Second International Symposium on Computational Particle Technology

and

Thirteenth International Conference on CFD in the Minerals and Process Industries

4-8 December 2018, Melbourne, Australia

PREFACE

Much of our environment and the benefits that we derive from our surroundings are strongly influenced by the interactions of the three primary phases of matter - solids, liquids, and gases. These interactions often occur at surfaces, with the individual phases being discrete in form. Particles and powders, which can be either wet or dry, and range in size from nanometers to centimeters, are one very important example of such a multiphase system. They have properties that are characteristic of each of the three primary phases. For example, under certain conditions they can withstand deformation like solids, flow like a liquid and exhibit compressibility like a gas. These features give rise to another state of matter – particulate/granular matter - that is poorly understood, posing a challenge to the scientific and engineering community for years.

Understanding the fundamentals governing particle and particle-fluid flows is of paramount importance to the design, control and optimisation of particulate and multiphase processes widely used in many industries. In the past, different measurement techniques have been developed, but there have been problems in probing the underlying physics and solving practical problems generally and reliably. Alternatively, a promising technique that can overcome these problems is computer simulation. This often involves a multiscale approach to understand phenomena at different length and time scales which, for particles, includes: (i) at the molecular/sub-particle scale to determine the interaction forces between particles, fluid and wall, and the transport behaviour between particles and/or pores; (ii) at the micro/particle scale to understand particle flow and force structures in relation to different flow conditions; (iii) at the meso/macro scale to formulate governing equations, constitutive relations and boundary conditions for continuum-based process modelling and simulation; and (iv) at the process equipment scale to quantify flow and process performance for control and optimisation. This consideration also applies to soft particles such as bubbles and droplets. There is also a need to consider the presence of fluid(s) and the coupling between fluid flow, heat and mass transfer. In the past two decades or so, with the rapid development of computer technology, many advanced computational technologies, either discrete- or continuum-based, have been developed and applied to tackle problems of various types.

The Second International Symposium on Computational Particle Technology, successive to the first one in Suzhou China in March 2016, aims to provide a forum to discuss the frontier and challenging problems in the modelling and simulation of complex particulate and multiphase processes, covering a wide spectrum from fundamental research to industrial application.

The Thirteenth International Conference on Computational Fluid Dynamics in the Minerals and Process Industries (CFD2018) is the eighth conference in this series to be held in Melbourne with SINTEF in Trondheim, Norway hosting the other five. Processing, be it in the Mineral, Metallurgical, Chemical, Oil & Gas or other related industries, often involves challenging fluid dynamics involving more than one phase and frequently other complex phenomena such as combustion, heat transfer, chemical reactions, non-Newtonian behaviour and phase change. Recognising the special challenges of these industries and that CFD was capable of tackling such problems, this conference series was established more than twenty years to provide a forum for discussing, promoting and advancing the application of CFD to the process industries.

The above two symposia or conferences are held together in Melbourne this time, representing a joint effort of two teams. As before, the joint conference is composed of plenary, keynote, oral and poster presentations. To be a high-level forum, world-leading scientists or experts from different countries are invited to deliver the plenary and keynote presentations at the event. There are also student sessions that offer an outstanding opportunity for PhD candidates to share their research and experience, important to the future developments in this exciting field.

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Liejin Guo, Xi'an Jiaotong University, China
Peter Witt, CSIRO, Australia

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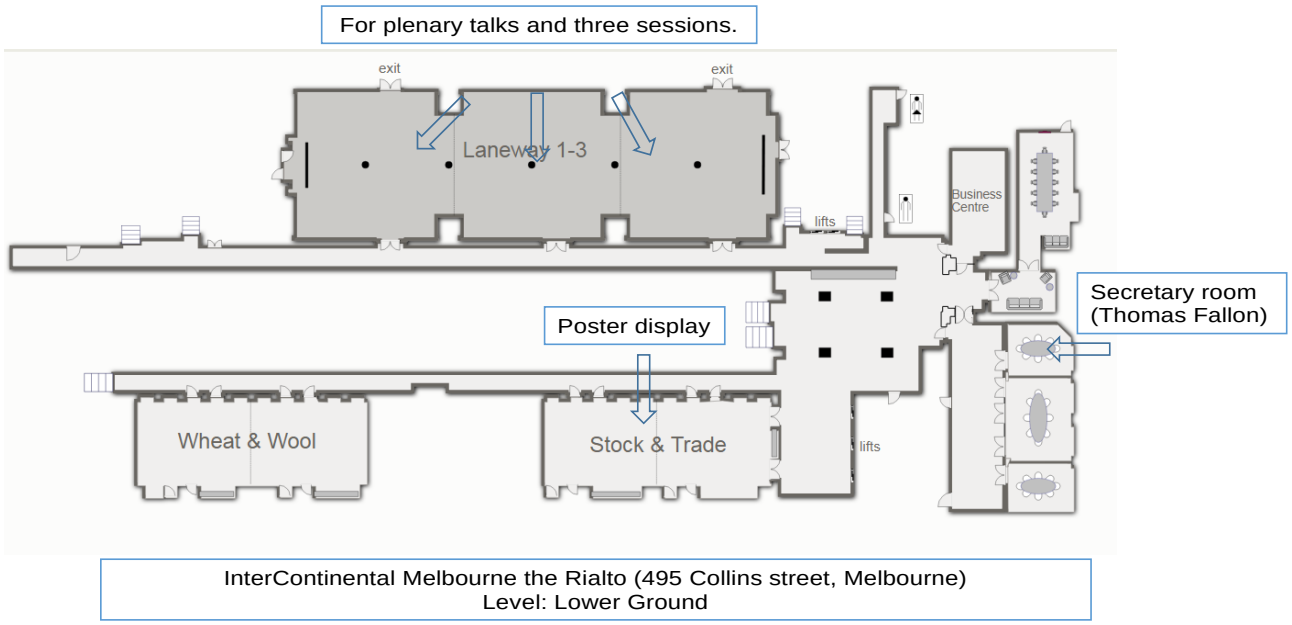
Longking, http://www.longking.com.cn/EnCMS/Home/index

Leap Australia, https://www.leapaust.com.au/

Computer Transition Systems, http://www.cts.com.au/newspage.html

Maps for the Conference and Dinner Venues

Conference Venue: InterContinental Melbourne the Rialto (495 Collins street, Melbourne CBD)



Dinner Venue: CQ Function Melbourne (123 Queen Street, Melbourne CBD)

CONFERENCE PROGRAM

Outline

Day 0 - Tuesday, 4 December 2018	
15:00 – 20:00	Registration/Cocktail Reception (Intercontinental Hotel: 495 Collins Street, Melbourne CBD)
Day 1 - Wednesday, 5 December 2018	
08:30 – 09:00	Conference Opening
09:00 – 10:30	Plenary Session
10:30 – 11:00	Poster Session/Morning Tea
11:00 – 12:30	Parallel Sessions
12:30 – 13:30	Lunch
13:30 – 15:30	Parallel Sessions
15:30 – 16:00	Poster Session/Afternoon Tea
16:00 – 18:00	Parallel Student Sessions
18:00 – 19:00	Poster Session And Happy Hour
Day 2 - Thursday, 6 December 2018	
08:30 – 10:00	Plenary Sessions
10:00 – 10:30	Poster Session/Morning Tea
10:30 – 12:30	Parallel Sessions
12:30 – 13:30	Lunch
13:30 – 15:30	Parallel Sessions
15:30 – 16:00	Poster Session/Afternoon Tea
16:00 – 18:00	Parallel Student Sessions
18:00 – 22:00	Conference Dinner (CQ Functions - 123 Queen Street, Melbourne CBD)
Day 3- Friday, 7 December 2018	
08:30 – 10:30	Parallel Sessions
10:30 - 11:00	Morning Tea
11:00 – 12:30	Parallel Sessions
12:30 – 13:30	Lunch
13:30 – 15:00	Parallel Student Sessions
15:00 – 15:30	Poster Session/Afternoon Tea
15:30 – 17:00	Plenary Session
17:00 – 17:30	Award Presentation, Wrap-Up And Conclusion
17:30 – 18:30	Happy Hour And Farewell
Day 4- Saturday, 8 December 2018 Post Conference Activities Are Cancelled Due To Lack Of Responses	

NB: (1) Time Allocated For Plenary - 45 Minutes, Keynote – 30 Minutes, Regular – 15 Minutes, And Students – 10 Minutes.
(2) Special Issues in Powder Technology for CPT /Applied Mathematical Modelling for CFD (may be limited to the presentations at the conference)

15:00-20:00	Day 0 (Tuesday, 4 December) Registration & Cocktail Reception (18:00-19:00) (Intercontinental Hotel)		
Day 1 (Wednesday, 5 December)			
08:30-09:00	Conference Opening Prof Aibing Yu (Monash University) Prof Robin Batterham (University Of Melbourne)		
	Plenary Session Chair: Peter Witt And Liejin Guo		
09:00-09:45	Discrete Simulation Of Granular And Particle-Fluid Systems (page:2) Professor Wei Ge Chinese Academy Of Sciences		
09:45-10:30	Modelling Subsea Gas Blowouts (page:5) Jan Erik Olsen SINTEF Industry		
10:30-11:00	Poster Session/Morning Tea		
	Laneway Room 1	Laneway Room 2	Laneway Room 3
	Simulation Methods Chair: Mikio Sakai, Qiang Zhou	Granular Dynamics Chair: Alain De Ryck, Paul Cleary	Fluid Bed Operations Chair: Peter Witt, Anthony B. Murphy
11:00-11:30	Keynote Using Failure Dynamics At The Mesoscale For Early Prediction Of Slope Failure From Data (page:7) Antoinette Tordesillas University Of Melbourne	Keynote Use Of 3D Printing For DEM Model Validation (page:45) Karen Hapgood Deakin University, Geelong Australia	Keynote Multi-Scale Modeling Of Reactive Dense Flows (page:190) Kun Luo Zhejiang University
11:30-11:45	12-Velocity Multiple-Relaxation-Time Lattice Boltzmann Model For Three Dimensional Incompressible Flows (page:9) Jiayi Hua, Wenhuan Zhang, Shibo Kuang, Aibing Yu, Baochang Shi, Yihang Wang (Ningbo University)	Segregation In Sheared Granular Matter (page:47) Gerald G Pereira And Paul W Cleary (CSIRO)	CFD-DEM Study of Mixing/Segregation of Particles in Fluidized Beds under Influence of Size, Density, and Shape (page:191) Esmaeil Abbaszadeh Molaei, Aibing Yu, Zongyan Zhou, Michael Small, Phillip Fawell (CSIRO)
11:45-12:00	A Solid-Stresses-Based Multiphase Particle-In-Cell Model For Gas-Particle Flow In Fluidized Beds (page:10) Vikrant Verma And Johan T. Padding (Delft University Of Technology)	Effect Of Vibrational And Geometrical Parameters On Granular Capillarity Induced By A Vibrating Tube (page:48) Fengxian Fan, Huateng Zhang, Eric J R Parteli, Thorsten Pöschel And Mingxu Su (University Of Shanghai For Science And Technology)	A Numerical Study Of The Solid Dispersion Behavior And Residence Time Distribution In A Circulating Fluidized Bed Methanation Reactor (page:196) Yuli Zhang, Rui Xiao, Mao Ye (Hohai University)
12:00-12:15	MP-PIC Simulation Of Blood Flow Across A LAD With High Stenosis (page:12) Jian Liu, Fan Yu, Yu Zhang (Tsinghua University)	Particle Based Modelling Of Metal Powder Flow In Additive Manufacturing Systems (page:49) G.W. Delaney, S. Gulizia, V. Lemiale, C. Doblin, A.B. Murphy (CSIRO)	System Design Of A Dual Fluidized Bed Pyrolysis Reactor (page:200) Reinhard Seiser And Robert Cattolica (University Of California San Diego)
12:15-12:30	Orientation Discretization In Discrete Modelling Of Non-Spherical Particles (page:14) Kejun Dong, Kamyar Kildashti, Bijan Samali And Aibing Yu (Western Sydney University)	Modeling Of Deformation Of Granular Pellet In Small-Scale "Unit Cell" DEM Simulations (page:50) Intan Soraya Shamsudin, Li Ge Wang And Rachel M. Smith (The University Of Sheffield)	EMMS Application In Rectangular Circulating Fluidized Beds (page:193) Qiuya Tu, Haigang Wang (Chinese Academy Of Sciences)
12:30-13:30 Lunch			
	Simulation Methods (Continued) Chair: Karen Hapgood, Alex Heath	Granular Dynamics (Continued) Chair: Jin Ooi, Fengxian Fan	Fluid Bed Operations (Continued) Chair: Vikrant Verma, Yansong Shen
13:30-14:00	Keynote Key Sub-Grid Quantities Affecting The Filtered Drag Force And The Derivation And Analysis Of Their Transport Equations (page:15) Qiang Zhou Xi'an Jiaotong University	Keynote DEM-FEM Coupled Modelling On The Compaction And Sintering Of Elemental And Composite Powders (page:51) Xizhong An Northeastern University	Keynote Application Of CFD For Operating Of Industrial Equipment: Take Ultra-Supercritical Coal Fired Power Plant Boiler For Example (page:197) Wenqi Zhong Southeast University
14:00-14:15	Simulation of particle dissolution in RANS simulations of turbulent (page:44) M. Philip Schwarz (CSIRO Mineral Resources)	Keynote Wall Effects In Powder Flow In Continuum Mechanics Modeling (page:53) Alain De Ryck IMT Mines Albi, France	Keynote CFD Study Of Ironmaking Blast Furnace: Recent Model Development And Application (page:199) Shibo Kuang Monash University
14:15-14:30	Impact Energy Dissipation Analysis During Ship Loading Of Iron Ore By Large-Scale MPI-GPU-DEM Simulation (page:17) Jieqing Gan, Tim Evans And Aibing Yu (Monash University)		
14:30-14:45	Designer Granular Materials - A Combined Discrete Element Method And Evolutionary Algorithm Approach (page:18) Gary Delaney And David Howard (CSIRO)	Modelling Of Particle Breakage In Grinding (page:54), Ebrahim Ghasemi Ardi, Cheng Lyu, Aibing Yu And Runyu Yang (University Of New South Wales)	The Phase Separation In Multi-Stage Fluidized Bed Reactors (page:131) Chenxi Zhang, Yao Wang, Weizhong Qian And Fei Wei (Tsinghua University)
14:45-15:00	Local Contact Point Treatment In Sphere Packings (page:20)	The Forces On Cylinders In The Free Molecule Regime (page:55) Jun Wang, Song Yu, And Guodong Xia (Beijing University Of Technology, China)	On Pragmatism In Industrial Modelling Part VI: Management, Retrieval And Analysis Of CFD Cases (page:202)

	Michael Harasek, Mario Pichler, Bahram Haddadi Sisakht, Hamid Reza Norouzi And Christian Jordan (TU Wien, Austria)		Josip Zoric, Stig Urheim And Kristian E. Einarsrud (SINTEF)
15:00-15:15	Just-In-Time Training (JITT) Paradigm For Granular Processes (page:22) Daniel N. Wilke, Nicolin Govender, Patrick Pizette (University Of Pretoria, South Africa)	Study Of Rheological Behaviour Of Granular Non-spherical Particle Suspensions Via CFD-DEM (page:93) Vinay V. Mahajan, Junaid Mehmood, Yousef M. F. El Hasadi and Johan T. Padding (Delft University of Technology)	Numerical Investigation On The Wake Of NACA0015 Hydrofoil (page:228) Sara Vahaji, Jiang Han, Sherman C.P. Cheung, Guan H. Yeoh And Jiyuan Tu (Deakin University)
15:15-15:30	Experimentally Validated Computational Models To Predict The Impact Of Humidity On The Flow Of Granular Mixtures (page:24) Koyel Sen, Raj Mukherjee, Mao Chen, Bodhisattwa Chaudhuri (University Of Connecticut, USA)	Grain-Based Discrete Element Method Modelling of Multi-scale Fracturing in Geomaterials under Dynamic Loading (page:58) Qianbing Zhang, Xiaofeng Li, Kai Liu And Wanrui Hu (Monash University)	Coupling Of CFD-DEM And Reaction Model For 3D Fluidized Beds (page:194) Jun Xie And Wenqi Zhong (Southeast University)
15:30-16:00	Poster Session/Afternoon Tea		
	Simulation Methods (Continued) (Student Session) Chair: Yijiao Jiang, Shibo Kuang	Granular Dynamics (Continued) (Student Session) Chair: Roberto Moreno-Atanasio, Baojun Zhao	Fluid Bed Operations (Continued) (Student Session) Chair: Sutthichai Boonprasop, Reinhard Seiser
16:00-16:10	Liquid Redistribution Upon The Liquid-Bridge Rupture Between Two Unequal Particles With A Minimal Energy Method (page:25) Dongling Wu, Ping Zhou, Baojun Zhao, Tony Howes, Geoff Wang (Central South University)	DEM Simulation Of Powder Packing Process In 3D Printing (page:69) Lin Wang, Aibing Yu, Zongyan Zhou (Monash University)	Predicting Minimum Fluidization Velocity For Vacuum Fluidized Beds (page:206) Lanka Weerasiri, Vishwanath Kumar, Subrat Das And Daniel Fabijanic (Deakin University)
16:10-16:20	Multi-Level Coarse-Grain Model In DEM And CFD-DEM Simulations (page:26) Daniel Queteschiner, Thomas Lichtenegger, Stefan Pirker, Simon Schneiderbauer (Johannes Kepler University Linz)	DEM Study of the Effects of Particle Shape and DRI-flap Shape on Burden Distribution in COREX Melter Gasifier (page:355) Yang You, Zhiguo Luo, Haifeng Li, Zongshu Zou, Runyu Yang (University of New South Wales)	A CFD-DEM Model For The Simulation Of Direct Reduction Of Iron Ore In Fluidized Beds (page:207) Mustafa Efe Kinaci, Thomas Lichtenegger, Simon Schneiderbauer (Johannes Kepler University)
16:20-16:30	A Numerical Study On The Reduction, Softening, And Melting Of Iron Ore Pellets And Dripping Of Molten Iron And Slag Using CFD-DEM (page:28) Mehdi Baniasadi, Maryam Baniasadi, Bernhard Peters (University Of Luxembourg)	Finite Element Investigation Of Briquetting Of Iron Ore Particles (page:63) Md Tariqul Hasan, C.L. Li, R.Y. Yang (University Of New South Wales)	Hydrogen Production In Fluidized Bed Membrane Reactors (page:209) Ramon J.W. Voncken, Ivo Roghair, Martin Van Sint Annaland (Eindhoven University Of Technology)
16:30-16:40	Numerical Study On Gas-Solid Two-Phase Flow In A Flue Gas Turbine (page:30) Jingna Pan, Jianjun Wang (China University Of Petroleum)	Experimental Study On Packing Densification Of Non-Spherical Particles Under Air Impact (page:64) Dazhao Gou, Xizhong An, Runyu Yang (Northeastern University)	Multiphase Direct Numerical Simulations (DNS) Of Oil-Water Flows Through Digitized Porous Rocks (page:211) H.V. Patel, J.A.M. Kuipers, E.A.J.F. Peters (Eindhoven University Of Technology)
16:40-16:50	Particle Scale Modelling To Study The Effect Of Bubble Dynamics On Orientation Of Ellipsoids (page:32) Siddhartha Shrestha And Zongyan Zhou (Monash University)	Shape Effects On Bulk Modulus Of Maximally Random Jamming Packing Of Intersecting Spherocylinders (page:65) Wei Deng, Lufeng Liu, Ye Yuan, Shuixiang Li (Peking University, China)	Determination Of The Minimum Fluidization Velocity In Fluidized Bed At Elevated Pressure And Temperature By CFD Simulation (page:223) Yingjuan Shao, Jinrao Gu, Wenqi Zhong, Aibing Yu (Southeast University)
16:50-17:00	A Continuum Model Of The Cohesive Avalanche Considering Stick-Slip Behaviours Of Granular Materials (page:34) LYM. Yang, Q.J. Zheng and A.B. Yu (Monash University)	Multi-Particle FEM Modelling On Hot Compaction Of Tic-316L Composite Powders (page:67) Defeng Wang, Xizhong An, Peng Han, Qian Jia (Northeastern University)	Simulation Of Combustion In Coal-Fired Circulating Fluidized Bed Boiler For Supercritical CO_2 Power Cycle (page:214) Ying Cui, Wenqi Zhong, Jun Xiang, Guoyao Liu (Southeast University)
17:00-17:10	Multi-Parameter Optimization Of Non-Catalytic Partial Oxidation Of Natural Gas Using Reduced Order Models And CFD (page:35) Philip Rößger, Yury Voloshchuk, Andreas Richter, Bernd Meyer (TU Bergakademie Freiberg)	Self-Assembly Of Granular Spheres Under One-Dimensional Vibration (page:68) Reza Amirifar, Kejun Dong, Qinghua Zeng (Western Sydney University)	Numerical Simulation Of Droplet Formation In Microfluidic Cross-Junction (page:221) Wei Gao, Wei Yu, Chengbin Zhang, Xiangdong Liu, Yongping Chen (Southeast University)
17:10-17:20	Modelling Biochemical Interactions In The Early Stage Formation Of Atherosclerosis Within The Arterial Wall (page:37) Ratchanon Piemjaiswang, Sargon A Gabriel, Yan Ding, Yuqing Feng, Pornpote Piumsomboon And Benjapon Chalermsinsuwan (Chulalongkorn University)	Waste-To- Energy Conversion Of Sewage Sludge Using Sorption-Enhanced Thermochemical Technology (page:57) Xiaoxia Yang And Yijiao Jiang (Macquarie University)	Direct Numerical Simulation Of Hot Spots In Packed Bed Reactors (page:217) V. Chandra, E.A.J.F. Peters And J.A.M Kuipers (Eindhoven University Of Technology)
17:20-17:30	On The Validity Of The Two-Fluid-KTGF Approach For Dense Gravity-Driven Granular Flows (page:38) Alexander Busch And Stein Tore Johansen (Norwegian University Of Science And Technology)	Shape Effects On Particle Segregation By Discrete Element Method (DEM) (page:70) Zhouzun Xie, Changxing Li, Xizhong An, Yansong Shen (University Of New South Wales)	Cluster-Induced Turbulence Closure Models For Momentum And Heat Transfer In Large-Scale Gas-Solid Flows (page:219) Stefanie Rauchenzauner And Simon Schneiderbauer (Johannes Kepler University)
17:30-17:40	Direct Numerical Simulations And Force Correlations Of Assemblies Of Non-Spherical Particles (page:41) Sathish K. P., Sanjeevi And Johan T. Padding (Delft University Of Technology)	Molecular Dynamics Simulation Of Silica Oligomerization (page:71) Malgorzata Kaminska, Frederic Gruy, Jules Valente (Ecole Des Mines De Saint-Etienne, France)	Numerical Investigation Of Gas Redistribution Effects By Raceways On The In-Furnace States And Performance Of Ironmaking Blast Furnace (page:220) Lulu Jiao, Shibo Kuang, Aibing Yu, Yuntao Li, Xiaoming Mao, Hui Xu (Monash University)
17:40-17:50	An Immersed-Grid Method For Simulation Of Viscous Flows (page:42)	Valid Local Quantities of Particle-fluid Flows for Constitutive Relations	A Numerical Approach For Generic Three Phases Flow Simulation (page:260)

	T.T.V. Le, N. Mai-Duy, K. Le-Cao, T. Tran-Cong (University Of Southern Queensland)	Qinfu Hou, Zongyan Zhou, Jennifer S. Curtis, and Aibing Yu (Monash University)	Son Tung Dang, Stein Tore Johansen And John Christian Morud (Norwegian University Of Science And Technology
17:50-18:00	Oxy-Fuel Combustion Behaviors In Fluidized Bed: Studied By Experiment And CFD Simulation (page:43) Qinwen Liu, Wenqi Zhong, Aibing Yu (*Southeast University)*	Numerical Investigation On The Rebound Mechanism Of Spherical Fine Particle Impacting Several Blade Materials (page:72) Juan DI, Shun-Sen WANG, Yong-Hui XIE (Xi'an Jiaotong University)	CFD Modelling Of Gas-Solid Fluidised Bed With Eularian Single Phase Air Coupled Explicitly With Eularian Solid Phase (page:213) Mst Farhana Diba, Md. Rezwanul Karim, Jamal Naser (Swinburne University Of Technology)
18:00-19:00	Poster Session & Happy Hour		

Day 2 (Thursday, 6 December)			
	Plenary Session Chair: Wei Ge, Hans Kuipers		
08:30-09:15	Using DEM To Develop Constitutive Models For CFD Simulations Of Particulate Flows (page:1) Professor Jennifer Curtis University of California, Davis		
09:15-10:00	DEM-CFD Analysis Of Contact Electrification Processes (page:3) Professor Chuan-Yu Wu University of Surrey		
10:00-10:30	Poster Session/Morning Tea		
	Laneway Room 1	Laneway Room 2	Laneway Room 3
	Particle-Fluid Flow & Multiphase Flow Chair: Runyu Yang, Hao Zhang	Granular Dynamics (Continued) Chair: David Pinson, Xizhong An	Multiphase, High-Temperature And Complicated Operations Chair: Benjapon Chalermsinsuwan, Yuqing Feng
10:30-11:00	Keynote Simulation And Modelling Of Ellipsoids In Particulate Systems (page:94) Zongyan Zhou Monash University	Keynote Reduced Stiffness Model For Cohesive Particles (page:73) Toshitsugu Tanaka Osaka University	Keynote The Mushy Zone In A Model Of Arc Welding Of Aluminium Alloys (page:224) Anthony B. Murphy CSIRO Manufacturing
11:00-11:15	Detachment Of Droplets On Solid Surface In The Surfactant Solution (page:95) Xinglong Shang, Zhengyuan Luo, Bofeng Bai (Xi'an Jiaotong University)	Keynote Transient Simulation Of Particle Segregation By Coupling Granular Flow Model And Diffusive, Segregating Fluxes (page:74) Qijun Zheng Monash University	Computational Models For Pyrometallurgical Phase Separation Problems (page:226) Quinn G. Reynolds, O.F. Oxtoby, M.W. Erwee, And P.J.A. Bezuidenhout (Mintek)
11:15-11:30	Computational Particle Fluid Dynamics Modeling Of Gas-Solids Flow In A Downer (page:96) Xingying Lan, Yingya Wu, Liqing Qin, Jinsen Gao (China University Of Petroleum, Beijing)		The Optical Properties And Electrical Field Enhancement Of Gold Nanospheres (page:204) Bin Chen, Linzhuang Xing, Dong Li, Wenjuan Wu (Xi'an Jiaotong University)
11:30-11:45	Interaction modelling for CFD-DEM simulations of floating particles (page:145) T.M.J. (Tim) Nijssen, K.A. (Kay) Buist, J.A.M. (Hans) Kuipers, J. (Jan) van der Stel and A.T. (Allert) Adema (Eindhoven University of Technology)	Advances in DEM simulations using GPUS: A focus on particle shape and number (page:16) Nicolin Govender, Charley Wu, Daniel Wilke, Johannes Kinhast (University of Surrey)	Mesoscale Modeling Of Drop Size Distribution In Rotor-Stator Devices (page:234) Ning Yang, Chao Chen, Xiaoping Guan, Ying Ren (Chinese Academy Of Sciences)
11:45-12:00	DEM-CFD Analysis On The Influence Mechanism Of Electrostatics On Single Bubble In Gas-Solid Fluidized Bed (page:100) Zhen Tan, Cai Liang, Junfei Li (Monash University)	Numerical Simulation Of Granular Flow Using Combined Discrete Element Model (page:78) Yongzhi Zhao, Huaqing Ma, Zihan Liu, Ying You, Changhua Xie, Yuan Zhao (Zhejiang University)	Characterization Of Size Resolved Atmospheric Particles In The Vicinity Of Iron And Steelmaking Industries In China (page:157) Vladimir Strezov, Tao Kan, Tim Evans, Xiaoxia Yang And Yijiao Jiang (Macquarie University)
12:00-12:15	Distribution Homogeneity Of Solid Particles In Slurry Taylor Flow (page:101) Zhengbiao Peng, Mohd. Mostafizur Rahman, Behdad Moghtaderi And Elham Doroodchi (The University Of Newcastle)	Liquid Film Modeling Within An Eulerian Multiphase Framework (page:79) Kshitij Neroorkar, Mohit Tandon, S. Jagan Mohan, And Raghavendra Krishnamurthy (Siemens Industry Software Computational Dynamics India Pvt Ltd)	Numerical Analysis Of The Component Interaction In A Hydrocyclone Treating Heterogeneous Mixture Using Multi-Phase CFD Model (page:230) Mandakini Padhi, Narasimha Mangadoddy (Indian Institute Of Technology)
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	Particle-Fluid Flow & Multiphase Flow (Continued) Chair: Qianbing Zhang, Nicolin Govender	Multiphase, High-Temperature And Complicated Operations (continued) Chair: Toshitsuga Tanaka, Qinfu Hou	Multiphase, High-Temperature And Complicated Operations Chair: G.W. Delaney, Josip Zoric
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14:00-14:15	Keynote Modelling And Optimisation Of Reacting Particle Flow: Examples In Ironmaking Industry (page:105) Yansong Shen University Of New South Wales	Keynote Particle Size Segregation For Fun And (Hopefully) Profit (page:148) David Pinson Bluescope Steel	High-Resolution Large Time-Step Schemes for Inviscid Fluid Flow (page:238) Sigbjørn Løland Bore and Tore Flåtten (Norwegian University of Science and Technology)
14:15-14:30			Euler-Lagrangian Simulations On Pyrolysis Oil Spray And Viscosity Effects On A High-Pressure Multi-Hole Injector Nozzle (page:247) Carlos Varas, A.E., Buist, K.A., And Kuipers, J.A.M (Eindhoven University Of Technology)
14:30-14:45	Numerical Prediction On The Drag Force And Heat Transfer Of Various Particles In Supercritical Water (page:109) Hao Zhang, Bo Xiong, Xizhong An (Northeastern University)	Predictive Optimization Of SAG Mill Performance Using DEM (page:149) Peter Rizkalla, Rahul Bharadwaj And Lucilla Almeida (LEAP Australia Pty Ltd)	Numerical Simulation On Flow Field Characteristics Of Backflow Controller (page:242) Huaizhong Shi, Jingfeng Tao, Heqian Zhao (China University Of Petroleum (Beijing))
14:45-15:00	An Investigation On Interactions Between Ultrasonic Waves And Particles Based On The Monte Carlo Method (page:108) Mingxu Su, Bingfa Huang, Fengxian Fan, Huinan Yang, Jun Chen And Xiaoshu Cai (University Of Shanghai For Science And Technology)	Numerical Investigation On Heat Transfer Characteristics Of Particle In Supercritical Water (page:152) Zhenqun Wu, Hui Jin, Liang Zhao, Liejin Guo (Xi'an Jiaotong University)	Strengthening Of Microalloying Spring Steels By Secondary Particles (page:158) Xiaodong Ma, Zongze Huang, Zan Yao, Zhouhua Jiang, Geoff Wang, Baojun Zhao (University Of Queensland)
15:00-15:15	A Multi-Scale Modelling Of Oscillatory Blood Flow And Mass Transportation In A Human Coronary Sargon A. Gabriel, Yan Ding, John A. Gear, Yuqing Feng (CSIRO)	Lattice Boltzmann investigation on the interactions between non-Newtonian fluid and ellipsoid particles Zheng Qi, Shibo Kuang, Aibing Yu (Monash University)	Numerical investigation of the effects of oxygen enrichment on an ironmaking blast furnace Haiqi Nie, Zhaoyang Li, Shibo Kuang and Aibing Yu (Monash-SEU JRI)
15:15-15:30	Numerical Investigation On Erosion Characteristics Of Double Elbows For Gas-Solid Flow (page:151) Yu Wang, Rongtang Liu, Ming Liu, Junjie Yan (Xi'an Jiaotong University)	Numerical Investigation On The Impacts Of The Evaporation Process On Cough Droplets Dispersions In An Enclosed Environment (page:154) Yihuan Yan, Xiangdong Li And Jiyuan Tu (RMIT University)	An Experimental Study Of Enhanced Heat Transfer Of Nano-Encapsulated Phase Change Material Slurry Embedded In Metal Foam (page:243) Wenqiang Li, Hao Wan, Peijin Liu, Guoqiang He, Fei Qin (Northwestern Polytechnical University)
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16:00-16:10	A DNS-DEM Coupling Methodology For Turbulent Non-Newtonian Suspension Flow (page:113) E.Z. Zheng, M. Rudman, S.B. Kuang, A. Chryss (Monash University)	Shape Optimization Of Axial Symmetrical Hoppers In The Discharging Of Granular Materials (page:80) Xingjian Huang, Qijun Zheng, Aibing Yu And Wenyi Yan (Monash University)	CFD Modelling Of A Lime Kiln Burner (page:249) Brad Wilson, Roger Hassold, Yvonne Yu, Renata Favalli, Jordan Parham (FCT Combustion Pty Ltd)
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16:20-16:30	Effect Of Lift And Hydrodynamic Torque On Fluidization Of Non-Spherical Particles: Experimental Validation (page:116) Ivan Mema, Vinay Mahajan, Kay Buist, Hans Kuipers, Johan T. Padding (Delft University Of Technology)	A Numerical Study On The Solid Flow Behavior In A Rotating Drum Based On An Eulerian-Eulerian Approach Using A Frictional Stress Model (page:83) Wenjie Rong, Yuqing Feng, Peter Witt, Phil Schwarz, Baokuan Li, Tao Song, Junwu Zhou (Northeastern University)	Droplet-Droplet Collisions In A Spray Dryer (page:252) Giulia Finotello, K.A. Buist, J.T. Padding, A. Jongsma, F. Innings, J.A.M. Kuipers (Eindhoven University Of Technology)
16:30-16:40	CFD-DEM simulation of particle-laden liquid-solid flow interacting with a resolved fixed spherical bubble (page:117) Linhan Ge, Roberto Moreno-Atanasio, Geoffrey (The University Of Newcastle)	Numerical Analysis Of Elongated Particles Flowing Through Shear Cell (page:84) M. Hossain, H. P. Zhu, A. B. Yu (Western Sydney University)	Numerical Study Of Droplet Generation Via Co-Flowing Microfluidic Device Under Electric Field (page:292) Lei Li, Jiayu Zhang, Chengbin Zhang (Southeast University)
16:40-16:50	Three-Dimensional Simulation Of Oxy-Fuel Combustion In A Circulation Fluidized Bed (page:126) Jinrao Gu, Wenqi Zhong And Aibing Yu (Southeast University)	DEM Study Of Copper Stave-Burden Interaction In The Ironmaking Blast Furnace (page:85) Joel Samsu, Zongyan Zhou, David Pinson, Sheng Chew (Monash University)	Numerical And Experimental Study Of Bubble Formation In Supersaturated Water (page:256) A. Battistella, S.S.C. Aelen, I. Roghair, M. Van Sint Annaland (Eindhoven University Of Technology)
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17:10-17:20	Direct Numerical Simulations Of Low-Reynolds-Number Flow Past Arrays Of Ellipsoidal Particles: Effect Of Particle Orientation On Drag Force (page:123) Xinyang Li, Ming Jiang, Zheqing Huang And Qiang Zhou (Xi'an Jiaotong University)	Axial Segregation Of Binary-Sized Mixture Of Ellipsoids In A Rotating Drum (page:89) Siyuan He, Jieqing Gan, Aibing Yu, David Pinson, And *Zongyan* Zhou (Monash University)	Three Phase Flows Using DSMC Method For Simulating Slurry Bubble Columns (page:262) S.S. Kamath, J.T. Padding, K.A. Buist, J. A. M. Kuipers (Eindhoven University Of Technology)
17:20-17:30	Analysis On Retention Capacity Of Liquid Bridge Between Two Particles Under Oscillation (page:124) Jian Chen, Kenneth Williams, Jie Guo (The University Of Newcastle)	DEM Study Of The Performance Of Screw Conveyor With An Inclined Screw Blade (page:90) Xin Li, Qinfu Hou, Jieqing Gan, Ruiping Zou, Aibing Yu (Monash University)	Assessing The Efficacy Of Inhomogeneous Thermal Conductivity To Enhance Heat Transfer Within Fusion Reactor Blankets (page:264) C. J. Camobreco, A. PothÉRat And G. J. Sheard (Monash University)
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09:45-10:00	Fluid Flow Through Unresolved CT Data-Sets – Can Gray-Scale LB Deliver Useful Results? (page:136) Gerald G Pereira (CSIRO)	Imaging Soft Matters and Interfaces at Nano-to-Micro Scale (page:304) Jing Fu (Monash University)	Modelling Of Diesel Spray Combustion For Top-Submerged-Lance Processes (page:277) Daniele Obiso And Sebastian Kriebitzsch (CIC Virtuhcon)
10:00-10:15	Non-spherical Particle Behaviors in a Spouted Bed (page:102)	Modeling Of Multiphase Flow And Particle Deposition Characteristics In Radiant Syngas	A Novel Tundish Design Based On CFD-DEM Study (page:279)

	Tianyu Wang, Xing Liu, Anxing Ren, Yurong He, Jiaqi Zhu (Harbin Institute of Technology)	Cooler Of Entrained-Flow Coal Gasification (page:160) Lei Wang, Yan Gong, Qinghua Guo, Fuchen Wang, Guangsuo Yu (East China University Of Science And Technology)	Vishnu Teja Mantripragada, Sabita Sarkar (Indian Institute O Ftechnology Madras)
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10:30-11:00	Poster Session/Morning Tea		
	Particle-Fluid Flow & Multiphase Flow (Continued) Chair: Hidehiro Kamiya, Yu Zhang	Multiphase, High-Temperature And Complicated Operations (continued) Chair: Vladimir Strezov, Haiping Zhu	Multiphase, High-Temperature And Complicated Operations Chair: Matt Sinnott, Ning Yang
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13:40-13:50	The Effect Of The Temperature On The Process Of Heterogeneous Condensation By Cloud-Air-Purifying (Cap) Technology (page:180) Yumeng Zhang, Guoyin Yu, Bo Wang (Lanzhou University)	Bubble Motion Characteristics Under External Disturbance During Water Splitting (page:168) Zhenshan Cao, Liejin Guo, Yechun Wang And Juanwen Chen (*Xi'an Jiaotong University)*	Sources Of Perturbation Growth In Cylinder Wake Instabilities (page:290) Z. Y. Ng, T. Vo, And G. J. Sheard (Monash University)
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	Ruizhi Jin, Erfan Keshavarzian, Bo Wang, Kejun Dong, Kenny Kwok, Ming Zhao (Western Sydney University)	Yu Qiu, Wenqi Zhong, Yingjuan Shao, Aibing Yu (Southeast University)	Helmholtz-Zentrum Dresden – Rossendorf, Institute Of Fluid Dynamics
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P014	The emerging and coupling of localized zones in sheared granular materials(page:321)	Wei Zhou, Yiao Li, Gang Ma, Jiaying Liu
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ABSTRACTS

Using DEM to Develop Constitutive Models for CFD Simulations of Particulate Flows

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Abstract

The discrete element method (DEM) is a powerful, yet computationally-intensive, simulation tool which provides the details of the flow of individual particles. A continuum treatment for the particle phase within a CFD framework is capable of simulating larger-scale processes yet requires constitutive models to describe averaged quantities associated with particle-particle and particle-fluid interactions. Granular kinetic theory well describes these interactions in dilute and dense-phase collisional flow although this theory is typically restricted to monodisperse, spherical particles. This presentation will outline the development of constitutive models for the collisional dissipation rate and the particle-phase stress in granular kinetic theory for particle assemblies that are comprised of non-spherical grains which are described (within DEM) either as perfect cylinders or disks of varying aspect ratio or described using a glued-sphere approach. This presentation will include DEM modeling of both rigid and flexible non-spherical particles. In the case of flexible particles, a bonded particle model is employed which includes normal and shear forces as well as the bending and torsional moments. These DEM simulations are validated via a variety of experiment measurements of both rigid and flexible particles in shear cells, hopper discharge rates, particle packing fraction measurements, and particle breakage in uniaxial compression and in agitated cylindrical mixers.

Brief Biography

Jennifer Sinclair Curtis is Distinguished Professor of Chemical Engineering and Dean of the College of Engineering at University of California, Davis. She is a Fellow of AAAS, AIChE and ASEE. Professor Curtis is a recipient of a Fulbright Senior Research Scholar Award, AIChE's Thomas-Baron Award in Fluid-Particle Systems, the AIChE's Fluidization Lectureship Award, the American Society of Engineering Education's Chemical Engineering Lectureship Award, the Eminent Overseas Lectureship Award by the Institution of Engineers in Australia, ASEE's Sharon Keillor Award for Women in Engineering, and the NSF Presidential Young Investigator Award. Professor Curtis received a B.S. in Chemical Engineering from Purdue University (1983) and a PhD in Chemical Engineering from Princeton University (1989). Professor Curtis' particulate flow models have been extensively adopted by both commercial and open source computational fluid dynamics (CFD) software packages.

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Discrete Simulation of Granular and Particle-Fluid Systems

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Abstract

Discrete methods following the trajectories of the individual particles, such as the discrete element method (DEM), are still the mainstream simulation methods for in granular and particle-fluid flows. However, to cope with the scale and complexity of industrial and engineering applications, many improvements and extensions are still required. This presentation will address three aspects of our researches in the direction, namely, the coarse-graining DEM for the discrete particle simulation of gas-solid flow, consideration of geometrical irregularity in DEM simulation of engineering applications, and the parallel implementation of discrete methods on heterogeneous supercomputing systems. With these efforts, industrial scale systems, such as the circulating fluidized beds for petrochemical processes, can be simulated in discrete methods within a reasonable time, and for lab scale systems, even interactive virtual operation will be possible.

Brief Biography

Prof. Wei Ge got his B. Sc in 1992 and then Ph. D in 1998, both from Harbin Institute of Technology, China. He has been professor of chemical engineering at Institute of Process Engineering, Chinese Academy of Sciences since 2006. He is mainly engaged in multi-scale simulation of multi-phase systems, including fluidization, micro-/nano-flow and transport, granular and porous media flows. He proposed pseudo-particle modeling for micro-scale simulation of macro-scale flow behaviors and improved the energy-minimization multi-scale model for gas-solid and gas-liquid flows. As project leader, he developed the Mole series multi-scale supercomputing systems to bridge simulations of molecular details to reactor performance. He is now working on virtual process engineering, trying to establish digital counterparts of real engineering processes through accurate realtime simulation and interactive realistic visualization on supercomputers.

He is author of over 160 journal papers and 5 monographs. He won the Outstanding Youth in Basic Science Award of Zhou Guangzhao Foundation in 2008, the P&G Outstanding Youth in Particuology of Chinese Society of Particuology in 2011, the National Science Fund for Distinguished Young Scholars in 2012, and Hou De-bang Innovation Award of Chemical Science and Technology of the Chemical Industry and Engineering Society of China (CIESC). He is associate editor of Chemical Engineering Science, Chairman of the Simulation & Virtual Process Engineering Committee, CIESC, council member of The Chinese Society of Particuology, and adversary board member of *Particuology*. He is director of the State Key Laboratory of Multi-Phase Complex Systems, China since 2015.

DEM-CFD Analysis of Contact Electrification Processes

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Abstract

Contact electrification is very common in powder handling processes, during which electrostatic charge can be transferred from one material surface to another during contacts. Triboelectric Charging can polarize particles and induce excess net charge. The presence of net charge and the induced electrostatic interaction can significantly affect the performance of powder handling processes and the quality of particulate products. Therefore, it is of fundamental importance to understand the influence of contact electrification and electrostatic interaction on powder handling processes.

In this talk, the influence of contact electrification and electrostatic interactions on powder handling processes will be analysed a coupled discrete element method with computational fluid dynamics (DEM-CFD). For this purpose, an in-house DEM-CFD code was adapted and advanced in four strands: (1) A condenser model is implemented to analyze the contact electrification of particles; (2) The Coulomb force model is incorporated to model the electrostatic interactions between particles; (3) A hybrid particle-cell (HPC) algorithm is developed to compare with the conventional direct truncation (DT) method to effectively model the long-range nature of the electrostatic interactions; (4) Symmetric and sphere-tree multi-sphere methods are also incorporated to investigate the effect of particle shape on contact electrification.

The advanced DEM-CFD is then used to explore electrostatic phenomena and dynamic behaviours of particles in various powder handling processes, including: 1) contact electrification of spherical particles during fluidization; 2) deposition of mono-charged and bi-charged particles; 3) contact electrification and electrostatic interactions of spherical particles during fluidization; 4) contact electrification of elongated particles in a vibrating container; and 5) contact electrification of particles with arbitrary shape in a rotating drum. It is demonstrated that the developed DEM-CFD is a very robust tool for analysing Triboelectric Charging phenomena in particle systems

Brief Biography

Prof. Chuan-Yu (Charley) Wu is a Professor of Chemical Engineering at the Department of Chemical and Process Engineering, the University of Surrey. UK. He is currently an executive editor for Powder Technology, a leading peer reviewed journal on particle systems. He recently co-authored a monograph on “Particle Technology and Engineering” published by Elsevier in 2016 and edited two books entitled “Discrete Element Modelling of Particulate Media” and “Particulate Materials: Synthesis, Characterisation, Processing and Modelling” published by RSC publishing. He also edited five journal special issues and published over 100 scientific papers. He has given more than 60 invited presentations and seminars at international conferences, industrial companies and universities worldwide. Prof. Wu is a member of the advisory and editorial board for “Particuology”, and “Acta Pharmaceutica Sinica B (APSB)”.

Prof. Wu has expertise in particle technology, discrete element methods, finite element analysis, modelling and simulations, pharmaceutical engineering and granular dynamics. His research has been supported by global pharmaceutical companies including Pfizer, AstraZeneca, Sanofi and MSD, in addition to EPSRC and EU. He recently coordinated a EU FP7 consortium on predictive modelling of roll compaction that consists of 14 partners and 15 researchers from 8 European countries, with a total budget of €3.8m and is also leading a new EU H2020 consortium (€4.2m with 15 partners) on thermomechanical analysis of particle systems.

Particle Resolved Simulations of Dense Gas-Particle Flows

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Abstract

Dense gas particle flows are frequently encountered in a variety of large scale processes for the production of functional powders, base chemicals and synthetic fuels. In the last decades considerable progress has been made in the modeling of these complex flows using Multiphase Computational Fluid Dynamics (MCFD) approaches. Both Euler-Lagrange (EL) and Euler-Euler (EE) models have been successfully used to predict hydrodynamics (gas bubbles behavior and solids motion) as well as mass and heat transport characteristics in dense particle laden flows.

The quality of these predictions strongly depends on the closures for mass, momentum and heat exchange between the suspended particles and the continuous phase (often a gas) which mostly have a strong empirical base. However, due to the ever increasing advancements in numerical algorithms and computing hardware, it has been recognized that ‘Particle-Resolved’ simulations offer an attractive alternative to obtain these closures especially for poly-disperse and non-spherical particles. In this presentation the focus will be on ‘Particle-Resolved’ simulation models based on the Immersed Boundary Method (IBM) to obtain a better understanding and quantitative description of mass, momentum and heat exchange in dense gas-particles flows.

Brief Biography

Hans Kuipers graduated in 1985 at the department of Chemical Engineering of the University of Twente. In December of the same year he started with his Ph.D. study at the Reaction Engineering group of University of Twente on detailed micro balance modeling of gas-fluidized beds. In June 1990 he received his Ph.D. degree in Chemical Engineering and was appointed as assistant professor in the Reaction Engineering group headed by Prof. W.P.M. van Swaaij. In 1994 he was appointed as associate professor in the same group. In 1999 he became fulltime professor in Fundamentals of Chemical Reaction Engineering at the University of Twente. From 2006 until 2010 he was Scientific Director of the Institute of Mechanics Processes and Control (IMPACT) at the University of Twente. Since August 2010 he is a fulltime professor at Eindhoven University of Technology and heads the group Multiphase Reactors. He teaches amongst others introductory and advanced courses on transport phenomena and multiphase reactors. His research interests are in the area of multiphase chemical reactors. He participates in the Gravitation Program Multi-scale Catalytic Energy Conversion (MCEC) and acts as program director Process Technology and member of the Executive Board (EB) of the Advanced Research Center (ARC) Chemical Building Blocks Consortium (CBBC).

Modelling Subsea Gas Blowouts

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Abstract

A subsea gas blowout can have catastrophic impact on human life and offshore assets. Understanding how the gas surfaces is vital for risk assessments and emergency planning. CFD is a valuable tool in quantifying the behavior of the bubble plumes resulting from these events. The particular challenge in modelling subsea gas blowouts is the large scales involved. Traditional bubble plume modelling is applied to reactors in with typical length scale of 1-2 meters and sometimes up to 7-8 meters, whereas a gas blowout can happen from depths below 1000 meters. This adds complexity to material properties and challenges with respect simulation resolution. An Eulerian-Lagrangian modelling concept has been developed for these large scale bubble plumes. The model is presented. Results are discussed with respect to experimental observations.

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Brief Biography

Jan Erik Olsen is research manager of the Flow Technology group at SINTEF in Norway. He holds a MD in physics and a PhD in mechanical engineering. He has practiced CFD for 15 years with focus on industrial applications, especially towards the metallurgical and oil and gas industry.

Single and Two-phase Hydrodynamics, Heat and Mass Transfer in Micro-channels: The Complexities of Laminar Flow

David F. Fletcher

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Abstract

Over the last two decades there has been a massive interest in miniaturisation for both analytical studies (Lab on a Chip) and process intensification. This presentation will draw together work performed over the last 15 years in this area and distil the important physics that must be modelled and numerics lessons learned. Whilst laminar flows appear simple, as soon as they become transient, two phase or contain heat/mass transfer at interfaces there are huge complexities. What might start as a very simple study often involves the need for advanced numerics, vast computing resources and great care to avoid results dominated by numerical error. The presentation will contain examples covering single phase heat transfer in complex geometries, Taylor bubble heat transfer, annular flow boiling and micro-mixing studies.

Brief Biography

David Fletcher is an Adjunct Professor at the University of Sydney, where he has performed CFD based research over the last 25 years. He is also a Visiting Professor at the Université de Toulouse, France, with whom he has been associated over the last 20 years. He has a long association with ANSYS, having used CFX when it was first developed at the UK Atomic Energy Authority and is the Senior CFD specialist at LEAP Australia. He has a wide interest in CFD modelling applied to the process industries involving complex chemistry and multiphase flow, as well as biomedical and pharmaceutical applications.

Using Failure Dynamics At The Mesoscale For Early Prediction Of Slope Failure From Data

Antoinette Tordesillas[1] and Robin J Batterham[2]

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Abstrac

Knowledge of granular failure is not only important in the design, control and optimisation of particulate processes in many industries, but also in risk assessment of natural hazards like earthquakes and landslides. This study uses knowledge and data assets on mesoscale failure dynamics in granular media to develop tools for early prediction of failure from small to large scales [1,2]. In particular, we present a new transdisciplinary approach, combining elements of artificial intelligence, complex networks, and granular media mechanics to examine spatio-temporal patterns from surface motion radar data for landslide monitoring. Two vastly different landslide behavior are studied: L1 exhibits quasi-brittle failure, while L2 presents a relatively slow ductile deformation preceding a collapse. The location of failure, spanning hundreds of meters for L1 (tens of kilometers for L2), is predicted two weeks in advance (ten weeks in advance) of the collapse. In the context of granular media failure, this study provides evidence for the "common principle of mesoscience" [3,4], especially its role as a key enabler of gap-jumping across scales towards understanding and predicting complex multiphysics phenomena.

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[2] S Das, N Kandhari, A Tordesillas (2019) A probabilistic machine learning algorithm for on-line quantification of risk of failure of a landmass (in preparation)
[3] J Li (2015) Mesoscales: the path to transdisciplinarity. Chem Eng J 277:112–5
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Brief Biography

Professor Antoinette Tordesillas conducts research across the domains of mathematics, engineering, physics and geophysics. She has been chief investigator on projects from a wide range of application domains, including: off-road vehicle mobility in terrestrial and extraterrestrial environments, sensor networks, infrastructure and geological materials, and biological structures. Her recent work is focused on granular data analytics with a focus on using failure dynamics to understand resilience in networked systems. These efforts involve international collaborations with multidisciplinary teams from the experimental and high performance computing fronts, with funding from US Department of Defense agencies like

the US Army and US Air Force. Recent highlights include a patented code on landslide prediction with Professor Robin Batterham, spotlighted by agencies around the world including the United Nations Office for Disaster Risk Reduction, The Australian Bulk Handling Review, The Smithsonian, US DoD Scientific Advisory Board Conference and UNESCO. Her work was recently recognized through a new grant from the *US DoD High Performance Computing Modernization Program* which supports transdisciplinary research into networked systems. The research will see Antoinette (lead CI) and her collaborators from Statistics and the School of Computing & Information Systems at the University of Melbourne combine their data analytics expertise and capabilities to develop new methods "Towards Designing Complex Networks Resilient to Stealthy Attack and Cascading Failure".

Professor Robin Batterham is one of Australia's leading scientists and researchers. Awarded an Officer of the Order of Australia his citation reads "For service to science, engineering and technology through promoting collaboration, excellence and innovation to enable Australian industry to remain internationally competitive and innovative." As Chief Scientist of Australia between 1999 and 2005, Robin advised the Australian Government on all matters associated with science, engineering and innovation. He was responsible for a major research review which produced the blueprint for government support for research in the early years of the 21st century. Robin worked at CSIRO for 18 Years as a chief scientist in the field of mineral and process engineering. His team of 240 scientists in four laboratories collaborated directly with mining and metallurgical companies to improve their performance. He joined Rio Tinto's resource and processing developments team, becoming vice president of research and technology, then global practice leader in innovation before becoming Rio's group Chief Technologist. In these roles Robin undertook or had overview of many innovative projects in all aspects of mining, including geotechnical interests.

Now Kernot Professor at the University of Melbourne he is responsible for strategic leadership of major projects in energy. His current areas of focus also include the stability of rock faces in mining.

12-Velocity Multiple-Relaxation-Time Lattice Boltzmann Model for Three Dimensional Incompressible Flows

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Abstract

This paper proposes a 12-velocity multiple-relaxation-time lattice Boltzmann model for the three-dimensional incompressible flows. This model in principle has higher computational efficiency than the commonly used 13-velocity multiple-relaxation-time lattice Boltzmann model, as proposed by Humières *et al*. (Phys. Rev. E, 63, 066702). The accuracy and stability of the 12-velocity and 13-velocity models have been compared using different simulations involving pressure-driven steady Poiseuille flow, periodically varying pressure-driven unsteady pulsatile flow, and lid-driven cavity flow. The result shows that the 12-velocity model has higher accuracy when applied to the Poiseuille and pulsatile flows, especially under the conditions of large pressure gradients. Also, the simulations of lid-driven cavity flow at different Reynolds numbers suggest that the new model can maintain the same stability as that of the 13-velocity model.

Brief Biography

Wenhuan Zhang obtained his BSc in statistics in 2008 and PhD in thermal power engineering in 2013 from Huazhong University of Science and Technology, P. R. China. In 2013, he joined Ningbo University as a lecturer until now. Currently, he is a visiting scholar in the ARC Research Hub for Computational Particle Technology, Department of Chemical Engineering at Monash University. His research is focused on the lattice Boltzmann modelling, discrete element simulation, and GPU computing for fluid/particle-fluid flow, heat and mass transfer.

A Solid-Stresses-Based Multiphase Particle-in-Cell Model for Gas-particle Flow in Fluidized Beds

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Abstract

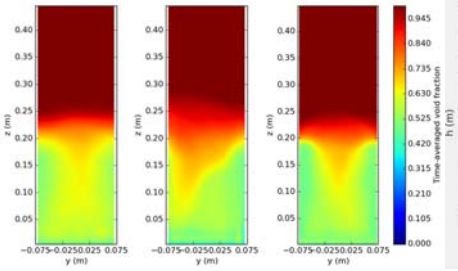
Fluidized beds are widely applied in the chemical, petrochemical, metallurgical, environmental and energy industries due to their favourable mass and heat transfer characteristics. In the past few decades, computational fluid dynamics has proven to predict hydrodynamics of gas-solid fluidized beds well. The Euler-Lagrange Discrete Particle Model (DPM) and Euler-Euler Two-Fluid Model (TFM) are the two most common modelling approaches for gas-solid flow in fluidized beds. TFM is the preferred model to study large scale fluidized beds, but the model suffers from high numerical diffusion. Moreover, the KTGF theory used in TFM assumes near-elastic collisions and is limited to spherical particles. DPM proves to be more accurate in the modelling of gas-particle flow. However, Lagrangian models quickly become computationally too expensive because of the large number of particle interactions. Therefore, coarse graining the interactions between discrete particles is an emerging approach to model large numbers of particles effectively. New coarse-grained model developments are of vital importance for the advancement of large-scale modelling of gas-particle flows that are flexible enough to be extended to polydispersity and non-spherical particles. In this study, a novel solid-stresses-based multiphase particle-in-cell (sMP-PIC) is developed for predicting dense particulate-fluid flow.

The solid-stresses-based multiphase particle-in-cell (sMP-PIC) model is an in-house developed particle solver, integrated with the OpenFoam fluid solver. The fluid phase is treated as a continuum and the solids are modelled by Lagrangian particles. The sMP-PIC model grew out of the MP-PIC model of Snider 2000, that employs a fixed Eulerian grid, and particles are traced in a lagrangian fashion, including a parcel approach where each simulated particle represents a large collection of real particles. Each parcel follows Newton's equations of motion, where inter-phase momentum transfer is accounted through mapping and interpolating quantities back and forth between parcel locations and the Eulerian grid. Particle collisions in MP-PIC are not fully resolved but are derived from particle pressure and, for the first time in this work, particle stresses based on the Harris and Crighton 1988 stress closure. In the sMP-PIC model, we implemented a functional form for the particle stress tensor where the coefficients are obtained computationally by means of DPM simulations. The idea is to extend the model from spherical particles to non-spherical particles, for which no KTGF theory is currently available in the literature. Efficient modeling of solid stresses and interpolation techniques from particle positions to Eulerian cells are proposed. The granular temperature dependent viscous stresses and random forces are typically ignored in classical MP-PIC models due to their assumed insignificant effect. Importantly, we incorporated viscous stresses and random forces, representing scattering of particles by mutual collisions, which are obtained from DPM simulations by measuring the actual variance. Details of the model development and validation are presented in this study.

Results from the sMP-PIC model are compared with MP-PIC from OpenFoam (MPPICFoam) and with DPM simulations from CFDEM-LIGGGHTS, respectively. A pseuduo-2D fluidized bed of dimension 0.015x0.15x0.45 m^3, with particles of density 2526 kg/m^3 and diameter 2500 micron equal

to the experimental setup of Goldschmidt et al. 2001 is considered for the comparison. Comparison is made on the basic of pressure drop, void fraction distribution, bubble size, granular temperature and solids motion. We studied the effect/sensitivity of particle stresses, drag force, grid size, and interpolation techniques in the newly developed sMP-PIC model. We observe that sMP-PIC is in much better agreement with DPM results than MPPICFoam (see Fig. 1 and 2). Unrealistic over-packing of solids is predicted in MPPICFoam. In sMP-PIC these limitations are overcome by new developments and no over-packing of particles occurs. Particle velocities and circulations are in good agreement with DPM results, where solids are moving upward in the center and downward near to the wall. Time-averages porosity plots from sMP-PIC in Fig.1 reveals the path of bubble motion, which is in agreement with results of DPM.

In conclusion, a novel solid-stresses-based multiphase particle-in-cell model is developed and validated to study gas-solid fluidized beds. Even for a parcel size 1, meaning that each particle is modelled, the model is 40-50 times faster in comparison with DPM, which allows us to handle a large number of particles. In future study, we plan to extend the model for dense flows of non-spherical particles.



(a) sMP-PIC (b) MPPICFoam (c) CFDEM

Fig. 1: Time-averaged porosity plots

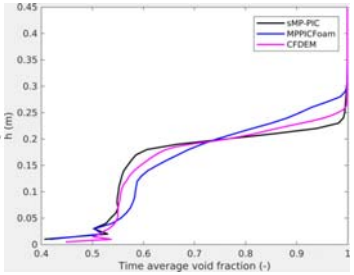


Fig. 2: Averaged void fraction vs. height of the bed

Acknowledgments

The authors thank the European Research Council for its financial support under its consolidator grant scheme, contract no. 615096 (NonSphereFlow).

Brief Biography

Dr. Vikrant Verma is a postdoc researcher in the Process & Energy department at Delft University of Technology. Prior to this he was a postdoc at National Energy Technology Laboratory, WV USA for two years. In the year 2014, he received his PhD degree in chemical engineering from Eindhoven University of Technology, Netherlands. He completed his B-Tech and M-Tech in chemical engineering from Indian institute of Technology, Delhi India. His research experience includes CFD modeling and simulations of gas-particle flows in fluidized beds.

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MP-PIC Simulation of Blood Flow across a LAD with High Stenosis

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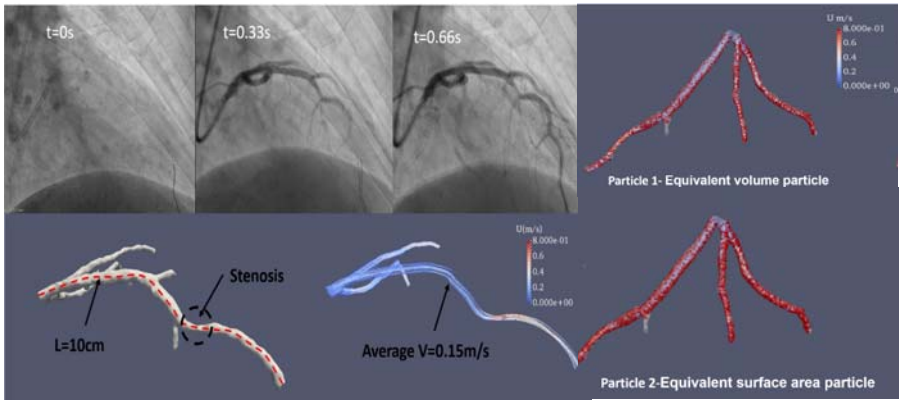
Abstract

Background: The CTA-based computational fluid dynamics (CFD) has been proposed as a non-invasive method to diagnose the coronary artery stenosis. Although blood contains a huge quantity of blood cells, the blood was still treated as a single-phase fluid in most of the CFD models, which may result in the inaccurate estimation of the pressure drop across an artery with stenosis.

Method: A male patient with high stenosis at his left anterior descending (LAD) was taken as a patient-specific model. The patient underwent a cardiac catheter examination of the pressure drop across the stenosis. A conventional single-phase model and a multiphase particle in cell (MP-PIC) model were chosen to simulate the pressure drop across the stenosis. In MP-PIC, two types of spherical particles were used to represent the non-spherical blood cells. Particle 1 has the same volume of a red blood cell while Particle 2 has the same surface area of a red blood cell.

Results: Single phase fluid model showed that the predicted pressure drop at the stenosis is 6mmHg that is smaller than the measured pressure drop (20mmHg). MP-PIC with Particle model 1 showed that the estimated pressure drop at the stenosis is 15mmHg, smaller than the measured pressure drop; while the MP-PIC with Particle model 2 showed that the estimated pressure drop is 25mmHg, greater than the measured pressure drop. It should be noted that the measured pressure drop is in the estimated range by Particle model 1 and 2.

Conclusion: Blood is a multiphase fluid; blood cell movement certainly influences the plasma flow. Single phase fluid simulation underestimates the pressure drop. MP-PIC simulation showed that the measured pressure drop falls in the estimated range using different particle models. This study indicated that in order to accurately estimate the blood flow, a reasonable multiphase flow model must be applied in the medical-image-based CFD simulation.



Blood flow in a coronary artery with high stenosis

Brief Biography

In June 2003, Dr. Zhang was awarded a Ph.D. degree in Mechanical Engineering from Tsinghua University, China. Since then he has worked in different research bodies, including Purdue University in USA (2005 to 2007), Chinese Academy of Sciences in China (2007 to 2010), Macquarie University (2010 to 2013) and Western Sydney University (2013 to 2014) in Australia. From 2007-2010, he worked in the Institute of Mechanics, Chinese Academy of Sciences as an Associate Professor. Since 2015, he is a Research Professor in the School of Medicine at Tsinghua University and in Tianjin Research Institute for Advanced Equipment, Tsinghua University. Since 2010, he started to use computational expertise and mechanical engineering knowledge to conduct cutting edge biomedical engineering projects, focusing on medical image based hemodynamic analysis, estimation of the outcome of intracranial bypass surgery, estimation of the outcome of intracranial stent deployment, estimation of coronary artery stenosis, and the design of a blood pump of extracorporeal assisted system.

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Orientation Discretization in Discrete Modelling of Non-spherical Particles

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Abstract

Discrete element method (DEM) has been widely used in studying particulate systems. However, the modelling of non-spherical particles is still a non-trivial issue. Compared to spherical particles, the difficulty for the modelling of non-spherical particles mainly lies in calculating the inter-particle forces, which are complicatedly dependent on the particle orientation due to the non-symmetries of the non-spherical shapes, and the dependencies are also rather different for different shapes. In fact, most current models for non-spherical particles need to solve high order equations by numerical iterations, with different algorithms used for different shaped particles. We have proposed the orientation discretization database solution (ODDS) to model arbitrary shaped non-spherical particles in a simple and universal way and used this method in different applications. In this paper, we review our recent studies related to this method. The concept is briefly introduced first. Then the packings of different non-spherical particles simulated by this method are discussed. Moreover, the method is also used to evaluate the existing contact force models, such as the common normal and geometrical potential methods for non-spherical particles. And based on the force database, the explicit force models for specific shapes have been constructed by Fourier series. In these studies, sub-particle scale finite element modelling (FEM) is used to obtain the precise inter-particle forces. Finally, the method is used in some theoretical analyses of the contact mechanics for different shaped particles. It is shown that ODDS is effective not only in simplifying the DEM simulations, but also in understanding the interaction between non-spherical particles.

Brief Biography

Dr Kejun Dong is currently a Senior Lecturer at the Centre for Infrastructure Engineering (CIE), Western Sydney University (WSU). He earned both his bachelor's and master's degrees from Department of Applied Physics, Hunan University (China) in 1996 and 1999 respectively, and received his PhD from School of Materials Science and Engineering, University of New South Wales (UNSW) in 2007. He then worked as a research fellow and Lecturer later in the Laboratory for Simulation and Modelling for Particulate Systems (SIMPAS) at UNSW, until he joined WSU in 2014. He has been awarded with Australian Postdoctoral Fellowship in 2009 and Australian Discovery Early Career Researcher Award (DECRA) in 2012. Dr Dong's main research interests are computer simulation and structural characterization of particulate systems, including granular materials and amorphous metal.

Key sub-grid quantities affecting the filtered drag force and the derivation and analysis of their transport equations

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Abstract

Based on numerous correlative analyses of fully resolved simulations, the filtered drag force is found to correlate well two sub-grid quantities: the drift velocity and the scalar variance of solid volume fraction, with the drift velocity as the primary marker. We refer to the drift velocity as the gas drift velocity since it is defined as the difference between the filtered gas velocity seen by the particle phase and the resolved filtered gas velocity and a drift velocity for the solid phase can be defined similarly. To date, various algebraic models for the gas drift velocity fail to give entirely satisfactory prediction of the filtered drag force. This makes a more elaborate model very desirable. In this study, the transport equation for the gas drift velocity was theoretically derived from the standard two-fluid model (TFM) equations. This leads to the appearance of several new unresolved sub-grid terms. The budget analysis of these new terms was performed by analyzing the data of fully resolved simulations. It shows that the production term due to micro-scale gradient of the gas volume fraction fluctuations and the source term accounting for the contribution of the inhomogeneous drag force at the micro-scale are both important for the transportation of the gas drift velocity. The new approach, though requires additional closures, is believed to have the potential to give better prediction of the filtered drag force for gas-solid fluidization problems. Furthermore, the dependence of the filtered drag force on sub-grid quantities are analyzed by employing the second order Taylor polynomial approximation to the microscopic drag coefficient. Through theoretical analyses of the coefficients of the new appearing sub-grid quantities in this approximation, it is found that, other than the gas drift velocity and the scalar variance of solid volume fraction, the solid drift velocity and a third-order moment defined as the covariance of squared solid volume fraction and the fluctuation of slip velocity, are significant for an accurate estimation of the filtered drag force at low Reynolds numbers. The data from fully resolved simulations support this finding and also reveal that the contributions of these four quantities vary at different solid volume fractions.

Brief Biography

Dr. Qiang Zhou received his Bachelor degree From Zhejiang University in 2004 and PhD degree from Tsinghua University in 2010. After that, He joined Prof. Liang-Shih Fan's group in The Ohio State University, where he worked first as a post-doctoral researcher and then as a research associate. In September, 2015, He joined Xi'an Jiaotong University as a professor and he is one of the recipients of the national "Thousand Youth Talents Plan". His major research interest is in the field of computational multi-phase flow with the focus on the effect of meso-scale structures on fluid-particle drag force. Dr. Qiang Zhou would like to present this work by oral talk.

Ming Jiang is a PhD candidate in the school of chemical engineering and technology, the Xi'an Jiaotong University. His research interests include the effects of meso-scale in gas-solid system, the modeling of filtered TFM and the application of high-performance computing in PR-DNS based on LBM and fTFM simulations. Ming Jiang has a BS in Energy Power System and Automation and a MA in Power engineering from Xi'an Jiaotong University. Contact him at jiang.k3d.kollo @stu.xjtu.edu.cn.

Advances in DEM simulations using GPUS: A focus on particle shape and number

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Abstract

The Discrete Element Method (DEM) is the most commonly used numerical methods for the modeling of granular material. However the computational cost of the DEM has limited the number and shape estimation of particles. In this paper we look at the Graphical Processor Unit (GPU) as an alternative computing platform to the CPU that has enabled detailed particle shapes such as polyhedra as well as an increase particle number to tens of millions. In particular we will consider the effect of particle shape in mills that is an important part in the processing of minerals as well as the charging process of blast furnaces in the steel making industry. We show that the effect of particle shape cannot be ignored and needs to be taken into account in the optimization of these process. It is also made apparent that the use of GPU computing enables a new performance level in DEM simulations make it more tractable to industrial applications and design optimizations.

Brief Biography

Dr Nicolin Govender is a Marie-Curie Research Fellow at the University of Surrey. He is the PI of the NVIDIA GPU Research Centre for Discrete Element Particle Modeling, which he established with the support from NVIDIA in 2013. This is the only research center specializing in GPU computing for particle systems. Dr. Govender is also associated with several world-leading institutes as an affiliated scientist. He is a member of the ATLAS Collaboration at CERN in Switzerland where he works on research projects associated with computing in High Energy Physics. He is also a visiting researcher at the Ecole Mines Douai in France and works on collaborative projects on granular mechanics with special application to Civil Engineering, and at the University of Utah working on collaborative projects related to Mining and Minerals Engineering as well as Tshingua University in China where he collaborates on Geo technical projects.

Dr Govender has over 8 years of experience on computational methods for particles and has been working on the GPU since the advent of general purpose GPU computing in 2008. During his PhD, he developed a novel approach for the implementation of DEM on the GPU using polyhedral particles. He has pioneered discrete element modeling of polyhedral particles on the GPU and is recognized as an international expert in this area and has received various awards. He has also reviewed numerous papers for international journals in the field of DEM and GPU computing, such as AICHE J, Chemical Engineering Science, Computer and Structures, Powder Technology.

Dr Govender has published over 50 journal papers spanning High Energy Physics, DEM and high performance computing with an H-factor of 45 (as of August 2016, Google Scholar). He also developed the academic GPU-based DEM code "BLAZE-DEM", that is hosted by Elsiever and is now used by a growing number of institutes, such as the University of Utah, University of British Columbia, Tshingua University, Chinese University of GeoSciences Beijing, Monash, Ecole Mines Doua, to name a few. This is currently the fastest DEM code for simulating polyhedral particles on the GPU.

Impact Energy Dissipation Analysis during Ship Loading of Iron Ore by Large-scale MPI-GPU-DEM Simulation

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Abstract

Degradation of the iron ore during handling and transportation results predominantly from impact from drops, such as the ship loading process. The lump ore degradation is directly related to the particle energy dissipation after impacts with wall or particles. Previous studies on iron ore degradation are mainly based on experimental drop tests, which cannot reflect the practical particle dropping processes where the particle contacts depend on the dropping history of the granular flow. Alternatively, discrete element method (DEM) can provide macro-scale flow behavior and micro-scale inter-particle and particle-wall interaction information. In this work, a graphical processing units (GPU) and message passing interface (MPI)-based DEM is developed for the large-scale iron ore ship loading process. The MPI-GPU-DEM model is then applied to analysis the particle impact and energy dissipation during the loading process. The effect of dropping height, belt speed and loading speed on energy dissipation are studied. The particle properties such as size distribution (with particle size from 3mm to 40mm) on segregation and cushion effect of degradation is also investigated. These studies provide useful guideline to the practical ship loading operation and material properties for iron ore exporter.

Brief Biography

Jieqing Gan is a postdoctoral research fellow with the Laboratory for Simulation and Modelling of Particulate Systems (SIMPAS), Department of Chemical Engineering, Monash University, Clayton VIC 3800, Australia (e-mail: Jieqing.gan@monash.edu). She received her doctorate of philosophy degree in Chemical Engineering in December 2015 at Monash University. Her research area refers to DEM/CFD-DEM modelling and simulation on fluid and granular flow, heat transfer and chemical reaction with spherical and non-spherical particles. She also develops GPU-MPI based DEM for large scale simulation of granular flow with arbitrary wall geometry, complex wall movement and non-spherical particles.

Designer Granular Materials - A Combined Discrete Element Method and Evolutionary Algorithm Approach

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Abstract

We apply a combination of particle based modelling and evolutionary algorithms to develop new custom granular materials that are tailored to specific applications. These applications range from determining optimal morphologies and compositions of granular materials for maximum density, through to more complex optimisation of material properties and device design for maximum performance.

We utilize a fully dynamic linear spring Discrete Element Method (DEM) simulation that allows for the specification of the particle properties including the sizes, masses, inter-particle friction, coefficient of restitution, particle shape and their interaction with arbitrary dynamic mesh objects. Further details of our DEM technique are given in ref. [1]. In our model particle shapes are represented as superellipsoids [2]:

$$\left(\frac{x}{a}\right)^m + \left(\frac{y}{b}\right)^m + \left(\frac{z}{c}\right)^m = 1$$

where we refer to m as the shape parameter, and a, b and c are the semi-major axis lengths. For $m = 2$, we recover the general formula for an ellipsoid [3], while larger values of m generate increasingly cubic shapes. This gives us the ability to investigate a broad range of particle shapes, smoothly transitioning through a range of surface curvatures and aspect ratios.

Evolutionary algorithms employ techniques inspired by biological evolution such as reproduction, mutation, recombination, and selection to optimise a population of candidate solutions (individuals) based on a specified fitness function [4, 5]. We start with an initial population of randomly created individuals and evaluate the fitness of each. We then select from the population based on the individuals fitnesses and breed new individuals using specified crossover and mutation operations to create new offspring. These new offspring are evaluated and replaced in the population based on their relative fitnesses. The process then repeats to iteratively improve the fitness of the population of candidate solutions.

Figure 1 shows an example evolution of the fitness (here specified as the packing fraction) of a population of bidisperse packings of superellipsoids, where we have allowed the shape parameter m and aspect ratios of each species to be varied. The evolutionary algorithm iteratively explores the parameter space, improving both the maximum and mean fitness of the population of candidate solutions, converging on final shapes that balance the relative contributions of surface curvature and aspect ratio for each species. This approach can be

used to optimise any desired properties of the granular material and the properties of simulated dynamic mesh objects that the material is interacting with.

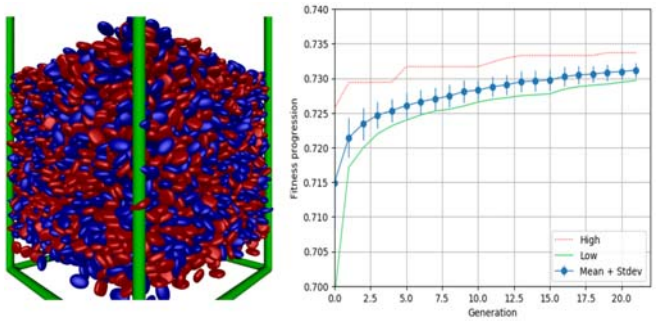

Figure 1: (Left) Image of a dense bidisperse packing of superellipsoids obtained via an evolutionary approach. (Right) Evolution of the fitness (packing fraction) over 21 generations for a population of bidisperse packings of superellipsoids.

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Brief Biography

Dr. David Howard is a Research Scientist at Data61 and leader of the Autonomous Design Testbed in CSIRO's AIM Future Science Platform. David's primary research interests include machine learning, evolutionary computing and autonomous robotics - robots that can flexibly learn and adapt to their surroundings by continuously updating their knowledge base in a self-guided manner.

Dr Gary Delaney leads Data61's Computational Modelling Group at the Commonwealth Scientific and Industrial Research Organisation (CSIRO) in Melbourne. Gary's primary research interests are in computational modelling and structural characterization of granular systems, and applications of Machine Learning in understanding and optimizing natural and industrial processes.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

Local Contact Point Treatment in Sphere Packings

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Abstract

CFD simulation of fully resolved packed beds has become a valuable tool to get deep insight into local phenomena in fixed bed columns. To get reliable simulation results special care has to be taken at particle-particle and particle-wall contact points when meshing such packings. Due to the complexity of the geometry highly skewed mesh cells can appear around contact points when using automated meshing tools without any contact point pretreatment.

Many authors have studied the influence of different contact point treatments on the porosity, pressure drop and heat transfer in packed beds consisting of spheres or cylinders. Using global modifications (reducing or increasing the particle size by 1-2%) has big influence on the porosity of the packing and therefore on the simulated pressure drop. Introducing small cylinders between particles and treating them as a solid or a fluid leads to the necks/bridges or caps method, respectively. Using the bridges method (shown in *Fig. 1*) with a bridge to particle diameter ration of d/D = 0.16 - 0.2 leads to the best prediction for pressure drop over packed beds of mono-sized spheres [1, 2]. However, previous studies have mostly focused on mono-sized particles.

The objective of this research is to study the influence of bridge size on the porosity and the pressure drop of randomly packed beds consisting of spheres with size distribution. Pressure drop experiments and numerical simulations for different bimodal mixtures of spheres and different flow rates was carried out (*Fig. 2*). An optimal bridge to particle diameter ratio d/D was found by variation of the bridges diameter in the simulation. A CFD simulation with multiple sphere sizes was run to validate the recommended d/D ratio for more complex particle beds.

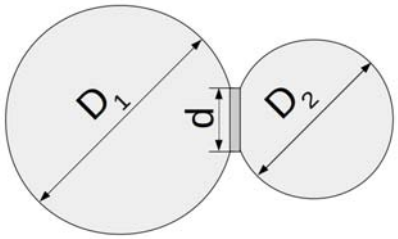

Figure 1: Bridges method: two spheres with different diameters (D_1, D_2) connected with a bridge of diameter d

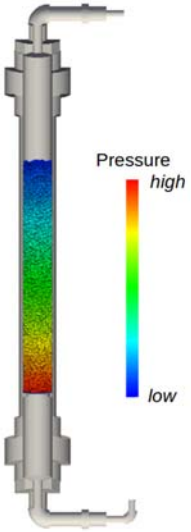

Figure 2: Simulated pressure drop over a packing

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Brief Biography

Dr. Michael Harasek received his PhD in Chemical Engineering from TU Wien in 1997. For more than twenty years, he has been working on the design of new processes and technologies in the process industries and related fields. A major part of his research work is dedicated to the development of environmentally friendly technologies and related fields as well as process intensification. Michael Harasek works on the application of CFD and experimental fluid dynamics in many fields of chemical engineering, and the implementation of multiscale and multiphysics capabilities for complex flow problems. As head of the research area „Thermal Process Engineering and Simulation" he guides a team of about 25 scientists at TU Wien, Institute of Chemical, Environmental and Bioscience Engineering.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

Just-In-Time Training (JITT) Paradigm for Granular Processes

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Abstract

The recent scientific and technological advancements in computing platforms and artificial intelligence has increased the demands for a more agile and responsive industrial work force. The rapid globalisation and porosity of international borders is allowing for an ever-increasing competitive market that attracts more and more projects with higher diversity and wider skill requirements. Current training paradigms of workshops and courses is being supplemented by online training material, but often these only focus on foundational knowledge. The demands for highly specialised training on highly specialised processes is ever increasing. This combined with a doubling over the last 20 years in the global average of the number of jobs within the first five years following graduation is putting pressure on sustainable and successful delivery of projects.

These pressures can be alleviated by a just-in-time training (JITT) paradigm that would allow new employees to build up an in-depth knowledge and fundamental understanding of specialised processes. Although various training models are available to achieve JITT, we are strong proponents of simulation based JITT for granular processes. Although this would have been unimaginable 20 years ago in granular processes, that were consistently dominated by two-dimensional analyses due to the computational cost of discrete element simulations, recent advances in graphical processing unit (GPU) computing platforms and artificial intelligence (AI) is making this a reality even for the discrete element method. GPUs allows for up to a hundred-times speed-up of DEM simulations [2] and AI allows for an accurate description of the process manifold that then allows the discrete element simulations to be replaced by responsive AI regression models.

The strategic deployment of tailor-made and validated simulation environments that utilise explicit time integration combined with a mature understanding of model fidelity is allowing engineers to apply real-time changes to simulations. Allowing engineers to interactively engage with a simulation to study the effect of various model parameters, geometrical changes of the environment with which the particles interact or changes in

boundary conditions in steady state processes or continuous bulk material handling processes is changing the paradigm from *analyse-wait-modify-analyse cycle (AWMAC) or batch-analyse-wait-modify-batch-analyse cycle (BAWMBAC)* to an active investigation. This naturally extends to an active learning tool and JITT environment when supplemented with a guided investigation protocol. This allows engineers to interact with the simulation to develop both quantitative and qualitative understanding. The role of this paradigm to allow for in-house training of new engineers or the use of this paradigm by experienced engineers to assess a process before an actual site visit may prove invaluable in a competitive and global market.

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Brief Biography

Daniel N. Wilke is a research fellow in the Center for Asset and Integrity Management (C-AIM) and senior lecturer in the Department of Mechanical and Aeronautical Engineering of the University of Pretoria, South Africa. His current research focuses on the development of interactive design optimisation technologies and just-in-time education and training environments that is powered by graphical processing unit (GPU) computing platforms and artificial intelligence. His artificial intelligence research extends from statistical learning, machine learning to deep learning for supervised, semi-supervised and unsupervised learning, which typically finds application in model calibration, industrial processes monitoring, degradation analysis and prognostic health-monitoring systems. He has co-authored over 70 peer-reviewed journal articles, full-length conference papers and book chapters. He is also the co-author of the 133rd book in the Springer Optimization and Its Applications Series, namely Practical Mathematical Optimization. At national advisory level, he served for five years on the Fluxion Specialist Working Group, which strategised the national development plan and focus areas of computational mechanics skills for the South African National Defense Force. He is a member of the South African Institution of Mechanical Engineering and the Society for Industrial and Applied Mathematics. He is actively serving on the Executive Committee of the South African Association for Theoretical and Applied Mechanics and the South African National Committee for the International Union of Theoretical and Applied Mechanics (IUTAM). In 2015 he was elected as an inaugural Tuks Young Research Leader Fellow.

Experimentally Validated Computational Models to Predict the Impact of Humidity on the Flow of Granular Mixtures

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Abstract

Moisture-induced flow variability in pharmaceutical mixtures lead to multiple impediments during manufacturing of tablets/capsules as the processing and storage humidity conditions can bear significant impact on the final product quality. Experimentally validated Discrete Element Method (DEM) based computational models has been developed to predict the effects of humidity on pharmaceutical powder flow by altering the cohesive forces based on granular bond numbers in simple geometries. Statistical formalism (Simplex Centroid Design) has been performed to understand the moisture induced cohesion in binary and tertiary mixtures at 20%, 40% and 60% RH. V-blending was applied to prepare the pharmaceutical blends, and mixing characterization was performed using a Raman PhAT probe. Optimum fill volume was established for the mixing conditions to minimize static charging due to blender wall interactions on the pharmaceutical powders. Statistical analysis predicted and quantified the non-linearity of the moisture-induced cohesion between the pharmaceutical powders within the blends, based on their systematic hopper discharge studies. A methodical implementation of these quantification tools was hence performed to validate a design space that enables an approach to the appropriate selection of blend concentrations that achieve minimum mixture flow variability across different humidity conditions.

Brief Biography

Bodhi Chaudhuri is an Associate Professor of Pharmaceutics, Chemical Engineering and Material Sciences at UConn. He got his PhD in Mechanical Engineering from NJIT after obtaining his MS and BS both in Chemical Engineering from Indian Institute of Science, Bangalore and Jadavpur University, Kolkata, respectively. He performed postdoctoral research in Chemical and Biochemical Engineering at Rutgers University and has 3 years of industrial experience. He has published more than 60 peer-reviewed journal articles, book chapters, conference proceedings and delivered more than 30 invited talks. He acts as an editorial board member for Advanced Powder Technology, Journal of Pharmaceutical Sciences, Asian Journal of Pharm. Sciences, and several other international journals in the areas of fluid mechanics, drug design, pharmaceutical sciences, and chemical engineering. His research has been funded by NIH, NSF, FDA, American Cancer Society, PhRMA, Pfizer, Genentec, Takeda, Astrazeneca, and several pharmaceutical companies. He regularly consults pharmaceutical, biotechnology, and engineering companies. He received Young Investigator Award from US-FDA, PhRMA Foundation Award, and several other prestigious awards.

Liquid Redistribution upon the Liquid-bridge Rupture between Two Unequal Particles with a Minimal Energy Method

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Abstract

For a polydisperse particulate system, the formation and the rupture of the liquid bridge between two unequal particles have significant effects on the local liquid distribution and subsequently the system performance. This work investigated the liquid redistribution upon the liquid-bridge rupture using a minimal energy method by means of the software Surface Evolver (SE). The calculated results, including the bridge rupture distance, the capillary force, and the transferred ratio, were compared with the previously published data obtained by numerically solving the Laplace-Young equation, showing good agreement. Based on this method, the effects of particle radii ratio, contact angle and the volume of the liquid bridge on the liquid transfer ratio were further examined. Using the grey relational analysis method, the effects of the radii ratio were found to be the most significant impactor, followed by the contact angle of the smaller particle. Two correlations between the liquid transfer ratio and the impactors were developed, which can be further implemented in numerical simulation of particulate systems.

Brief Biography

I am a Ph.D. candidate at Central South University (CSU) in China, and also a visiting Ph.D. candidate at The University of Queensland (UQ) in Australia supported by the China Scholarship Council (CSC).

Focusing on developing multiscale models to simulate multiphase flows at different time and length scales in the ironmaking blast furnace, I am now a participant for two projects. One of them is supported by the Natural Science Foundation of China (61573383) “Method of online monitoring and optimization of blast hearth inner profile by molecular and multi-physical field simulation” supervised by Professor Ping Zhou at CSU. The other one is the ARC Hub (IH140100035) Project - Multi-scale modelling of erosion and deposit formation in pulverized coal conveying and combustion supervised by Professors Geoff Wang and Baojun Zhao at UQ.

Multi-Level Coarse-Grain Model in DEM and CFD-DEM Simulations

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Abstract

The discrete element method (DEM) [1], often used in combination with computational fluid dynamics (CFD) [2], has proven to be a viable tool for the analysis of granular flows. In a broad range of industries, DEM and CFD-DEM simulations are successfully used to support process design and optimization. On the downside, the DEM is a computationally demanding method, due to actually resolving the contact between particles, and thus making it difficult to apply to large-scale systems.

The coarse-grain (CG) model of the DEM [3] relaxes this computational restriction by replacing multiple equal particles by a single coarser (pseudo) particle, thus significantly decreasing the number of particles involved in the computations. However, due to the violation of geometric similarity, this approach fails to capture effects that intrinsically depend on particle size. Particularly, this becomes an issue in multi-scale systems typically found in large industrial facilities.

Seeking for a computationally feasible description of such large-scale systems, we have developed a method which concurrently couples multiple coarse-grain levels to adjust the resolution of the simulation as required. Spatially confined sub-domains of finer scale are embedded into coarser representations of the system and coupled by exchanging volumetric properties of the granular flow, such as mass flow rate, particle velocity and size distribution. On one side the coarse-grained data enables us to impose proper boundary conditions in each sub-region and at the same time the fine-scale information may be used to enhance the more inexact coarse-grain simulation. By this means it is possible to preserve the particulars of the granular system in spatially confined regions while keeping the benefit of the speedup of the coarse-grain model, where a lower level of detail is sufficient.

We have extended this multi-level coarse-grain (MLCG) model to CFD-DEM simulations where the DEM component is typically taking up the major part of the computational resources. On the CFD side, each coarse-grain level of the granular

model is treated individually using appropriately scaled drag laws and an adequate mesh resolution. The DEM part merges the different levels via the coupling procedure described above.

We have applied the model to various systems with constrictive and obstructive geometries that significantly influence the granular flow to investigate the applicability of the technique. The method was validated through comparison of the statistical properties of fine-scale reference simulations with the properties of the corresponding multi-level coarse-grain systems. Generally, the results showed very good agreement while the speedup achieved with our model was nearly proportional to the amount of saved particles.

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Brief Biography

Daniel Queteschiner is a Research Assistant (PhD Candidate) at the Department of Particulate Flow Modelling at the Johannes Kepler University Linz. He is a member of the Christian Doppler Laboratory for Multi-Scale Modelling of Multiphase Processes. He received his master’s degree in Physics from the Johannes Kepler University Linz. His research interests include the theoretical and numerical modelling of particulate flows with special emphasis on multi-scale systems and large-scale processes. His recent publications include “Coupling resolved and coarse-grain DEM models”, *Particul. Sci. Technol.* (2018) and “Multi-level coarse-grain model of the DEM”, *Powder Technol.* (2018).

A Numerical Study on the Reduction, Softening, and Melting of Iron Ore Pellets and Dripping of Molten Iron and Slag Using CFD-DEM

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Abstract

Various processes involving physics, chemistry, thermodynamics, and fluid mechanics take place inside a blast furnace to produce liquid iron. Iron ore particles begin to reduce in the shaft and complete reduction might occur in the cohesive zone (CZ). Reduced iron ore pellets become soft due to the softening reluctance in the presence of the high-temperature ascending gas and the weight of burden above the CZ. As a result of softening, the void spaces among particles decrease which results in the deviation of the flow of ascending gas and pressure drop. With the increase of temperature, the softened and reduced ore particles start melting and producing two hot liquids, primary slag and molten iron, which are dripping through the layers of coke particles in the dripping zone.

Numerical modellings, in particular, Computational Fluid Dynamics (CFD)-Discrete Element Method (DEM) proved to be practical tools to understand the phenomena occurring in the blast furnace (BF) [1, 2]. The eXtended Discrete Element Method (XDEM) as a numerical simulation platform based on the CFD-DEM models is used to model the processes mentioned above. The XDEM is extended and enhanced with heat and mass exchanges between particle and fluids to be able to model particle’s heat up, reduction, softening, and melting processes. The particle's softening, temperature, shrinking, and melting as well as the gas temperature, concentration and pressure drop along with the flow of fluids are examined. Moreover, FactSage version 7.0 software [3] was used to compute the melt onset temperatures, specific heats, and the viscosities of liquid phases.

Brief Biography

Mehdi Baniasadi

A graduate in Chemical Engineering (BSc, MSc) from Bahonar University of Kerman, he is currently a PhD candidate at the engineering department of the University of Luxembourg. After collaborating with several industrial projects in the field of metallurgy and gas network, and teaching of heat and mass transfer and fluid mechanics in various universities, he joined the LuXDEM group in 2015 as a PhD student. His current research focuses on the blast furnace modelling and additive manufacturing using the numerical methods, in particular, CFD –DEM.

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Numerical Study on Gas-solid Two-phase Flow in a Flue Gas Turbine

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Abstract

Flue gas turbine is the crucial equipment in a Fluid Catalytic Cracking (FCC) energy recovery system. It plays a dominant role in the whole material balance and economic benefits by recycling energy of pressure and heat from flue gas. Catalyst particles will stick to the blade surface under the joint action of high-speed rotation and eutectic salt. Due to the particle fouling on the blade, the flue gas turbine is prone to breaking down. The issue of particles and blade wall surfaces is really complicated and relies on lots of factors, such as particle size and gas flow characteristics. In order to study the complex two-phase flow based on numerical simulation and experiment research, we establish a model that is 2.5 times smaller than the actual flue gas turbine. Its structure is shown in Fig. 1. Fig. 2 illustrates the computational domain of flue gas turbine geometric model and boundary conditions.

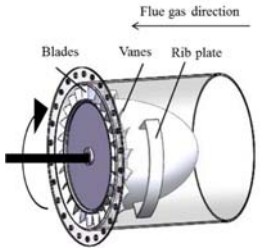

Fig.1. Structure of flue gas turbine.

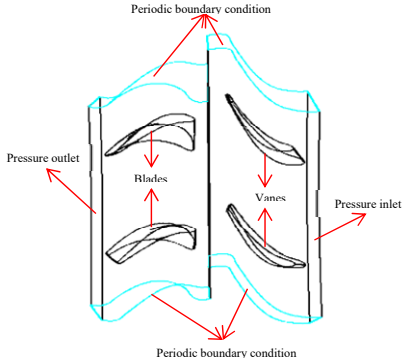

Fig.2. The schematic of computational domain and boundary conditions.

In the simulation, the flue gas and catalyst particles flow is studied by means of Eulerian-Lagrange. The turbulence is modeled by RNG k-epsilon model with standard wall functions, and particles motion is simulated by Discrete Phase Model (DPM) with User Defined Function. The flow characteristics of flue gas and catalyst particles are depicted in Fig.3~Fig.5, respectively. The results show that flue gas accelerates along the direction of vanes bending and decelerates around rotating blades. There are two distinct vortexes at the trailing edge of vanes suction surfaces. Particles collide

repeatedly with the leading edge and pressure surfaces of blades. The numerical results are in good agreement with experimental data of PIV and high-speed photography in the flue gas turbine.

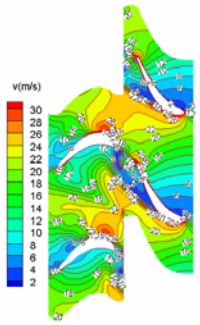

Fig.3. Gas velocity distribution.

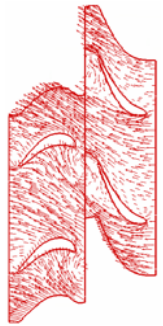

Fig.4. Gas velocity vector.

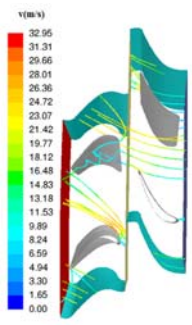

Fig.5. Particle trajectory.

Brief Biography

Jianjun Wang, associate professor, master tutor, received his PhD from University of Petroleum in 1993, is now an associate professor of department of process equipment and control engineering. His research areas are separation technology of multiphase flow, testing technology of multiphase flow, numerical simulation of multiphase flow, resistance reduction technology of chemical equipment and pipeline flow, physical parameters measurement of industrial powder. Earlier, his doctoral study is on particle separation mechanism in axial guide vane cyclone tube. And his current research mainly focuses on gas-solid two-phase flow in the three-stage cyclone separator and flue gas turbine, gas-liquid two-phase flow in the mist eliminator of desulphurization tower.

Jingna Pan, graduated from department of process equipment and control engineering, China University of Petroleum at Qingdao in 2016, is now a postgraduate of third year, and will obtain the Master's degree in 2019. Her research area is multiphase flow. And her work mainly focuses on gas-solid two-phase flow in a flue gas turbine by means of numerical simulation, building and optimizing the deposition model of catalyst particles. She also suggests how to prevent particles deposition to ensure the safe and long-period operation of flue gas turbines (for example, through agglomeration of catalyst fine particles). All work about this research is supported by the Shandong Provincial Natural Science Foundation of China (ZR2015EM026).

Particle Scale Modelling to Study the Effect of Bubble Dynamics on Orientation of Ellipsoids

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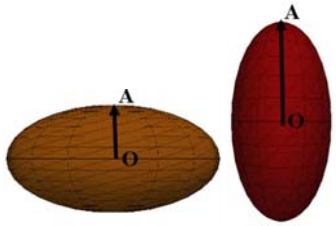
Abstract

Gas-solid fluidized beds are widely encountered in many industrial applications due to their excellent mixing and heat and mass transfer characteristics. The fluidization process has been extensively studied, both experimentally and theoretically, in the past. However, most of the studies focus on spherical particles while in practice, particles used in gas-solid fluidized beds are generally non-spherical. The gas-solid flow behavior such as fluidization quality, flow regime transitions, pressure drop, and minimum fluidization velocity, is greatly influenced when a bed of non-spherical particles is employed compared to spherical particles. As such, the effects of particle shape on dynamics of fluidized bed are required to be fully understood for practical applications. For convenience, spheroids/ ellipsoids can be used, which can describe particle of different shapes by one single shape parameter – aspect ratio. In our previous simulations bubble formation process of ellipsoids of aspect ratio 0.5 (oblate) and 2 (prolate) was successfully generated by CFD-DEM in fluidized bed operated by a single jet. The bubble formation process starts at the bottom of the bed atop distributor which rise through the bed and burst at the top of the bed. The mechanisms of bubble splitting and coalescence were found strongly dependent on particle shape. In addition, the bubbles for ellipsoids were widely distributed on both sides of the bed centre. This behaviour closely relate to the particle orientation of ellipsoids. Spheres are homogenous in all directions and thus do not have preferred orientation, whereas ellipsoids show preference to align in the bed horizontally or vertically in the direction of fluid flow. Particle orientation can affect particle-fluid interaction forces because of the changed projected area to the flow direction of fluid. Therefore, it is interesting to investigate how particle orientation is related to bubble properties. In this paper, the particle orientation of ellipsoids of aspect ratio 0.5 and 2 is investigated as the bubbles are rising through the bed by CFD-DEM simulations. Simulations are carried out in a slot model of fluidized bed operated with a single jet. In the present simulations, the initial orientation is randomly assigned, then its orientation in the fluidization process is tracked by the vector **OA**. Initially before the jet is injected through the bed, most of the ellipsoids are oriented horizontally and as the bubble formation process starts, the ellipsoids align themselves vertically to allow the bubble to rise through them. Over time, the number of the ellipsoids taking up the preferred orientation increases as the ellipsoids line up side by side or atop each other. It was found that ellipsoids change the orientation with the movement of the bubble. In the nose and wake of the bubble

ellipsoids were mostly oriented horizontally while the ellipsoids surrounding the bubble were mostly oriented vertically. In addition, 20 oblate and prolate particles at different locations in the bed are tracked from the initial packing state. The particles at the centre bottom of the bed are found to travel to the top while the particles situated at the top of the bed are found to reach the bottom showing that the bubble movement can significantly affect the internal circulation of ellipsoids and their trajectory. During the trajectory, the orientation of the ellipsoids changed dynamically at certain timings. Further investigation of the timings shows that the particle orientation of the oblate ellipsoids changes from 0° (horizontal) to 90° (vertical) and vice versa for prolate ellipsoids with the passage of bubble. At this instance the particle fluid interaction force acting on the particle also transformed dynamically because of the change in the projected area to the direction of the flow. The findings obtained from this study can aid to understand the fluidization dynamics associated with the non-spherical particles.



(a) α = 0.5 (obalte) (b) α = 2 (prolate)

Brief Biography

Siddhartha Shrestha is a PhD student at Monash University since 2016 under the supervision of Dr. Zongyan Zhou. He is working on the project titled "Particle scale study of bubble dynamics in gas-solid fluidization". The simulation technique used in the study is CFD-DEM and the particles used in the simulations are fine non-spherical particles. He completed his undergraduate degree in Chemical Engineering from Bangladesh University of Engineering & Technology in 2011. He obtained his Master's degree in Engineering (Chemical Engineering) by research from University of Malaya in 2015.

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A Continuum Model of the Cohesive Avalanche Considering Stick-slip Behaviours of Granular Materials

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Abstract

The cohesive particles behave quite differently from cohesionless particles due to the complicated consequences of interparticle adhesive forces, such as capillary force and van der Waals force. This work proposes a continuum model for the intermittent flow of wet particles in a rotating drum. We start with the basic Mohr-Coulomb theory and, use the Rumpf model theory to correlate the microscopic structures and adhesive forces to the macroscopic cohesion. This basic model is shown to work well in slow quasi-static rotation of drum, offering a good prediction of the maximum stability angle of particle bed, unlike previous studies where is was reported to give an overestimation. This basic Mohr-Coulomb-Rumpf model, however, obviously underestimates the stability angle at moderate to high rotational speeds. We attribute this rate-dependency to the dissipative stick-slips occurring between particles, whose time scale, of 0.1-1 s, can be comparable to the period of drum rotation. A visco-elasto-plastic model is proposed to describe the stick-slips and shown to satisfactorily capture the frequencies, peaks and decays of cohesive avalanches in rotating drum.

Keywords: wet particles; cohesive avalanche; rotating drum; Eulerian approach; continuum modelling; FEM

Brief biography

Liuyimei Yang

Ph.D. candidate, Chemical engineering, Monash University

Liuyimei Yang is current PhD student in ARC Hub for Computational Particle Technology and Lab for Simulation and Modelling of Particulate Systems (SIMPAS) in Monash University. She received her bachelor degree from University of Saskatchewan (Canada) in Chemical Engineering, petroleum program. Her research interest mainly focuses on particle simulation, powder mixing, finite element method, as well as the development and application of macroscopic model using FEM for particle flow and granular dynamics.

Multi-Parameter Optimization of Non-catalytic Partial Oxidation of Natural Gas using Reduced Order Models and CFD

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Abstract

The development and optimization of reactors and burners for non-catalytic partial oxidation of natural gas can be rapidly accelerated by the use of numerical models. While the process is influenced by several parameters, e.g. reactor geometry and process parameters, a multi-parameter optimization is required resulting in several hundreds or thousands of necessary calculations [1]. However, CFD calculations are computationally expensive. Alternatively, reduced order models as fast predictions can be used for process optimization. Based on a detailed CFD-based analysis of the POX process, a ROM model [2] was developed that comprises several zones. These zones represent the different conversion steps in the flame and post-flames zones as well as in the recirculation zone and the plug-flow region of the reactor. The different zones and a general model scheme are shown in Figures 1 and 2.

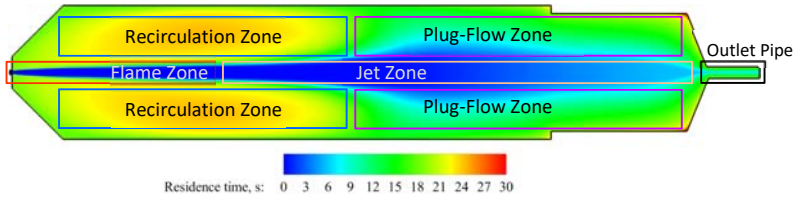

Fig 1. Residence time distribution in CFD [4] and corresponding zones

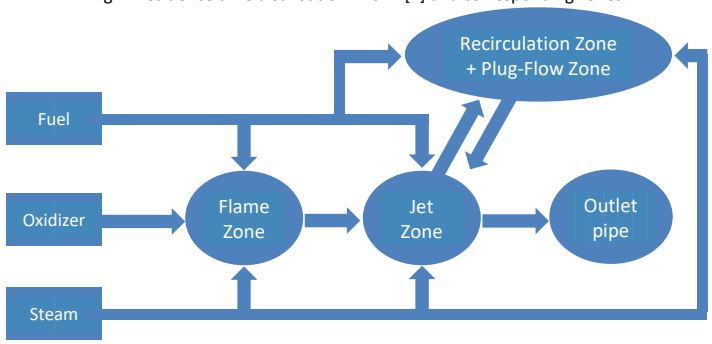

Fig 2. Reduced order scheme [3]

The reduced order model is validated against experimental and numerical results for different reactor geometries and process conditions [3, 4]. The influence of fuel slip, mixing process and recirculation is analyzed in respect to the methane content and temperature at the outlet.

Based on the reduced order model a fully automated optimization strategy is developed. The residence times of the different zones are taken from fast non-reactive CFD simulations. Therefore, the reduced order model is coupled with automated mesh generation and non-reactive CFD simulations. A multi-parameter optimization is performed and first results are discussed.

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Brief Biography

Since 2015, the author is a research associate at the Department of Energy Process Engineering and Chemical Engineering at TU Bergakademie Freiberg in Germany. His research is focused on the development of CFD based optimization tools for high temperature processes and the model utilization for highly loaded particle systems.

Modelling Biochemical Interactions in the Early Stage Formation of Atherosclerosis within the Arterial Wall

Ratchanon Piemjaiswang[1], Sargon A. Gabriel[2], Yan Ding[2], Yuqing Feng[3] ,
Pornpote Piumsomboon[1,4], and Benjapon Chalermsinsuwan[1,4*]

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[2] Mathematical Sciences, School of Science, RMIT University, Victoria 3001, AUSTRALIA
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Abstract

Atherosclerosis is a degenerative disease of the arterial wall, and is well associated with leading causes of death, such as heart attacks and stroke. In the present study, a three-dimensional model of the critical biochemical reactions that drive the formation of atherosclerosis within the arterial wall is developed, and solved using ANSYS Fluent solver. The Navier-Strokes equations are used to govern flow transport within the arterial lumen, whereas Darcy's law is used to govern flow within the porous arterial wall. In both the arterial wall and lumen, the transport of species is modelled by the advection-diffusion-reaction conservation equations of passive scalars. The flux of species across the endothelium interface is modelled with the three-pore model, with additional sets of species transports and reactions taking place thereafter within the arterial wall layers. In order to capture the detailed behavior adjacent to the endothelium interface, special wall treatments are applied with customized user-defined functions in the solver. The 3D model geometry is taken within a diseased human coronary artery with a stenosis present. For the present investigation, the time-evolution of the biochemical reactions is studied, though a steady flow of blood is assumed, with a shear-rate dependent Carreau viscosity model. The species concentration inside the intima layer is examined as a sign of the early stage development of atherosclerosis. Results show compromised locations where the accumulation of atherosclerosis are likely to occur. Therein, elevated concentrations of low density lipoprotein (LDL) are observed, as the accumulation progresses over time. Foam cells which are critical cause to the biochemical inflammatory process are also observed to significantly buildup, as is the deposition of the excessive cholesterol which is formed according to the interactions of monocytes, oxidized LDL, macrophages and cytokines.

Keywords: atherosclerosis; cardiovascular flow; multi-layered artery wall; species transport; biochemical reactions.

Brief Biography

Ratchanon Piemjaiswang is currently a doctoral candidate at Chulalongkorn University in the department of Chemical Technology, Faculty of Science, under the supervision of Assoc. Prof. Dr. Benjapon Chalermsinsuwan. His current research focuses on the mass transfer and multiphase flow for biomedical applications using computational fluid dynamics investigation. He holds a M.S in Chemical Technology from Chulalongkorn University and a B.Eng. in Petrochemical and polymeric material from Silpakorn University.

On The Validity Of The Two-Fluid-KTGF Approach For Dense Gravity-Driven Granular Flows

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Abstract

As a subproblem of solid transport in wellbores, we have investigated the cliff collapse problem by means of the Two-Fluid-Model (TFM), where the rheological description of the second phase (sand with density ρ_s = 2560 kg/m³) is governed by the Kinetic Theory of Granular Flows (KTGF) for the loose (collisional/kinetic) regime (solid volume fraction $\alpha_s < 0.5$, index c/k), and additionally by closures from soil mechanics (Johnson and Jackson 1987; Schaeffer 1987) for the dense (frictional) regime ($\alpha_s \geq 0.5$, index f). Using ANSYS Fluent R17.2, we have studied the influence of the aspect ratio and scale of the initial cliff ($a = y_0/x_0$ = 2, 3, and x_0 = 0.1, 1 ,10 m, respectively), the scale of the particle size (d_p = 10^{-4}, 10^{-3}, 10^{-2} m), four different interstitial fluids (air, water, and two viscous but shear-thinning solutions, namely PAC2 and PAC4, obeying a Cross (1965) material function), and the role of the initial conditions (ICs) such as α_s and solid pressure p_s fields.

Most of the results were obtained by establishing ICs in a first simulation, where solids were patched into a smaller domain (width $w = x_0$) with α_s = 0.54 and allowed to settle and build up a solids bed in dynamic equilibrium with $\alpha_s \approx 0.59$. This solution was then used as IC in the actual domain ($w = 10 \cdot x_0$). Depending on the fluid type, simulations were run for 4 s (air) or 100 s (all liquids) to obtain the final shapes.

In case of air, the final deposit heights at t_f = 4 s fit the scaling of Lube et al. (2005) very well for all the large cliff scales, while this is not so for the smaller cliff scales, where the predicted deposit height is under-, and the run-out length overpredicted (Table 1).

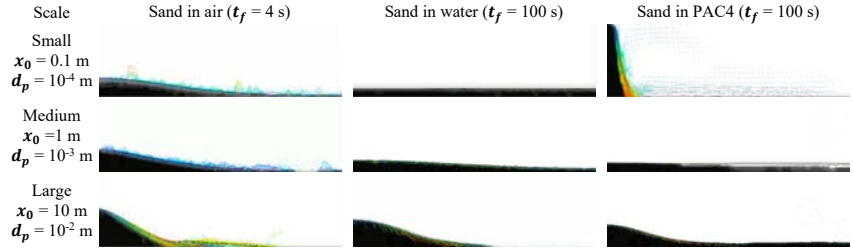

Table 1: Final shapes for a = 3. Black colored areas indicate the maximum magnitudes of frictional viscosities $\eta_{s,f}$=10^5 Pa·s, colors indicate magnitudes of solid velocities. Click on pictures for videos.

However, if the deposit height at t_f = 1 s is used instead, the scaling of Lube et al. (2005) is fairly well met. An explanation for the mismatch is that after the collapse a macroscopic steady-state is achieved in < 1 s in the case of air and > 2 s in the case of all liquids. However, as opposed to experimental results, the outer layer of the collapsed cliff (just as the top layer of the bed in the IC simulations) features a non-zero velocity. Hence, microscopically, the outer layer remains flowing and consequently the shape of the collapsed cliff is continuously changing, albeit on a much larger time scale in the later part of the simulations. We suspect this non-zero velocity to be a consequence of the numerical solution procedure which is based on pressure-velocity coupling of the phases on a collocated grid. The introduction of the additional state equations $p_s = p_{s,c/k}(\alpha_s) + p_{s,f}(\alpha_s)$ results in an overdetermined system (Laux 1998). Obtaining α_s from p_s instead may be a way to remedy this problem (Laux 1998).

The water and PAC cases qualitatively fit very well the experimental results of Rondon et al. (2011) and Thompson and Huppert (2007). Again, due to the surface sheet flow there is no true steady-state, resulting in a planar final shape (Table 1) for d_p = 10^{-4} m for water.

In case of water as the interstitial fluid, the collapse happens in about 2-3 s. For a liquid first phase, the initial solid volume fraction of the cliff is known to have a drastic effect on the dynamics of the collapse (Rondon et al. 2011). Our results obtained with the pre-simulated settled solid bed in dynamic equilibrium ($\alpha_s \approx 0.59$) are equivalent with the loose solid bed ($\alpha_s \approx 0.55$) of Rondon et al. (2011). Hence, the model needs to be tuned such that the pre-simulations result in settled beds with $\alpha_s \approx 0.55$.

In case of PAC as the interstitial fluid, the cliff slowly erodes from its top leading edge resulting in a vertical erosion flow disintegrating the cliff slowly on time scales T > 60 s. This behavior is comparable to the dense states of Rondon et al. (2011), indicating that the Cross (1965) material function with its zero-shear viscosity and shear-thinning property has a similar effect on the dynamics of a cliff collapse than a pre-compacted and dense bed. However, because of the much higher viscosity level, the cliff does not actually disintegrate in the time scale of observation in case of d_p = 10^{-4} m (Table 1). Nevertheless, in case of d_p = 10^{-2} m, the collapse is rather abrupt (T < 20 s), due to the larger gravity-induced normal stress.

Overall, the TFM-KTGF framework in conjunction with a pressure- and shear-rate-dependent rheology model for the solid frictional stress provides satisfactory results, especially when tuning of model parameters is conducted. However, depending on the numerical solution procedure, the concept of a non-horizontal final deposit may depend on the time scale of observation and correspondingly on the spatial scale of the cliff due to the ongoing sheet flow in the outer layer.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

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Brief Biography

Alexander Busch is a PhD candidate at the Norwegian University of Science and Technology (NTNU). Previously, he worked for Dräger Safety AG & Co. KGaA as a Systems Engineer. His research interests include multiphase flow modeling, non-Newtonian rheology and system simulation. Busch has authored and coauthored more than ten technical papers and holds seven patents. He holds a M.Sc. degree in development and simulation methods in mechanical engineering from Hochschule für Technik und Wirtschaft (HTW) Berlin.

Direct Numerical Simulations and Force Correlations of Assemblies of Non-spherical Particles

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Abstract

Particle resolved flows are performed around static assemblies of random orientations of non-spherical particles using a multi-relaxation-time lattice Boltzmann method. The parameter space for static assemblies of spherical particles are relatively simpler. They are just limited to different Reynolds numbers (Re) and solids-volume fractions (ε_s). However for non-spherical particles, it is also needed to know the mutual orientation of the particles in the simulation domain and also their mean orientation with respect to the flow direction. Therefore, we propose two parameters S1 and S2 to measure the mutual orientations of the particles and also the incident angle φ with respect to the incoming flow. We investigate the dependencies of drag, lift and torques as functions of Re, ε_s, S1, S2 and φ. From the data obtained, we propose accordingly the correlations for drag, lift and torque coefficients, which can be used to simulate larger scale CFD-DEM simulations of non-spherical particles fluidization.

Brief Biography

Sathish K. P. Sanjeevi is a doctoral researcher at the Delft University of Technology, Netherlands. His doctoral research focuses on direct numerical simulations of flows around non-spherical particles. Sathish holds bachelors in Mechanical Engineering from Amrita University, India. After graduation, he worked at Larsen and Toubro, India on the design and construction of supercritical thermal power plants for two years. Later, he pursued his masters in Simulation Sciences (a.k.a Computational Engineering) at the RWTH Aachen University in Germany. Subsequently, he moved to Eindhoven to start his doctoral research in the group of Prof. Hans Kuipers and Johan Padding. His research is funded by European Research Council and the funded project is about developing a multi-scale modelling strategy for fluidization of non-spherical particles.

An Immersed-Grid Method for Simulation of Viscous Flows

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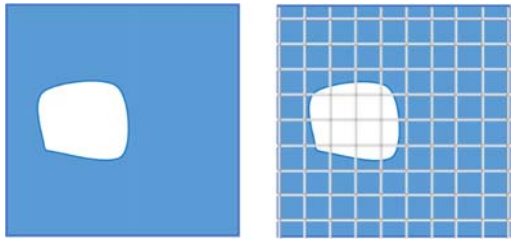
Abstract

This paper reports an efficient immersed grid method for numerical simulation of viscous flows in multiply-connected domains (Figure 1a). The basic feature of non-boundary-fitted-grid/mesh-based methods is to extend the problem defined on a geometrically-complex domain to that on a larger, but simpler shaped domain (Figure 1b) [1]. Cartesian grids are employed to represent the extended/computational domain and one dimension integrated radial basis function IRBFs which are constructed through integration rather than the usual differentiation [1], are then utilised to approximate the field variables. A body force is introduced into the momentum equations to represent the inner boundaries. The interesting features of the proposed method include (i) simple pre-processing (uniform Cartesian grid); (ii) the extended domain can be regular or irregular; (iii) high convergence rate can be achieved [2] (IRBF high-order approximation); (iv) system matrices can be kept unchanged when handling with moving boundaries. Several kinds linear and nonlinear test problems are conducted to demonstrate the efficient of the proposed technique.



(a) (b)

Figure 1. A multiply-connected domain (a) and its typical discretisation (b)

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Brief Biography

I am Miss Van Le, from Ho Chi Minh City, Viet Nam. I am doing PhD in Computational Engineering at the University of Southern Queensland in Australia. In 2015, I have started the PhD research. In 2013, I have got the Master of Science degree in Applied Mathematics from University of Technology- Ho Chi Minh City, and in 2010, I have got the Bachelor of Science degree in Mathematics and Computer Sciences from University of Science- Ho Chi Minh City. I have worked as a researcher in the Institute of Applied Mechanics and Informatics (IAMI) - Ho Chi Minh City, Viet Nam from 2010 to 2014.

Oxy-Fuel Combustion Behaviors in Fluidized Bed: Studied by Experiment and CFD Simulation

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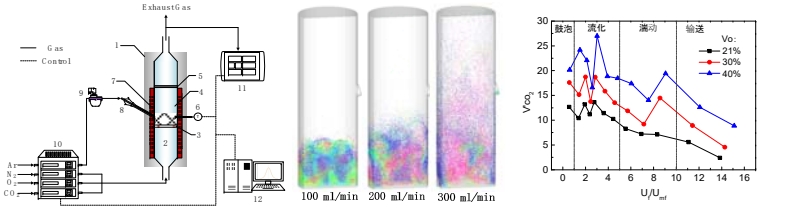
Abstract

Oxy-fuel combustion is one of the most promising carbon capture technologies. In order to fully understand the oxy-fuel combustion behaviors in fluidized bed, a micro-fluidized bed reactor with an online mass spectrometry were established. The effects of oxygen concentration, temperature, gas-solid flow pattern on main combustion characteristics were experimental investigated. Besides, 3D Eulerian−Lagrangian simulation based on the multiphase particle-in-cell (MP-PIC) scheme were carried out. The gas phase was modelled by a large eddy simulation (LES) and the particle phase is described by discrete particle method. A comprehensive reaction model including devolatilization, combustion of char and volatiles, production of pollutant is incorporated into the scheme. Based on CFD simulations, some interesting findings, which are difficult to be obtained only from experiments, are presented, e.g. the effect of flow patterns on the Oxy-fuel combustion.



(a) Experimental setup (b) CFD simulations (c) Flow pattern with CO2 concentration

Brief Biography

Qinwen Liu, female, is a Mast student in Thermal Engineering, Southeast University. She is supervised by Professor Wenqi Zhong and Professor Aibing Yu.

Simulation of particle dissolution in RANS simulations of turbulent flow

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CSIRO Mineral Resources

Stirred tanks and other agitated vessels are often used to dissolve solid particles. Particle tracking is often used within RANS (Reynolds averaged Navier Stokes) CFD (Computational Fluid Dynamics) models of such agitated tanks to simulate the rate of dissolution. The assumption generally used is that the dissolution rate is mass transfer limited, so that standard formulas for Sherwood number (Sh) as a function of Reynolds number (Re) and Schmidt number (Sc) similar to Ranz - Marshall correlation can be used. In the calculation of Sherwood number, the relative velocity is taken to be the difference between the mean particle and liquid velocities, in the sense of Reynolds averaged velocities. Finally the driving concentration difference is taken to be the difference between the surface concentration and the average local concentration, again in the Reynolds averaged sense. Both these assumptions are questionable, and in the case of relative velocity, almost certainly leads to an underestimate of dissolution rate in a highly agitated vessel, because the relative mean velocity is less than the average instantaneous velocity difference, when account is taken of turbulence in the flow field external to the particle. Three different techniques are proposed to account for this effect, corrected formulas are derived, and simple calculations are used to estimate the magnitude of the effect.

Use of 3D Printing for DEM Model Validation

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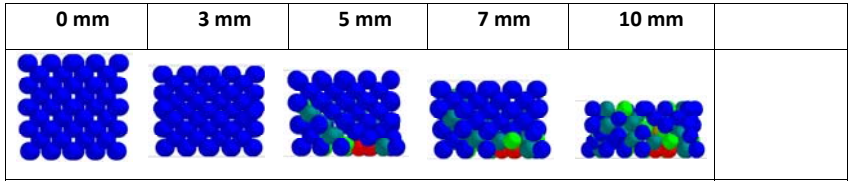
Abstract

One of the long-term barriers to accurate DEM particle modelling is the lack of tunable "calibration" particles that can be used for validation. Despite increased computing power, it is difficult to produce an accurate prediction of the behaviour of a simple particle system (varying size or density). Highly complex industrial powders are far more complex. Ideally, we need hundreds of identical copies of particles or agglomerates with realistic sizes, shapes, densities and structures, and to be able to systematically vary the particle and/or test conditions to achieve reproducible data. To date, this has not been possible via experimental particle production techniques.

We have designed and 3D printed *multiple, identical* copies of agglomerates, and compared their deformation and breakage behaviour in DEM simulations. The agglomerates are printed on a "PolyJet" printer, which prints multiple polymers simultaneously, including rigid or rubber-like flexible materials with well-defined mechanical properties. Agglomerates are designed in CAD or in DEM, and exported to the printer to produce multiple, identical for experiments.

This paper summarizes ongoing work on printing tunable agglomerates for DEM simulations[1]. Rigid particles with ductile cylindrical inter-particle bonds (representing "dried liquid bridges") were printed and the structure and the strength of agglomerates were systematically varied by changing the design or the polymer used to print the bonds. DEM modelling using the TBBM[2] bond model in EDEM™[3] software package has shown a better match between quasi-static compression and experimental data than has previously been achieved (see Figure 1). We will also outline other potential applications of the 3D printing approach for producing a wide range of particles with varying shape, size and densities (for example), for use in calibrating other types of DEM simulations. We anticipate that 3D printing will be routinely used as an experimental aid in a wide range of simulations.



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[3] DEM Solutions, Edinburgh, UK

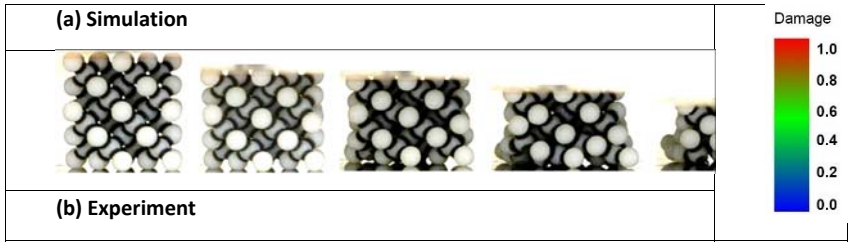

Figure 1. Simulated and experimental breakage results for a cube shaped agglomerate with ordered, tetrahedral internal structure as a function of the displacement (in mm) of the upper platen. (Ge, Ghadiri, Zhou, Hapgood, unpublished data, work funded by IFPRI & ARC)

Brief Biography

Professor Karen Hapgood is Executive Dean of the Faculty of Science Engineering & Built Environment (SEBE) and Vice President at Deakin University. Her career has criss-crossed between industry and academia. After graduating as a chemical engineer from the University of Queensland in 1993, she spent 2.5 years as a control engineer. She returned to UQ to complete her PhD in chemical engineering and then spent 5 years working for Merck & Co, as a Senior Research Chemical Engineer in the US and a Pharmaceutical Technical Operations Engineer at Merck Australia, before starting as a Senior Lecturer at Monash University in 2006. She became the Head of the Department of Chemical Engineering at Monash in 2012, and moved to Deakin University in Geelong in 2017 as the Head of School of Engineering. In July 2018, she became the Executive Dean of the Faculty of Science, Engineering and the Built Environment.

Her professional research interests include powder technology, pharmaceutical manufacturing, 3D printing, and promoting diversity in engineering. Professor Hapgood received an Office of Learning and Teaching Citation for her Outstanding contribution to Student Learning in 2010, an Australian Davos Connection (ADC) Australian Leadership Award in 2011 and an Australian and New Zealand Federation of Chemical Engineers (ANZFCHE) Caltex award for Teaching Excellence in 2013. She is a Fellow of IChemE, Engineers Australia and RACI and a Graduate of the Australian Institute of Company Directors.

Segregation in Sheared Granular Matter

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Abstract

When dry granular mixtures which are composed of particles with different size, density, or shape flow they will tend to segregate. We consider segregation that occurs when a granular mixture is sheared, such as when it flows down along an inclined slope. A partially filled cylindrical drum which is slowly rotated about its axis (which is perpendicular to gravity) is a popular test-bed to examine sheared granular segregation. Here we consider simulation (Discrete Element Method, DEM), experiment and continuum theories to understand the segregation that occurs.

Using DEM simulations we can clearly determine the underlying causes of segregation which intimately depend on intrinsic particle properties. We compare these DEM simulations with both experiments and continuum theories, for a number of these properties, and find very good agreement. It will be shown that segregation arising from differences in particle size is the strongest, with stable asymptotic states being reached after only one or two cylinder rotations. Density segregation is the next strongest followed by segregation due to particle shape, where segregation takes of the order of 10 rotations. The underlying physical mechanism leading to segregation is different for each of these properties. We compare and contrast these mechanisms in detail.

Brief Biography

Dr Gerald G Pereira holds a PhD in Applied Mathematics from Melbourne University and currently works at CSIRO in Clayton. His areas of scientific interest include application and development of numerical models to describe the flow behavior of granular materials; algorithmic development of numerical methods for fluids especially the lattice Boltzmann (LB) method; application of computational fluid dynamics (CFD) methods to a variety of physical systems including porous media, microfluidics and processing devices; and statistical mechanics of soft condensed matter especially polymers and liquid crystals.

Effect of Vibrational and Geometrical Parameters on Granular Capillarity Induced by a Vibrating Tube

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Abstract

When a narrow tube inserted into a static container filled with particles is subjected to vertical vibration, the particles rise in the tube. This phenomenon is termed as granular capillarity, because of its resembling the capillary effect of liquid. As the granular capillarity is driven by the convective motion of the particles in the container due to the vibrational motion of the tube, the dynamics of granular capillarity in terms of the steady-state capillarity height and the average ascending rate could be affected by the granular convection behaviors, such as the convection velocity and the convection region. To gain insights on the effects of vibrational and geometrical parameters on the convective motion of particles in the container and thus on the granular capillarity dynamics in the tube, we numerically investigated the particle system using the Discrete Element Method (DEM). We obtain the phenomena of granular capillarity under different vibration intensity, frequency and container diameter, and analyze the capillarity height, the ascending rate as well as the convection behaviors. Our simulation results show that when the vibration frequency keeps constant, with the increase in vibration intensity the granular column in the tube experience no ascending, monocyclic and multi-cyclic (period-doubling and period-quadrupling) ascending. When the vibration intensity keeps constant, lower vibration frequency leads to higher steady-state capillarity height and greater ascending rate. The container diameter has a significant effect on the ascending rate, while it affects little on the steady-state capillarity height. Moreover, our results for the granular convection behaviors suggest that the convective motion of particles in the container is one major factor that determines the dynamical behavior of the granular capillarity phenomenon.

Brief Biography

Dr. Fengxian Fan is an associate professor in School of Energy and Power Engineering at the University of Shanghai for Science and Technology, China. She obtained her BSc in Thermal Energy and Power Engineering from Henan University of Science and Technology, and her PhD. in Thermal Energy Engineering from School of Energy and Environment at Southeast University (Nanjing, China) in 2008. She worked as a lecturer from September 2008 to June 2011, and as an associate professor since July 2011 at the University of Shanghai for Science and Technology. She was invited to work as an academic research professor in the Computational Fluid Dynamics Laboratory at Kyung Hee University from June 2012 to February 2013. She worked as a visiting scientist in the Institute of Multiscale Simulation at the University of Erlangen-Nuremberg from December 2013 to December 2013, supported by the China Scholarship Council.

Dr. Fan has expertise in modelling and simulations of gas-solid two-phase systems in energy and environment field, fine particle emission control, discrete element methods, and granular dynamics. She has published more than 50 scientific papers. She is a frequent reviewer for over 10 top journals in the areas of particle technology, chemical engineering, energy and environment. Her research has been supported by the National Natural and Science Foundation of China, Shanghai science and technology commission, and renowned companies.

Particle Based Modelling of Metal Powder Flow in Additive Manufacturing Systems

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[2]CSIRO Manufacturing, Clayton South, VIC 3169, Australia;

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***Gary W. Delaney presenting author. Oral Presentation.**

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Abstract

Particle based modelling is a powerful tool for studying the complex flow behavior of granular systems in modern industrial devices, allowing for precise specification of the detailed geometry of the device, the particle morphology and the interaction properties of the individual particles. We present results of a discrete element method (DEM) model of metal powder flow in an additive manufacturing device. In powder-bed based metal additive manufacturing applications, the addition of the powder layers is the crucial first step in building up of the part in 3D and has a significant impact on final part quality. A common technique employed is to add successive layers of metal powder by raking a new layer across the existing surface. Understanding this raking process and how the properties of the powder particles (e.g. size, shape, density, interaction properties) and process parameters (e.g. height of powder layer, rake geometry, rake speed) affect the properties of the bed after raking is crucial in optimizing the performance of the system and ensuring the quality of the 3D-printed part. Our DEM model directly incorporates the powder's particle size distribution, particle shapes and experimental measurements of the powder flowability. Results will be presented of the raking of both Arcam Titanium powder and CSIRO manipulated titanium powder, with comparisons to detailed experimental data characterizing the powder bed structure after the addition of a powder layer.

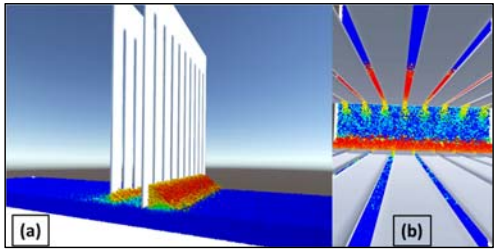

Figure 1: Flow images from a DEM simulation of raking of a reference Ti-6Al-4V metal powder with particles coloured by velocity. Images are shown from (a) side view and (b) top view positioned between the two rakes.

Brief Biography

Dr Gary Delaney leads Data61's Computational Modelling Group at the Commonwealth Scientific and Industrial Research Organisation (CSIRO) in Melbourne. Gary's primary research interests are in computational modelling and structural characterization of granular systems, and applications of Machine Learning in understanding and optimizing natural and industrial processes.

Dr. Vincent Lemiale is a Senior Research Scientist and Team Leader at CSIRO Data61. He specializes in Computational Solid Mechanics using both grid based (Finite Element) and mesh free (Smooth Particle Hydrodynamics, Discrete Element, Material Points) methods. Over the last 10 years, he has applied his expertise to a wide range of areas including manufacturing, geomechanics, materials modelling and food processing.

Dr. Tony Murphy is a Chief Research Scientist at CSIRO Manufacturing and leads the Materials and Process Modelling Team. He has worked mainly on the physics, chemistry and applications of thermal plasmas such as welding arcs. Tony has published over 240 papers in refereed journals, and has presented over 80 invited, keynote and plenary lectures at international scientific conferences. He has won several awards and holds editorial positions with four international journals, including Editor-in-Chief of Plasma Chemistry and Plasma Processing.

Stefan Gulizia is a Research Group Leader in CSIRO's Metal Industries Program. Stefan has over 30 years of research experience in materials research and technology. Stefan's current research interests include strategic and applied research in Cold spray, Powder Manipulation and Additive Manufacturing (AM) technologies. Stefan has developed a wide range of industrial coatings and AM technologies directed towards the manufacturing aerospace, bio-medical, defence, die-casting, printing, powder and metal processing industries. He co-pioneered Cold spray and EBM AM technology in the Southern Hemisphere and continues to develop new research fields in direct powder manipulation and Cold spray Additive Manufacturing technology.

Dr Christian Doblin is a Senior Research Scientist in CSIRO's Metal Industries Program. Christian's research interests include gas-solids processing and separation, fluidized beds, the development of novel metal powder production processes and process scale-up.

Modeling Of Deformation Of Granular Pellet In Small-Scale "Unit Cell" Dem Simulations

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Abstract

The wet granulation process can be conceptually split into three simultaneou rate processes: nucleation and wetting, growth, and breakage. Wet granule breakage is a particularly important rate process in high shear granulation, however, it is very difficult to predict.

In this work, small-scale "unit cell" DEM simulations are used to study the hydrostatic and deviatoric stresses experienced by a granular pellet undergoing shear in a dynamic shear cell. A section of the annular shear cell with periodic boundary conditions represents the unit shear cell. The granular pellet surrounding by some particles was generated inside the unit shear cell. Simulations were performed using Hertz-Mindlin with no slip contact model. The influence of types of granular pellet, shear velocity, normal load and the size of the surrounding background particles on both stresses will be studied.

The simulation results will be used to predict the deformation of the granular pellet with von Mises failure theory. The von Mises yield stress results will be directly compared with the yield stress of real materials, allowing the prediction of pellet deformation.

In conclusion, a new method for predicting the deformation of granular pellets will be presented, using a combination of numerical and theoretical tools.

Brief Biography

Dr. Rachel Smith is a senior lecturer at the University of Sheffield, with a speciality in particle technology. Her research is focused on improving the manufacturing and processing of solid and particulate materials. In particular, she is interested in studying particle-particle and particle-fluid interactions, and using this understanding to develop useful tools, models and guidance for bulk processing. She conducts research into a wide range of processes, including granulation, particle and powder coating, fluidized bed processes, drying and spherical agglomeration. This research is applicable to many industries, including foods, detergents, consumer products, pharmaceuticals, and agrichemicals. Her research uses a broad range of experimental and computational tools.

Dr. Smith received her BEng in Chemical Engineering at the University of Queensland, Australia, in 2000. She went on to receive her Doctorate from the same institution in 2008. In the same year, Rachel joined the Department of Chemical Engineering as a post-doctoral research fellow, at Monash University, in Melbourne, Australia. In early 2012, she joined the University of Sheffield's Department of Chemical and Biological Engineering as a lecturer, and was awarded as a Royal Society Industry fellowship in 2015.

DEM-FEM Coupled Modelling on the Compaction and Sintering of Elemental and Composite Powders

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Abstract

Compared with other manufacturing methods, powder metallurgy (PM) becomes increasingly attractive in fabricating structural and functional materials with the advantages of high accuracy, low cost, easy operation, and mostly importantly the net shape or near net shape forming. With this method, each stage included in PM (from initial packing before compaction to final sintering) is equally important; therefore, properly controlling these stages are the precondition for the PM production of elemental or composite granular materials with superior quality. Even though in the past decades much effort was paid in the research on the PM production of different powders both numerically and physically, most of them were focusing on the physical experiments, fewer studies were on numerical simulations. And the currently existed numerical work was only carried out from macro-continuous scale with the assumption that the initial structure is considered to be uniform, which makes them unable to reproduce the powder compaction and sintering from particulate scale. However, in real case, the PM process is principally dominated by individual particle behavior like rearrangement, deformation, and even partial melting, while the researches in this regard are limited.

In this paper, the compaction process and sintering process of various elemental metallic powders (e.g. pure Al and pure W) and composite powders (e.g. Al/SiC, W-Cu alloy and FeAl intermetallics) under different compaction methods (such as die compaction, cold isostatic pressing, and high velocity compaction) and solid state sintering conditions were numerically reproduced by using multi-particle finite element method (MPFEM) from particulate scale. The effects of powder initial packing structures, composition, compaction mode, compaction pressure/velocity, and sintering temperature on the densification of each powder mass were systematically investigated. Various macro- and microscopic properties of the compacts and sintered parts were characterized and compared. And the densification dynamics and mechanisms were also analyzed and identified. The results show that the initial packing structure, compaction mode, compaction pressure/velocity, and sintering temperature can greatly influence the structure and properties of the compacts and sintered components. Compared with the mechanically mixed composite powders, the composite powder with core/shell structure is preferable for the compacts with high relative densities, uniform local density and stress distributions. Dynamics and mechanism analyses indicate that MPFEM is effective in dealing with the whole PM process from particulate scale.

Take the PM production of pure tungsten material as an example, Fig. 1 gives the MPFEM modelling results on the whole PM production process of tungsten powder from particulate scale. It shows that for the hard refractory materials like W, the initial packing structure plays an important role in determining the subsequent compaction and sintering processes as well as the structure and properties of the final sintered part, which is also affected by the size of powders. Therefore, properly choosing the powder size, improving the initial packing density

and uniformity, controlling the compaction and sintering conditions are the precondition for the production of high performance of tungsten material.

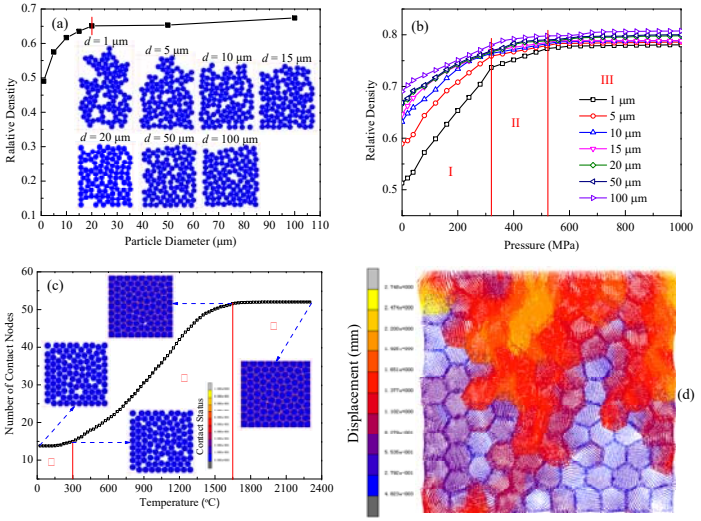

Fig. 1 2D MPFEM modelling on the full PM process of pure tungsten material, where: (a) initial packings; (b) compaction; (c) sintering; (d) displacement variation in the final sintered component.

Brief Biography

Dr. Xizhong An got his Ph.D degree from University of Science and Technology Beijing in 2002, and currently he is working as a full professor in School of Metallurgy, Northeastern University. Prof. An's research interests include numerical and physical study on particle packing, granular matter, and powder metallurgy. In recent years, he has undertaken more than 20 projects. More than 90 papers were published, where over 60 were in SCI journals such as Phys. Rev. Lett., Soft Matter, J. Alloy & Compd., Powder Technol., Adv. Powder Technol., Europhys. Lett., Comput. Phys. Commun., Euro. Phys. J. E, Nanotechnology, Sensors & Actuators: B. Chemical, Appl. Phys. A, AIP Adv., RSC Adv., Metall. Mater. Trans. A, Metall. Mater. Trans. B, Granular Matter, Particuology, Particul. Sci. Technol., J. Min. Metall. B, Nanoscale Res. Lett., Diam. Relat. Mater., et al. More than 20 patents were applied, where five were authorized. His honors and awards include: Candidate for "Liaoning Hundred, Thousand, and Ten Thousand Talents Engineering", Hundred Level (2009); Candidate for "New Century Outstanding Talents" of Ministry of Education of China (2010); "Outstanding Scientific and Technological Worker" of Liaoning province (2014); "Longchuan Talent" of Yangzhou City (2015); "Shuangchuang Doctor" of Jiangsu Province (2016); "Science and Technology Progress Award (second prize)" of Chinese Society of Particuology (2016); "Lingjun Talent" of Shenyang (2017); "Natural Science Award (second prize)" of Chinese Society of Particuology (2018). He is the executive director of National Materials New Technology Development Research Institute; Director of Chinese Society of Micro-Nano Technology; Youth Director of Chinese Society of Particuology; Director of Liaoning Society of Particuology. Member of Editorial Board for four international journals.

Wall Effects in Powder Flow in Continuum Mechanics Modeling

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Abstract

The handling of particulate solids needs the knowledge of the bulk friction properties but also of the wall-particles friction interactions in order to properly design the devices used in process engineering. It is particularly important in silo storage, for which the Janssen distribution of vertical stresses, due to the arching effect, depends closely to the capacity of the walls to maintain by shear friction resistance a fraction of the particle weight. The presence of the walls has also a tremendous impact when the size aperture is of order a tenth of particulate diameter, since it may lead to a mechanical blockage.

First we present here a research in the case of roll compaction, using continuum mechanics modeling and simulation, where the impact of the sealing system design (fixed cheek plates or walls attached to one roll) on the tablet mechanical properties is investigated. The difference of wall shear induced by these designs leads to a difference of pressure distribution and consequently of density distribution in the tablet that cannot be observed by a 2D-simulation. The results of the simulations are then compared with experimental observations.

Then we investigate the role of the walls in the case of confined flows, i.e. when the typical size for the flow is of order the tenth of particle sizes, and how this confinement effect may be taken into account in effective constitutive equations for continuum mechanics modeling and simulations. To that purpose, we review the physical origin of the confinement effect as induced by frustrated dilation and particle reorganization. The latter study quantifies the confinement phenomenon in a similar manner than the intrinsic cohesion proposed by Weir. This effective cohesion, of order the pressure exerted by one particle, is then introduced in a continuum modeling of flows in narrow channels of different particle size-channel width ratio. The results obtained compare well with experimental data.

Brief Biography

Alain de Ryck graduated from École polytechnique, Paris (1990), a leading French Engineering Grande École. He obtained a MSc in solid physics at the Université Paris-Sud, Orsay (1991) and a PhD in physics at the Université Pierre-et-Marie-Curie, Paris 1994, with a thesis on the dynamic wetting of fibers. After the PhD, he worked with a Marie-Curie Fellowship at the Instituto pluridiscplinar, Universidad Complutense, Madrid, before to join IMT Mines Albi, France in 1996. He is currently Professor at the Rapsodee Center, UMR CNRS 5302. with a Professional Visiting Fellow at the School of Materials Science and Engineering, UNSW Sydney during 2007. Since 2015, he is also the Associate Dean for the Engineering studies of IMT Mines Albi. His domain of research is the experimental or modelisation in the physics and mechanics of granular media. Some research programs are the study of stick-slip shear instabilities in granular friction, the slope stability of cohesive bulk materials, the dense flows of partially wetted or cohesive particulate solids, the particulate solids-air interactions during chute flows, and compaction. He is also Editorial board member of the Proceedings of the Institution of Mechanical Engineers, Part E: Journal of Process Mechanical Engineering.

Direct DEM Modelling of Particle Breakage in Grinding

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Abstract

Grinding is an important size reduction process in many industries which is known as an intensively power-consuming, low-efficient and complex process. Modelling and simulation have been used widely to understand the grinding and, more precisely, particle breakage mechanisms. DEM has been recognized as a powerful tool to achieve this purpose, as it is capable of providing valuable micro-scale information of particle interactions. However, direct DEM modelling of particle breakage using particle replacement method is the recent development of this field, but still immature.

This study aimed to integrate particle breakage into an in-house DEM model to develop a generic direct DEM model of particle breakage. A validated breakage probability model was employed to determine the breakage point of particle based on impact energy and minimum required energy. For those particles determined to be broken, the size distribution of daughter particles was calculated using an employed breakage function. Then, the progeny cluster was determined and replaced in parent position. Finally, the particle list was updated at the end of every time-step and the DEM simulation proceeded using the updated list.

The proposed frame work is distinguished with other studies by its straightforward structure, capability of determining the true point of single particle breakage, generically determination of progeny distribution and their position inside the original particle and being able to practically apply for any grinding environment. To validate the proposed model, the model was implemented to investigate the breakage behaviour of a packed bed of particles inside a virtual box whilst the bed was hitting regularly by a grinding ball at determined time interval. The examination of collision energy distributions, breakage rates, and PSDs showed that breakage rate can deviate from the first order kinetic. For feed particles, the deviation was appeared as deceleration in the breakage rate. Grinding time and magnitude of impaction energy were demonstrated to be the effective factors in breakage rate deviation. The existing model for representing the time-dependent breakage rate was modified to include the impact energy. The results also proved the necessity of a DEM based model capable of simulating the grinding similar to its real environment, and independent from the variation of grinding parameters.

The model was then applied to simulate grinding in a pilot-scale ball mill. Applying the direct DEM modelling of particle breakage in the mill showed that findings were in line with experimental study from the literature. The simulation results could predict the final size distribution trend very well. It was shown that by increasing the mill rotation speed the particle flow regime changes from mostly dominant by charge rolling at rising side of the mill to intensely projected streams. Energy consumption and mean velocity increase as mill speed increases. Increasing the mill speed also influences the collision energy spectra in case of energy magnitude and collision frequency. Breakage rate increases as mill rotates rapidly. The PSD curves moves to finer regions as the rotation speed increases.

In Summary, a direct modelling of particle breakage based on DEM was developed which is capable of simulating the grinding similar to its real environment and independent from the variation of grinding parameters. Developed model was successfully employed to modelling grinding in various conditions.

Brief Biography

Ebrahim completed his B.Sc. in Mining Engineering in 2008 and M.Sc. in Mineral Processing in 2011. His enthusiasm for grinding modelling led him to choose an industrial project as M.Sc. thesis. As a part of the project, he carried out a comprehensive study to simulate and optimize the grinding circuit of cement clinker. After the graduation, he improved his professional knowledge and experience by working in some distinguished mining companies in Middle East to design and develop process flowsheets for base and precious metals with mainly focusing on comminution process. He moved to Australia, in 2014, to pursue his studying in PhD degree under the supervision of A/Prof. Runyu Yang at UNSW. His Thesis topic was “DEM Modelling of Particle Breakage and its application to ball milling”. Since then he has tried to investigate the single particle breakage behaviour under multiple different impactions and then apply the obtained information in developing a DEM based Model to directly and generically model the particle breakage in grinding processes.

The Forces on Cylinders in the Free Molecule Regime

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Abstract

Theoretical formulae for the forces on cylinders in the free molecule regime are derived based on the gas kinetic theory. For a simple gas in non-equilibrium state with temperature or velocity gradients, the second-order approximation of the gas molecule velocity distribution function reads [1,2]

$$f = f_0\left(1+\Phi\right), \tag{1}$$

where f_0 is the equilibrium Maxwellian velocity distribution function, and Φ is the correction owing to nonequilibrium contribution. Consider a cylindrical particle of length L and radius R_0 (L>>R_0) moving in a simple rarefied gas. As shown in Fig. 1, we introduce a global coordinate system {X, Y, Z} with its origin located at the center of the particle, a local coordinate system {x, y, z} fixed to the surface element of the particle, and an auxiliary coordinate system {X_1, Y_1, Z_1} with its origin fixed at the center of the particle. The force acting on the particle can be obtained by integrating the elementary force components over the whole surface of the particle [3,4]. The elementary force components (normal and shear forces) produced by the incident and outgoing gas molecules can be calculated by an integration of the gas molecule velocity distribution function, which consists of two contributions: momentum exchange due to the impact of the incident gas molecules and that due to the reflection of the molecules.

In the linear shear flow field, the drag force on the cylinder is given by [5,6]

$$\boldsymbol{F}_{\mathrm{D}} = n\sqrt{2\pi m k_B T}R_0 L\left[\sigma_\tau \boldsymbol{U}_{//} + \left(2-\sigma_p+\frac{\pi}{4}\sigma_p+\frac{\sigma_\tau}{2}\right)\boldsymbol{U}_{\perp}\right], \tag{2}$$

and the shear lift force reads

$$\boldsymbol{F}_{\mathrm{SL}} = -\frac{5\pi}{32}\rho\lambda R_0 L U_0 \boldsymbol{G}\left[2\sigma_\tau \sin^2\psi + \left(2-\sigma_p-\frac{3\sigma_\tau}{2}\right)\left(3\cos^2\psi\cos^2\theta+\sin^2\theta-\cos^2\psi\right)\right], \tag{3}$$

where n is the number density of gas molecules, m is the mass of single gas molecule, k_B is the Boltzmann constant, ρ and λ are the density and mean free path of the gas, and the subscripts "$\perp$" and "//" indicate the components perpendicular and parallel to the cylinder axis, respectively. In Eq. (3), the transverse force of shear lift force has been neglected for simplicity. However, it is found that can even be larger than the shear lift force under some particular orientations [5].

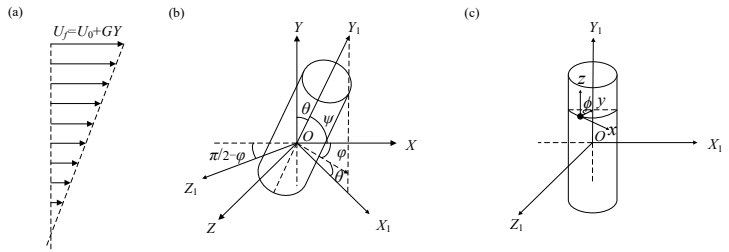

FIG. 1. The reference systems for cylindrical particles moving in shear flow of a rarefied gas: (a) the flow gradient; (b) the global and auxiliary coordinate systems; (c) the auxiliary and local coordinate systems.

Under a nonuniform temperature field [6], the thermophoretic force on the cylinder is given by

$$\mathbf{F}_{\mathrm{T}} = -\frac{\kappa}{5}\sqrt{\frac{2\pi m}{k_B T}}R_0 L\left[\sigma_\tau \nabla T_{//} + \left(2-\sigma_p+\frac{\sigma_\tau}{2}\right)\nabla T_{\perp}\right], \tag{4}$$

where κ is the thermal conductivity of the gas, and T is the gas temperature. The thermophoretic velocity can be also obtained by the balance between the thermophoretic and drag forces, which deviates from the opposite direction of the temperature gradient ∇T about 10.7°.

In summary, we derived the formulae for the shear lift, and thermophoretic forces for cylinders in the free molecule regime. It is found that the pitching effect of the nonspherical particles results in a transverse force, which is non-negligible and substantially affect the transport of the nonspherical particles.

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Brief Biography

Professor Wang received his B. S. degree in Engineering Thermophysics from University of Science and Technology Beijing in 2004 and his PhD degree in Theoretical Physics from Beijing Normal University in 2009. He was a postdoctoral fellow at Hong Kong Baptist University from 2009 to 2010, and a postdoctoral research associate at the Hong Kong University of Science and Technology from 2010 to 2012. Then, he joined Beijing University of Technology. He is now an Associate Professor in the Department of Energy Science and Engineering. His research interests lies in the interdiscipline between the statistical physics and Engineering Thermophysics, including nanoparticle transport in dilute gases, thermal Rectification, heat transfer in micro- and nano-scale. He has published over 30 refereed papers in these areas.

Waste-to- Energy Conversion of Sewage Sludge Using Sorption-Enhanced Thermochemical Technology

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Abstract

With the rapid growth in sewage sludge generation, conventional treatment approaches, like landfill and land application, are becoming less viable considering the land shortage and environmental concerns. Efficient approaches to treat sewage sludge in an environmentally benign and sustainable manner is in urgent demand. To date, one promisingly alternative solution would be the thermochemical technology, which could not only lead to an effective minimization of sludge, but also convert sludge into energy, syngas. Syngas which consists mainly of hydrogen (H_2) and carbon monoxide (CO) has gained increasing interests due to its high calorific value and wide application as feedstock for green chemical manufacturing. Upon introduction of the lime (CaO)-based carbonation-decarbonation loop, we put forward a new two-stage thermochemical technology of sewage sludge conversion (Figure 1) to separate the production of H_2 and CO, and importantly, intensify the utilization of carbon in the sewage sludge through recovering the CO-rich syngas. The technical feasibility of the proposed process was experimentally demonstrated by temperature-programmed thermochemical conversion of sewage sludge with and without CaO, showing that H_2 and CO can be easily separated at 550 °C and 750 °C, respectively. In addition, the syngas production by varying CaO contents was investigated. The results indicate that 50% of CaO content was the optimal value for CO-rich syngas production. We found that the presence of CaO could intensify carbon utilization efficiency via promoting CO_2-gasification of sludge to produce CO. The carbon remained in sludge reduced by 21 % with the addition of CaO, and the carbon conversion efficiency into CO was 13 % higher than that without CaO. In summary, this two-stage thermochemical process opens a way to turn waste into energy and valuable chemicals.

Brief Biography

Dr Yijiao Jiang received her PhD in Chemical Technology from University of Stuttgart, Germany in 2007. Since 2014 she has been a Senior Lecturer in the School of Engineering at Macquarie University (MQ), Australia. She is leading a dynamic research group currently with 1 MQ Research Fellow, 1 visiting professor and 7 PhD students. She has secured *ca.* AUD$4m in research grants from ARC DECRA, ARC DP, and ARC Research Hub, EU Marie Skłodowska-Curie Research Grant, etc. Yijiao's research interests mainly focus on the development of better catalytic/photocatalytic systems for green chemical processes, renewable energy and environmental protection. She has developed various in situ and operando spectroscopic techniques including NMR, EPR, IR, UV-Vis and Raman for achieving breakthroughs in catalysis research.

Grain-Based Discrete Element Method Modelling of Multi-scale Fracturing in Geomaterials under Dynamic Loading

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Abstract

This study aims to explore dynamic behaviour of fracturing and damage evolution of geomaterials at the grain scale. A series of dynamic tests is conducted on geomaterials to investigate dynamic responses under multiaxial pre-stress states using a novel triaxial Hopkinson bar. A high-speed camera at the frame rate of 200,000 fps with a resolution of 256 × 256 pixels is used to capture the fracture characteristics. Full-field strain and strain-rate fields of rock materials under dynamic compression are determined by the high-speed three-dimensional digital image correlation (3D-DIC) method. A grain-based discrete element method (GB-DEM) is proposed to reveal microscale characterisation and mineral grain compositions of geomaterials realistically. Comprehensive numerical simulations are conducted to compare with dynamic experimental results obtained by the Hopkinson bar. The 3D imaging of fracture networks in the damaged/fractured specimens is acquired via the X-ray computed tomography (CT) system. Combined with crack strain and acoustic emissions of numerical modelling, we also study the rate dependency of crack initiation stress threshold and crack damage stress threshold. The dynamic damage evolution in the form of Weibull distribution is distinctively different from that in static tests and the shape/scale parameters are presented as functions of strain rate.

Brief Biography

Dr. Qianbing Zhang is a Senior Lecturer in Geomechanics Engineering of Department of Civil Engineering at Monash University. Dr. Zhang received his PhD in Mechanics from Swiss Federal Institute of Technology in Lausanne (EPFL) in 2014. Prior to joining Monash, he was a postdoctoral researcher at EPFL and Cavendish Laboratory, University of Cambridge. Dr. Zhang's research group focuses on the development and application of experimental techniques and multiphysics computational tools to understand the progressive failure of geomaterials and structures under extreme conditions such as natural hazards (e.g., earthquake, landslides and explosive volcanic activity) and human-made disasters (e.g., nuclear power plant explosion, terrorist attacks, rock bursts and induced earthquakes). Dr. Zhang is a Co-Editor-in-Chief of *Tunnelling and Underground Space Technology* (Elsevier, Impact factor 2.418). He has published more than 40 international journals in the fields of geomechanics, tunnelling and impact engineering.

CFD modelling of air and particle flows in different airway models

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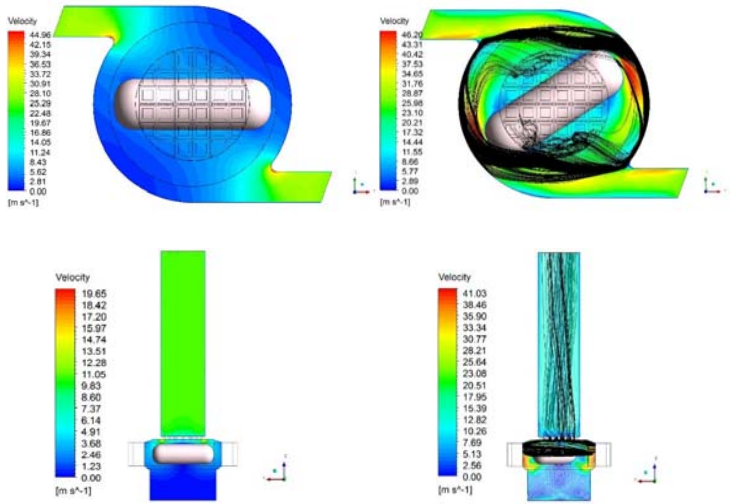
Abstract

De-agglomeration mechanism of the cohesive pharmaceutical particles in aerosolization process is a major interest particularly for the carrier-based dry powder inhalers (DPI) such as Foradile^® Aerolizer. Cohesive characteristic of microparticles can be useful in the device for increasing the device performance as it participates as a synergistic effect to the emitted dose. However, particles agglomerate causing the increase of particles' aerodynamic diameter eventually results poor penetration of mouth-throat. Therefore, appropriate de-agglomeration of cohesive particles prior to the dispersion from the device is significant process for obtaining necessary emitted doses.

The investigation on the effect of design modification is important in the aim of achieving particle de-agglomeration which eventually influences the device performance of DPI. Many CFD simulations on various DPIs in conjunction with design modifications are attempted to investigate device performance variation and dispersion mechanism [1-2]. Similarly, the CFD-DEM coupling method is previously adopted to see agglomerate breakage particularly for DPIs of the carrier based pharmaceutical ingredients [3-5]. However, the effect of device design modification to the breakage of particle agglomerates using CFD-DEM coupling method is not much previously attempted.

The conventional Aerolizer design consisting of grid and capsule chamber which allows capsule containing pharmaceutical ingredient to arbitrarily move during patients' inhalation is still being incompetent for particles to be efficiently de-agglomerated. The Aerolizer consisting of bumpers in capsule chamber is proposed for device design modification to observe the particle de-agglomeration process. The CFD-DEM coupling is employed to model the unsteady continuum phase in the Aerolizer as well as particle agglomerate modelling. Capsule sliding motion under one degree of rotation in dynamic mesh method is enabled to investigate the influence of capsule motion to the aerosolization and dispersion processes [6]. The simulation results including resistance, emitted dose and fine particle fractions of Aerolizer with modified design will be compared with the simulation results of conventional Aerolizer design.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia



(a) (b)

Fig 1. Top and front view of velocity contour (peak flowrate at 60 L/min) with capsule motion at; (a) t=0 s, and (b) particle injection at t=0.55 s.

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Brief Biography

Yun Hwan Kim is currently a Ph.D. candidate at the School of Materials Science and Engineering, UNSW Sydney. He has earned B.E. in Aerospace (2014) and M.Phil. in Materials Science (2016) from the same institute and has worked as an analyst at Hyundai Motor Group prior to pursuing the research degree at UNSY Sydney in 2015. His research has been focused on the CFD modelling of fine powders in the respiratory tract and CFD-DEM modelling of the dry powder inhalers using advanced turbulence model.

Dynamic modelling and analysis of the sintering of fine powders

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Abstract

Powder sintering is a key process in powder metallurgy. Powder sintering includes particle packing, compaction and heat treatment. Although extensive experimental studies have been conducted, it is still lack of microscopic information to understand the theory of compaction and sintering due to limited capabilities of experiments.

In the present study, a DEM model consisting of the contact force model, Van der Waals force model, sintering force model and the viscous force model, was implemented to study die compaction and free sintering of powders. The parameters in the model were calibrated by previous experimental and numerical results.

In the die compaction of particles (Fig. 1a), densification was initiated at the top punch and propagates to the bottom stationary punch. The densification near the top was larger than that at the bottom. In the die compaction of binary mixtures, the extent of densification due to particle rearrangement in binary mixture compaction was higher than that in mono-sized particle compaction. Plastic deformations in the mixture compaction were larger than those in mono-sized particle compaction. As large particles were mostly surrounded by small particles, small-small particle contact, and large-small particle contact patterns dominated the process.

In the sintering process (Fig. 1b), for a loose packing of powders, friction can help increase densification rate and tensile stress through preventing extra particle rearrangements and increasing average coordination number (Martin et al. 2015). However, if the compact was densified, friction took little effects on the evolution of free sintering behavior. The mechanisms of compaction dominate the evolution of contact radius at the initial stage of sintering, whereas the mechanisms of sintering take over the process after the initial stage of sintering. The evolution of anisotropy in shrinkage was highly dependent on the initial conditions of green compacts at the initial stage of free sintering. However, after sintering, the anisotropy tended to reduce largely to near isotropy (Boccaccini and Trusty 1998).

In summary, the DEM model in this study has shown its capabilities to simulate the process of die compaction and sintering. The effectiveness of our DEM model has been verified by previous experimental and numerical results.

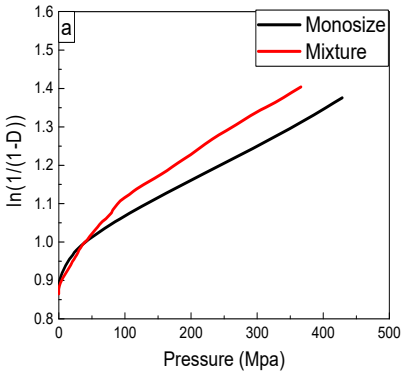

Fig. 1 a) Comparison between the Heckel plot of mono-sized particle compaction and mixture compaction for pressure-density relation. b) Evolution of relative density at stage A (loose packing), stage B (maximum load), and stage C (after compaction) — comparison with numerical results from (Parhami and McMeeking 1998)

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Brief Biography

Yaoyu Li is currently a Master of Research candidate at School of Materials Science and Engineering, the University of New South Wales UNSW. He obtained his Bachelor degree from Harbin Institute of Technology in 2016. His current research is focusing on dynamic modelling of compaction and sintering.

Finite Element Investigation of Briquetting of Iron Ore Particles

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Abstract

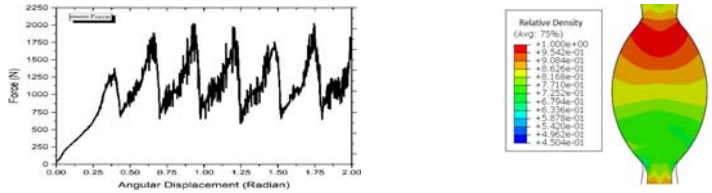
Briquetting is a compaction technique which can produce a solid briquette with definite size and shape by compressing loose powders. This technique is widely used in different industrial fields such as pharmaceuticals, mining, ceramics and food industries. During this process, forces and properties of the materials change significantly inside the briquette. Several factors can affect the steady production of compacts, including particle size and moisture content and operation condition such as coefficient of friction, feeding pressure, roll speed, roll gap. Comprehending the behavior of briquette is very significant for predicting the product properties and improving the control process.

In this current work, the properties of briquettes are analyzed by Finite Element Method (FEM) and Drucker-Prager Cap (DPC) model has been opted as a constitutive model. The model parameters for the briquetting simulation is determined by die compaction test, uniaxial compression and diametrical test of iron powders. A 4-node plain strain element (CPE4R) is used.

The exerted compaction force is one of the most important pointer used to explain the forming process. Figure 1a shows the simulated compaction force acting on the center of the roll. The forming process become stable very quickly as all the peaks are almost the same after the first peak. Most of the energy is utilized for the torque of the roll compaction in briquetting process. Figs. 1b shows the contour plot of the relative density at the maximum compression stage in the briquetting process. The density is higher at the upper part and decreases to the lower part. Higher relative density is because of higher pressure on powder materials during compression. Therefore, the top part of the briquette is much more compact than the lower part.

The effect of friction is also investigated. The results that the average relative density increases with increasing the coefficient for friction. The higher compacted area is difficult to compress leads a higher compaction force which is the reason for higher relative density.

In summary, the mechanism and densification process of briquetting was investigated by using FEM. The force and torque histories during compaction, structural states, plastic flow pattern and cracking and failure criteria inside the briquette were analyzed. Density as well as force can be influenced by coefficient of friction and an optimized coefficient of friction is necessary to achieve a higher and homogenous briquette density.



(a) (b)

Figure 1 (a) variation of force with angular Displacement; and (b) spatial distributions of compact density.

Brief Biography

I, Md Tariqul Hasan, received my BSc degree in Mechanical Engineering from Chittagong University of Engineering & Technology (CUET), Bangladesh, and MSc at University of Ulsan, South Korea. I also worked as an Assistant Director in one of the most renowned Engineering company in Bangladesh. Now, I am currently pursuing my PhD supervised by Associate Professor Runyu Yang at University of New South Wales, Sydney Australia. I am working on Finite Element Modeling of Briquetting of Iron-ore coal particles.

Experimental study on packing densification of non-spherical particles under air impact

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Abstract

Particle packings are ubiquitous in both industrial production and our daily life, which has rendered wide applications in many areas such as materials, metallurgy, chemical engineering, and so on. It is known that the densification of particle packing can be realized through the input of external energy like mechanical vibration, pressing, and air impact, etc. In comparison, the air impact has its own advantages, including uniform density distribution in the final packing, high densification efficiency and easy operation. Thus, air impact has been successfully used in foundry industry for the compaction of molding sands. Previous studies about packing densification under the air impact are mainly focusing on sphere particles, and few studies have focused on the densest random packings of non-spheres subjects to air impact. In this paper, the packing densification of various non-spherical particles under air impact is systematically investigated by physical experiments in our self-designed equipment. As shown in Fig. 1, the high-speed air (supplied by air compressor) enters from the inlet (A) of the cylinder, then interacts with the spheres in the cylinder and densifies the packing, and finally flows out of the porous bottom plate (7). In the whole process, the macro- and microscopic properties (e.g. packing density, distribution of air pressure in the container and force distribution in granular layer) for different packings are comprehensively characterized and compared. The results show that the air impact can realize the transition of packing from random loose to random close state at appropriate pressure for each shaped particles. The optimal air pressure for the RCP of each kind of particles is determined by both the material properties and particle shape, a correlation has been identified. The distribution of forces (measured by force sensor) in granular layer gradually decreases with height, while the air pressure (measured by pressure sensor) gradually increases.

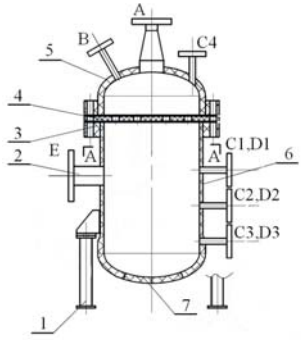

Fig. 1 Schematic view of the air impact equipment. A, inlet; B, pressure relief valve; C, force sensor; D, pressure sensor; E, window; 1, bracket; 2, support lug; 3, flange; 4, spreader plate; 5, upper head; 6, cylinder and 7, porous bottom plate.

Brief Biography

Gou Dazhao, PhD candidate in Northeastern University since 2016 in Northeastern University (NEU), got the Master Degree of Engineering from NEU with the major of Ferrous Metallurgy. Until now, 8 papers have been published, where 3 are in SCI journal and 3 are in EI journal. One patent is in application. And one project titled 'CFD-DEM modelling on the packing densification of particles when subjected to air impact' (supported by Fundamental Research Funds for the Central Universities of China) is undertaken. Mr. Gou's research interest is about the packing densification of granular matter under air impact, including physical experiments and CFD-DEM numerical modelling on the densification behavior, dynamics, and mechanisms of spherical and non-spherical particle packings.

Shape Effects on Bulk Modulus of Maximally Random Jamming Packing of Intersecting Spherocylinders

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Abstract

Granular materials have been arisen in a variety of scientific and industrial applications. The use of granular materials as building materials has many advantages such as easy assembly, transportation and disassembly. More particularly, aggregates made of non-convex particles are an emerging material of researches. They may have fairly low packing densities which save materials and rather high stability. It is well known that a small change in particle shape can lead to a large variation in the final assembly configuration as well as distinct mechanical properties. Furthermore, the mechanical properties are also related with the initial packing state of the assemblies. Therefore, it has great significance to study the particle shape effects on the mechanical properties of the assemblies at the same initial states. However, the effects of initial packing state and non-convex shape effects are rarely investigated in previous studies. In this work, we investigate the mechanical properties of the maximally random jammed (MRJ) packings of frictionless spherocylinders, two-dimension (2D) and three-dimension (3D) intersecting spherocylinders with different aspect ratios and branches. In the MRJ state, the packings are disordered but strictly jammed and mechanically stable. We use the adaptive shrinking cell algorithm to generate the initial structures of intersecting spherocylinders which are close to the MRJ state. Then the Discrete Element Method is used to stabilize the initial structures to reach a real jamming state, as shown in Fig.1. Afterwards, the packing structure are compressed isotopically to measure their bulk modulus. Our results show that the effects of aspect ratio on bulk modulus have the same tendency for spherocylinders, 2D and 3D intersecting spherocylinder. The bulk modulus first increases and then decreases with the increase of the aspect ratio, the maximum is achieved around the aspect ratio of 0.5 which is also the peak location for the packing density, as shown in Fig.2(a). Moreover, the bulk modulus increases with the packing density and have little relevance with the particle morphology. In another words, the bulk modulus of the packings of frictionless spherocylinders, 2D and 3D intersecting spherocylinders have almost the same value when they have the same packing density in the MRJ state, as shown in Fig .2(b). These results are helpful in the granular material design.

Keywords: Intersecting spherocylinder, Non-convex particle, Bulk modulus, MRJ state

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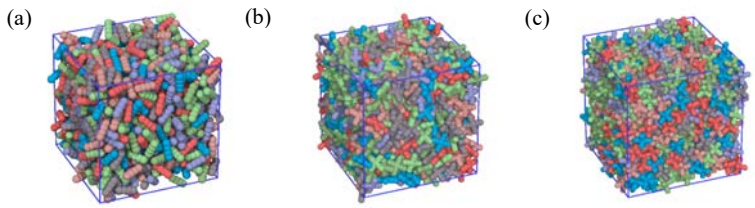

Fig.1.The packing structures of spherocylinders(a), 2D (b) and 3D (c) intersecting spherocylinders with the aspect ratio of 2.5

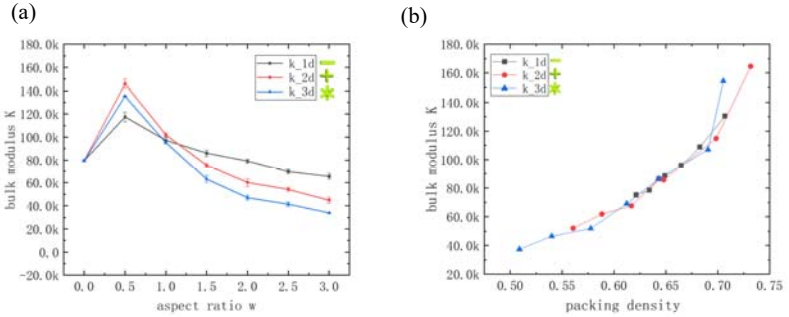

Fig.2.The effects of aspect ratio (a) and packing density (b) on the bulk modulus of spherocylinders, 2D and 3D intersecting spherocylinders.

Brief Biography

Mr. Wei Deng is a second-year Ph.D. student of Department of Mechanics and Engineering Science, College of Engineering, Peking University. He obtained his BE in Mechanics and Engineering Science from Peking University in 2017. His main research interests are particles packing and mechanical properties of the granules materials. His supervisor is Prof. Shuixiang Li in the same department of Peking University.

NOTICE:

Thanks for the acceptance of my abstract, I prefer both oral and poster presentations at this symposium. The speaker will be Mr. Wei Deng.

Multi-particle FEM modelling on hot compaction of TiC-316L composite powders

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Abstract

316L stainless steel (abbreviated by 316L) has been applied in many key industrial areas due its outstanding properties like corrosion resistance, ductility and biocompatibility etc., however, the relatively low strength and wear resistance of this material limited its further application. The introduction of TiC particulate reinforcement into 316L matrix can slove this problem, which can effectively improve the strength, stiffness, wear resistance and high temperature strength. In present work, hot compaction of TiC-316L composite powders in a closed die is numerically reproduced by multi-particle finite element method from particulate scale in 3D. The evolution of macroscopic and microscopic properties during compaction is systematically characterized and analyzed, and the densification dynamics and mechanisms are identified. The results show that hot compaction can not only significantly decrease the compaction pressure, but also alleviate the stress concentration in the final compacts. With the increase of compaction temperature, the equivalent von Mises stresses in the compacts get smaller. Large stresses are mainly concentrated within the TiC particles and the contact regions with 316L particles. In the whole compaction process, the equivalent von Mises stresses concentrated within the 316L particles firstly increase with the relative density of the compact at the initial stage of compaction and then decrease, which can be attributed to the increase of equivalent plastic strain of 316L particles. The equivalent von Mises stresses concentrated within the TiC particles gradually increase with the relative density since no obvious deformation can be found in TiC particles. While, larger contact normal forces are concentrated in the contact regions between the particles and the die, and larger contact friction forces are concentrated in the contact regions among 316L particles.

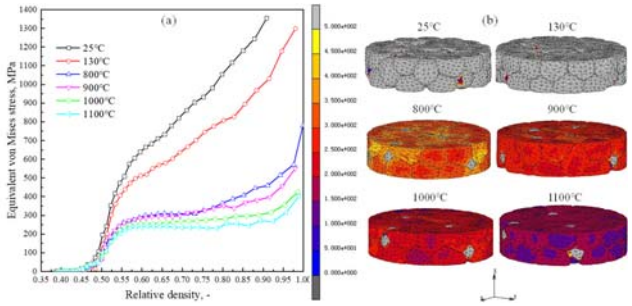

Fig. 1 (a) Variation of equivalent von Mises stresses with relative density in the compacts during compaction; (b) Morphologies of the final compacts under different compaction temperatures.

Brief Biography

Defeng Wang, a Ph.D candidate at Northeastern University (NEU) since 2015, got the Master Degree of Engineering from NEU with the major of Metallurgical Engineering. Until now, 2 papers have been published in SCI journals, 1 patent is in application and 1 submitted paper is under review. Mr. Wang's research interest is about the multi-scale numerical modelling on the compaction and sintering of different powders in powder metallurgy process.

Self-assembly of Granular Spheres under One-dimensional Vibration

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Abstract

Granular particles are often in disordered structures, but can change to ordered structures under certain conditions. This is related to the self-assembly, an interesting yet intricate phenomenon happening in different systems. Despite many experimental and numerical studies conducted, the fundamentals governing the self-assembly of granular particles, including the transitions of phases, order/disorder and jamming states are yet to be understood more clearly. In this work, the continuous self-assembly of uniform granular spheres from the initial random packing subjected to one-dimensional (1D) vibration is numerically studied by use of discrete element method (DEM). A wide range of the vibration amplitude and frequency is investigated. The structures of the packings are analyzed in terms of the packing fraction and microscopical structural parameters, including the coordination number and bond-orientational orders, and particularly the ordered clusters by the adaptive common neighbor analysis (a-CNA). It is shown that 1D vibration can also result in the self-assembly of particles with the packing fraction exceeding the random close packing (RCP) limit. The final packing would be a mixture of both FCC and HCP structures while their total fraction can reach nearly 100%. Moreover, the effect of the boundary, including the periodic boundary conditions (PBC) and containers of different shapes, is also studied. It is shown that certain boundaries can enhance the self-assembly by initiating the local ordered structures and directing the packing towards self-assembly as demonstrated via a cluster analysis. These results not only present a clearer picture for the self-assembly of granular spheres under vibration, but also help improve our understanding on the fundamentals of granular materials and jamming states.

Brief Biography

Mr. Reza Amirifar earned his bachelor and master degrees in Mechanical Engineering from Amirkabir University of Technology and Isfahan University of Technology, respectively (Iran) and now is a PhD student at the Centre for Infrastructure Engineering, Western Sydney University (Australia), under the principal supervision of Dr. Kejun Dong. His research interests include computer simulation of particulate systems, structural characterization of particulate systems and particle packing.

DEM Simulation of Powder Packing Process in 3D Printing

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Abstract

3D printing is a rapidly developing manufacturing method. The powder packing process in 3D printing aims to spread layers of material powders by a recoater onto the previous part for the subsequent sintering or melting. The packing density and homogeneity of the powder bed are proved to be important for the sintering or melting efficiency during the fabrication and affect the fabrication efficiency and part quality. Particle-based study is needed for identifying the powder bed structure under different conditions. In this work, particle-based DEM is used to simulate the powder packing process with considering the friction and adhesion between powder particles. The effects of recoater type, operating parameters and powder properties on the powder bed structure are analyzed.

Brief Biography

Mr. Lin Wang is a PhD student of Chemical Engineering of Monash University. He got his bachelor and master degrees from Northeastern University of China in 2014 and 2017 respectively. His present research work is on the modeling of powder handling process in 3D printing.

Shape Effects on Particle Segregation by Discrete Element Method (DEM)

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Abstract

Particle segregation is one important issue in many industries which deal with granular materials. In this work, the packing systems of spheres and cuboids with a range of aspect ratios are used to study the segregation phenomenon under three-dimensional vibrations by the discrete element method (DEM). The effects of some key variables, including vibration conditions, particle size and shape, on segregation are dynamically investigated. Based on the results, the underlying segregation mechanism will be discussed. The results indicate that, with the optimal vibration condition for each case, in a mixture of particles with different shapes but with equal volumes, the particles which tend to have a higher packing fraction, segregate to the bottom. However, when mixtures of particles with different volumes are simulated, the larger particles tend to move upwards. Therefore, particle segregation behavior comes from a combined effect of particle shape and size.

Brief Biography

Zhouzun Xie is a PhD candidate in School of Chemical Engineering of University of New South Wales. He received his BEng and MEng degree from Northeastern University (China). His research interest is non-spherical particle packing as well as flow and applications in water treatment.

Molecular Dynamics Simulation of Silica Oligomerization

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Abstract

Silica is a mineral applied in many fields of everyday life, for instance as a reinforcement filler for the tires or an animal feed additive. Thus, full understanding of the process of its production is of great interest not only to scientists but also to the industry. The important part of the research on silica precipitation is analyzing the influence of experimental conditions on the final product morphology.

Amorphous silica is a product of precipitation by neutralization of basic solution of sodium silicate with sulphuric acid. Its synthesis consists of few principal stages: mixing of the reactants, nucleation of silica, growth and agglomeration. Most of the studies found in the literature give insight into the final stages - aggregation and agglomeration of already formed silica clusters. At the same time, although, the events occurring at the beginning of precipitation are crucial for the following steps, they are not yet fully discovered. The problem lies in the nanometric size scale of the nucleating systems that is on the limit of detection of experimental methods with most of the processes appearing below it.

Bearing in mind limitations of experimental techniques, another tool is required to complement and confirm obtained results. Hence, computer simulations are applied to act as a bridge between the nanometric time and length scales of nucleation and the macroscopic scales of the laboratory.

Having a good understanding of the effect of operating parameters on the final product depends upon studying nucleation kinetics, mechanisms and clusters' morphology. As a result, what a considered simulation method should provide, is not only the access to the time and size scale of nucleation but also to the details such as morphology of the clusters during oligomerization.

The choice of a method satisfying all the aforementioned conditions is a difficult task. Nevertheless, it was stated that Molecular Dynamics (MD) simulation can provide at least partial information about the temporal evolution of the system of interest, as well as kinetics and mechanisms concerned.

The purpose of this study is to bring better understanding to the initial stages of silicic acid oligomerization to serve as a starting point in the investigation on silica nucleation. In the series of simulations, using ReaxFF reactive force field, the effect of the initial sodium silicate concentration and pH on the distribution of species with time was studied. The obtained results were compared with the literature data.

Brief Biography

Małgorzata Kamińska is currently a PhD student in the department of Process Engineering at École des Mines de Saint-Étienne, France. Her current research revolves around the first instants of silica precipitation with the special focus on kinetics and morphology of the nucleation process. Her thesis is performed in collaboration with silica producers and it includes a combination of experimental and computational methods. Prior to starting her PhD she had been working in the research group of Prof Bałdyga on application of chemical reactions to study micromixing in the chemical reactors. She holds an MA in Industrial Biotechnology from Warsaw University of Technology, Poland.

Numerical Investigation on the Rebound Mechanism of Spherical Fine Particle Impacting Several Blade Materials

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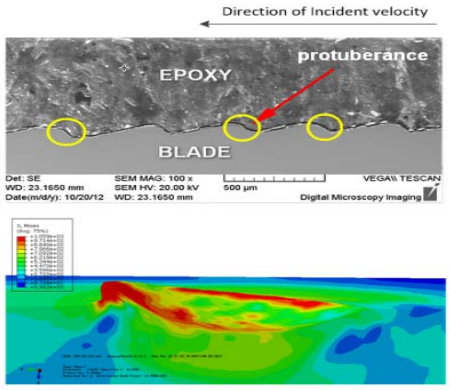
Abstract

Fine particles impacting blades with high velocity generally occur in turbomachinery component due to particulate matter ingestion, which always affects the life and operation safety of the equipment. In the present work, the rebound characteristics of several blade materials were investigated systematically using the ABAQUS/explicit code. A detailed study was conducted to investigate the effects of particle velocities, impact angles, particle sizes, temperatures, impact numbers and particle initial spins on the particle rebound characteristics and particle-wall interaction mechanism. The results showed that the tangential restitution coefficients of the three steels decreased with the increase of the impact angle and velocity. The normal restitution coefficients decreased with the increase of impact angle. For the collision of multiple particles, the tangential restitution coefficient gradually decreased with the increase of collision number, and eventually stabilized. The normal restitution coefficient increased with the increase of collision number and finally tended to be stable when the impact angle is less than 60°. Moreover, the effect of collision number on normal restitution coefficient can be ignored when the impact angle is larger than 60°. Tangential COR was found to generally decrease with an increase in temperature. The effect of particle size should be negligible. In general, the effect of positive spins on velocity restitution coefficient was greater than that of negative spins.

Keywords: Spherical particle; Rebound characteristics; Numerical simulation; Velocity restitution coefficient; Turbomachinery



Reduced Stiffness Model for Cohesive Particles

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Abstract

When we make a DEM simulation of granular flow, it is required to reduce the computational time to reduce the calculation cost. The method of reducing the spring constants in DEM contact force model which is proposed by the present author's group for the DEM-CFD simulation of gas-fluidized bed[1],, has been widely used for this purpose. The author's group found that this reduced stiffness model could not predict the flow of cohesive particles in gas-fluidized bed, and proposed a novel reduced-stiffness model, called dynamic adhesion/cohesion model, for cohesive particles[2].

Dynamic adhesion/cohesion model was developed analytically based on the binary collision process, and it can reproduce the fluidized behavior of Geldart-A-particles and aggregates formation in granular shear flow. In this keynote speech, the fundamentals of dynamic adhesion/cohesion model and its application to fluidized bed and granular shear flow will be given.

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Brief Biography

1. Education
Doctor of Engineering: Osaka University, 1994/ Master of Engineering: Osaka University, 1984/ Bachelor of Engineering: Osaka University, 1982

2. Professional Experience
2003-present, Full Professor, Osaka University/ 1996- 2003, Associate Professor, Osaka University/ 1984-1996, Research Associate, Osaka University

3. Major Research Interest
- Physics of Fluid-Particle Two-Phase Flow and Granular Flow
- Discrete Particle Modeling of Fluid-Particle Two-Phase Flow and Granular Flow

4. Service to organizations
- President of "The Japan Society of Multiphase Flow", 2018-present.
- Vice President of "The Society of Powder Technology, Japan", 2017- present.

Transient simulation of particle segregation by coupling granular flow model and diffusive, segregating fluxes

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[2] Monash-Southeast University Joint Research Institute, Suzhou, China

Abstract

Particles of different sizes or densities can segregate when mobilised. The segregation counteracts the effect of self-diffusion resulting from randomised interparticle collisions, and discourages well-mixing of particles. Several types of models have been proposed to simulate this phenomenon, which, based on different theoretical treatises, possesses different scopes of applicability. A new continuum model is formulated in this paper to simulate the segregation of bidispersed sphere mixture in rotating tumblers. The mixture is modelled as a single phase, whose averaged flow properties are assumed to constant irrespective of the variation in material constitution. This model is featured with a coupling of dense granular flow model, which permits the simulation of transient particle transportation and the applicability in configurations with complex loading or geometrical conditions.

Keywords: particle segregation; rotating tumbler; Eulerian approach; continuum modelling; FEM

Biography:

Dr Qijun Zheng is currently a research fellow in ARC research hub for computational particle technology, chemical engineering, Monash University. He obtained Phd degree from Material Science and Engineering, University of New South Wales in 2013, Master and Bachelor degrees from the Engineering Mechanics, Xi'an Jiaotong University, China. Dr Zheng's main research interest and expertise are simulation and modelling of granular flow, mixing and particle-structure interactions using continuum-based finite element method and discrete element method, with a focus on the civil/chemical processes of silo, rotating drum, blast furnace et al.

Computational and Experimental Investigations on Silicon Particle Growth in Silane Pyrolysis System

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Abstract

At present, the polysilicon market is facing excess production capacity however, the long term expectation to photovoltaic industry will inevitably stimulate polysilicon consumption in the future. The Siemens process has been the workhorse of polysilicon industry, with the disadvantages of batchwise operation and high energy consumption hindering further reduction of cost. As an alternative, the fluidized-bed process can run continuously and is less-energy-intensive, thus attracts more players engaged in it.

Our group has been working for 10 years on silane and silane based polysilicon. In an early phase, we investigated silane CVD (chemical vapor deposition) process in a fluidized bed reactor by means of CFD technique. Due to complexities of multiphase flow and reaction mechanism in this system, a CFD-PBM (population balance model) coupled model was proposed to predict the gas-solid flow hydrodynamics and the evolution of particle size distribution. The influences of silane pyrolysis kinetics, aggregation, and operating condition on silicon particle growth were studied. The predictions of flow parameters and growth rates were verified by empirical values and experimental data.

The flow hydrodynamic simulation showed that the EMMS-based drag model had remarkable advantages in predicting the "core-annular" flow structure and mesoscale flow characteristics, compared to the Gidaspow model. For the polydisperse particle system, when the aggregation effect was included, segregation with a rich layer of small particles at the top and near wall regions was accurately predicted, and when a higher fluidization ratio was applied, more diluted regions formed due to the enhanced drag force. Surface deposition, cluster scavenging, and aggregation were considered in calculating particle growth, and the results showed that the scavenging effect was responsible for the particle growth, and the growth rate agreed well with the experimental data when the scavenging factor was set to 0.1 under the condition of 923K and atmospheric pressure. Moreover, the formation of light silicon hydrides by silane homogeneous pyrolysis in the dilute phase was also investigated in the form of CHMEKIN mechanism, which showed that disilane turned to be the main silicon hydride and the silane conversion was under estimated by 12.5%. The effect of operating conditions on growth rate was studied in detail with the observation of defluidization phenomenon during the evolution of particle growth. The effect of silane pyrolysis kinetics was also analyzed and the results showed that the growth rate agreed well with Hsu's experimental data under the combination kinetic models of Hogness' homogenous and Furusawa's heterogeneous ones, in which a complete silane decomposition was almost achieved, but the impractical growth result was obtained as inlet silane mole fraction higher than 0.5. Moreover, the interphase mass transfer of silane surface deposition and cluster scavenging was also focused, which showed that silane surface deposition tended to occur at the solid dense bottom region with higher mass transfer rate and cluster scavenging happened in almost the whole solid phase.

In a secondary phase, silicon powders were prepared experimentally from silane pyrolysis in a horizontal quartz tube reactor. The effect of sintering treatment on the powder was investigated. Both the as-prepared and the sintered samples were characterized to determine the crystallite size, hydrogen bond structure, and morphology. The results showed that the higher sintering temperature and lower pressure were more favorable to the growth of silicon crystallites and the liberation of hydrogen from silicon hydrides. The crystallite size increased significantly with a critical low FWHM when the sintering temperature was at 750 °C, and the hydrogen releasing from polysilanes and OSiH took place remarkably with a relative flat IR spectrum when the vacuum condition was implemented. Moreover, the particle aggregation was strengthened with broad particle size distribution when long sintering duration or high temperature applied, and the fusion occurred as the temperature was high enough but still with good crystallinity.

Brief Biography

Prof. Wen-De Xiao is a Distinguished Professor at Shanghai Jiao Tong University. He received his B.S. (1985), M.S. (1988) and Ph.D. (1991) degrees in Chemical Engineering from East China University of Science and Technology, and worked there after graduation and was promoted to Professor in 1997. In 2009 he was invited to join the Department of Chemical Engineering at SJTU. He was awarded the "Excellent Young Talent Program of Trans-Century" by MOE in 1995, the "Cheung-Kong Scholar Program" by MOE, MOF, and the Cheung-Kong Holding Limited in 1999, and the "State Allowance for Outstanding Contribution" by the State Council in 2000.

He experts on chemical reaction engineering and catalysis related to environment, energy and materials. His current research interests include: photovoltaic materials such as large-scale production of silane and silane-based polysilicon (catalyst, mechanism, and reactor), clean coal technologies such as flue gas de-SO_2 and de-NO_x (reactor and catalyst), syngas to liquid such as Fischer-Tropsch synthesis to fuel and olefins (reactor and catalyst) and methanol to olefins (catalyst, mechanism, and reactor).

Closure Modeling of Particle Laden Flows with Machine Learning

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Abstract

The objective of this work is to describe particle laden flows with two-fluid equations with the unclosed terms closed by using machine learning models trained from particle-resolved direction numerical simulation (PR-DNS) data. As a starting point, we follow the work of Ma et al. (2015, 2016) on bubbly systems, with our improvements on the machine learning methodology and adaptation for particle laden flows. The focus of this work is on the regime of shear-thickening as delineated in Lashgari et al. (2014), which is featured by moderate Reynolds number (Re between 2000 and 5600) and solid volume fraction of approximately [0.15; 0.5], i.e., the cyan parts in Figure 1.

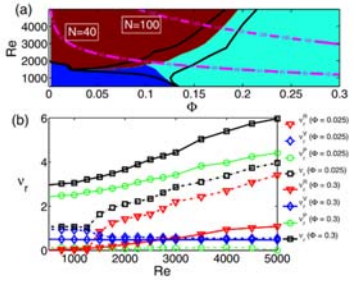

Figure 1 The regime of particle-laden flows that are the focus of this study. Figure reproduced from Lashgari et al. (2014)

Notes the coordinate system (following the convention of Ma et al.): the channel is vertical and flow goes upward. Further,

- x is the wall-normal direction, the only non-homogeneous direction of the system;
- y is the ow direction; gravity g acts in the -y direction only;
- z is the out-of-plane direction, which is periodic.

The PR-DNS data will be used to build the machine learning functions M : q — Y. Direction numerical simulations will be performed on the plane channel flow case. To start with, we will vary the following parameters:

- Reynolds number (based on half channel width): Re = 2000, 3500, 5000
- Solid volume fraction: Φs = 0:1, 0.2, 0.4
- Density ratio: 1, 10, 100
- Initial distribution of particles: linear distribution, uniform (yet random), sinusoidal (Φs (x) = cos(π x), assuming the channel walls are located at x = 0 and x = 2).

We regard the parameter in the middle (emphasized) as the “baseline", Then we change the parameters one at a time along each parameter cases. The particles are fixed initially with the specified distribution. When the flow field is fully developed, we release the particles at t = 0 and observe the evolution of the particles. During the simulation, the instantaneous field is plane averaged (averaged in the y and z plane to obtain a profile of the variables along the non-homogeneous x direction. It is possible that some temporal filtering can be done as well, i.e., the profile is output every n^{th} step or averaged every n^{th} step.

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Brief Biography

Dr. Guichao Wang obtained his Ph.D from the University of Newcastle under the supervision of Professor Geoffrey Evans, Graeme Jameson, J.B. Joshi. He is currently a research assistant professor at Southern University of Science and Technology. His present research interests encompass complex multi-phase flow systems with specific interest on hydrodynamics and particle dynamics. Exploring turbulence-particle interaction mechanisms involving interplay of various governing forces using experimental and LBM tools is an ongoing research activity. Another area of research is understanding particle detachment in a bubble-particle aggregate system due to interactions with turbulent flow structures i.e. eddies and coalescence among bubbles releasing surface ripples which has direct application in flotation based mineral processing. A new interest has emerged to explore study closure problems of particle laden turbulent flows with machine learning.

Numerical Simulation of Granular Flow Using Combined Discrete Element Model

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Abstract

DEM (Discrete Element Method) is an effective way to study the physics of granular materials because it can simulate the micro-dynamic behavior of granular material on an individual particle scale and the motion of every particle can be traced. Since DEM was first considered, many modified discrete element models have been developed. However, most existing DEM models are just for spherical particles or a specific type of non-spherical particles. In this work, a combination of several types of discrete element models including spherical model, super-ellipsoid model, polyhedron model, multi-sphere model, multi-super-ellipsoid model, multi-polyhedron model, and bonded-sphere model were used to simulate the flow of granular materials with many different shapes. And all the above models can be used together in one simulation. The accuracy of different models are different, and the simpler shapes have the higher model precision. The calculation speed of different models are also different, and the simpler shapes have the faster calculation speed. Several simulation cases including the flow of particles in tumblers, blenders, and other devices were performed to validate the modeling approaches. The simulation results show that it is practical and efficient to combine different discrete element models together for simulating both spherical and non-spherical particles in granular systems with quite high accuracy.

Keywords: DEM (Discrete Element Method), Non-spherical particle, Super-ellipsoid model, Multi-sphere model, Granular flow

Brief Biography

Dr. Yongzhi Zhao

Associate Professor in College of Energy Engineering at Zhejiang University, China. He received his Bachelor’s degree in Chemical Machinery and Equipment in 1998, Master’s degree in Chemical Process Equipment in 2001, and Doctor's degree in Power Engineering and Engineering Thermal Physics in 2005, all from Xi’an Jiaotong University, China. Afterwards, he started his postdoctoral research in Department of Chemical Engineering at Tsinghua University, China. In 2007, Dr. Zhao began teaching and researching in Zhejiang University. Dr. Zhao became an Associate Professor at the end of 2007 and a doctoral supervisor in 2015. From 2014 to 2016, he joined Northwestern University in the U.S. as a visiting scholar. The research subjects of Dr. Zhao include the numerical model and simulation of the particle system (including spherical and non-spherical DEM model and simulation, CFD-DEM model and simulation, and SPH model), fluidization, and new energy utilization (hydrogen energy). Up to now, he has got 8 national funding (including the funding from NSFC, National 863 Project, National 973 Project, and so on.) over 10 million Chinese Yuan (RMB) and has published over one hundred journal papers on *Powder Technology*, *AIChE Journal*, *Chemical Engineering Science*, *Granular Matter* and so on, among which 55 papers are indexed by the Web of Science core collection.

Liquid Film Modeling Within an Eulerian Multiphase Framework

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Abstract

Liquid films appear in many industrial applications like boiling water reactors, internal combustion engines, liquid atomizers, refrigerant flows in evaporators, etc, and the modeling of films is extremely important for design and analysis of these systems. For conducting a complete simulation of these liquid films, a number of physical phenomena have to be modeled accurately. These include the modeling of the formation of liquid films due to the flow of droplet-laden gas, and the consequent deposition of these droplets onto solid surfaces. As the liquid film flows along the surface, waves are generated due to its interaction with the gas flowing over it, and can lead to entrainment of droplets from the film into the gas. Additionally, as the film flows over complex geometries, it can encounter sharp corners which can also lead to further "stripping" of droplets from it. Another important phenomena associated with films is due to heat transfer from the wall leading to a depletion of the film through evaporation and boiling. Eventually, when the film is completely depleted, a condition known as dryout is achieved which has significant consequences in many industrial applications.

In the StarCCM+ solver, there are multiple methods to model multiphase flows, and the current work focuses on the Two-Fluid approach for modeling droplet-laden flows. Models have been implemented for capturing the deposition of droplets onto solid surfaces, stripping off of droplets from the film due to surface waves, and to capture the effect of sharp geometries. Since the Two-Fluid model considers both the gas and droplet phase as two inter-penetrating continua, two separate sets of transport equations are solved for both these phases. The liquid film modeling in StarCCM+ is performed by using a 2D-Laminar approximation for the film with a parabolic profile for the velocity across it. The transfer of mass between the droplet phase and liquid film is captured by calculating the mass lost/gained by the film, and converting it into an appropriate source/sink term in the corresponding phase transport equation. A few validation studies have been conducted and will be presented in the current work. The next step in this work will be the implementation of the heat transfer effect which will provide a complete framework for modeling of fluid film effects on droplet-laden gas flows.

Brief Biography

Kshitij Neroorkar completed his PhD in Mechanical Engineering from the University of Massachusetts Amherst in 2011. Following which, he worked as a visiting researcher at the propulsion system research lab in the General Motors Research Center in Michigan for 2 years on cavitation and flash boiling in fuel injectors. Since 2011, he has been working for CD-ADAPCO (now known as Siemens Industry Software Computational Dynamics India Pvt Ltd) as a developer for the StarCCM+ solver.

Shape Optimization of Axial Symmetrical Hoppers in the Discharging of Granular Materials

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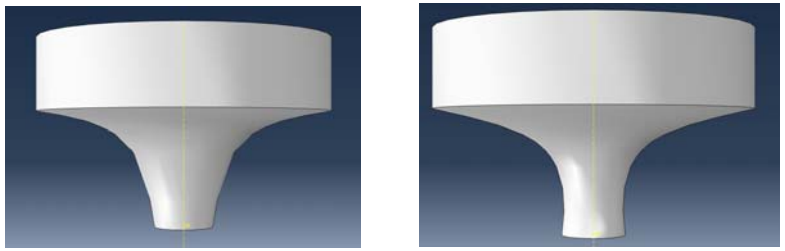
Abstract

Background/Aim: Mass discharge rate (MDR) of hoppers is an important parameter to evaluate hopper's performance. Beverloo equation and its extended series of correlation equations have described the relationship between MDR and many factors, e.g. diameter of hopper orifice, diameter of particle, hopper half angle and wall friction. In terms of the effect of hopper geometry, these empirical correlations offer an acceptable prediction on MDR of some typical shapes of hoppers such as flat-bottomed, conical or wedge hoppers. However, few studies have assessed the MDR of a hopper with a more complicated funnel wall rather than these normal surfaces. In the case when loading environment restricts the geometry of hoppers such as hopper height, diameter of orifice and diameter of hopper's upper opening, how we can optimize the wall surface of hoppers to improve the loading efficiency becomes an interesting question to investigate. In this study, we introduced shape optimization on wall surface geometry of hoppers, with the objective of increasing MDR.

Methods: This paper used Coupled Eulerian-Lagrangian (CEL) method to model the discharging process of granular materials from a hopper. This elastoplastic finite element method (FEA) model was validated by both discrete element method (DEM) and experiment, which shows good estimation of MDR in different cases. In terms of the optimization process, Genetic algorithm and gradient descent method were used respectively. Genetic Algorithm is a typical heuristic algorithm that imitates the mechanism of evolution in nature, which can avoid local optimal results but with low efficiency to reach an optimal solution. Gradient descent is a typical derivative based algorithm that has better efficiency but may converge to a local optimal solution frequently. The implementation of the heuristic optimization algorithm provided a reference, which was used as a guide of reaching to a global optimal for the derivative based gradient descent method. The combination of these two methods lead to an improved gradient descent method, which is converged faster and avoids local optimal solutions. This gives a pathway to conduct large-scale parametric study on different cases further.

Results: In our case study, the optimization was based on an initial conical hopper in the half angle of 45 degree, with the fixed geometry in the diameter of the orifice, the hopper height and the diameter of the upper opening of the hopper. The MDR increased 91.4% from the optimal design based on genetic algorithm, and 101.6% from the optimal design based on gradient descent method. The optimal shapes of the funnel walls from the two methods are consistent in a certain degree. The results of parametric study in different cases will update in the near future.



(a) *(b)*

Figure 1. Optimal design a) based on genetic algorithm and b) based on gradient decent method.

Conclusions: The combination of genetic algorithm and gradient descent method presented an efficiency optimization process. Our case study shows that the optimization reached to a globally optimal design with the computational time dropped from days to hours. It also demonstrates that shape optimization on wall of hoppers can increase MDR dramatically than normal designs with conical hoppers. Our research provides a potential solution for those hopper discharging challenges in process engineering, which are restricted by external conditions but are desired to have a higher loading efficiency.

Brief Biography

Xingjian Huang received his joint bachelor degree of transportation engineering from Central South University and bachelor degree of mechanical engineering from Monash University in 2016. He is currently a PhD candidate in the Department of Mechanical & Aerospace Engineering at Monash University since 2017. His PhD research topic is about structural optimization of hoppers in discharging of granular materials and related optimization algorithm.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

DEM Study on Granular Mixing in a Double-Screw Conical Mixer

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Abstract

Granular mixing is a common process observed in lots of industries such as chemical processing, food handling, pharmaceutical manufacturing, etc. Double-screw conical mixers are widely used in these industries for its high mixing quality and mixing rate. However, a deeper understanding as well as a large-scale simulation about the granular mixing in this kind of mixer is still lacking. In this work, discrete element method (DEM) is utilized to investigate the flow pattern of particles and their mixing performance in a double-screw conical mixer with the number of particles from 0.5 to 1.1 million. There are two asymmetric screws with short one and long one in the mixer, which maintain both rotation and revolution in operation. Combination of rotation and revolution of the screw contributes to a three dimensional particle mixing containing three mechanisms, convection, shearing and diffusion. The convection, shearing and diffusion of the particles will result in increasing the extent of mixing, increasing local mixing quality and attaining the overall homogeneous condition, respectively. Effects of the rotation and revolution speeds on mixing efficiency are studied. Different particle diameter ratios are also investigated to reveal the mixing performance of the double-screw conical mixer. Deeper analyses of the spatial distribution of the different components are done for improving the mixing efficiency to reduce the dead zone and inhomogeneity of the mixing.

Keywords: granular mixing; flow pattern; double-screw conical mixers; large-scale; DEM (Discrete Element Method)

Brief Biography

Ruihuan Cai

He is a PhD Student in College of Energy Engineering at Zhejiang University, China. He received his B. Sc. Degree in Process Equipment and Control Engineering in 2016 from Zhejiang University of Technology, China. In the same year, he joined Institute of Process Equipment at Zhejiang University, China, as a graduate student, majoring in Chemical Machinery and Equipment. His research interests and expertise range from diffusion, granular flow, granular mixing to large scale DEM simulation. He focuses on the diffusion of bidisperse particles in order to figure out the flow pattern of particles, which is fundamental to the intrinsic investigation of granular flow. He also has done some researches to improve the algorithm for DEM for better used in large scale engineering applications. The modified algorithm contains memory saving and efficiency improving. Here, he studies the granular mixing in a double screw conical mixer in a large scale DEM simulation to improve the mixing efficiency of the industry. Flow pattern of the particles in the mixer are also studied. In future works, he will continue to investigate the diffusion for deeper understanding of the granular flow as well as the large scale simulations for further engineering applications. His works are supported by two national funding (funding from NSFC).

A Numerical Study on the Solid Flow Behavior in a Rotating Drum Based on an Eulerian-Eulerian Approach Using a Frictional Stress Model

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Abstract

The dynamic behavior of solid particles in a rotating drum, operating in the rolling regime, is strongly influenced by particle to particle forces due to close packing of the particles. In Discrete Element Method (DEM) models these inter-particle forces arise naturally from particle and wall collisions. In continuum based models these forces are typically averaged leading to solids stress and pressure terms. The kinetic theory of granular flow (KTGF) provides a model for calculating solids stresses but has limitations in densely packed regions such as mills, kilns and rotating drums. The Eulerian-Eulerian multiphase model coupled to the kinetic theory of granular flow (KTGF) is evaluated in the present work. An additional frictional stress models are added in dense region and their suitability evaluated.

For the evaluation, a rotating drums at three rotational speeds (20 rpm, 42 rpm and 65 rpm) was analyzed. The simulated results were compared with Positron Emission Particle Tracking (PEPT) measurement data and simulated results by Discrete Element Method (DEM) from literatures. Unlike fluids, particles can and in the experiment did slip at the wall. A partial slip boundary condition incorporating a specularity coefficient was applied as boundary condition between particles and the rotating wall. Johnson and Jackson's model and Schaeffer's model for the frictional stress both show a lower angle of repose than observed in the PEPT measurements or DEM results regardless of the wall boundary condition used. A new frictional viscosity model based on solid pressure was implemented. By adjusting the specularity coefficient in the wall boundary condition results for the present model agreed well with the PEPT and DEM results in terms of angle of repose and spatial velocity fields. It was also observed that the frictional viscosity decreased as rotational speed increased.

Brief Biography

Wenjie was born in Inner Mongolia, China. She received her bachelor and master degrees from Northeastern University in 2014 and 2016, respectively. Then, she begins her Ph.D. study in Engineering Thermos-physics at the same university. During the first year of her Ph.D. period, she published two papers about energy and exergy analysis for different industrial sectors. After that, she came to CSIRO in 2017 funded by the Chinese Government Scholarship for a two-year project. She is currently working as a visiting Ph.D. student supervised by Dr. Peter Witt and Dr. Yuqing Feng in CSIRO Mineral Resources Computational Fluid Dynamics team. She is focusing on developing CFD models of multiphase flows to better understand and solve problems in mineral process.

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Numerical Analysis of Elongated Particles Flowing Through Shear Cell

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Abstract

It is essential to comprehend granular flow dynamics as particles are present in almost all aspects of our daily lives. The majority of such particles are non-spherical, which is a crucial feature that affects the nature of flow. Accordingly, the research on non-spherical particle flows is immensely significant. However, previous numerical studies were mainly focused on spherical particles. In this work, flow of ellipsoidal particles in a shear cell was analysed at the microdynamic level based on discrete element method simulations. In a stress-controlled double-shear condition, the flow was studied by varying the aspect ratio of ellipsoidal particles and compared with the flow of spherical particle assembly in terms of some key properties, such as particle velocity, contact force network and energy distribution. It was found that particle alignment towards shear flow direction has strong influence on overall flow pattern. Particle elongation primarily impacts its restriction of rotational displacement through preferential alignment which causes percolation of force across the flow become more uniform. The regime transition of particle flow was also investigated for spherical and ellipsoidal particles with various aspect ratios. The correlations among elastically and kinetically scaled stress, kinetically scaled stiffness and volume fraction were examined and a regime map was obtained for all specimen particle assemblies.

Brief Biography

Muzahid Hossain is a PhD candidate in School of Computing, Engineering and Mathematics, Western Sydney University (WSU). He is currently involved in research projects related to flow of non-spherical particles with Dr. Haiping Zhu at WSU where he is primarily working with elongated ellipsoidal particles in virtual platform in a comparative analysis with spherical particles and identification of distinguishing features of non-spherical particles especially in regard to regime transition. He is also a mechanical engineer with experience in construction of single cycle gas-fired power station operation of combined cycle gas-fired power station including desalination plants.

DEM Study of Copper Stave-Burden Interaction in the Ironmaking Blast Furnace

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Abstract

The influence of copper stave design on the material descent in the ironmaking blast furnace is not well understood. Staves are water cooled elements that fully cover the internal surface of the blast furnace shell and provide both its working lining and thermal protection. Current stave designs commonly exhibit protruding ledges which are exposed to the descending burden. In this study the effect of stave geometry, on burden descent phenomena such as the resulting wall forces and burden segregation has been explored. The discrete element method (DEM) simulation technique was applied to investigate these phenomena at a particle scale. Different arrangements of the ledges on the stave working surface as well as process parameters such as the particle size distribution, burden flow rate and various material properties were investigated with regards to their influence on the resulting material flow patterns and force profiles inside the blast furnace. The consideration of staves in the model greatly influenced the burden descent, especially along the walls of the blast furnace and the obtained wall stress profiles highlighted potential regions of high wear. This has implications for the gas distribution close to the furnace wall as well as the stave operating life. It is therefore necessary to consider the presence of copper staves in the simulation of blast furnace burden flow when studying near wall phenomena.

Brief Biography

Joel Samsu received his BSc and MSc degrees in Process Engineering from the University of Leoben, Austria in 2012 and 2014, respectively. He is currently a PhD candidate at the Laboratory for Simulation and Modelling of Particulate System (SIMPAS) at Monash University, Clayton, Australia. His research interests are the application of computer simulation of burden flow in the ironmaking blast furnace.

Charge Material Distribution Behavior in Blast Furnace Charging System

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Abstract

The productivity and stability of blast furnace smelting processes can be achieved largely by optimisation of both internal state in-furnace processes (chemical reactions) within the reactor and peripheral operations such as meticulous control of raw materials quality and appropriate burden distribution at stock-line level [1, 2]. A considerable amount of research has been conducted to better and improve the understanding of burden distribution characteristics at charging of the blast furnace and stock-line profiling. Such efforts include the works of various researchers [3, 4]. The afore-mentioned works provide both physical and numerical burden distribution models with principle investigations into the behaviour of blast furnace charge material as a function of the particle properties, methods of operation and geometrical effects.

However, the handling of bulk solids in any form has a challenge in terms of maintenance of homogeneity. Bulk solids dynamics still poses critical knowledge gaps in science despite numerous studies [5]. With particular applications in blast furnace charging system which has a network of equipment and mechanisms designed to charge materials into the furnace, understanding of how charge materials mix and segregate (de-mix) during multiple handling points is of substantial interest. Although numerous past studies have focused on characterising granular mixing and segregation (de-mixing) by defining a mixing and/ or segregation index based on lumped sample and measure particular variance [6], though quite informative, the major drawback of such characterisation is the averaging over a domain of measurement while neglecting the particle-particle distribution variation which remains undiscovered [7].

This work implements a near-neighbour distance method approach to investigate the effects of polydispersity on mixing and segregation (de-mixing) in the blast furnace charging system. The near-neighbour distance method approach gives useful inferences on segregation and dispersion as it provides an unprecedented quantification of the particle-particle scale distributions of particle types relative to others with time in the system.

A 1:5.8 lab-scale 3-D DEM model framework of a blast furnace charging system was developed. The particles were tracked in space and time by explicitly solving Newton's second law of motion equations while a soft sphere linear-spring dashpot model was used to model the particle contacts [8]. In order to investigate the influence of polydispersity on the mixing and segregation behaviour of the charge material along the charging system, four initial scenario packing arrangements of raw materials were studied. Sinter and pellets materials of different sizes and distributions were initially charged into weigh-hopper (WH) in alternating layers (completely segregated). The materials were allowed to undergo various flow movements in the system units under the influence of gravitational or mechanical (vibration) forces. Quantification of near-particle neighbour distributions with time was done. Analysis of the near-particle neighbour distributions has shown that, over time along the system, the raw materials subsequently approaches a mixed state irrespective of initial position. The developed DEM and near-neighbour distance method characterisation have proved to be a powerful tool to further the understanding of charge material dispersion with time over prolonged and multiple handling stages of the charging system.

Brief Biography

Deside Chibwe is a holder of BSc. (Honours) and MSc. in Extractive Metallurgical Engineering, from the University of Zimbabwe and University of Stellenbosch respectively. He has previously worked in ferrous and non-ferrous pyro-metallurgical smelting operations in various capacities. Key interests and activities mainly involved the application of fundamental research to improve smelting operations. He is currently undertaking PhD at the University of Newcastle under the supervision of Prof. Geoffrey Evans (Academic) and Dr David Pinson (Industrial). The study is looking at optimization of burden (charge material) delivery for blast furnaces operation. Particular interest is in furthering the understanding of particle dynamics in relation to mixing and segregation of handling of burden materials of variable size, size distribution and densities. Discrete element modelling (DEM) is the key technique being currently applied.

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Analysis of Factors Affecting Funnel-shaped Moving Bed

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Abstract

Granules are widely found in nature and have a wide range of applications in industry, agriculture and tertiary industries. Granular materials are aggregates of discrete solid particles. The number of particles is large, and their size, shape and properties are different. It is a typical complex system. The movement of particulate materials is very different from the common gas and liquid flows. As a reactor for realizing gas-solid phase or liquid-solid phase reaction process, moving bed is widely used in industrial energy-saving industries, and the fluidity of granular materials has a great influence on the heat transfer performance of moving bed. In this paper, the discrete element method (DEM) is used to study the effect of particle size, opening width of funnel-shaped moving bed and moving bed half cone angle on particle mass flow rate of funnel-shaped moving bed. The results show that the particle size, the funnel-shaped moving bed half cone angle and the bottom opening width have a great influence on the particle flow rate. The mass flow rate of the particles is positively correlated with the particle size; the mass flow rate of the particles increases exponentially with the increase of the slope of the discharge port; the mass flow rate of the particles increases with the increase of the opening, and meets the requirements of MYERS ME, SELLERS M. Correction formula for the square exit of the Beverloo empirical relationship of the flat-bottom moving bed.

Brief Biography

Dawei Sang, PhD student of University of Science and Technology Beijing.

Lin Qiu, Associate Professor, School of Energy and Environmental Engineering, University of Science and Technology Beijing. Member of the American Society of Mechanical Engineers (ASME), member of the "Scientific Reports" (Nature Publishing Group, IF=5.578) Editorial Board, In recent years, more than 40 academic papers have been published by the first author or correspondent author, including 23 articles in SCI and 9 articles in EI.

Yanhui Feng，Professor /Deputy Dean, Department of Thermal Engineering, School of Energy and Environmental Engineering, University of Science and Technology Beijing ,Secretary General of the China Society of Metals Energy and Thermal Engineering. She Received the Excellent Youth Science Fund Project established by the National Natural Science Foundation of China. In the past 5 years, a total of 58 SCI papers have been published, including 1st of the 1st correspondence author's thesis; the paper was cited 343 times by SCI, and the 1st correspondence author's paper was cited 189 times by SCI.

XinXin Zhang, Professor , School of Energy and Environmental Engineering, University of Science and Technology Beijing ,Deputy Director of the Energy Dynamics Teaching Guidance Committee of the Ministry of Education, Director of the Thermal Engineering Foundation Teaching Guidance Subcommittee, Deputy Director of the Engineering Thermophysical Committee of the Higher Education Institute of China Higher Education, and Chief Scientist of the 2011 973 Program. He published more than 350 papers.

Axial Segregation of Binary-Sized Mixture of Ellipsoids in a Rotating Drum

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Abstract

Rotating drums play an important role in industry for mixing, milling, coating and drying process. Both radial and axial segregation due to different particle properties, such as size and shape, could happen in the mixing process. The studies on the axial segregation of spherical particles have been carried out extensively. It was found that axial segregation tend to happen slowly after the rapid formation of radial segregation. However, particles shape could have an influence on the formation of axial segregation, which has received limited studies. In this work, discrete element method is used to study the axial segregation of binary-sized mixtures of ellipsoidal particles in a rotating drum. The segregation patterns for both spheres and ellipsoids are presented. The effects of rotating speed and aspect ratio of ellipsoids on the evolution of axial segregation are investigated. For both spheres and ellipsoidal particles, the revolution of the drum gives rise to the bands of fine particles, i.e. axial segregation, in the vicinity of end walls. Particularly, the bands of fine spheres continue to form in the central region with the increasing revolutions. As the aspect ratio deviates from the unity, i.e. elongated or platy shape-type, axial segregation forms more slowly with lower extent at the equilibrium state. It could be explained by the effects of particle shape on the diffusion of fine particles between radial cores. Furthermore, the effects of rotation speed on axial segregation are examined. It is found that in rolling or cascading regime, increasing rotating speed leads to faster formation and larger extent of axial segregation at the steady state for both spheres and ellipsoids.

Biography

Siyuan He is a third year PhD student in the Department of Chemical Engineering, Monash University. He obtained his bachelor degree in Qingdao Technological University. He finished his master study in Ocean University of China. He is currently focusing on DEM simulation for the flow of aspherical particles in rotating drums.

DEM study of the performance of screw conveyor with an inclined screw blade

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Abstract

Screw conveyors, as a transport equipment, are used in many industries, such as agriculture, ironmaking, pharmaceutical, plastic, and mining industries. They can transport and/or elevate particles continuously at controlled and steady rates while reducing the risk of environmental pollution. Screw conveyor can be operated at all angles, from horizontal to the vertical. Because of the effects of gravity and centrifugal force, particles will roll backwards relative to the mainstream, giving the so-called backflow. To reduce the backflow and increase the flow rate under different inclinations, newly designed screws with an inclined blade are adopted. The performance in terms of flow rate, power draw, energy dissipation is examined by the Discrete Element Method (DEM) under different operation conditions such as different rotation speeds and inclination of the screw conveyors. The results demonstrate that the inclined blade can reduce the backflow and hence increase the flow rate in a wide range of inclination. The degree of blade angle plays an important role and a slightly inclined blade may improve the performance of the screw conveyor system significantly. This work, through the cost-effective numerical examination of new screw designs, provides a comprehensive guid for screw conveyor design and operation.

Keywords: Inclined screw blade, Screw conveyor, DEM

Biography

Xin Li is currently a PhD candidate in ARC Research Hub for Computational Particle Technology at Monash University. She obtained her Bachelor's degree at Nanjing University in 2006 and Master's degree at the University of Science and Technology Beijing in 2012. Her PhD project is focused on improving screw feeding system performance by proposing new designs, by utilizing the cost-effective DEM-based numerical simulation.

Numerical study of vibration induced size segregation

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Abstract

Segregation in granular systems is primarily a practical concern of many industries. A better understanding of segregation will help solve the handling and processing of these industrial issues. Among all processes that may cause segregation, vibration can drive large particles to move upward within bulk solids of small particles. This phenomenon has been well studied considering various particle properties, here we further extend the study of segregation nature with the help of DEM simulation. In this work, different vibrated binary systems contain both ellipsoidal and spherical particles are investigated. The binary granular materials are charged into the vessels separately, and vibrations are introduced after all particles settle down. Aspect ratio of ellipsoids is used to quantitatively determine the particle shape. Other factors including vibration amplitudes, frequencies and size ratio are also tested. Several results have been addressed through the research. It was found that vibration conditions are the triggering factors of the Brazil Nut phenomenon while size ratio and aspect ratio can affect the segregation degree. And for special conditions, this segregation presents a come-back behavior as the large particles will once again sink inside the bulk solids. These patterns are further studied based on overall bed porosity, averaged coordination number and local porosity. The profiles exclusively offer a new idea about the nature of vibration segregation that the overall bed state show a vibrated phenomenon which is consistent with the movement of the large particle.

Brief Biography

Dizhe Zhang is a full time Ph.D student affiliated with the Department of Chemical Engineering at Monash University, Australia. His study focus on the numerical study of particle behaviors in segregation systems. Dizhe Zhang earned his BSc from School of Energy and Power Engineering at Beihang University, China.

Ab Initio Molecular Dynamics Study of Properties in Supercritical Water

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ABSTRACT

Water above the critical point T=647 K, P=22.1 MPa, and ρ=0.32 g/cm^3 has been found successful applications in supercritical water gasification (SCWG) in the last few years. Within SCWG reaction, supercritical water is a very attractive media, which may dissociate, dissolve or hydrolyze more hydroxide anion than conventional steam. Contrary to the ordinary liquid state, at supercritical conditions the hydrogen bond network is destabilized to various extend and the continuous breaking, which is demonstrated by changing curves of mean number of hydrogen bonds per water molecule. The reformation of hydrogen bond structures allows large dipole fluctuations that can significantly affect the dielectric properties of the solvent.

Actually, it is very hard to measure the physical properties of supercritical water directly, because of the super worse experimental environment. In this respect, computational simulation is used to study the intrinsic property of supercritical water. However, classical molecular dynamics simulation is not sufficient to obtain the dipolar and dielectric properties of supercritical water. Although many articles about ordinary or critical state water are interpreted by classical molecular dynamics, there are still many shortcomings within these water potential models, due to the lack of significant polarization and charge transfer effects, which makes it inadequate for correctly describing the liquid at supercritical conditions. Also, for chemical reactions within supercritical water, the electronic structure of both reactants and solvent must be treated at the same level. Therefore, we notified Car–Parrinello molecular dynamics (CPMD), which has already been proved to be a good approach to studying in an unbiased way water at extreme thermodynamical conditions. CPMD is one of ab initio molecular dynamics (AIMD) methods, which could well combine molecular dynamics and first principle methods. In this approach, dynamic equations of motion are solved for the ions with the inter-ionic forces computed from the valence electron density, which is solved using density functional theory.

On the other hand, infrared (IR) adsorption is one of the main tools for investigating the dynamical properties of condensed systems. Theoretical interpretations of the IR spectrum have so far been mainly based either on qualitative arguments or on molecular dynamics simulations. In this case, CPMD can give a detailed description of the ionic motion and calculations of the IR spectrum of water.

Here, we analyze the structural, dipolar and spectral properties of water above the critical point, and compare them with the ordinary liquid state. The calculations were performed using CPMD packages. The goals of this work are presenting a method for investigating unique properties of supercritical water which is more accurate and economical, as well as extending the computational scale for water, which is applied for further investigation in reaction. Furthermore, studying chemical reactions involving supercritical water in SCWG is our further objective. We demonstrate that the experimentally observed peculiar behavior of the IR spectra for water is well reproduced in our computational scheme.

BRIEF BIOGRAPHY

Ms. Song earned her bachelor's degree in the Institution of Energy and Power Engineering at Shandong University in 2015, Jinan, China. She is studying as a Ph.D. under the guidance of Prof. Liejin Guo, in the State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University, Xi'an, China. During the Ph.D. period, she devotes herself to study the unique properties of supercritical water comparing to ambient water, and thus understand the reaction mechanism of supercritical water gasification (SCWG). She chose Car-Parrinello molecular dynamics (CPMD) for her research. Her research topics include structural, dipolar and spectral properties of water above the critical point, as well as compares them with ordinary liquid water. She is also working to find appropriate tools for studying supercritical water and investigate the unique properties of supercritical water. One important goal of these researches has been to provide reliable results comparing with experiments to apply in hydrogen production by SCWG. Another major goal is to extend the computational scale for the critical state. Furthermore, to study chemical reactions involving supercritical water in SCWG is her further objective. Based on some previous works, she got a second-class scholarship and a third prize in energy saving & emission reduction contest in college. Moreover, she is very proficient in using some instruments, such as STA (TG-DSC) and Automatic Titrator.

Study Of Rheological Behaviour Of Granular Non-spherical Particle Suspensions Via CFD-DEM

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Abstract

Non-inertial (or colloidal) suspensions of non-spherical particles have been studied extensively. However, the rheology of inertial (or granular) suspensions of non-spherical particles is rarely investigated. The rheological behavior of relatively large elongated granular particles is therefore not well known. In this work, we study suspensions of rod-like particles of aspect ratio 4 subjected to shear flow in a low-density Newtonian fluid. We perform CFD-DEM simulations for a periodic shear box for a range of shear rates and volume fractions of particles, which are practical for fluidized bed applications. We demonstrate the verification of our predictions via a comparison with granular kinetic theory developed for sheared spheres. We discuss the dependence of rheological properties like stress, pressure and relative viscosity on volume fraction, shear rate, granular temperature and the particle orientation. Perhaps surprisingly, the granular rods show shear thickening behavior. These results provide insights into the macroscopic rheology of suspensions of randomly oriented and oriented granular rods. This study can further be extended to develop a stress closure for use in a coarser grid models like MP-PIC which can simulate an industrial fluidized bed reactor of non-spherical particles.

Brief Biography

Vinay Mahajan is a PhD Researcher at Technical University Delft, Netherlands with experience in CFD/DEM modeling and experiments of particle-laden flows. He is currently investigating “Non-spherical particles in pseudo-2D fluidized bed: Experiments and Simulations”. He has Master’s degree in Process Engineering from Technical University Eindhoven, Netherlands with a thesis on “Granular flow on inclined rotating chutes”. His prior work experience includes a short term assignment with Tata Steel, Ijmuiden, as an Intern and a 2 year assignment with National Chemical Laboratory, Pune as a Research Assistant. He completed his Bachelor’s in Chemical Engineering from National Institute of Technology, Rourkela, India.

Simulation and Modelling of Ellipsoids in Particulate Systems

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Abstract

Particle science and technology is a rapidly developing interdisciplinary research area with its core being the understanding of the relationships between micro- and macro-scopic properties of particulate matter. In particular, discrete particle simulation has been widely used to tackle fundamental problems in particle research. However, so far, most of the simulation studies deal with spherical particles. The resulting findings are useful, but may have limitation in addressing practical problems. It is well recognized that particle shape significantly affects the packing/flow structures of particles. Hence, many efforts have been made to develop further understanding of particle shape effects on particulate systems. In our work, ellipsoidal particles are used as they can represent a range of different shapes varying disk-type to cylinder-type. The approach used is on the basis of discrete element method, an advanced numerical method that can capture particle dynamics at a particle scale. In this presentation, we give a brief review of studies of ellipsoidal particles on the basis of discrete element method, and examine the effects of particle shapes in some typical particulate systems, including: (1) particle packing, focusing on how aspect ratio affects packing density and structure for coarse and fine ellipsoids; (2) particle flow in hoppers and rotating drums, demonstrating the dependence of discharging rate and flow regimes on particle shapes; (3) sandpile formation, focusing on how aspect ratio affects the angle of repose, stress dip distribution and shape or size-induced segrgation; and (4) fluidization, illustrating how particle shape affects the bed permeability, orientation, and bed flow/force structures. The results show that discrete element method for ellipsoids provides a useful approach to investigate shape effect on the behavior of granular materials.

Biography

Dr Zhou, PhD (2007, UNSW), specialises in the modelling of multiphase flow, heat and mass transfer, and particulate systems. Dr Zhou has made significant contributions in the theoretical developments of advanced numerical models for complex particle-fluid systems, particle scale approach for heat and mass transfer modelling, and modelling of non-spherical particles. Dr Zhou has successfully won 7 ARC grants, 4 industry sponsored projects, and been involved in many other projects. He has published more than 70 journal papers in learned journals, with the total citations more than 2800 times (SCOPUS data). Dr Zhou has been actively engaged with international conferences by giving keynote/invited presentations, chairing/organising mini-symposiums, and acting as symposium secretary. Dr Zhou was the ARC APD fellow (2007-2010), members of AIChE and Engineers Australia, and currently acts as the vice director of ARC Hub for Computational Particle Technology (2016-2021).

Detachment of droplets on solid surface in the surfactant solution

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Abstract

The motion of droplet on solid surface displaced by another continuous fluid with additives encountered in many applications such as oil detachment. In the petroleum industry, the performance of enhanced oil recovery technology is strongly dependent on the mobility of oil droplets/film attached to the rock surface. In addition to change the interfacial tension of oil-droplet interface, the adsorptions of additives, e.g., surfactants, also have significant influence on the wettability of solid surface. The main challenges of available numerical methods associated with the two-phase flow is to incorporate the surfactant effect into the dynamic description of moving contact line, for instance, the inclusions of interfacial tension and contact angle into the slip boundary condition. In the present paper, we extended the GNBC-based front-tracking method to simulate the detachment of droplets displaced by a shear flow in the surfactant solution. For the droplet adhered to the solid surface, the variation of surface surfactant concentration, and the effect of Marangoni flow induced by the nonuniform surfactant concentration on the droplet interface are investigated and compared with the clean droplet. Then the behavior of moving contact line (i.e., equilibrium, dynamic contact angles and velocity) for wetting droplet and non-wetting droplet and its effects on the onset of detachment are investigated in the presence of surfactant. It is found that the increasing contact angle in the presence of surfactants at the contact line have a great effect on the wetting droplet in comparison with the non-wetting droplets. Due to the increase in the surface force and equilibrium contact angle, detachment is preferred to occur early in the surfactant solution in comparison with the clean droplet in the shear flow.

Brief Biography

Xinglong Shang is currently a Ph. D. candidate in the State Key Laboratory of Multiphase Flow in Power Engineering at Xi'an Jiaotong University. He received his M. Sc. degree from Dalian University of Technology in 2014. His current research interests include DNS of two-phase flow, droplet dynamics, moving contact line modelling and the computations of droplets with complex interface in the presence of surfactant.

Computational Particle Fluid Dynamics Modeling of Gas-solids Flow in a Downer

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Abstract

Gas and solid phases move concurrently downward in a downer, thus displaying distinctive fluid dynamic properties compared with those in a riser, such as more uniform flow field, better heat and mass transfer performance, and shorter residence time of particles, which provide significant advantages for downer in catalytic cracking, high-temperature cracking of pulverized coal, cracking and synthesis of biomass, and especially in coal pyrolysis. For such high temperature and rapid reaction processes, the gas-solid flow behavior, the effect of inter-particles mixing and the heat transfer in downer are the key problems to facilitate the reaction. Therefore, it is of great significance to fully understand the gas-solid flow, mixing, heat transfer and reaction characteristics in a downer to promote the industrial application of downer reactors.

A gas-solid flow model was developed by means of computational particle fluid dynamic method (CPFD), and the size of mesh, density of parcels, wall boundary conditions and drag models were fully investigated, and with special attention to the effect of particle inlet conditions on gas-solid flow field. Then, the gas-solid hydrodynamic characteristics in the downer were analyzed in detail and the influence of operating conditions was investigated. The results show that the gas-solid flow behavior in the downer is very sensitive to the inlet conditions and the inhomogeneous particle inlet boundary conditions can describe the particle distribution at the inlet of the downer more accurately. The radial distribution of particles concentration in the downer is not very uniform. From the center to the side wall, the particle concentration increases at first and then decreases, with the maximum value at the position near the wall. As the superficial gas velocity increases, the particle concentration decreases and the velocity of particles increases. As for the residence time of particles, with the increase of superficial gas velocity, it becomes shorter, and the particles' residence time curve becomes narrower with a higher peak value. With the increase of particle circulation rate, the concentration and velocity of particles and their inhomogeneity of radial distributions all increase.

Keywords: Gas-solid flow; Downer; CPFD

Brief Biography

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Research

- Simulation of reaction multiphase flows
- Design and optimization of multiphase rectors
- Computational fluid dynamics
- Chemical reaction engineering

Awards

- Prize for outstanding youth of science and technology, China Petroleum and Chemical Industry Federation, 2017

- National Natural Science Foundation--Outstanding Youth, 2016
- The first prize of progress of science and technology, China Petroleum and Chemical Industry Federation, 2013
- The first prize of natural science award, Ministry of Education, 2011

Research Funding

- Petroleum chemical, NSFC, 2017-2019.
- High density circulating fluidized bed, NSFC, 2016-2019.
- Meso-scale structure and its effect in RFCC risers, NSFC, 2014-2016.
- CFD Modeling of flow and combustion in commercial furnaces, SINOPEC, 2014-2017.
- CFD Modeling of gas-solid flow and reaction in an commercial riser, SINOPEC, 2013-2016.

Publications

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Numerical Simulation of the Filtration Characteristic in the Pleated Filter Media Using CFD-DEM

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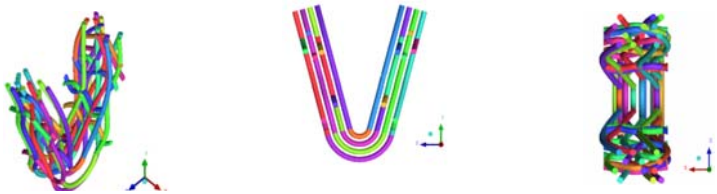
Abstract

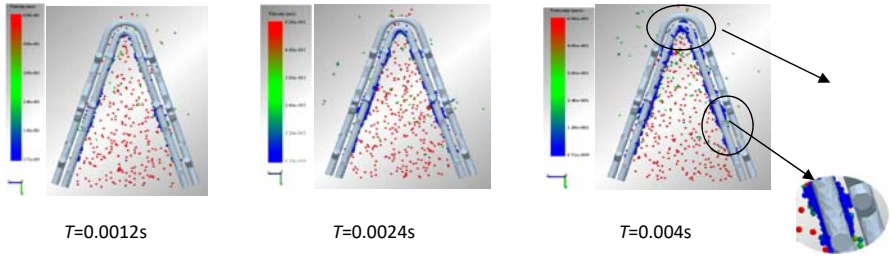
In this study, the microscopic random pleated models had been established in order to analyze the filtration performance of the pleated filter media. One of the illustrations of the pleated filter media models is shown in Figure 1.The CFD-DEM simulation of gas-solid two-phase flow was used to study the deposited state of the particle in the pleated filter media during the filtration process. The deposited particles on the pleated filter were visualized, and the effect of deposition of particles on pressure drop was analyzed. Figure 2 presents an apparent phenomenon of agglomeration and deposition in the pleated filter media, which indicates that the arrangement of fibers affects the deposition morphology of the filter media, which also points out the direction for further studying the performance of the pleated filter media.

The collision effect between particles to particles and particles to fibers was fully taken into account in this study. As shown in Figure 3, the total number of particles shows a linear increasing trend with the filtration time, and part of the particles are collected by fibers and deposited on the surface of the fibers. The deposited particles increase nonlinearly with the filtration time, it is due to that some of particles form pronounced dendritic structures, and the dendritic structures act as new fibers to impede airflow movement. Figure 3 also shows that the number of collision particles first increase and then decrease with the filtration time, this is because that the particles deposit in the gaps of the filter media in the initial stage of the filtration, the gap is blocked gradually with the filtration process, so the number of collision increases continuously, then decreases in the later stage because of the certain injection number (total number is set to 2000 because of the influence of calculation time and calculation accuracy). As shown in Figure 4, the total force on geometry increases with the filtration time, which can be attributed to that, deposited particles increase frequently. More and more particles adhere to the surface of the fiber, due to their own weight and the force from fluid, and the total force on geometry increases constantly with the filtration time. Compared with the particle collision mechanism, the total energy loss of particle collision presents the same trend, which indicates a positive correlation between the loss of kinetic energy and particle collision.



(a) isometric view (b) left view (c) front view

Figure 1. 3D model of the fibrous media and the view of different direction



T=0.0012s *T*=0.0024s *T*=0.004s

Figure 2. Changes of DEM simulation results with filtration time

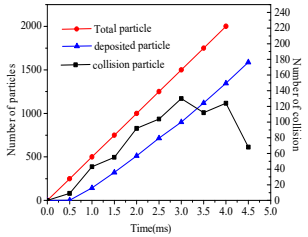


Figure 3. The relationship between total particles, deposited particles

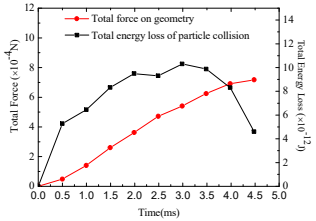


Figure 4.Mechanical property with non-dimensional time

Brief Biography

Fuping Qian, male, PhD, professor, vice dean of the School of Civil Engineering and Architecture and director of the Institute of Ventilation and Purification in Anhui University of Technology.

DEM-CFD Analysis on The Influence Mechanism of Electrostatics on Single Bubble in Gas-solid Fluidized Bed

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Abstract

Electrostatics occurs in the gas-solid fluidization processes, it influences the hydrodynamics of gas-solid flow. However, few specific research has investigated the influence mechanism. In this work, the influence of electrostatics on the single bubble was investigated by means of Digital Image Analysis (DIA). The experimental results showed that, in the high charged system, the aspect ratio of bubble gradually decreased as the bubble rose and bubble collapses were discovered at the end of rise. To study the influence mechanism of electrostatics on single bubble, a discrete element method coupled with computational fluid dynamics (DEM-CFD) was developed to simulate both mono-charged system and bipolar-charged system. Numerical simulations interpreted the deformation of bubbles from the magnitude and direction of the electrostatic force on particles, as well as the stream traces of gas in the flow field. The simulation results showed that, the electrostatic force affected the particle's movement tendency. In mono-charged system, this caused the drop of particles from the roof of bubble, whereas in bipolar-charged system, this led to the split of the bubble.

Brief Biography

Dr. Zhen Tan obtained his B.E. Degree in thermal energy and power engineering at Nanjing Normal University in China in 2009, and completed his MEng and Ph.D. in power engineering and engineering thermophysics at Southeast University in China in 2013 and 2018 respectively. He joined Institute for Process Modelling and Optimization as a postdoctor in July 2018. His main research direction during his Ph.D. was the influence mechanism of electrostatics on the hydrodynamics of gas-solid flow. The main research methods in his studies are experimental analysis and numerical simulation. Numerical simulation methods include Two Flow Model (TFM) and Discrete Element Method-Computational Fluid Dynamics (DEM-CFD). Until now, he has published 2 patent applications and 3 papers.

Distribution Homogeneity of Solid Particles in Slurry Taylor Flow

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Abstract

Reactors of Taylor flow with a slurry contact mode was firstly proposed in 2005 where solid particles are dispersed in the liquid slugs and remained in motion in a stable flow under the effects of the symmetrical vortices present in each slug. Just recently, a few studies have been directed towards addressing mass and heat transfer characteristics amongst the gas-liquid-solid phases. Nevertheless, a good understanding of this micro reaction technology is largely lacking. In particular, the distribution homogeneity of solid particles in the liquid slug between two consecutive bubbles is of great interest to researchers as it directly dictates the interactions between solid particles and the liquid phase and those between liquid and the bubbles, hence the overall performance of the system. However, the liquid flow exhibits the feature of high non-linearity and interactions between solid particles and the toroidal vortices are very complex. It is always a challenging task to predict the distribution of solid particles for specific operating conditions.

In this study, the distribution of solid particles under different operating conditions is investigated. Interactions amongst solid particles and those between particles and confined tube walls are directly solved using the discrete element method (DEM). Critical fluid forces are solved based on the Taylor flow profile which is analytically solved. Considering the low Stokes numbers in the context of this study, a one-way coupling between the fluid flow and the particle motion is implemented, i.e., only the effect of fluid flow field on the particle flow has been considered. Dependence of particle motion on the fluid flow field and the total solid inventory is examined and quantified. Experiments are conducted to collect benchmark data for validating the model.

The results show that the distribution homogeneity of solid particles strongly depends on the intensity of the vortices which is jointly determined by the liquid flow rate and the aspect (height to diameter) ratio of the liquid slug. There is a critical value of the aspect ratio of the liquid slug for a given particle Stokes number to achieve the homogeneous distribution of solid particles. Subsequently, a map that relates solid distribution to operating conditions (expressed as dimensionless numbers) is proposed.

Brief Biography

Upon completion of his PhD studies in 2009, Dr Peng commenced his academic research as a postdoctoral research associate in the School of Engineering at The University of Newcastle, Australia. Dr Peng's principal area of expertise lies in areas of fluid mechanics, particle/powder technology, heat transfer and chemical reaction in multiphase processes, as specifically applied to chemical looping combustion systems, methane-air deflagrations, gas-solid/liquid-solid fluidised bed reactors, froth flotation processes, abatement of particulate matters, and bulk materials handling.

Non-spherical Particle Behaviors in a Spouted Bed

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Abstract

Spouted beds are widely used in chemical engineering, such as pyrolysis, coating, mineral processing and granulation. It is found that the gas channel is one of the most important factors to dominate the overall particle behaviors. With the changing of operation conditions, there will be different types of gas channels in the bed. And in some researchers' work, the instability of gas channels is observed in experiments. For the spouted bed with non-spherical particles, the instability phenomenon has not been studied yet. As most particles in industry and nature environment is non-spherical, the research on non-spherical particles is of specific significance because variety of particle behaviors are different from that in spherical particle systems.

Thus, in this study, the experimental and numerical investigations on spouted bed with non-spherical particles are conducted to study the particle behaviors. The PIV and non-spherical particle modeling by hard sphere method are applied. The instability phenomenon, which has only been studied in spherical particle systems, is numerically and experimentally investigated.

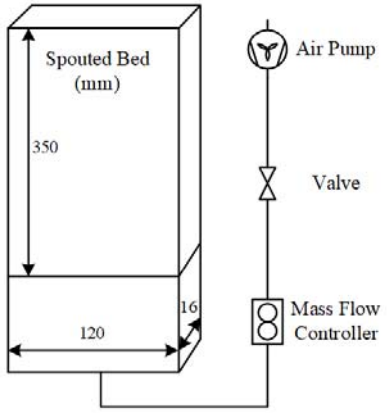

Figure 1 Sketch of the experimental platform

The sketch of the experimental platform is shown in Figure 1. After recording the results, a post process software in PIV system is used to obtain the detailed particle distribution and movement. The dimensions of the spouted bed are also shown. For the non-spherical particles used in this work, green beans are chosen in similar shapes.

The results show that the simulated and experimental data match with each other well, and the spring-like particle movement was shown, which is a typical particle motion in spouted bed. A s-shaped gas channel is in the middle of bed, proving the presence of instability in the spouted bed with non-spherical particles.

Acknowledgements

This work is financially supported by the National Natural Science Foundation of China (Grant No. 51706055, 51322601), the China Postdoctoral Science Foundation (Grant No. 2017M611366), the Heilongjiang Postdoctoral Fund (Grant No. LBH-Z16058) and the Fundamental Research Funds for the Central Universities (Grant No.HIT.NSRIF.201844).

Brief Biography

Dr. Tianyu Wang is a lecturer in the School of Energy Science & Engineering, Harbin Institute of Technology. He was a Research Fellow in the University of New South Wales(2017-2018). He obtained his Ph.D. in Thermal Power Engineering in 2016 from Harbin Institute of Technology. His research interests are the multiphase flow and heat transfer and the development of new energy. He has published over 30 papers in refereed journals and conference proceedings.

Multi-scale modeling of multiphase complex flows: Bridging the gap between fundamentals and industrial applications

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Abstract

With advances in computing speed and parallelization technology, improved software and multiphase algorithms, computational fluid dynamics (CFD) modelling is playing an increasingly important role in design, control and optimization of many industrial processes nowadays.

Most of the industrial flow systems are intrinsically multi-scale - that is, there are widely separated characteristic length and time scales that are of importance to the behaviour of the system as a whole. The ability to feasibly model all important scales simultaneously is a technical challenge that increased computing resources alone will not solve. Average approaches are not sufficient for characterizing these structures and related behaviors, while discrete approaches based on very detailed mechanisms are limited to capability and cost of computation. Using a multi-scale modelling approach, the detailed micro- modelling information of a real system, such as the detailed particle and/or bubble dynamics, can be used to build constitutive correlations to improve macro- or process scale modelling accuracy. This multi-scale modelling approach is proved to be promising and powerful, and has received increasing interest in the study of complex multiphase flow systems. CSIRO CFD team has been working on the application of CFD models to new and existing plant in the mineral processing, metal production and energy industries for decades. The broad application of CFD has the potential to save companies many millions of dollars per year.

This presentation will discuss the multi-scale modelling methodologies CSIRO has worked on during the past 10 years. For gas-liquid flow systems, current work on CFD modelling of the aluminium smelting process will be presented, including a micro-bubble model for studying detailed bubble dynamics, time-averaged macro- gas-liquid flow models for simulation of bath flow and alumina mixing in a full reduction cell, and the linkage between the micro- and macro- models. For gas solid systems various models has been developed and will be discussed in reference to applications in mineral processing and other process industries. Techniques discussed will include direct numerical simulation (DNS), discrete element method coupling with CFD (CFD-DEM), Particle-in-Cell Model, Eulerian-Eulerian (E-E) or two fluid model (TFM), and recently developed hybrid DEM-TFM model, and how these have been used in applications such as froth flotation, grinding mills and a coal beneficiation fluidized bed.

BRIEF BIOGRAPHY

Dr Yuqing Feng (B Eng, 1992; M Eng, 1995; Ph D, 2004, UNSW, Australia) is a principal research scientist at CSIRO Mineral Resources, leads in the development and application of advanced computational fluid dynamics (CFD) models for complex multiphase flow systems involving bubbles, particles and droplets, with a focus on their applications in process industries, including light metal production, mineral processing & extractive metallurgy, chemical and petroleum engineering. In addition to provide practical advice for reliable scale-up, design and control/optimization of different multi-phase complex flow systems, he has been co-supervising over 10 PhD students in conjunction with several universities and published 3 book chapters, over 130 scientific papers and 31 industrial reports.

Modelling and Optimisation of Reacting Particle Flow: Examples in Ironmaking Industry

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Abstract

Reacting particle flows are involved in many manufacturing industries, including ironmaking industry. The understanding and optimisation of the reacting flows are essential to maintain the competitivity and sustainability of ironmaking industry under increasingly demanding conditions. Mathematical modelling, facilitated by physical modelling, provides a cost-effective way for process understanding and control. In particular, cross-scale modelling is widely used in academia and industry for their effectiveness. This report will overview some recent CFD and DEM-based process models and discuss their roles in the development of new technologies for sustainable ironmaking. Some recent examples are used: 3D modelling of blast furnace with raceway, 3D modelling of pulverised coal injection, and 3D modelling of cokemaking. It is demonstrated that mathematical modelling indeed plays a significant role in process understanding and optimisation, vital to sustainable modern ironmaking.

Brief Biography

Dr Yansong Shen is an Associate Professor in the School of Chemical Engineering at University of New South Wales (UNSW). He obtained his BEng and MEng degrees at Northeastern University (China) and PhD degree in UNSW. His research interests include process modelling and simulation of reacting flows, with applications in process metallurgy, black/brown coal upgrading and utilisation, water treatment, and renewable energy process designs. He published over 100 peer-reviewed papers in the field of process engineering with H-index 17 as of 2017, secured over A$3M research funding including over 15 national-level ARC, ACARP and ARENA projects as lead investigator or investigator, established long-term industry engagements in Australia and overseas, and won several honours/fellowships including ARC Postdoctoral Fellowship and ATSE Emerging Future Leaders in Low Emissions Coal Technology Fellowship. He is the member of Chartered IChemE, TMS, AIST, and invited/plenary speakers in several international conferences.

CFD modelling of Fluid Flow and Particle Separation in Electrostatic Separator

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Abstract

An electrostatic precipitator (ESP) is a device used to separate fine particles from dust laden gases by charging the particles using electrostatic forces and driving them towards the collecting plate. ESP's are widely used to control the particulate emissions from power stations, cement industries and industrial process sources. Very complex interaction mechanisms between the electric field, fluid flow, and particulate flow can be found in an industrial ESP. In the last two decades, experiments were conducted in an ESP to understand the fluid and particle behavior at wide range of operating and design conditions (Choi and Fletcher, 1997; Böttner, 2003; Skodras *et al.*, 2006; Arif *et al.*, 2016). Experiments being cumbersome and expensive, researchers utilized computational tools to simulate the flow behavior for better understanding thereby the possible design modifications can be made virtually.

Because of the complexity of flow inside ESP, a detailed numerical model is yet to evolve. Moreover, many simplifications are necessary in order to keep both the computational time and cost in a balanced level. Accuracy of calculations is affected by the considered turbulence and multiphase models and various idealizations of the process used for simulation. Computationally most intensive component of the simulation is probably to predict the influence of electro hydrodynamics on particle collection efficiency in an ESP. Authors like (Choi and Fletcher, 1997; Böttner, 2003; Skodras *et al.*, 2006; Arif *et al.*, 2016) investigated the particle transportation and collection in an ESP.

The present study aims to develop a CFD model that describes the flow of particle laden gas, particle charging and collection in an ESP. A single wire plate [2D] unit ESP is chosen to investigate the interaction between the primary flow and the secondary flow (electric wind or ionic wind) and their effect on particle collection in an ESP. The dimensions of wire-plate ESP are 0.65 [m] in length, height 0.1 [m], wire spacing 0.15 [m], and wire dia 0.005 [m]. The top boundary is a wall, the bottom is a symmetry plane and wires are taken as walls. The secondary flow arises due to the significant transfer of momentum from corona-generated ions to the gas. The model considers all the mechanisms which affect an industrial ESP process such as three coexisting fields of gas flow, particle dynamics and electrostatic field, which have been implemented using the User Defined Functions (UDFs) in ANSYS's FLUENT. Numerical calculations for the gas flow are carried out by solving the Reynolds-averaged Navier–Stokes equations using the k–ε turbulence model. A finite-volume approach is utilized to solve the coupled equations for the electrostatic field and charge transport equations. The Discrete Phase Model (DPM) is used to simulate the particle phase. The simulated results provide the particle trajectories inside an ESP under the influence of primary and secondary flows. Validation of CFD model against the literature data (Skodras *et al.*, 2006) is attempted and found them in good agreement. This method can be applied to a full scale industrial ESP to gain an insight into collection efficiency along with performance optimization for better collection efficiency in an ESP.

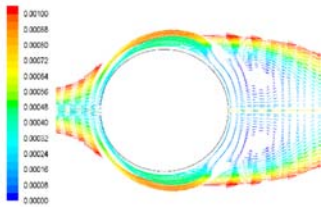

Fig 1 (a): stream function in [kg/s]

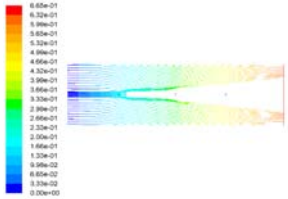

Fig 1 (b): particle tracks [sec]

Figure 1 (a), (b) displays the CFD simulated flow filed stream function and the DPM particle tracks of (2µm). Boundary layer starts to grow from the inlet along the plate and later it is suppressed by the growing wakes behind the wires (recirculation region with lower velocity), with turbulence at edge of layer. The deviation of particles from their path starts at first wire and successively continues to deflect along the subsequent wires. Few particles are trapped at the collecting plate and some manage to escape through the outlet.

Key words: Electrostatic precipitator, Fluid Flow, Eclectic field, Magneto hydrodynamics, DPM approach, Particle Separation

Acknowledgments: The authors express thanks to Dr. Sainath Koneru, Srikanth Koneru and Dr. Shreekanta Aradhya of Clair Engineers Pvt. Ltd, India, for their support in the work.

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Brief Biography

Dr Narasimha Mangadoddy is an Associate Professor & HoD in the department of Chemical Engineering, IIT Hyderabad, India. He received PhD in 2010 from the JKMRC, University of Queensland (Australia). Before joining IIT he worked at R&D-TATA Steel India, JKMRC-Australia on various mineral processing projects. Dr Narasimha's areas of interest include CFD, CFD & DEM for multi-phase flows, particulate technology, mineral processing, slurry rheology, transport processes of separation devices. He has two international patents and 55 referred journal and conference publications. He is the recipient of 2010 & 2016 IIME KHARE best paper award and excellence in teaching award in 2011 & 2015 by IIT Hyderabad.

An investigation on Interactions between Ultrasonic Waves and Particles Based on the Monte Carlo Method

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Abstract

Ultrasonic attenuation spectroscopy plays a very important role in particle size characterization. This method is usually based on several necessary processes such as forward theoretical model, attenuated signal detection and mathematical inversion, where the forward model is obviously a particularly important and difficult part. Since the ultrasonic wave itself is a mechanical wave, which inevitably brings complexity to the interaction problem with particles. For the study of predicting ultrasonic attenuation of mixed particles and exploring the underlying behavior of interaction, the Monte Carlo method was investigated to establish a particle size characterization model in concentrated particulate system and serve as a probability and statistics technique to probe the intrinsic ultrasonic events during the ultrasound propagation. In addition, the extension of the well-established single-particle theory of Epstein, Carhart, Allegra, and Hawley (ECAH), by incorporating the couple phase model from a hydrodynamic point of view was also accounted for the ultrasonic attenuation characteristics in the two-phase system of suspensions and emulsions with different particle sizes, ultrasonic frequencies and concentrations. After verifying its feasibility, such a method is then applied into mixed particle system with various ratios. It is shown that as the particle volume concentration is up to 10%, the variation of the ultrasonic attenuation coefficient with mixing ratio yields a nonlinear tendency. At higher concentrations, this model was validated that the attenuation in two-phase system of suspensions and emulsions agreed well with the experimental results of literature, which presents a novel approach in calculating the attenuation in high particle volume concentration of even over 50% and provides a numerical modeling of particle size measurement in the complex particle-particle interaction condition.

Brief Biography

Prof. Su Mingxu received his degree in Power Engineering from Nanjing University of Aeronautics and Astronautics in 1996 and his PhD in Thermal Engineering from the University of Shanghai for Science and Technology, USST in 2002. In the same year, he got a postdoctoral position at UMR 6614 - CORIA in Rouen, France. After a year of investigation on the wet steam testing by using light extinction method, he went back to the USST being a teacher till now. His main research interests are methods of particle size characterization based on ultrasonic spectroscopy and light scattering, as well as the industrial applications on particulate two-phase flow measurement.

Numerical prediction on the drag force and heat transfer of various particles in supercritical water

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Abstract

Using supercritical water (SCW) as the working fluid to achieve the fluidization of coal and biomass particles for producing high-quality fuels is more and more popular since SCW has many advantages such as high reaction efficiency and H_2 selectivity[1,2]. However, people know no much about the complex chemical reaction and heat transfer characteristic on the particle scale and temperature and component distributions on the reactor scale during the solid gasification process in SCW circumstances. The lack of this knowledge generates difficulties in the design and scaling techniques of SCW devices. This work contributes to provide some important information and the prediction on the drag force and heat transfer of solid particles in SCW like drag coefficient (Cd) and average Nusselt number (Nu).

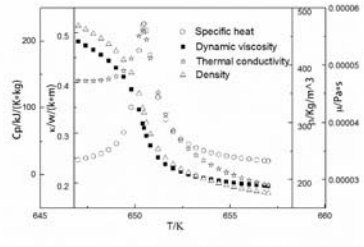

Figure 1. Property of SCW in the pseudo-critical zone, $P = 23MPa$.

We consider the forced convention process of an isolated particle with different shapes in SCW. Navier-Stokes equations are solved to numerically simulate the momentum and heat transfer process. Cd and Nu under different working conditions are obtained. Note that the key of this set of numerical simulations on SCW, which is different with the conventional fluid, lies on the variation physical parameters of SCW with temperature and pressure as shown in Figure 1. These parameters include fluid density, dynamic viscosity, thermal conductivity and specific heat capacity. Finally, new correlations for Cd and Nu are proposed including Reynolds number and particle shape as the key factors. Figure 2 shows several temperature distribution patterns of SCW under selected working conditions.

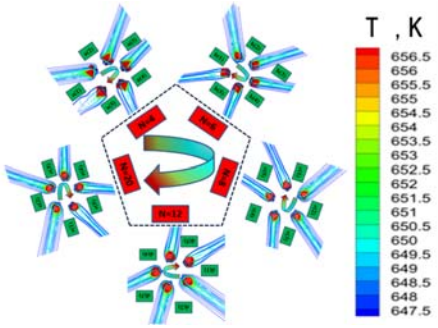

Figure 2. Temperature distributions in different cases.

New correlations are proposed for ellipsoids with different aspect ratio and Platonic particles. For the ellipsoids, the effect of the incident angle is also taken into account. The prediction capability of these correlations is demonstrated good for facilitating the phase coupling in further multi-phase flow modelling.

Brief Biography

Hao Zhang obtained PhD from Technical University of Catalonia. He is currently an associate professor in Northeastern University in China and a visiting scholar in Monash University. His research mainly focuses on numerical modelling of process metallurgy (heat transfer, multiphase flow, chemical reaction and non-spherical particles), air pollution control and efficient and high quality transfer of renewable energy (hydrogen production based on supercritical water). As a result, he is the author of more than 70 publications, 30 of them are published in international journals.

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Numerical and Experimental Analysis of Particle Mixing in a Liquid Fluidised Bed Based on Individual Particle Tracking

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Abstract

Solids mixing in fluidised beds is a significant phenomenon that determines the rate of energy and mass exchange between phases and can contribute to the final conversion of chemical reactions where applicable [1, 2]. A common parameter that defines the degree of mixing in fluidised beds is the mixing index (ratio) which varies between 0 (for completely segregated) to 1 (for fully mixed) in the system.

In this study, the mixing of 8 mm glass particles in a fluidised bed operating at a superficial liquid velocity of $u_{sf} = 0.184$ m/s was investigated through simulations and experiments. The simulations of the fluidisation process was carried out using a new DEM approach originally developed by Abbasfard et al. (2018)[3]. In this approach, the fluid velocity is considered to be made of a mean and a fluctuating parts with a standard deviation that follows a Gaussian Probability Density Function (PDF). Comparison with volume fraction versus superficial velocity measurements and predictions (e.g. Richardson-Zaki equation) showed that the proposed DEM-only model suffices to predict the hydrodynamics of a fluidised bed to a reasonable accuracy.

The mixing ratio can be defined by the ratio of the visited space to the whole bed space over the time. Two experimental and numerical methods to quantify the mixing ratio were introduced and named as: position-based and path-based. In the position-based method the mixing ratio was only dependent on the position of the particle center while in the latter method it depended on both the position as well as the travelled path of the tracer particle. In both methods the bed space was discretised into multiple cells to determine the number of visited/un-visited cells. A post-processing code was developed to analyse the mixing process using the DEM results based on the abovementioned methods.

Experimentally, a dark colored glass particle, with the same size and density as the other particles, was used as a tracer particle. The motion of this tracer was recorded with a high-speed camera in the form of series of 2-D images. The images were then analysed using an in-house image processing code to extract the position of the tracer particle at each time frame. Having the positions of the tracer particle, the mixing ratio was quantified through the above-mentioned methods for a given 2-D projected area.

The experimental (2-D, projected area) mixing time measurements were well-matched by both 2-D simulation, position- and path-based approaches. However, for the 3-D simulations, the mixing time was computed to be much longer than that for the 2-D, projected area (both experimental and simulation) approach. The inference from this result is that mixing time estimates obtained from project-area measurements (or simulations) is likely to under-predict the true mixing time for a real (3-D) fluidised bed.

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Brief Biography

Hamed Abbasfard has recently submitted his thesis for a degree of PhD in Chemical Engineering at The University of Newcastle. He also worked at the same university as Research Associate and Casual Tutor. He currently works at Rio Tinto as a Process Engineer.

Before commencing his PhD, Hamed Abbasfard was working in Petrochemical industries against various roles for several years since 2005. His main area of expertise includes process engineering and design, operations control and supervision, mathematical modelling and simulation (DEM/CFD/MATLAB/ANSYS/Fluent), water/wastewater treatment, drying and particle technology, environmental and green engineering, failure analysis, etc.

A DNS-DEM Coupling Methodology for Turbulent Non-Newtonian Suspension Flow

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Abstract

Currently there is a move towards higher concentration tailings disposal due to its environmental, economic and political benefits. These high concentration non-Newtonian suspensions often occur with a broad size distribution including coarse solids that can settle, and typically exhibit shear-thinning behavior along with the presence of a yield stress. The interaction between non-Newtonian rheology and coarse particle transport in high concentration suspension is still poorly understood, particularly in the transitional and turbulent flow regimes.

This lack of understanding motivates us to develop a DNS-DEM coupling methodology for investigating the underpinning fundamentals of turbulent non-Newtonian suspension. DNS is applied to capture the unsteady turbulent flow structure, and the DEM is used for modelling the detailed particle-particle interaction. We implement our model using an open-source coupling library CFDEM, which couples OpenFOAM and LIGGGHTS. The method includes a diffusion-based approach to deal with the presence of the coarse particles in DNS-DEM, with an appropriate smoothing length scale for smoothing the exchange fields to be determined.

The Herschel-Bulkley (H-B) model is applied to describe the non-Newtonian rheology. Initially we have chosen to replace the Newtonian viscosity in the drag correlation with the H-B viscosity. This simplification will be modified and the effects of the H-B carrier rheology, applied shearing and solids concentration on the drag correlations will be included. Once these improved drag correlations are implemented in CFDEM, the results will be validated against experimental suspension data including pressure drop, flow rate and concentration profile.

Despite the current simplifications, preliminary simulations of turbulent non-Newtonian suspensions have been found to be qualitatively correct. The methodology developed in this project will allow an extended understanding of the interaction between non-Newtonian fluids and particle transport to be determined, as well as

provide guidance for LES-DEM studies of turbulent non-Newtonian suspension with higher Reynolds number in the future.

Brief Biography

E.Z. Zheng is currently a Ph.D. student in the Department of Mechanical & Aerospace Engineering, Monash University. He is working on a project entitled “Modelling Extreme Suspension Flow”, which focuses on numerical simulation of turbulent non-Newtonian suspension flow in a horizontal pipe. Enzu’s core areas of strength include understanding and experience with multiphase flow modelling and turbulence modelling, plus a mathematical background with some experience in programming and development of numerical codes for solving equations.

Enzu obtained his Master of Science degree in Mining Engineering from University of Alberta in 2015, where he worked on the project “CFD Modelling of Oil Sand Multiphase Flow in At Face Slurry System”. This project focused on developing the mathematical models governing the friction loss associated with the flexible pipe system. CFD modelling of oil sand multiphase flow using ANSYS-FLUENT was conducted. A flexible arrangement of pipe loop imitating the system was set up in the laboratory to test the accuracy of CFD modelling.

For the past two years (2015~2017), Enzu had been working as a Finite Volume Analysis R&D Engineer in China Nuclear Power Design Co., Ltd, where he was in charge of the project “Self-development of a computer code for the transient thermal-hydraulic analysis of the EPR (European Pressurised Water Reactor) steam generator”. This project mainly involved the interpretation of the geometrical model, conservative equations, code execution and numerical techniques adopted in a technology transferred FORTRAN code that calculated pressure, temperature, flow rate and heat transfer coefficient of ERP steam generator.

Analysis of Two-Phase Dusty Williamson Nanofluid Flow With Marangoni Convection

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Abstract

Fluid flow which contain identical non-miscible inert solid particles is known as two-phase fluid system. Examples of two-phase flow include bubbles, rain, waves in the sea. This fluid system has numerous application in various natural processes like blood flow in arteries, dust in gas cooling systems, sand or other suspended particle in sea beaches. Dusty fluid model flows have been a subject of special interest in recent studies. From past few decades, researchers have been focusing on the behavior of heat and mass transfer characteristics of dusty nanofluid through different channels. The marangoni effect refers to the variation of surface tension of liquid with temperature (thermo-capillary) or with the concentration of a surfactant (solutal marangoni effect). Marangoni effect is divided into the thermal marangoni effect (EMT) and the solutal marangoni effect (EMS). Theory of EMT is utilized in the present work. Pearson created the initial model and criterion. Experiments showed that the surface tension of fluid is connected to the temperature, in most of the cases the surface tension decreases with increase in temperature. Some of the non-Newtonian fluids such as blood, honey, starch, molten plastics, artificial fibres, food stuffs and slurries exhibit shear-stress-strain relationships which are distinct from Newtonian model. Mostly non-Newtonian models involve some form of modification in the viscous term in momentum equation. In the category of non-Newtonian fluids, the Williamson fluid has distinguishable features. Williamson fluid model describes the flow of shear thinning non-Newtonian fluid. It is used in modeling of biological fluid in small passages and have many other applications in chemical and biological science, geophysics and petroleum industries. The present paper investigates the heat transfer characteristics of dusty williamson nanofluid with marangoni convection. The mathematical model of the physical problem invoke equations of continuity, momentum and energy equations for solid and fluid phase, separately. The non-linear partial differential equations are normalized to ordinary differential equations and solved by Galerkin Finite Element Method. Influence of pertinent parameters that are radiation parameter, dust particle mass concentration parameter, thermal dust parameter are analyzed. It has been observed that velocitiy and temperature decrease with increase in dust particle concentration parameter.

Brief Biography

I, **Madhu Aneja** pursuing **Ph.D** (Reg. number 901511008) in Applied Mathematics from Thapar Institute of Engineering of Technology, India. I recieved my masters degree in Mathematics & Computing (C.G.P.A = 9.01) from Thapar University, India, in 2011. In Dec 2011, I joined Department of Applied Sciences, RIMT, India, as Assistant Professor. I qualified "**GATE**" in 2012 which is one of the reputed test in India. I am appointed as a Junior Research Fellow (JRF) in **Department of Science and Technology (DST)**, **Fast Track Project**. entitled "**Higher order Discontinuous Gelerkin Method for Unsteady Incompressible Navier Stokes Equations : Analysis and Simulation".** My research topic is "**Modeling and Numerical Analysis of Heat and Mass Transfer Phenomenon in Fluid Flow**". I am working on the problems of Heat and Mass Transfer. **Finite Element Method** is used for the solution of Incompressible Navier Stokes equations. Also, I am working on **Discontinuous Gelerkin Method.** I hold good command in computer languages (C, C++, Matlab, FreeFem++) and modified a number of codes for studying fluid dynamics. I attended workshops on "**Hyperbolic Conservation Laws**" and "**Numerical Methods for Partial Differential equations**" held in India related to my research work. I presented my research work in "**19th International Conference in Computing Science & Mathematics**", Melbourne, Australia.

Effect of Lift and Hydrodynamic Torque on Fluidization of Non-Spherical Particles: Experimental Validation

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Abstract

In recent years, we have witnessed an increasing tendency to use fluidized beds for biomass gasification. Numerical models of the fluidization processes usually approximate the particles as spheres. However, spheres are not a good representation of dried and milled biomass particles, which are usually characterized by an elongated shape. So far, there is only limited literature available in relation to hydrodynamic forces experienced by non-spherical particles under fluidized conditions. When suspended in a gas flow, non-spherical particles will not only experience hydrodynamic drag, but also torque and lift forces.

In this study we investigate the effect and importance of lift forces and hydrodynamic torque in dense gas-fluidized conditions. The CFD-DEM code used in this research is based on open source engine CFDEM, which uses the OpenFOAM computational fluid dynamics (CFD) solver to describe the fluid component and LIGGGHTS to implement discrete element method (DEM) calculations. These open source codes were adapted by us to take in to account elongated non-spherical particles. In the simulations, we employ lift and torque correlations derived from previous DNS simulations by Sanjeevi et al. [1]. Simulations of a 3D fluidized bed with different hydrodynamic forces considered are compared with experimental results obtained with MPT (Magnetic Particle Tracking) technique, a non-invasive 3D experimental technique. In this study we show that when simulating fluidization of elongated particles, lift forces and hydrodynamic torque can no longer be neglected.

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Brief Biography

Ivan Mema was born on November 8th 1989 in Vrsac, Serbia. In 2008 he started studying chemical engineering on Faculty of Technology and Metallurgy in Belgrade, Serbia. He finished bachelor studies in 2012 and master in 2013 in the same university. In his fourth year of studies Ivan, did an internship at Universidade Estadual de Campinas (Unicamp), Brazil, on the study of heterogeneous catalytic reactions. During his studies he received special recognition of Serbian Chemical Society and award for excellent success during studies. After his studies he worked as process engineer in "Prava Iskra-Namenska A.D." in Belgrade. In December 2015 he started his PhD project on "Multiphase modeling of dense gas-fluidized flows of non-spherical particles" under the guidance of dr.ir J.T.Padding in the Process & Energy group at Delft University of Technology in The Netherlands.

CFD-DEM simulation of particle-laden liquid-solid flow interacting with a resolved fixed spherical bubble

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Abstract

Particle-bubble interaction occurs in various multiphase reactors such as gas-liquid or gas-slurry bubble columns and gas-liquid/slurry-solid fluidised bed systems. As an essential process of these systems, the complex fluid dynamics and physical-chemical interactions determine the heat and mass transfer, mixing and segregation, and aggregation behaviour. For a system with large bubbles and small particles, as in a typical flotation process, particles are selectively attached to the bubble surface depending on their surface properties (hydrophobicity) and then carried by the bubble to be collected as a desired product. The hydrodynamics around the bubble, e.g. boundary layer and wake, in this case, strongly affects the overall performance of the system.

Conventional flotation modelling has defined particle-bubble capture probability as first order kinetics where the rate constant is determined by three sub-processes namely: collision, attachment and detachment. The models for each of these sub-processes are either statistical or semi-empirical which are process/unit specific.

Advances in numerical simulations provide an alternative solution to model particle-bubble interaction by resolving the hydrodynamics of the system from first principles. Since particles and bubbles exist as dispersed phases in flotation systems, the Eulerian-Lagrangian (E-L) framework, is inherently the best option to model the system. Mostly, in applying the E-L approach, the fluid is treated as a continuum, the particles as discrete elements, and the bubble as a fixed spherical wall boundary. The fluid flow is resolved by either direct numeric simulation [1] or turbulence models [2]. Particle-bubble collision is modelled under both laminar and turbulence flow conditions using one-way coupling mode where only the influence of the fluid on the particle is considered [2].

In our previous work [3, 4], the E-L methodology has been applied to resolve the surface forces for particle-bubble interactions explicitly. However, only simple hydrodynamic conditions, e.g. quiescent and stokes flow were solved by using streamline function. The significance of the fluid pattern around bubble intuitively leads to a demand for the combination of CFD and DEM models to resolve the hydrodynamics and surface chemistry simultaneously. However, conventional CFD-DEM coupling model requires the mesh cell size to be as large as 1.6~6 d_p [5] which contradicts the multiscale nature of the particle-bubble interaction system.

In this paper, we propose a four-way CFD-DEM model to simulate the particle-laden liquid-solid flow that interacts with a fixed spherical bubble and resolve the flow field around the bubble without concern about the fluid cell size restriction. The capability of the CFD-DEM model was examined at different mesh size, mesh uniformity, and dense and dilute particle phase condition. The results showed that the CFD-DEM model could achieve mesh-independent results with different mesh size and uniformity which is critical for the simulation in the presence of a boundary layer and wake. The simulations of single particle settling and fluidised bed prove the model capability to predict particle dynamics at the dilute or dense condition. Finally, the bubble collision efficiency, particle sliding and wake interactions at various hydrodynamic conditions were predicted by the CFD-DEM model. It is demonstrated that the four-way feature of this model makes it possible to consider all factors that can affect the particle-bubble interaction, such as surface chemistry or turbulence modulation effect of particles, in future studies. It is also noted that the model as a basic framework can also be used to simulate other particle-bubble systems or capture of particles by a magnetic collector.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

Brief Biography

Linhan Ge obtained his Master of Engineer degree in mineral processing Engineering from China University of Ming and Technology (CUMT) in 2015. Afterwards, he began his PhD study at the Department of Chemical Engineering of the University of Newcastle under the supervision of Prof. Geoffrey Evans and Dr. Roberto Moreno-Atanasio. His PhD research project is to model particle-bubble interactions under different hydrodynamic environments as applied to many industrial processes especially to the froth flotation in mineral processing field. The major methods he applied include unresolved CFD-DEM coupling, interface resolved Volume of Fluid (VOF)-DEM coupling and fictitious domain methods to resolve the dynamics at different length and time scales.

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Numerical Simulation of Solid-Fluid Interaction in a Supercritical Water Fluidized Bed

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Abstract

With the energy crisis and stricter environmental requirements, finding a sustainable energy technology has become a hotspot worldwide. Hydrogen production from supercritical water gasification (SCWG) of organic matters, such biomass and coal, is of great interest in recent decades. Supercritical water shows great potentials as a high quality solvent and reactant for organics, with unique properties of high diffusivity and low viscosity. Matsumura and Minowa firstly proposed a concept of supercritical water fluidized bed reactor (SCWFBR) with SCW as the fluidization medium to overcome the plugging problem in tubular reactors. Later, Lu developed SCWFBR reactor for biomass gasification. After that, SCWFBR was applied to gasify kinds of biomasses and coals and achieved encouraging results in gasification efficiency and avoiding plug.

Although the SCWFBR achieved a great success in lab experiments, hydrodynamics in the bed is little studied as the conventional measurements are limited in supercritical condition. Duo to the extreme operating conditions, computational fluid dynamics (CFD) provide a useful way to obtain detailed information inside the SCWFBR. In this work, a two-fluid model was developed to simulate the hydrodynamics of SCWFBR. General speaking, gravity force, drag force and buoyance force are three major forces in the fluid-solid system. The drag force model is vital for the success of this model. Under supercritical pressure, solid particle (biomass particle or coal particle) feed are transported by cold water into the reactor. Solid particle feed entrained by cold water tend to aggregate like strands after ejecting from the reactor nozzle and concentrate at the bottom of the reactor. As heterogeneous structure exists in the fluid-solid system, a structure-dependent drag force model is needed. Since most of the present drag force model are derived from the experimental data on fixed bed or homogeneous liquid-solid fluidized bed, they can't provide accurate information as the heterogeneous structures occur. The energy minimization multi-scale (EMMS) model might yield comprehensive understanding of both heterogeneous structure and particle-fluid flow behaviors. Taking into consideration the properties of water under supercritical pressure, the original EMMS model was modified to suit the conditions in this work. Drag force model derived from the modified EMMS model is incorporated with the two-fluid model. Kinetic theory of granular flow (KTGF) is introduced for the closure of solid stress term. Simulation results showed the flow regime consisted of a dense solid-rich section at the bottom and a dilute SCW-rich section at the top. SCW-solid interaction was dependent on the flow structure. Properties of water significantly influenced the flow behavior of water when encountering SCW. This work reasonably revealed the hydrodynamics of SCWFBR, and provided a beneficial exploration for reactor optimization.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

Brief Biography

My name is Changsheng Ren, from State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong Universty, Xi'an 710049, China. I'm working in professor Liejin Guo's team on hydrogen production of supercritical water gasification and multiphase flow concerned. Experiment and theory are combined in my research. Up to date, I filed three patent applications with respect to the nozzle design of supercritical water reactor. Poster was made about the mass and heat transfer of particles and supercritical water (SCW) on UK-China International Particle Technology Forum Ⅵ. And the research on the interaction between subcritical water jet and SCW was submitted into the 16th International Heat Transfer Conference. At present, my research focus on the mass and heat transfer of particles and fluid in supercritical water environment, and the neural network algorithm is used to predict the heat transfer coefficient and drag coefficient between solid-fluid systems. Thank you!

Convective Heat Transfer Coefficient for a Rod-like Particle in Forced Flow

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Abstract

Rod-like particles are widely encountered in the industry, *e.g.*, the biomass utilization, and it always involves the heat transfer in forced flow. However, the researches about the convective heat transfer coefficient, *i.e.*, the Nusselt number, for rod-like particle are rare. Under this circumstance, this work is therefore devoted to develop a Nusselt number relation for rod-like particle in forced flow. To do so, a hot stationary rod-like particle that is passed by the cold continuous fluid flows is simulated by the three-dimensional Lattice Boltzmman Method (LBM). In the LBM, two lattice Boltzmman equations are solved side by side: one is to simulate hydrodynamics using multiple-relaxation-time (MRT) collision model, and the other is to simulate thermodynamics using Bhatnagar-Gross-Krook (BGK) collision operator. This in-house numerical model is then validated against available state of the art Nusselt number correlations proposed for spherical particle, ellipsoidal particle and cylindrical tube. Subsequently, the fluid flow and the heat transfer between the fluid and solid phase are simulated while changing the shape (*i.e.*, the aspect ratio) and the orientation of the rod-like particle as well as the Reynolds number. Based on the simulation results, the Nusselt number can be quantitatively obtained. From these obtained data, the Nusselt number correlation that takes the particle shape, particle orientation and Reynolds number into consideration is established for quantitatively describing the convective heat transfer between the fluid and rod-like particle and further for providing the closure correlation for CFD-DEM (Computational Fluid Dynamics - Discrete Element Method).

Keywords: Rod-like particle; LBM (Lattice Boltzmann Method); Nusselt number; Convective heat transfer; CFD-DEM (Computational Fluid Dynamics - Discrete Element Method)

Brief Biography

Huaqing Ma

PhD Student in College of Energy Engineering at Zhejiang University, China. He received his B. Sc. Degree in Process Equipment and Control Engineering in 2015 from Anhui University of Science and Technology, China. At same year, he joined Institute of Process Equipment at Zhejiang University, China, as a graduate student. His research interests involve the numerical investigation of the flow and heat transfer of rod-like particles by DEM and LBM, which the research background is the biomass utilization and are supported by two national funding (funding from NSFC). He had made the relatively thorough investigations in regard of the flow of rod-like particles by DEM, and seven papers had been published in *Chemical Engineering Science*, *Powder Technology*, etc. By his investigations, how the particle shape and the superficial velocity in the fluidized bed or the rotation speed of the drum in the rotating drum affects the flow of rod-like particles could be found. The fluidization behaviors of the binary mixtures had also been numerically investigated in his work. Now, his research focus is putting on the heat transfer of rod-like particles. Here, he will use LBM to derive some closure correlations about the heat transfer, *e.g.*, the Nusselt number relation, for rod-like particles. And the derived closure correlation will be incorporated into the CFD-DEM for a more thorough investigation of the heat transfer between rod-like particles and fluid flow.

Effect of Anisotropic Microstructures on the Drag Force for Low-Reynolds-Number Flows Past Static Spheres

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Abstract

Direct numerical simulations show that assemblies of particles containing anisotropic micro-structures produce appreciable different drag force when flows pass them in different directions. In this study, we focus on investigating the effects of anisotropic micro-structures on the drag force solely in homogeneous fixed beds at low Reynolds numbers. The anisotropy of micro-structures is quantified by a second-order structure tensor. The tensor is determined with a directionally dependent mean-free path length and is able to capture the principal nature of the microstructure. The anisotropic micro-structures are obtained by stretching isotropic structures with different stretching ratios in one direction or simultaneously in two perpendicular directions. The isotropic structures used for generating the anisotropic structures are body-centered-cubic (BCC), face-centered-cubic (FCC) and random arrangements. It is found that, with a fixed solid volume fraction, the difference between the normalized drag force in one principal direction in anisotropic assemblies and that in corresponding isotropic assemblies correlates well with the product of the eigenvalues in the other two principal directions divided by the second invariant of the structure tensor. It is also found that the drag force deviates from the flow direction when the flow does not follow the three principal directions determined by the structure tensor. Considering the superposition principle of low-Reynolds-number flows, a drag relation containing an anisotropic friction coefficient tensor is formulated to predict the normalized drag force for flows through anisotropic micro-structures in arbitrary directions.

Brief Biography

Teng Ma started his doctoral study in Prof. Qiang Zhou's group in the School of Chemical Engineering and Technology at Xi'an Jiaotong University, Xi'an in 2016. His current research focuses on evaluating the fluid-particle drag force in anisotropic assemblies as well as in heterogeneous assemblies. The numerical method he adopts is mainly particle-resolved direct numerical simulations. This paper is going to be presented both by oral talk and by poster. The presenter will be Teng Ma.

Direct Numerical Simulations of Low-Reynolds-Number Flow Past Arrays of Ellipsoidal Particles: Effect of Particle Orientation on Drag Force

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Abstract

A second-order immersed boundary-lattice Boltzmann method (IB-LBM) is used to study the effect of particle orientation on flows through fixed random arrays of ellipsoidal particles at low Reynolds numbers. Herman's orientation factor and Beta distribution are introduced to quantify the mean orientation and orientation deviation of a random array of ellipsoidal particles. First, the immersed boundary-lattice Boltzmann method model is validated by simulating low-Reynolds-number flows passing a single ellipsoidal particle with various aspect ratios. Then, arrays of mono-disperse ellipsoids are simulated at solid volume fractions from 0.1 to close-packed limits at eight different Herman's orientation factors. The simulation results show that the effect of particle orientation is profound especially when the solid volume fraction and the aspect ratio are large. The current simulation results are compared with wildly used traditional drag force correlations in the literature. The comparisons show that the traditional drag force correlations significantly under-predict the drag force on random arrays of ellipsoidal particles. Based on current simulation results, a new relation are proposed for predicting the drag force on random arrays of ellipsoidal particles at arbitrary aspect ratios, Herman's orientation factors and solid volume fractions.

Brief Biography

Xinyang Li, born in China in 1994, got his bachelor's degree in the School of Mechanical Engineering and Automation at Northeastern University (China) in 2016. From 2016 to now, he is studying for his doctorate degree in the School of Chemical Engineering and Technology at Xi'an Jiaotong University. The supervisor is Prof. Qian Zhou and the research subject is direct numerical simulations of gas-solid flow for ellipsoidal particles. The major research is focusing on (1) generation of ellipsoidal particles with specific particles' mean orientation, orientation deviation and solid volume fraction; (2) the drag force model for ellipsoidal particles in gas-solid flows. This paper is going to be presented both by oral talk and by poster. The presenter will be Xinyang Li.

Analysis on Retention Capacity of Liquid Bridge between Two particles under Oscillation

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Abstract

Liquid bridge is the water existing among particles due to surface tension and adhesion. Because of its significant influence on the material flowability, liquid bridge plays an important role in bulk material handling and processing, especially for wet and sticky materials. The shape and volume of the liquid bridge generally vary during material handling with the alteration of the distance between particles. Meanwhile rupture and reconstitution of the liquid bridges can occur, which leads to uneven moisture distribution within bulk materials associated with inhomogeneous flowability. This study investigates the liquid bridge from a microscopic view. The liquid bridge shape and volume between two particles for various particle sizes and particle distances were studied in the static condition under the effect of gravity. Additionally, an oscillation motion was applied to the liquid bridge and the corresponding ruptured liquid bridge shape and volume were investigated.

Brief Biography

Mr. Jian Chen is a PhD candidate from the University of Newcastle. Before his PhD study, he went Southeast University for bachelor study in mechanical engineering and Zhejiang University for master study in mechatronics engineering. His main research in master study was hydraulic power transmission and control, typically the hydraulic power transmission system of concrete pump. Mr. Jian Chen went to the University of Newcastle for his PhD study in mechanical engineering in 2014. His main research area in PhD is unsaturated water flow in particulate system in dynamic condition. During these years of study, he developed a theoretical model and a simulation model (DEM-SPH) for the unsaturated flow in bulk materials under oscillation. His research interests including but not limited to simulation (DEM, VOF and SPH) and infiltration theories. He is also doing some casual research in his research centre - Centre for Bulk Solids and Particulate Technologies, such as coal self-heating.

Till now, Mr. Jian Chen has one SCI paper published and one SCI paper accepted, as well as a few under review. Mr. Jian Chen would like to take this great opportunity to give an oral presentation about his further work on microscopic liquid bridge and liquid bridge rupture under oscillation.

Study of Particle Velocity Distribution and Mixing Index in Single and Multiple Jets Fluidized Bed: Comparison of Model Predictions with Experiments

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Abstract

Fluidized bed is widely used in industrial applications. The mixing efficiency, which depends on jets number and location, is important in successfully designing fluidized bed. In this research, particle velocity distribution and mixing index in gas-solid fluidized bed are measured with both computational simulation and experimental method. For experimental method, particle image velocimetry (PIV) system is employed to measure the particle velocity in a pseudo-fluidized bed. For computational simulation, discrete particle modelling (DPM) is used to simulate particle velocity around a single bubble. And based on the same total gas velocity (superficial gas velocity), cases with different jets number are also compared in terms of maximum bed pressure drop, bed height, mixing index. The results show that particle velocity distribution around a single bubble is the linear superposition of multiple peak distributions. On the other hand, different jets number will result in different flow pattern and this will severely affect the mixing efficiency. The mixing efficiency in one jet (spouted-bed) case is higher than other cases. This may result from the higher jet velocity and umbrella-type flow pattern that promote particle exchange between bottom and top. For the multiple jets cases, bubbles and vortex will form and promote particle mixing to some extent but not as efficient as that in one jet case. However, particle contact number distribution in multiple jets cases is more evenly than that in one jet case. That means from the perspective of particle heat transfer, multiple jets may be better than one jet

Brief Biography

Runjia Liu received his B.S degree in 2014, from the School of energy and environment, Southeast University, China. He studied in Dalian institute of chemical physics, Chinese academy of sciences in 2016. Now he is joint Ph.D. candidate in Monash and Southeast University. His general research interests are the simulation and experiment for gas-solid fluidized bed.

Three-Dimensional Simulation of Oxy-Fuel Combustion in a Circulation Fluidized Bed

Jinrao Gu[1,2], Wenqi Zhong[1*,2] and Aibing Yu[2,3]

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2. Center for Simulation and Modelling of Particulate Systems, Southeast University-Monash University Joint Research Institute, Suzhou, P.R. China

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Abstract

A three-dimensional Eulerian−Lagrangian was developed to perform the full-loop simulation of the oxy-fuel CFB combustion process. The gas phase was simulated by a large eddy simulation (LES) and the particle phase is described with the Multi-Phase Particle-In-Cell (MP-PIC) scheme. A conversion model for the coal particles was implemented which covers the devolatilization processes. The model was satisfactorily validated by the experimental data from a pilot-scale 0.1MW_{th} CFB combustor. Then, the gas-solid flow behaviors and combustion characteristics in the oxy-fuel CFB were numerically investigated. The findings, which are difficult to achieve with experiments, are important for the structural design and operation optimization of the oxy-fuel CFB.

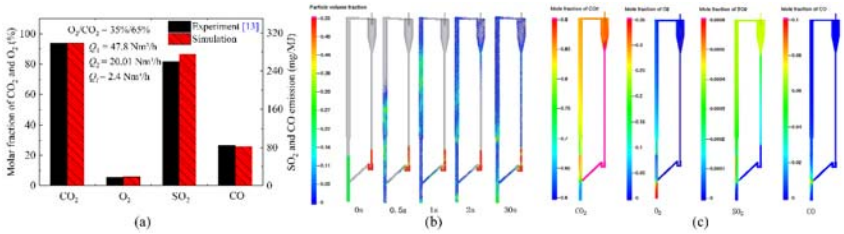

Fig.(a) Comparison of outlet gas composition between simulation and experiment, (b) the particle circulation and (c) concentration distribution of main gas compositions in the whole CFB. (Q_1 = 47.8 Nm^3/h, Q_2 = 20.01 Nm^3/h, Q_l = 2.5 Nm^3/h, O_2/CO_2 = 35 %/65 %.)

Brief Biography

Jinrao Gu, Male, is a first-year PhD candidate in Thermal Engineering and Engineering Thermophysics, Southeast University. He is supervised by Prof. Wenqi Zhong and Prof. Aibing Yu.

Ash adhesion behavior characterization and control at high temperature in energy and environmental systems

Hidehiro Kamiya

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Abstract

The characterization and control of the adhesion and deposition behavior of fine ash particles at high temperatures is one of the most important technology for the stable operation of coal, biomass, and solid waste combustion and gasification as well as for gasification in power plants and other industrial plants. Original two kinds of characterization method and apparatus for adhesion force measurement and analysis of adhesion force increase under high-temperature conditions were designed and prepared by using split type tensile strength tester[1)] and computer-controlled FE-SEM/EDS system[2)]. Based on the results for adhesion behavior and the results of other characterizations, the mechanism underlying the increase in adhesion force between the particles, such as liquid bridge force etc., was analyzed by combined approach using thermodynamic calculation and DEM simulation[3)]. The effect of liquid and solid bridge formation on the dust detachment phenomena on ceramic filter and tensile strength test of ash powder bed at high temperature were simulated by DEM/CFD method with liquid bridge force. Some strategy for controlling the ash adhesion behavior at high temperature condition was discussed about some kinds of additives for chemical and physical effects between ash particles, and confirmed each effect by laboratory level experimental approaches,

Key notice & instructions: Ash deposition, Ash agglomeration, Pulverized coal combustion, Sewage sludge combustion, High temperature gas cleaning, Ceramic filter

Reference

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3) Y. Shao, N. Aoki, Z. Tong, W. Zhong, A. Yu, H. Kamiya, ibid., 27, 215-222 (2016)

Brief Biography

Dr. Hidejiro Kamiya was chief editor of Journal of Society of Powder Technology, Japan, during 2012-17 and is editorial board member of "Powder Technology". He received B.C. degree (1981) and PhD (1986) in Department of Chemical Engineering at Nagoya University, Japan. He has published over 200 papers about fine and nano- particles and powder science and technology. His fine particle technology has also been applied in various fields, such as "Energy and Environmental" subjects, DDS, cosmetics, pigment and toner based on collaboration with many industrial companies. Professor Kamiya has received various award included the SCEJ Award for Outstnding Research (2007) and Technology (2016) Achievement, Society of Chemical Engineers, Japan, and Advanced Powder Technology, Distinguished Paper Award. (2013)

CFD-DEM Modelling on Spouting Behaviors of Cylindroid Particles

Xuejiao Liu[1,3], Wenqi Zhong[1*,2], Jieqing Gan[3], Aibing Yu[2,3]

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2. Center for Simulation and Modelling of Particulate Systems, Southeast University-Monash University Joint Research Institute, Suzhou, P.R. China

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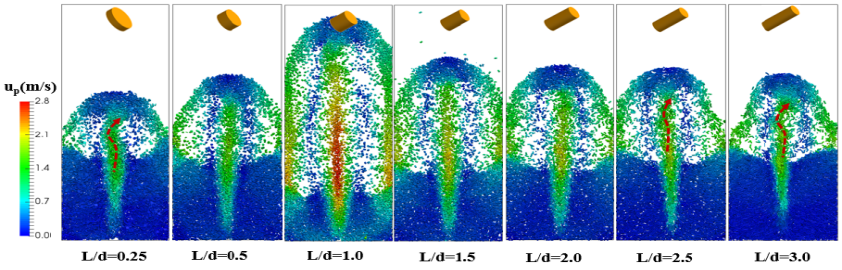
Abstract

The Computational Fluid Dynamics-Discrete Element method (CFD-DEM) approach for cylindroid particles was developed to study the effects of particle shape on spouting behaviors in a flat-bottomed spouted bed. The gas motion was modelled with *k-ε* turbulent model, and the particles ware represented with realistic cylindroid shapes. The drag force model and various contact forces for cylinders were comprehensively involved to describe the particle motions more accurately. With the aspect ratio of particle varying from γ=0.25 to 3.0, spouting behaviors including flow pattern, particle velocity, orientation and contact details were investigated. Results found that cylindroid particles tend to put their longer dimension vertically in spout, while in annulus the orientation tendency is contrary. The particle with γ=1.0 obtains the maximum projected area in spout and thus the largest drag force and particle velocity. When particle shape becomes more flat or long, the particle projected area in spout accordingly decreases, resulting in the decreasing particle velocity and particle circulation rate. On the other hand, when aspect ratio deviates from 1.0, the obviously increasing particle contact number in annulus reflects their increasing interlocking effects and worse flowability.

Keywords: gas-solid flow, cylindroid particle, spouted bed, CFD-DEM



The different flow behaviors of cylindroid particles with varying aspect ratios (u_g=6 m/s, H_0=0.21 m, ρ_p=1200 kg/m^3, V_p=42.39 mm^3)

Brief Biography

Dr. Xuejiao Liu is a research staff at Southeast University and she specializes in multiphase flows, computational fluid dynamics, clean coal combustion technologies and biomass thermal transformation.

Discrete simulation of particle manipulation in micro-fluid with acoustic force

Wenjing YANG, Peijin LIU, Qiang LI and Guoqiang HE

Science and Technology on Combustion, Internal Flow and Thermo-Structure Laboratory, Astronautics School, Northwestern Polytechnical University, China

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Abstract

In recent decades, particle manipulation becomes more and more important for many lab-on-a-ship applications such as flow cytometry, single molecular detection, protein folding, cell sorting and enzymatic kinetics. For microflow, particle focusing can be quite difficult, since the laminar nature of microfluidic flow predominantly determines the particle motion following the fixed streamlines. Thus the lateral forces are necessary to change the original path of particles, involving hydrodynamic force, electro-kinetic force, dielectrophoresis force and acoustic force. To date, the standing surface acoustic wave (SSAW) shows the unique abilities in focusing particles in micro-channel. Based on particle size, density and shape, with proper application of SSAW, particle focusing can be done meeting various demands. However, each single particle motion in microscopic level is not easy to be studied by experimental method and conventional continuum method, therefore, the discrete element method (DEM) plays irreplaceable role to study the particle focusing phenomena with SSAW. In this paper, the polystyrene particles are described by DEM, the flow (water) is simulated by computational fluid dynamics (CFD). The acoustic force acted on each particle in implanted into DEM based on Gorkor theory.

In order to validate the mathematical model in this work, the experimental setup used shown as Fig.1 For the sake of comparison, the particles in simulation are presented in green color without specific physical meaning. The simulation results are compared with the experiments in Fig.2, which indicates the focusing behavior of particles is consistent between simulation and experimental photos. As mentioned in reference, in the experiment the particles are gradually focused into a narrow region (5μm) after a certain distance, which is around 300μm. Accordingly, in our simulation, the particles similarly focus into a thin layer of 4.1μm at 350μm, which shows satisfied consistency. Furthermore, when we put our attentions on the focused layer (Fig.2), the uniformly arranged particles agree with the smoothed line in experimental photo, which also emphasizes the merits of discrete model. In Fig.2 the particle is colored by the acoustic force acted on the particles, smaller in the central line and larger near the wall. Based on the comparison, CFD-DEM shows good accuracy in numerical study of particle focusing with acoustic wave, along with the microscopic information of each single particle which is difficult to obtain either by experiments or continuum simulation.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

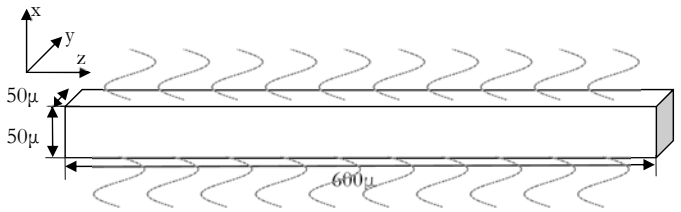
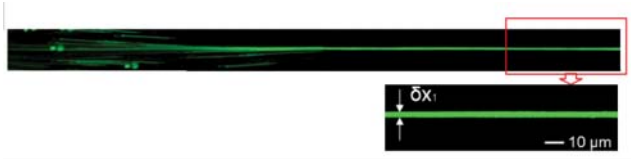
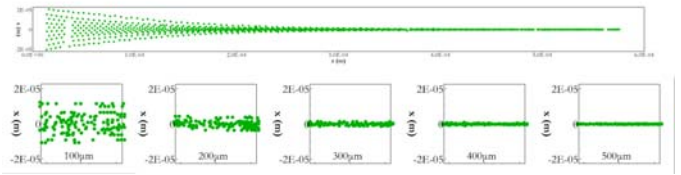


Fig.1 Geometry of micro channel and schematic diagram of SSAW



(a)



(b)

Fig.2 Comparison between experimental photo (a) and simulations (b)

Brief Biography

Dr. Wenjing YANG, an associate professor in Science and Technology on Combustion, Internal Flow and Thermo-Structure Laboratory, Astronautics School, Northwestern Polytechnical University, works in gas-particle flow, gas-solid heat transfer, and multi-phase flow in solid rocket motor for years, which have been supported by several national fundings. Dr. YANG got Doctor Degree from University of New South Wales in 2014, Master degree from Tsinghua University in 2009 and bachelor degree from Hefei university of technology. Dr. YANG published 12 journal papers, including Chemical Engineering Journal, Powder technology, Industrial & Engineering Chemistry Research and Metallurgical and Materials Transactions B.

The Phase Separation in Multi-stage Fluidized Bed Reactors

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Abstract

The multi-stage fluidized bed (MSFB) reactor consists of several stages connected in series, obtaining excellent gas-solids interaction in each stage and thus has a favorable capability of heat remove, while at the same time effectively preventing gas and solids back-mixing between each stage to gain the plug-flow reactor performance. In addition, different process steps can be accomplished by establishing different temperatures and/or concentration in a single reactor. Therefore, as shown in Figure 1 multi-stage fluidized bed reactors are acknowledged as novel and flexible multi-phase flow reactors for heterogeneous catalytic processes, especially with the intermediates as the desired products.

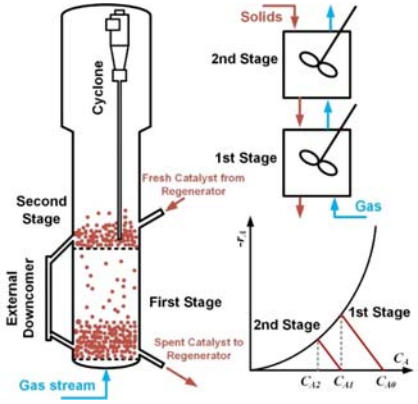

Figure 1. The conceptual design of multi-stage fluidized bed reactors (MSFB)

The unique capability of suppression of gas solids back-mixing in MSFB come from the formation of the 'gas cushion'. In this study, the phase separation through nozzle i.e. the change of flow density, is determined by the compressibility of gas solids mixture in dense system, treated as supersonic flow (Ma>1) as shown in Figure 2. The degree of gas solids separation through the narrow throat can be calculated. Then, this theory is examined by a cold test in a 300 mm diameter.

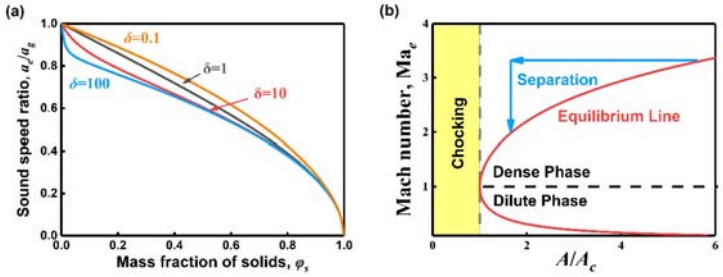

Figure 2. (a) The effect of mass fraction of solids on equilibrium speed of sound for gas solids flow, where γ = 1.4; (b)Phase separation of gas solids flow through nozzle.

At last, typical process developments in the industry involve the methanol to aromatics (MTA), regeneration in fluid catalytic cracking (FCC) and hydrogenation of nitrobenzene to aniline. The purpose of this article is to provide a comprehensive review of the fundamental researches as well as particular industrial applications on multi-stage fluidized bed reactors in Fluidization Laboratory of Tsinghua University (FLOTU).

Brief Biography

B.E. (Chemical Engineering) Tongji University, China (2009)

Ph.D. (Reaction Engineering) Tsinghua University, China (2017)

2017-now Research Associate, Department of Chemical Engineering, Tsinghua University, China

List of Publications

1. Zhang C.X., Wang Q., Jia Z., Muhammad U., Qian W.Z., and Wei F.* (2016) Design of parallel cyclones based on stability analysis. AIChE Journal, 62: 4251-4258.

2. Zhang C.X., Qian W.Z., and Wei F. (2017) Instability of uniform fluidization. Chemical Engineering Science, 173: 187-195.

3. Zhang C.X., Li P.L., and Lei C., Qian W.Z., and Wei F.* (2018) Experimental study of non-uniform bubble growth in deep fluidized beds. Chemical Engineering Science, 176: 515–523.

4. Wang Q., Zhang C.X., Zhu Z.X., Muhammad T.A., Yang L., and Wei F.* (2016) Comparison study for the oxidative dehydrogenation of isopentenes to isoprene in fixed and fluidized beds. Catalysts Today, 276: 78-84.

5. Jia Z., Zhang C.X., Cai D.L., Blair E., Qian W.Z., and Wei F.* (2017) The analysis of hot spots in large scale fluidized bed reactors. RSC Advances, 7: 20186.

Understand Solids Loading Effects in Dense Medium Cyclone

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Abstract

Industrial cyclones, such as gas, hydro and dense medium, are widely used in chemical, mineral and process industries to separate particles from fluids or classify particles by size, density or other solid properties. It is well known that the loading of particles can significantly affect fluid flow in such cyclones but the specific effect can be confusing due to a limited fundamental understanding of the working mechanisms involved. In this work, the effect of solids loading effect in dense medium cyclone (DMC) is discussed by mainly analyzing the simulation data obtained from a combined approach of Computational Fluid Dynamics (CFD) and Discrete Element Method (DEM) (CFD-DEM). It suggests that the effect of solids loading rate heavily depends on particle properties (which includes coal particle size and density distributions and other solids properties such as particle shape and particle surface roughness). The most notable finding is that particles of different density/size have different trajectories in the cyclone (e.g., Figure 1), leading to different spatial distributions of solid particles and thus different spatial distribution of volumetric particle-fluid interaction forces which cause different effects on the fluid flow. A universal rule to describe the specific effect of solids loading rate in DMCs is very difficult to develop. This is because, even for given/constant solids loading rate, the flow and DMC performance can still vary significantly with properties of particles. In other words, the specific effect of solids loading rate depends on particle material properties. In the future, the effect of solids loading rate for different particle properties can be better defined with the CFD-DEM approach as the major tool and the support of physical experiments. The findings should be useful for developing a better understanding the working mechanisms of solids loading effects in DMCs and also in other similar swirling multiphase flow systems.

Brief Biography

Dr Kaiwei (Kevin) Chu is specialized in the modelling and simulation of complex particle-fluid flows that are ubiquitous in nature and industries. He carried out extensive pioneering work to elucidate the fundamentals of complex particle-fluid flows by developing and applying combined approach of computational fluid dynamics and discrete element method (CFD-DEM), leading to >80 publications, with total citation times of 1955 and H-index of 21 (as at 8 Nov. 2018 via google scholar). He has 3 first-authored articles belonging to “Most Cited Articles” and 7 first-authored articles

belonging to “Top25 Hottest Articles” in their respective journals. He obtained his PhD degree from UNSW Australia in 2010 and is current a Research Fellow at Monash University of Australia.

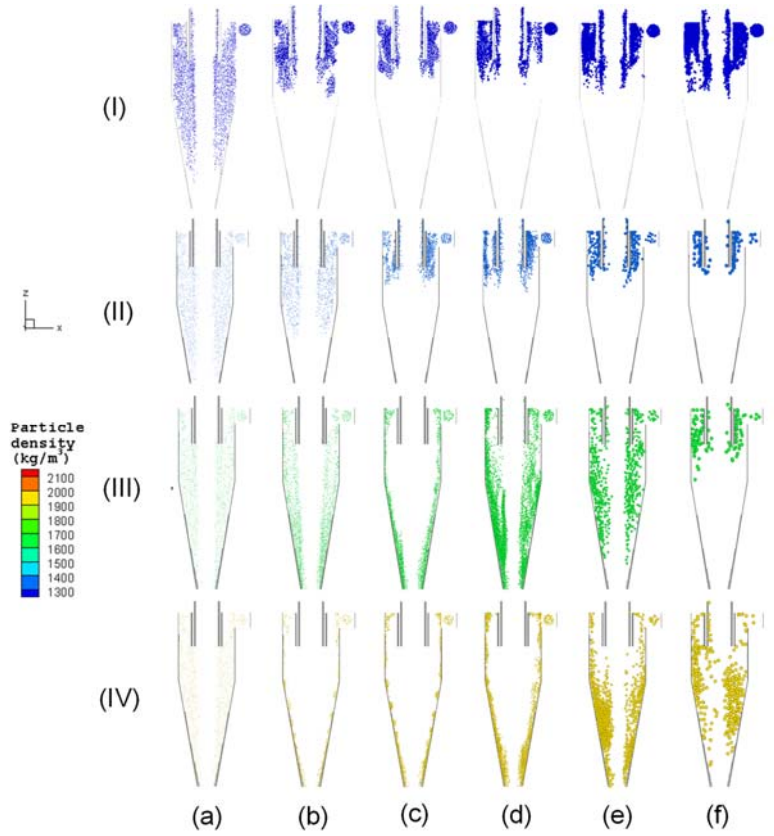

Figure 1. Spatial distribution of particles of different size and density: (I) 1200 kg/m^3, (II) 1400 kg/m^3, (III) 1700 kg/m^3 and (IV) 2000 kg/m^3; and (a) d = 0.25 mm, (b) d = 1 mm, (c) d = 5 mm, (d) d = 20 mm, (e) d = 40 mm, and (f) d = 60 mm (Chu et al., 2017).

HIGmill Modelling by DEM and CFD

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Abstract

HIGmills are stirred media mills for fine grinding applications, typically used for high-value concentrate streams that have already been ground by a ball mill. A HIGmill consists of a stationary vertical tank partially filled with ceramic beads around 2-5 mm diameter and agitated by a central shaft with a number of grinding rotors. Feed slurry enters the bottom of the tank and overflows at the top.

HIGmills have been modelled by first DEM, and subsequently multiphase CFD. Initially DEM was used to solve a grinding rotor wear issue with early installations, leading to the development of a castellated rotor. However, while DEM captures much of the bead particle physics it is a dry bead model and does not include the fluidisation and other effects from the slurry.

Subsequently a 4-phase Eulerian CFD model was developed, with phases for beads, fine and coarse ore particles, and the liquor. Model development includes drag laws for the phases, rheology for the non-Newtonian bead phase, and a grinding model that converts coarse particles to fine particles based on the local grinding energy. Various additional scalar transport equations are also required to track aspects of the particle phase history as it travels through the mill. Convergence was unsurprisingly difficult, and solution strategies are also discussed.

Brief Biography

Alex is a researcher with 25 years experience in the Australian mining industry. He has a PhD in chemical engineering and population balance modeling from Murdoch University. He spent 14 years at the CSIRO in various roles, but predominantly doing CFD and other numerical modeling as part of the AMIRA P266 project. For the last 10 years he has been at Outotec, a mineral processing equipment supplier, working on a number of projects in both the thickener and mills product lines.

Fluid Flow Through Unresolved CT Data-Sets – Can Gray-Scale LB Deliver Useful Results?

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Abstract

Understanding and controlling the flow of fluids through porous media such as rocks, fibres, granular media and paper is of fundamental significance to a variety of industries such as oil and gas, chemical production, health and sanitary products. Numerical modelling of this physical process can be difficult not only because of the complex, three-dimensional topology of the porous medium but also because of computational limitations. For example, shale rocks which is now being intensively investigated for its oil and gas resources have porosity over a wide range of length scales from nano-metres up to millimetres. It has been shown that the micro-porosity is fundamental to the fluid movement through the rock. However, current numerical models, which work off computed tomo-graphical (CT) scans of the rock will be excessively large if they are to fully model all length scales which may span six or more orders of magnitude.

Here we consider the development of a lattice Boltzmann (LB) technique which may be able to solve the fluid flow over a wide range of length scales. In the past LB techniques have proven to be ideal to model fluid flow in complex porous media since it can readily import and process digital data from CT scans. Hence the fluid flow field is quickly determined and permeabilities can be predicted. However, when the CT data contains micro-porosity, the conventional LB method is not applicable and a modified LB method needs to be developed. Here we consider a gray-scale LB method which operates on voxels which are not fully void or solid but something in between, i.e. each voxel is partially resistant to fluid flow.

We develop models not only for single phase fluid flow, but also multiphase fluid flow (i.e. water and oil). We calculate relative permeability and capillary pressure curves on a tight rock CT data-set. It is shown that the gray-scale LB model gives realistic predictions for these quantities and thus could be a useful computational tool for fluid flow through multiple length scales – a difficult computational problem which is of increasing significance in many real-world applications

Brief Biography

Dr Gerald G Pereira holds a PhD in Applied Mathematics from Melbourne University and currently works at CSIRO in Clayton. His areas of scientific interest include algorithmic development of numerical methods for fluids especially the lattice Boltzmann (LB) method; application and development of numerical models to describe the flow behavior of granular materials; application of computational fluid dynamics (CFD) methods to a variety of physical systems including porous media, microfluidics and processing devices; and statistical mechanics of soft condensed matter especially polymers and liquid crystals.

Model Driven Design in Particulate Products Manufacturing

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Abstract

The manufacture of particulate products is widespread in many industrial sectors. Manufacturing processes such as granulation or milling remain poorly understood, primarily because of the complexity of a typical particulate system involving particle–particle and particle–fluid interaction phenomena. Modelling of such particulate systems has become increasingly popular as a powerful means to gain insight into the phenomena that govern the particulate processes. Despite significant advances in many computational and analytical modelling approaches, very few models developed within academia have been implemented in industrial practice.

This paper describes an academic–industrial partnership project to develop a Model Driven Design (MDD) framework to enable industry to implement the best available models, taking twin screw granulation as an exemplar case study. A multi-scale modelling approach is adopted, using Discrete Element Method (DEM) to provide particle-scale physics and inform the process-scale using Population Balance Model (PBM). The multi-scale information is exchanged between the DEM and PBM models to extract the maximum benefits of two different methods with complementary strengths.

In consultation with industrial partners and the Centre for Process Innovation UK (CPI), a best-practice guide of developing and implementing a multi-scale modelling approach to help transfer the academic models into industry and facilitate model-driven design of particulate processes and products is presented. The guide proposes a rigorous verification and validation procedure to verify the appropriateness of a multi-scale model before establishing the predictive capability of the model for a particulate process.

Brief Biography

Jin Ooi received his B.Eng. Honours degree from The University of Auckland as a Senior Scholar and his Ph.D. degree from The University of Sydney. He has been the Professor of Particulate Solid Mechanics at the University of Edinburgh since 2005. He also holds the position of Qiushi Chair Professor at Zhejiang University and Distinguished Adjunct Professor at Shandong University. With over 30 years of experience in particulate solid mechanics and bulk solids handling, his research covers both computational and experimental studies of solids behaviour and industrial problems in bulk handling and processing. He has published over 200 journal and conference papers and has delivered many keynote lectures around the world. He is on the Editorial Board of the Canadian Geotechnical Journal and edited special issues in Powder Technology and Granular Matter. He co-founded DEM Solutions Ltd with the EDEM discrete particle simulation software and Particle Analytics Ltd with the Iota data analytics software, bringing impact of his research on many industrial and scientific challenges.

Effects of Diffusion of Metal Vapour in an Argon TIG Welding Plasma

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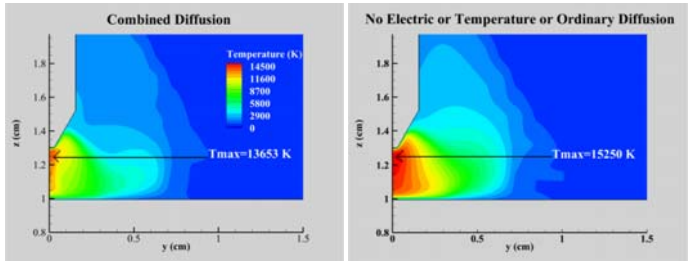
Abstract

Tungsten inert-gas (TIG) welding is widely used to join metals. In the TIG process, an electric arc is initiated and maintained between a tungsten cathode and a metal anode workpiece, melting the workpiece and forming a weld pool. Metal vapour is generated from the weld pool once the liquid nears its boiling point, affecting the arc welding process. Previous studies have found that metal vapour diffusion is strong in a helium arc, and diffusion driven by the electric field between the electrodes is found to be the main mechanism for metal vapours penetrating upward through the arc (Park *et al.* 2017). In the present work, we investigate metal vapour diffusion in an argon arc with a stainless-steel workpiece and assess how each diffusion driving force affects the overall transport of metal vapour in the TIG process.

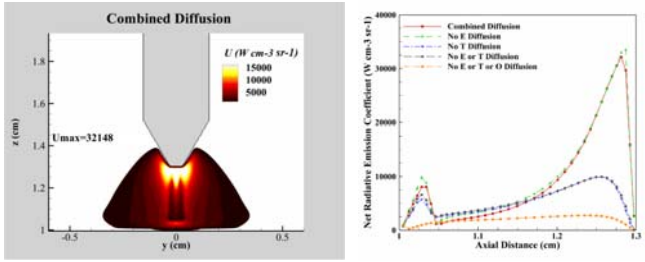
An axisymmetric computational model incorporating the arc and the weld pool is applied to treat the transport of iron and chromium vapour in the argon arc plasma, using the combined diffusion coefficient method (Murphy 2014), which takes into account ordinary diffusion, temperature diffusion, pressure diffusion and electric field diffusion at the same time. Our results show that in an argon arc, electric field diffusion is weaker than in a helium arc, and diffusion due to the temperature gradient dominates metal vapour transport. The effect of ordinary diffusion is also significant, especially in the region close to the weld pool. When all the diffusion effects are included, the arc temperature is predicted to be significantly reduced due to the enhanced radiative cooling associated with the presence of the metal vapour. Compared to results obtained when ordinary, temperature and electric field diffusion are set to zero, the full calculation shows that the maximum arc temperature drops by more than 1500 K (Figure 1) and the maximum net radiative emission coefficient is increased by more than a factor of eleven (Figure 2).

The results demonstrate that the effect of the metal vapour on the arc plasma is significant in argon TIG welding. This is in contrast to previous modelling studies for argon, which have only considered ordinary diffusion, and which found that the metal vapour was only present near the workpiece. Only by including diffusion due to temperature gradient and the electric field is it possible to obtain an accurate prediction of metal vapour distribution and arc temperature.



(a) (b)

Figure 1 Distribution of temperature in arc plasma calculated (a) with full combined diffusion coefficient treatment and (b) with electric field, temperature and ordinary diffusion neglected



(a) (b)

Figure 2 Distribution of net radiative emission coefficient in the arc (a) in a vertical cross-section calculated using full combined diffusion coefficient treatment and (b) along a line in the axial direction at a radius of 0.005 cm using several combinations of diffusion coefficients

Reference:

A. B. Murphy (2014). "Calculation and application of combined diffusion coefficients in thermal plasmas." Scientific Reports **4**: 4304.
H. K. Park, M. Trautmann, K. Tanaka, M. Tanaka and A. B. Murphy (2017). "Mixing of multiple metal vapours into an arc plasma in gas tungsten arc welding of stainless steel." Journal of Physics D: Applied Physics **50**(43): 43LT03.

Brief Biography

Dr. Junting Xiang is currently a postdoctoral fellow in CSIRO Manufacturing, focusing on computational modelling of arc welding and computational fluid dynamics in general. He has worked on a variety of government and industry-funded projects including gas turbine engine optimisation, particle-laden flow simulation, drag reduction design for marine vessels and tungsten inert-gas (TIG) welding calculations. He is enthusiastic about using CFD and scientific modelling tools to solve real-world problems.

Coupled CFD-Material Bed Modelling for Optimised Rotary Kilns Performance

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Abstract

The performance of a kiln burner has a great influence on kiln output, product quality, NOx emissions, creation of rings and cycles and many other process factors. Up until recently, burners were designed from experience, trial and error and empirical rules. FCT Combustion has advanced its modelling capability to combine two-way coupling of CFD with Material Bed (CFD-MB) modelling, resulting in a greater understanding of how the burner design is interacting with the material bed in the kiln. An operational coal-fired lime kiln, processing calcium carbonate (CaCO3) is used as a case study. A visual on-site observation of the flame showed a long black plume of unburnt coal particles. This indicates an ignition delay, which is one of the challenges addressed in this study.

The CFD-MB predictions are used to redesign the burner to shorten the ignition-delay distance, and enhance the utilisation of the latent capacity in the bed to increase the production rate. The modification has resulted in reduced ignition-delay distance by approximately 5*m* (Fig.1), which consequently reduces the heat transfer from the inner refractory and the material bed to the secondary air, without affecting the shape of the wall heat flux profile. The predictions of the original burner showed that calcination is completed approximately 6*m* before the material reaches the cooler chute, which leads to an initial sharp rise in bed temperature. That is, the heat transfer from the gas is being converted into sensible energy in the material bed, rather than been used for material calcination. The bed temperature then starts to decrease closer to the burner as this sensible heat is transferred back from the bed to the secondary air. This section of the bed with the temperature rise, provides an opportunity to increase the production rate by utilising the embedded sensible bed energy. Accordingly, the feed rate is increased to 120% and later to 130%. A complete calcination is achieved when the feed rate increased to 120% of its original feed rate. This implies that the current firing capacity (using the redesigned burner) is sufficient to handle the additional feed. The prediction also showed that the embedded sensible heat in the bed is no longer wasted, which indicates improved process heat utilisation. The production of CaO is increased by 20%. The efficiency of the actual-to-theoretical $CaCO_3$/CaO conversion is also increased from 81% to 90%. Further increase in the feed rate to 130% of the original rate, however, (without increasing the firing rate) has resulted in an incomplete calcination of 5.5% of the feed material. This case study is a demonstration of the powerful impact that CFD-MB modelling has on enhancing and optimising the performance of rotary kilns.

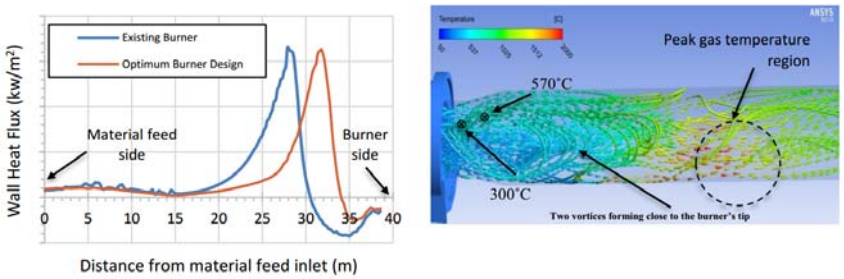

Figure 1: (left) wall heat flux profiles of the flame produced by the optimum burner design and that with the original burner, (right) flow streamlines coloured by gas temperature for the optimised burner design.

Brief Biography

Farid C. Christo is an experienced researcher in combustion and thermal-fluids, and also has a significant applied research and industry experience in the Defence and private industry sectors. Farid holds BSc & MSc degrees in Aerospace Engineering and a PhD from the University of Sydney. Farid is currently Group Leader of the thermal energy research group at Deakin University.

Yvonne Yu is a CFD Modelling Engineer at FCT since 2015. She is graduated in Mechanical Engineering and International Economy and Trade, holding two master degrees, from University of Adelaide, in Mechanical and Aerospace Engineering. Yvonne has worked with renewable fuels and is an experienced CFD Modelling Engineer, developing CFD projects for kiln and calciner burners in the cement, lime and iron ore pellet industries, as well as for ceremonial flame applications and R&D projects.

Roger Hassold is the general manager and is at FCT since 2014. Graduated in Chemical Engineering and holding a certificate in Advanced Management Program, he is an experienced combustion engineer, designing, installing and commissioning advanced burner systems for industrial clients and solving complex pyro-processing problems with the use of CFD modelling. Roger is also an experienced Production Manager, Technical Manager and Process Engineer in the cement and lime industry and has worked with a large range of kiln technologies and product types.

Multi - scale Simulation of Pressure Loss in the Pleated Fibrous Media

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Abstract

At present, the pleated fibrous media has been widely used as filtration material in air purification devices because of its large filtration area, high filtration efficiency and small space volume. With the development of computational fluid dynamics (CFD) technology, a lot of scholars have applied CFD method and its related software to study the filtration characteristics of fibrous media. However, when using CFD software for numerical calculation, the relevant parameters of the fibrous media such as porosity, viscous drag coefficient and the like are usually empirically obtained. Whereas there is no doubt that this method will increase the calculation error. Therefore, this study builds the data relationship that transfers the pressure loss of the pleated fibrous media from the micro and macro perspectives. The research process can be divided into two stages, in the first stage, a micro-three-dimensional mimicry model of pleated fibrous media is established, as shown in Figure 1, and the pressure loss of the pleated fibrous media is calculated, the relevant parameters of the fibrous media are obtained by developing a fitting equation of flow rate and pressure loss, which is shown in Figure 2. In the second stage, a macroscopic model of the fibrous media is established, as shown in Figure 3, which is also simulated based on the property parameters obtained from the microscopic model. Additionally, the simulation results are compared with the empirical formula, and the contrast results are shown in Figure 4.The results of this study illustrate the feasibility of data transmission between the microstructure and macrostructure of the pleated fibrous media, so that provides a basis for optimizing the pleated fibrous media based on the macroscopic model. The results of this study will be of important theoretical and practical significance for expanding the research methods of fiber filter media and optimizing its structure.

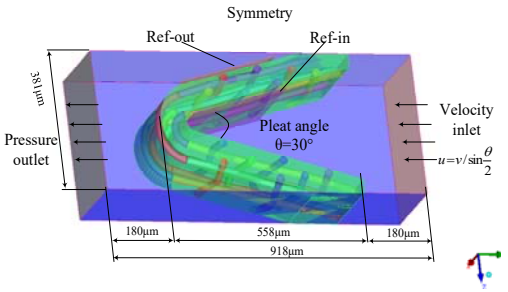

Figure 1. Boundary conditions of the pleated fibrous media based on micro-model

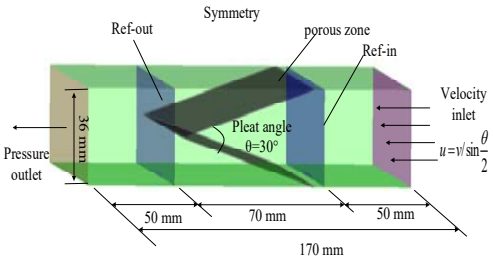

Figure 3. Boundary conditions of the pleated fibrous media based on macro-model

Figure2. The curve of filtration velocity and pressure loss of the pleated fibrous media

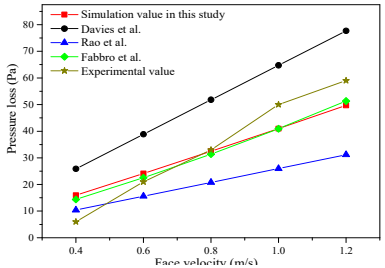

Figure 4. Results analysis diagram of the macro-scale simulation

Brief Biography

Fuping Qian, male, PhD, professor, vice dean of the School of Civil Engineering and Architecture and director of the Institute of Ventilation and Purification in Anhui University of Technology.

DNS of coupled heat and mass transfer in slender packed bed reactors: Effect of particle to column diameter ratio on heat transfer

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Abstract

Catalytic tubular fixed bed reactors are one of the most widely used reactors in chemical and process industries. Inside these reactors, the chemical reactions take place on the surface of solid catalyst particles. The overall pressure-drop, species conversion, and temperature control are some of the major design considerations for these fixed bed reactors.

The temperature control inside the reactor is of importance as it affects the performance of the catalyst. In case of exothermic reactions, the rate of the reactions and thereby the rate of heat generation is an exponential function of temperature. If no proper heat removal system is employed in the reactors, the temperature could increase very rapidly along the length of the reactors which can damage the catalyst. This uncontrolled rise in temperature can cause thermal runaway conditions. This could lead to operational safety issues.

Multi-tubular slender fixed bed reactors are used for improved thermal management of systems. They consist of large number of parallel tubes places inside a cooling jacket. The diameter of these tubes is of the same order as that of catalyst particle diameter, and this offers a higher specific heat transfer area.

Due to their industrial importance, modeling and simulation of slender packed bed reactors is of great importance and has been an industrial priority for decades. With the advances in the field of computational sciences, it is now possible to perform fully resolved simulation of fluid flow along with heat transfer inside a fixed bed with realistic catalyst packings.

In this paper, we study the fluid flow and heat transfer inside a slender packed bed reactor by means of fully resolved direct numerical simulations (DNS). We also include an exothermic heterogeneous reaction in the model to analyze the effect of heat generation on the heat transfer inside the reactor. In one of the major improvements over the past similar studies, we include fully resolve the solid wall of the catalyst particles and the temperature inside the solid particles is solved by a conjugate heat transfer (CHT) model.

We use the developed model to study the effect of the ratio of column diameter (D) to particle diameter (d). The column-to-particle diameter ratio (N) is varied along with particle Reynolds number (Re). We analyze these results to determine the possibility of thermal runway and formation of heat spots inside the slender fixed bed reactor.

Brief Biography

Saurish is a Researcher, Fluid flow and reactor engineering (2017 to date) at Shell Technology Center Bangalore, India. He is currently working on developing novel computational models for new energy business for Royal Dutch Shell (RDS) and at the same time providing high-end technical consulting for several assets of RDS. His currents research focus includes numerical simulation for packed bed reactors, novel catalyst design, electrochemistry modelling, predicting internal corrosion and erosion, fluid-structure interaction, rapid prototyping etc.

Saurish did his PhD (2013 to 2017) from Technical University Eindhoven, Netherlands. During his PhD, he worked on developing CFD code for gas-liquid transport phenomena through complex porous media. Prior to enrolling at TU Eindhoven, he worked for two years (2011 to 2013) as a multiphase flow expert in Ansys Fluent Pvt. Ltd. In Ansys he had worked on numerical models for boiling heat transfer, turbulence flow modelling, three-phase flows etc. He holds a master's degree (2009 to 2011) in Mechanical Engineering from IIT Bombay, India and a bachelor's degree (2005 to 2009) in Mechanical Engineering from Jadavpur University, Kolkata, India. He has co-authored more than twenty peer-reviewed journal articles and conference proceedings and delivered talks in several international conferences. In his free time, Saurish enjoys bird watching and photography.

Simulation Of Floating Particle Bed Dynamics Using CFD-DEM

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J. (Jan) van der Stel[2] and A.T. (Allert) Adema[2]

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Abstract

Beds of floating particles can be found in multiple industrial processing units, such as the ironmaking blast furnace and the slurry bubble column reactor. Typical of these systems is the interaction between a discrete particle phase and multiple continuous phases. The unresolved CFD-DEM method provides an efficient way of simulation the interaction between particles and a surrounding fluid phase. Being computationally less expensive than Direct Numerical Simulation, CFD-DEM allows for the study of macroscopic behaviour of multiphase systems. This makes it a particularly powerful method for developing closures to be used in more coarse, industrial-scale models (e.g. Two Fluid Model) [1].

In order to simulate free-surface flow, the CFD-DEM method is extended to accommodate multiple continuous phases. This is done by the Volume Of Fluid (VOF, [2]) methodology, in which a single set of Navier-Stokes equations and a scalar transport equation for the volume fraction are used to describe multiple fluids. The specific solver used in this work [3] is derived from the OpenFOAM solver interFoam [4].

Unresolved CFD-DEM has been applied to gas-solid systems successfully many times (e.g. [1]). In order to simulate liquid-solid systems additional measures must be taken to obtain accurate momentum exchange between the phases, as the continuous phase density can no longer be neglected. A total interaction force model is presented in which next to the drag, pressure gradient and viscous forces, also lift [5], virtual mass [6] and Basset forces [7] are taken into account. This enables the CFD-DEM method to be used to simulate dynamic behaviour of liquid-solid systems and floating beds.

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Brief Biography

Tim Nijssen is a PhD candidate in the Multiphase Reactors group of Professor Hans Kuipers at the Eindhoven University of Technology in The Netherlands, department of Chemical Engineering and Chemistry. He did both his bachelor and master in Chemical Engineering in the same department, focussing in Chemical Process Technology and graduation on the fluidisation behaviour of non-spherical particles. Starting his PhD project in September 2017, Tim is working on an unresolved CFD-DEM method for the simulation of solid particle bed dynamics in liquids. Of special interest in this project is the ironmaking blast furnace, in the bottom-end (the hearth) of which the interaction of floating coke particles and liquid iron free-surface flow generates flow patterns causing erosions of the refractory lining. Due to harsh conditions rendering measurements virtually impossible, simulations are used to gain deeper insight in the phenomena at play in this complex system.

Key technologies for industrial granular flow simulations

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Abstract

The discrete element method (DEM) [1] is often employed in a numerical simulation of a granular flow. Very recently, novel models has been developed to perform a DEM simulation in an industrial system [2]. The DEM has been applied to a granular flow in an industrially complex shaped vessel thus far, e.g., a ribbon mixer [3], a twin screw kneader [4] and a screw conveyer. When the complex shaped vessel is created, usage of signed distance functions (SDF) [5] is helpful. This is because the boundary wall could be created without meshes. The SDF is scalar function and hence contact detection became very simple in the collision between the particle and wall. When the simulation of solid-fluid mixture system is performed, combination of SDF and immersed boundary method (IBM) [6] is useful. The combination of SDF and IBM makes it possible to create the wall boundary by simple operation, specifically, only opening CAD data and entering number of CFD grids. Applicability of the SDF/IBM has been proven in a die-filling system [7]. When the DEM simulation is performed using a single PC, number of the calculated particles is substantially limited, namely, the number of particles is a few millions. Coarse graining model of the DEM [8] has been developed to perform a large-scale particle system efficiently, where the coarse grain particle represents group of the original particles. In the coarse grain model, total energy is modeled to be equivalent between original particles and the coarse graining particle. Adequacy of the coarse grain model has been proven in a pneumatic conveyer [8], a fluidized bed [9] and spouted bed [10]. Consequently, SDF, SDF/IBM and coarse grain model are shown to be key technologies to apply the DEM to a simulation of an industrial system.

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Brief Biography

Dr Mikio Sakai is currently Associate Professor in the Resilience Engineering Research Center in The University of Tokyo. He earned his Ph.D. degree from The University of Tokyo in 2006 and joined the Department of Quantum Engineering and Systems Science as Assistant Professor in 2007. He then became Associate Professor at the Department of Systems Innovation in 2008, Department of Nuclear Engineering and Management in 2012 and Resilience Research Engineering Center in 2013. He has been Visiting Reader at Imperial College London since 2016. His interests include general computational granular dynamics (gas-solid flows, solid-liquid flows, gas-liquid-solid flows, granular flows and colloidal suspensions with hydrodynamic interactions) and the parallel computing techniques. At present, he is Associate Editor of Chemical Engineering Science.

Particle Size Segregation For Fun and (Hopefully) Profit

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Abstract

Within a typical integrated steelmaking plant, the primary ironmaking operations (sintermaking, cokemaking and blast furnace) are dominated by granular handling problems. For example, the blast furnace ironmaking process is fundamentally driven by permeability management, achieved through spatial control of granular materials. Inherent to the process is the feeding of a collection of ores, fuels and fluxes that while segregated into layered batches are still mixtures within a given batch. Critically, the goal in such processes is often to maintain size or material segregation to optimize a process outcome. However, the majority of equipment and practices are heavily dependent on empirical knowledge and small scale physical experiments. Occasionally fullscale testwork is possible, although the ability to make measurements during operation is typically severely limited. Discrete particle methods have made great advances in understanding key aspects of these phenomena, but we are still a long way from being able to directly simulate the time and length scales involved. Such poorly understood or controlled segregation dominated processes provide many interesting problems worthy of fundamental research.

Brief Biography

Dr Pinson has worked on industrial ironmaking problems for more than 20 years. It is an industrial sector dominated by large-scale, multiphase, particulate based unit processes which have mostly reached design maturity. However, this relative process equipment maturity isn’t matched by an adequate understanding of the multiphase thermochemical processes within them. Over the recent time-period, technologies like discrete particle simulation have grown into a practical problem solving and design tool in both plant operations, asset management and process understanding. In these areas he has worked on many problems of coupled particle-fluid problems, wide size ranges, cohesive materials and large time and physical scale problems. In addition he has also worked in process support for sintermaking, blast furnace ironmaking, and by-product management and recycling. Experiences with sinter waste gas treatment by activated carbon adsorption demonstrate the ongoing need for research into highly coupled modelling approaches for heat, mass and fluid flow in reacting granular systems.

Predictive Optimization of SAG Mill Wear using DEM

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Abstract

Semi-Autogenous Grinding (SAG) mills are the technology of choice for reducing primary hard-rock ore to feed size for use in a secondary crusher. In these mills, cascading ore undergoes impact breakage against grinding balls in a rotating cylindrical shell. Continuous operation of these mills is disrupted when the mill liner, comprising lifter bars plates intended to protect the parent shell and provide necessary lift for the grinding action, wears out after months of processing abrasive material. In light of this, it can be a very costly exercise when maintenance intervals, and thus downtime losses, become too frequent. In the mining sector, these losses can be quite substantial. For example, a trained professional crew may require up to 120 hours to replace the worn liner of a SAG mill with each hour costing tens or even hundreds of thousands of dollars, depending on the size of the mill and the plant in which it operates.

Mining companies can realize significant cost savings simply by slowing peak wear rate without compromising throughput, an outcome that calls for optimizing both the liner design and operating process parameters. Likewise, changes to the mill lifter design and/or its operation can result in reduced power draw and therefore energy costs. As SAG and other types of mills are power hungry, even a marginal reduction in power draw can translate to massive energy savings. Conventional approaches to achieve these goals are based on a combination of practical experience and 'trial-and-error' studies that modulate design features and/or operating conditions.

However, it is not feasible to perform a comprehensive experimental design, especially when the mill is in constant operation. Discrete element method (DEM) simulations, which are based on first principle physics, have proven very helpful in such cases by enabling increased process insight and evaluation of a large number of possible solutions. Using a commercial DEM software like Rocky, an engineering team can easily evaluate changing process variables, such as speed and fill level, or a new lifter design that incorporates changed face angle and height with a high degree of accuracy. This article highlights how Rocky DEM software can help in predicting liner wear and fine-tuning optimum conditions for SAG mill operation.

Brief Biography

Dr. Peter Rizkalla

Peter Rizkalla studied Aerospace Engineering at RMIT and graduated with first-class honors in 2001. He then completed his PhD with Robert Bosch in Germany where developed a numerical model using Computational Fluid Dynamics (CFD) to predict erosion rates of high pressure abrasive slurries in diesel injector nozzles. Peter is currently working at LEAP Australia in WA as Product Manager for their flagship Discrete Element Modelling (DEM) package, Rocky, and is engaged in sales, account management, technical support, training and consulting related activities in both the DEM and CFD lines of business. Since joining LEAP, he has had over 10 years' experience in providing engineering solutions across a wide range of industries.

Dr. Alex Potapov

Alex obtained his Masters in Geomechanics and PhD in Physics and Mathematics at the Moscow Institute of Physics and Technology. He first joined Conveyor Dynamics Inc (CDI) in 1998 where he spent 3 years there as a project manager. In 2001 he joined Metso Minerals as a Senior Scientist where he developed several CFD and DEM codes. He has a wealth of knowledge and experience in breakage simulations including particle comminution and attrition and has developed several unique programs to simulate size reduction of particles in crushers and grinding mills. After spending almost 10 years at Metso he returned to CDI and started development of Rocky for commercial use. He is currently Chief Technical Officer at ESSS and is leading the core-solver development of Rocky.

Dr. Saurabh Sarkar

Dr. Saurabh Sarkar is an Applications Engineer for the Rocky DEM Business Unit. Prior to joining ESSS, Dr. Sarkar worked as an Adjunct Faculty at Rutgers University and an on-site Consultant at Sunovion Pharmaceuticals where he supported drug formulation and process development activities. He obtained his Ph.D. in Pharmaceutics from the University of Connecticut where his focus was understanding and optimization of different pharmaceutical unit operations using DEM and CFD tools in projects with multiple industrial and government collaborators. He is a Senior Member of the AIChE and serves as an expert reviewer for several journals.

Numerical Investigation on Erosion Characteristics of Double Elbows for Gas-Solid Flow

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Abstract

The continuous layout of elbow is common in pipe system of coal-fired power plants. The flow and erosion characteristics of pipe wall have significant influence on the dependability of pipe system. And the flow in flue ducts and pulverized-coal pipe is high-Reynolds number flow. Numerical simulation of solid particle erosion of double elbows was conducted by computational fluid dynamics method.

The erosion distribution and magnitude was presented. Results illustrate that maximum erosion position occurs on the convex of the first elbow. And erosion distribution presents a falloff to surrounding zone. The particles distribution in double elbows was also displayed. As the flow direction of gas changes, particles collide with pipe wall on various positions due to the inertia. Particles concentrated on the convex wall of elbows. And particles distribution is symmetric in the first elbow but asymmetric in the second elbow. Correspondingly, the erosion of the first elbow is symmetric but asymmetric of the second elbow. The influence of inlet velocity, particle size, particles concentration and connection length between elbows on maximum erosion rate was obtained. The maximum erosion rate of double elbows increases exponentially with flow velocity and increases linearly with particles concentration; the maximum erosion rate increases with increasing particles diameter in present range.

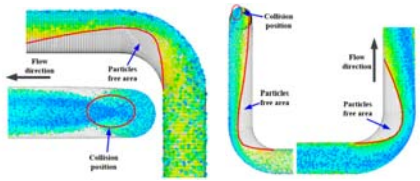

Fig.1 Particles distribution in double elbows

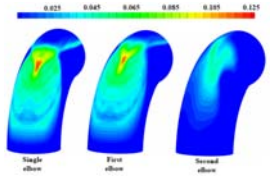

Fig. 2 comparison of erosion contour between single elbow and double elbows

Brief Biography

Junjie Yan

Prof. Yan is currently the dean for the School of Energy and Power Engineering at Xi'an Jiaotong University of China. He received his Ph.D. degree in Engineering from Xi'an Jiaotong University in 1994. He was a senior visiting scholar in the department of mechanical engineering at Yokohama National University from Sep. 2001 to Mar. 2002. Prof. Yan is a well-known researcher in the areas of thermal system energy saving, multiphase flow and heat transfer. He authors or co-authors of 4 books and more than 300 peer-reviewed journal papers, about half of which are in international journals. He holds more than 40 patents. He is a committee member of several international conferences including ISMF, ASTFE, et al. He has also delivered more than 10 invited/keynote lectures in international conferences. He won the 2nd Class National Award for the Study in Progress in Science and Technology (2010), the 1st Class Award for Advances in Science and Technology of Shaanxi province (2008, 2016).Prof. Junjie Yan is the Yangtze River Scholar Professor, the winner of China National Funds for Distinguished Young Scientists by NSF of China, the expert enjoying the special allowance of the State Council, et al. He is a member of Multiphase Flow Special Committee for Chinese Society of Engineering Thermophysics, a member of Thermal Power Generation Special Committee of Chinese Society of Electrical Engineering, et al.

Numerical Investigation on Heat Transfer Characteristics of Particle in Supercritical Water

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Abstract

The technology of coal gasification in supercritical water (SCW) for hydrogen-rich products is a novel way for the efficient and clean usage of fossil energy. From the previous study, the temperature is the major factor of gasification efficiency and the incomplete gasification of coal particle is mainly caused by the insufficient heat transfer. So the study of the heat transfer characteristics of particle in SCW has a fundamental significance, which is the key to enhance the gasification efficiency from the heat transfer prospect. For the drastic change and singularity of water properties at the large specific heat capacity zone, the accuracy of the numerical study has a great dependency on the calculation of water properties. Considering the common methods, polynomial or piecewise liner fitting, can't reflect the change characteristics, the IAPWS-IF97 equations was inserted into the numerical model to updated the water properties during the computed process. In this work, influences of the pressure, temperature and velocity of inlet flow and the particle surface temperature and heat flux were taken into account. The simulated results were compared to the calculated ones by the empirical correlations. A new model applicable for the heat transfer including the large specific heat capacity zone was obtained through regression fitting of the simulated results.

Heat transfer un-involving the large specific heat capacity zone

When the large specific heat capacity zone was not involved in the heat transfer process, as the water properties changed with temperature approaching linear, the simulated results of Nu are consistent to that calculated by the empirical correlations.

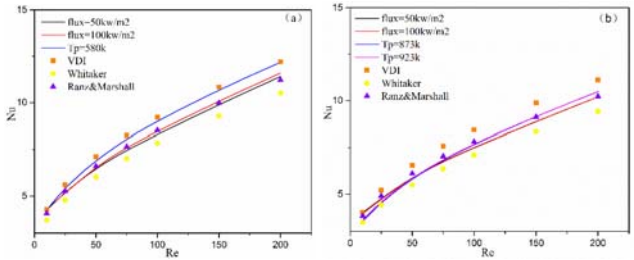

Fig 1. Simulated results of Nu comparing to calculated results (a) 23MPa, 630K; (b) 23MPa, 973K.

Heat transfer involving the large specific heat capacity zone

When the large specific heat capacity zone was involved in the heat transfer process, the heat transfer characteristics were much different. When the temperature interval was small and didn't cross the critical point, the simulated results were closed to the calculated ones. With the increment of temperature interval, especially crossing the critical point, the heat transfer got obvious enforcement.

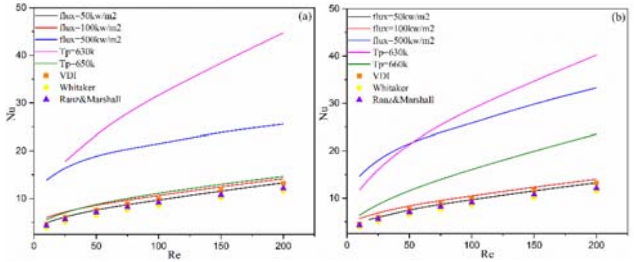

Fig 2. Simulated results of Nu comparing to calculated results (a) 23MPa, 680K; (b) 25MPa, 690K.

Heat transfer model

Through regression fitting of the simulated results, a new heat transfer model involving the large specific heat capacity zone was obtained as following:

$$Nu = 2 + 1.090 Re^{0.434} \overline{Pr}^{0.215} \left(\frac{\rho_w}{\rho_p}\right)^{-0.971}$$

Where $\overline{Pr}$ was calculated by the averaged specific heat capacity $\overline{Cp}$:

$$\overline{Cp} = (H_w - H_p)/(T_w - T_p)$$

The subscripts f w and p were referred to inlet water and particle surface respectively.

Brief Biography

Zhenqun Wu was born in Shandong, China, on May. 10, 1991. He received his bachelor's degree from the Xi'an Jiaotong University in 2010. After that, he is a PhD candidate in State Key Laboratory of Multiphase Flow in Power Engineering of Xi'an Jiaotong University and learn from Pro. Hui Jin so far.

His research area is the coal gasification in supercritical water for hydrogen-rich gas. The main research direction is the granular flow behaviours and heat and mass transfer in supercritical water fluidized bed in multi-scale. As the extreme operating condition in supercritical water fluidized bed, the researches were mainly conducted by numerical simulation. In the particle (micro-) and particle cluster (meso-) scale, the open source computational fluid dynamic software of OpenFOAM is used and the research is included the drag force and heat transfer of particle in supercritical water. The particle reaction, especially on the particle surface, are the research interest in the future. In the reactor (marco-) scale, the computational particle fluid dynamic software of Barracuda is used. The research has been done included the fluidization characteristics in supercritical water fluidized bed considering the real particle size distribution. And a swirling flow distributor for supercritical water fluidized bed is also studied. The next research interest is the multiphase flow and reaction of coal particle and supercritical water, with the help of the study in micro- and mesoscale.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

Numerical Investigation on the Impacts of the Evaporation Process on Cough Droplets Dispersions in an Enclosed Environment

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Abstract

Cough droplets being expelled through coughing contains water and small amount of non-volatile compounds. The droplets could reduce to much smaller nuclei due to the droplets evaporation process. This study used a multi-component Eulerian-Lagrangian approach to model the evaporation and dispersion of cough droplets in an enclosed space, while real droplets size distribution of coughing from 3 μm to 750 μm was investigated. The size of the droplets significantly reduced nearly 75 % of the initial sizes due to the evaporation process, which led to a dramatic percentage increase of respirable droplets that would easily penetrate deeper into the respiratory system. The numerical results also indicated strong impacts of the evaporation process on the instantaneous droplets transport characteristics. Droplets tended to be suspended long in the air after evaporation, while the rate of evaporation process was found very sensitive to the relative humidity of the local environment.

Brief Biography

Dr Yihuan Yan is a research officer in School of Engineering, RMIT University. His research focuses on the air quality, the HVAC systems, contaminants transport and infection risks assessments in indoor spaces.

Particle methods in comminution: models for understanding process performance, scale-up and optimisation

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Abstract

Particle methods, specifically the Discrete Element Method (DEM) and Smoothed Particle Hydrodynamics (SPH) are critical tools in the simulation of grinding processes. DEM allows the prediction of media and coarse feed and product particles for which collisional interactions are dominant. SPH allows interstitial slurry including fine feed and product fractions to be coupled to the coarse particle motion predicted by DEM allowing transport, mixing and classification to be predicted. Breakage of particles by combinations of five mechanisms allow the life cycle of particles within mills to be understood and predicted. A broad range of examples of mill models with be used to demonstrate the predictive power of these models. Use in understanding scale-up of mill designs from small to large scale will be explored. Finally, the role of such models in the design and optimisation of mills will be discussed.

Brief Biography

Paul Cleary is a Chief Research Scientist at CSIRO Data61. His research interests are focused on particle based modelling for industrial, geophysical and biophysical applications and the development of the Workspace framework to support the commercialisation of software tools developed in a research environment.

Keynote presentation

Development of a DEM-CFD Multiphysics Model for Predicting Powder Behavior in a Dry Powder Inhaler

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Abstract

Monodose dry powder inhalers (DPI) are widely used for delivering solid drug product formulations to the lungs. The use of such a device is relatively straightforward, involving only placing a pre-filled capsule in a molded cavity, piercing both of its ends with built-in self-retracting needles, and then inhaling from the device mouthpiece. As with many other pharmaceutical processes, particulate phenomena involved herein are complex; factors important to the drug delivery process, such as the modes by which solids are discharged from the capsule and the dynamics of solid particles in the device and their interplay with the air flow, are not well understood. In addition, the effects of solid properties on device performance is relatively unknown. As a result, the efficiency of DPI's is often poor with little means to improve it.

This work highlights the development of a coupled computational fluid dynamics (CFD) and discrete element method (DEM) model of a spinning capsule filled with powder in a DPI. Commercial software ANSYS Fluent and Rocky DEM were used for, respectively, performing the CFD and DEM computations. The primary focus of the talk will be on the role that air flow plays in the process: on the one hand, the in-device swirling air flow provides the necessary momentum to spin the capsule, which in turn provides the centrifugal acceleration that forces powder to exit the capsule. On the other hand, the presence of high velocity air at the capsule ends impedes the rate of powder discharge from the capsule. In addition, air flow into the capsule, the magnitude of which increases as fewer and fewer particles remain in the capsule, combined with the dome shape of the capsule ends, causes a small amount of powder to be inevitably retained within the capsule. The predicted location and approximate quantity of in-capsule powder retention are found to be in reasonable agreement with experimental data. Further, the result of the coupled simulations may also be used to determine the most likely locations of in-device powder retention. In silico parametric studies also identified material attributes critical to powder retention and discharge rates, providing insights into how solids formulation may be optimized to minimize the former and maximize the latter. Lastly, different fluid/particle interactions resulting from different types of multi-physics coupling and how they in turn affect the predicted powder discharge behaviors from the capsule and the device, as well as the limitations of the current state of the art and future work will also be discussed.

Biography

Ariel R. Muliadi received his bachelor's, master's, and doctorate degrees from the School of Mechanical Engineering at Purdue University. Subsequent to receiving his doctorate degree, Ariel pursued post-doctoral training under the guidance of Prof. Jim Litster, also at Purdue University. Armed with nearly a decade of higher and post-graduate education, he then bravely entered the pharmaceutical industry. He spent his first five years in the industry at Vertex Pharmaceuticals in Boston. Driven by his desire to move as far away as possible from the harsh New England winters, Ariel joined Genentech in South San Francisco as a Scientist in the Small Molecule Pharmaceutical Sciences (SMPS) Group in 2017, where he has remained since. Ariel's work revolves around modeling and measurements of granular materials and liquid sprays in various pharmaceutical processes. More ambitiously, he strives to apply his modeling and experimental background to enable more mechanistic approaches to drug product developments.

Characterization of Size Resolved Atmospheric Particles in the Vicinity of Iron and Steelmaking Industries in China

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Abstract

China currently faces environmental challenges of lower air quality, partly as a result of industrial activities. The aim of this study was to investigate the role of iron and steelmaking facilities to regional air quality in four selected industry dominated urban centres in China. Nine different particle size ranges present in atmospheric particles collected from four sites (KM, WH, NJ and NB) were analysed and compared with particles collected at one background site (UN) with very little industrial influence in China. Similar mass concentration levels of $PM_{2.1}$ and $PM_{1.1}$ were found at the three sites near older iron and steelmaking plants (KM, WH and NJ). Significantly lower levels of $PM_{2.1}$ and $PM_{1.1}$ were collected at the fourth site (NB), which is near to a modern and coastal iron and steelmaking plant. The particles collected have the highest mass concentration in the aerodynamic diameter range of 3.3-9.0 μm for all sites, expect for the background site (UN). Scanning electron microscopy equipped with energy-dispersive X-ray spectroscopy was used to determine the surface morphology and particulate chemistry. Mg, Al, Si, Fe, Na, K and Ca were found as the most abundant elements in all samples. The possible anthropogenic effect on the elemental concentrations was assessed by elemental enrichment factors. This study will assist development of improved particle monitoring programs in the vicinity of industrial areas and also establish an elemental modality dataset which can be incorporated in the exposure and risk assessments of atmospheric particles.

Brief Biography

Prof. Vladimir Strezov earned his PhD in Chemical Engineering from the University of Newcastle, Australia in 2000. Since 2015, he has been a professor in the Department of Environmental Sciences at Macquarie University, Australia. He has research interests in renewable and sustainable energy, industrial ecology, control of environmental pollution and designing sustainability metrics of industrial operations. He has established research links with primary industries aiming to reduce their environmental impacts and improve energy efficiency. He is advisory panel member for the Australian Renewable Energy Agency (ARENA) and Fellow of the Institution of Engineers Australia. He is Associate Editor of the Journal of Cleaner Production and editorial member for the journals Sustainability, Environmental Progress & Sustainable Energy, and International Journal of Chemical Engineering and Applications.

Strengthening of Microalloying Spring Steels by Secondary Particles

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Abstract

Addition of single or combination of V, Nb, and Ti elements is a promising way to increase the strength of spring steels. In this study, the solubilities of carbides and nitrides with single addition of V, Nb and Ti in 55SiCr steel were first examined at 1000 °C. The effects of microalloying elements (V, Nb and Ti) on the strength and hardness of 55SiCr steels have been experimentally investigated in lab scale to optimise the conditions. Based on the results obtained in the lab scale, two new spring steel grades with 2050 MPa and 2100 MPa have been developed with the addition of V and Nb in plant scale. The microstructures of the spring wires were measured by TKD and the second phase particles were analysed by SEM and TEM. The strengthening mechanisms including solid solution strengthening, grain refinement and precipitation strengthening were calculated to understand the contributions to the yield strength of steel.

DEM-CFD Coupled Simulation of a Mill: Effects of Slurry Filling and Mill Speed on the Power Draw and Load Behavior

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Abstract

Autogenous and Semi-Autogenous Grinding (AG/SAG) mills are widely used in mineral processing industries. In these tumbling mills, cascading ore undergoes impact breakage against grinding balls in a rotating cylindrical shell. Very often water is fed along with the ore charge, forming a slurry phase when mixed with the fine particles, helping the material transport to the grinding zone and facilitating the discharge of the grinded ore particles out of the mill. The increased throughput of the mill and lower power requirement per ton of material ground when, compared to dry grinding, are the main advantages of the wet milling.

Depending on the operating conditions and water amount added, a pool of slurry forms at the base of the ball mill charge, sometimes referred to as pooling. The efficiency of a wet mill is dependent on the size of the slurry pool formed. A higher amount will dampen the impact force on the particles, whereas a low slurry amount may cause unnecessary wear of the mill lifters. Detailed information of the charge motion and slurry flow through the mill is imperative for improving the efficiency of wet milling circuits.

The scope of the present work is to provide a coupled DEM-CFD model that accurately predicts the complex multiphase dynamics of charge, air and slurry for modeling wet grinding in mills, providing invaluable insight into overall mill performance. In the coupling, the charge motion is modeled using the Discrete Element Method within Rocky. The slurry phase is treated as a continuum and both slurry and air phases are solved by a Computational Fluid Dynamics approach using ANSYS Fluent. The coupling between the solid and fluid phases is accomplished by inter-phase momentum transfer terms due to the interaction between phases.

The influence of the slurry filling on the load orientation is evaluated by comparing the pool, toe and shoulder angles for different slurry fills for a conceptual overflow mill. The power draw obtained numerically is computed for each case and compared with the values predicted by Morrell's correlation. In order to assess the influence on breakage, energy spectra analyses are performed by examining the normal and shear specific power.

Brief Biography

Dr. Lucilla Almeida

Lucilla holds a BE (Chemical) undergraduate degree, an M.Sc. in Chemical Engineering and a Ph.D. in Nuclear engineering from the Federal University of Rio de Janeiro. She joined ESSS in 2008 and has spent 5 years focused on applying CFD to solve common engineering problems in the Oil and Gas industry, dealing with turbulent and multiphase flow simulations. Since 2013, she is an Application Engineer for Rocky DEM, supporting users, working on consultancy projects and validating models implemented for the CFD-DEM coupling.

Dr. Rahul Bharadwaj

Dr. Rahul Bharadwaj is the Vice President of Rocky Business Development and Technical Services at ESSS. He has over a decade of experience in the development, validation, and application of computational tools such as Discrete Element Modeling (DEM), CFD and FEA. After completing his Ph.D. in Mechanical Engineering at Purdue University, he was a senior scientist at Pfizer R&D and senior engineer at Jenike and Johanson Inc, where he has several years of consulting experience in the field of bulk material handling. He is also an active member of the American Institute of Chemical Engineers (AIChE), the American Association of Pharmaceutical Scientists (AAPS), and is the founder and past-chair of AAPS's Process Modeling and Simulation Focus Group.

Dr. Peter Rizkalla

Peter Rizkalla studied Aerospace Engineering at RMIT and graduated with first-class honors in 2001. He then completed his PhD with Robert Bosch in Germany where developed a numerical model using Computational Fluid Dynamics (CFD) to predict erosion rates of high pressure abrasive slurries in diesel injector nozzles. Peter is currently working at LEAP Australia in WA as Product Manager for their flagship Discrete Element Modelling (DEM) package, Rocky, and is engaged in sales, account management, technical support, training and consulting related activities in both the DEM and CFD lines of business. Since joining LEAP, he has had over 10 years' experience in providing engineering solutions across a wide range of industries.

Modeling of Multiphase Flow and Particle Deposition Characteristics in Radiant Syngas Cooler of Entrained-flow Coal Gasification

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Abstract

Radiant Syngas Cooler (RSC) can recover heat from the entrained-flow coal gasifer raw syngas by membrane wall as the raw syngas flows through the RSC. The design of division walls can efficiently enhance the heat transfer of syngas and coolant. But division walls would change the space structure of the RSC, and affect multiphase flow field as well. In this study, effects of different division wall structures on slag particle motion and impact characteristics in the RSC of the RSC type entrained-flow coal gasification process are carried out by a numerical method. The gas phase flow field is calculated by Realizable k-ε model in Eulerian coordinates while the discrete random walk is applied to trace the particles, and the interaction between gas and particles is considered by two-way coupling model. The radiation heat transfer is simulated by the P-1 radiation model; and the radiative properties of syngas are calculated by the Weighted-Sum-of-Gray-Gas Model (WSGGM). Comparing simulated data with industrial measured data, the maximum relative error is 3.7% and the reliability and accuracy of the mathematic models are validated. Comparing with different configurations of division wall tubes, the results indicated that increasing radical length of the division wall decreases the central heat exchange region, which results in the enhancement of the recirculation in the top region of RSC. Reducing the radical length directly decreases the heat exchange area which leads to the increase of outlet temperature, but improves the distribution of annular surface temperature. When the radical length of the division wall tubes increases, the particle impact rate as well as the impact area will be increased correspondingly, which effectively weaken the slagging phenomenon in the industrial RSC. The surface temperature of division wall reaches the maximum value near the axis of RSC, especially at 12 to 15 m height where the average temperature is higher than 950 K, and the rate reaches the maximum value, 0.015 kg/(m^2s). The simulation results of different division wall configurations in the RSC can provide theoretical guidance for industrial RSC type entrained-flow coal gasification technology.

Brief Biography

Dr. Qinghua Guo, an associate Prof. from East China University of Science and Technology (ECUST), won Shanghai Pujiang Scholar in 2015. He worked on coal gasification technology since he graduated from ECUST in 2009, and participated in R&D, and optimization of the Opposed Multi-burner (OMB) Coal-water Slurry gasification technology developed by ECUST. He involved in onsite technique support for the OMB commercial projects with gasifier's capacity ranging from 1000 t/d to 4000 t/d.

Research interests are mainly focus on fundamental research and development of entrained-flow coal-water slurry gasification technologies with both quenching process and Radiant Syngas Cooler process. Published more than 30 academic papers and granted more than 10 Chinese patents.

Conversion Characteristics of a Single Coal Char Particle with High Porosity Moving in a Hot O2/CO2 Atmosphere

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Abstract

Based on pseudo-steady-state approach, the conversion characteristics of a single coal char particle moving in high temperature O_2/CO_2 atmosphere was simulated to analyze the particle conversion mechanism. The particle size and porosity were variable in the range of 0.1-1.0 mm and 0.5-0.9 respectively. The particle structure model is developed referring to experimental coal char particle pore structure. Two different char structures were used for particles with different porosity. The Navier-Stokes equations, energy and species conservation equations were combined to solve the problem. Stefan flow, Maxwell-Stefan equation and Soret effect were considered for mass transport. Water-gas-shift reaction, CO oxidation reaction and four heterogeneous reactions were taken into account. The results show that with the increase of particle size, the temperature difference between internal and external surface increases and the temperature gradient decreases. The specific carbon consumption rate decreases along with the enhancing of the particle size and porosity. The flame sheet attaches to the particle surface when the particle size is small. Additionally, the detaching of the flame sheet and the endothermic Boudouard reaction causes the surface temperature of the large particle decreases.

Brief Biography

Prof. Guangsuo Yu is an expert on clean coal technology with over 20 years' experience in entrained-flow gasification, high temperature processing of fossil and biomass resources for production of power, chemicals and fuels, etc.

Extracting 3D velocity fields within opaque granular media using dynamic X-ray radiography

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Abstract

X-ray micro- and nano-CT technologies have been developed to extract non-obtrusively detailed maps of internal density fields and three-dimensional geometrical structures inside opaque particulate materials. However, these established techniques offer only limited insight into the dynamic properties of granular media since they can only be applied to non-deforming, stationary samples. We present a new X-ray method that provides such insight, being able to reconstruct the full three-dimensional velocity field of flowing material using only three sets of sources and detectors. The technique is based upon each detector recording a series of high-speed radiographs, giving information about the evolving integrated density field as particles move. By applying the mathematical principles of correlation and convolution to the subsequent images, we are able to deduce the set of particle displacements that have taken place inside the sample but, if taken in isolation, insufficient details about precisely where these displacements have taken place. Combining the results from the different scanning directions using a novel optimisation algorithm allows the displacements to be arranged accordingly, giving a three-dimensional reconstruction of internal velocities. The technique has been validated for steady-state granular flows by repositioning a single X-ray tube and detector through different angles, but can also be applied to transient regimes if three simultaneous sources are available. In addition, similar algorithms can be used to reconstruct the evolving internal particle size or particle orientation distributions, making our approach a potentially powerful tool to inform models of many different aspects of soil mechanics.

Brief Biography

Itai Einav is working at the University of Sydney as a professor of geomechanics. He is the Director of Sydney Centre in Geomechanics and Mining Materials (SciGEM), and the founder of its state-of-the-art Particles and Grains Laboratory and the DynamiX facility. Itai is a world leader in granular physics and theoretical mechanics. Apart from holding a professorship from the University of Sydney since 2012, he also holds an Honorary Professorship from University College London. Einav's research is multi-disciplinary, with many publications in premier journals in Physics, Geophysics, Geotechnics, Solid Mechanics and Fluid Mechanics. His work in the area of granular materials has led to discoveries in breakage, heat transfer, mixing, segregation, shape realignment, melting and solidification. His work in theoretical solid mechanics has resolved the structure of effective stress in partially saturated soils, unified previously considered contradictory theories in plasticity, and disclosed new dynamic patterns in crunchy soft matter. His work in theoretical fluid mechanics has established links between hydraulic jumps in various complex fluids. Most recently, his group in Sydney has established DynamiX, the world's first facility for fast 3D X-ray velocimetry of bulk disordered materials flows.

Industrial scale simulations of tablets on GPUs: A validation study

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Abstract

Tablet coating is a widely used technology in pharmaceutical industry. During this process tablets are covered with a film that fulfills both functional and non-functional purposes. Coating uniformity is a critical property to assess the quality of the final product, thus to determine whether e.g. a batch can be accepted or not. Therefore, the coating process has to be optimized in order to achieve the desired uniformity and reduce manufacturing costs. Understanding how process parameters (such as spray properties, drum geometry, etc.) influence the coating process is a key step in process scale up and optimization.

A new approach how to detect contacts between bi-convex tablets in DEM (Discrete Element Method) will be presented, especially suited to parallel architectures like GPUs (Graphics Processing Units), avoiding examination of the contact in a case-by-case fashion. Such elements facilitate a more realistic representation of the real physics in discrete matter compared to widely used multi-sphere approaches. Simple and efficient geometrical representations allow for highly efficient simulations of such tablets.

Some verification and validation cases are presented, followed by a demonstration of the capability of massively parallel GPU architectures (Graphics Processing Unit) to simulate industrial scale coaters (processing more than 10 mill. tablets or granules) via single workstations.

Brief Biography

Hermann Kureck studied Information and Computer Engineering at Graz University of Technology (TU Graz). The main goal of his master's thesis was the development of advanced neighbor search algorithms as well as neighbor list structures for the Discrete Element Method (DEM) on GPU platforms. He is currently employed at the Research Center Pharmaceutical Engineering (RCPE GmbH) as a specialist in GPU based software development, with emphasis on the implementation of non-spherical particle shapes in DEM as well as large scale simulations.

A Mechatronics Model Approach To Vehicle Dynamics On Granular Off-road Surfaces

Matt D Sinnott and Paul W Cleary

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Abstract

Realistic virtual models of vehicle dynamics on dry, flat, rigid surfaces are commonly used in driving simulators and computer games. However, real off-road surfaces (soil/rocks/sand) consist of granular materials that can: compact under load, destabilize and flow around moving wheels, and experience large discontinuous deformations due to wheel-track sinkage. These have a major effect on wheel traction and so pose a challenge for simulating a vehicle driving over an unsteady terrain.

Here, we simulate a detailed mechatronics model representation of a Toyota Hilux 4WD coupled to a loose dry, granular terrain of non-spherical rocks modelled using the Discrete Element Method (DEM) (see Figure 1). DEM is a powerful numerical method that is at the leading edge for modelling granular materials at the particle scale. Key aspects of the vehicle's mechanical control are included in the model as drivetrain, braking, and suspension sub-models. The drivetrain and braking sub-models make use of scheduled real-world inputs such as throttle, gear, and brake pedal pressure to generate wheel torques. The vehicle model also has independent suspension defined for each wheel which consists of a number of mechanical components linked together by joints and springs. The parametric nature of the mechatronics model is easily extensible and additional/alternative modules can easily be added to represent a broader family of different vehicles.

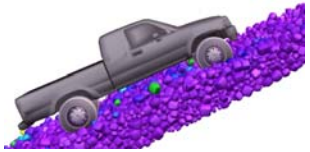

Figure 1: Simulation of vehicle driving up a 25 deg inclined slope of coarse rocks. Wheel torque (and simple tyre tread) are insufficient for vehicle to drive up the incline and significant wheel sinkage occurs for the front wheels.

Brief Biography

Matt Sinnott is a Senior Research Scientist with CSIRO Data61. He has 16 years commercial experience in advancing the science of world-leading particle-based computational models of industrial scale engineering devices and biomedical applications. Publication of over 50 peer-reviewed journal articles with over 700 citations in areas including process engineering, comminution, bulk materials handling, food/digestion, and cardiovascular flows.

Paul Cleary is an elected Fellow of the Australian Academy of Technological Sciences (ATSE) in 2015 for his significant impact on the development and worldwide adoption of particle-based methods for modelling fluid and particle flows. Seven CSIRO, national and international commercialisation and research awards, including the 2005 CAST CRC Commercialisation award for CASTfill and 2017 Victorian iAward for Dive Mechanic. Member of Scientific Committees for 18 international conferences. Invited/keynote speaker at international conferences or workshops on 32 occasions. Strong interest in software development processes and leads the Workspace development project. Holder of three patents and a member of three journal editorial boards.

Coke collapse behavior and its optimization in blast furnace top based on discrete element method

Mingyin Kou, Zhibin Hong, Zhehan Liao, Zongwang Zhang, Shengli Wu, Heng Zhou, Jian Xu

Abstract

In a blast furnace, coke layer collapses when the ore is dumped onto the coke surface. This results in the changes of burden distribution and the radial ore to coke ratio. The burden permeability and gas distribution are then affected and further the gas utilization. The coke collapse phenomenon is inevitable in blast furnace. Therefore, the coke collapse is significantly important to the burden and gas distribution, and further affects the gas utilization and CO_2 emission. It is imperative to investigate the coke collapse in blast furnace. The present work built a three dimensional model of bell-less top blast furnace based on discrete element method (DEM). This model is then used to investigate the effects of different burden matrixes on the coke collapse charateristics. The results show that coke profile changes much after collapse at different burden matrixes. The burdens impacted on the turning point between the platform and the funnel affects the coke collapse amount and the coke collapse region. The coke collapse can be optimized by increasing the rings a little in the first several angles in order to charge the burden on the platform and move over the turning point between the platform and the funnel.

Brief Biography

Dr Mingyin Kou is now a lecturer with the School of Metallurgical and Ecological Engineering of USTB. He received his B.Eng. degree and PhD degree from USTB, Beijing, China in 2009 and 2015. He also studied in the University of Queensland for one year as a joint PhD student with the support of China Scholarship Council. His current research includes the numerical simulations of ironmaking process based on CFD and DEM, efficient utilization of iron ore, physiochemical characteristics of slag, and so on. He received the National Scholarship for Postgraduate Student award in China. He has published more than 20 papers in Chemical Engineering Science, MMTB, ISIJ International and so on. He is also the reviewer of Journal of American Ceramic Society and Steel Research International.

Wall Treatment Type Turbulence Damping at Large Scale Interface of Two-Phase Flow in Conduit

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Abstract

Multiphase flows are found in variety of industrial applications. Such flows are markedly different from single-phase flows due to presence of interface, across which fluid-properties change as well as mass, momentum and energy interaction occur. From the analysis point of view, multiphase flows can be classified based on the increasing spatial scales of interface into dispersed (bubbly flow, droplet flow), mixed/intermittent (slug flow, churn flow) and separated/stratified (film flow, annular flow, horizontal stratified flow). The Large Scale Interface (LSI) model developed within the two-fluid model formulation provides a criteria based on local phase-distribution to distinguish between regimes characterized by small and large scale interfaces, see Gada et al., (2015). Appropriate closures for momentum, energy and mass are specified for each regime. Weighted sum of these closures is then used to close the interaction between the phases.

In the present work, the turbulence modelling in the vicinity of large interface is studied. In the literature, it has been shown that a boundary layer develops in the vicinity of large scale interface and flow is close to laminar. Thus, the turbulence needs to be damped at the large interface. Egorov et al. (2004) and Lo & Tomasello (2010) suggested the use of source term based low Re wall like treatment to model turbulence near the large interface. Such a source term based formulation operates in a region close to the interface and not just at the interface, thus the damping is spread-out close to the actual large interface. Such spreading of the turbulence damping introduces its own error. In the present work, the focus is to ensure that the turbulence is damped only at the interface. To achieve that, three step procedure is followed. Firstly, the large interface is detected to a single cell layer, thereafter interface distance is calculated in the vicinity of the detected interface cell layer and finally, wall treatment is applied in one cell on either side of the detected interface. This approach is validated employing three test cases of two-phase flow in conduits. Two among the three cases have co-current flow and the third case has counter-current flow.

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Brief Biography

Mohit Tandon completed his PhD in Chemical Engineering from the University of Utah in 2007. Following this, he started as a Development Engineer with CD-adapco which has now been acquired by Siemens PLM and currently is the manager responsible for development of multiphase models in STAR-CCM+.

Comprehensive Modelling of Blast Furnace Including Pulverised Coal Injection and Hot Metal Tapping

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Abstract

In the iron-making process, due to the severe environment and economic feasibility, it is extremely hard, if not impossible, to clarify the inner state of a blast furnace (BF) with experiments. As an alternative to the experimental studies, numeric simulation, mainly the CFD method, has been the most prevailing method during the past several decades to investigate the in-furnace conditions and flow regimes. Although numerous efforts have been put toward the simulation of the BFs, because of the complexity of the whole process, such as the multiphase (gas-liquid-solid-powder) interactions in the form of momentum, heat and mass transfer, which are attributed to the redox reactions and coal combustion, few works have been reported regarding the integrated modelling of the whole furnace structure. Instead, researchers usually isolate their model within the regions they concern the most (e.g. Raceway, Shaft and Hearth etc. referred to sub-models).

The current BF models, to a large extent, successfully reproduced the performance of the specific regions in a blast furnace, both quantitively and qualitatively. Nevertheless, most of those models did not consider the Raceway (RW) directly, which is a cavity caused by the interactions between the blast flow and solid particles. The problem is that the flow pattern and mass distribution in RW may have an unignorable effect on the inner state of a BF, which needs further validation. In addition, when the powder coal injection is practised, it is unable for those models to make a reasonable prediction because of the dispersion of coal powders. Besides, the hot metal velocity and temperature distribution in the Hearth model greatly rely on the inlet conditions, which is normally assumed but can be acquired with BF model. Therefore, it is necessary to integrate those sub-models into a comprehensive one.

However, for different regions, the calculation length scale varies. For instance, in the Raceway, the behavior of injected coal particles is the key to the performance of combustion efficiency, thus the length scale should be at the particle level. On the contrary, the BF model is supposed to be on the process scale, since the micro information of solid particles is of less interest. This intrinsic problem becomes the bottleneck of integrating those models into a single case. To address this issue, a new approach is proposed in the present report, which combines those submodels into an organic unity, with the PCI and iron tapping process being considered. Using this approach, it is possible to understand and optimize the in-furnace flow-thermo-chemical characteristics at the whole process level.

Brief Biography

Lingling Liu is currently a PhD candidature at Monash University. His research interests are multiphase flow and CFD simulation. He received his master degree from Sichuan University, China in 2016. During his time at Sichuan University, he worked towards the mitigation of particulate matter in industrial exhaust through the wet scrubbers.

Bubble Motion Characteristics under External Disturbance during Water Splitting

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Abstract

Gas desorption in photoelectrolysis water splitting is a typical interfacial phenomenon. Hydrogen and oxygen gas bubbles form on the photocathode and photoanode respectively, and the evolution of oxygen bubble is a key issue for water splitting, not only representing the way in which the gas is collected, but also influencing the effective surface area and conversion efficiency. A significant part of the losses during water splitting are associated with the formation and attachment of gas bubbles on the electrode, which could decrease the effective contact area between the photoelectrode and the electrolyte, block the electron transfer, increase the ohmic loss, and therefore increase the electric resistance of the whole photoelectrocatalysis water splitting system. Studying the motion characteristics of gas bubbles evolved from photoelectrodes provides an effective method to understand the solid-liquid-gas interface interaction and reaction product transportation during photoelectrochemical process. To date, the interaction between a gas bubble and a surface has received limited attention, especially the bubble motion under external disturbance during photocatalytic process has rarely been discussed in the literature. Herein we investigate the bubble motion characteristics and the effects on the mass and heat transfer and the catalytic reaction near the photoelectrode surface.

In this paper, a study of oxygen bubble motion behaviors especially the bubble bouncing behavior under external disturbance was conducted. The experimental system, which is shown in Fig. 1(a), consisted of four components, the illumination system, the external disturbance system, the reaction system and the camera system. For the external disturbance system, the electronic shutter controlled by a precision timer as an optical chopper, which switch time was adjustable, was applied to cut the laser beam that irradiated the electrode surface.

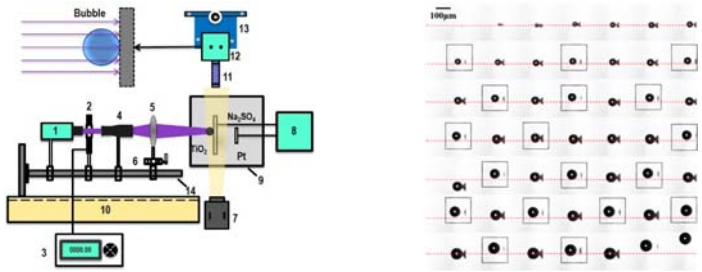

Figure 1. (a)Schematic diagram of experimental system: 1-Laser, 2-Shutter, 3-Timer, 4-Beam expander, 5-Lens, 6-Displacement table, 7- LED light, 8-Electrochemical workstation, 9-Photoelectrochemical cell,

10-Optical guide, 11-Microscope, 12-High-speed Camera, 13-Adjustable platform; (b) Snapshots of a bubble bouncing on vertical surface

Bubble bouncing behaviors appeared when the shutter close time was short enough. One example of the bubble bouncing behavior was shown in the Fig. 1(b). The bubble detached from the surface when the shutter closed and then rebounded immediately when the shutter opened. The bubble may jump-off and return many times by changing the shutter switching time before the final detachment. The laser irradiation variation with time caused by chopping induced the local temperature and concentration gradient Marangoni convection changing with time. Then a force balance model to analysis the bubble bouncing behaviors including Marangoni force was built, and Fig. 2 shows the force analysis of bubble bouncing process.

Fig. 3 shows the bubble departure diameter ratio under chopping in different conditions. Bubbles detached earlier with chopping than of the bubble growth without chopping, so the chopping bubble departure diameter was smaller. With the increase of the laser power, the bubble departure diameter ratio decreased, the influence of the chopping increased. But with the increase of the bias, the bubble departure diameter ratio increased, the influence of the chopping decreased.

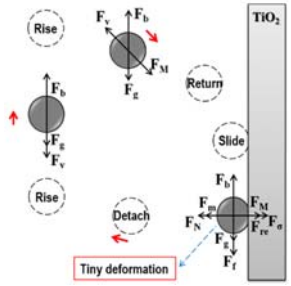

Figure 2. Force analysis of bubble bouncing process

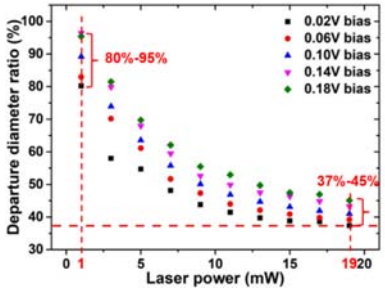

Figure 3. Bubble departure diameter ratio under chopping in different conditions

In this paper, a method to control the bubble motion characteristics on the electrode surface under external disturbance has been proposed. We designed and built an external disturbance experimental system and showed some typical examples of bubble behaviors, including collision, coalescence and sliding. The oxygen bubble may detach and rebound several times by controlling the chopping mode. We explored the dynamics of oxygen bubbles during the bouncing process, such as the bubble growth, the bubble center trajectory, the rise velocity and corresponding photocurrent. A force balance model to analysis the bubble bouncing behaviors including Marangoni force was built. Finally, the bubble motion characteristics and their influences on the mass and heat transfer and the catalytic reaction were explored.

Brief Biography

Zhenshan Cao was born in Tianjin, China in 1990. He received his B.S. degree in 2014 from School of Science, and he is now a Ph.D. student in State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University (supervised by Professor Liejin Guo). He is mainly engaged in the research of photocatalysis water splitting and multiphase flow, especially in bubble dynamics.

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Numerical Study of Coal Gasification in Integrated Supercritical Water Reactor Using Eulerian-Eulerian Multiphase Model

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Abstract

Coal gasification in supercritical water (SCW) coupling subsequent products oxidation as heat source in integrated supercritical water reactor (ISWR) is a sophisticated reacting multiphase flow process. Flow and heat transfer characteristics of coal gasification in ISWR is essential for reactor design and process optimization. In this paper, a numerical study of coal gasification in a novel ISWR was conducted using Eulerian-Eulerian model with the kinetic theory of granular flow (KTGF) introduced to take non-ideal particle-particle collisions and gas–particle drag into account. An eleven-step reaction kinetic model including volatile pyrohydrolysis, fixed carbon reforming and water-gas shift was used to describe the coal gasification and products oxidation process in ISWR. The result of this numerical model was in agreement with experiment study.

Detailed physical and chemical field distribution (temperature, velocity and reaction rate distribution, gas composition profiles, fluid-particles flow behaviors) in ISWR were analyzed and typically shown as Fig.1. Results show that swirling flow formed below feed inlet due to the buoyancy force becomes violent with the increases of heat released from the oxidation reaction around the coal slurry nozzle, which promotes the species transport increases the particle residence time effectively.

Moreover, factors affecting the state of coal gasification in ISWG including coal slurry and oxygen supply method, flow rate of feedstock, thermal boundary condition of wall, structure of the injector were discussed. The results show that oxidation of gas products as inner heat source can promote the gasification reaction with only slight or even little maximum temperature increase of the pressure-bearing wall. Coal feeding rate and oxygen supply method impact a lot on the physical and chemical field distribution. Multi-injection coal slurry supply method suppresses the low temperature in the jet region and promotes a more uniform distribution of coal particles. And multi-injection oxygen supply method provides a more uniform temperature field for operation safety but lower heat transfer temperature difference. The carbon gasification efficiency (CGE) in the gasification zone can easily reach up to 99% under mild conditions (less than 650℃) directional controlled by appropriate coal slurry and oxygen supply method. This numerical model This study gives a deep insight into the flow and heat transfer

behaviors of particle inside the ISWR reactor, and the results may be useful for system optimization and reactor scale-up as well as further in-depth study of detailed mechanisms.

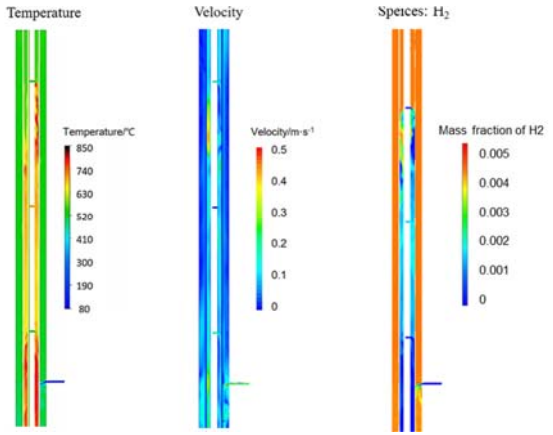

Fig. 1. Typical distribution of temperature, velocity and species in ISWR

Brief Biography

Zhisong Ou is a Ph.D. candidate under supervision of Prof. Liejin Guo in State Key Laboratory of Multiphase Flow in Power Engineering (SKLMF), Xi'an Jiaotong University, in China. He has been committed to the research and development of supercritical water gasification (SCWG) technology since he received his bachelor degree in energy and power engineering from Wuhan University of Technology (WHUT) in 2015.

His main research interests lie in the reactor design and optimization for coal gasification in supercritical water. So far, he has conducted a wide study about supercritical water gasification of coal involving numerical and experimental studies on flow and heat transfer characteristics, heat management, structural optimization of reactor. In his research filed, he has attended 2 international conference and has 1 paper published and 1 under review till now.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

A CFD-DEM Study of the Effects of Grain Properties on Drying and Shrinkage of Food Grain in a Fluidised Bed

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Abstract

Drying is one of the key preservation techniques for food materials. One of the most important physical changes that the food grain suffers in a drying process is the volumetric change or shrinkage. Drying and related shrinkage are usually controlled by the various operational conditions and grain properties like grain size, density and initial moisture content in the fluidized bed. The effects of these grain properties on drying and shrinkage are investigated in this study by the developed computational fluid dynamics-discrete element method (CFD-DEM) drying model with shrinkage. First, the contribution of different heat transfer modes on fluidised bed drying are investigated and found that the convective heat transfer is dominant but the conductive heat transfer become important at low air velocity. Then, the effects of grain size, density and initial moisture content on drying rate are quantified here for the first time. It is revealed that the drying rate decreases exponentially with increasing of particle size but a slight slower drying rate is observed with decreasing the initial moisture content and grain density. The shrinkage rate, resembling of drying rate decreases with increasing grain size or decreasing initial moisture content and grain density. This grain scale drying model with shrinkage should be useful for the design and control of many drying processes of food grains. Finally, the effects of these grain properties on the drying quality quantified by the uniformity of moisture and reduced grain size distribution are evaluated here by the grain scale information. The results reveal that increasing grain size, decreasing initial moisture content or grain density increase the uniformity of moisture and reduced grain size distribution. The findings should be useful for better understanding of a drying process and predicting the drying process in the fluidised bed.

Brief Biography

Jannatul Azmir is a PhD student at the ARC Research Hub for Computational Particle Technology, Department of Chemical Engineering, Monash University, working with Professor Aibing Yu. Her research area includes the development of a combined computational fluid dynamics (CFD)-discrete element method (DEM) model for a fluid-particle food grain drying process. The model is incorporated with a water evaporation model in resemblance to a chemical reaction, thus requiring less model parameters. By such a model, detailed and verified predictions of temperature and moisture content in both fluid and particle phases are generated. Following the initial development of the drying model, Jannatul has extended the model by incorporating a linear shrinkage model to consider more complicated and realistic drying consequence i.e., particle shrinkage during drying. The model has the capability to study transient drying and particle shrinkage behaviours in a fluidised bed and to investigate the effects of some important parameters such as operating conditions, grain properties and bed geometries on drying and shrinkage rate, and dried product quality related to particle moisture and diameter distribution. Jannatul is optimistic that the model will be able to provide detailed information for design and optimisation of drying processes and to make significant contribution to the sustainability in the energy intensive food drying sector.

CFD-PBM Modelling Of Mixer Settler

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Abstract

Mixer settler is widely applied in rare earth element separation industry. How to reduce the loss of the reagents and the occupied areas and achieve efficient separation in the settler is a challenging task. In this work, we report numerical simulations of liquid-liquid flow in a stirring-settler and their experimental validation. A 3D CFD-PBM coupled module in Fluent17.0 was developed further to investigate the liquid–liquid flow characteristics and settling performance in the stirring-settler. The predicted dispersion band thickness by the Turbulent aggregation model was in good agreement with the experimental measurements. The effects of total liquid flow rate and initial droplet average diameter on the settling characteristics were investigated. It was found that the dispersion band thickness increased significantly with the decreased of droplet diameter. The dispersion band thickness decreased with the total liquid flow rate decreased. The research showed that the CFD-PBM coupled model was promising in designing large-scale stirring-settlers and optimize their settling performance.

Key words: Mixer-settler; Solvent extraction; Droplet coalescence; Population balance model; Computational fluid dynamics

Brief Biography

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9,2016~present：Northeastern University, doctoral candidate, major in nonferrous metallurgy

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Work Experience:

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Publications:

[1] GUO Xu-huan, ZHANG Zi-mu, ZHAO Qiu-yue, ZHANG Ting-an. Numerical Simulation of Liquid Phase Flow in a Self-Stirring Reactor. Journal of Northeastern University Nature Science, 2018, 39(3): 357-361, 366. DOI: 10.12068/j.issn.1005-3026.2018.03.011.

Combustion Optimization of M701F4 Gas Turbine based on CFD Numerical Simulation and Artificial Intelligence

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Abstract

Gas turbines are widely applied in the modern industries,for example,the Power generation,Aviation,Shipbuilding,Automotive,Chemical industry and so on.Under the background of the shortage of natural gas resources and gradually increasing environmental requirements,how to improve the efficiency and stability of gas turbine combustor and reduce pollution emissions has become an increasingly concerned and urgent problem.In this study,a method for optimizing the combustion in M701F4 gas turbine is developed to achieve the higher operation efficiency and stability, as well as the lower emissions.In this method,the data generated from Computational Fluid Dynamics (CFD) simulation and the history data collected from power plant are combined to build a more convincing training database. To improve the accuracy and efficiency of the predictions,the PauTa Criterion is adopted to remove the outliers and the Kernel Principal Component Analysis (KPCA) is used to reduce the impact of data dimensions on data extraction.With the inputs including the actual load,gas composition,bypass valve opening and fuel ratio distribution,and the outputs of the thermal efficiency,NOx emissions, and maximum amplitude of pressure pulsation,three Least Squares Support Vector Machine models (LS-SVM) are respectively established to predict the operating efficiency,stability and emission characteristics of the gas turbine combustor. Based on the predictions of LS-SVM models,the Genetic Algorithm (GA) is used to optimize the operating conditions including the optimal fuel proportional distribution scheme and the opening setting of the bypass valve.The three prediction models established show good consistency with the plant data, with the average error of 0.015%,0.153 ppm and 0.067KPa,respectively.The results indicate that the use of CFD data can help generalize the LS-SVM models.This method provides an effective tool for multi-objective optimization of gas turbine combustion performance, achieving the goal of improving thermal efficiency,reducing NOx emission and decreasing pressure pulsation amplitude.

Key words: Multi-objective optimization; CFD simulation; LS-SVM-GA；Gas turbine combustor

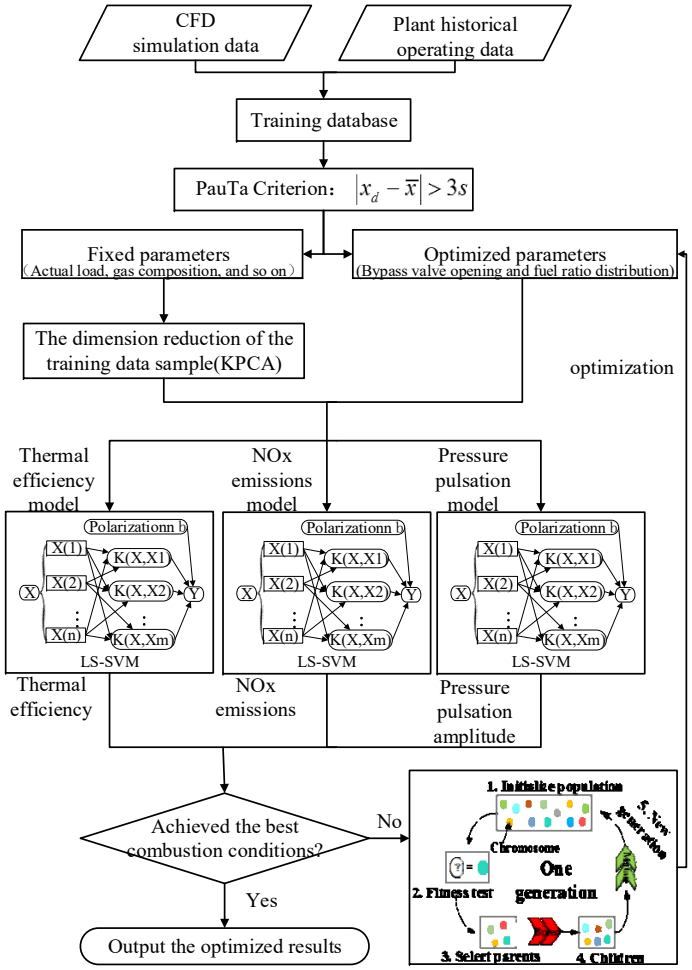

Fig.Flow chart of the combustion optimization scheme of gas turbine

Brief Biography.

Gu Qi, female, is a second-year postgraduate in Thermal Engineering, Southeast University. Dr. Wenqi Zhong, a professor at Southeast University, is specialized in multiphase flows, computational fluid dynamics, clean coal combustion technologies and biomass thermal transformation.

Molecular Dynamics Simulation of Coal Oxy-Fuel Combustion

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Abstract

There have been a lot of experimental researches on the macroscopic phenomena of Oxy-fuel combustion, but few of them show the thorough understanding of microscopic reaction characteristics. In this study, the microscopic molecule motions and reaction behaviors were simulated to study the coal combustion in O_2/CO_2 atmosphere by the Molecular Dynamics method, with the molecular structure of coal being represented by the Wiser coal model and molecule interactions modeled by the ReaxFF force field. The generation path of carbon dioxide was explored and the effects of temperature (3000K, 4000K and 5000K) and oxygen concentration (21%, 25%, 30% and 35%) on the main products and reaction rates were investigated. As the results, the main mechanism of CO_2 generation can be summarized as the dehydrogenation and oxygenation. The higher temperature promotes the conversion of CO_2 to CO with the main path being $CO_2 \rightarrow CO + O$, resulting in the increase of O radical and thus the reduction of O_2 consumption. The number of CO_2 and CO decreases with the increasing of O_2 concentration.

Keywords: Molecular dynamics simulation; Oxy-fuel combustion; ReaxFF reactive force field; oxygen concentration

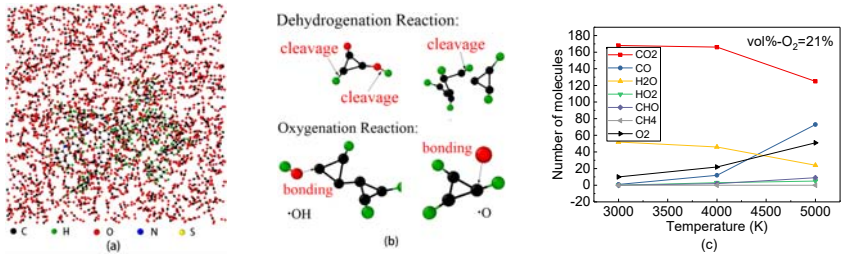

Figure Molecular dynamics simulation of coal oxy-fuel combustion: (a) reaction system, (b) dehydrogenation and oxygenation reaction in the generation process of CO_2, (c) distribution of main molecules at different temperature.

Brief Biography

Qiu Yu, female, is a third-year PhD candidate in Thermal Engineering, Southeast University. Dr. Wenqi Zhong, a professor at Southeast University, is specialized in multiphase flows, computational fluid dynamics, clean coal combustion technologies and biomass thermal transformation.

Gas Effect on Particle Flow Trajectories in Bell-less Top Blast Furnace Burden Distribution

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Abstract

Burden distribution plays a key role in the determination of an ironmaking blast furnace performance. Modern blast furnaces have converged on a rotating chute to distribute materials circumferentially around the furnace throat offering the potential to vary the ratio of ferrous and coke materials across the furnace radius and significantly influencing the cohesive zone shape and furnace gas flow distribution. In the real blast furnace operation, the ascending gas flow has a strong influence on the burden falling trajectory, which is important for size segregation, burden profile, layer formation and pile peak location. Granular materials in burden trajectory are prone to segregate spatially with different sizes, densities, shapes or particle resilience. Different particle sizes for sinter and coke were selected in order to investigate the individual behavior of each material under gas flow. The predictions of gas flow pattern, size segregation, burden trajectory and impact point are achieved and analyzed by CFD-DEM method. In this work, we start with mon-sized particles to study the effect of gas flow on different particle sizes, and extend the results to multi-sized system both in sinter and coke particles. It can be proved that the particle trajectory is significantly influenced by the in-furnace gas flow and the effect on different particle kinds varies. The range of particle size, which will be seriously influenced by the gas flow, is identified in the simulation process. The trajectory information resulted from the CFD-DEM simulation could be used as input parameters for other parts of blast furnace operation.

Brief Biography

Mr. Yinxuan Qiu is a PhD candidate in the Chemical Engineering Department, Monash University. Currently, his project is the development of a fundamental particle scale approach to modeling blast furnace charging phenomena. His research focuses on the granular system in the upper part of the blast furnace, seeks to reveal the principles of the burden distribution. His research interest mainly involves using CFD and DEM modeling method to describe the particle behavior and coupled fluid flow in the blast furnace.

Heat Exchange Inside A Moving Porous Media

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Abstract

Rising energy prices and environmental restrictions lead to improvements of waste gas recovery processes. In the steel production, hot waste gases leave many furnaces and reactors. The thermal energy can be used in recuperation systems or for the steam production. More efficient is the preheating of the scrap that has to be remolten. There are different concepts of scrap preheating devices, like vertical towers, chambers or horizontal tunnels.

To predict the efficiency of the preheating process and prevent overheat and partial melting of the scrap numerical simulations are a helpful tool for the dimensioning. The scrap is typically modelled as porous media with the hot off-gas flowing through it. To calculate the heat exchange between hot off gas and cold scrap several parameters like material properties, porosity and permeability have to be known. The permeability respectively the pressure drop through the scrap is the most difficult parameter, due to several varying circumstances. Normally, only a rough approximation of the bulk density is known while the exact shape of the scrap pieces can vary in wide range. Nevertheless, laboratory tests and approximations lead to reasonable results for batch preheating processes.

In case of a continuous preheating system, the scrap moves through the reactor while it is heated up by the off-gas counter flow. In all known CFD solvers the porous media consists of a solid zone and fluid zone at the same location. The fluid zone represents the off-gas whereas the solid zone embodies the scrap. For stationary simulations a movement of the solid zone is not possible and therefore the convective flow of scrap enthalpy would be neglected.

To implement the convection of the scrap a second fluid zone with a defined velocity is set up at the same location. Source terms calculated in user defined functions manage the correct temperature distributions of the zones. Additionally, this kind of configuration offers the possibility to implement radiation along with the porous media, which is not possible with the given setting options of for example ANSYS Fluent.

Brief Biography

Moritz Eickhoff, M.Sc. is the group manager for high temperature flows of the Department for Industrial Furnaces and Heat Engineering at RWTH Aachen University in Germany. He focusses on numerical and physical modelling of metallurgical reactors and industrial furnaces.

Moritz studied materials engineering at RWTH Aachen University since 2008, focusing on industrial furnaces as well as aluminum and steel design. Actually, he is working on his Ph.D. thesis concerning the vacuum arc remelting process.

CFD study of pulverised coal combustion in an ironmaking blast furnace: Effect of tuyere angle

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Abstract

Pulverized coal injection (PCI) is widely used in ironmaking blast furnaces (BFs), where blast and pulverized coal is introduced into BFs through tuyeres. In this study, numerical simulations are conducted to study the effect of tuyere angle on coal combustion under real BFs conditions using a recent three-dimensional (3D) full-scale computational fluid dynamics (CFD) model. In this model, the blowpipe-tuyere-raceway region and the surrounding coke bed are treated as a cavity and a porous media, respectively. The models are validated against the experimental measurements. Using this model, the simulations of PCI operations with inclined tuyere and non-inclined tuyere are compared. The results showed that when the tuyere is configured at an inclined angle, the raceway depth is enlarged while the raceway height is maintained. As a result, the coal plume has a larger inclined angle. The devolatilization then starts further away from the lance tip and last for a longer distance. The gas species distributions change with the tuyere angle. For example, the position of peak CO_2 concentration became lower and further away from the lance tip. It is indicated that the proper downward inclination of tuyere is useful for raceway extension and coal combustion. This study provides an effective way for understanding and improving PCI practice in BFs.

Brief Biography

Yiran Liu is currently a PhD student in the School of Chemical Engineering, The University of New South Wales. She received both BEng and MEng in Metallurgical Engineering from University of Science and Technology Beijing. Her major research interests are carbothermic reduction process and biomass injection in ironmaking blast furnace.

The effect of the temperature on the process of heterogeneous condensation by cloud-air-purifying (cap) technology

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Abstract

Recently we proposed the Cloud-Air-Purifying (CAP) technology which combines electro-acoustic ultrasonic nebulization with a cyclone dust collector to purify the industrial gases. The technology has shown a significant improvement in collecting fine particles than previous gas cyclones. To further explore and understand how it works on different temperature, in this work, the effects of the temperatures of water vapor and mixed gases are studied in a lab-scale CAP system. The effects of the temperatures on the performance of the cyclone is investigated in terms of the overall and grade removal efficiencies. Furthermore, the SEM is employed to examine themorphology change of the dust particles, which demonstrates the particle growth due to heterogeneous condensation and agglomeration. Results indicate that the collection efficiency is significantly improved when the vapor is added to the system, and a higher improvement is observed when the temperature of water vapor is relatively higher. As a smaller surface tension for water vapor with higher temperature, causing the critical free energy and critical supersaturation of heterogeneous condensation are both lower, thus particles are easier to be activated as condensation nucleus. Consequently, the increase of the removal efficiency by the centrifugal force can be achieved owing to the enlarged size of the particles. On the other hand, the overall and grade removal efficiencies of particles are decreased with the temperatures of mixed gas increased, this is attributable to the supersaturation degree and the condensable water vapor are both in decline, which is disadvantageous to the growth of the particles in the CAP environment.

Brief Biography

Yumeng zhang is a Ph.D. candidate under the supervision of Prof. Bo wang in the Key Laboratory of Western China's Environmental Systems of Lanzhou University. He received his Bachelor's degree in Environmental Engineering from Dalian Polytechnic University in 2015. His current research focuses on the efficiency removal of fine particles，especially the CFD and experimental study on cyclone. The research group proposed the Cloud-Air-Purifying (CAP) technology for industrial dust particles removal, which has widely used in China's catalyst industry.

Model Study of Central Coke Charging Patterns on Ironmaking Blast Furnace Performance

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Abstract

Ironmaking blast furnace (BF) remains the dominant reactor for production of hot metal worldwide presently. Central coke charging (CCC) operation is a promising technology for BF stable operations and it needs reliable process design. In this work, a multi-fluid BF model with the consideration of respective chemical reactions in respective coke- and ore- layers is further developed to investigate the flow-thermal-chemical phenomena of a BF under the central coke charging conditions. The simulation results show that the gas flow pattern and cohesive zone's shape and location are significantly affected by central coke charging operations. When increasing the width of central coke platform, the average gas velocity is increased, and the pressure drop is decreased; the heat load becomes even heavier near the furnace center while the reduction load shows the opposite trend; the carbon solution reaction is further suppressed near the furnace center while the gas utilization becomes lower at the furnace top. Then, the fuel rate is increased, and the hot metal productivity is decreased. The model is useful for coke central charging design and optimization in BF practice.

Brief Biography

Xiaobing Yu is a PhD candidate of chemical engineering at the University of New South Wales. He received a Master degree in ferrous metallurgy from Northeastern University in China. He is interested in modelling of innovative operations of blast furnace.

CFD-DEM study of effect of operating conditions on spout deflection in a flat-bottomed spout fluidized bed

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Abstract

Spout deflection is a typical instability phenomenon in spout fluidized beds. It could damage spout quality and thus should be well characterized and then controlled. However, quantitative characterization of spout deflection is limited in the past. In this study, the effects of several key operating conditions on spout deflection are investigated at particle scale by CFD-DEM method. The key variables include static bed height, background velocity and bed width. The model is validated by experimental data from literature. Typical alternating spout deflection is captured by adjusting spouting velocity. The so-called spout angle is defined and used to characterize the behaviour of alternating spout deflection. The simulation results show that the static bed height has an insignificant effect on deflection intensity of the spout within the investigated range of alternating deflection. Secondly, as the background velocity increases, within the investigated range of alternating deflection, the magnitude of spout angle increases slightly and then drops slightly at 2.0 m/s, and the frequency reduces slightly. Thirdly, effect of bed width is investigated under two conditions. Under the condition of keeping the static bed height unchanged, as bed width is changed in the range of 0.12 m-0.13 m, non-alternating spout deflection will appear instead of alternating spout deflection; as the bed width increases from 0.14 m to 0.18 m, alternating spout deflection will appear when the magnitude of spout angle not change much. The similar results can be observed when changing the bed width under the condition of keeping particle loading unchanged. Moreover, it is found the magnitude of the spout angle is always lowerest when the bed width is 0.16 m regardless of the static bed height or solid loading. This finding indicates that bed with is a critical parameter to control delfection intensity of alternating deflected spout. This work is useful for controlling spout deflection and optimising spout fluidized bed operation in industrial applications.

Brief Biography

Yuanhe Yue is a PhD student in School of Chemical Engineering at University of New South Wales, Australia. He received his Bachelor and Master degrees from China University of Mining and Technology. His research interest is instability phenomena of spouted bed by CFD-DEM method.

Numerical Modelling of Low-Rank Coal Briquettes pyrolysis in a Gas Heat Carrier Pyrolyzer

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Abstract

Gas heat carrier pyrolyzer is a dominant reactor for low-rank coal upgrading and has been widely employed worldwide. It is a complex high temperature fixed bed reactor involving counter-, cross-current flows of gas and solid, coupled with heat and mass transfer and chemical reactions. In this study, a two-dimensional CFD model is developed to simulate the flow and thermochemical behaviours related to coal pyrolysis under industrial-scale gas heat carrier pyrolyser conditions. The effects of low-rank coal briquette shape (ellipsoidal) and gas heat carrier conditions on furnace performance are examined, in terms of pyrolysis efficiency and gas products distribution. The simulation results indicate that the ellipsoidal briquettes helps improve the interphase heat transfer between heating gas and coal bed and thereby improve the pyrolysis efficiency. Also, the gas carrier's temperature and composition play a significant role in determining the gas products yield as well as pyrolysis efficiency. The recycled pyrolysis gas as the supplemental heat source for coal bed should be preheated for enhancing the subsequent gas combustion in the pyrolysis chamber and the efficiency of production. The model provides a cost-effective tool for understanding and optimising the operation of pyrolyser for low rank coal upgrading.

Brief Biography

Yuting Zhuo is a PhD candidate in School of Chemical Engineering of University of New South Wales. He received his Bachelor degree from the University of Science and Technology Liaoning. His research interest is process modelling of low-rank coal upgrading and conversion process.

Numerical Study on Air Purifying by Gas Cyclone with Supersaturated Vapour

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Abstract

A recent proposed technology, the cloud-air-purifying (CAP) method shows that by introducing the supersaturated vapour into a gas cyclone, the cyclone can effectively collect fine dust particles and be used to purify industrial waste gases. This paper presents a numerical study to understand the effect of the supersaturated vapour on the performance of such a cyclone. The multiphase (air-vapour-particle) flow in the cyclone is simulated based on computational fluid dynamics (CFD) coupled with other numerical models using FLUENT software. Air flow is modelled by Navier-Stokes equations with the Reynolds stress model (RSM) for turbulence. Vapour phase is simulated by the species transport model, and the condensation of vapour on the wall is simulated by the Eulerian wall film model. Particle flow is modelled by Lagrangian particle tracking model (LPT), and the vapour condensation on the surfaces of particles is modelled via user-defined-function (UDF), which can consider the material properties of dust particles. The model has been used to investigate the performance of the cyclone under different operational conditions. The effect of the amount of the supersaturated vapour on the pressure drop and collection efficiency is analysed. Generally the collection efficiency is improved by the addition of the supersaturated vapour without increasing the pressure; as such environment leads to the condensational growth of particles. In addition, the air, vapour and particle flow patterns have been analysed based on the microscopical information obtained from the numerical simulations. Finally, a previous predictive model is adapted to consider the new cyclone. These studies can help improve the fundamental understanding of the multiphase flow and particle collection in the CAP cyclone, and also provide guidance to optimize the CAP technology, such as for the water consumption.

Brief Biography

Mr Ruizhi Jin earned his bachelor degree in Environmental Engineering from Lanzhou University in China and now is a candidate of Master of Philosophy at the Centre for Infrastructure Engineering, Western Sydney University (Australia), under the principal supervision of Dr Kejun Dong. His research interests are numerical study on particle-fluid dynamics and its application in air purifying technology.

Numerical Simulation of Inner Vortex Eccentricity in Gas Cyclone

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Abstract

The characteristics of three-dimensional complex and strong swirling flow in cyclone separators have been the focus of many researchers. For a single tangential inlet cyclone (such as the Lapple cyclone used in this study), the asymmetry of the geometry will lead to the asymmetry of the flow field, resulting in the eccentricity of the inner vortex (also called the processing vortex core phenomenon), which means the center of rotation of the inner vortex does not coincide with the geometric center of the cyclone. This kind of flow pattern will have a negative impact on both the separation efficiency and pressure drop of the cyclone, so it is necessary to conduct in-depth research on it. Compared with the present experimental methods, the computational fluid dynamics (CFD) method can capture this phenomenon more conveniently and clearly. In this study, the flow field and particle motion are simulated, respectively, by means of a Reynolds stress model (RSM) and a Lagrangian particle tracking (LPT) model. Firstly, the impacts of inlet velocity and geometric height on the eccentricity of inner vortex are studied and the corresponding changes in the performance of cyclone are analyzed. Then, based on the consideration of improving symmetry, the vortex eccentricity of the cyclone with single tangential inlet, double tangential inlet and quadruple tangential inlet are studied. Finally, to optimize the performance of cyclone, the feasibility of the method of deviating the vortex finder is verified. The results improve the fundamental understanding of the phenomenon of inner vortex eccentricity in gas cyclone.

Brief Biography

Mr. Sijie Dong is a second-year postgraduate student of Lanzhou University, PR China. He was awarded the bachelor' degree in environmental engineering from Lanzhou University in 2017 and in the same year he continued to pursue the master's degree in environmental engineering at Lanzhou University as a recommended postgraduate. He is mainly engaged in numerical modelling and simulation of cyclone separators and in charge of a scientific research training project entitled "Mechanism of particle growth in Cloud-Air-Purifying technology". His graduate thesis entitled "Numerical simulation of fine particles growth in a supersaturated humidity environment in cyclone" was named as outstanding undergraduate graduation thesis. He also won the first-class academic scholarship for graduate students in 2017. Now, Mr. Sijie Dong, as a research student, is visiting "Centre for Infrastructure Engineering" in Western Sydney University in Australia.

Numerical Study on Flow and Heat Transfer of Slag Particles in the Slag-discharge Process of Supercritical Water Gasification

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Abstract

Supercritical water gasification (SCWG) of organic matters for hydrogen production as a novel hydrogen production technology is getting increasingly attention. Generally, raw organic matters are accompanied by some inorganic components, which will form slag particles after the SCWG is completed. The efficient and energy saving discharge of slag particles from the reactor under supercritical conditions will be one of the major problems that must be solved before the large-scale application of SCWG technology. However, there is little research on the slag-discharge process of SCWG. A comprehensive three dimensional Eulerian two-fluid model accompanying with heat transfer is developed in this study to simulate the slag-discharge process of supercritical water (SCW) fluidized bed reactor in a range of 400~600 ºC under 26 MPa. Factors that affect the performance of slag-discharge, such as slag-discharge pressure, position of slag-discharge outlet, cooler temperature and reactor temperature, are systematically studied. Results show that the slag particles can be carried out of the reactor smoothly under the pressure difference. Large pressure difference can enhance slag-discharge efficiency, but it will have a great impact on the flow field of the reactor inside. When the slag-discharge outlet is closer to the bottom of the reactor, a large amount of SCW will enter the reactor, which will decrease the slag-discharge efficiency. Reasonable fluid temperature in the cooler helps to improve slag-discharge efficiency and reduce wear and corrosion in the cooler. The current 3-D slag-discharge model can reasonably describe the flow and heat transfer of slag particles in the slag-discharge process, which may provide a theoretical basis for the design of lock hopper and the choice of slag-discharge parameters.

Mathematical model

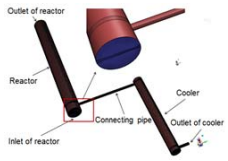

Fig. 1 Mesh structure of geometric model.

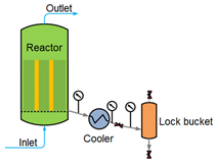

Fig. 2 Schematic diagram of slag-discharge system for SCW fluidized bed reactor

In this study, the geometric model consists of a SCW fluidized bed reactor and a slag cooler. Fig. 1 shows the mesh structure of geometric model. The specific dimensions of geometric model are based on the physical system built by our laboratory. Fig. 2 shows the schematic diagram of slag-discharge system. In the geometric model, the preheated water (SCW) enters the reactor from the reactor inlet located at the bottom of reactor, causing the slag particles to form a bubbling fluidization state in the SCW fluidized bed reactor. During the slag-discharge process, the valve at the outlet of the cooler is opened. Under the action of pressure difference, the slag particles enter the slag hopper after being cooled by the slag cooler. This study mainly researches the dynamics and heat transfer of multiphase flow during the slag-discharge process after the valve is opened.

Brief Biography

Zening Cheng

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Supervisor: Prof. Liejin Guo, Academician of Chinese Academy of science

Mr. Zening started his postgraduate studies from September 2013. For more than four years, he has been working on the research of SCWG of organic matters (including coal and biomass). His research focuses on SCWG characteristics of organic matters, SCWG process kinetics, design and optimization for the SCWG reactor, large-scale application of the technology of SCWG, and numerical study of dynamics and heat transfer for the slag-discharge process of SCWG.

Currently, Mr. Zening has shown a good development potential in his own research field. And, he has published 5 papers and has applied for 3 patents. At the same time, as one of main members, he participated in a number of research projects, including two projects supported by the National Science and Technology Major Project of the Ministry of Science and Technology of China, one project supported by the National Basic Research Program of the Department of Science and Technology of Shaanxi Provincial, and two projects supported by some companies.

Education

Vesiting Ph.D. student

Western University, Canada Sep. 2017 ~ Present

Ph.D. Candidate

Xi'an Jiaotong University, China Sep. 2013 ~ Sep. 2017

Bachelor

Taiyuan University of Technology, China Sep. 2009 ~ Sep. 2013

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

Numerical Studies on Pollutant Dispersion around a High-rise Building

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Abstract

Pollutant dispersion in urban environment is of great concern to city civilians, especially for those living in high-rise buildings during the outbreak of airborne diseases. Numerical model based on Computational Fluid Dynamics (CFD) to simulate the pollutant dispersion around high-rise buildings is helpful to the understanding and hazard control of such processes. However, as the processes involve wind-particle flow, the complicated wind-structure interaction and pollutant particle properties need to be considered in an integrated model. In this paper, we attempt to develop such a model in multi steps. Firstly, a wind flow CFD model is developed and calibrated based on the available experimental data from wind tunnel tests. From this model, different parameters from wind-structure point of view, such as wind direction, location of pollutant sources around the building and height of the building are investigated. Secondly, the dispersion of pollutant particles is considered in the model, which enables us to study the particulate pollutant properties like particle size, density, and morphology, etc. Choosing appropriate multiphase model to consider the pollutant particles is essential to accurately predict their dispersions even the CFD model for the wind flow is reliable. We compare several approaches to model particles. Generally they all belong to two groups: Lagrangian approach and Eulerian approach. Our simulations show that although the Lagrangian approach can explicitly consider particle properties, it is not easy to directly predict of pollutant concentration. On the contrary, the "scalar transport model" as a simplified Eulerian model commonly used in the literatures is not able to consider particle properties. The Eulerian-Eulerian model as one of the comprehensive multiphase models is comparatively more suitable for the study of particle pollutants dispersion as the wind-particle interactions including the drag, lift, virtual mass, and turbulent dispersion forces, etc, can be considered.

Brief Biography

Erfan Keshavarzian is a PhD candidate in the Centre for Infrastructure Engineering in Western Sydney University working on the CFD simulations of pollutant dispersion in urban areas. He obtained his BA and MA in Mechanical Engineering at Shiraz University (2011) and Amirkabir University of Technology (Iran) (2014) respectively. Erfan is a member of the research group led by Dr. Kejun Dong focusing on the simulation and modelling of particulate systems.

Comparison Of Extrusion Simulations Within Various Numerical Methods And Experiments

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Abstract

This is a numerical study on mixing in extrusion processes. Simulation of extrusion processes are already done, using for example Finite Element Method or Finite Volume Method [1, 2]. The results look promising, however validation of these studies are hardly available. The goal of this project therefore is to create a good comparison of discretization methods (here FEM and FVM) and their numerical techniques for rotating machinery (here the Sliding Mesh Interface and the Immersed Boundary Method). This is done by experimental and theoretical validation of pressure drop in the various sections of a single screw extruder.

SMI is often used with rotating machinery that has a rotating fluid domain inside a stationary fluid domain. The meshes of both domains are sliding over each other on the interface between these domains. The sliding of the meshes can be the reason of inaccuracies in the results. SMI cannot be used with the simulation of an intermeshing twin screw extruder and various mixing elements.

IBM is a method that can be used with the simulation of intermeshing twin screw extruders. IBM has a rotating solid domain in a stationary fluid domain. The rotation of the solid domain causes elements to change in time between solid and fluid. The geometry of the solid will change with the structuration of the mesh in time. The finer the mesh at the fluid solid transition, the less change of geometry. This change of geometry can be the reason of inaccuracies in the results. Therefore IBM needs to be validated first on a single screw and after successfully validated it can be used in simulations for twin screw extruders and mixing elements. If IBM is not accurate than remeshing needs to be done, but this is a time consuming process.

Brief Biography

The Professorship for Polymer Engineering of Windesheim University of Applied Sciences Zwolle is focused on research on sustainable processing of polymers. Cristian Hummel has a Bachelor in Mechanical Engineering and is an instructor in CAE at the Windesheim University. Cristian Hummel is graduating at the Master in Polymer Engineering on this project. Tijmen Mateboer graduated in 2017 as Master in Polymer Engineering at Windesheim University. Tijmen Mateboer researched numerical prediction of tire rubber extrudate swell and co-authored a paper on this subject [3]. Tire rubber extrusion experiments and simulations with wall slip is part of the graduation project of Tijmen Mateboer. Jakob Buist is a researcher who's main specialism is numerical fluid dynamics.

Multi-scale Modeling of Reactive Dense Flows

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Abstract

In large-scale industrial processes involving coal/biomass gasification and combustion, reactive dense particulate flows coupled with mass, momentum, and heat transfer are frequently encountered. Both inter-phase and intra-particle interactions need to be considered, because these interactions govern the key features of dense particulate flows, such as solid mixing, cluster, and regime transitions. Therefore, these interactions prevail at different length scales and consequently a multi-scale approach is adopted to achieve a quantitative description of these complex flows. Specifically, the relevant details of particle-resolved direct numerical simulation (PR-DNS) and discrete element model (DEM) are used to develop closure laws to feed two-fluid model (TFM) which can be used to simulate dense flows on a much larger (industrial) scale. In recent years, such research has been rapidly developed worldwide. This talk will present an overview of the work in this direction at Zhejiang University. Specifically, a parallel immersed boundary method is developed and applied to explore a simplified experimental shallow fluidized bed and a laboratory bubbling fluidized bed coupled with a soft-sphere model. The developed PR-DNS approach shows a better agreement with experimental measurements compared with coarser approaches. Besides, an unresolved CFD-DEM approach with the capability of high performance parallel computation is developed and validated to explore the dense particulate flows in fluidized beds. Moreover, this approach is extended to combine heat and mass transfer, used to simulate biomass pyrolysis and gasification in fluidized bed reactors. Finally, the coarser approaches (coarse grained CFD-DEM, MPPIC, and TFM) are also developed for industrial applications.

Brief Biography

Dr. Kun Luo has been engaged in the study of multiphase flow since 2000. He got his Ph. D from Zhejiang University in 2005. From 2007 to 2009, he visited the Center for Turbulence Research, Stanford University. His work mainly involves in developing high-resolution numerical methods for high-fidelity simulations of intra-phase and inter-phase transport phenomena of mass, momentum and energy in non-reactive/ reactive multiphase flows, and investigating the underlying multi-scale physics and models for particle-turbulence interactions, particle-particle interactions, and particle-flame interactions as well as related applications in energy and environment engineering.

CFD-DEM Study of Mixing/Segregation of Particles in Fluidized Beds under Influence of Size, Density, and Shape

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Abstract

In most of the multiphase operations in the fluidized beds, the properties of the particles, i.e. size, density, and shape can differ from each other either from the beginning of the operations or they may change during the process because of attrition, coalescence or chemical reactions. The differences in particles properties can result in segregation or mixing phenomena in fluidized beds. Segregation is a popular phenomenon for granular materials and can be observed in various particulate systems due to the property differences. In this work, two types of segregation phenomenon were chosen to investigate. The first one is called layer inversion phenomenon and the second one is segregation under influence of particles shape.

In terms of layer inversion phenomenon, even though substantial studies have been conducted, limited efforts are made to explain the segregation mechanisms behind this peculiar phenomenon. In principle, the motion of particles is governed by forces acting on them, including particle-particle, particle-wall, and particle-fluid interaction forces. Thus, the layer inversion must be controlled by these interactions, and quantifying these interaction forces is crucial to reveal the segregation mechanism. Unfortunately, these interaction forces are difficult to measure experimentally. This difficulty, however, can be overcome by the combination of Computational Fluid Dynamics and Discrete Element Method (CFD-DEM). Therefore, the aim of the first part of the work was to use this approach to address what causes layer inversion and provide a thorough explanation of this phenomenon. The force analysis revealed that the particle-fluid interaction force is responsible for the occurrence of the layer inversion phenomenon. Furthermore, the comparison of different drag force correlations revealed that Di Felice (1994) drag model failed to predict the inversion phenomenon while Rong et al. (2014) drag model predicted the inversion velocity with the best accuracy. Finally, a mathematical model was proposed to predict the inversion velocity. The new mathematical

model predicted the inversion velocity with average error of 14% which is consistent with the best available model in the literature.

In the second part of the work, the particles shape effects on fluidized beds behaviour and also on the mixing/segregation phenomenon was studied. In the simulations, ellipsoidal particles were used as they can represent a wide range of particle shapes from oblate to prolate particles. It was observed that particles shape significantly affects the solid flow behaviour in liquid fluidizations of mono-sized particles. The spherical particles exhibited highest minimum fluidization velocity while the oblate and prolate particles had less minimum fluidization velocity. A uniform pressure gradient distribution was observed for spherical particles confirming their uniform expansion in the bed while changing the particles shape from spherical to oblate or prolate ones distorted the pressure gradient distribution. For the oblate and prolate particles, a maximum pressure gradient happened somewhere between the bottom and middle of the bed. Force analysis as well as particles orientation and terminal velocity analysis revealed that the changes of particle orientations is responsible for the entrainment phenomenon.

A modified drag force correlations was proposed for the mixtures of polydisperse systems of non-spherical particles. There has been no such a drag model so far. The modified drag force provides more consistent results with experiments than the drag model developed based on mono-sized particles. On the other hand, according to analysis of mixtures of spheres and ellipsoids it was found that particles shape clearly affects the mixing and segregation phenomenon in liquid fluidized beds. Increase in liquid superficial velocity results in decreasing the mixing index. Nonetheless, for the mixtures of spheres and oblate particles, the mixing index remains constant after specific liquid velocity. The reason behind the segregation due to particle shape effect was found to be the role of the particles shape on the amount of the drag force that a particle receives when particle shape varies. The oblate and prolate particle have larger projected area compared to spherical particles and this leads to receiving larger drag force than that of spherical and hence a driving force is created and segregation happens.

Brief Biography

Esmaeil finished his PhD in Chemical Engineering at Monash under Dr Zongyan Zhou and Prof Aibing Yu in Jan 2018. He employed combined CFD-DEM to elucidate mixing and segregation phenomena of spherical and non-spherical particles. Esmaeil is currently a joint postdoctoral research fellow between CSIRO and University of Western Australia. In his project, Esmaeil is numerically studying the turbulent flow mixing of high solids concentration slurries with viscoelastic polymer solution in flocculation processes in which long chain polymers are used to aggregate and settle the suspended particles. He is also working on the arbitrary shape aggregates settling velocities in gravity thickeners. He will be using both continuum (CFD) and discrete approach (DEM) to study the process. Esmaeil is skilled in computational and mathematical modeling of particle-fluid systems, programming languages such as C++ and Fortran, computational fluid dynamics (CFD), discrete element model (DEM), OpenFoam, and ANSYS-CFX.

EMMS Application in Rectangular Circulating Fluidized Beds

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Abstract

Konwlton (2013) mentioned: "scale-up of fluidized beds is difficult because it is widely known that the hydrodynamics of small fluidized beds can be significantly different than the hydrodynamics of larger beds". The typical scale-up steps are lab scale, pilot-plant scale, demonstration plant scale and commercial scale. Normally, it is easy to get the data for the first two scales from simulation and experiment, which can give good hints for the further scale-up.

Flows inside circulating fluidized beds (CFBs) are multiphase, involving at least one fluid phase and one solid phase. Computational fluid dynamics (CFD) simulation is an efficient tool for the CFBs design, optimization and scale-up. But the simulation accuracy is largely determined by the drag models employed, which are classified mainly in two types, one is the conventional drag model, like Wen-Yu, Ergun etc., which is true for the homogeneous flow, the other is the heterogeneous drag model, such as energy minimization multi-scale (EMMS) etc., which considers the existence of particle clusters and bubbles inside the flow, is suitable for the non-homogeneous flow. Flow inside CFBs is complex, includes heterogeneous flow in the bottom dense region, homogenous flow in the top dilute region and transition region, EMMS drag model developed by Wang and Li (2007) can resolve this phenomena effectively by introducing the heterogeneity index into the Wen-Yu drag model.

In this study, two full-loop CFBs will be simulated with the application of Wen-Yu and EMMS/matrix drag models, respectively. Both risers have the rectangular cross section, one of them is in the lab-scale, has the dimension of 6.7 cm X 20.1 cm X 200 cm; while the other is in the pilot scale, has the dimension of 42 cm X 92 cm X 580 cm. Computational particle fluid dynamics (CPFD) software Barracuda will be employed as the simulation platform. The simulation results are analyzed in terms of full loop pressure drop, particle volume fraction distribution and particle circulation flux etc., and compared with available experimental data. Through the comparison, it can give guidance to the CFB scale-up.

Brief Biography

Qiuya Tu obtained her Bachelor and Master degrees from Beijing Institute of Technology in China in 2004 and 2006, respectively. After the graduation, she continued her study in US, and obtained her PhD from University of Florida in the major of Mechanical Engineering, then she joined the company of Halliburton in US as a mechanical engineer, focusing on the CFD simulation of new tools development and old tools optimization. In 2015, Qiuya joined the lab of circulating fluidized bed in Institute of Engineering Thermophysics, Chinese Academy of Sciences, working on the CFD simulation of gas-solid multiphase flow in circulating fluidized beds and experimental measurements.

Coupling of CFD-DEM and Reaction Model for 3D Fluidized Beds

Jun Xie and Wenqi Zhong*

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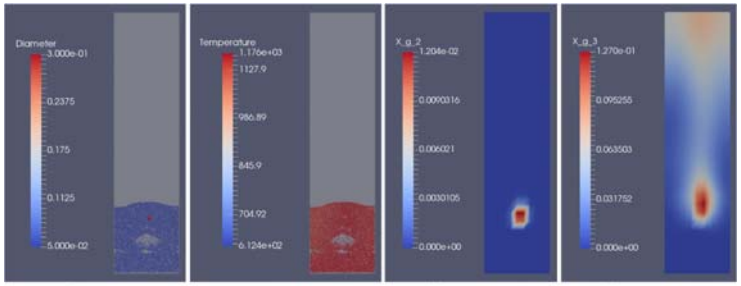
Abstract

In this paper, a three-dimensional (3D) numerical model coupling of CFD-DEM with chemical reaction has been developed to study the combustion process in a lab-scale bubbling fluidized bed. The gas phase is modeled with *k-ε* turbulent model and the solid phase is modeled with discrete element method (DEM). The dense gas-solid flow, heat and mass transfer, and comprehensive chemical reaction are simultaneously considered. The reactive submodel includes the fuel pyrolysis, combustion of char and volatiles (CO, H_2, CH_4, tar), formation and reduction of gaseous pollutants (NO, N_2O, and SO_2). The parallel computing can also be realized in present model.

The established model is first validated by the simulation of the combustion of single char particle in a quasi-3D fluidized bed. The temperature of char particles increases rapidly in the initial reaction stage, and then remains stable. With the increase of temperature, the particle size gradually decreases, while the variation amplitude increases. In general, the predicted values compared well with experimental results. Based on model validation, the simulations are performed to study the coal combustion in a 3D fluidized bed. The solid flow pattern, profiles of voidage, temperature, and concentrations of gas composition inside the reactor are obtained, as shown in Fig. 1. The effects of excess air ratios on the particle combustion and gaseous pollutants emissions are also analyzed. The results show that coal combustion rate of initial stage increases with the increasing air ratio, accelerating the rise of coal temperature. An increase in excess air ratio causes the increase of emissions of NO, N_2O, and SO_2.



(a) flow pattern (b) particle temperature (c) CO concentration (d) CO_2 concentration

Fig. 1 The contours of particle pattern, temperature, concentrations of gas compositions.

Brief Biography

Dr. Jun Xie obtained BEng in 2007 and PhD in 2015 from Southeast University. He is currently working in Southeast University as an associate research fellow.

CPFD study on pressurized high-density circulating fluidized bed

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Abstract

3-D full-loop numerical simulation of solids circulation is conducted in a high-density circulating fluidized bed, which consists of a riser, a gas-solid separator and a return feeder. The Large Eddy Simulation turbulence model is used for gas phase, and the multiphase particle-in-cell model is used for solid phase. The effects of operating conditions (i.e. operating pressure, fluidized air velocity, aeration rate in the return feeder and bed inventory, etc.) on the gas-solid hydrodynamics in a high-density CFB are numerically studied using the computational particle fluid dynamics approach. Finally, the scale up law of operating parameters on the high-density circulating fluidized bed were obtained.

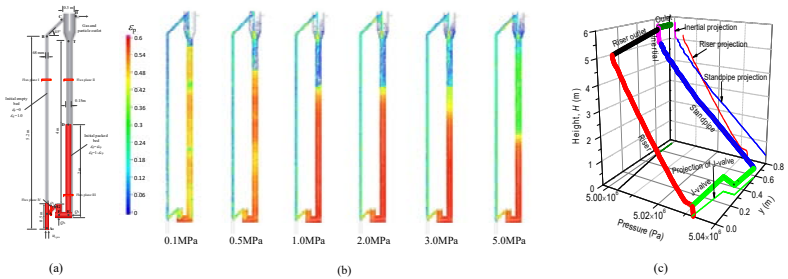

Fig. (a) Sketch of high-density circulating fluidized bed, (b) Particle volume fraction distribution in high-density circulating fluidized bed under various operating pressures, (c) Pressure profile in the high-density circulating fluidized bed at operating pressure of 5.0 MPa.

Brief Biography

Dr. Shangyi Yin, female, is a postdoctoral scholar at Southeast University and an instructor at School of Energy and Mechanical Engineering at Nanjing Normal University. Dr. Wenqi Zhong, a professor at Southeast University, is specialized in multiphase flows, computational fluid dynamics, clean coal combustion technologies and biomass thermal transformation.

A Numerical Study Of The Solid Dispersion Behavior And Residence Time Distribution In A Circulating Fluidized Bed Methanation Reactor

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Abstract

Methanation of the syngas from biomass gasification is one of the key processes in the biomass-to-SNG technology. Circulating fluidized bed reactor turns to be suitable for the operation of methanation reaction with high exothermicity. The methanation reaction involves a substantial reduction in the gas volumetric flow, which may bring about different fluidization behaviors. An exploration of the solid dispersion behaviors can help to interpret the relationship between the reaction, hydrodynamics and mass transfer in the circulating fluidized bed methanation reactor. In this research, a numerical study is applied to characterize the solid dispersion and residence time distributions in a circulating fluidized methanation reactor. The effect of solid flux, superficial velocity, pressure, reaction rate are considered in the study. This research can provide a theoretical basis for the optimization and scale up of methanation circulating fluidized bed reactor.

Brief Biography

Yuli Zhang received her Ph.D. degree in power engineering and engineering thermophysics in 2017, from the School of Energy & Environment, Southeast University, China. Since fall 2017, she has been worked in the College of Energy and Electrical Engineering, Hohai University, China. Her general research interests are in the area of fluidization. And her current research focuses on numerical simulation and measuring technologies for investigation of the gas-solid fluidization behavior in fluidized bed reactors.

Application of CFD for operating of industrial equipment: take ultra-supercritical coal fired power plant boiler for example

Wenqi Zhong[1*], Aibing Yu[2], Xi Chen[1], Jie Li[3], Longhai Liu[3], Guoyao Liu[4], Wanjun Tian[5]

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Abstract

CFD has been successfully developed to accelerate the design process in aviation, automobile, chemical, and energy industry. However, the application of CFD in equipments operating in aforementioned fields still lacks. How to make the time-consuming CFD satisfy with the real-time demand of equipment control, is not only a challenge in science and technology, but a meaningful question for industry field as well. Our group has worked on application of CFD for operating of industrial equipment for a long time and achieved some significant developments. In this study, we take an ultra-supercritical coal fired power plant boiler for example, to demonstrate the application of CFD for operating.

One application is rapid probing and online display of boiler combustion status in arbitrary position, which cannot be realized through conventional method. Accurate and detailed combustion status in boiler is the prerequisite for boiler sophisticated control. Based on large numbers of CFD simulations, a database containing temperature and chemical component (including NO_x and O_2) distribution field under various conditions, e.g. coal properties, load, air distribution scheme, and other operating parameters, was established in the on-site boiler control system. The database can provide query results containing key combustion data according to current operating parameters, which will be reconstructed and displayed as images by the system. These images then can offer guidance for staff to operate the boiler more efficiently.

The other application is the combustion optimization. At present, the combustion control of ultra-supercritical coal fired power plant boiler relies on the transfer function model, which cannot fulfill the combustion control task under complicated circumstances when coal properties and load frequently vary. To solve this problem, the aforementioned CFD database was extended with historical operating data first. Then, Artificial Neural Network (ANN) was used to proceed data mining in the database and boiler efficiency and pollution emission characteristics models were established. The two models took coal properties, load, air distribution scheme, and other operating parameters as inputs,

and outputted boiler efficiency and NOx emission, respectively. Then Genetic Algorithm (GA) was used to optimize the air distribution scheme to achieve a higher thermal efficiency and lower emission simultaneously based on the ANN models. The performance of the optimization method was validated by a third party inspection institution (Xi'an Thermal Power Research Institute Co., Ltd.). It is found that when the load was 600 MW, 500 MW, and 400 MW, the boiler thermal efficiency increased by 0.50%, 0.51%, and 0.52%, and NOx emission decreased by 10.51%, 16.68%, and 16.72%, respectively.

Both applications have been implemented by software and successfully embedded in the on-site boiler control system of Datang Nanjing Power Plant, which can realize the real-time display of the combustion status in the boiler and the online optimization of the air distribution scheme.

Brief Biography

Professor Wenqi Zhong focuses on multiphase flow and numerical simulation, industrial process optimization, and thermal conversion of coal and biomass. His group has been funded by over 65 projects, with a total funding of over 50 million RMB supported through the NSFC, Ministry of Science and Technology (China), Jiangsu province, and industrial partners. He has received over 4 national, provincial, or ministerial level awards in science and technology. To date (Nov 2018), the number of citations for his 92 collected SCI publications is over 1700, with an H-index at 23 according to the Web of Science. And also, he has 22 patents granted as the first inventor.

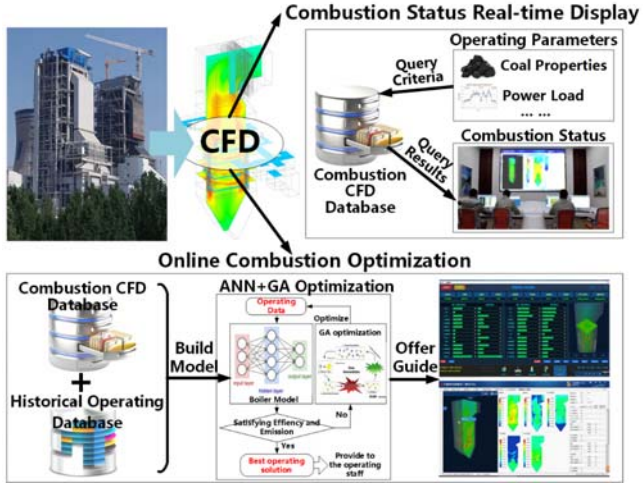

Figure 1. Use of CFD in combustion status real-time display and online optimization

CFD Study of Ironmaking Blast Furnace: Recent Model Development and Application

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Abstract

The design and control of blast furnace (BF) ironmaking must be optimized in order to be competitive and sustainable, particularly under the more and more demanding and tough economic and environmental conditions. To achieve this, it is necessary to understand the complex multiphase flow, heat and mass transfer, and global performance of a BF under different conditions. Mathematical modelling, often coupled with physical modelling, plays an important role in this area. This talk will present an overview of CFD studies of BF in our laboratory, focused on the recent model development and application. The model development is discussed in terms of model formulation, new features and model validation. Then, the usefulness of the CFD process BF model is demonstrated through some case studies related to BF optimization and new technology development.

Brief Biography

Dr. Shibo Kuang is currently a research fellow in ARC Research Hub for Computational Particle Technology at Monash University. His research has been focused on the development and application of numerical models at different time and length scales, with the support of physical experiments, for the fundamental and applied research on particle-fluid flow and granular dynamics. The specific topics include particle transportation, particle separation, and multiphase reacting flows in the process engineering. In this area, he has published over 70 papers including 50 journal papers (40 in the past five years) collected in Web of Science. The number of citations from these publications is > 980 (H-index=18) according to Google Scholar.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

System Design of a Dual Fluidized Bed Pyrolysis Reactor

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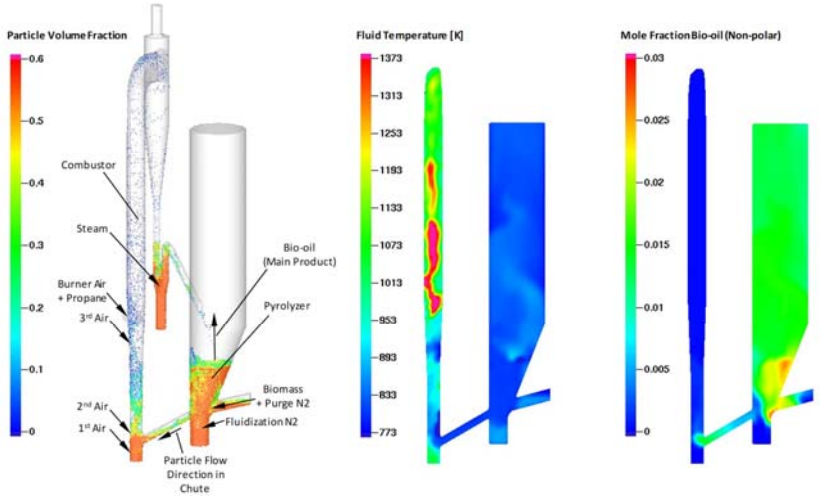
Abstract

A modeling study is performed on a dual-fluidized-bed reactor to evaluate its use for catalytic fast pyrolysis. The geometry of the reactor is that of an existing pilot-scale dual-fluidized-bed gasifier. Compared to gasification, the temperature for pyrolysis is lower, e.g. 870K instead of 1070K. To maximize the liquid yield, high heating rates and short residence times are desired. Low heating rates would increase the amount of char, and long residence times would increase the gaseous products. Instead of steam, nitrogen is used for pyrolysis. Using a catalytically active bed material can reduce the oxygen content of the pyrolysis oil. In this study, a pyrolysis system design is investigated that is similar to an original gasification plant, but with operating parameters to maximize liquids production. Here, the pyrolysis occurs in the bubbling bed and the oxidation of the char occurs in the riser. Barracuda 17.3.1 is used for the modeling of the two-phase flow employing chemical reactions and heat loss to the reactor walls. Figure 1a shows the system configuration and the results of the computed particle volume fraction employing a bed material similar to a FCC catalyst. Figure 1b shows the fluid temperature inside the reactor vessels, and Figure 1c shows the mole fraction of the non-polar portion of the pyrolysis oil vapors.

The dual-fluidized bed reactor allows for the variation of many parameters, foremost the flow rates of all input gases. The balance of the gases through various inlets determines the distribution of bed material, including circulation rate. The circulation rate is also influenced by bed height in the bubbling bed, pressure difference between the vessels, and type of bed material. The circulation rate is inversely linked to the temperature difference between the vessels, since the pyrolysis in the bubbling bed is endothermic, and the combustion in the riser is exothermic. The circulation rate is computed by recording the particle mass flow across the chute from pyrolyzer to combustor. It is generally increased with increased fluidization in the pyrolyzer (fluidization N_2), and bottom of the combustor (1st and 2nd air), within certain limits. Fluidization is also improved by higher temperature (higher gas viscosities) or gas production from reaction. A second bed material with a larger particle size was also studied in the simulation. Flow rates were adjusted to yield similar circulation rates. Since the larger-sized bed material requires higher flow rates for fluidization, residence times are shorter. The selection of the bed material is therefore an important factor. Table 1 shows some of the key differences between the two cases for a biomass feed rate of 228kg/hr. The larger bed material requires larger flows of nitrogen and air to maintain fluidization and achieve a similar circulation rate (50x biomass feed) and temperatures (830K in pyrolyzer, 1050K in combustor). The residence time in the pyrolyzer is therefore reduced and the pyrolysis gas more diluted.



(a) (b) (c)

Figure 1: Results of simulation of pyrolysis system with FCC-type bed material: a) Particle volume fraction and description of inlet flows. b) Fluid temperature. c) Mole fraction of the non-polar fraction of the bio-oil.

Bed material		FCC catalyst	Carbo EconoProp 30/50
Bed material diameter	[micron]	200	473
Nitrogen flow	[kg/hr]	39	186
Air Flow	[kg/hr]	527	727
Mass Fraction Bio-oil (non-polar)		0.154	0.083
Residence time in pyrolyzer	[s]	3.340	1.670

Table 1: Comparison of flow rates and residence times for two bed materials.

Brief Biography

Dr. Reinhard Seiser, associate project scientist, is the lead resident UC San Diego scientist at the Woodland Biomass Research Center in Woodland, CA. He has a Ph.D. in Chemical Engineering from the Technical University Graz, Austria. He conducts research on the thermochemical conversion of biomass for applications in power, renewable fuel production, and chemical synthesis, most recently focused on the methanation of producer gas.

Dr. Robert Cattolica, Professor of Engineering Physics at UC San Diego, is the Director of Research at the Woodland Biomass Research Center. He has BS, MS, and Ph.D. degrees from the University of California Berkeley. He conducts research on biomass gasification to include: the development of reforming catalysts, CFD modeling of multiphase gasification systems, the chemical synthesis of mixed alcohols, and most recently the development of new methanation catalysts.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

On Pragmatism in Industrial Modelling

Part VI: Management, Retrieval and Analysis of CFD Cases

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Abstract

This work in progress addresses case repositories for management, retrieval and analysis of pragmatic industrial models (Zoric et.al., 2014, 2015). Two use cases (UC) have been used for this practical design and implementation study: UC1 – CFD modelling in cardiac simulations, focusing on the case repository (CR) design and implementation, and UC2 – theoretical CFD calculations, used to evaluate case metadata processing and modelling orchestration functionality. We present the CR design and implementation results, practical experience and roadmap for future functional improvements.
Keywords: Industrial modelling, pragmatism, case repository, CFD.

INTRODUCTION

A framework (FW) for pragmatic industrial modelling was suggested and demonstrated on industrial use cases (UCs) with a process centric approach (Zoric et al., 2014). The framework was further elaborated (Zoric et al., 2015) with focus on metadata for modelling and experimental processes. Their organization, syntax, and semantics were exemplified on a UC related to drilling of oil & gas wells (Johansen et al., 2017), where principles of pragmatic industrial modelling described in (Zoric et al., 2014) have been applied.

This work focuses on a Case Repository (CR), an important part of pragmatic industrial modelling frameworks. In addition to case management and retrieval functionality, CR gives a foundation for data analyses and machine learning processes (based on the stored experimental, technical design data, CFD modelling and simulation results). By mock-up based practical implementation tests, we evaluate CR design issues, implementation alternatives and functional solutions. We provide some results of the functional tests, evaluate design variants and suggest future improvements.

DESIGN REQUIREMENTS AND FUNCTIONAL CONSIDERATIONS FOR THE CR

Our preliminary focus has been on the following basic functional requirements:

Information management and retrieval functionality

Administration and retrieval of hybrid CFD cases, a combination of: (i) experimental results, (ii) results from field trials / extracts from industrial designs, (iii) CFD modelling and simulation cases and (iv) relevant "State-of-the-art research results".

Informative representation of the case history, i.e.: (a) previous workflows, actions, research items, (b) status of the case / workflow / analyses, and (c) other CR concepts (some illustrated in Figure 1). It should be noted that some CR entities can be accessed many times (e.g. case, workflow, activity) to carry out new analyses, improve the results and add the new information.

All activities should be quality assured by proper logging and security mechanisms.

The CR should provide a foundation for various methods of information retrieval, data analyses and Augmented Intelligence.

We are aiming at a pragmatic, case-based, recommendation/ decision support system, as illustrated by one of the possible usage areas in health services (Figure 2).

MOCKUP-BASED TESTS AND EVALUATIONS

We have carried out a series of tests and evaluations to demonstrate the above-mentioned functionality. Different CFD UCs have been used for this purpose, because not all of them needed/supported all the required functionality:

UC_1 - evaluated the basic CR retrieval and management functionality by e.g.:

CR lists: cases and related workflows, actions and related research Items, files and Uniform Resource Identifiers (URIs), metadata and metadata tags, system administration functionality.

Case Management and Retrieval functionality. UC_2 – processing the CR information:

Extraction of simulation results for (a) data processing and analysis, and (b) extracting and storing the summary of CFD cases in the CR, and Metadata-driven orchestration of CFD simulations

Our CR design included rich set of metadata and data processing mechanisms to orchestrate various existing tools and analyses, e.g.:

Information duality and redundancy – realised by a combination of database solution and Flat File System (FFS) functionality:

Repository import/export functionality (FFS and compressed files).

Information cut/paste functionality - hybrid information clipboards.

Information patterns retrieval: (i) search for information patterns, (ii) detect information patterns.

Various design/implementation techniques: (i) decorator pattern, (ii) function intercept, (iii) rich logging functionality

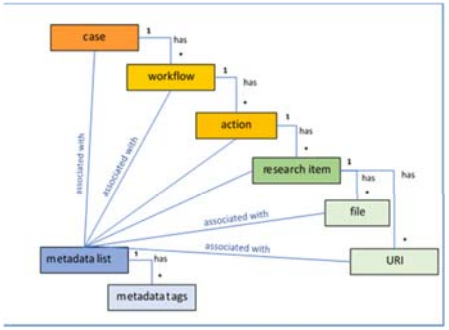

Figure 1. Sketch of some concepts (the high-level metadata schema) used in the Case Repository modelling activities

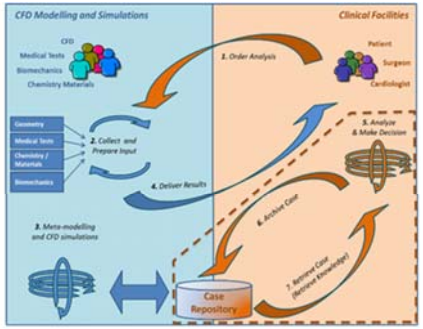

Figure 1. UC_2 - Use Case related to medical use of CFD

The CR design and implementation approaches have been tested in realistic UCs, e.g. UC_1 – medical use of CFD in cardiac interventions, tested in several hospital procedures (anonymised patient intervention scenarios, carried out at Haukeland University Hospital Bergen). They were essential for specifying the domain specific metadata (Figure 1), the crucial element of well-functioning CR. UC_1 included all the health treatment activities, starting with the initial medical examination of the patient and concluding with the final surgical procedure. Based on the used practical cases we have extracted 16 workflow variants (explaining various types and phases in medical procedures) with 23 different activity types. The medical workflows generated the set of the CFD analyses (Figure 2) for which the necessary input health information (metadata and various raw multimedia data) had to be prepared, anonymised and exported. This specific UC_1 required that 4 various heart intervention alternatives/suggestions, get calculated in 40 different geometrical situations, resulting in a CFD metamodel, comprising the total of 120 calculations. After the CFD calculations, the modelling results have been processed and the recommendation (formalized as metadata and various geometry parameters for the surgical intervention) was prepared and delivered to surgeons and cardiologists.

CONCLUSION

The CR (work in progress) is an essential part of many pragmatical modelling frameworks. We will continue improving it, finetuning its functionality, and semantics and syntax of the involved information/knowledge. For that we will use various industrial UCs. They often impose different and sometimes new functional requirements, challenging different aspects and parts of the pragmatic modelling frameworks (Zoric et.al., 2014, 2015).

ACKNOWLEDGEMENTS

The project CardioSIM (Strategic SINTEF Institute Programme) and SINTEF Industry are gratefully acknowledged for funding and supporting this work.

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Brief Biography

Presenter, Dr. Josip Zoric is VP for Digital Research Infrastructure at SINTEF Industry (one of the Institutes at SINTEF AS). Digital R&D Infrastructure activities include digital systems for experimental R&D and field trials, modelling and simulation work (including HPC), data analysis and SW engineering. This work is a continuation of strategic and operative activities on pragmatic industrial modelling, addressed together with several SINTEF's groups, including the CFD, health and process engineering group.

The Optical Properties and Electrical Field Enhancement of Gold Nanospheres

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Abstract

Gold nanospheres (GNPs) with the size between 1 and 100 nm have attracted significant interests in biomedical applications, such as sensing, imaging, and photothermal therapy. The unique optical properties of GNPs play an important role in their various applications. The aim of this study is to investigate the optical properties and electrical field around the surface of GNPs to provide the guide for the choice of morphology of GNPs and corresponding laser parameters in clinical application.

In this study, the discrete dipole approximation (DDA) [1] approach was employed to calculate the optical properties and electrical field of GNPs. In our calculations, the structure of GNPs is similar to a sphere and the diameter is the only structure parameter of GNPs (Fig. 1). The bulk dielectric constants of gold are obtained from Ref. [2]. The general ambient medium is water with the refractive index of 1.333.

The results showed that GNPs had one extinction peak in visible range which was dependent on the diameter of GNPs and the ambient medium. When the diameter increased from 5 nm to 40 nm, the extinction peak increased from 521 nm to 528 nm, and the extinction absorbance also increased. With the increment of refractive index of ambient medium from 1.0 to 1.8, the extinction peak changed from 509 nm to 567 nm (Fig. 1). The electrical field around the surface of GNPs relied on incident laser wavelength, diameter of GNPs, and ambient medium. The electrical field enhancement occurred at two sides of GNPs parallel to the polarization direction of the incident light. At off-resonance wavelength, the electrical field enhancement is much smaller than that at the resonant wavelength where the maximum electrical field can be obtained (Fig. 2). At the resonant wavelength, the largest field enhancement is a function of diameter and ambient. With the increment of diameter from 5 nm to 25 nm, the maximum electrical field increased from 31.4 to 37.0. Besides, the maximum electrical field displayed a significant exponential shift with the increment of refractive index of ambient medium (Fig. 3).

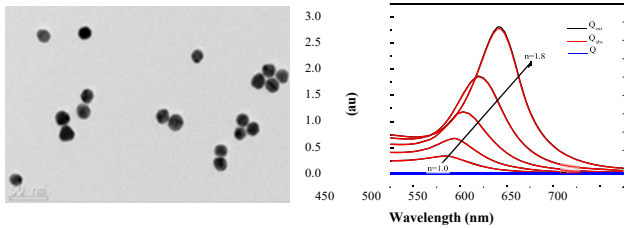

Figure 1. TEM image of GNPs with diameter of 18 nm (left) and refractive index of ambient medium dependent extinction spectra of GNPs (right).

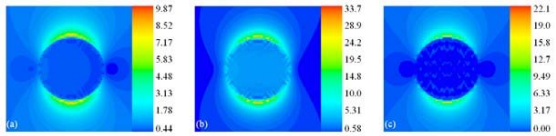

Figure 2. Electrical field enhancement contours of GNPs at different incident laser. (a) at off-resonance wavelength of 422 nm, (b) at resonance wavelength of 523 nm, (c) at off-resonance wavelength of 622 nm.

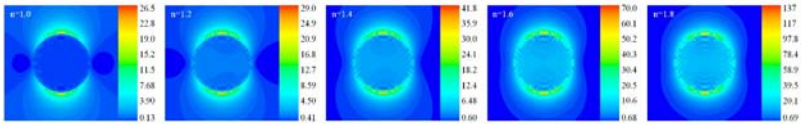

Figure 3. Electrical field enhancement contours of GNPs at different ambient medium (n).

Acknowledgement

This work is financially supported by National Nature Science Foundation of China (51727811).

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Brief Biography

Dr. Bin Chen is now a full professor and vice director in State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University. For more than a decade, Dr. Chen has devoted his efforts to the research of computational heat transfer with application in bio-medical engineering, especially laser dermatology. He has published over 60 peer-reviewed journal papers and was invited for more than 20 keynote speeches.

Predicting Minimum Fluidization Velocity for Vacuum Fluidized Beds

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Abstract

Fluidised beds exhibit excellent hydrodynamics and thermal characteristics due to mixing and homogenisation. The mathematical models that are reported, so far, heavily rely on drag correlations from the experimental data. The hydrodynamics of vacuum fluidized beds has not been investigated extensively due to the lack of sufficient experimental data. Many argue that at reduced pressure, the particle-particle and particle-fluid interactions are complex due to slip-velocity, changing the overall hydrodynamics including the onset fluidization. Thus, the influence of solid-fluid-mixture properties on the hydrodynamics due to vacuum has not been clearly distinguished. In this work, CFD simulations are carried out to predict the minimum fluidization velocity under vacuum pressure conditions. A wide range of sub-atmospheric pressures (P_{gauge} = 50, 75, 90 and 97 kPa) are investigated using both Kumar [1, 2] and Gidaspow [3] drag models. The predicted minimum fluidization is validated with our experimental data. The pressure drop across the bed height are compared for all range parameters. The results show that Gidaspow drag model under-predicts the minimum fluidization velocity at reduced pressure conditions.

Methodology

A two-dimensional computational fluidized bed (125 x 1000 mm) was model and solved transiently on Ansys Fluent. Gas was introduced from the bottom of the bed as the source of superficial velocity to the bed. The simulations were carried out for a range of bed pressures (P_{gauge} = 50, 75, 90 and 97 kPa) with increase in superficial velocity from 0.02 to 0.14 m/s. The pressure drop within the bed was monitored at bed heights of 70 and 950 mm. The models were solved for both Gidaspow and Apruv (slip flow) drag models.

Results

The numerical models were solved until the pressure drop within the bed was stable. The minimum fluidization velocity was determined using the pressure-superficial velocity plots for each parameter. We found that the numerical model with Gidaspow drag law was not sensitive to vacuum pressure change, however, the Apruv drag model showed that the superficial velocity increased with reducing pressure conditions.

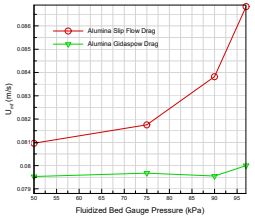

Figure 3. Predicted minimum fluidization velocity for vacuum pressure fluidized beds.

Brief Biography

Mr. Lanka Weerasiri received his Masters by Research degree in Mechanical Engineering from Deakin University in 2016. Thereafter, he has worked as a research assistant in Computation Fluid Dynamics for Deakin University on industrial projects. Simultaneously, he has collaborated on other research fields for publications on microfluidics, fluidized beds, droplet impact studies. He is expected to commence his PhD in Fluidized beds at Deakin University in early 2019.

A CFD-DEM Model for the Simulation of Direct Reduction of Iron Ore in Fluidized Beds

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Abstract

The research on the reduction of iron ore has received much attention in the past few decades, because of the increasing cost and low availability of raw materials. Due to harsh conditions and limited accessibility for measurements, computer simulations have become one of the most important tools for optimizing the iron making processes. One such tool is the CFD-DEM coupling method, in which the gas phase reactions and governing equations are determined on the Eulerian (CFD) side, while the reduction reactions occurring on the particles are calculated on the Lagrangian (DEM) side.

In this work, two of the most prominent types of mathematical models to represent particles submerged in fluids, the Shrinking Particle Model (SPM) and the Unreacted Core Model (UCM) [1], are implemented into the open-source CFDEMcoupling library [2]. While in the SPM the solid particles reacting with the reactant gas are reduced in size, in the UCM they form a layer of product around themselves and impede the reduction. In the metallurgical process of iron ore reduction, oxygen is removed according to thermodynamic equilibrium conditions. The gaseous reduction of iron oxides with CO/H_2 can be expressed with the following mechanism [3]

$$Fe_xO_y + y\,CO/H_2 \leftrightarrow xFe + y\,CO_2/H_2\,O.$$

The iron ore reduction will go through different reaction steps, since the reducing iron oxide forms a product laye. The Hematite ore reacts and forms Magnetite, whereas the reacting Magnetite forms Wustite. Finally Wustite reacts with incoming gas flow and produces Iron. The gaseous reactant diffuses through the porous product layers, while simultaneously reacting at the interfaces of every layer. The UCM is thus considered to be an able model to represent these intermediary steps, as it can represent the resistance that affect the reduction process. The implementation of the mathematical models is carried out such that only the required data is communicated between the two phases with an adaptable communication interval.

The models have been validated by comparing the reduction degrees of iron ore from experimental work with CFD-DEM simulations. First, the reduction process of a single

particle is investigated. In the experiments, a vertical reduction aggregate has been used with various incoming gas concentrations starting with 40% CO to 60% N_2, and decreasing the CO content and adding CO_2 and H_2 to the gas composition. For validation, the total reduction degree depending on time has been compared for every case. Also the reaction rate determining steps has been investigated and compared with the results from available literature. The adjustable parameters that affect the reduction such as the particle porosity, pore size diameter and tortuosity as well as the gas composition and velocities were investigated. After the successful validation of single particle models, the direct reduction of iron ore inside a fluidized bed reactor was investigated with the same model, where the results were also compared with available experimental work. A total iron ore amount of 165 gr that was used in the experiments has been represented with 49325 coarse-grained particles in the DEM side. A gas composition consisting of H_2, H_2O, CO, CO_2 and N_2 was blasted at 750 °C into the bed. The simulations were carried out for every reaction step starting from Hematite to Magnetite, Magnetite to Wustite, and Wustite to Iron. The gas composition has also been altered for every reaction step according the experimental works. The simulation results were then compared with the experimental data allowing us to gain an insight on the reduction process.

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Brief Biography

Mustafa Efe Kinaci is a research assistant and a PhD student at the Department of Particulate Flow Modelling in the Johannes Kepler University, Austria. He has finished his masters in Mechanical Engineering in the University of Duisburg-Essen in Germany, where he worked on the investigation of drag forces on particles in Non-Newtonian flows. His current research as part of the Christian Doppler Laboratory for Multi-Scale Modelling of Multiphase Processes is on the direct reduction of iron-ores in fluidized bed reactors, where he utilizes the CFD-DEM coupling method. His latest works are the "Direct Reduction of Iron-Ore in Fluidized Beds" in Proceedings of the 28th European Symposium on Computer Aided Process Engineering and "Reduction Modeling of Iron Oxides with Carbon Monoxide and Hydrogen using CFD-DEM" in the 14th Mini-symposium Chemical and Process Engineering and 5th Particle Forum. He also gave presentations in the World Congress on Particle Technology, Orlando and in 12th international Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries, Trondheim.

Hydrogen Production in Fluidized Bed Membrane Reactors

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Abstract

Hydrogen is expected to play a major role in the journey towards a more sustainable energy future. Hydrogen is industrially mostly produced via Steam Methane Reforming (SMR) carried out in multi-tubular packed bed reactors. First, methane reacts with steam to form carbon monoxide and hydrogen at temperatures around 900 °C. Consecutively, the formed carbon monoxide reacts with steam to form carbon dioxide and hydrogen via the Water Gas Shift (WGS) reaction. Traditionally, WGS is performed after SMR in separate reactors, which consist of two stages; in the first reactor most of the CO is converted at 300-450 °C and in the second reactor the remaining CO is converted at 200-300 °C. However, to produce hydrogen efficiently, low hydrogen concentrations are required to achieve high CO conversions.

Fluidized bed membrane reactors (FBMRs) have been proposed as alternative reactor systems for hydrogen production via SMR. In FBMRs, the reaction and separation steps have been integrated in one single unit; ultra-pure hydrogen is obtained from the reactor by extracting it from the gas mixture with modern high-flux hydrogen perm-selective supported palladium-based membranes. The hydrogen extraction drives the reaction equilibrium towards the product side, which will increase the reaction rate and reactant conversion. A fluidized bed membrane reactor with hydrogen extraction via membranes performs very well at 550-600 °C. Temperatures above 600 °C should be avoided when using palladium-based membranes, because the membrane's chemical/mechanical stability will be affected.

For the industrial application of FBMR systems, high pressure fluidization is a very interesting research topic, because the reaction rates will increase at higher pressure. Furthermore, high pressure significantly changes the fluidization behavior from fairly structured bubbling fluidization to a more (visually) turbulent movement of the particles. Finally, high pressure will also affect the hydrogen flux through the membrane, but there has been no detailed study on the effects of high pressure on the local hydrogen flux around a membrane.

Two-Fluid Model (TFM) simulations of hydrogen production via Steam Methane Reforming (SMR) in pseudo-2D fluidized bed reactors with horizontally immersed membranes have been performed at 550 °C at various pressures. Systems with horizontally immersed membranes have great potential for industrial applications, because the membranes do not only extract hydrogen, but they also improve the solids mixing in the bed by breaking up large bubbles, which could be beneficial for catalytic reactive systems. Furthermore, they are good learning systems and a significant amount of simulation time is saved by using pseudo-2D systems compared to full 3D systems.

The TFM simulations show that the extraction of hydrogen via membranes clearly increases the reaction rates near the membranes, which moves the reaction away from its equilibrium and overall allows 20% higher methane conversion than systems without membranes at 550 °C. The reactions are consistently away from their equilibrium around the membranes, which is expected according to Le Chatelier's principle. Reaction rates averaged around active membranes are significantly higher than between the membranes and they reduce only 15% in magnitude axially. The reaction rates between active membranes reduce about 50% axially, whereas switched off the membranes reduce the reaction rates 75% axially. Simulations at pressures up to 32 bar show that high pressure does not only increase solids mixing, but it also increases the reaction rates and hydrogen flux through the membranes. Combining the hydrodynamic, mass transfer and reactive effects of high pressure can improve the reactor performance and makes the fluidized bed membrane reactor an attractive option for industrial hydrogen production.

Brief Biography

The Chemical Process Intensification group of the Eindhoven University of Technology focuses on the development of novel reactor concepts for sustainable energy and chemicals production, such as the fluidized bed membrane reactor. The group develops intensified reactors for relevant industrial processes, such as hydrogen production via Steam Methane Reforming (SMR), and combines Computational Fluid Dynamics (CFD) models with phenomenological models and detailed experimental investigations to understand the physical phenomena occurring in the systems. This numerical investigation has been performed by PhD student Ramon Voncken under the supervision of dr. Ivo Roghair prof. Martin van Sint Annaland.

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Multiphase Direct Numerical Simulations (DNS) of Oil-Water Flows through Digitized Porous Rocks

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Abstract

Multiphase flows through complex solid geometries are encountered widely in nature and technology. Examples include water flooding for oil recovery, trickle bed reactors, microfluidics devices, chemical reactors etc. During the primary oil recovery process, oil comes out of the porous rocks automatically due to its own natural pressure. Gradually, the natural pressure of the oil reduces and the automatic flow of the oil stops. There is still a large amount of oil which remains trapped in the porous rocks. To recover this residual oil various secondary and tertiary processes are used. Water flooding is a commonly used secondary oil recovery process which uses pressurized water to recover oil from porous rocks.

The present study focuses on fully resolved pore-scale level multiphase Direct Numerical Simulations (DNS) of oil-water flows through digitized porous rocks. A 2nd order direct forcing implicit immersed boundary method (IBM) by Das et al. (2016) is used to resolve complex geometries, employing the finite volume method on a staggered grid. The main advantages of IBM over the traditional unstructured body conformal grids are simplicity in grid generation and discretization of the Navier-Stokes equations, ease of code development, less memory requirement to store the grid information and higher computational efficiency. The fluid-fluid interface is tracked by a mass conservative sharp interface volume of fluid (VOF) method proposed by Young (1982). The fluid-fluid interface is reconstructed using piecewise linear interface calculation (PLIC) method. Volumetric surface tension force is computed using continuum surface force (CSF) model by Brackbill et al. (1992). To reduce the parasitic currents during simulations pressure and surface tension forces are discretized at the same location using the balanced-force approach of Francois et al. (2006). Fluid-fluid interfaces in contact with solid boundaries produce a three-phase contact line and contact line dynamics plays a major role in fluid motion. IBM and VOF are coupled by prescribed apparent contact angle boundary condition at contact line by Patel et al. (2017) to simulate contact line dynamics at macroscopic length scale.

The coupled IBM-VOF solver can work with any arbitrarily shaped complex solid surface mesh and is validated using a variety of benchmark test cases. Simulations of water flooding process through digitized porous rocks are performed based on typical pore-scale capillary and Reynolds numbers. The effect of porosity on the mobility of oil-water flows through porous rocks is quantified.

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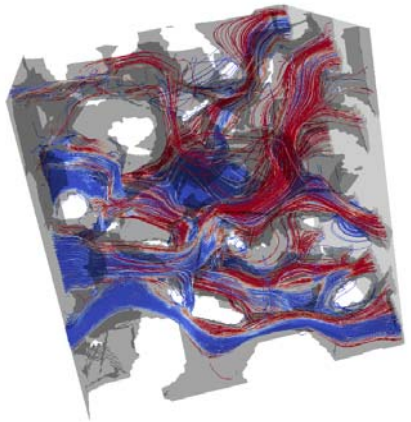

Figure 1: Flow streamlines for a sample water flooding simulation from the digitized porous rock of porosity ~0.15. Oil (in red) from the porous rock is being displaced by water (in blue) at capillary number 0.1.

Brief Biography

Harshil Patel was born on 30th January, 1991 in Mehsana, India. After finishing his high school in Surat, India in 2008, he joined an undergraduate program in the department of Mechanical Engineering at SVNIT Surat. He was awarded the Bachelor degree in Mechanical Engineering with distinction in 2012. After graduation, he worked in the Equipment Design department of Linde Engineering, Vadodara, India for a year. He then started his postgraduate studies in Thermal and Fluids engineering at the department of Mechanical Engineering, IIT Bombay, India in year 2013. His master's thesis on "Development of Fluid Structure Interaction Solver using Ghost Cell based Immersed Boundary Method" was guided by Prof. A. Sharma. He received the degree in Master of Technology in year 2015 with the highest score (1st rank) in his batch. He also earned the Institute Silver Medal for his accomplishments in academia and extra-curricular activities. Immediately after completing his masters, he started his PhD project on "Interfacial Dynamics in Multiphase Flow through Porous Rock" under the supervision of dr. E.A.J.F. Peters and prof. J.A.M Kuipers in the Multiphase Rectors Group at TU Eindhoven, The Netherlands. He is currently in 3rd year of his PhD and published 3 peer reviewed journal papers. Overview of his research work is available at https://www.researchgate.net/ profile/Harshil_Patel20.

CFD Modelling of Gas-Solid Fluidised Bed with Eularian Single Phase Air Coupled Explicitly with Eularian Solid Phase.

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Abstract

Gas-solid fluidised bed has extensively been used in different sectors such as chemical, petroleum, mineral, fuel gasification and combustion due to its uniform mixing property, consistent heat and mass transfer and temperature homogeneity. Flow dynamics has significant impact on the design of fluidised bed and therefore, it is necessary to understand its complex behavior comprehensively to scale up fluidised bed. Experimental investigation is considered as the most effective way of studying this type of experiment to solve practical problems but at the same time, it is expensive, time consuming and technically challenging as well. On the other hand, Computational Fluid Dynamics (CFD) is an efficient tool for designing and analysing the method which can give better insights into the flow and other phenomena occurring inside each individual particle of solid. Therefore, Computational Fluid Dynamics (CFD) simulations can be used to study the hydrodynamic characteristics of a fluidised bed in detail by combining different theoretical methods and experimental results.

In this work, a complete numerical model was used to exercise the process of flow dynamics in the fluidised bed. It is crucial to predict the size and shape of the rising bubbles to model the degree of mixing of solid particles, as the performance of a fluidised bed depends strongly on bubble dynamics behavior. A qualitative validation has been made with available experimental results to compare the characteristics of predicted flow dynamics obtained from a gas-solid fluidised bed using digital image analysis technique. The predicted flow dynamics were in reasonable agreement with the experimental results. A commercial CFD code, AVL Fire version 2017 has been used in this simulations. The bed was considered as a porous media and the solid phase variables were presented in the CFD through the User Defined Functions (UDFs) platform. Extensive FORTRAN subroutines were written to explicitly couple the solid phase with the air phase. Comprehensive subroutines were developed to solve the momentum and continuity of the solid phase and then explicitly coupled with the Eularian air phase available in AVL Fire 2017. Relevant parameters like pressure, shear stress and friction force for the solid phase were calculated and integrated with the solution process for momentum and continuity of the solid phase. The pressure for the solid phase was obtained from the continuity of the solid phase in an analogous way as done in the SIMPLE algorithm used in conventional CFD practice.

Brief Biography

Mst Farhana Diba is currently a PhD student in Swinburne University of Technology at Faculty of Science, Engineering and Technology (FSET), Melbourne, Australia. She is pursuing her research on Computational Fluid Dynamics (CFD) in Fluidised bed. Farhana is tutoring as well as a sessional staff for Faculty of Science, Engineering and Technology in Swinburne University of Technology, Australia.

Farhana received her Masters of Science in Maritime Affairs from World Maritime University (WMU), Malmo, Sweden awarded with the Sasakawa Fellowship scholarship from Ocean Research Policy Foundation (OPRF), Japan. She completed her Bachelor of Science in Mechanical Engineering from Rajshahi University of Engineering and Technology (RUET), Bangladesh awarded with Technical Scholarship. Farhana is a Senior Instructor at Bangladesh Institute of Marine Technology under the Ministry of Expatriates' Welfare & Overseas Employment of the People's Republic of Bangladesh Government (currently on study leave). There she was responsible to tutor the subjects like Fluid Mechanics, IC Engine Principle and Thermodynamics and involved in supervising the final year projects. She has four years of working experience at the RingTech Limited as an assistant Engineer.

Farhana has visited different countries like UK, France, the Netherlands, Portugal, Japan, South Korea and Malaysia to attend several study tours, training programs and conferences. She attended the IMO conference at IMO headquarter, London, UK. Farhana went to the Maritime Simulation Training Centre (MSTC) in The Netherlands for a training on "Train the Trainer according to STCW 2010 on Maritime Simulators".

Simulation of combustion in coal-fired circulating fluidized bed boiler for supercritical CO_2 power cycle

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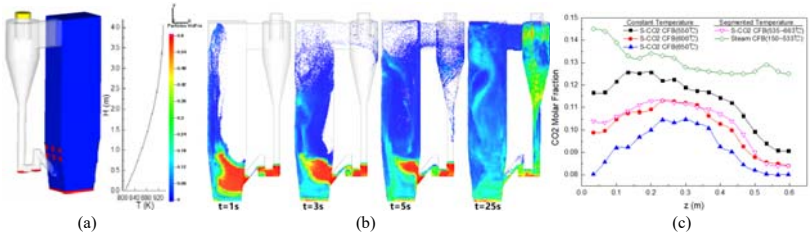
Abstract

Supercritical carbon dioxide (S-CO_2) power cycle is promising to integrate with the coal-fired circulating fluidized bed (CFB) boiler. The changes of boiler shape and boundary conditions with the S-CO_2 power cycle lead to the unclear combustion characteristics. A three-dimensional Eulerian-Lagrangian model was established to simulate the combustion process in a designed S-CO_2 CFB boiler (H=4.080 m, S=0.6×0.6375 m^2) and the effects of different thermal wall boundary conditions including constant temperature, segmented temperature, constant heat flux and segmented heat flux on the combustion characteristics were investigated. On the basis of the multiphase particle-in-cell (MP-PIC) scheme, the large eddy simulation (LES) approach for gas phase and discrete particle method for solid phase were adopted and reaction models including devolatilization and combustion of char and volatiles were incorporated into the scheme. Results show that with increasing the wall temperature, temperature range in S-CO_2 CFB furnace became narrower and the emissions of CO_2 and CO decreased. Optimized operation suggestions were proposed according to the investigation.



(a) (b) (c)

Figure. S-CO_2 CFB boiler and its simulated combustion characteristics: (a) Sketch of the S-CO_2 CFB boiler with its segmented wall temperature, (b) flow pattern transformation in S-CO_2 boiler, (c) radial distributions of CO_2 molar fraction at H=1.5m in z-direction.

Brief Biography

Ying Cui, female, is a first-year PhD candidate in Thermal Engineering, Southeast University and Dr. Wenqi Zhong is a professor at Southeast University specializing in multiphase flows, clean coal combustion technologies and biomass thermal transformation.

A Numerical Approach for Generic Three Phases Flow Simulation

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Abstract

In this paper, we introduce numerical methods that can simulate complex multiphase flows. The finite volume method, applying Cartesian cut-cells (Kirkpatrick et al., 2003; Yoann Cheny et al., 2016) is used in the computational domain, containing gas, liquid and solid, to conserve mass and momentum. With this method flows in and around any geometry can be simulated without complex and time consuming meshing. The interaction between each phase is treated simply by wall function models or jump conditions of pressure, velocity and shear stress at the interface (Kang et al., 2000; Vukčević et al., 2017). The sharp interface method "Coupled Level Set and Volume of Fluid"(CLSVOF) is used to represent the interface between the two fluid phases (Chakraborty et al., 2013; Sussman and Puckett, 2000). This approach will combine some advantages of both interface propagation methods, such as excellent mass conservation from volume of fluid and good accuracy of normal computation from level-set function. In order to resolve interacting lines created by gas-liquid-solid, the first CLSVOF will be generated to reconstruct the interface between solid and the other materials. The second one will represent the interface between liquid and gas. Several benchmark test cases are performed to validate numerical results.

The first test is a dam break flow which is designed to investigate the two-phase flow. The water column is initialized with 0.3m height and 0.6m width inside an 0.6x1.61 rectangular tank. Due to gravity, water travels along the horizontal bed and generates a downstream wave. The evolution of the free surface is shown in figure 1.

The next test is a water entry simulation which is used to demonstrates the capability of our numerical method to handle three-phase flow. The shape of a wedge object and initial stage of simulation is presented in figure 2. For simplicity, the item is kept standstill and the free surface is let moving with a velocity being equivalent to a water entry velocity. Figure 3 displays a comparison of numerical result, experimental data and theoretical method for splash expansion and splash tip velocity. As shown in this figure, our numerical method can predict fairly accurate the characteristics of splash.

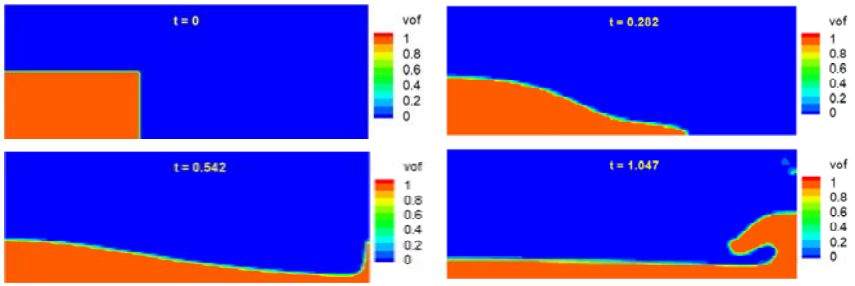

Figure 1. The Temporal Development of Air-Water Interface (time t in seconds)

Figure 2. The Schematic Diagram of Water Entry Problem and Splash Formation

$\alpha = 90^o$ $\alpha = 120^o$

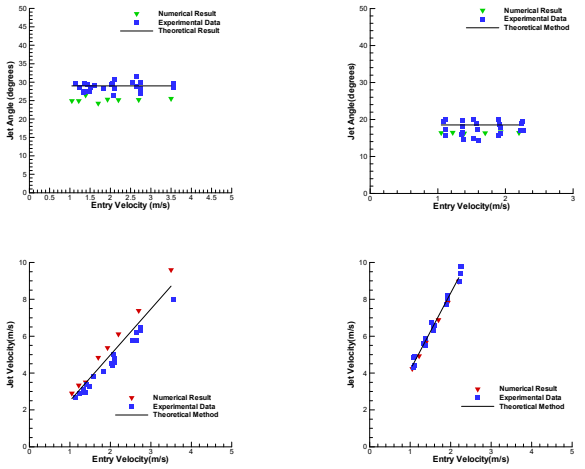

Figure 3. Wedge jet root expansion angle and jet velocity

Brief Biography

Son Tung Dang was born in Namdinh, Vietnam, in 1990. He received the B.E. degree in mechanical engineering from the Hanoi University of Science and Technology, Hanoi, Vietnam, in 2013, and the M.Sc in mechanical engineering from the Pusan National University in 2016. Since April 2016, he has been Phd candidate at Department of Energy and Process Engineering, NTNU, Trondheim, Norway. His current research interests are multiphase flows and immersed boundary methods.

Direct Numerical Simulation of Hot Spots in Packed Bed Reactors

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Abstract

Tubular packed bed reactors have been used in the chemical process industry for over a century and are very popular in various applications (Methane reformation and Fischer-Tropsch) even today. Tubular reactors are generally preferred when performing highly exothermic reactions as the tubular jacket provides an efficient cooling mechanism to ensure a uniform temperature gradient in both the axial and radial direction. Though there exists many efficient mechanisms to uniformly cool the reactor bed, the reasons for the formation of 'hot spots' in packed bed reactors are still being widely researched[1]. Many studies have shown that the Arrhenius dependency of the rate of reaction and the heat of production which govern the highly exothermic reactions are the essential cause for the formation of these hot spots. However, while some studies have shown that the primary factor for the formation of hot spots is the kinetic parameters governing the reaction[1], other studies have speculated that the packing structure of the catalysts and the local heterogeneities may be the root cause for the formation of these hot spots[2].

In this contribution we employed Direct Numerical Simulation (DNS) where the fundamental continuum governing equations are solved on a single uniform Cartesian domain with the transport in the fluid and solid phases both accounted for in a fully resolved manner. The appropriate fluid-solid interface coupling is enforced using a second-order accurate sharp interface Immersed Boundary technique as described by Das et. al[3]. It is assumed that the solid phase is an active catalytic material where the diffusing reactants are converted into products following irreversible first order kinetics. Furthermore it is also assumed that the reaction is highly exothermic and the first order rate constant has an Arrhenius dependency thus replicating a thermally autocatalytic system. In Figure 1 we show the classic Weisz and Hicks case[4] where pure diffusion and non-isothermal reaction is studied in a single catalyst pellet. It is observed that a large dimensionless adiabatic temperature rise is seen within the catalyst pellet accompanied with sharp concentration and temperature gradients due to the highly exothermic reaction with almost complete conversion of the reactants.

In order to investigate the formation of hot spots we perform as well DNS in a dense array of spheres where the packing is generated using the Discrete Element Method. The packing is enclosed by a cylindrical tube where the tube acts as a cooling jacket to ensure that the system does not experience thermal runaway.

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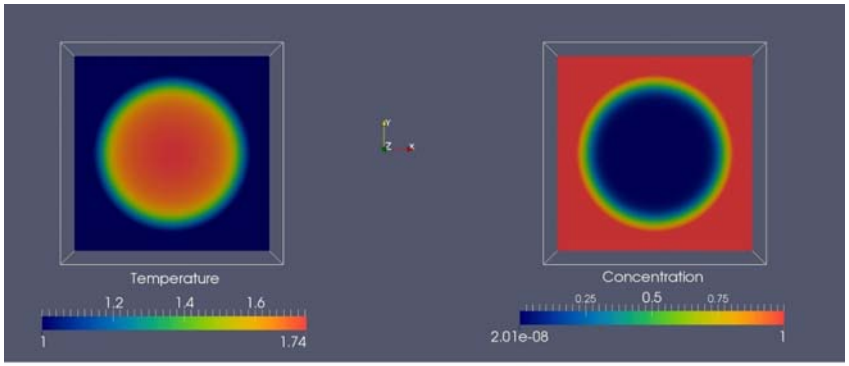

Figure 1: Non-isothermal diffusion and reaction in a single spherical catalyst pellet

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Brief Biography

The oral presentation shall be given by Vishak Chandra. V. Chandra is a PhD student in the Multiphase Reactors Group in the Department of Chemical Engineering and Chemistry at Eindhoven University of Technology, Netherlands. Chandra's research focusses on the numerical analysis of transport phenomena in packed bed reactors where the interplay between heat, mass and momentum transfer is investigated using Direct Numerical Simulation techniques and is supervised by Dr.ir. E.A.J.F. (Frank) Peters and Prof.dr.ir. J.A.M. (Hans) Kuipers.

Cluster-Induced Turbulence Closure Models for Momentum and Heat Transfer in Large-Scale Gas-Solid Flows

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Abstract

Gas-solid flows, like fluidized beds or risers, are used for a wide range of applications, from food drying and polymer production to the direct reduction of iron ore. While for small scale fluidized beds, simulation is quite feasible, the occurring physical phenomena cannot be fully numerically analyzed in large scale reactors yet, due to a large range of involved scales. In fluidized bed reactors of several meters in height, the smallest stable structures are usually only several particle diameters wide [1]. Thus, the microscopic behaviour of individual particles, i.e. gas-solid drag, intra- and interphase heat transfer between the particles and the gas, as well as collisions cannot be fully resolved due to computational limitations. However, the unresolved heterogeneous structures have a significant influence on the flow properties. The velocity fluctuations around particle clusters give rise to turbulence, i.e. cluster induced turbulence [6, 7]. An overestimation of the gas-solid drag force by not accounting for this turbulence leads to an overestimation of the bed expansion [5].

A model accounting for the unresolved terms can be derived by spatially averaging the kinetic theory based two-fluid model equations [4]. The filtered gas-solid drag can be, for example, approximated by the filtered drag coefficient times the filtered slip velocity corrected by a drift velocity [2, 3]. The drift velocity can be viewed as the gas-phase velocity fluctuations seen by the particles. Additionally, the drift velocity and, thus, the filtered drag force depend on the turbulent kinetic energy of the gas phase, as well as on bulk density fluctuations [3]. Closures for the turbulent kinetic energies of both phases and the bulk density fluctuations are derived [4, 8].

Finally, the spatially averaged two-fluid model will be extended to include a model for heat transfer and, therefore, filtered energy equations are derived. The effective heat transfer coefficient divided by the solid's volume fraction is approximated by its zeroth order Taylor series expansion about the filtered variables. This gives rise to a similar construct as the drift velocity. The temperature difference between both phases is corrected by a 'drift temperature' stemming from phase averaging. Closure models for this 'drift temperature', as well as for other unresolved terms in the filtered energy equations are derived following the concepts outlined in [4]. A comparison of the presented closure models with fine grid simulation data shows fairly good agreement.

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Brief Biography

Stefanie Rauchenzauner is a research assistant and PhD student at the Department of Particulate Flow Modelling of the Johannes Kepler University in Linz, Austria. She received her MSc from Vienna University of Technology, studying Technical Mathematics and Technical Physics, where she worked on models for capillary free-surface flows. As a part of the Christian Doppler Laboratory for Multi-Scale Modelling of Multiphase Processes, her research focuses on multi-scale modelling of large-scale, dense gas-solid flows. Currently she is working on mathematical closure models for mesoscale unresolved terms in coarse grid, large scale simulations of dense gas-solid flows, with focus on momentum and heat transfer. Latest results are included in "Spatially-Averaged Models for Heat Transfer in Gas-Solid Flows", presented at the 2018 AIChE Annual Meeting.

Numerical Investigation of Gas Redistribution Effects by Raceways on the In-furnace States and Performance of Ironmaking Blast Furnace

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Abstract

The transport properties within raceways significantly affect the performance of ironmaking Blast Furnace (BF), but were generally studied as isolated local phenomena. To date, our knowledge about the influences of raceways on global BF performance is not fully established. This paper presents a numerical study of the inner states and global performance of BF, with special reference to the effect of gas distribution by raceways. The model is based on our newly developed parallel three-dimensional CFD BF process model, which is integrated with the recent developments in modelling the layered burden structures, the stockline variation, and the liquid flow in the dripping zone. Also, it explicitly considers the presence of raceways that are treated as boundaries in the model. With this development, the global performance and in-furnace states of BF can be quantified with respect to different sized and shaped raceways resulting from different blast conditions. For the first time, the importance of the reducing gas distribution by raceways to BF performance is clarified in a quantitative manner.

Brief Biography

Lulu Jiao, obtained his bachelor and master degree in University of Science and Technology Beijing in 2013 and 2016 respectively. After that, he, as a Ph.D. candidate, joined ARC Hub for Computational Particle Technology, Department of Chemical Engineering in Monash University, Australia. His Ph.D. project focuses on the development and application of three-dimensional blast furnace process model.

Numerical Simulation of Droplet Formation in Microfluidic Cross-Junction

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Abstract

Based on the VOF (Volume of Fluid) liquid/liquid phase interface tracking method, an unsteady model of the droplet formation process in the cross-junction microchannel is established. The hydrodynamic behavior of the droplet formation process is studied by numerical simulation. By analyzing the flow field information of typical flow patterns and the evolution of their deformation parameters in detail, the internal mechanism of typical flow patterns is clarified, and the flow patterns at different intersection angles are given. The effects of flow ratio and intersection angles on droplet length, generation frequency and monodispersity are also discussed. Finally, a prediction formula for predicting the length of droplets generated in a squeezed flow pattern in a cross-junction at different intersection angles is proposed.

The results show that the competition between the control forces (such as viscous force, inertial force and surface tension) of different phase fluids under different working conditions is different, which leads the phases flow and phase interface evolution behavior to present different characteristics during emulsification. Different characteristics result in four typical flow patterns, namely, squeezing, dripping, jetting and wiring. The change in the angle of intersection θ directly changes the force characteristics of the dispersed phase fluid in the cross-area and its outlet, so that the growth and neck of the flow pattern are developed during the expansion and extrusion stages of the extruded flow pattern occurring in this region. The interfacial dynamic behavior in the growth and necking stages of the dripping pattern has important effects.

However, under the jetting flow pattern, the droplet formation position is downstream of the main channel far from the intersection area and the flow field downstream of the main channel has become uniform at different intersection angles, so the intersection angle has little effect on the interfacial morphology and evolution during droplet formation. In addition, for the working conditions studied in this paper, the change of the intersection angle is not enough to change the internal mechanism of droplet formation, so the bifurcation angle has less influence on the flow pattern. When the continuous phase capillary number is constant, the increase of the flow ratio affects the droplet length, the generation frequency and the flow pattern transition. The monodispersity of the droplet formation under the squeezing and drippng flow pattern is good, while it under the jetting flow pattern is the worst monodisperse. When θ deviates from 90°, the variation of the droplet length under the dripping flow pattern is significantly different from that of θ = 90°. Finally, this paper proposes a formula for reliable prediction of droplet (bubble) generation length in a cross-junction microfluidic device with different intersection angles under squeeze flow.

Keywords: droplet formation, microfluidic cross-junction, intersection angles, VOF method, numerical simulation

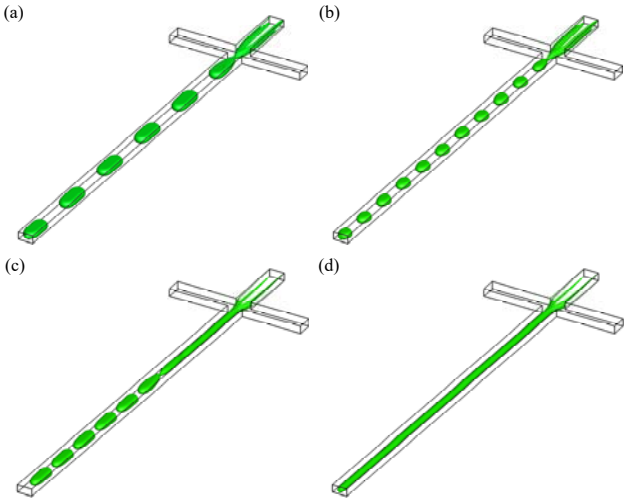

Fig. 1. Four flow regimes of droplet formation in a microfluidic cross-junction with $\theta = 90°$.

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Brief Biography

Wei Gao is a 3rd grade Ph.D. candidate of power engineering and engineering thermophysics in School of Energy and Environment, Southeast University. His major research interest is focused on the area of computational fluid dynamics and the experiment investigation on droplets and particles generation, manipulation and application. His current research project involves droplet formation mechanism in different channels. He has published five papers on international journals which are SCI sources, including *Lab on a chip* (1), *Science Advances* (2), *Angewandte Chemie International Edition* (1) and *Advanced Functional Materials* (1). One of his work "Three-dimensional splitting microfluidics" has been published in *Lab on a Chip* as inside cover letter. He has applied for 11 Chinese invention patents (2 patents has authorized).

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Determination of the Minimum Fluidization Velocity in Fluidized Bed at Elevated Pressure and Temperature by CFD Simulation

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Abstract

The minimum fluidization velocity (U_{mf}) is one of the most important parameter for the design and operating of fluidized beds. This parameter is difficult to experimentally measure at elevated pressure and temperature. In this paper, a three-dimensional Eulerian−Lagrangian simulation was employed to predict the minimum fluidization velocity. The results of simulation were validated with correlations reported in literatures. The detailed influence of pressure, temperature, particle density and particle size distribution on the minimum fluidization velocity was also systematic investigated.

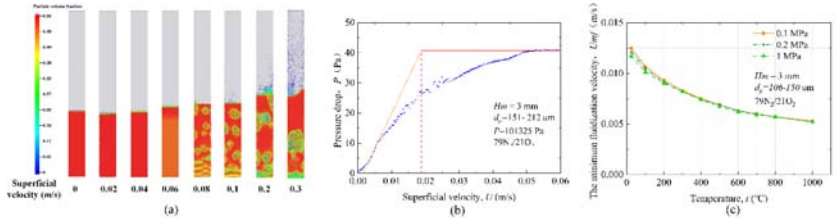

Fig.(a) Particle volume fraction at different superficial velocity, (b) estimate the minimum fluidization velocity by CFD data, (c) the changes of U_{mf} with temperature and pressure.

Brief Biography

Dr. Yingjuan Shao, Female, an associate professor at Southeast University, is specialized in multiphase flows, computational fluid dynamics, clean coal combustion technologies and biomass thermal transformation.

The Mushy Zone In A Model Of Arc Welding Of Aluminium Alloys

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Abstract

Arc welding is widely used to join metal components, using the intense heat flux from by the arc plasma to partially melt the metal. There are many variants of arc welding, of which metal inert-gas (MIG) welding is the most important in manufacturing industries. In MIG welding, the upper electrode is a metal wire anode and the lower electrode is the workpiece cathode. The wire is melted by the arc, forming droplets that pass through the arc into the weld pool (the molten region of the workpiece).

A three-dimensional computational model of MIG welding of aluminium alloys that includes the wire electrode, arc plasma, weld pool and workpiece in the computational domain has been developed [1]. The model combines equations for the conservation of mass, momentum and energy, with equations derived from Maxwell's equations to account for current continuity and to calculate electromagnetic fields. Equations describing the transport in the arc of metal vapour (formed at the liquid metal surfaces) and mixing of the wire alloy and workpiece alloy in the weld pool are also solved.

The mushy zone, the region between the solidus and liquidus temperatures in metal alloys, has recently been included in the model. This required three main changes. First, the solidus and liquidus temperatures and latent heat of melting had to be calculated as a function of the local composition of the workpiece, which depends on the fraction of the workpiece alloy and the wire alloy at that position. Values of other thermophysical properties of the metal, such as thermal and electrical conductivity, also had to be calculated in the mushy zone. Second, influence of the latent heat of melting had to be included in the mushy zone; the method of Prakash et al. [2], extended to the case of a moving heat source, was adopted to ensure numerical stability. Third, since the mushy zone impedes the flow of molten metal, the influence of the mushy zone on flow had to be considered; this was done using the Carman–Kozeny equation [3].

Figures 1 and 2 show results obtained for welding of 3-mm-sheet Al–Mg alloy AA5754 with a wire composed of Al–Si alloy AA4043 with an arc current of 95 A in argon shielding gas. Figure 1 shows a vertical cross-section of the welded metal, perpendicular to the weld direction, indicating the mushy zone thickness is about 0.2 mm for a weld depth of 1.7 mm. Figure 2 shows a vertical cross-section through the weld pool during welding, showing that the flow in the weld pool is strongly impeded in the mushy zone. Results comparing weld pool dimensions and temperature and flow distributions, including and neglecting the mushy zone will be presented. The importance of considering the mixing of the wire and workpiece alloys will also be examined.

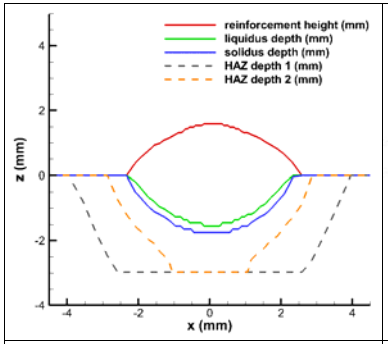

Figure 1. Vertical cross-section of the welded metal, showing the regions that reached the liquidus and solidus temperatures, and the heat-affected zone (regions that reached temperatures of 400 and 500°C).

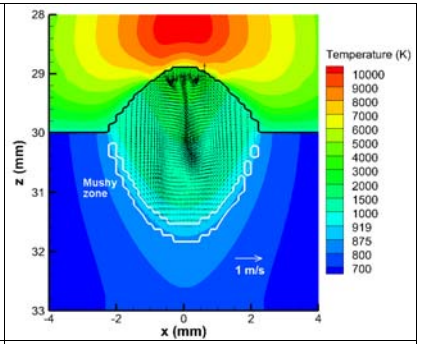

Figure 2. Temperature distribution in a vertical cross section through the centre of the arc and weld pool. The black arrows show the flow in the weld pool (a reference vector is given), and the boundaries of the mushy zone are shown in white.

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Brief Biography

Tony Murphy is a Chief Research Scientist and Team Leader at CSIRO, which he joined in 1989 following a postdoctoral fellowship at Max Planck Institute for Plasma Physics in Munich and a PhD in physics at University of Sydney. His research focuses on computational modelling of thermal-plasma and additive-manufacturing processes, and applications of atmospheric-pressure plasmas. He is Editor-in-Chief of *Plasma Chemistry and Plasma Processing*, a member of the Editorial Board of three other journals, and has won research awards from the Australian Academy of Science, Institute of Physics (UK), Australian Institute of Physics and Royal Society of NSW. He is currently President of the International Plasma Chemistry Society.

Computational Models for Pyrometallurgical Phase Separation Problems

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Abstract

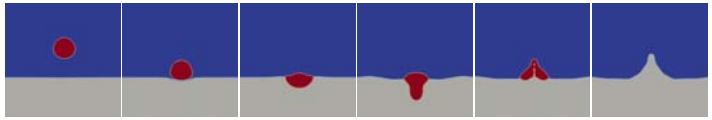
Pyrometallurgical smelting processes account for a significant portion of the world's production of industrial commodities such as iron and steel, ferro-alloys including ferrochromium, ferronickel and ferromanganese, high-value materials such as platinum group metals, and many others. Smelting furnaces operate at sufficiently high temperatures that the material being processed is in the molten state, typically over 1500°C. The products from the thermochemical reactions inside the furnace form immiscible liquid phases, and a key part of the operation involves ensuring adequate separation of the valuable product phase, generally a metal alloy or matte (a mixture of metal sulphides), from the waste phase, generally slag (a mixture of metal oxides). This separation may occur directly inside the smelter, or in special-purpose settling furnaces or ladles as a secondary processing step. Separation may be complicated by the unusual properties of the molten fluids including very high interfacial surface tensions and a wide range of viscosities and densities – this can result in poor separation characteristics (Eidem et al. 2015) which ultimately have a negative impact on the process operability and economics.

In the present work, the behaviour of droplets of a generic metal product separating from a slag waste was examined using computational modelling. Separation occurs in two stages – first the dense metal droplets must settle through the lighter, more viscous slag phase under gravity, and second, the droplets must join with each other (and the main pool of metal) via a process which includes the creation and drainage of thin films of slag. To study both effects, a volume-of-fluids multiphase flow model together with a multiple marker approach (Coyajee & Boersma 2009) was developed and combined with several different empirical and theoretical sub-grid film drainage and rupture models. The model was implemented using the OpenFOAM® open source computational mechanics framework.

Model optimization and validation was conducted using data obtained from an experimental study of single droplets of mercury falling into a quiescent pool through fluids of different viscosities. The optimized models were used to conduct an analysis of the droplet separation problem's sensitivity to various parameters such as metal and slag properties, droplet size and fall distance, and film sub-model. Preliminary results from model cases representing more typical industrial conditions, in which many droplets interact and separate simultaneously, are also presented.

(a) 24.00 ms (b) 31.25 ms (c) 40.50 ms (d) 62.25 ms (e) 69.25 ms (f) 74.75 ms

Figure 1: High-speed photography of a mercury droplet 3 mm in diameter falling into a mercury pool from 16 mm above the interface, through silicone oil at 0.096 Pa.s viscosity. The interfacial film between the droplet and the pool ruptures at frame (e).



(a) 25 ms (b) 35 ms (c) 40 ms (d) 60 ms (e) 70 ms (f) 75 ms

Figure 2: Phase fields from a computational model of the experiment in Figure 1, using an empirical film drainage and rupture sub-model. The mercury droplet and pool are shown in red and grey respectively. Film rupture occurs between frames (e) and (f).

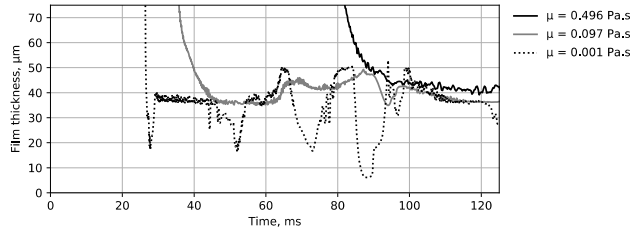


Figure 3: Sensitivity of film thickness evolution to different light-phase viscosities for the model case shown in Figure 2 (Reynolds-equation-based film drainage model with rupture disabled).

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Brief Biography

Quinn Reynolds holds degrees in engineering and a PhD in applied mathematics. He is employed as a Technical Specialist at Mintek, a national research institute serving the extensive mineral processing and metallurgical industry in South Africa. His interests include the mathematical and computational modelling of complex coupled problems in high-temperature processes, in particular the application of high performance computing to phenomena arising in the field of pyrometallurgy.

Numerical Investigation on the Wake of NACA0015 Hydrofoil

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Abstract

Two-phase bubbly flows occur widely in nature and are extensively applied in industry. Cavitation is one type of two-phase flows that occurs in many hydrodynamic applications (e.g. hydrofoils, hydrodynamic pumps, propellers, etc.). It happens when the pressure is dramatically reduced - typically due to high-speed flow or existence of a sharp object in the flow - where the liquid medium breaks down leading to creation of some cavities in the liquid or vaporous bubbles. Cavitation could lead to bubbly flows during the underwater ventilation - where the air is entrained inside water – for example in turbine aeration. Clearly, waters in lakes, rivers, reservoirs and underground aquifers are of most importance for people and to the world's ecological systems [1]. However, hydroelectric facilities discharge water with low dissolved oxygen, which impacts on the downstream water quality, especially at greater depths. The most important influencing factors for optimization design of Auto-venting turbines (AVTs), for solving the low level of dissolved oxygen (DO) in the discharged downstream water, are the quantity of entrained air, the bubble size distribution resulting from coalescence and breakage processes, and the rate of oxygen transfer from the bubbles. In order to better understand the influencing flow conditions on the bubble size distribution, in this paper a numerical investigation for flow around NACA0015 hydrofoil is carried out.

The numerical simulations require the consideration of the dynamic behaviors of two-phase flow and bubbles undergoing coalescence and breakup. For this purpose, the ensemble-averaged mass and momentum transport equations for continuous and dispersed phases are modeled within the two-fluid modeling framework. These equations are coupled with population balance equations (PBE) to aptly account for the coalescence and break-up of the bubbles. In this paper, the turbulent random collision is considered for the bubble coalescence proposed by Prince & Blanch [2], and bubble binary break-up under isotropic turbulence situation is considered for the bubble breakage proposed by Luo and Svendsen [3].

Experimental data of Karn et al. [4] is used in this study for investigating the bubble size distribution at the wake of the hydrofoil at different flow conditions. The experiments were conducted in the SAFL high-speed water tunnel at University of Minnesota.

Two-phase gas-liquid flows in the wake of NACA0015 at different conditions were simulated to study the effects of air discharging configurations on the interactions between

the carrier fluid flow and bubbles. The resultant bubble size, normalized velocity and void fraction distributions for different flow conditions including angle of attack (AOA), air-entrainment coefficient, and Reynolds number are presented and discussed. The results show that varying AOA has the most significant impact on the distribution of the bubbles in the wake. The bubble size is reduced by increasing the angle of attack due to the higher turbulence imposed by larger AOA. Change in AOA also creates a drift in the location where the minimum velocity occurs in the wake, which is an upward drift by increasing the AOA. Also, by increasing the AOA, the bubbles are dispersed more effectively within the wake. Increasing the air-entrainment coefficient results in production of smaller size bubbles due to higher collision and break-up rate of bubbles. Also, with higher air-entrainment coefficient, larger areas with higher void fraction are observed downstream the hydrofoil. Changing the Reynolds number does not have significant influence on the average bubble size in the wake of the hydrofoil. Similarly, the void fraction distribution is not drastically changed by varying the Reynolds number. However, Reynolds number has direct impact on the bubble size distribution at the wake of the hydrofoil.

Brief Biography

Dr. Sara Vahaji is a lecturer in Mechanical Engineering at Deakin University. She received her B.Sc. (Hons) (2003) degree in Chemical Engineering from Amirkabir University of Technology and her Ph.D. (2017) degree in Mechanical Engineering from RMIT University. She worked in industry as a chemical engineer for seven years before she started her PhD candidature. She then performed research as a research fellow in the School of Engineering, at RMIT University. Dr. Vahaji's research interests are mainly on numerical and experimental modelling and design of systems with two-phase gas/liquid flows. Her research outcomes to date are published in 21 high-ranking journals and prestigious national and international conferences. She has been the recipient of several awards including APA scholarship, fund from DST Group for performing high quality research, and travel grants for presenting her research outcomes at international conferences.

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Numerical analysis of the component interaction in a hydrocyclone treating heterogeneous mixture using multi-phase CFD model

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Abstract

In mineral industry, the extraction of the pure minerals from the ore are very crucial. While the equipment become main factor of choice for the high efficiency separations, the material or ore properties plays a vital role as well. The ore having the inherent heterogeneous component mixture influences the performance in a hydrocyclone classifier and increases the particle misplacement [1]. In this study, an improved Algebraic slip mixture (ASM) approach with the enabled granular options is used for the hydrocyclone classification performance and particle segregation in 75 mm cyclone. The specific focus of this study is to understand and quantify the interaction of the individual components due to the different sizes; densities in hydrocyclone treating dual component mixture consist of magnetite and silica in different proportions. Predicted component classification performance data is compared with the experimental performance data is found in close agreement. An interaction is observed between the components during the classification leading to an increased component cut-size and reduced component recoveries in a mixture compared to when it is classified individually. At similar particle sizes, the heavier density component influences the lighter component to migrate towards forced vortex region and shifts the locus of zero vertical velocities towards forced vortex causing a significant increment in the lighter particle cut-size. Separation characteristics of the silica and magnetite particles are explained fundamentally using the equilibrium radius concept via numerical simulations. This concept can be utilized to develop the understanding of the particle performance in the industrial scale during the natural ore beneficiation.

Keyword: Hydrocyclone, Heterogeneous feed, Particle-interaction, Lagrangian particle tracking, Misplacements.

Methodology

The continuity and momentum equations are solved using the unsteady segregated solver with a time step of $5x10^{-5}$s [2],[3]. The geometry and the mesh of the hydrocyclone was created using ICEM. SIMPLE is used for pressure velocity coupling, PRESTO for pressure and QUICK for the VOF equation, solving the water- air phase initially. The momentum equations used QUICK with the Bounded Central Differencing with LES. Followed by the "full water" simulation, at a fixed inlet flow rate and integrate in time until the swirl created an axial region of negative pressure forming the air-core. The secondary phases, i.e. lighter and denser phases with different degree of mixing are injected from inlet and solved using ASM model with the viscosity modification including the fines correction [4],[5]. For the proof of concept, 3-inch experiments conducted at laboratory and simulation data are validated against the numerical data. Followed by which the different size and density proportion of particles are assessed at higher percentage of solids in a larger scale 10-inch hydrocyclone to understand the influence of solids on the component interaction.

Results

Table 1: Design and performance parameters from the numerical analysis:

Mixture	Cut-size (d_{50}) (microns)			Solid Recovery (Rs) (%)			Water split (Rf)(%)
S: M	Mixture	Mag	Silica	Mixture	Mag	Silica	Mixture
100:0		-	16.98	-	-	60.5	12.6

10:90	12.37	7.09	14.54	56.4	74.6	54.7	11.1
20:80	13.64	9.87	15.09	55.4	75.5	51.1	10.2
50:50	15.37	11.26	15.8	67.7	87.1	51.3	9.7
0:100		9.94	-	-	83.1	-	10.6

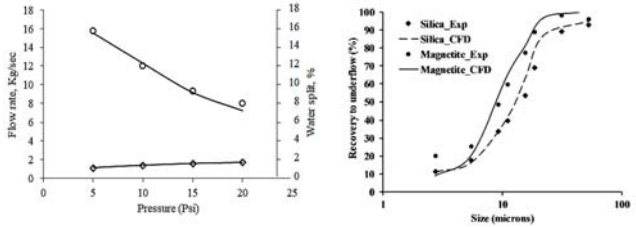

Figure 1: (a) Water split and flow comparisons with experiment (b) Performance curve comparisons of pure component, experimental verses numerical.

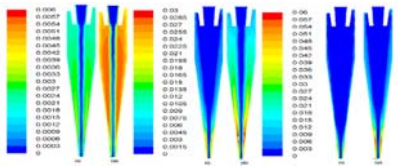

Figure 2: The volume fraction distribution of particles at 10 Psi, and 10 % solids, where (i) heavier particles and (ii) lighter particles.

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Brief Biography

Dr Narasimha Mangadoddy is an Associate Professor & HoD in the department of Chemical Engineering, IIT Hyderabad, India. He received PhD in 2010 from the JKMRC, University of Queensland (Australia). Before joining IIT he worked at R&D-TATA Steel India, JKMRC-Australia on various mineral processing projects. Dr Narasimha's areas of interest include CFD, CFD & DEM for multi-phase flows, particulate technology, mineral processing, slurry rheology, transport processes of separation devices. He has two international patents and 55 referred journal and conference publications. He is the recipient of 2010 & 2016 IIME KHARE best paper award and excellence in teaching award in 2011 & 2015 by IIT Hyderabad.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

Integrated Hydrodynamic and Kinetic CFD model for Column Flotation

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Abstract

Froth flotation is widely used beneficiation process for separating fine valuable minerals from gangue particles using air bubbles in aqueous medium. Column flotation is believed to be effective than mechanical flotation cells due to its inherent advantages such as froth washing system and prevailing quiescent operating flow regime. In the past, Computational Fluid Dynamics (CFD) models were developed for mechanical flotation cell in which significant level of turbulence prevails, however turbulence is not fully developed for the column flotation. In this research work, we focused on the development of CFD model by integration of hydrodynamic parameters with kinetics. Experimentation was carried out in a laboratory flotation column made up of Perspex cylinder having diameter of 0.1m and height of 2.5m. The hydrodynamic parameters such as gas and solids hold-ups are measured using Electrical resistance tomography (ERT) and Sature mean bubble size measured using photographic technique. CFD model was developed using Eulerian-Eulerian approach with k-ε turbulence model for the liquid phase by considering mono sized bubbles and mean particle size. The CFD predicted hydrodynamic parameters were validated with experimental values. First order rate equation was incorporated by user defined functions to calculate probability of collision (P_c) probability of adhesion (P_a) and probability of detachment (P_d). Rate equation was developed for the pulp zone of the flotation column. The model predictions are validated against the published experimental rate constants for coal and chalcopyrite mineral particles and found them in close agreement. This model is having capability to study detailed particle separation dynamics for various flotation process parameters thereby a possibility of design and optimizing flotation column.

Key words: Column flotation, Hydrodynamics, Kinetics, Hydrophobic particles, Eulerian-Eulerian approach, first order rate equation

Brief Biography

I, Prasad Kopparthi have been working in R&D, Tata Steel Ltd as a Principal Researcher. I have 10 years of research experience in the field of mineral processing. Earlier of my carrier, mostly focused on the experimental investigation & optimization of coal flotation processes. Presently, extended to modeling to analyze the flotation process comprehensively. Interested research areas are Interphase science especially coal flotation and gravity separation of fines (Reflux Classifier, Spirals and Tables) and CFD modelling of mineral beneficiation processes such as mechanical flotation cell, column flotation, external sparger and Reflux Classifier. To my credit, I have published 2 papers in international peer reviewed journals, 10 papers in international conferences. I have one granted patent and also 3 filed patents. Currently, pursuing as an external Ph.D at IIT, Hyderbad, Chemical Engineering Dept. I am leading the project to demonstrate 10 TPH Column Flotation with inhouse designed external sparger with dewatering system at one of the Tata Steel captive coal mines site.

Study on the Characteristics and Influence Factors of Air Core inside Hydrocyclone

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Abstract

As an important phenomenon of rotational flow field, air core was always an emphasis in studies of hydrocyclone. For a pretty long period, air core was considered as negative effects, and some methods to eliminate or reduce air core were investigated. Nowadays, with the development of computational fluid dynamics (CFD) simulation method, a clearer and more detailed understanding of air core can be assessed. It was found that unnecessary energy was consumed, but no extra perturbation was brought into flow field by air core. Additionally, air core can reflect the characteristics of flow field and separation performance inside hydrocyclone. In this paper, with the combination of CFD simulation and experimental validation, the forming process and characteristics of air core were investigated. Systematic studies of effects of different structural and operational parameters of hydrocyclone on air core were conducted. On this basis, optimum ranges of parameters of hydrocyclone can be recommended, which had good agreements with recommendations of traditional models.

Keywords: hydrocyclone, air core, influence factors, parameter optimization, CFD simulation

Brief Biography

Dr Baoyu Cui is holding a lecturer position at Northeastern University, China, after he completed his PhD study in mineral processing from the same university in 2014. He has been a joint PhD candidate of Northeastern University, China and CSIRO Mathematics, Informatics and Statistics, Australia from 2010 to 2011. His research interest has now focused on mineral processing theory, beneficiation of Iron Ore, as well as CFD modelling on a wide range of mineral processes.

Mesoscale modeling of drop size distribution in rotor-stator devices

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Abstract

Droplet size distribution represents one of the key parameters of emulsification products and emulsification efficiency. Precise and rational control of droplet size distribution (DSD) is important in emulsification for target oriented product design. While there is a large number of computational fluid dynamics and population balance model (CFD-PBM) simulation for droplet size distribution in various emulsification devices, fitting parameters or empirical correlations were always involved to generate the reasonable simulation. To develop a complete DSD model, crossing the two mesoscales of two different levels is of great significance, viz., the emulsifier adsorption at interfacial level (Mesoscale 1) and the droplet breakage and coalescence in turbulence in rotor-stator device level (Mesoscale 2). While the first mesoscale can be simulated by coarse-grained molecular dynamic (CGMD), the second has been investigated in computational fluid dynamics and population balance model (CFD-PBM) simulation through the Energy-Minimization Multi-Scale (EMMS) approach in Part I. The so-called mesoscale energy dissipation for droplet breakage was derived to close the population balance equations through a breakage rate corrector. The correction factor was then integrated into the fully-coupled CFD-PBM simulation for a surfactant-free MCT-oil/water system. Compared to the original Alopaeus breakage model or the combination of Alopaeus model and Prince coalescence model, this new model could greatly improve the prediction of droplet size distribution, Sauter mean diameter, median diameter and span of size distribution for both the dilute and the dense systems of dispersed oil phase. We then developed a model framework in Part II, coupling CGMD and CFD-PBM simulation through surfactant transport equations in bulk phase and at interface, with source terms taking account of emulsifier adsorption parameters. The parameters including maximal adsorption amount, diffusion coefficient and adsorption/desorption kinetic constants are acquired from CGMD. The coalescence efficiency is then corrected by the interfacial area fraction not occupied by surfactant and fed into the coalescence kernel functions in PBM. Compared to traditional CFD-PBM simulation, the coupled model can greatly improve the simulation of DSD, Sauter mean diameter, median diameter and span for high dispersed phase amount (DPA), and correctly reflect the influence of DPA, surfactant concentration and rotational speed of rotor-stator (RS) devices. While the simulation cases validate and demonstrate the advantage of this new model framework, it is also promising to incorporate different types of surfactant in future.

Reference:

Chen, C., Guan, X., Ren, Y., Yang, N.*, Li, J., Kunkelmann, C., Schreiner, E., Holtze, C., Mülheims, K., Sachweh, B. Mesoscale modeling of emulsification in rotor-stator

devices: Part I: A population balance model based on EMMS concept. Chemical Engineering Science, 2019, 193,171-183.

Chen, C., Guan, X., Ren, Y., Yang, N.*, Li, J., Kunkelmann, C., Schreiner, E., Holtze, C., Mülheims, K., Sachweh, B. Mesoscale modeling of emulsification in rotor-stator devices: Part II: A model framework integrating emulsifier adsorption. Chemical Engineering Science, 2019, 193, 156-170.

Brief Biography

Ning Yang received a B.S. degree and a M.S. degree in mineral processing in 1996, and a Ph.D degree in Chemical Engineering in Chinese Academy of Sciences in 2003. His research interests covers the meso-scale modeling of gas-solid, gas-liquid and gas-liquid-solid flow in chemical and process industries. He also worked in the Institute of Fluid Mechanics of Toulouse as a post-doctoral fellow and Oak Ridge National Laboratory as a visiting scholar. He has many collaboration with industrial partner (e.g., BASF, TOTAL, BP, Unilever, SinoPec, Synfuel China, etc.). He obtained the Excellent Young Scientist Fund from National Natural Science Foundation of China in 2012, Qiushi Outstanding Young Scholar Award for Research Achievements and Transformation in 2013 and SCEJ Award for Outstanding Asian Researcher and Engineer in 2016. He is also the plenary or keynote speakers of ISCRE, APT and GLS conferences. He is the chair of the 14th International Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering (May 30-June 3, 2019).

Recent Works:

Chen, C., Guan, X., Ren, Y., Li, J., Kunkelmann, C., Schreiner, E., Holtze, C., Mülheims, K., Sachweh, B., Mesoscale modeling of emulsification in rotor-stator devices. Part I: A population balance model based on EMMS concept, Chemical Engineering Science, 2019, 193,171-183.

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2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

Bubble dynamics in Hydrogen Production by Photocatalytic Water Splitting

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Abstract

To become a viable fossil-fuel alternative, solar energy requires a cost-effective utilization way. Hydrogen production by photocatalysis water splitting is one of the promising ways for carbon-free energy. Although lots of endeavors have been devoted on design and synthesis of more active and stable photocatalyst, few researches have been carried out on the mass transfer process at the interface of photocatalyst. In fact, this interfacial mass transfer process, which is characterized by bubble evolution, plays an important role in determining the efficiency. The hydrogen and oxygen gas bubble evolution on the photocatalyst surface is a typical interfacial phenomenon controlled by the interfacial interactions and mass-transfer process. In order to optimize the interfacial mass and energy transfer on the photocatalyst surface, understanding of the bubble evolution process is required.

Herein, we studied the bubble dynamics on photocatalyst surface with special emphasis on the effect of light irradiation and surface morphology, and then proposed a method to control the bubble behaviors. The in-situ experimental system that combines the photoelectrochemical measurement and high-speed imaging technique has been conducted. Based on the thermodynamic models of bubble nucleation on the nanostructured surface, the impact of the dimension of morphology has been explored. It has been presented that the wicking nanostructured photocatalyst benefits mitigating the bubble-induced local blockage by forming a reactive liquid film. The coupling effects between bubble and light irradiance have been explored. It was found that the bubble scatter effect changed the light intensity distribution and increased the local photocurrent. We have established a bubble growth model that combines molecular diffusion theory with the surface renewal theory. A modified force balance model including Marangoni force has been built, which is more accurate in predicting the bubble departure diameters on photoelectrode and their variations with light intensity. Finally, for enhancing the conversion efficiency and catalytic reaction rate in the system, we developed a technique for the control of bubble motion dynamics by external disturbance.

Brief Biography

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Prof. Liejin Guo is an academician of the Chinese Academy of Sciences, a scientist of engineering thermophysics and energy utilization and one of the leading academic leaders in China's energy power multiphase flow and hydrogen energy discipline. His current research concentrates on multiphase flow and heat and mass transfer, high efficient clean energy-power system and thermal power conversion process, multiphase flow thermophysics and key technologies of in exploitation and mixed transportation of oil and gas, high efficient conversion and utilization of renewable energy such as solar energy, biomass energy, and the mass production and use of hydrogen energy. He has been serving as member of Scientific Committee of the International Centre for Heat and Mass Transfer, member of the International Information Center for Multiphase Flow, member of the International Association for Hydrogen Energy. He serves in the editorial boards of several international journals including International Journal of Hydrogen Energy, International Journal of multiphase flow and Applied Thermal Engineering, etc. He has published more than 400 papers in journals and conferences, given over 30 invited or keynote lectures in international conferences. He has been awarded with Second Class Prize of National Technology Innovation Awards in 2009 and Second Class Prize of National Natural Science Awards in 2007 and 2017 respectively. He was awarded the global highly cited scientist for more than 10 years from 2002 to 2016 by Thomson Reuters. And he had been selected as a highly cited Chinese scientist from 2014 to 2017 in the energy field by Elsevier.

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High-Resolution Large Time-Step Schemes for Inviscid Fluid Flow

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Abstract

In 2014, SINTEF Materials and Chemistry, in collaboration with the Norwegian University of Science and Technology, received funding from the Research Council of Norway to develop a framework for complex 3D multiphase and multiphysics flows (SIMCOFLOW). The target for this development was to simulate the flow of air, oil and water in an operated oil boom interacting dynamically with wind, waves and sea current. As a supporting activity, more specialized investigations into efficient and accurate numerical models for some simpler flow submodels were performed within this project.

In this presentation, we extend previous works on explicit Large Time Step (LTS) schemes. The generalization is based on the previous work in [1,2,3]. Starting from a general LTS scheme, a set of sufficient conditions for conservative, consistent, and total variation diminishing (TVD) LTS schemes are derived. Second-order accuracy away from discontinuities is achieved by a modified flux approach. Such an approach is shown to be TVD whenever a supplementary condition is satisfied. The full set of criteria constitutes a new framework of sufficient conditions for high-resolution LTS. By application of this framework on the large time-step Roe scheme (LTS-Roe1), a new second-order version (LTS-Roe2) is proposed. Further, to overcome the problems of LTS-Roe1 and LTS-Roe2 with transonic rarefaction, a hybrid scheme of LTS-Roe and Lax-Friedrichs is proposed (Hybrid). The methods are investigated and compared against the second-order LTS-Harten [2] applied to the Euler equations modelling one-phase inviscid fluid flows. Numerical tests for continuous initial conditions show the expected second-order convergence. For discontinuous initial conditions LTS-Roe2 has better accuracy than LTS-Roe1- however, this difference becomes small for high CFL-numbers. LTS-Roe2 is shown to have a very good resolution of discontinuities, but for high CFL-numbers it produces spurious oscillations for the Euler equations. Hybrid is more diffusive, but has no problems with transonic rarefaction. Tests show that LTS-Harten consistently gives good results with less oscillations than LTS-Roe2, but it has, however, a tendency to smear out discontinuities when the CFL-number is increased.

Figure 1 illustrates the ability of LTS-Roe2 to provide high resolution for large time steps, i.e. we avoid excessive oscillations near discontinuities while retaining second order accuracy for smooth solutions. On the left, a Courant number C=4 was used, whereas on the right C=8; i.e. the sonic waves propogate through 8 cells per time step.

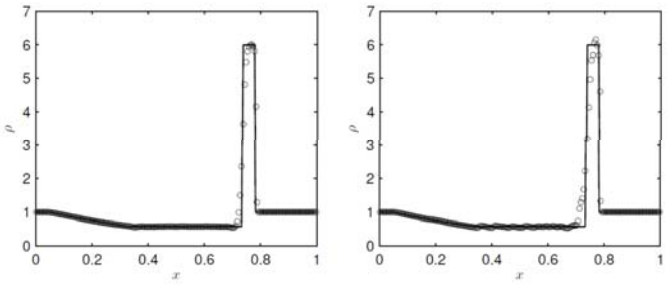

Figure 4: Shock tube problem for the Euler equations. Density plot.

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Brief Biography

Tore Flåtten received his PhD degree in Computational Fluid Mechanics from the Norwegian University of Science and Technology, Trondheim, Norway in 2004. Since then, he has been affiliated with several Norwegian research institutes, performing contract research with a particular focus on the numerical and mathematical analysis of multiphase flows. Herein, he has supervised 7 Master and 5 PhD students and published 28 papers in peer-reviewed journals.

Sigbjørn Løland Bore holds master's degrees in mathematical physics from both the Pierre and Marie Curie University in Paris and the Norwegian University of Science and Technology in Trondheim, Norway. He is currently completing his PhD studies in computational chemistry at the University of Oslo, Norway.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

Computational fluid dynamics (CFD) investigation of the AOD process with six submerged side-wall tuyeres

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Abstract

A compressed injection flow model was developed in a Eulerian multiphase flow approach by using a three-dimensional (3-D) unstructured orthographic grid system. The model considers the AOD converter with six submerged side-wall tuyeres to investigate the influence of injection pressure and bubble size on the jet behavior, the flow pattern, the stirring height and the mixing efficiency. The investigations show that inlet pressure significantly affects the jet behavior. Increasing the pressure boosts the velocity of the gas phase, thereby increasing the penetration depth of the jet. The bubble plumes are located close to the side wall, and a vortex appears on each side of the bubble plume, namely, the bulk vortex and the corner vortex. In addition, the former has an opposite direction vector against the later. Bubble size has a pronounced impact on the flow pattern, stirring height and mixing efficiency. Increasing the bubble size within a certain range can improve the penetration depth and reduce the mixing time. This model can be further extended to consider the chemical reactions in the AOD reactor.

Brief Biography

Dr. Zhongfu Cheng is a postdoctoral research fellow in Department of Materials Engineering at KU Leuven. He received his B.Sc. degree in metallurgy engineering in 2010, and his PhD degree in ferrous metallurgy in 2016, all from Northeastern University (NEU, Shenyang, P.R. China). His PhD project mainly focuses on the development of the bottom powder injection for refining ladles. During his degrees, he took on two academic projects as the leader: The 3rd National University Student Innovation Program, thesis: Study on the flow characteristic and the control of interfacial behavior of steel/slag in wide and thick slab continuous casting model (2008-2009), and Graduate Research and Innovation Program, thesis: Development of bottom powder injection device for refining ladle (2012-2014). After that, Dr. Cheng joined the research group for high temperature processes and industrial ecology at KU Leuven.

His study interests are mainly in the areas of simulation, slag engineering and plasma fuming, focusing on the aspects of CFD simulation of multiphase flow behavior for AOD refining processes and plasma fuming disposal for metallurgical residues. He has already published 8 papers and also obtained 8 patents authorized.

Free Surface Lattice Boltzmann Method and Large Eddy Simulation modeling of Free Surface at the top of the Continuous Casting Mold

Zhao Peng[1, 2], Shaoli Yang[1], Lanhua Zhou[1] and Zongshu Zou[3]

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[2] *State Key Laboratory for Vanadium and Titanium Testing, Panzhihua, 61700, China.*

[3] *School of Metallurgy, Northeastern University, Heping District, Shenyang, 110819, Liaoning, China.*

Email: zhaopeng@research.neu.edu.cn

Abstract

Behavior of free surface at the top of the continuous casting mold can strongly affect the slag entrainment, which is associated with final quality of the continuous casting slab. Free surface is simulated by the three-dimensional models of Free Surface Lattice Boltzmann Method and Large Eddy Simulation (FSLBM-LES). The model is verified by the good agreement between the calculated result and the measurement. The effect of various operating conditions on the fluctuation of free surface is also investigated. The result show that FSLBM-LES model can offer a promising way to study the fluctuation of free surface and related complicated phenomena inside the mold.

Brief Biography

I am Peng Zhao, Ph.D., graduated from School of Metallurgy, Northeastern University. My major is Ferrous Metallurgy. I am engaged in the macroscopic and mesoscopic numerical simulation of continuous casting, and the comprehensive development of the vanadium-titanium magnetite as well as the efficient utilization of secondary resources at Panzhihua University, China.

Numerical simulation on flow field characteristics of backflow controller

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Abstract

Efficient and safe drilling is an important issue in the drilling industry and a concern for drilling engineers, especially for hard formations. Based on techniques of underbalanced drilling and coiled tubing drilling, the authors propose a new technology of partial underbalanced drilling modulated by coiled tubing which increases the rate of penetration and ensures safe drilling. In this technology, a method of cooperating with a coiled tubing and drill pipes is adopted to form an annulus between the drill pipe and the well wall and a micro annulus between the drill pipe and the coiled tubing. The coiled tubing is connected to the bit directly through the pipes. The reflow controller is an important part of the technology connecting the annulus and the micro annulus. The flow field characteristics of the backflow controller are studied by numerical simulation. The DDPM model was used to simulate the cuttings transport through the backflow controller, and the Realizable k-ε model was used to simulate the flow of drilling fluid. The cuttings movement is simulated at different rotational speed, different flow rate of drilling fluid and different size of cuttings. The residual cuttings is defined, the cuttings in the fluid domain, to represent the cuttings carrying capacity at various parameters. The results of numerical simulations show that the backflow controller has a pressure drop of about 2 MPa when the flow rate varies from 12 L/s to 16L/s. The flow rate rises suddenly as the fluid approaches the holes of the backflow controller. And the increase of the rotational speed or the size of cuttings leads to the decrease of the cuttings-carrying ability. On the contrary, the increase of the flow rate enhance the cuttings transport of the backflow controller. The flow characteristics of the backflow controller were obtained through numerical simulation, which provides a basis for studying the partial underbalanced drilling modulated by coiled tubing technology.

Brief Biography

Huaizhong Shi is a senior engineer at the China University of Petroleum (Beijing), China, focusing on the efficient drilling technology, fluid mechanics in petroleum engineering, high pressure water jet, and so on. He has MSc and PhD degrees in oil and gas-well engineering from China University of Petroleum (Beijing), and visited University of Louisiana at Lafayette as a visiting scholar for a year. He has published more than 20 papers in his research field. CFD is used by him to calculate solid-liquid two phase flow in drilling process.

An Experimental Study of Enhanced Heat Transfer of Nano-encapsulated Phase Change Material Slurry Embedded in Metal Foam

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Abstract

Nano-encapsulated phase change material slurry (nano-PCMS) has the merits of high latent heat and high surface area, and overcomes the defects of supercooling and volume expansion that exist in most organic/inorganic PCMs. Subjected to the low thermal conductivity, the thermal management systems using nano-PCMS are highly dependent on slurry's convection coefficient, which cannot be guaranteed in the condition where the natural convection is constrained. Here, we proposed a novel thermally stable and efficient hybrid PCM that infiltrating nano-PCMS into metal foam for passive thermal management. The experimental results indicated that the addition of metal foam could reduce the heated surface temperature by maximum 38% in regardless of heated angle, while this contribution was 24% achieved by natural convection of pristine nano-PCMS. The flow convection of nano-PCMS was completely suppressed in the foam cells due to the high viscosity of slurry and flow resistance of foam matrix. Higher porosity composite obtained lower heat transfer efficiency and more pronounced thermal non-equilibrium effect attributed to its lower effective thermal conductivity and less interfacial area. This newly-proposed foam/nano-PCMS composite not only provides high heat transfer efficiency, but reduces the dependency on the convection coefficient of nano-PCMS.

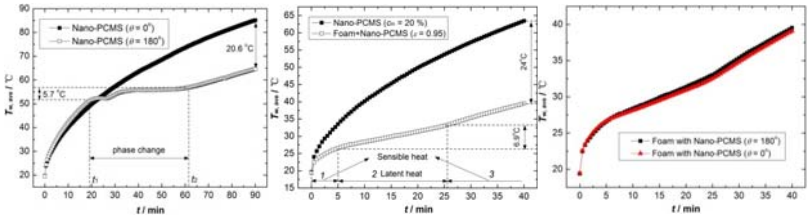
Experimental

Figure 1 shows experimental system and the test rigs for evaluating the flow and thermal characteristics of the foam/nano-PCMS composite. The composite was caged in a plexiglass cavity An electric-insulated film heater was attached onto the copper substrate using a silver glue The whole test rig was then thermally-insulated by polyurethane foam plates (k_{in} = 0.03 W/m·K). In this study, the influence of flow convection of slurry on the thermal performances of pristine nano-PCMS and foam/nano-PCMS composite was also evaluated. We positioned the experimental setup in two sets of angles, i.e. θ = 180° representing heated from top and θ = 0° representing heated from bottom. θ is the angle between heatflux and positive *y*. A constant heat power 7 W was provided by a D.C. stabilizer, which was connected to the film heater. We stuck five T-type thermocouples on the film heater and calculated the arithmetic mean value as the average surface temperature. The temperature signals were measured every 30s using Agilent data logging system.

Fig.1 Experimental system and test rigs

Results

As Fig.2(a) shows, for pure slurry, surface temperature increased at a dramatic rate in condition of heated from top(θ= 180°). Comparatively, for the case heated from bottom(θ = 0°), the heat transfer was enhanced due to the slurry flow convection, which triggered more internal PCM particles to phase change and more latent heat to absorption. The maximum temperature was reduced by 24.2%. For foam/slurry composite(Fig.2b), the foam/nano-PCMS combination presented much better thermal control capability. The surface temperature was reduced by 38% compared with the pure nano-PCMS. In Fig.2(c), the two curves almost overlapped in the temperature range considered with their maximum difference of less than 0.4 °C. This implied that in bottom-heated condition (θ = 0°), the heat transfer mechanism was still dominated by combined heat conduction of the composite and the slurry's convection was almost suppressed by foam strut.



(a) (b) (c)

Fig.2 Performance of nano-PCM and nano-PCM/foam composite

Brief Biography

Wenqiang Li is the associate professor of department of Key Lab of Science and Technology on Combustion, Internal Flow and Thermal-structure at Northwestern Polytechnical University in China. He obtained the Ph.D in department of Energy and Power Engineering at Xi'an Jiaotong University. His research interests center on the enhanced heat transfer in porous material, thermal storage and management with phase change material, and their applications in the cooling for electronic devices.

DEM-based Virtual Experimental Blast Furnace Model and Its Applications

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Abstract

Intensive heat and mass transfer between continuum fluids and discrete particulate materials is quite common in many chemical processes. To understand and improve the operation of these processes, discrete particle models are very helpful when they are combined with flow, heat and mass transfer and chemical reaction models. However, due to the high computational cost with discrete particle models, it is not practical until now to study long transient processes. A transient discrete element method-based virtual BF model is developed recently through scaling and allows the study of the transient process at a particle scale (Fig. 1). The scaled model is able to simulate the process two orders faster and makes it practical to track the whole process of iron ore reduction from burden charge to the cohesive zone. This work will introduce the transient discrete element method-based virtual BF model and its applications to the study of the effects of burden batch weight and distribution. The results demonstrate that the scaled virtual BF model can reasonably predict in-furnace flow state, temperature distribution, iron ore reduction and the characteristics of the cohesive zone (Fig. 2).

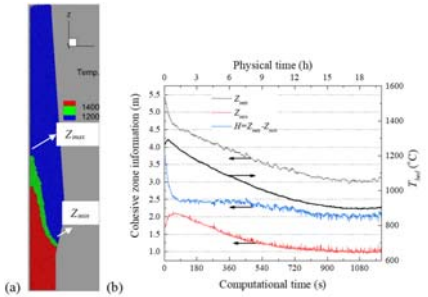

Figure 1. (a) The cohesive zone according to temperature field (1200~1400°C) and the evolution of key parameters (Z_{max} is the Z coordinate of the highest particle within the temperature range, Z_{min} for the lowest; H for the cohesive zone height, and T_{bed} for the bed temperature).

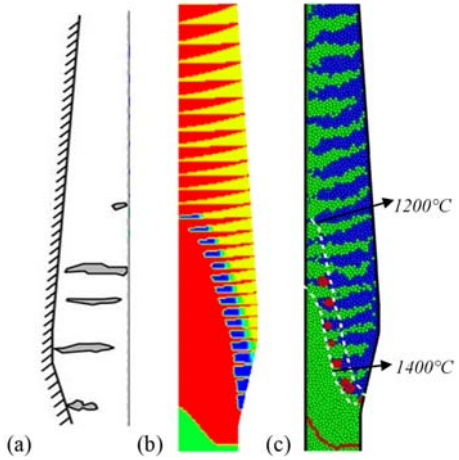

Figure 2. The cohesive zone: (a) from experiments (*Watakabe et al., ISIJ Int., 2013*) (b) from CFD model and (c) from the present particle scale simulation (coke particles are green and iron ore particles are blue).

Brief Biography

Dr Hou is a current ARC DECRA Fellow and Research Fellow in the Department of Chemical Engineering at Monash University. He was awarded a PhD at UNSW of Australia in 2012, ME and BE in 2003 and 2000 respectively from Northeastern University of China. Aiming to formulate safe, energy efficient and sustainable processes involving granular materials, his research mission and passion centre in the understanding of the mechanics and thermochemical behaviours of granular (and multiphase) flows and their impact on structures and environment through rigorous cutting-edge multiscale modelling techniques, experiments and theoretical analysis. The knowledge can be applied to solving energy and water issues in the industry including chemical, metallurgical, mineral processing, agriculture, pharmaceutical and geotechnical engineering. His main research areas include: (i) heat transfer and chemical reactions in gas-solid flows, (ii) multiphase flows in water treatment, (iii) granular flow stability pertinent to segregation and mixing, and (iv) development of numerical techniques and virtual process models. Dr Hou has published 60+ articles, and attracted over A$2M research funds. Dr Hou has also received various awards in the past, reflecting the recognition at different stages, and been invited to give talks at different international conferences. He has also involved in the co-supervision of 4 PhD candidates (one graduated in 2018) and undergraduate teaching at UNSW and Monash University.

Euler-Lagrangian Simulations On Pyrolysis Oil Spray And Viscosity Effects on a High-Pressure Multi-Hole Injector Nozzle

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Abstract

Pyrolysis oil is becoming a promising alternative to traditional fossil fuels to power diesel engines for Combined and Heat Power (CHP) units[1]. Pyrolysis oil has a higher viscosity and the spray hydrodynamics is expected to change due to larger viscous energy dissipation in the droplet-droplet interactions, promoting more coalescence. The efficiency of fuel spray combustion on diesel engines heavily depends on the droplet size distribution and the fuel mass that wets the combustion chamber walls before its evaporation. A larger exposed droplet surface area to the surrounding gas phase, is key to have high droplet evaporation rates and therefore reduce the fuel ignition time. In this work, an insightful computational work has been performed in order to elucidate more insight about the influence of viscosity on the outcome of binary droplet collisions by means of a benchmarking droplet collision model[2] where viscosity effects are accounted for in terms of the Ohnesorge number $\left(Oh = \frac{\mu}{\sqrt{\rho \sigma d_d}}\right)$.

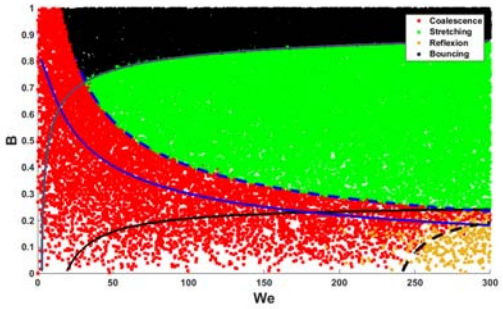

Figure 5 Regime boundary map for Oh=0.44. Ashgriz and Poo boundaries (dashed) and Finotello regime boundaries (solid lines)[2].

An Euler-Lagrangian model has been utilized to perform a sensitivity analysis about the influence of viscosity on the flux size distribution. In Figure 2, it can be observed that viscous forces only play a significant role at relatively low injection pressures (16 bar), while at 200 bar the viscosity influence is hardly perceived.

Besides, a parametric study on the far-field spray dynamics is performed, where droplet interactions are relevant and primary and secondary breakup effects are not considered. In this work, it is shown that other operating spray conditions rather than fluid viscosity such as fuel density or ambient pressure play a more significant role on the spray characteristics (droplet size and velocity) due to droplet collisions. Denser fluids or/and higher ambient pressure lead

to more coalescence events, increasing the Sauter Mean Diameter (SMD), while an increase on the fluid viscosity only leads to an almost negligible increase in the SMD.

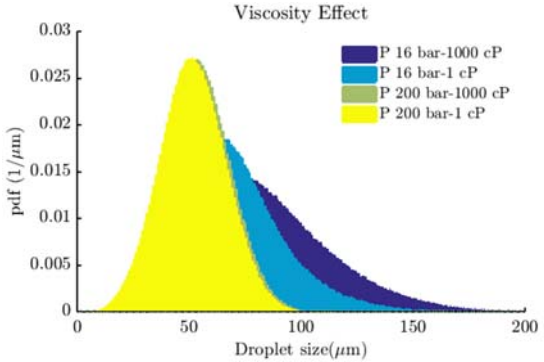

Figure 6 Flux size pdf. Yellow: Injection pressure at 200 bar and μ= 1 cP. Green: Injection pressure at 200 bar and μ= 1000 cP. Blue: Injection pressure at 16 bar and μ= 1000 cP. Cyan: Injection pressure at 16 bar and μ= 1 cP.

This study also shows evidence about how the injection angle and the piston chamber design play a key role on the internal circulation patterns, which locally determine the nature of the collisions' outcome. Furthermore, we assess the influence of the fuel physicochemical properties on the fluid-wall impingement times on a high-pressure combustion chamber of a multi-hole injector nozzle. These results show that denser fluids than diesel lead to shorter droplet free paths, decreasing the droplet residence time without hitting the chamber walls.

Author's Biography

The author (A.E. Carlos Varas) is a Spanish chemical engineer who has received his doctorate degree in 2017 in the group of Multiscale Modelling of Multiphase Reactors at Eindhoven University of Technology under supervision of J.A.M Kuipers and E.A.J.F. Peters. The title of his PhD thesis was "Experimental and numerical studies on riser hydrodynamics and mass transfer". Earlier steps on his professional career were taken in the industrial sector. The author joined International Flavors and Fragrances (Spain) as a chemical operator, and he was promoted to the Research and Development department as Processes technician. In 2010, he decided to pursue new professional challenges abroad and started the Process Engineering MSc at Eindhoven University of Technology. After the completion of his MSc degree, he joined the Multiphase Reactors Group in January, 2013 to start his PhD. Currently, he is leading a post-doctoral research project about CFD modelling and experimental validation of pyrolysis oil spraying.

1. **B.V.Beld, E.Holle and J.Florijn**. *Applied Energy* (2013) 102, 190-197

2. **Finotello G., Kooiman R.F., Padding J.T., Buist K.A., Jongsma A., Innings F. and J.A.M. Kuipers.** *Experiments in Fluids* (2018) 59:17

CFD Modelling of a Lime Kiln Burner

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Abstract

CFD modelling was used to assist a lime kiln burner operation upgrade. CFD was used to model the performance of the existing and new burner before it was installed, to demonstrate that the design objectives would be met, in particular:

- Improve the thermal performance (heat transfer) from the burner;
- Ability to operate successfully on 100% gas and co-firing up to 50% waste oil with the new burner;
- Controllable and adjustable burner operation;
- No increases in NOx emissions.

The software used in the simulations was Fluent, from ANSYS Inc. The computational domain includes kiln hood and a 45 meters long rotary kiln. A polyhedral mesh was build with appropriate mesh size refinements where large gradients should exist. The models and the chemistry mechanisms used in this study were:

- K−ω SST model for turbulence;
- Two step reaction mechanism for methane combustion, and one-step reaction for both ethane and waste oil combustion;
- Finite rate and eddy dissipation model for turbulence-chemistry interaction;
- Discrete ordinate model for radiation, with WSGGM for radiation absorption.

Previously to the modelling stage, a site survey was conducted to provide information on the process and on kiln operation, such as feed and firing rates, secondary air temperature, primary air flow rates, etc. The boundary conditions for the CFD modelling were established based on these measurements and a mass and energy balance of the system.

CFD was used to assess the kiln aerodynamics, gas temperature, species, heat of reaction and wall heat flux profiles for all cases considered in the project. From these results the adjustability of the FCT burner can be observed by varying the gas swirl in order to change the amount of heat transferred to the bed between heat flux peak and kiln discharge. It was also demonstrated that FCT's burner can operate with different fuels, either separately or by co-firing them. A reduction in fuel consumption was demonstrated though a better heat recovery of secondary air in the cooler for the FCT burner as it uses substantially less cold primary air then the existing burner.

NOx calculations were modelled using a post-processing approach. Thermal, prompt and fuel NOx pathways mechanisms for NOx formation were used, with thermal NOx being identified as the main pathway. The predicted NOx concentrations for all FCT burner cases are lower than the existing burner benchmark.

Brief Biography

Brad Wilson is the lead process engineer at FCT since 1998. Graduated in Chemical Engineering and holding a TUV certificate in Functional Safety Engineering, he is the combustion engineering specialist, with extensive engineering and site experience in Australia and around the world for heat transfer equipment such as rotary kilns, multiple hearth furnaces, dryers and flash calciners in a broad range of process industries including cement, lime, alumina, magnesia and iron pellet.

Roger Hassold is the general manager and is at FCT since 2014. Graduated in Chemical Engineering and holding a certificate in Advanced Management Program, he is an experienced combustion engineer, designing, installing and commissioning advanced burner systems for industrial clients and solving complex pyro-processing problems with the use of CFD modelling. Roger is also an experienced Production Manager, Technical Manager and Process Engineer in the cement and lime industry and has worked with a large range of kiln technologies and product types.

Yvonne Yu is a CFD Modelling Engineer at FCT since 2015. She is graduated in Mechanical Engineering and International Economy and Trade, holding two master degrees, from University of Adelaide, in Mechanical and Aerospace Engineering. Yvonne has worked with renewable fuels and is an experienced CFD Modelling Engineer, developing CFD projects for kiln and calciner burners in the cement, lime and iron ore pellet industries, as well as for ceremonial flame applications and R&D projects.

Renata Favalli is a CFD modeller at FCT since 2017 but has been developing CFD projects for pyro-processing industries as well as for the environmental control sector since 2007. For the year of 2004, she held an academic visitor position at Imperial College, London, shortly after her Ph.D. graduation at IPEN – Research Institute on Energy and Nuclear Power, a Brazilian autarchy associated to the University of Sao Paulo.

Jordan Parham is the CEO since 2017 but has been working at FCT since 2002. He is graduated in Mechanical Engineering and has a Ph.D. in combustion and fluid dynamics, with extensive experience with FCT as a combustion engineer, designing and installing advanced burner systems for industrial clients, including research and development of the GyroTherm burner technology which FCT has an exclusive license to market worldwide.

Modelling of Effect of Gas Flow rate on Open-eye Formation and Mixing Time of Nickel Alloy in Argon Stirred Industrial Ladle

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Abstract

In secondary metallurgy, argon gas stirring and alloying of elements are very important in determining the quality of the steel. The argon gas is injected through the nozzle located at bottom of the ladle into the molten steel bath, this gas breaks up into gas bubbles and breaks up the slag layer creating an open-eye. Additions to the molten steel are performed through the open-eye to attained the desired steel composition. In this work, physical modelling measurements are conducted to study the effect of gas flow rate on the open-eye size and mixing time of nickel alloy dissolution. The mixing time of nickel alloying with the liquid steel in the ladle within the range from 7.99 to 8.04 was investigated. The physical modelling results show that the open-eye area and mixing time increases with increase in the gas flow rate. A new mathematical model is developed to study the air-liquid metal-slag-nickel alloy four-phase flow in the ladle. The Eulerian volume of fluid (VOF) model is used for tracking the liquid metal-slag- air interface and the Lagrangian discrete particle model (DPM) is used for describing the movement of dissolution of nickel. The simulation results of open-eye area and mixing time of nickel alloying showed a good agreement when compared to experimental results measured.

Brief Biography

Mr. Eshwar Kumar Ramasetti is a third year doctoral student at the University of Oulu, Finland. This PhD program is a part of Marie Sklodowska Curie Horizon 2020 project funded by European Union. As part of the program the author will be working half time at University of Oulu (academic partner) and at Outokumpu research center (industrial partner) during the three-year period. The author received Master's degree in Mechanical engineering from Manchester Metropolitan University, United Kingdom. The author also received Post Graduate diploma in Thermal Power Fluid Engineering from University of Manchester, United Kingdom. The research interests of the author include the CFD application to multi-phase flows in the areas of oil & gas flows, metallurgical flows, minerals engineering, food and process industries.

Droplet-Droplet Collisions in a Spray Dryer

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2 Intensified Reaction and Separation Systems, Department of Process and Energy, Delft University of Technology, The Netherlands

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Abstract

In this work we investigate droplet-droplet collision interactions in a spray dryer. An Eulerian-Lagrangian model with coupled gas phase and droplet heat and mass balances is used to study air flow dynamics, temperature and humidity profiles at different positions of the spray. Moreover we study the combined effect of droplet collisions and their response to turbulent dispersion in a spray. The quality of the final powder produced in a spray dryer is indeed strongly dependent on the processes of coalescence, leading to droplets with larger sizes, and break-up, leading to smaller droplet sizes.

The dispersed phase is treated with Lagrangian transport of droplets and the turbulent gas flow using large eddy simulation (LES). A Direct Simulation Monte Carlo (DSMC) method is used to stochastically model the collisions between droplets. The outcome of a binary collision is described by collision boundary models by Finotello et al. (2018) for water and milk concentrates. A turbulence dispersion model, based on the Langevin equation, accounts for the stochastic subgrid fluid velocity fluctuations along the droplet trajectory. Nijdam et al. (2006) compared the Eulerian and Lagrangian approach to include turbulent dispersion and coalescence in a spray. They demonstrated the importance of applying a turbulent dispersion model and indicated the Lagrangian approach as the most flexible in applicability. To model the droplet drying, the reaction engineering approach (REA) by Cheng et al. 2013 is used.

The effect of the inlet air conditions and of droplet viscosity on the droplet size distributions are analyzed. In the axial direction, most of the heat and mass transfer occurs in the vicinity of the droplet inlet. The radii of the droplets increase, both in the axial and radial direction, because of the high frequency of coalescence in the whole droplet spray. The particle size distributions are affected by evaporation in the vicinity of the nozzle while, at larger axial distances, the effect is less visible. The domain in which heat and mass is transferred is very small, so the amount of evaporation is still low. The droplet size distributions for water and milk concentrates present only small differences. We observe that collisions increase the Sauter Mean Diameter because of coalescence occurring in a wide volume of the spray. This has a strong implication for evaporative processes, where the mechanism of mass and heat transfer between a drop and the fluid medium is influenced by the interface area. The changes of the droplet phase due to the turbulent dispersion are analyzed in terms of number and frequencies of collisions. Droplet-droplet collision outcomes are studied in the entire spray with non-dimensional parameters (Weber, Reynolds and Ohnesorge numbers). For our system, in the presence of turbulent dispersion, the collision rates of all the regimes are enhanced and the total number of collisions increases by 25%, while the overall dynamics of the spray, such as spray angle and width, are not modified. The distributions of We, Re and Oh numbers show that the spatial evolution of collisions strongly depends on their position in the spray, see Fig. 1. With increasing the droplet viscosity the coalescence is promoted and, as a consequence, the number of droplets available for collision decreases and the collision frequency reduces.

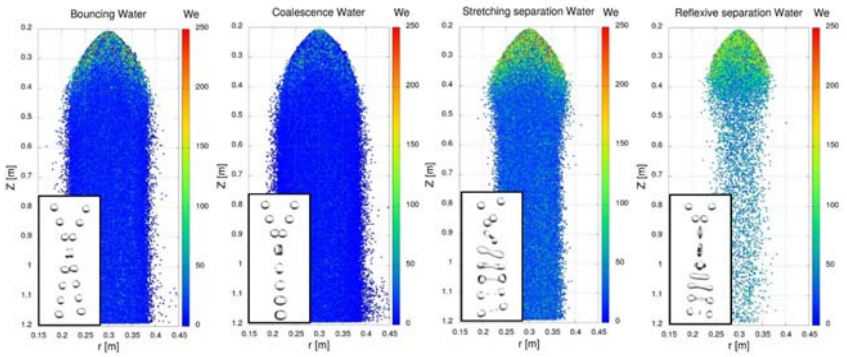

Fig.1 Weber number of the droplets in the entire spray dryer for coalescence, bouncing, stretching separation and reflexive separation.

The results obtained in this work can be used to better describe droplet collisions in sprays when drying and dispersion is included.

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Biography

Giulia Finotello was born on 14th July 1989 in Torino, Italy. She completed her Bachelor degree in Chemical Engineering in Politecnico di Torino, Italy in 2011 with great honor. In the same year she started the Master of Chemical Engineering at the same university. In 2013 she started a trainee in the Fluid Dynamics team of BASF, Ludwigshafen, Germany. She received her Master degree in 2014 with a thesis on simulation of the effect of coalescence and break-up on the mass transfer in stirred tanks. From November 2014, Giulia is a PhD candidate in the Multiphase Reactors Group of Eindhoven University of Technology, The Netherlands with a project in collaboration with Tetra Pak Heerenveen, The Netherlands.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

Front Tracking of the free surface in an Euler-Lagrange gas-liquid model

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Abstract

Bubbly flows represent a widely distributed category of multi-phase flows in the process industry, as for instance in Fischer-Tropsch reactors, waste water treatments or electrolytic processes. Despite the applications are known since several decades, detailed knowledge of the underlying transport phenomena is still lacking, due to the complexity of the hydrodynamics, especially in heterogeneous flows. Computational Fluid Dynamics (CFD) has demonstrated to be a promising way of gaining fundamental insights in such flows, overcoming known experimental limitations.

Several scales have been acknowledged in the framework of CFD, ranging from detailed but computationally expensive Direct Numerical Simulations (DNS) to widely adopted Euler-Euler simulations. At the meso-scale, Euler-Lagrange models allow to describe the motion of bubbles and their interactions in a Lagrangian manner, while reaching a relatively larger scale compared to DNS. In such models, rarely the top free surface dynamics is accurately tracked, ranging from being neglected in most in-house codes to being described with a diffuse interface in available commercial software. Generally, the inherent assumption is that the interface dynamics does not influence the flow field, unless considering the vicinity of the free surface. However, in particular cases, as for instance when dealing with flat columns, an accurate description of the free surface is needed to avoid instabilities.

For these reasons, a Front-Tracking free surface (Roghair, van Sint Annaland and Kuipers, 2013) has been implemented in an in-house Euler-Lagrange model (Lau, Bai, Deen & Kuipers, 2013). The free surface consists of tracer points connected in a triangular mesh. Remeshing has been implemented to smooth imperfections and maintain an optimal mesh. In this work, the free surface has been carefully validated with simplified test cases, as the filling of a tank or Rayleigh-Taylor instabilities (Figure 1). In addition, a multiphase test case has been compared with the available experimental results and with the Euler-Lagrange code without the free surface, to understand the influence of it on the flow field.

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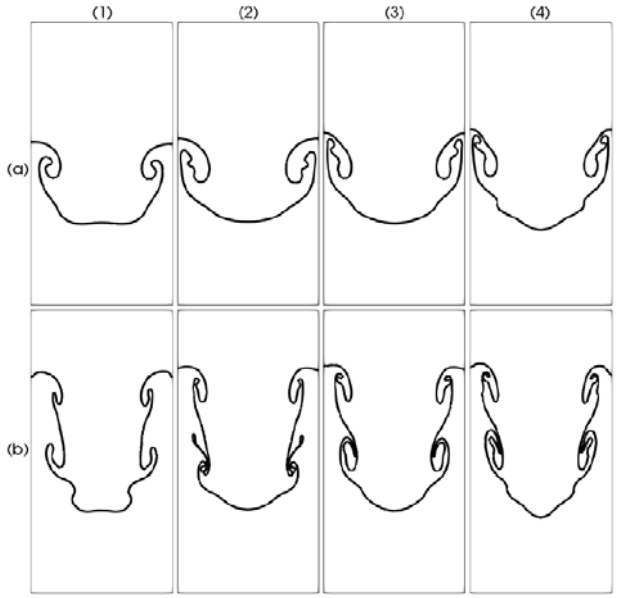

Figure 7 Rayleigh-Taylor instabilities. (a) horizontal slice along the center of the domain (b) diagonal slice, corner to corner. 1-4 represent increasing grid resolutions.

Brief Biography

Alessandro Battistella was born on the 22nd of April 1990 in Merate, Italy. He started his bachelor degree program in Chemical Engineering in 2009, at Politecnico di Milano, Italy, where he graduated in 2012. Soon after he started his Master of Science program in Chemical Engineering at the Eindhoven University of Technology, the Netherlands, where in 2014 he successfully defended his MSc thesis titled "Membrane Assisted Chemical Looping Reforming process modeling for H_2 production", within the group of Prof. Martin van Sint Annaland.

After his graduation, he joined SABIC for a 6 months traineeship in Geleen, the Netherlands, where he worked on reaction kinetic modeling. In September 2015, he decided to pursue a doctoral degree in the group of Prof. Martin van Sint Annaland, under the guidance of him and Dr. Ivo Roghair in the Multiphase Reactors group at the Eindhoven University of Technology in the Netherlands. His research project, funded by the Netherlands Organisation for Scientific Research (NWO) deals with CFD modeling of bubbly flows, and in particular with the fundamental understanding of the interlinks between mass/heat transport and phase transition with the hydrodynamics. The results of this work are part of his research.

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Numerical and experimental study of bubble formation in supersaturated water

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Abstract

Phase transition is a natural phenomenon which occurs in everyday life as well as in many relevant industrial applications. The formation of gas bubbles as a consequence of supersaturation represents a common situation in, for instance, electrolytic processes or in industrial fermenters. Thus, detailed knowledge of the fundamental transport phenomena and their interactions with the hydrodynamics is required for the further design and optimization of such systems.

The predominant mechanism for bubble formation is heterogeneous nucleation (Jones, Evans and Galvin, 1999), and while it has been studied on the micro-scale (e.g. Enriquez et al, 2013), the influence of bubble nucleation on the meso-scale performance of bubble column reactors is still scarcely investigated. In this work, a meso-scale Euler-Lagrange model accounting for bubble nucleation in a supersaturated liquid is described.

The Discrete Bubble Model (DBM) is a meso-scale Euler-Lagrange model where bubbles are treated as point particles and tracked in a Lagrangian fashion, while considering their interactions such as collisions, coalescence and breakage (Lau, Bai, Deen & Kuipers, 2013). The model has been expanded to include discrete nucleation sites, initialized as conical cavities with defined radius and depth. On each site, a gas pocket can form, allowing for the nucleation, growth and detachment of gas bubbles.

With this model, the formation of CO_2 bubbles in supersaturated water has been studied on different surfaces. The influence of surface properties on the hydrodynamics of a nucleating flow has been linked with experimental data, in order to gain fundamental insights on the phase transition process.

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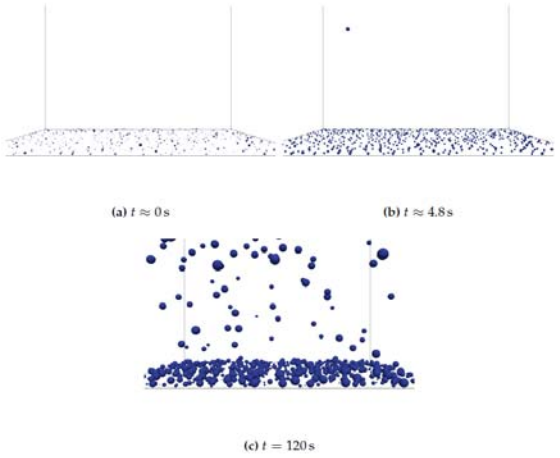

Figure 8 Snapshot of the bubble nucleation process in the DBM: (a) initial gas pockets, (b) first detachment and (c) pseudo-stationary.

Brief Biography

Alessandro Battistella was born on the 22nd of April 1990 in Merate, Italy. He started his bachelor degree program in Chemical Engineering in 2009, at Politecnico di Milano, Italy, where he graduated in 2012. Soon after he started his Master of Science program in Chemical Engineering at the Eindhoven University of Technology, the Netherlands, where in 2014 he successfully defended his MSc thesis titled "Membrane Assisted Chemical Looping Reforming process modeling for H_2 production", within the group of Prof. Martin van Sint Annaland.

After his graduation, he joined SABIC for a 6 months traineeship in Geleen, the Netherlands, where he worked on reaction kinetic modeling. In September 2015, he decided to pursue a doctoral degree in the group of Prof. Martin van Sint Annaland, under the guidance of him and Dr. Ivo Roghair in the Multiphase Reactors group at the Eindhoven University of Technology in the Netherlands. His research project, funded by the Netherlands Organisation for Scientific Research (NWO) deals with CFD modeling of bubbly flows, and in particular with the fundamental understanding of the interlinks between mass/heat transport and phase transition with the hydrodynamics. The results of this work are part of his research.

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Forces Acting on a Particle Moving Near a Wall at Low *Re* Numbers

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Abstract

In suspension flows, particles flowing along a channel move towards or away from the channel walls and accumulate at different equilibrium distances from the wall. In the absence of inter particle collisions (ie, a dilute suspension), this particle migration is caused by hydrodynamic lift forces. These forces are significant in applications such as cancer-detecting and cell sorting in microfluidics, and in flow cytometery [1]. In the biological flow context, theses wall induced forces contribute towards the separation between platelets and red blood cells that results in a Cell Free Layer (CFL) forming adjacent to blood vessel walls. CFL development is crucial for blood clot formation, as the presence of this layer increases the platelet concentration near (damaged) vasculature walls, enhancing the coagulation process [2].

Lift forces act in a direction normal to the flow and are due to small but finite inertial effects. In a linear unbounded flow, a neutrally buoyant particle can experience lift due to slip (relative velocity of particle), combined with shear or rotation. Near a wall, the presence of the wall induces extra flow disturbances, resulting in increased lift forces [3]. In unbounded linear flows, a freely translating neutrally buoyant particle moves at the same velocity as the fluid (ie, zero particle slip) and hence, there is no slip induced lift component. However, in wall bounded flows, a shear induced drag force causes particles to lag the fluid near the wall. This generates a finite particle slip velocity in the vicinity of the wall that results in a slip induced lift force that drives neutrally buoyant particles away from the wall. Additionally, a neutrally buoyant particle moving near a wall experiences a shear-based wall induced lift force, irrespective of its slip.

As part of a continuing project on developing a multiphase model for dilute particle migration, this single particle study examines the effect that wall induced drag forces have on neutrally buoyant rigid spherical particles moving freely in a linear flow, close to and parallel with a wall. The slip velocities are obtained under low inertial conditions ($Re_\gamma = 0.1$) and in the near the wall region of $1.2 \leq l/a \leq 10$ by setting the net drag force on the particle to be zero. The velocities closely follow the previously reported values calculated under Stokes and low inertia conditions [4,5].

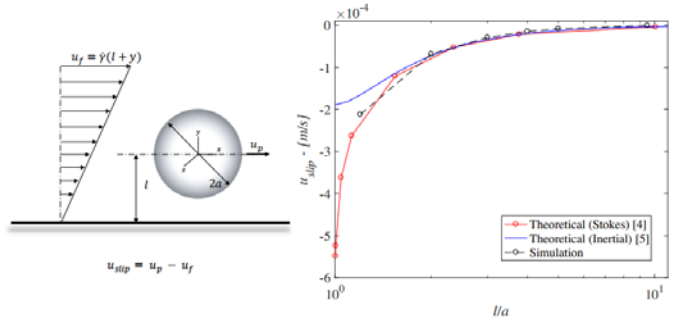

Figure 1. Slip velocity variation of a freely translating particle near a wall at $Re_\gamma = 0.1$. Here $Re_\gamma = \gamma a^2/\nu$ and γ, a, ν are shear rate, particle radius and kinematic viscosity respectively.

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Brief Biography

I am Nilanka Ekanayake, a third-year PhD student at The University of Melbourne. My research focuses on modelling blood-cell migration using computational fluid dynamics relevant for thrombus formation. I also collaborate with CSL for experimental investigation in the particle migration in microfluidics. Before undertaking the doctoral studies, I worked as a senior tutor in Chemical and Process Engineering at the University of Peradeniya, Sri Lanka. My main research interests are multiphase modelling, suspension rheology, bio-fluids and microfluids.

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A Numerical Approach for Generic Three Phases Flow Simulation

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Abstract

In this paper, we introduce numerical methods that can simulate complex multiphase flows. The finite volume method, applying Cartesian cut-cells (Kirkpatrick et al., 2003; Yoann Cheny et al., 2016) is used in the computational domain, containing gas, liquid and solid, to conserve mass and momentum. With this method flows in and around any geometry can be simulated without complex and time consuming meshing. The interaction between each phase is treated simply by wall function models or jump conditions of pressure, velocity and shear stress at the interface (Kang et al., 2000; Vukčević et al., 2017). The sharp interface method "Coupled Level Set and Volume of Fluid"(CLSVOF) is used to represent the interface between the two fluid phases (Chakraborty et al., 2013; Sussman and Puckett, 2000). This approach will combine some advantages of both interface propagation methods, such as excellent mass conservation from volume of fluid and good accuracy of normal computation from level-set function. In order to resolve interacting lines created by gas-liquid-solid, the first CLSVOF will be generated to reconstruct the interface between solid and the other materials. The second one will represent the interface between liquid and gas. Several benchmark test cases are performed to validate numerical results.

The first test is a dam break flow which is designed to investigate the two-phase flow. The water column is initialized with 0.3m height and 0.6m width inside an 0.6x1.61 rectangular tank. Due to gravity, water travels along the horizontal bed and generates a downstream wave. The evolution of the free surface is shown in figure 1.

The next test is a water entry simulation which is used to demonstrates the capability of our numerical method to handle three-phase flow. The shape of a wedge object and initial stage of simulation is presented in figure 2. For simplicity, the item is kept standstill and the free surface is let moving with a velocity being equivalent to a water entry velocity. Figure 3 displays a comparison of numerical result, experimental data and theoretical method for splash expansion and splash tip velocity. As shown in this figure, our numerical method can predict fairly accurate the characteristics of splash.

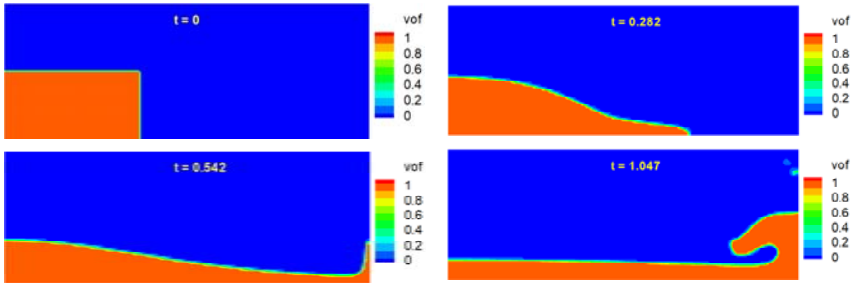

Figure 1. The Temporal Development of Air-Water Interface (time t in seconds)

Figure 2. The Schematic Diagram of Water Entry Problem and Splash Formation

$\alpha = 90^o$ $\alpha = 120^o$

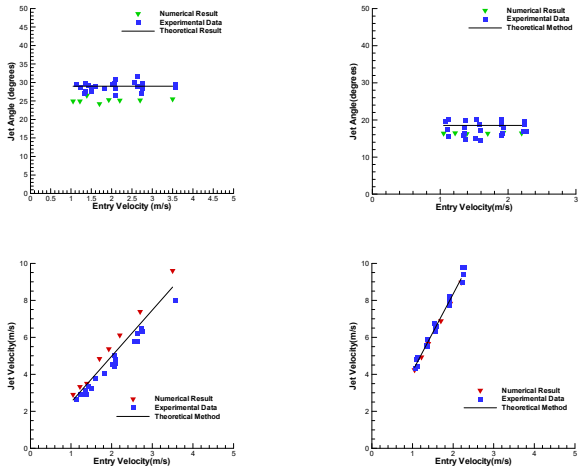

Figure 3. Wedge jet root expansion angle and jet velocity

Brief Biography

Son Tung Dang was born in Namdinh, Vietnam, in 1990. He received the B.E. degree in mechanical engineering from the Hanoi University of Science and Technology, Hanoi, Vietnam, in 2013, and the M.Sc in mechanical engineering from the Pusan National University in 2016. Since April 2016, he has been Phd candidate at Department of Energy and Process Engineering, NTNU, Trondheim, Norway. His current research interests are multiphase flows and immersed boundary methods.

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Three Phase Flows Using DSMC Method For Simulating Slurry Bubble Columns

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Abstract

Slurry bubble columns are widely used in the chemical industry because of their simple design and high efficiency. The scale-up of these kinds of columns is challenging. They are operated in the heterogeneous bubbling regime where the flow is complex and turbulent. Design of such columns is also done using CFD simulation techniques which can resolve physics at different scales. Multi fluid models (MFM) can in principle simulate large scale columns but have limitations with respect to prediction of bubble size distribution and resolution of bubble-bubble interactions. The Discrete Bubble Model (DBM) does resolve the bubble-bubble interactions but the deterministic detection and treatment of bubble collisions makes this method computationally too expensive for larger scale bubble columns.

Direct Simulation Monte Carlo (DSMC) method treats the bubbles in a discrete manner while stochastically handling the collisions in a very efficient manner. As a proof of concept, the DSMC model has been verified with the DBM and validated with experimental data from Deen et al. [1]. The mean flow velocity and the root mean square of the velocity fluctuations in the column are correctly predicted, due to the right estimation of the collision frequency within different regions of the system. This is true even for highly dense regions. The method is proven to be 100 times faster for dense flows with up to 30 percent overall gas fraction and more scalable compared to the DBM [2], [3].

In this work, the DSMC method has been extended to simulate three phase systems with catalyst particles added into the bubble column making it a slurry bubble column. Along with the 4-way coupling (liquid-bubble-bubble) previously achieved using the volume-averaged Navier-Stokes equations, bubble-particle and particle-particle interaction is added. The model and closures for the particle system are verified using a sedimentation problem. The bubble-particle interaction is restricted to bouncing. Moreover, a particle concentration based viscosity is introduced for cells with large particle concentrations.

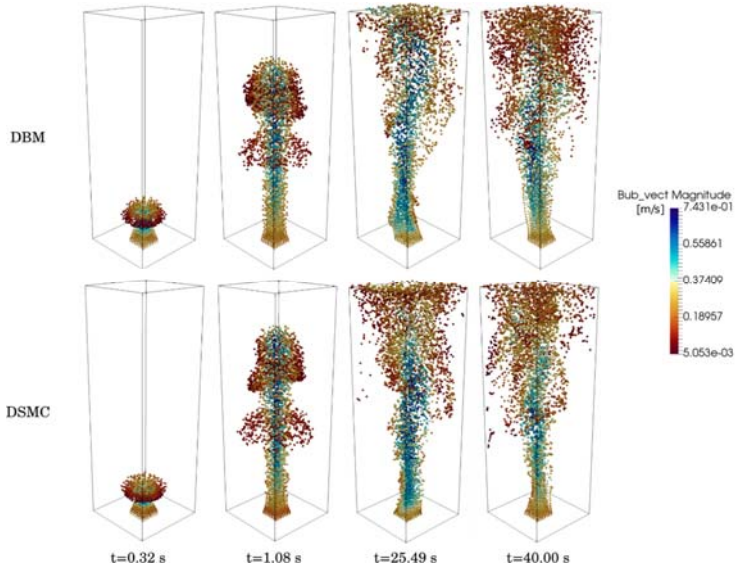

Figure 9: Evolution of the bubble plume in a bubble column comparison: DBM vs DSMC [2].

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Brief Biography

Satish Kamath is a PhD student working in the group of prof. Hans Kuipers at Eindhoven University of Technology in the department of Chemical Engineering and Chemistry. His daily supervisors are dr. Johan Padding and dr. Kay Buist. His research topic is "Numerical Modeling of Large Scale Bubble-Columns using Stochastic Euler Lagrange Methods".

Assessing The Efficacy Of Inhomogeneous Thermal Conductivity To Enhance Heat Transfer Within Fusion Reactor Blankets

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Abstract

Poloidal blanket modules within magnetic confinement fusion reactors must generate tritium fuel and exhaust large thermal loads, while exposed to extreme temperatures at the plasma-facing wall. This necessitates the use of liquid metals, which exhibit rapid rates of thermal diffusion (Prandtl numbers of order 10^{-2}). As thermal energy is preferentially diffused, rather than advected, this work focuses on thinning the thermal boundary layer, by disrupting its formation, through inhomogeneity in the thermal conductivity of the wall. This also avoids any increase in viscous pressure drop.

The plasma-confining magnetic field introduces a great deal of complexity. The electrically conducting breeder liquid experiences a Lorentz force, $\boldsymbol{j} \times \boldsymbol{B}$, where $\boldsymbol{j}$ represents the current density, and $\boldsymbol{B}$ the magnetic field. The Lorentz force greatly increases the pressure drop, and equalizes velocities within the core of the duct, which results in a flat, slug flow velocity profile. To the further detriment of heat transfer, the Lorentz force suppresses turbulent mixing. Hence, within fusion reactor blankets, improving the efficiency of conduction may be more effective at enhancing heat transfer, as attempts to increase the convective velocity must overcome the strength of the magnetic field.

However, the heat flux directly applied by the plasma, as well as from absorption of neutrons into the breeder liquid, can locally drive high-velocity buoyant flows. Although the pressure drop still scales with the strength of the magnetic field, strongly buoyant flows provide an excellent means of highlighting the capabilities of inhomogeneous thermal conductivity. It is also highly relevant to the design of reactor blankets. The Richardson number, which quantifies the ratio of buoyant to inertial forces, may be of the order of magnitude of 10^{-4} (strongly inertial) to 10^{2} (strongly buoyant) for various blanket designs.

Simulations were performed with a spectral element solver employing the SM82 model, proposed for quasi-two-dimensional flows. Such an approximation is valid for reactor blankets as the strength of the magnetic field, and hence Lorentz force, causes rapid diffusion of momentum along magnetic field lines, enforcing two-dimensionality. The relative strengths of forced and natural convection were varied, in the Rayleigh number and interaction parameter ranges of $10^2 < Ra < 10^4$ and $100 < N < 1600$, which respectively govern the strength of buoyant to viscous, and electromagnetic to inertial, forces.

It was found that heat transfer was promoted when buoyant forces were sufficiently stronger than electromagnetic forces (low N, high Ra), when comparing a duct with reduced conducting area, to an unmodified duct, at the same blanket conditions (N, Ra). A peak Nusselt number ratio of $Nu_R = 3.5460$ was observed at $N = 100$, $Ra = 10^4$, with 6.25% of the heated face conducting (93.75% insulating). As the natural convective velocity was found to linearly scale with the ratio of conducting to total area, this indicates that the efficiency of conduction requires significant improvement before convective effects (streamwise velocities) become the limiting condition. Furthermore, the effect of inhomogeneous thermal conductivity on pressure drop was also considered. The increase in pressure drop for a flow directed against gravity exactly matched that for a flow directed with gravity (with the same fraction of conducting area). For blankets with multiple ducts, this makes the system highly efficient. Overall, the application of inhomogeneous thermal conductivity can provide significant benefits to heat transfer; however, it remains highly dependent on the working conditions.

Key notice & instructions: oral presentation by C. J. Camobreco

Brief Biography

C. J. Camobreco is a first year PhD student, under the supervision of G. J. Sheard and A. Pothérat. He graduated from Monash University in 2017, with H1 Honours in a Bachelor of Aerospace Engineering. His PhD work is an extension of his FYP.

G. J. Sheard is an Associate Professor of Mechanical and Aerospace Engineering, and Director of the Sheard Lab at Monash University. He received his PhD from Monash University in 2004, winning the Faculty of Engineering Kenneth Hunt Medal and Monash Universities' Mollie Holman Doctoral Medal for the year's best PhD thesis, before securing an Australian Postdoctoral Fellowship. Dr. Sheard has authored over 150 research publications, editorials and patents, and has secured over $1.7 million in nationally competitive grant funding, including extensive time allocations on national high performance computing facilities.

CFD modelling of bubble-particle collision efficiency in froth flotation

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Abstract

In order to improve understanding of the interaction between bubbles and particles during the flotation process, the interaction between the various factors that affect the collision efficiency has been analyzed. In this paper, four kinds of mineral particles (quartz, chalcopyrite, copper sulfide and galena) were investigated. Particle-bubble collisions between bubbles with size ranging from 0.6μm to 2.0μm and particles with diameter from 31μm to 150μm were examined. The results of the CFD model are compared with the existing mathematical model to analyze the advantages and disadvantages of the existing mathematical model, as a description of the collision process of the flotation process. The results show that the GSE model fits the CFD predictions well in the particle size range below 74 microns. The Schulze model exhibits a good fit to the CFD predictions when the particle density is greater than 4200 kg/m3 (especially 4200–5600 kg/m3). It would be expected that the CFD model would be more exact than either semi-theoretical model, given that it involves fewer assumptions. In this paper, the influence of bubble diameter on particle– bubble interaction is analyzed in detail from the theoretical point of view, and a computational fluid dynamics model, which is expected to be applicable over a wide range of parameters, is established.

Brief Biography

Shuofu Li is currently a doctoral candidate at University of Science and Technology Beijing, Faculty of minerals processing, and a visiting student at CSRIO. His current research focuses on the bubble-particle collision in froth floatation.

Characteristics of Axial Velocity Wave Zone and Internal Particle Movement in Hydrocyclones

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Abstract

Grinding-classification circuit is one of the most common applications of hydrocyclones in classification duty, where the cut-size d_{50} and classification sharpness C_s are two critical control indicators. Axial velocity wave zone (AVWZ) which is evolved from the locus of zero vertical velocity (LZVV), is also a general form of inner and outer swirl interface in conventional hydrocyclones. Its spatial distribution and the momentum transfer between the liquid and solid phases affect the d_{50} and C_s of hydrocyclones. Based on the principle of liquid-solid two-phase momentum transfer and the validation of LDA and high-speed camera test, a computational fluid dynamics (CFD) method was established to investigate the characteristics of the AVWZ and the internal particle movement. The simulation results were analyzed in terms of the distributions of pressure, density, viscosity, velocity components, and particle volume fraction as well as the force analysis of particles. The results demonstrated that the particles with diameters close to d_{50} are collected in the AVWZ, reducing the efficiency of classification. This is mainly due to the radial force characteristics of the particles in the AVWZ region. By changing the structure of the cyclone, the relationship between the AVWZ characteristics and C_s was finally determined.

Keywords: hydrocyclone, classification, axial velocity wave zone, force analysis, CFD simulation

Brief Biography

Mr. Qiang Zhao is a Ph. D. Candidate at Northeastern University, China. His doctoral topic is “Characteristics of Axial Velocity Wave Zone and Its Influence on Separation Performance of Cyclones”. His research interests mainly focus on the numerical simulation, fluid-solid coupling, and industrial application of hydrocyclones.

1D Channel Flow Patterns in Shallow Enclosure Horizontal Convection

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Abstract

Horizontal convection is a distinctive class of natural convection, where non-uniform heating and cooling occurs along just one horizontal boundary of the enclosure. Studies ofhorizontal convection have been inspired by the transport of warm fluids in the oceanic circulation [1] and engineering processes, like glass melting in furnaces [2]. Previous experimental [3, 4] and numerical [2, 5] studies informed the heat transfer scalings and flow dynamics considering a change of Rayleigh numbers (Ra) for a fixed or a narrow range of aspect ratios (ratio of height to length, A). The lowest reported aspect ratio ($A = 0.16$) is at least two orders of magnitude larger relevant to the oceans. This study aims to emphasise shallow enclosure horizontal convection flow dynamics and heat transfer scalings by varying aspect ratios and explores the connection with the 1D-channel flow. A water-filled rectangular enclosure of length L and height H is studied. The flow with buoyancy modelled using a Boussinesq approximation is driven by imposing a linear temperature profile on the bottom boundary of the enclosure, and insulating temperature conditions on the remaining boundaries. The 2D incompressible Navier–Stokes equations augmented by a buoyancy term in the momentum equation and a scalar advection-diffusion transport equation for temperature were solved by a high-order in-house solver, which employs a spectral-element method for spatial discretisation and a 3rd-order time integration scheme based on backwards-differencing.

Numerical simulations are conducted for a wide range of aspect ratios ($0.001 \leq A \leq 0.16$) and Rayleigh numbers ($10 \leq Ra \leq 10^{17}$) maintaining a fixed Prandtl number ($Pr = 6.14$), representative of water. The logarithmic values of the calculated Nusselt number (Nu) and $RRRR$ are presented in figure 1(a), which depicts that increasing $RRRR$ governs the flow from a diffusion-dominated regime ($Nu \sim A$) via a transition regime ($Ra \sim A^{-4}$) towards a steady-state convection-dominated regime ($Nu \sim Ra^{1/4}$). Figure 1(a) is rescaled in 1(b) based on the obtained scalings, which plots $\log(Nu\ /A)$ against $\log(RaA^4)$ and illustrates a collapse for all A values at low-Ra. The grouping RaA^4 implies a modified Ra controlling this collapsed regime, which is expressed as

$$Ra_H = RaA^4 = \frac{g\alpha(\delta\theta_H)}{\nu\kappa_T}H^3 \qquad (1)$$

Here, $\delta\theta_H$ is the temperature difference along a portion of the bottom boundary of length H, which indicates that horizontal convection at very shallow enclosures will be controlled by the enclosure height and adjacent the horizontal temperature gradient at low-Ra. The horizontal velocity component and the temperature relative to a local bottom wall temperature of this collapsed regime are extracted at various location at the bottom boundary from the

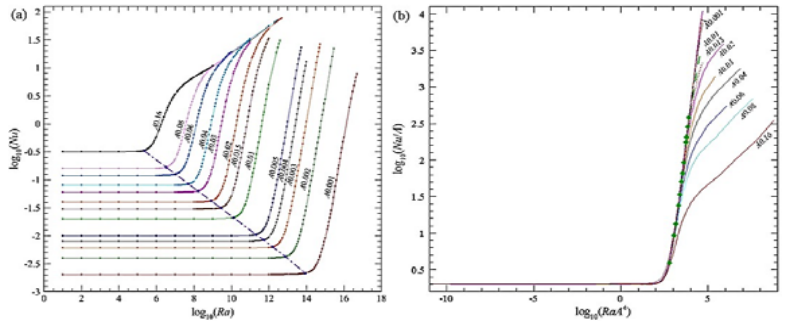

Figure 1: (a) $log\ Nu$ vs $log\ Ra$ is plotted for all aspect ratios, where the purple line marks the onset of transition regime. (b) Rescaled plot of (a), where the low- Ra values collapsed into a single curve.

hot sidewall of the enclosure. Polynomial fits to these velocity and temperature plots are found to agree with the obtained analytical solution for a 1D-channel flow driven by a linear temperature gradient. The analytical solutions for horizontal velocity U and temperature θ'S.H. is supported by MIPRS and MGS scholarships from Monash. This work was supported by the ARC Grants, titled DP150102920 and DP180102647, and was undertaken using NCI by a grant under the National Computational Merit Allocation Scheme (NCMAS).

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Brief Biography

Sajjad Hossain is a PhD student of Monash University studying natural convection flows. He completed BSc. in mechanical engineering from BUET, Bangladesh in 2011. His thesis was on CFD analysis of novel techniques to reduce friction factor in u-type wavy tubes. He worked as a project engineer in BanglaCAT, the largest electric power generation dealer for Caterpillar in the Asia Pacific, whereby he was engaged to design and installation of two 100 MW HFO-based power plants and over 30 gas and diesel captive power plants. He completed Masters from University of Malaya, Malaysia. There he conducted heat transfer and combustion analysis of renewable and sustainable fuels, like gas-to-liquid (GTL) and biodiesels. He has published 15 ISI Q1 journal papers in the field of energy and heat transfer.

Modeling of Complex Liquid-Solid Flow of Swelling Particles

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Abstract

Particle swelling has a significant influence on the liquid-solid flow of swelling particles. It is of practical significance for reactor troubleshooting or optimization to develop a swelling-dependent fluid dynamics model that is able to reasonably depict these effects. However, the lack of knowledge on microscale particle swelling and mesoscale particle aggregation makes it difficult to directly simulate these complex behaviors. This work heuristically developed a STFM model to account for the swelling effects on fluid dynamics. A swelling-dependent two-fluid model (STFM) is developed for the liquid-solid flows of swelling particles in polyethylene reactors. The model integrates the two-fluid model (TFM) with a species transport equation (STE) to account for the diffusion of alkane molecules from the liquid bulk to the amorphous region of particles, and a population balance equation (PBE) to consider the aggregation of swelling particles. Simulations show that only the TFM fails to capture the main features of swelling systems. By contrast, the STFM captures the gradual increase of power consumption due to particle swelling and aggregation, which agrees with the experiments in a stirred tank. The STFM predicts also the slug formation and a sharp increase of power consumption in a slurry loop reactor as well as the solid accumulation behind pump. The difference of model prediction for stirred tanks and loop reactors suggests the potential of reactor optimization by enhancing local mixing while still keeping high solid concentration for productivity.

Reference:

Zhou, R., Chen, J., Yang, N.*, Li, J., Fernandez, A., Ricoux, P. Modeling of complex liquid-solid flow of particle swelling in slurry loop reactors, Chemical Engineering Science, 2018, 176, 476-490

Brief Biography

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

Ning Yang received a B.S. degree and a M.S. degree in mineral processing in 1996, and a Ph.D degree in Chemical Engineering in Chinese Academy of Sciences in 2003. His research interests covers the meso-scale modeling of gas-solid, gas-liquid and gas-liquid-solid flow in chemical and process industries. He also worked in the Institute of Fluid Mechanics of Toulouse as a post-doctoral fellow and Oak Ridge National Laboratory as a visiting scholar. He has many collaboration with industrial partner (e.g., BASF, TOTAL, BP, Unilever, SinoPec, Synfuel China, etc.). He obtained the Excellent Young Scientist Fund from National Natural Science Foundation of China in 2012, Qiushi Outstanding Young Scholar Award for Research Achievements and Transformation in 2013 and SCEJ Award for Outstanding Asian Researcher and Engineer in 2016. He is also the plenary or keynote speakers of ISCRE, APT and GLS conferences. He is the chair of the 14th International Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering (May 30-June 3, 2019).

Recent Works:

Chen, C., Guan, X., Ren, Y., Li, J., Kunkelmann, C., Schreiner, E., Holtze, C., Mülheims, K.,Sachweh, B., Mesoscale modeling of emulsification in rotor-stator devices. Part I: A population balance model based on EMMS concept, Chemical Engineering Science, 2018, in press

Chen, C., Guan, X., Ren, Y., Li, J., Kunkelmann, C., Schreiner, E., Holtze, C., Mülheims, K.,Sachweh, B., Mesoscale modeling of emulsification in rotor-stator devices. Part II: A model framework integrating emulsifier adsorption, Chemical Engineering Science, 2018, in press

Zhou, R., Chen, J., Yang, N.*, Li, J., Fernandez, A., Ricoux, P. Modeling of complex liquid-solid flow of particle swelling in slurry loop reactors, Chemical Engineering Science, 2018, 176, 476-490

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Yang, N.*, Xiao, Q., A mesoscale approach for population balance modeling of bubble size distribution in bubble column reactors, Chemical Engineering Science, 2017, 170, 241-250.

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Hydrodynamic and Stability Behaviour of a Plunging Jet Downflow Bubble Column

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Abstract

Bubble columns of many different designs are used in minerals and process industries for carrying out gas-liquid operations. In mineral processing, the plunging liquid jet bubble column, known as the Jameson Cell, is widely used in mineral processing. Briefly, in the downcomer of the Jameson Cell (see Fig. 1) the liquid is introduced as a high-speed free jet that entrains gas into the mixing zone where fine bubbles are generated as a result of the high energy dissipation rate. Once formed, the bubbly mixing is transported downward into the pipe flow zone and exits from the base of the column. It is in the pipe flow zone that the transition from homogeneous (bubbly) to heterogeneous (churn-turbulent) flow can occur, which greatly influences the performance of the system.

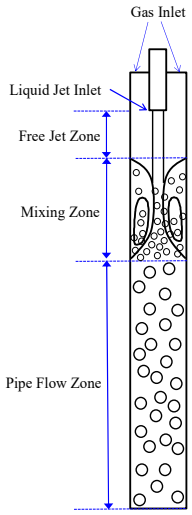

Fig. 1. Schematic of a plunging jet bubble column (Evans, 1990).

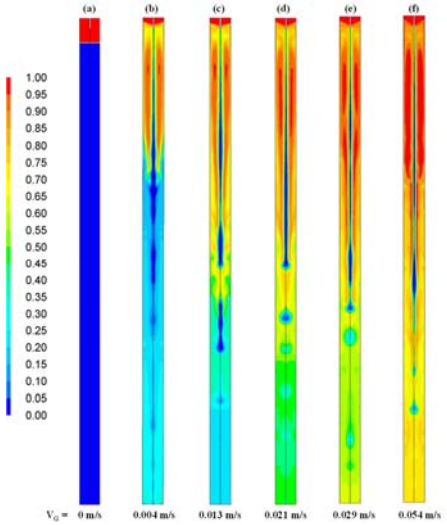

Fig. 2. Contours of gas volume fraction for U_L = - 0.033 m/s and at different gas superficial velocity, V_G.

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In this study, CFD analysis based on the Euler-Euler framework was used to model the two phase (air-water) flow behaviour. It was found that use of the Tomiyama (1998) drag model was successful in capturing the flow hydrodynamic behaviour and of all three (free jet, mixing, and pipe flow) zones when compared with the experimental data of Evans (1990). For example, as shown in Fig. 2 for steady-state CFD simulations (200s) it can be seen that, as expected, for a given liquid jet velocity and diameter the volume of the gas-filled headspace increased with increasing gas inlet flow rate. The length of the headspace corresponded well with the free jet length measurements. The simulations were able to predict the gas void fraction profiles and highlighted the mixing zone, where the determined boundary again well matched with those obtained from the experimental pressure profile. Finally, the CFD-predicted energy dissipation rates were combined with appropriate drift-flux and linear stability (Joshi et al., 2001) analyses to determine the critical gas volume fraction at which the homogeneous to heterogeneous flow regime transition was seen to take place during the experimental observations. For example, for a gas superficial velocity of 0.013 m/s the critical gas volume fraction was at 0.416. As part of the study, comment is made on the influence of influent velocity fluctuations on the gas volume fraction at which regime transition takes place.

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Brief Biography

Dr Md. Shakhaoath Khan is currently working as a Research Officer at the School of Engineering, RMIT University. He obtained his Doctor of Philosophy degree from the University of Newcastle in November 2017. Dr Khan is actively involved in fundamental and applied research into fluid dynamics and multiphase flow systems. The research aims to develop an increased understanding of the principles of intermixing-segregation in a multiphase reactor (e.g., fluidised bed, bubble column) and to use this knowledge to optimise its use in mineral processing. Dr Khan has worked on several research projects (thesis and fellowship) in Bangladesh and Australia. His present research is focusing on process design, optimisation and evaluation of pyrolysis reactors. Research involves a combination of experimental measurement, mathematical modelling and CFD simulation.

Modelling Heat Loss in Metal Runner During Furnace Tapping

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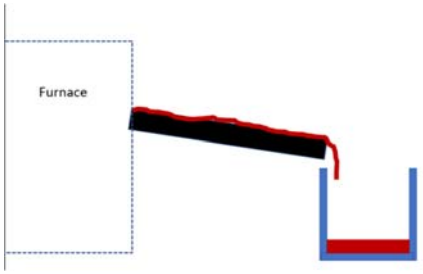
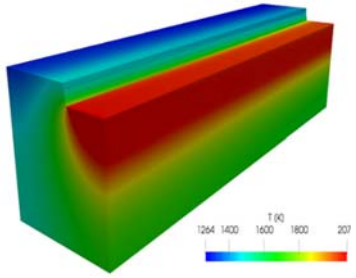
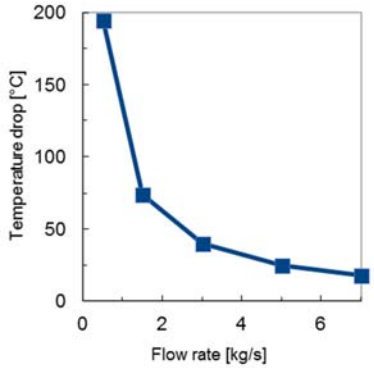
Abstract

When metal is tapped from the furnace it flows from the tap-hole down a runner before it falls into a ladle (see figure below). The runner is an open channel typically circular in shape. During its residency in the runner the metal loses heat to the runner block and the surroundings. This heat loss can also be quantified by mathematical modelling. A CFD model accounting for metal flow, heat conduction, heat convection and radiation are presented together with results from model simulations. The example studied is tapping from a ferrosilicon furnace. The runner is 800 mm long and made of graphite which is fairly conductive. The temperature leaving the furnace is normally 1600-1900ºC and thus radiation from the metal surface is significant. This is accounted for. The case of the metal runner from ferrosilicon metal production is simulated using OpenFOAM 5.0 with the solver *chtMultiRegionFoam*.

Simulations provide results on fluid velocity and temperature in metal and runner. A typical temperature field is illustrated on the left in the figure on the following page. The tapping rate (i.e the inlet mass rate) is a parameter which is difficult to control, and it varies significantly. The influence of tapping rate on heat loss is thus studied. We see on the figure on the right-hand side on the following page that the temperature drop in the metal from inlet to outlet in metal runner is significantly influenced by tapping rate. The results show that radiation is significant, but not the dominating heat transfer mechanism. Heat loss by conduction to the runner is more significant. These and other results will be presented.







Brief Biography

Dr.Jan Erik Olsen is research manager in the Flow Technology group at SINTEF Industry. He holds a PhD in continuum mechanics from NTNU in Trondheim and has over 15 years of experience with CFD. He works on industrial challenges, including metallurgical applications.

Debottlenecking of Flow in a Hot Strip Mill Walking Beam Furnace

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Abstract

The operation of Port Kembla Steelworks (PKSW) hot strip mill (HSM) walking beam furnace #2 (WBF#2) is investigated to evaluate the feasibility of increasing its slab heating capacity by increasing the ability to push more flue gases through the recuperator. Given that the pressure drop across the recuperator is rather constant under a given set of conditions, it becomes necessary to achieve a lower negative pressure at the end of the recuperator, just before entering the stack, for a higher flowrate of flue gases to go through the system. A higher suction (more negative pressure at the end of recuperator) is required to allow an increase in the flowrate of gases from the furnace and subsequently through the recuperator.

A Venturi injector uses the Venturi effect of a converging-diverging nozzle to convert moving fluid pressure energy to velocity energy which creates a low-pressure zone that draws in and entrains a suction fluid. Velocity energy is subsequently converted back to pressure energy in the diverging section of the Venturi. A typical Venturi injector is shown in Figure 1. It is widely used in industry and especially for pneumatic transport of solids, spraying of fertilisers, etc.

The stack of the WBF#2 follows the same principle shown above, with the air coming from the induction fan acting as the 'motive fluid' and the 'inlet gas' coming from the recuperator. This means for the WBF#2 case, the motive fluid enters at 180° with the gas inlet from the recuperator.

The stack consists of a cylindrical structure equipped with a Venturi injector. The stack main diameter is 3.1 m and its total height is 45 m. The Venturi consists of a 3.4 m long converging section, a 1.604 m diameter Venturi throat (6.5 m long) and a 3.4 m long diverging section. An induction fan ejects at the bottom end of the throat through a 0.541 m nozzle. The motive fluid is that coming in from the induction fan.

The suction capacity through a Venturi injector depends on several factors including: (i) throat diameter, (ii) nozzle location, (iii) nozzle diameter, (iv) Venturi diameter and (v) motive fluid flowrate.

Flow and heat transfer in the stack of HSM WBF#2 have been simulated using CFD for the existing 1.6m diameter Venturi case including buoyancy effects.

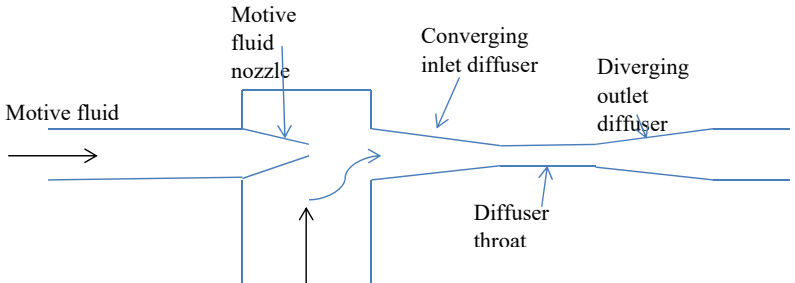

Figure 1: A typical Venturi injector arrangement

Results show that flow in the stack is made complex by the obstruction caused by the nozzle from the fan. Pressure predictions at inlets from recuperator and fan are in line with plant measurements and calculated values by a third party. The main recommendation of this work is that lowering the location of the nozzle will result in a lower pressure at the inlet to the stack from the recuperator and consequently a capacity to push more gas through the recuperator and furnace. Lowering the location of the nozzle from the start of the throat to the start of the converging section resulted in a decrease in the pressure at the exit from the recuperator by more than 400 Pa. This is likely to increase the capacity to push more gas through the furnace and consequently through the recuperator. This change in design was implemented and the performance after the debottlenecking agreed with the CFD predictions.

Other conclusions found include that (i) increasing the Venturi throat, (ii) increasing the nozzle diameter and (iii) increasing the flow rate from recuperator did not result in any significant positive effect on the capacity to push more gas through the recuperator.

The paper presents a full discussion of the modelling details and benefits achieved by the debottlenecking.

Brief Biography

Dr Habib Zughbi is a Senior Technology and Development Engineer in the Coke and Ironmaking Technology Section of BlueScope. His activities include applying CFD simulations to a wide range of flow and heat transfer problems across the steelworks. He also focusses on energy and environment related projects using process integration.

Modelling of Diesel Spray Combustion for Top-Submerged-Lance Processes

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Abstract

The Top-Submerged-Lance (TSL) technology is nowadays widely used in pyrometallurgical processes. Its high flexibility allows the usage in a large range of metal production chains such as tin, copper, lead, nickel or zinc. The TSL furnace is successfully implemented also in secondary processes and will play a key role in the route towards recovery and recycling for the achievement of a circular economy in the metallurgical industry.

Despite the wide application, there is still a lack of fundamentals and in-depth scientific understanding of the TSL process. At CIC Virtuhcon, a detailed CFD model of a TSL copper smelting furnace is currently in development to contribute to the comprehension and the development of a reliable and efficient technology.

In this work the authors focus the modelling of the diesel spray injection and combustion in the lance of a small-scale TSL furnace operating at TU Bergakademie Freiberg (Fig. 1).

Fig. 1: Internal view of the lance geometry

The air flows in the outer annular section of the lance, encountering a swirling component which confers a high angular velocity before entering the combustion zone. The fuel oil comes from the inner tube at high pressure conditions and is injected through a pressure-swirl atomizer nozzle in the reactive region, where the flame will develop. An Eulerian-Lagrangian approach is used within ANSYS Fluent® to investigate in detail the performances of the lance combustion. Two aspects of the flow are mainly highlighted:

The fuel spray injection: the combustion of evaporating diesel droplets is highly dependent on the droplet size distribution. A validation of the DPM model for liquid fuel spray is carried out in order to determine the applicability of this approach.
In Fig. 2 a droplet diameter distribution of the liquid fuel spray injection is shown.
The combustion of evaporating diesel droplets: different modelling approaches are tested, comparing the equilibrium and kinetic conditions.

The results obtained with this research activity represent a decisive element towards the modelling of the submerged combustion inside the liquid slag, where the combustive injection interacts with bubbling flow.

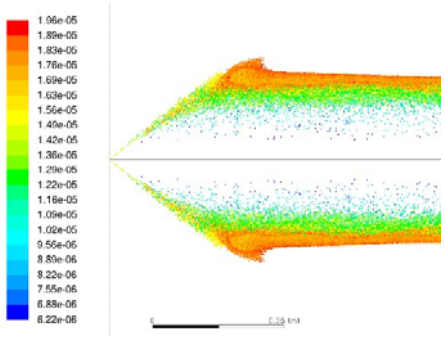

Fig. 2: Fuel droplet size distribution

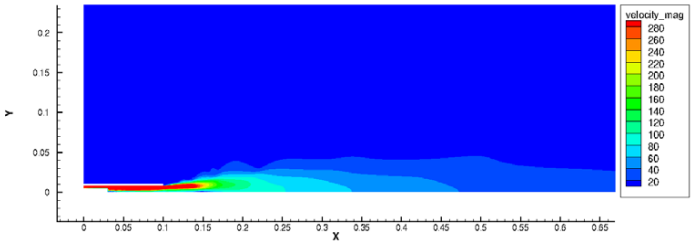

Fig. 3: Velocity field of the combusting flow in the lance

Acknowledgements

The German Federal Ministry of Education and Research (BMBF) has funded this research within the framework of the Centre for Innovation Competence Virtuhcon (project number 03Z22FN11). The authors are responsible for the content of the publication.

Brief Biography

Dr. Sebastian Kriebitzsch got his degree in chemical engineering (Diplom-Ingenieur) from the University of Dortmund in Germany in 2006. From 2006 to 2012 he worked in the group of Prof. J.A.M. Kuipers on the direct numerical simulation of dense gas-solid flows, first at Twente University than at Eindhoven University of Technology in the Netherlands. In 2013 he joined the CFD department of the Institute of Fluid Dynamics of the Helmholz-Zentrum Dresden – Rossendorf, Germany to work on the modelling and simulation of disperse bubbly flows. Since 2016 is heading the research group multiphase models of the CIC Virtuhcon at the Technische Universität Bergakademie Freiberg, Germany.

A Novel Tundish Design Based on CFD-DEM Study

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Abstract

A novel design of a single slab caster tundish for the separation of non-metallic inclusions from molten steel was proposed. The inclusion separation efficiency was quantified using a combined CFD-DEM approach. The dimensions of the new design were optimized for the maximum separation of inclusions. The modified design is more efficient in separating the inclusions than a traditional tundish of similar capacity with flow modifiers. The tundish with the modified design can directly replace the tundishes in the industries.

1. Introduction

Presence of non-metallic inclusions affects the processing as well as the final properties of steel. The last stage of separation of inclusions in steel is done in a tundish, which acts as an intermediate buffer vessel to convert batch process to continuous process. The traditional designs of the tundish, that are currently being used in the industries employ separate flow modifiers such as weir, dam, turbo stop etc.[1-3] to direct the flow towards the surface and thus improve the inclusion separation efficiency. However, existing tundishes are only effective in separating inclusions up to 50 µm. Further improvement of the inclusion separation efficiency is necessary for clean steel production.

2. Current Formulation

In the current work, a novel design of a single slab caster tundish was considered, which naturally facilitates surface driven flow behavior thereby eliminating the utilization of separate flow modifiers [4]. The schematic of the cross-section of the proposed tundish is shown in Figure 1.

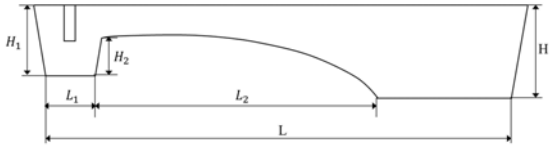

Figure 1: Schematic of the modified design tundish cross-section

The optimal design, for achieving the maximum inclusion separation efficiency was obtained, by changing the different dimensions of the tundish. To compare the separation efficiency of the current tundish with that of various existing tundishes available in the literature, the current design was scaled for the same capacity as a physical model of an existing tundish. Water was used as the continuous phase liquid and LLDPE particles were used for modeling the inclusion behavior. Physical modeling was done using Froude number similarity criteria and the particles are assumed to follow the Stokes law [5,6]. A mathematical modeling approach was chosen to quantify the separation efficiency, using a combined CFD-DEM approach.

3. Results and discussions

The residence time for the tundish was obtained by tracing a die having the same properties as those of the continuous phase. A steady-state flow profile was first obtained, in which 6g of LLDPE particles were injected for 3 seconds [2]. The particle trajectories were tracked for a time thrice the residence time, and the separation efficiency was calculated. The steady state velocity profile in the cross-section is shown in Figure 2(a).

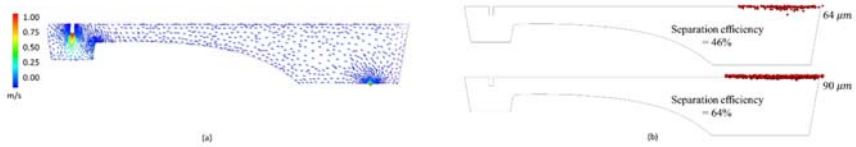

Figure 2: a) Velocity profile in the cross-section, b) Particle separation efficiency

Recirculating flow can be seen in the left end of the tundish, which slows down the liquid significantly as it enters the central neck region. A stream lined flow is seen in the central region, which allows the particles to rise to the top due to buoyancy. The outlet located at the bottom of the right end has the same head as that of existing tundishes. So, the outflow rate and hence the casting rate is not affected. The positions of two different sized particles and the corresponding separation efficiencies after a time of thrice the residence time, are shown in Figure 2 (b). The separation efficiency was found to be greater than that of a traditional tundish with flow modifiers [3].

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Brief Biodata

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- 2009-2013: Bachelor of Engineering, Department of Mechanical Engineering, Osmania University, Hyderabad, India.

Research Interests Computational and experimental fluid dynamics, Process Modeling.

Dr. Sabita Sarkar

- 2009 - till now: Assistant Professor, Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, India.
- 2008-2009: Research Scientist, SINTEF Materials and Chemistry, Norway.
- 2006-2007: Post-Doctoral Researcher, the University of Twente, The Netherlands
- 2000-2006: Ph.D. from Indian Institute of Science, Bangalore, India.

Research Interests Process modeling, design intensification of metallurgical and chemical processes.

Application of Scale-Resolving and RANS Approaches to the Simulation of Fluid Mixing and Residence Time in an Industrial Crystalliser

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Abstract

Process vessels used in the Bayer process to produce smelter-grade alumina are characterised by their large scale and the requirement to process slurries with wide particle size distributions and high solids loadings. Precipitation vessels are a good example and are critical to the process as they are used to crystallise aluminium trihydroxide from solution. An understanding of the flow and residence time behaviour in these vessels is critical to addressing design considerations, such as impeller selection, off-bottom solids suspension and crystallisation yield. In the current study, Computational Fluid Dynamics (CFD) models were used to predict the flow field and residence time in a laboratory-scale alumina precipitator, with the predictions compared with Laser Doppler Velocimetry (LDV) and residence time measurements taken in the same system.

RANS and URANS approaches using the k-ε, RNG k-ε, SST, SSG Reynolds Stress and explicit algebraic Reynolds Stress models (EARSM) were assessed. Most of the models are found to perform poorly in this system and over-predict the reattachment height. This is consistent with observations that RANS models typically under-predict the shear stress in separating shear layers. The SST model, which is intended to combine the best features of both the k-ε and k-ω models, significantly over-predicts the reattachment height and it is found that the high eddy viscosity generated in the separating shear layers exiting the draft tube, together with the recirculated turbulence in this geometry, suppresses the correct behaviour of the SST blending functions. The best agreement with the experimental LDV data is achieved using the k-ε and k-ε EARSM models, however these models result in a steady solution which is inconsistent with the large-scale unsteadiness observed in the full-scale system. As a result, residence time predictions with these models show poor agreement with the experimental data.

Hybrid RANS-LES approaches using the Scale Adaptive Simulation (SST-SAS) and Stress-Blended Eddy Simulation (SBES) models were also assessed. The SBES model, which utilises an explicit switch between a RANS model in the boundary layer and an algebraic LES model in the freestream, was found to transition to scale-resolving mode at the draft tube exit faster than SST-SAS, which results in better agreement with the experimental LDV data on moderate mesh sizes. However, further mesh refinement results in comparable results from both models.

Both models resolve significant large-scale unsteady structures in the flow, and residence time predictions carried out with the SBES model show an ability to predict both the average residence time response in the vessel, and the variation in response when tracers are injected at different points in time. The ability to predict both the time-averaged flow, and the range of residence time outcomes experienced, is a significant result for the modelling of industrial crystallisers.

Brief Biography

Mr. Brown currently holds the position of Global Technology Manager – Simulation and Digital in Alcoa's Refining Centre of Excellence. In this position he leads a team of engineers and scientists developing and utilising chemical process simulations, computational fluid dynamics and advanced analytics to optimise Alcoa's global refining operations and equipment. Mr. Brown is a past recipient of the James A. Brodie medal from the Institution of Engineers Australia and is author on 15 peer-reviewed journal and conference papers in the areas of computational fluid dynamics and process simulation. Mr. Brown is also a PhD candidate at the University of Western Australia, where he is studying the application of scale-resolving turbulence modelling to the simulation of fluid mixing, residence time and particle suspension in industrial process vessels.

Numerical Simulation of Submerged Arc Furnace for Ferrochromite Production

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Abstract

Submerged arc furnace is simulated by computational fluid dynamics (CFD) method to understand the role of electromagnetic and temperature field inside for ferrochromite smelting process. The finite element model of 75MVA submerged arc furnace has been established. The current density, magnetic induction intensity, Joule heat and temperature are analyzed by magnetic vector potential models. With different polar circle diameter, the temperature of material layer, slag layer and ferrochromium alloy layer are investigated. The results show that the skin effect of three phase alternating current has great influence on the distribution of current density. When the polar circle diameter increased, the temperature value of the arc zone decreased in the furnace. Also, the electromagnetic and temperature field inside of the submerged arc furnace can be obtained to reflect the rate of reduction reaction.

Brief Biography

Baokuan Li, Professor, work for the School of Metallurgy, Northeastern University, Shenyang, Liaoning, China. Researches focus on high temperature melting multiphase flow thermophysics, industrial furnace thermal engineering, combustion technology and fluid power engineering.

Key notice & instructions:

Baokuan Li will present the paper in oral format.

Application of Mathematical Models for Different Electroslag Remelting Processes

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Abstract

Electroslag remelting is widely applied in manufacture of high grade special steels and super alloys with the character of high cleanliness, homogenous composition and compact structure which have been used in many industrial fields such as aerospace, aviation, energy, ship building, electronics, petrochemical industry, heavy machinery, transportation and so on. Due to the difficulties of precise measurements in a high temperature environment and the excessive expenses, mathematical models have been more and more attractive in terms of investigating the transport phenomena in ESR process.

To understand the interplay of associated transport processes (electromagnetic field, fluid flow, heat transfer and mass transfer) and phase transformation, as well as to establish the link between the operational parameters and resulting structural and chemical effects is becoming more important in both fundamentals and practice. Mathematical models of the ESR process often provide an efficient approach for analyzing such process.

In this paper, the numerical models for different ESR processes made by our lab in last decade have been introduced. The first topic deals with traditional ESR process predicting the relationship between operating parameters and metallurgical parameters of interest. To predict the relationship between operating parameters (such as power input and type, fill ratio, depth of electrode immersion, amount of slag and melt rate) and temperature fields, pool profiles and local solidification time (LST). The second topic is concerning the new ESR technology process including ESR with current-conductive mould (CCM), ESR hollow ingot technology, electroslag casting with liquid metal(ESC LM), electroslag remelting of bimetallic rolls and so on. Finally, the numerical simulation of solidification microstructure with multi-scale model is presented, which reveals the formation mechanism of microstructure. The computed results agree well with the experiment, which provide effective guide for the determination of process parameters.

Moreover, the worldwide recent research progress of numerical modeling during ESR process is introduced. Unsteady state simulation of ESR process with a dynamic mesh-based approach, simulation of droplet behavior and formation of slag skin will be particularly addressed. For better illustration and process understanding, some visualization results are given. The needs and the challenges ahead for ESR process modeling are also discussed. Finally the future works for simulation of ESR process have been proposed.

Brief Biography

Dr. Zhouhua Jiang is currently a professor and head of Ferrous Metallurgy Department in the School of Metallurgy at Northeastern University, China. His research is concentrated in special steels and nickle-based alloy metallurgy, including electroslag remelting, vacuum induction melting, electric furnace steelmaking, secondary refining, steel solidification and modelling.

He leads research projects from various funding sources, including The Ministry of Science and Technology of China and National Natural Science foundation of China and many Chinese steel companies. He has contributed over 300 journal publications, 48 patents and many plenary/keynote/invited presentations. He has won some prestigious awards, e.g."1906"Award from International Electrotechnical Commission (IEC) 2005, National Award of Science and Technology Progress 2006, National Award of Science and Technology Progress 2014, Chinese Award of Science and Technology Progress in Metallurgy 2018.

SPH modelling of laser metal additive manufacturing

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Abstract

Laser additive manufacturing is a process whereby a structure is created by the selective melting of metallic powder. A bed of fine powder is maintained by addition of metallic grains followed by a raking process. A laser then passes over the bed following a path the represents the cross-section of the structure to be created at that height. The laser heats the grains and solid metal below (from previous passes of the laser) causing localized melting which lead to flow of the liquid metal. The flow increases the density of the metallic material bonding it to lower layers and creating a new layer of the structure. The way in which the laser heats the bed, the melting and liquid flow and grain movement that results, end as the conductive heat transfer cools the melted material leading to solidification. This process is repeated leading to the buildup of the full structure.

Smoothed Particle Hydrodynamics (SPH) is a Lagrangian particle based continuum method that is well suited to the challenges of metal laser additive manufacturing. An SPH model which includes grains and grain motion, laser heating (with deposition controlled by a ray tracing method), metal melting and solidification (including temperature dependence of material properties and mushy zone behaviour between solidus and liquidus temperatures) is developed.

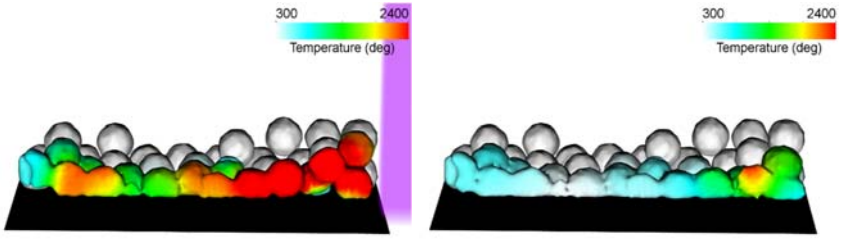

Figure 1: Shows melting of grains within a bed heated by the passage of the laser (purple) with the material coloured by its temperature.

This model is first demonstrated on a small section of a linear laser track of grain. Here the metal grains are of order 50 micron diameter and the SPH resolution is 5 micron. The laser,

which is convergent and has a non-uniform energy density, is 100 microns in diameter at the height where it intersects the powder bed. The ray tracing for the deposition of the radiative energy from laser beam on the grains assumes an average reflectance/absorption. Heat is deposited where the rays intersect the grains which allows for realistic deposition of heat into the grain bed. Figure 1 shows the progress of the melting and metal flow following the passage of the laser. Figure 2 shows the melt track from above for the base case and when the laser travels at half the speed.

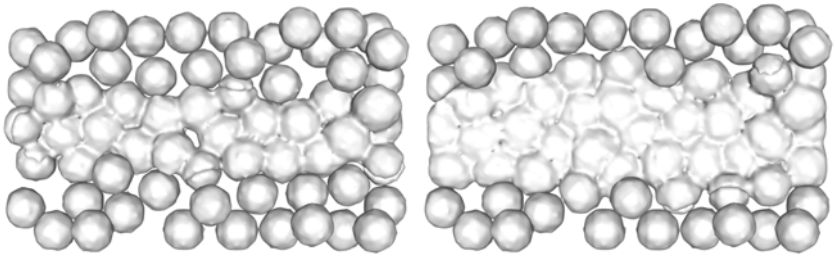

Figure 2: View of the melt track across the grains following solidification for (left) the base case, and (right) when the laser travels at half the speed.

The model will then be demonstrated for a larger more complex tile. The inclusion of surface tension effects, volumetric expansion and residual stress option are explored.

Brief Biography

Paul Cleary is a Chief Research Scientist at CSIRO Data61. His research interests are focused on particle based modelling for industrial, geophysical and biophysical applications and the development of the Workspace framework to support the commercialisation of software tools developed in a research environment.

Numerical Model for Co-Firing of Solid Recovered Fuel in a Cement Rotary Kiln

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Abstract

In the production of cement clinker, substitution of conventional solid fuels such as coal and coke with fuels derived from waste is increasing because of economic and environmental reasons. Solid Recovered Fuel (SRF) is one such fuel prepared from non-hazardous waste materials. However, due to irregular particle shape and inhomogeneous nature, the combustion of SRF has a direct impact on the performance of the cement burner-kiln system. High degree of substitution is possible when a high degree of energy conversion is obtained in the burning zone while still maintaining a stable condition in the kiln. Numerical simulation, with appropriate models for SRF combustion incorporated, is a useful tool for the control and investigation of the co-combustion process. In this study a pragmatic modelling approach for the combustion of SRF is presented. Physical characterization including particle size, weight, shape factors and composition of SRF particles was derived based on physical sorting, wind sieve tests and 2D imaging of particles. This characterization was used as an input for computational fluid dynamic analysis. The particles were classified into six different size fractions according to their terminal velocity. Specific shape factors were attached to each size fraction to account for the aerodynamic and thermodynamics behavior. The SRF fuel was further classified as biomass, plastics and inert particles. Separate combustion mechanism and combustion kinetics was used for conversion of biomass and plastics. Influence of variation in fuel moisture, substitution rate and particle size distribution was evaluated using this proposed methodology. The flame temperature, species concentration and heat output provide useful conclusions regarding the maximal allowed substitution rate for stable kiln operations.

Brief Biography

FLSmidth is a leading supplier of equipment and services to the global cement and minerals industries. FLSmidth supplies everything from single machinery to complete cement plants and minerals processing facilities including services before, during and after the construction. Development of FLSmidth's capabilities in simulating burner and calciner operation with different alternative fuel properties is a key part of the MiCeTech platform project being made in collaboration with Innovation Fund Denmark and the Technical University of Denmark (DTU).

Coupled analysis of flow, temperature and stress in radiant tubes

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Abstract

In the field of industrial furnace construction, critical parameters for parts to use are mostly stability and resilience. For a profitable use, a long life span is crucial. Therefore, the life span of construction parts is the most decisive parameter to choose between different options of layout. Especially mechanical stress reduces the life span of single components critically. One major reason for components to break are temperature gradients within an assembly, caused by the need to operate processes at high temperatures. If a critical limit is reached, stress may lead to plastic deformation and creep. If the stress will be held upright over a long time, the construction part may collapse.
A coupled simulation between a CFD part and a structural analysis in ANSYS Fluent offers the possibility to estimate the life span of a component under certain circumstances. Especially when stresses result from pressure of a fluid flow or temperature gradients in a flow field. The method of coupled simulation offers the chance to gain further information about the effects of a fluid flow on surrounding parts.
This work deals with the example of a radiant tube in a galvanizing line. Radiant tubes are used in industrial furnaces when it is crucial to separate the atmosphere of the oven from the product e.g. to protect it from surface failures. A burner heats up the tube from the inside for an indirect heat treatment of the product through radiation. While being heated up the tube is exposed to enormous strain. Small changes in the temperature distribution may lead the stress to exceed and make the tube break.
In the first part of the simulation, the fluid flow will be calculated. In the second part, a chemical reaction will be implement to simulate the flame inside the tube, the amount of radiation and convection, and generate a temperature profile at the outer wall of the radiant tube. During the second part, the temperature profile at the outer wall of the tube will be linked to a structural analysis. Different programs will be tested for the compatibility with fluent data export. Advantages and disadvantage will be compared for certain software.
In the end, a stress profile will be generated to make a statement about the place and amount of highest stress. Furthermore, a prediction will be made about the life span of radiant tubes regarding different process temperatures. In advance, the results of the stress profile lead to recommendations regarding the shape of radiant tubes in industrial furnaces.

Brief Biography

Daniel Brykarczyk, M.Sc. works as a research associate at the Department for Industrial Furnaces and Heat Engineering at RWTH Aachen University in Germany. He focusses on numerical modelling of various radiant tubes used in heat treatment plants. For validation, he builds models of furnaces to compare experimental and numerical results
Daniel studied materials engineering at RWTH Aachen University since 2012, focusing on industrial furnaces and heat treatment processing. Now he is working on his Ph.D. thesis concerning the use of special structures to improve the life span of furnaces components.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

Sources of Perturbation Growth in Cylinder Wake Instabilities

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Abstract

Flows past cylindrical obstructions have been the subject of keen research interest owing to their ubiquity, importance to engineering structures under aero- or hydrodynamic load, and the fascinating flow patterns they produce. These flows undergo a systematic sequence of transitions, each of which incur a change in their dynamics. This study focuses on the instabilities associated with bifurcations to three- dimensional flow. Although these transitions have been investigated extensively in the past (see report by Barkley & Henderson[1] and review by Williamson[2]), this study approaches the problem from an energetics perspective through the consideration of the out-of-plane averaged perturbation kinetic energy (PKE) equation in an attempt to understand the sources feeding the growth of the linear modes.

For this study, two-dimensional base flow solutions are computed from the incompressible Navier—Stokes equations evaluated at the transition Reynolds numbers for modes A and B. Spatial discretisation is achieved through a nodal spectral-element method, and the equations are evolved forward in time using a third-order-accurate time integration scheme based on backwards differentiation[3]. The linearised equations are also evolved using the same numerical scheme, and the Floquet modes determined using an Arnoldi package (ARPACK). Terms in the out-of-plane averaged PKE equation are then computed.

The oral presentation will discuss the contributions of each term of the PKE equation toward the instability growth, comparing the cases for both modes A and B. The period- averaged terms of the total PKE equation show that the perturbation growth in both modes A and B are predominantly accelerated through terms containing the cross-flow gradient of the base-flow velocity, while viscous dissipation dampens its growth as expected. A key difference between the mean energy exchange rates of the two modes are in the magnitudes of each term's contribution relative to the total perturbation kinetic energy; mode A draws PKE at a significantly lower rate than mode B. Dynamically, each contributing term for mode A either distinctly accelerates or delays PKE growth over the shedding cycle, unlike mode B where PKE production through streamwise gradients of the base flow switches between phases of promoting and impeding the instability growth, albeit at negligible amplitudes.

The locus of the dominant production terms' maxima for mode A locate its origins in the core of the forming vortex in the wake, and it develops according to the description provided in Thompson *et al.*[4] in demonstrating the co-operative elliptical instability mechanism for mode A. For mode B, the maximum production rate occurs within the highly strained region of the near wake. As the vortex is being shed, these regions of high production rate are drawn into the forming vortices, facilitating the feedback reflected in the symmetry of mode B. Contributions from these terms appear negligible downstream where the vortices are relieved from most of the strain induced from the shedding. The perturbations then weaken primarily due to the action of viscosity unlike mode A where the transport terms carry some perturbation out of the domain.

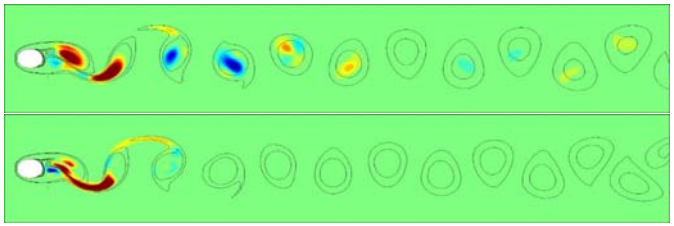

Figure 1: Distribution of the dominant production terms (u'v'dU/dy + v'v'dV/dy) corresponding to events of the base flow. Red (blue) contours indicate net positive (negative) contribution to the PKE growth rate, and the solid lines draw the vortices in the two-dimensional vortex street of the base flow. The top image corresponds to the case for mode A, while the bottom image corresponds to mode B.

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Brief Biography

Zhi is a PhD student at Monash University investigating the dynamics of transitions in bluff body wakes.

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Numerical Study of Droplet Generation via Co-Flowing Microfluidic Device under Electric Field

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Abstract

Applying active control of electric field on the preparation of micro-droplets via the traditional microfluidic technology has attracted great attention because it can effectively improve the controllability of the preparing process. Therefore, a full understanding of mechanisms underlying microdroplets generation via the microfluidic technology under electric field will provide interesting possibilities to actively control preparation of required microdroplets in real applications. A transient theoretical model is developed via coupling of phase-field method and electrostatic model to numerically investigate generation of the single-phase droplets in a co-flow microfluidics device under control of a uniform direct electric field. Via the numerical simulations based on the transient model, the control mechanisms of the electric field on dynamic behaviors of droplets generation are revealed, and the influences of flow and electric parameters on the droplets generation characteristics is elucidated. The results indicate that the electrostatic field is able to generate an electric field force toward the inner phase in the normal direction of the interface between two-phase fluids with different electric parameters (see Fig. 1). The electric field force enhances necking and breakup of the inner fluid interface, which accelerates the droplet generation, increases droplet deformation degree, and decreases droplet size. As the electric capillary number increases under the same hydrodynamic capillary number, the droplet formation pattern is transformed from dripping regime with only a single droplet formed per cycle to another dripping regime with one main droplet formed together with the following satellite droplets per cycle.

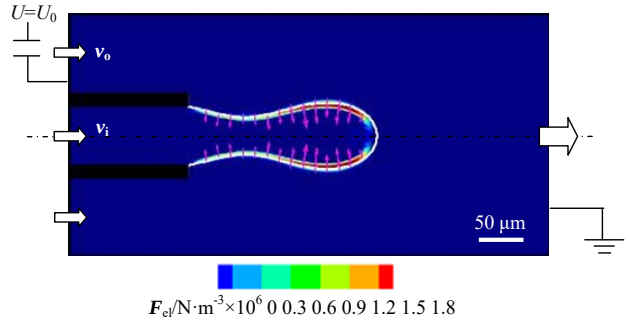

Fig. 1. Electric force on interface, where the purple arrow indicate electric force vectors.

Brief Biography

Lei Li was born in Inner Mongolia, China. She graduated from China University of Petroleum and got her Bachelor degree in 2015. Her major was thermal and energy engineering. With a top ten percent of school achievement, she was recommended to continue her further study in Southeast University. At present, Lei Li is a doctoral candidate of power engineering and engineering thermophysics in school of energy and environment, Southeast University. Her research interests lie in the area of computational fluid dynamics. She has studied the CFD method for almost three years. And her current research projects involve droplet generation, deformation and manipulation under control of an electric field using the finite element method. Specifically, she studied droplet behavior in microfluidic device under the control of a uniform direct current electric field via the coupling of phase field method and electrostatic model. Some of her works are published on conferences and SCI journals as listed below:

1. Lei Li, Xiangdong Liu, Chengbin Zhang Formation of single droplets in co-flowing microfluidic device under electric field 2016 *Lab on a Chip International Symposium: Droplet-based Microfluidics*

2. Lei Li, Chengbin Zhang Mechanism for regulation and control of emulsion droplet

Boundary Layer Resolved Simulation Framework Using Adaptive Grids

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Abstract

Boundary layers can arise in the transport of momentum, mass or heat. Specifically, in multiphase systems, boundary layers also occur at gas-liquid (eg. bubbly flows) or gas/liquid-solid (eg. flows thorough a bed of particles) interfaces[1,2]. In a direct numerical simulation, the grid requirements are often decided by the thinnest of these boundary layers. The study of mass and heat transfer in gas-liquid-solid systems requires resolving the different boundary layers. Because of large Schmidt and Prandtl numbers, the concentration and temperature boundary layers are much thinner than the momentum boundary layers. In a uniform grid approach the resolution of these small scales would demand an overall refinement, which requires an immense computational effort. We present a hybrid mesh approach which uses a fixed Cartesian grid for the hydrodynamics and an octree mesh[3,4] for scalar transport which can be adaptively refined. Since in any CFD calculation, most of the computational time is spent on solving the Poisson equation, our methodology takes the benefit of fast and efficient solvers which incorporates the benefits of Cartesian grids thus reducing the overall computational complexity.

In the present study we will demonstrate the methodology for rigid interfaces which are encountered in gas-solid or liquid-solid flows. The methodology consists of tree-structure based adaptive mesh refinement framework for the convection-diffusion equation for one or more passive scalars, a communicator framework for efficient exchange of flow field from Cartesian grid and staggered velocity interpolations for divergence free adaptation. Tree based adaptive refinements commonly suffer from low order accurate numerical schemes. A higher order finite volume scheme[5] on a parallel tree data structure for solving the convection-diffusion equation has been implemented using an implicit formulation. The resulting set of linear algebraic equation are then solved with a matrix solver from the AMG class. We present detailed validation cases for each module and present results for high Prandtl number flows over single and multiple solid particles. The present study will demonstrate the robustness of this framework to capture sharp boundary layers and its extension to multi core parallel architectures.

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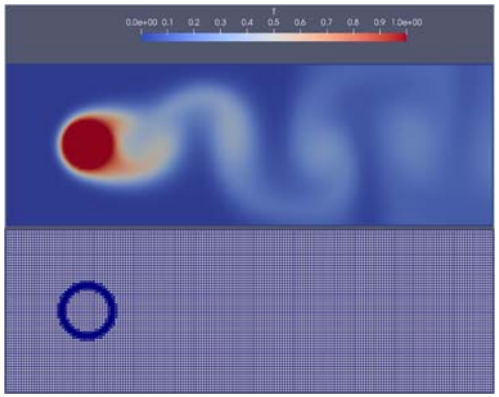

Figure1: Scalar contour plot for flow around a sphere with the respective adaptive grid refined at the interface shown at the bottom

Brief Biography

Aniruddha Panda is currently working as a PhD Researcher working in the area of multiphase flow systems specifically looking at heat and mass transport in bubbly flows. His research interests lie in developing computational framework for resolving boundary layers using adaptive mesh refinement. His research group viz. Multiphase Reactors group headed by Prof. Hans Kuipers has competencies spanning multiple areas covering both experimental as well as numerical work. He joined the group in 2015 prior to which he was working in the fields of data analytics for industrial process control systems and CFD studies on the synthesis of nanoparticles using aerosol flame reactors. He completed his master's studies from Indian Institute of Technology, Delhi from the department of Chemical Engineering where he worked on the numerical study of nanoscale transport phenomena of colloidal particle deposition in microchannels under the guidance of Prof. Rajesh Khanna. Prior to this he completed his bachelor's from University of Pune, India (2nd Rank) and his bachelor's project was on process simulation of amine treatment unit and rating of heat exchangers.

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Numerical Simulation of a Large Scale Bubble Column on Massively Parallel Computers

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Abstract

Bubble (slurry) column reactors (BCRs) are known as efficient and relatively simple reactors used in the Fischer-Tropsch synthesis as well as in waste water treatment, absorption and many other processes. However, their efficient design and scale-up directly depends on understanding of dynamics of multiple phases and impact of multi-scale turbulent structures. In investigating BCRs numerical simulations are increasingly used as an alternative to expensive and sometimes troublesome experiments. However, providing theoretically boundless abilities, numerical techniques are limited by available computational power and quality of models and their embedded closures. In our work we are developing new models and a new highly-parallel numerical code aimed to simulate industrial-scale BCRs with local gas fraction up to 40%.

The main approach used in simulations of large-scale BCRs is the Euler-Euler (EE) approach in which all phases are represented as continuous interpenetrating media. The EE approach has proven to be applicable to industrial scales due to its relatively low computational costs. However, it demands careful formulation of the closures for the interfacial exchange of mass, momentum and heat. Also, due to the loss of information on the scale of individual bubbles incorporation of break-up and coalescence (which are essential in large scale systems) constitutes a challenging problem.

To overcome limitations of EE approach and preserve the same computational expenses, we are using Direct Simulation Monte Carlo method (DSMC) - a modification of the Discrete Bubble Model (DBM), proposed by Kamath et al. [1]. Both models allow to track bubbles as individual objects. However, DSMC incorporates stochastic rules for the determination of collision partners, while DBM uses the conventional deterministic approach. As a result, DSMC demonstrates significant boost in performance (more than 100 times faster compared to DBM). The DSMC model was successfully tested on various problems and its robustness and accuracy was demonstrated. An example of the time-average axial velocity profile from a simulation of a square bubble column is shown in fig. 1.

Apart from computationally inexpensive and accurate models the simulation of large scale system demands for a highly parallel and efficient numerical implementation. Thus, we have designed and developed a new MPI-based CFD framework. The new numerical code demonstrates linear scalability up to 1000 tested cores proving its applicability for large scale problems. With the parallelized DSMC, we are able to simulate BCRs with several millions of individually tracked bubbles on a fine computational grid. In this work we are presenting results

of our test simulations for various middle-scale bubble columns highlighting the potential and efficiency of our numerical framework. As an example of one of the tested heterogeneous bubbly flow systems a snapshot of the corresponding bubble configuration is shown in fig. 2.

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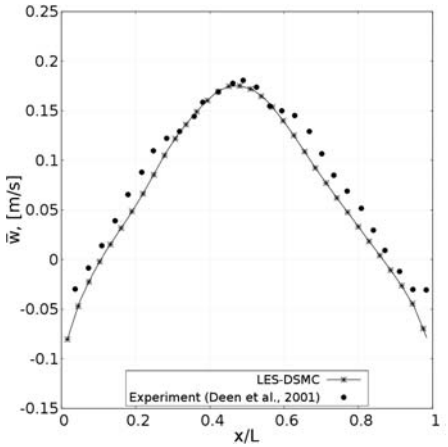

Fig. 1. Comparison of numerically obtained and experimental profiles of time-average axial liquid velocity in a square bubble column [2]. Numerical results are obtained with Vreman subgrid-scale model and DSMC.

Fig. 2. An example of bubble distribution in a square bubble column of size 0.4x0.4x3.6 m containing O(10^6) bubbles.

Brief Biography

Maxim Masterov has obtained his MSc in applied physics and mathematics at the Peter the Great St. Petersburg Polytechnic University in 2011. From 2010 to 2015 he worked in NPO CKTI as an engineer and was responsible for conducting numerical (using Ansys Fluent and CFX) and physical experiments on a different scale hydro turbines and steam turbines. In 2015 Maxim started his Ph.D. at the Eindhoven University of Technology in the Multiphase Reactors Group.

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Bubbly Flow in Stirred Tanks: Euler-Euler / RANS Modeling

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Abstract

Aerated stirred tanks are frequently used equipment in industries ranging from chemical engineering and biotechnology to minerals processing. In principle, CFD simulation of such equipment on industrial scales is feasible within the Euler-Euler framework of interpenetrating continua. Practical application, however, requires suitable closure models to account for phenomena on the scale of individual bubbles, which are not resolved in this approach. The present work applies a set of closure relations that was previously used with good success to describe bubbly flows in pipes and bubble columns. It turns out that model extensions are needed concerning turbulence and the drag force. To validate the model a comprehensive set of experimental data including gas fraction as well as liquid velocity and turbulence has been assembled from different literature sources. The finally proposed extended model compares reasonably well with this dataset.

Keywords: aerated stirred tanks, dispersed gas-liquid multiphase flow, Euler-Euler two-fluid model, closure relations, Reynolds-stress turbulence model, CFD simulation

Brief Biography

Pengyu Shi is a thermo-physics engineering graduate of the Central South University (China, M.S., 2016 and B.S., 2013). He is currently a Ph.D candidate at Technische Universität Dresden in the faculty of Mechanical Engineering under the supervision of Dr. Roland Rzehak at HZDR. His research interest has now focused on multiphase flow, turbulent dispersion, bubble/particle induced turbulence, and interfacial momentum transfer through computational and experimental investigations. This work has been funded Chinese Scholarship Council.

Comparison Of Extrusion Simulations Within Various Numerical Methods And Experiments

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Abstract

This is a numerical study on mixing in extrusion processes. Simulation of extrusion processes are already done, using for example Finite Element Method or Finite Volume Method [1, 2]. The results look promising, however validation of these studies are hardly available. The goal of this project therefore is to create a good comparison of discretization methods (here FEM and FVM) and their numerical techniques for rotating machinery (here the Sliding Mesh Interface and the Immersed Boundary Method). This is done by experimental and theoretical validation of pressure drop in the various sections of a single screw extruder.

SMI is often used with rotating machinery that has a rotating fluid domain inside a stationary fluid domain. The meshes of both domains are sliding over each other on the interface between these domains. The sliding of the meshes can be the reason of inaccuracies in the results. SMI cannot be used with the simulation of an intermeshing twin screw extruder and various mixing elements.

IBM is a method that can be used with the simulation of intermeshing twin screw extruders. IBM has a rotating solid domain in a stationary fluid domain. The rotation of the solid domain causes elements to change in time between solid and fluid. The geometry of the solid will change with the structuration of the mesh in time. The finer the mesh at the fluid solid transition, the less change of geometry. This change of geometry can be the reason of inaccuracies in the results. Therefore IBM needs to be validated first on a single screw and after successfully validated it can be used in simulations for twin screw extruders and mixing elements. If IBM is not accurate than remeshing needs to be done, but this is a time consuming process.

Brief Biography

The Professorship for Polymer Engineering of Windesheim University of Applied Sciences Zwolle is focused on research on sustainable processing of polymers. Cristian Hummel has a Bachelor in Mechanical Engineering and is an instructor in CAE at the Windesheim University. Cristian Hummel is graduating at the Master in Polymer Engineering on this project. Tijmen Mateboer graduated in 2017 as Master in Polymer Engineering at Windesheim University. Tijmen Mateboer researched numerical prediction of tire rubber extrudate swell and co-authored a paper on this subject [3]. Tire rubber extrusion experiments and simulations with wall slip is part of the graduation project of Tijmen Mateboer. Jakob Buist is a researcher who's main specialism is numerical fluid dynamics.

Viscoelastic Rubber Extrusion Simulation With Wall Slip And Comparison To Experiments

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Abstract

Unvulcanized rubber extrusion is a key process in the tire industry. In recent studies flow problems are often addressed with numerical simulations with viscoelastic models and the balance equation. Traditionally, in such flow problems, it is assumed that the fluid adheres to the wall surface: "no slip" condition. However, in some studies the no slip assumption leads to a discrepancy between experiments and simulation [1-5].
This study was focused on simulations of rubber extrusion with slip and verification with industrial extrusion experiments. Both a butadiene rubber and a tire rubber compound were used. Extrusion experiments with both rubbers were performed at a wide range of flow rates.
Slip velocities were determined by comparing rheological measurements with a rheometer with grooved surfaces and a rheometer with smooth surfaces [reference to be submitted].
The rheological behavior (G', G'') was measured with the RPA2000 cone-cone oscillatory rheometer. A PTT model was fitted onto the measurements in order to describe the viscoelastic behavior of the rubber. Viscoelastic extrusion simulations were performed with slip and simulations without slip. The simulation of butadiene rubber without slip overpredicts the pressure drop inside the die. The simulations with slip are for a large range of flow rates in agreement with the experiments. The extrusion simulation of the tire rubber compound without slip overpredicts the measured pressure drop. The pressure drop decreases when slip is included in the simulation, but the simulated pressure drop is still greater than the measured pressure drop.

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Brief Biography

The Professorship for Polymer Engineering of Windesheim University of applied sciences is focused on research of polymer processing. Tijmen Mateboer graduated in 2017 as Master in Polymer Engineering at Windesheim University. Research of Tijmen Mateboer is focused on modeling polymer melt flow, viscoelastic simulations, wall slip and modeling of polymer mixing. Tijmen Mateboer researched numerical prediction of tire rubber extrudate swell and co-authored a paper on this subject [1]. Tire rubber extrusion experiments and simulations with wall slip is part of the graduation project of Tijmen Mateboer.

A Numerical Study on Concentration Polarization In 3D Cylindrical Fluidized Beds With Vertically Immersed Membranes

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Abstract

Hydrogen is recognized as an important alternative energy carrier to move towards a more sustainable future, as well as an important feedstock for chemicals. Hydrogen is commonly produced by Steam Methane Reforming (SMR) in (multi-tubular) packed bed reactors. Methane reacts with steam to form CO and hydrogen at temperatures around 900 °C, after which the formed CO reacts with steam to form additional hydrogen and CO_2 in separate reactors. To ensure a high methane conversion, high temperatures and low hydrogen concentrations are required, and complex and energy intensive separation units such as pressure swing adsorption columns (PSA) are required to separate the hydrogen from by-products like CO_2.

To circumvent the disadvantages of the current industrial methods for hydrogen production, the fluidized bed membrane reactor can be used, which is a novel reactor concept in which hydrogen is both continuously produced and separated from the reaction mixture with modern high-flux palladium-based hydrogen perm-selective membranes. Using a fluidized bed removes the pressure drop limitations from the system and enables usage of small catalytic particles with a higher surface-to-volume ratio. Next to obtaining a pure hydrogen stream at the permeate side of the membrane, hydrogen removal drives the chemical reaction equilibria towards the product side, increasing the reaction rate and allowing reactor operation at lower temperatures (around 550-600 °C) compared to the conventional industrial process.

When injecting binary H_2/N_2 gas mixtures into a fluidized beds with state-of-the-art high flux vertically immersed palladium membranes, mass transfer limitations from the bulk of the bed to the membrane surface (also known as concentration polarization) occur, which reduces the performance of the membranes. Palladium-based membranes are expensive, so they should be utilized as good as possible with as little as possible performance reduction. Next to concentration polarization, placing membranes too close to one another can cause reduced system performance due to the membranes competing for hydrogen with each other, leading to areas in the reactor with strongly reduced hydrogen concentrations, again leading to poor membrane performance. Furthermore, if the membranes are placed too far apart, there will be a lot of hydrogen bypassing, so a balance should be found between concentration polarization and membrane competition.

This work is a numerical study on concentration polarization in 3D cylindrical fluidized bed reactors with vertically immersed membranes. The goal of this work is to identify, describe and explain how concentration polarization manifests itself in fluidized beds with vertically immersed membranes. Full 3D Two-Fluid Model simulations of cylindrical lab-scale fluidized beds with single and multiple vertically immersed cylindrical membranes were performed to quantify concentration polarization, to study how multiple vertically immersed membranes compete for hydrogen.

Reduced hydrogen concentrations occur mostly within 1 cm from the membrane surface, and have disappeared within about 2 cm from the membrane surface. Comparison of a 3D simulation and a Cartesian 2D simulation that represents a slice of the 3D system showed that the 2D simulation did not fully capture the hydrodynamics and radial mass transfer effects of 3D cylindrical fluidized bed membrane reactors, and overestimated the severity of concentration polarization and densified zones near the membrane. The severity of densified zones is also affected by particle size, because for smaller particles (250 μm) the emulsion phase density near the membrane surface is higher than for larger particles (500 μm), which results in increased concentration polarization and a reduced extractive hydrogen flux, so using particles of at least 500 μm in fluidized beds with modern high flux membranes is advised.

In fluidized beds with multiple membranes, interaction between concentration polarization zones of each membrane was observed. The interaction becomes more significant at smaller inter-membrane distances, especially below 2 cm, and decreasing the bed diameter decreases the system performance even more due to hydrogen depletion. Vertically immersed membranes also affect the fluidized bed hydrodynamics by reducing bubble size and increasing the number of small bubbles.

Brief Biography

The Chemical Process Intensification group of the Eindhoven University of Technology focuses on the development of novel reactor concepts for sustainable energy and chemicals production, such as the fluidized bed membrane reactor. The group develops intensified reactors for relevant industrial processes, such as hydrogen production via Steam Methane Reforming (SMR), and combines Computational Fluid Dynamics (CFD) models with phenomenological models and detailed experimental investigations to understand the physical phenomena occurring in the systems. This numerical investigation has been performed by PhD student Ramon Voncken under the supervision of dr. Ivo Roghair prof. Martin van Sint Annaland.

CFD simulation of a cold model inter-connected three fluidized reactors applicable to chemical looping hydrogen production

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Abstract

Nowadays, hydrogen is a crucial gas which is widely used to produce various petrochemical products. Moreover, it is also considered as clean energy carrier for the future. The hydrogen production process using chemical looping is a new approach to produce both the energy and hydrogen. In general, it consists of three reactors which are air reactor, fuel reactor and steam reactor. The metal oxide such as iron oxide with different oxidization states is circulating between reactors, acting as oxygen source and heat transfer media.

In this study, the cold-flow behavior of a typical chemical looping hydrogen production is simulated using computational fluid dynamics. The simulation model is implemented on open source code, namely MFIX. 2D Cartesian coordinate geometry includes air reactor, fuel reactor, steam reactor, loop seal and cyclone. The geometry is implemented using the cut cell technique with optimal mesh cells. The air reactor and steam reactor are operated in fast fluidization regime. In contrast, the fuel reactor is operated in bubbling fluidization. The 200 µm-glass bead particles are fluidized in air. The hydrodynamics profile is emphasized to provide the system behavior such as solid circulation rate, gas leaking, pressure drop and mass distribution of each unit when the operating parameters are varied. In conclusion, the study has validated the model as well as showing the effect of operating parameters on hydrodynamics profiles of the interconnected 3 reactors system. The simulation results aim to provide the useful model and serve as the baseline understanding of the process.

Keywords: chemical looping hydrogen production, three fluidized bed reactor, CFD simulation

Brief Biography

Tarabordin Yurata is currently a PhD candidate at Department of Chemical Technology, Faculty of Science, Chulalongkorn University. Supported by Royal Golden Jubilee PhD scholarship by The Thailand Research Fund, he joins the Energy Business Unit of CSIRO as PhD student. He has background both of computational fluid dynamics and process simulation. Now his researches focus on chemical looping combustion and H_2 purification process.

Imaging Soft Matters and Interfaces at Nano-to-Micro Scale

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Abstract

High resolution imaging of soft materials, particularly their porous microstructures and solid-liquid interfaces, provides crucial information for designing novel materials and optimizing the transport of liquid and particles inside. We demonstrate the recent progress of imaging hydrated and biological specimens at nano-to-micro scale, and the computational tools used to support the development and implementation of the techniques:

(1) X-ray ultramicroscopy (XuM) based on phase contrast is employed to image, reconstruct and analyse the 3D porous structures of hydrogel. This Scanning Electron Microscopy (SEM) based X-ray system produced projection images of ~ 1 µm pixel size, and the reconstruction of the tomographic series provides a complete geometry of individual pores and their spatial distribution and interconnectivity. By further incorporating Atomic Force Microscopy (AFM), the elastic modulus of the hydrogel was determined and mechanical modelling of individual pores and the bulk scaffold also proved to be feasible.

(2) We have also researched on using 2D material (graphene) to encapsulate hydrated and biological specimens followed by various imaging studies including AFM, Electron Microscopy (EM) and Atom Probe Tomography (APT). A computational framework has been developed to understand the detailed encapsulation process, as well as the nanoindentation process on the encapsulated specimens. The successful establishment of controlled graphene encapsulation offers a new route for probing and imaging hydrated specimens and biological cells at nanoscale.

Brief Biography

Dr Jing Fu received Ph.D. from the Pennsylvania State University in 2008, with concentration on manufacturing processes particularly at nano-to-micro scale. From 2008 to 2010, he was awarded a postdoctoral fellowship by the National Institutes of Health (NIH) to continue his research towards biomedical applications. In 2010, Dr Fu joined the Faculty of Engineering at Monash University and currently works as a senior lecturer in the department of Mechanical and Aerospace Engineering. His main research interests are to combine nanoengineering tools, particularly charged particle beams to solve the structural and chemical maps, and to understand various interactions occurring on soft matters and their interfaces. His group has been developing imaging technologies including Focused Ion Beam (FIB), Atomic Force Microscopy (AFM) and Atom Probe Tomography (APT) for imaging and exploring cell-material interfaces.

Hydrodynamic and Stability Behaviour of a Plunging Jet Downflow Bubble Column

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Abstract

Bubble columns of many different designs are used in minerals and process industries for carrying out gas-liquid operations. In mineral processing, the plunging liquid jet bubble column, known as the Jameson Cell, is widely used in mineral processing. Briefly, in the downcomer of the Jameson Cell (see Fig. 1) the liquid is introduced as a high-speed free jet that entrains gas into the mixing zone where fine bubbles are generated as a result of the high energy dissipation rate. Once formed, the bubbly mixing is transported downward into the pipe flow zone and exits from the base of the column. It is in the pipe flow zone that the transition from homogeneous (bubbly) to heterogeneous (churn-turbulent) flow can occur, which greatly influences the performance of the system.

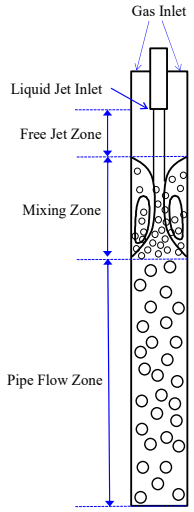

Fig. 1. Schematic of a plunging jet bubble column (Evans, 1990).

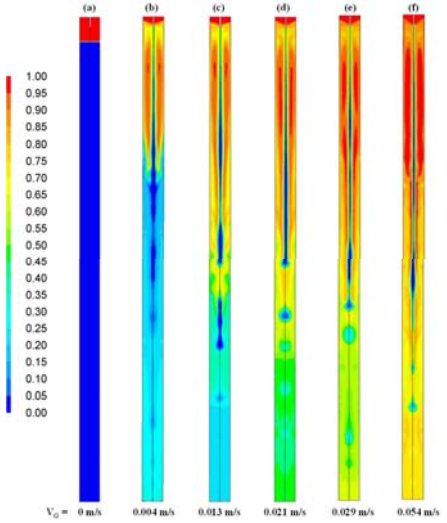

Fig. 2. Contours of gas volume fraction for U_L = - 0.033 m/s and at different gas superficial velocity, V_G.

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In this study, CFD analysis based on the Euler-Euler framework was used to model the two phase (air-water) flow behaviour. It was found that use of the Tomiyama (1998) drag model was successful in capturing the flow hydrodynamic behaviour and of all three (free jet, mixing, and pipe flow) zones when compared with the experimental data of Evans (1990). For example, as shown in Fig. 2 for steady-state CFD simulations (200s) it can be seen that, as expected, for a given liquid jet velocity and diameter the volume of the gas-filled headspace increased with increasing gas inlet flow rate. The length of the headspace corresponded well with the free jet length measurements. The simulations were able to predict the gas void fraction profiles and highlighted the mixing zone, where the determined boundary again well matched with those obtained from the experimental pressure profile. Finally, the CFD-predicted energy dissipation rates were combined with appropriate drift-flux and linear stability (Joshi et al., 2001) analyses to determine the critical gas volume fraction at which the homogeneous to heterogeneous flow regime transition was seen to take place during the experimental observations. For example, for a gas superficial velocity of 0.013 m/s the critical gas volume fraction was at 0.416. As part of the study, comment is made on the influence of influent velocity fluctuations on the gas volume fraction at which regime transition takes place.

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Brief Biography

Dr Md. Shakhaoath Khan is currently working as a Research Officer at the School of Engineering, RMIT University. He obtained his Doctor of Philosophy degree from the University of Newcastle in November 2017. Dr Khan is actively involved in fundamental and applied research into fluid dynamics and multiphase flow systems. The research aims to develop an increased understanding of the principles of intermixing-segregation in a multiphase reactor (e.g., fluidised bed, bubble column) and to use this knowledge to optimise its use in mineral processing. Dr Khan has worked on several research projects (thesis and fellowship) in Bangladesh and Australia. His present research is focusing on process design, optimisation and evaluation of pyrolysis reactors. Research involves a combination of experimental measurement, mathematical modelling and CFD simulation.

Arc Welding Modelling Software Benchmarking For Parameter Optimisation

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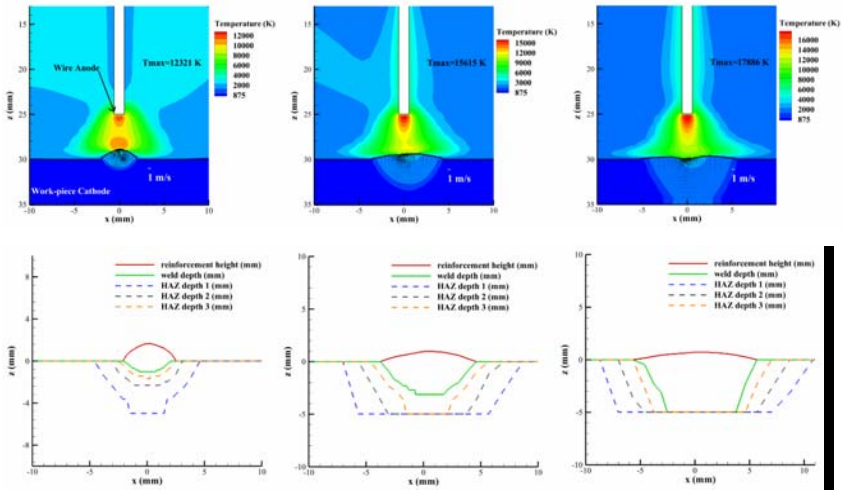
Abstract

Metal inert-gas (MIG) welding is a widely used arc welding process to join metal pieces together using the high temperature and heat flux that is generated by an electric arc between a wire anode and a workpiece cathode. The MIG welding process involves many parameters, such as arc current, workpiece geometry and wire feeding rates, that can influence the weld quality. Computational approaches have been developed to model the interaction between the arc plasma and the workpiece, taking into account these processing parameters [1, 2]. The numerical MIG welding model has been streamlined as a user-friendly software tool for research and industrial use [3].

This work presents a benchmarking study on the MIG arc welding software in order to quantify the relationships between welding processing parameters. The objective of the study is to gain a better understanding of the arc welding process through theoretical modelling and numerical analysis, and ultimately provide critical information and practical guidelines for welding process optimisation. A series of benchmark tests were designed and conducted to study the interrelationships of arc current, workpiece thickness and geometry, welding speed, wire feeding rates, gas flow rates, as well as material selection for the wire electrode and workpiece metal. An example case involving arc current and workpiece thickness for bead-on-plate (flat plate) workpiece geometry is presented here to demonstrate our benchmarking method and the model's capabilities.

Arc current is a very important parameter in MIG welding. The electric arc between the consumable wire electrode and metal workpiece creates a circuit that produces the heat to melt and join metals. The size of the arc current affects the magnitude of the current density, the magnetic field induced by the current and the temperature field. Figure 1 shows the temperature distributions and weld profiles of a 5-mm-thick aluminium-alloy AA5754 workpiece for currents of 95, 150 and 200 A. It shows that, as the current increases from 95 to 200 A, the maximum temperature in the arc increases from 12 300 to 17 900 K, while the weld pool becomes deeper and wider. Further analysis reveals that the ratio of the weld-depth to the workpiece thickness is 0.2 for 95 A, over 0.6 for 150 A and 1 for higher current. This suggests that for 5 mm workpiece (AA5754), 150 A is an appropriate current value to apply. The current of 95 A generates insufficient heat for significant penetration of the weld, while 200 A generates an overly large molten region that penetrates through the bottom of the workpiece.

This work demonstrates the feasibility of a quantitative analysis of MIG welding parameter interdependence using the arc welding model, combined with benchmarking tests. The examples presented show an effective way to identify key parameters in the complicated welding process and quantify their effects on the welded products. The results show the potential of model-based parameter optimisation to assist process engineers in practical improvement of the welding process.



a) 95 A b) 150 A c) 200 A

Figure 1: Comparison of temperature (top row) and weld profile (bottom row) for workpiece thickness 5 mm and different arc currents for bead-on-plate geometry; the 'HAZ depths' correspond to the heat affected zone reaching temperatures of at least 300, 400 and 500°C.

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Brief Biography

Dr. Fiona Chen is an applied mathematician and computational scientist. She has worked for both industrial and government research organisations and conducted various multi-disciplinary projects ranging from MRI imaging analysis, signal processing, sound recognition, to commercial R&D X-ray instrument development for wood microstructure characterisation. In recent years, her research has focused on computational design of aerospace coatings, multi-scale corrosion modelling, material structure and transport property modelling and molecular structure-property relationship modelling (QSPR).

Computational Fluid Dynamics of Sulfur Dioxide and Carbon Dioxide Captures using Mixed Feeding of Calcium Carbonate / Calcium Oxide in Industrial Scale Circulating Fluidized Bed Boiler

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Abstract

The sulfur dioxide (SO_2) and carbon dioxide (CO_2) emissions from fuel combustion in coal-fired power plant are the main reason that harms to living life and environment. Therefore, the SO_2 and CO_2 should be captured before releasing into the atmosphere. However, the competitive of SO_2 and CO_2 captures using mixed feeding of calcium carbonate ($CaCO_3$) / calcium oxide (CaO) solid sorbents is still unclear. In this study, the unsteady state computational fluid dynamics model for gas-solid particle flow in industrial scale circulating fluidized bed boiler, integrating with heterogeneous combustion, carbonation, calcination and desulfurization chemical reactions using mixed feeding of $CaCO_3$ / CaO solid sorbents, was developed in two-dimensional circulating fluidized bed riser to investigate the competitive of SO_2 and CO_2 captures. Then, the effect of operating variables and appropriate guidelines for SO_2 and CO_2 captures were proposed using statistical experimental design method. The considered operating parameters were mixed feeding solid sorbent particle size, mixed feeding solid sorbent position and proportion of inlet fuel velocity. For the mixed feeding of $CaCO_3$ / CaO solid sorbents, the mixed feeding solid sorbent particle size had the significant effect on the SO_2 capture while the interaction between mixed feeding solid sorbent particle size and mixed feeding position of $CaCO_3$ and CaO had the significant effect on the CO_2 capture. About the competitive of SO_2 and CO_2 captures, the reaction rate of CO_2 capture was higher than the reaction rate of SO_2 capture. For the SO_2 capture, the CaO was reacted with SO_2 higher than $CaCO_3$. For the CO_2 capture, both CaO and $CaCO_3$ had higher carbonation reaction rate than calcination reaction rate. In addition, the overall SO_2 and CO_2 captures with mixed feeding of $CaCO_3$ / CaO solid sorbents were higher than the ones with pure CaO solid sorbent.

Brief Biography

Dr. Benjapon Chalermsinsuwan is an Associate Professor of Department of Chemical Technology at Faculty of Science, Chulalongkorn University. He holds a Bachelor of Science degree in chemical engineering from Chulalongkorn university and Doctor of Philosophy degree in chemical technology from Chulalongkorn university. His research interest relates to computational fluid dynamics simulation, experimental design and analysis, carbon dioxide capture and circulating fluidized bed technology. He has published more than 50 articles in professional journals and published 1 book.

Numerical Study on the Coordination Numbers of Particle Mixtures

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2 Monash University-Southeast University Joint Research Institute, Suzhou, China
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Abstract

Coordination number (CN) is an important microscopic parameter in describing the packing of particles. However, little information is available for particle mixtures because of the difficulty in generating data experimentally. This paper presents a numerical study on the CNs of particle mixtures by means of the discrete element method (DEM). In this paper, the DEM results are used to assess the applicability of three most popular analytical models in the literature, which are the models of Dodds, Suzuki & Oshima, and Ouchiyama & Tanaka. It has shown that the model of Ouchiyama & Tanaka differ from the simulated CN significantly thus is not recommended. The Dodds model generally produces a more precise prediction than the Suzuki & Oshima model but their estimations are similar. These two models are able to estimate the variation trends of average CNs for various particle size distributions but their predictability reduce with the increase of the most significant size difference of the packing. In particular, the Dodds model becomes numerical unsolvable when such size ratio is smaller than 0.154. Therefore, modifications or a new model are required for better prediction of the CNs of the packings of multisized systems.

Keywords: multisized particle packing; coordination number; analytical models; discrete element method

Brief Biography

Ruiping Zou is an Associate Professor (Research) at Department of Chemical Engineering, Monash University Australia (2016-). She received B.Eng. (1986) from North-Eastern University China, M.Eng. (1990) from University of Wollongong Australia and PhD (1998) from UNSW Australia. She was an ARC Australian Postdoctoral Fellow (1998-2000), Research Fellow/Adjunct Lecturer (2001-2008) and Senior Research Fellow/Senior Lecturer (2008-2016) with UNSW Australia. Her work mainly focuses on particle characteristics and porosity prediction; particle-structure-property relations; processing and handling of bulk/particulate materials; simulation of particulate systems, and applications in mineral/metallurgy/material industries.

Dr Zou has authored 130 Journal papers, book chapters and conference papers including 76 referred Journal papers; attracted~$1.8M research grants through various university and ARC competitive schemes; graduated 8 PhD and 9 MEng (as co-supervisor or supervisor) and been referee for ARC grant applications and various learned journals including Powder Technology, Chemical Engineering Science, and Industrial & Engineering Chemistry Research.

An Experimental Study of Die Filling of Pharmaceutical Powders using a Rotary Die Filling System

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Abstract

Die filling is a critical process step in pharmaceutical tablet manufacturing. Mass and content uniformity of the tablets as well as the final production throughput depend upon the die filling performance of the formulations. The efficiency of the die filling process is influenced by powder properties, such as flowability, cohesion, particle size distribution and morphology, as well as the process conditions. The purpose of the present study is to systematically investigate powder flow behaviour during die filling. For this purpose, both a linear and a rotary die filling systems were developed to model the die filling process. The linear system consists of an interchangeable stationary die and a moving rectangular powder container (*feed shoe*) driven by a pneumatic drive. The die can be fitted with a moving piston connected to a second electromechanical drive to model the suction filling processes. The rotary die filling system consists of a round die table of 500 mm in diameter, equipped with a rectangular die. The die table can rotate at an equivalent translational speed up to 2 m/s. The filling occurs when the die passes through a stationary shoe positioned above the die table. Using these two systems, die filling behaviours of seven commonly used pharmaceutical excipients with various material characteristics (e.g. include particle size distribution and sphericity, morphology, air permeability, cohesion, and flowability) were examined. The efficiency of die filling was evaluated using the concept of critical filling speed. It was found that the critical filling speed is strongly dependent on such properties as cohesion, flowability, average particle size and air sensitivity index. In particular, the critical filling speed increased proportionally as the mean particle size, flow function and air sensitivity index increase, while decreased with the increase of specific energy, average pressure drop and cohesion. It was also demonstrated that the suction filling can significantly improve the efficiency of die filling.

Population Balance Modelling of Ribbon Milling with a New Mass-based Breakage Function

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Abstract

Dry granulation through roll compaction followed by milling is a widespread pharmaceutical process. The material properties of powders and the process conditions affect the strength of ribbons, and subsequently the granule size distribution of milled ribbons. Accurate prediction of granule size distribution from ribbons with different properties is essential for ensuring tablet quality in the final compaction stage. In this study MCC ribbons with precisely controlled porosities were made and milled in a cutting mill. A population balance model with a new breakage function based on the Weibull function was developed to model granule size distribution from the ribbon milling process. Model parameters at different milling conditions were obtained and their sensitivity analysis were also performed. The parameter sensitivity analyses lead to a simplified model with only one model parameter that is directly related to ribbon porosity. Very good agreement between modelling results and experimental data were obtained. The developed model was also validated with experimental data that were not used for model estimation and the it can predict granule size distribution (GSD) really well. This shows that the model has great potential and can be used for quality by design of dry granulation process.

Two- and Three- dimensional Hydrodynamic Modeling of a Pseudo-2D Turbulent Fluidized Bed with Geldart B Particle

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Abstract

This study presents two- and three- dimensional hydrodynamic modeling of a thin turbulent fluidized bed with Geldart B Particle. Based on the Euler-Euler approach and the EMMS-based drag model, 2D and 3D CFD models are established, the sensitivities of these two models to restitution coefficient and specularity coefficient are analyzed, and the 2D and 3D hydrodynamic simulations are performed and then compared. The simulation results show: (1) 3D simulations are much more sensitive to the restitution coefficient and the specularity coefficient than 2D simulations in the pseudo-2D TFB with Geldart B particle. For different model parameters, there exsit some qualitative and quantitative differences between the 2D and 3D hydrodynamic simulations. (2) At the beginning of fluidization preocess, 2D simulations predict greater bubble and higher bed expansion than 3D simualtions. When complete fluidization are achieved, 2D models exhibit higher solid concentrations than the 3D models in the middle and the upper regions. The fluidization process in 2D simulation develops more quickly than that in 3D computation. (3) Both the 2D and 3D simulations capture the global flow behavior in the bottom dense-phase region reasonably. With increasing the bed hiehgt, the discrepancies between the 2D and 3D results tend to increase. In the middle and the upper regions, however, the 2D models overestimate the solid concentratiion and particle velocity, while the 3D simulations give better hydrodynamic predictions. (4) For the present pseudo-2D TFB with Geldart B particle, the bottom dense-phase region resembles 2D flow and 2D simulations may be adequate. However, the middle and upper regions exhibit 3D flow structure and full 3D simulations are needed.

Brief Biography

Dr. Jian Chang graduated in Petroleum Engineering from the Daqing Petroleum Institute and held his B.Sc. in 1996. From 2001 to 2004, He served as a master in Zhengzhou University, Henan province, China. He was awarded a Ph.D. in Chemical Engineering and Technology from China University of Petroleum in 2007. Then, he spent two years as a postdoctoral researcher in the Refining and Chemical Department at Luoyang Petrochemical Engineering Corporation, SINOPEC, China, working on the computational fluid dynamics (CFD) modeling of FCC process. He dedicated to the multi-phase flow research since 2004 with activities focusing on industrial applications of multi-phase chemical reaction engineering and technology, CFD modeling and process design. He has published near 30 papers on the multi-phase flow and its numerical simulation research.

Particle-scale Investigations of Fluidized Beds with Chemical Reaction Based on CFD-DEM Coupling Method

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Abstract

Fluidized beds have been widely used in the industrial applications of solid fuel energy conversion. Though efforts have been taken to investigate reactive fluidized beds under various conditions, there is still a lack of thorough understanding on the interplays among the gas-solid hydrodynamics, heat transfer, and chemical reactions. It is noted that most previous numerical studies on the reactive fluidized beds were based on the continuum-based simulations, in which it is difficult to arrive the particle-scale information. Comparatively, the coupling of computational fluid dynamics (CFD) and discrete element method (DEM) gives predictions with higher accuracy and resolution, which facilitates the researches of mechanisms in fluidized beds.

A computational framework of CFD-DEM for the dense reactive gas-solid flow has been developed, which includes comprehensive sub-models for the gas-solid momentum, energy and species exchanges. The proposed mathematical methods are first validated against a series of experiments, which shows good agreement between the predictions and measurements. In present study, three typical reactive applications operated under the bubbling fluidization regime are investigated, namely the (i) biomass fast pyrolysis, (ii) coal gasification and (iii) coal combustion. By the virtue of the CFD-DEM, two fundamental aspects are explored: (i) the role of each heat transfer mechanism and (ii) the effect of the gas-solid mixing on the performance of the reactor. The results show that these applications, which differs in the time-scale and characteristics of the reactions, shows distinct patterns of particle entrainment, gas-solid mixing and heat transfer. It demonstrates that the type of the reaction process greatly affects the gas-solid hydrodynamics and heat transfer behaviors. The brief descriptions of the predictions in three applications are shown in **Figure 1**.

Brief Biography

Chenshu Hu majored in new energy engineering and science and got his bachelor's degree from Zhejiang University. He is currently in his fifth year as a PhD student majored in engineering thermophysics under the guidance of Professor Kun Luo, who is an expertise in modelling reactive multiphase flow with turbulence and multi-physics. Chenshu is working to apply the Euler-Lagrangian methods (including the CFD-DEM, coarse-grained CFD-DEM and MP-PIC) to investigate the reactive dense gas-solid system at the commercial scale, aiming to improve the design and operations of the reactors (e.g., chemical looping reactors, oxy-fuel fluidized bed combustor, biomass fluidized bed gasifier, etc.) towards a low-emission and high-efficiency energy conversion.

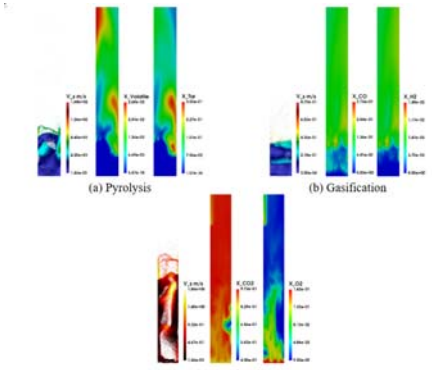

Figure 1 Instantaneous solid distributions and gas species distributions in three applications

Modeling of metal melt, slag and Inclusion Behavior in Electroslag Remelting Process

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Abstract

Electroslag remelting (ESR) is a secondary refining technique with consumable-electrode used in manufacturing high performance and high added-value materials. The ingot quality depends on the macrosegregation of solute elements and distribution of inclusions. A mathematical method has been developed to understand the solute transport and inclusion motion behavior. A finite volume method is used to solve the transient Maxwell equations, heat transfer and fluid flow equations, the slag-metal interface is tracked with the volume of fraction (VOF) approach; the permeability of mushy zone is defined by Blake-Kozeny equation. The solute redistribution at the solidification front is escribed by the lever rule, with the consideration of shearing stress, thermal buoyancy and solute buoyancy; the dynamical mesh technique is used to model the ingot growing process. The numerical results indicate the positive segregation is in the center, and the negative segregation in the outer-radius region of ingot. The trajectories of inclusion particles in liquid metal pool are tracked by the Euler-Lagrange approach. With the VOF-DPM coupled method, the inclusion removal process is revealed, the final positions of inclusions can be defined based on the entrapment criterion.

Key words: Multi-phase Flow, Macrosegregation, Inclusion, Electroslag remelting

Brief Biography

Baokuan Li, Professor, School of Metallurgy, Northeastern University, Shenyang, Liaoning, China. Research interest is Modeling of Multi-phase flow of high temperature melt metal and slag in metallurgical processes.

Atomization and Flame Characteristics of Coal Water Slurry in an Impinging Entrained-Flow Gasifier

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Abstract

Based on the bench-scale impinging entrained-flow gasifier with coal water slurry (CWS) as the feedstock and the development of advanced visualization techniques, the in-situ atomization and flame characteristics of CWS were investigated. A new imaging system was applied to capture the images around the burners in the operating condition. After image post-processing, the instantaneous flame, time-averaged flame and oscillation of the flame were discussed. With the statistical method, the droplet size distribution, oscillation of the droplet concentration and time-dependent droplet size were obtained to analyze the efficiency and stability of the atomization process. The instantaneous flame shows that the atomization and gasification process is turbulent. The time-average CWS flame shows that the atomization angle decreases with an increase in the ratio of elemental oxygen to elemental carbon (O/C ratio). The oscillation of the flame and the atomization process demonstrate that in-situ atomization is closely related to the CWS flame. The diameter and number of droplets after primary atomization decrease with the increase of the O/C ratio. The decreases in median diameter and unconsumed CWS rate demonstrate that the increase in O/C ratio improves the efficiency of the atomization process. The reduction in oscillation scopes of the droplet concentration and size demonstrates that the increase in O/C ratio improves the stability of the atomization process. In addition, the droplet concentration c in three different O/C conditions is 17.8 kg·m-3, 5.9 kg·m-3 and 1.6 kg·m-3 which demonstrates that the CWS is the dilute phase in the OMB gasifier.

Brief Biography

Dr. Yan Gong is a researcher on clean coal technology with 10 years' experience in flame/particle visualization, flame temperature/structure reconstruction, refractory failure diagnosis in gasifier and coal gasification technology, etc.

The Investigation of Drying Characteristics on Flexible Fibrous Particles in Rotary Kilns

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Abstract

Biomass is an important part of renewable energies and characterized by physical properties and structures, including high moisture content, heterogeneous size, and low density. Wet flexible fibrous biomass particle drying was performed in a rotary kiln, aiming to get the appropriate moisture content. To investigate the drying characteristics of fibrous particles, a mathematical model on the heat and mass transfer was proposed, as shown in **Fig.1**. Experiments with fibrous particles under selected conditions were compared to simulations and the feasibility of mathematical models was verified. Furthermore, the transfer of heat and mass between the wet flexible fibrous particle and gas flow was described in terms of rotary drum temperatures, gas flow velocities and gas temperatures. The aim was to gain more information on temperature, moisture content, and the moisture evaporation rate of particles within a rotary kiln during drying processes. The simulation results indicated that the drum temperature could greatly affect the drying behaviors of particles, as shown in **Fig.2**. The temperature and moisture content of particles were marginally affected by properties of the gas flow. The results show that the proposed models offer effective methods to investigate the drying characteristics of flexible fibrous biomass particles.

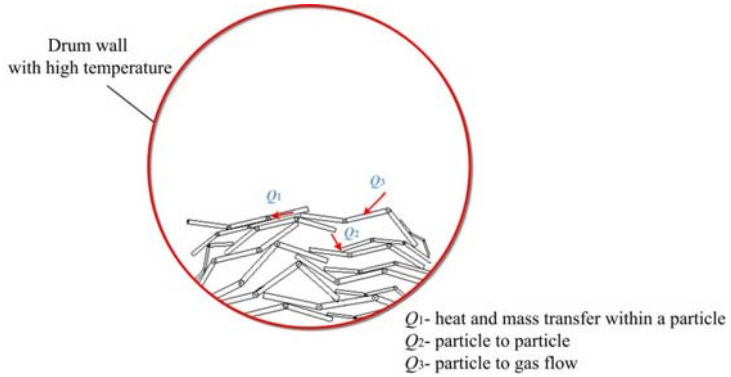

Fig.1 Modeling on heat and mass transfer of flexible fibrous particles in a rotary kiln

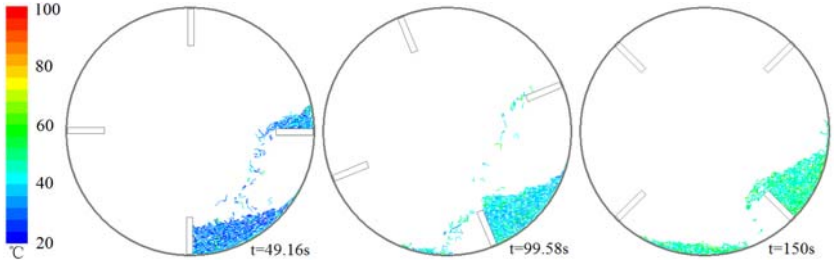

Fig.2 Heat transfer between hot gas flow and flexible fibrous particles in a rotary kiln

Brief Biography

Conghui Gu is a lecturer of the school of energy and power at Jiangsu University of Science and Technology, which is located in Zhenjiang, Jiangsu Province of China. Dr. Gu was born in Jiujiang, Jiangxi, in 1990. She earned her Ph.D in Engineering from the school of energy and environment, the key Laboratory of Energy Thermal Conversion and Control of Ministry of Education at Southeast University, researching the dynamics characteristics and heat and mass transfer on flexible fibrous particles in rotary kilns and fluidized beds. She has also studied at the key Laboratory of Tobacco Processing Technology, Zhengzhou Tobacco Research Institute of China National Tobacco Corporation, Zhengzhou. Since 2013, Dr. Gu has participated in multiple National Natural Science Foundation projects, National 973 projects and 863 projects. She has studied the mean residence time of flexible fibrous particles during drying processes in rotary dryers, and summarized a new corrected formula. The results has been published in Powder Technology, 2016.

So far, Dr. Gu has published about 15 academic papers in various journals, such as *Powder Technology, Fuel Processing Technology, International Journal of Food Engineering*. More than 9 of which collected in SCI/EI Indexes. She has written a textbook on Thermodynamics for international students that study in Jiangsu University of Science and Technology.

Experimental and Numerical Study on Packing Densification of Binary Sphere Mixtures under 3D Vibrations

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Abstract

This paper studies the packing densification of binary sphere mixtures under three-dimensional (3D) vibrations using DEM simulations and physical experiments. The key variables including frequency ω, size ratio r, and volume fraction of large particles X_L are systematically investigated. The results indicate that for a given size ratio r, the dense packing can be achieved by proper control of vibration frequency; and the packing density is much higher than that of mono-sized spheres. The results also show that an ordered structure is readily formed by the large particles, and the small particles are filled in the voids among the large particles. Through the extrapolation on packing densities obtained in different sized containers, the maximum packing density of binary sphere mixtures (without wall effect) is able to reach 0.9013.

Keywords: Particle packing; binary sphere mixtures; densification; 3D vibration; size ratio

Brief Biography

Dr Changxing Li is a research assistant in School of Chemical Engineering of University of New South Wales. He received his Bachelor degree from Shenyang University of chemical Technology (SYUCT), and Master degree from Northeastern University (NEU), and PhD degree from University of New South Wales (UNSW). His research interests include: packing of spherical and non-spherical particles, particle segregation in a blast furnace, and particle transportation under microgravity.

Influence of Cohesion on the Angle of Repose of Iron Ore Granules

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Abstract

Humidity always accompanies different kinds of ores in mining activities that causes various amounts of cohesion force between non-cohesive particles and usually boosts adhesion characteristics of sticky materials. These forces are generally neglected in many researches about granular assemblies. In this research work we have investigated the effects of the magnitude of the cohesion force between particles of different sizes together with varying rolling frictions on macroscopic characteristics of particulate systems particularly angle of repose. In order to achieve this aim, an in-house developed DEM code was used that takes advantage of the Hertz model for contacts between particles and the JKR model for simulating the cohesion force. Particle sizes of 10 and 7 mm were considered. Simulations were carried out for each individual particle size and for different mixtures of the two types of particles. A cubic box with two chambers in the vertical direction has been used to investigate pile formation characteristics. Particles were randomly generated in the upper chamber and then the side walls were removed slowly, so that particles discharged to the lower part of the box and the pile formed at the bottom of the top chamber.

In the absence of cohesion (i.e. surface energy was zero j/m^2), by increasing rolling friction coefficient, the repose angle of formed piles showed a significant rise for all mono-sized and multi-sized particulate systems. Measured angles for rolling friction coefficient between 0.05 and 0.1 were in good agreement with the ones reported by Zhou et al (Zhou, Xu, Yu, & Zulli, 2002). Moreover, keeping the ratio of the box thickness to particle size constant, the value of the repose angle for the smaller particle size were relatively higher than the bigger one that has been previously mentioned by Zhou et al (2002).

In presence of cohesion force the simulation results for the mono-sized systems demonstrated that the cohesion force had a significant influence on the pile characteristic of small particles and resulted in considerable increase in the repose angle. In addition, small amount of cohesion force also changed the behavior of the particulate systems with relatively large particle size (10 mm) and increased the repose angle of piles. Furthermore, after applying cohesion force it was observed that when the surface energy increased, both the number of particles that contribute in pile emergence and the average coordination number of the formed piles rose considerably. Changing particle size from 10 mm to 7 mm generally showed an increase in the value of the coordination number for the whole range of cohesion force (0 to 0.6 J/m^2).

Investigation of the particulate systems with mixture of the two particle sizes revealed that when the proportion of smaller particles increased from zero to 25% and then 50%, although the average coordination number of piles increased, the repose angles decreased. This was attributed be as a result of the formation of a looser structure caused by increase in smaller particles portion (Jia, Zhang, Chen, & He, 2012).

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Brief Biography

Dr Roberto Moreno-Atanasio is currently a Lecturer in Chemical Engineering and a Member of the Priority Research Centre for Advanced Particle Processing and Transport at the University of Newcastle, Australia. His main area of research involves the multiscale theoretical and computational modelling of particulate systems including flotation, granulation, segregation and colloidal suspensions. He has recently extended his research interests to the process intensification of particle fabrication and surface functionalisation. Dr Moreno-Atanasio obtained his PhD in 2003 from the University of Surrey, UK and previously worked at the Institute of Particle Science and Engineering, University of Leeds as a postdoctoral researcher.

The Emerging and Coupling of Localized Zones in Sheared Granular Materials

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Abstract

A series of true triaxial tests with designated constant *p* and constant *b* loading path is simulated using discrete element method (DEM), which provides thorough insights into granular materials on both micro- and macroscopic scales. The macroscopic failure is observed within the particle assemblies when localized deformation emerges. Of great interest in this paper is the coupling of localized zones before the onset of the shear banding. Several measures, such as particle temperature, non-affine deformation, and local militancy angle, are adopted to quantify localized and nonaffine deformation. By calculating the correlation coefficient matrix of different measures, it's evident that non-affine deformation correlates well with other indicators, which confirm the key role that one plays in distinguishing strain localization. Thus, a best-fitted parameter related to trigger position of sheared localization is put forward, which is used for the exploration of the emerging localized deformation pattern in sheared granular materials before the onset of stable shear bands. The simulation results demonstrate that as the loading proceeds, the increase of Moran's *I* indicate a more clustered granular system before the generation of obvious shear bands.

Brief Biography

Prof. Wei Zhou received his Master's degree and Doctor's degree from Wuhan University in 2001 and 2004, respectively. He was a visiting scholar in University of Alberta from 2010 to 2011. Currently, he is a professor in State Key Laboratory of Water Resources and Hydropower Engineering Science, Wuhan University, and a New Century Excellent Talent, Ministry of Education, China. His research interests include mechanism and numerical methods for granular material, thermal analysis of concrete structure and stability analysis of high dam foundation.

Prof. Zhou has been engaged in the research of numerical analysis methods and deformation control of high rockfill dams for a long time. He proposed a refined description method for the meso-structural features of rockfill granular materials, established a stochastic discontinuous deformation model of rockfill materials, developed a numerical simulation technique based on continuous-discrete coupling for particle crushing and complex particle shape, and developed a large-scale FEM/DEM coupled numerical analysis platform for stress and deformation analysis of high rockfill dams.

Prof. Zhou has served as journal reviewer of Applied Mathematics and Computation, Earthquake Engineering and Engineering Vibration, Energy, Engineering and Structures and Computers and Geotechnics. He has been supported by a series of the National Natural Science Foundation of China, as well as Talent Supporting Program, and he is a recipient of the Naional Science Fund for Distinguished Young Scholars.

Relationship between packing density and randomness for packing of ellipsoids

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Abstract

Granular packing of different particle properties pervade the pharmaceutical, chemical, agricultural, mining, building materials, explosives, and food industries. For packing of spheres, the bed can transit from disordered to ordered and meanwhile from loose to dense under properly controlling vibrational and charging conditions. However, the relationship between packing density and ordering in packing of ellipsoidal particles is still not clear for. In this work, this relationship has been examined for packing of fine ellipsoids and vibrated system with coarse ellipsoids at both macro-and micro- scales by DEM. The shapes considered are oblate and prolate spheroids, with aspect ratio varying from 0.15 to 4.0. It is shown that under the poured packing conditions, for poured packing of coarse ellipsoids, flat or elongate particles show strong orientation preference on the horizontal direction. For packing with different particle sizes, when increasing particle size, packing density increases, orientational order increases. For the cases of packing under one-dimensional vibration with periodic boundary condition and cylindrical wall conditions, after vibration, packing density increases, but orientational order decreases. For spheres, denser packing leads to more (positional) ordered. For ellipsoids, denser packing can either be more (orientational) ordered/random packing, which implies it does not necessarily be ordered packed to obtain higher packing density.

Brief Biography

Jieqing Gan is a postdoctoral research fellow with the Laboratory for Simulation and Modelling of Particulate Systems (SIMPAS), Department of Chemical Engineering, Monash University, Clayton VIC 3800, Australia (e-mail: Jieqing.gan@monash.edu). She received her doctorate of philosophy degree in Chemical Engineering in December 2015 at Monash University. Her research area refers to DEM/CFD-DEM modelling and simulation on fluid and granular flow, heat transfer and chemical reaction with spherical and non-spherical particles. She also develops GPU-MPI based DEM for large scale simulation of granular flow with arbitrary wall geometry, complex wall movement and non-spherical particles.

Lattice Boltzmann Investigation on the Interactions between Non-Newtonian Fluid and Ellipsoid Particles

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Abstract

Non-Newtonian fluid flows through packed beds are commonly encountered in many industries and have been extensively studied, either experimentally or theoretically in the past decades. In recent years, the sub-particle scale simulation approach, lattice Boltzmann (LB) method, has been developed and successfully applied to study the important interaction forces between non-Newtonian fluid and particles in the mixture systems. To date, such studies of non-spherical particles are rare for non-Newtonian flow systems. In this work, we extend our recent studies of non-Newtonian fluid-sphere particle systems to the packed beds with ellipsoid particles. The LB model will be firstly used to validate the drag force coefficient of a single ellipsoid. Then, the validated model will be used to study the particle shape and porosity on fluid flows and quantify the interactions between non-Newtonian fluid and ellipsoid particle in packed beds. The aspect ratio of the ellipsoid varies from 0.25 to 4, which represent from disk-type to cylinder-type particle, covering a wide range of engineering conditions. The flow structure and the distributions of drag on particles are analyzed relating to the non-uniform structure and shear-dependent viscosity of non-Newtonian fluids. Based on simulated data, a new equation is proposed to calculate the drag force on particles.

Biography

Mr. Zheng Qi obtained his BEng in 2011 from Tsinghua University, MEng in 2014 from UNSW and PhD in 2018 from Monash University. He is currently a research fellow in ARC Research Hub form Computational Particle Technology at Monash University. His research has been focused on the development and application of numerical models at different time and length scales, including using CFD, LBM-DEM to study particle-Newtonian/non-Newtonian fluid flows and particle separation.

CFD-DEM study on mixing behavior of cohesive particle in a spouted bed

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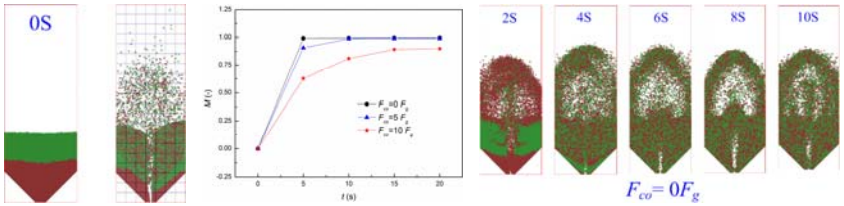
Abstract

Spouted bed, which is a special fluidization reactor, can be extensively used in various industrial fields. Cohesive force between solid particles widely exists in a lot of industrial processes and influences particle behavior greatly. However, the effect of cohesive force on particle mixing behavior in the spouted bed has not been well understood. In the present work, a numerical model was developed using discrete element method to study the mixing behavior of cohesive particles in the spouted beds. The evolutions of flow patterns during mixing processes with different magnitudes of cohesive force were obtained. Particle mixing index and particle circular fluxes were also compared. The mixing rates at the same spouting gas velocity were found to decrease as the increasing of the cohesive force due to the fact that particle diffusive motion in the annular zone was hindered by the cohesive force.



Brief Biography

Dr. Huibin Xu is a research staff at Jiangsu University. His research focuses on the CFD-DEM simulation of cohesive/wet particles in dense gas-solid multiphase systems.

CFD-DEM Investigation of Mixed Layer Formation and its Effect on the Performance of a Blast Furnace

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Abstract

Gas flow distribution in a blast furnace (BF) plays a significant role in BF smooth operation, productivity and thermal efficiency. It is affected by the distribution of burden materials composed of alternating coke and ferrous ore layers. While moving downward coke and ferrous layers of different sizes can mix and form the so-called mixed layers. Generally, the porosity is lower and hence the pressure drop is higher in the mixed layers. These variations can change the gas flow distribution and BF performance. Previous work tried to quantify the effect of material properties and process conditions on the formation of mixed layers and the resulting local porosity variation. However, these studies were often conducted under simplified conditions. Few were dedicated to the formation of mixed layers in a BF and its effect on BF performance. This work studies the formation of mixed layers in an experimental BF by using a combined computational fluid dynamics and discrete element method approach. The effect on BF performance is evaluated under different operational conditions including different size ratios of coke and iron ore particles, burden distribution and batch weight, and discharge rate. The corresponding thermo-chemical behaviors are observed and discussed. The results are helpful to optimize burden charge for improving BF performance.

Brief Biography

Dianyu E is currently an associate professor in the Institute for Minerals, Metallurgy & Materials, Jiangxi University of Science and Technology. He received his bachelor degree from the University of Science and Technology Liaoning, master degree from the University of Science and Technology Beijing, and PhD from Monash University. His main research interests are modelling and simulation of the multiphase flows in chemical engineering processes at different scales for optimal design and operation.

Detailed Analysis of Multicomponent Adsorption Using CFD

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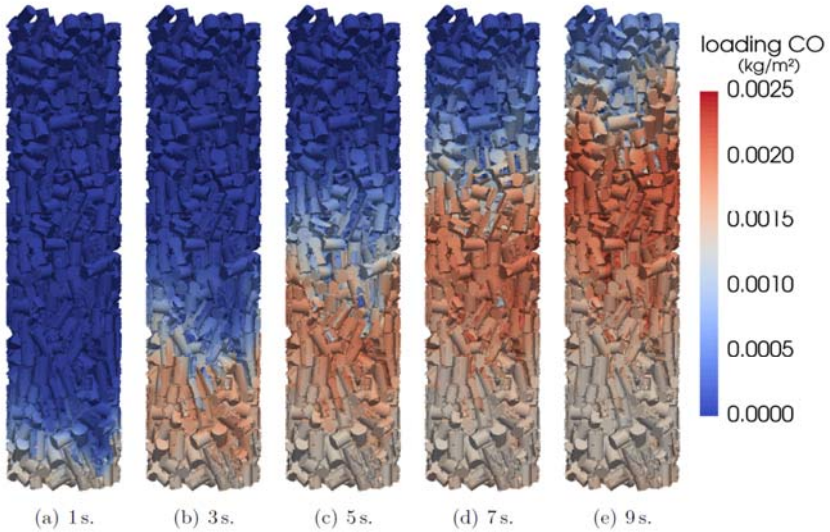
Abstract

Adsorption is a well-developed technique in separation and purification of process streams. It is common that more than one component of a mixture adsorbs on the adsorber, and a competitive behavior during the separation of multicomponent mixtures can be observed. CFD simulation of adsorption phenomena can give a very detailed insight into these phenomena and helps with improving the design of adsorption columns and devices. In this work, multicomponent adsorption models have been implemented in computational fluid dynamics solver adsorpFoam [1] developed at TU Wien based on the open-source code OpenFOAM®. For this, two multicomponent equilibrium models, the Extended Langmuir Model ELM and the Ideal Adsorbed Solution Theory IAST, are used. They solely depend on single-component isotherm data. For interspecies-dependent kinetics, a diffusion-based approach is chosen [2].

At the beginning, the equilibrium and kinetics models were tested using a zero-dimensional approach. The quality of prediction of equilibria is dependent on the chosen system of species. The model predictions are compared with experimental data of multicomponent systems. If experimental data are available, a simple extension to the ELM is possible. This is done by introducing empirical interaction coefficients to account for competitive adsorption, which improves the prediction of most systems. For this approach, data of multicomponent adsorption experiments have to be obtained.

The implementation in OpenFOAM (adsorpFoam) includes the adaptation of the governing equations, calculation of actual and equilibrium adsorption loading and rate of adsorption. Additionally, the adsorption enthalpy is added as heat source term to the adsorbent. As a first step towards multicomponent mass transfer, using the adsorpFoam multicomponent adsorption of hydrogen, methane, carbon monoxide and carbon dioxide in a packed bed was simulated and the competitive behavior of the gases on their adsorption was studied. The loading of CO on the packing at different times can be seen in the following figure.



Distribution of the adsorbed amount of carbon monoxide in a packed bed for different simulation times.

[1] Haddadi, Bahram, Christian Jordan, and Michael Harasek. "Cost efficient CFD simulations: Proper selection of domain partitioning strategies." Computer Physics Communications 219 (2017): 121-134.

[2] Do, Duong D. Adsorption analysis: equilibria and kinetics. Vol. 2. London: Imperial college press, 1998.

Brief Biography

Dr. Michael Harasek received his PhD in Chemical Engineering from TU Wien in 1997. For more than twenty years, he has been working on the design of new processes and technologies in the process industries and related fields. A major part of his research work is dedicated to the development of environmentally friendly technologies and related fields as well as process intensification. Michael Harasek works on the application of CFD and experimental fluid dynamics in many fields of chemical engineering, and the implementation of multiscale and multiphysics capabilities for complex flow problems. As head of the research area „Thermal Process Engineering and Simulation“ he guides a team of about 25 scientists at TU Wien, Institute of Chemical, Environmental and Bioscience Engineering.

Numerical Simulations of Fluid Flow past a Superelliptic Cylinder

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Highlights

- Cylinders with superelliptic cross sections were studied in the flow simulations.
- The drag coefficient and Nusselt number of the superelliptic cylinders were estimated.
- Adaptive octree meshes were used to resolve the surfaces of the superelliptic cylinders.

Introduction

As a classic problem of flow past a blunt body, flow past a circular cylinder has always been the focus of attention and research for its important engineering significance and theoretical value. Moreover, drag reduction and inhibition of Vortex-Induce-Vibration are the key in practical engineering application. Therefore, it is of great importance to explore the flow mechanism and related physical nature, and then to find an effective method to reduce the drag, control the flow and improve heat transfer efficiency based on the relevant physical mechanism.

Currently, the studies on the fluid flow past blunt bodies mainly focuses on cylinders of regular-shaped cross section, such as circular, elliptic and squared. To our knowledge, few researches have been made to estimate the drag force and heat transfer of cylinders with complex cross sections. However, in some chemical engineering applications, say catalytic reactors and adsorbent beds, the fluid-solid relative motion of irregular bodies is always involved. So, it is of great significance to study the drag and heat transfer characteristics of superelliptic cylinders.

In this work, a series of superelliptic cylinders were constructed for the numerical simulations. To highly resolve the geometrical shape of the cylinders and save computational cost, a technique of adaptive octree mesh was used. Based on the simulated results, correlations were formulated between the drag coefficient and Nusselt number of the cylinders, and Reynolds number, geometric shape and incident angle.

Methodology

In the present work, the cross sections of cylinder studied are in superelliptic shape, which can be described using Lame curve. In the Cartesian coordinate system, the set of all points (x, y) on the curve satisfy the following equation:

$$\left|\frac{x}{a}\right|^n + \left|\frac{x}{b}\right|^n = 1 \qquad (1)$$

Here, a、b、n are positive numbers. As shown in Fig.1, we set $a = b$ and $1/2 \le n \le 2$ in the simulations. It is obvious that as n increases from 1/2 to 2, the shape of superellipse will gradually change into a circle.

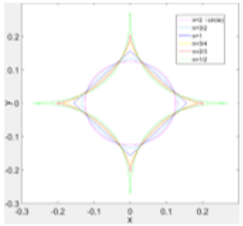

Fig.1 Superelliptic cylinders of identical cross area but in different shapes used for simulations.

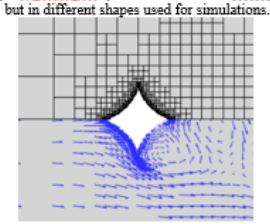

Fig.2 Adaptive meshes and velocity field near the superelliptic cylinder at n=2/3 and R_e=200.

It is difficult to highly resolve the surface of superelliptic cylinders with traditional mesh technique because of their complex geometrical shapes. So a technique of adaptive octree mesh was used here. As shown in Fig.2, The meshes are automatically refined during the calculations. In addition, velocity field of the fluid flow near the superelliptic cylinders was also showed.

Results and Discussion

In Fig.3, we compared the surface pressure coefficients of different superelliptic cylinders under the same condition to illustrate the influence brought by geometric parameter n. Clearly, the surface pressure gradient become greater as n reduces from 2 to 1/2. In Fig.3, the dimensionless pressure coefficient is defined as

$$C_p = \frac{P - P_\infty}{\frac{1}{2}\rho U_\infty^2} \qquad (2)$$

with ρ, U_∞, P and P_∞ being the fluid density, fluid velocity, surface pressure and far-field pressure, respectively.

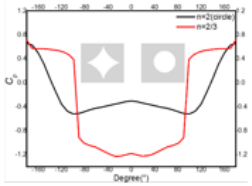

Fig.3 Pressure coefficients around the surfaces of superelliptic cylinders for n=1/2 and n=2 when R_e=200.

The analysis of variation of drag force with Reynolds number is a classical topic for studying the flow past an object. The dimensionless drag coefficient in 2D is defined as

$$C_D = \frac{F_X}{\frac{1}{2}\rho U_\infty^2 D} \quad (3)$$

where F_X , D are the drag force and characteristic length, respectively.

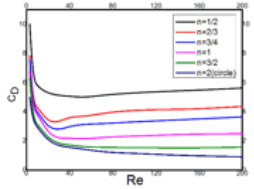

Fig.4 Variation of C_D with Reynolds number at different n.

As shown in Fig.4, drag coefficients sharply decrease as Reynolds numbers increase from 3 to 20 and gradually become gentle as Reynolds number increase to 200. In addition, in spite of the same variation trends, the extreme values of drag coefficients reduce as n increases from 1/2 to 2.

The heat and mass transfer characteristics are also significant for studying the fluid flow past an object. In this paper, we use dimensionless Nusselt number to reflect the intensity of convective heat transfer. Nusselt number is defined as:

$$N_u = hD/k \quad (4)$$

With h being heat transfer coefficient and k being thermal conductivity of stationary fluid.

The Nusselt number is almost linear growth with Reynolds number and also increase with n at same Reynolds number, as shown in Fig. 5.

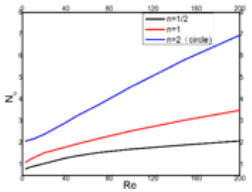

Fig.5 Variation of N_u with Reynolds number at different n.

Conclusion

Fluid flow past superelliptic cylinders have been simulated. Based on adaptive octree mesh, the finite volume method was used to solve two-dimensional incompressible viscous N-S equations. The effects of Reynolds number, geometric parameters and incident angles on the drag force and heat transfer of superellipses are studied.

The method developed here was proved to be effective. We hope that based on the simulated results for superelliptic cylinders, we can explore the fluid flow past three-dimensional superellipsoid in the future.

Brief Biography

Dr. Liangwan Rong is now working at the School of Civil Engineering and Transportation at South China University of Technology (SCUT) in Guangzhou, China as a lecturer. He obtained his PhD (2010) in Fluid Mechanics from Sun Yat-sen University, and worked as a postdoctoral fellow at the University of New South Wales, Australia, from 2011 to 2014. Dr Rong's research interests are mainly the simulation and characterization of fluid flows in porous media and the modeling of fluid-particle interactions for particle-fluid flow systems. His current research project is: The micro-mechanism of fluid flow in porous media and the correlation between flow and pore-structure, supported by the Natural Science Foundation of Guangdong Province.

Numerical investigation of the effects of oxygen enrichment on an ironmaking blast furnace (BF)

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Abstract

The enrichment of oxygen content in an ironmaking BF can help to increase the productivity. However, an excessive increase of oxygen content in hot blast lead to an increased fuel rate due to the small thermal flow ratio in-furnace and consequently insufficient heating-up of burden materials To overcome this problem, a previously developed multiphase flow BF process model was used to study the effects of oxygen enrichment in hot blast on BF performance. The study was carried out under the condition that the temperature and flow rate of reducing gas generated from raceway were kept constant throughout the simulations. Model study reveals that optimum oxygen enrichment exists for the BF operated with specified operational and materials conditions. Below this value, the heat loss from wall for processing unit HM is increased and indirect reduction of iron ore is inhibited. Above it, the heat exchange between burden materials and reducing gas is deteriorated due to the intensified interphase movement. To increase the optimum value of oxygen enrichment and hence productivity of the BF, typical burden distribution patterns were examined at different oxygen enrichment. It is shown that as the radial burden distribution becomes more uniform, the optimum value of oxygen enrichment is increased. This is attributed to the lowered down gas-soli relative velocity when the radial distribution of burden materials becomes more even.

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Valid Local Quantities of Particle-fluid Flows for Constitutive Relations

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Abstract

There are continuum and discrete approaches to describe granular flows. A continuum approach relies on local average quantities which can be derived through an averaging method based on a discrete approach. But the selection of an averaging domain and the validity of local quantities for constitutive relations are not well established, particularly for transient particle-fluid flows. Here, we demonstrate that converged local quantities such as stress and solid volume fraction can be achieved on an averaging domain with proper spatial and temporal sample sizes. Furthermore, the relation between solid pressure and solid volume fraction is established which agrees qualitatively but is different from all the existing monotonic ones in the literature (Fig. 1). It shows a bifurcation at a high solid volume fraction, essentially linked to the variation of short and enduring contacts among particles with flow state and solid volume fraction. This bifurcation must be properly recognized in developing constitutive relations for granular materials.

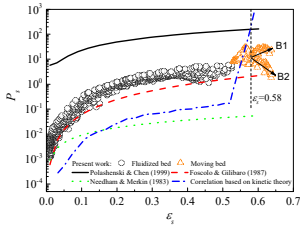

Figure 1. The relations between P_s and ε_s in fluidized and moving beds. L_t and L_p are temporal and spatial sample sizes. Circle and triangular symbols are from the averaging method with L_t = 180 and L_p = 3. The relations are from literature.

Brief Biography

Dr Hou is a current ARC DECRA Fellow and Research Fellow in the Department of Chemical Engineering at Monash University. He was awarded a PhD at UNSW of Australia in 2012, ME and BE in 2003 and 2000 respectively from Northeastern University of China. Aiming to formulate safe, energy efficient and sustainable processes involving granular materials, his research mission and passion centre in the understanding of the mechanics and thermochemical behaviours of granular (and multiphase) flows and their impact on structures and environment through rigorous cutting-edge multiscale modelling techniques, experiments and theoretical analysis. The knowledge can be applied to solving energy and water issues in the industry including chemical, metallurgical, mineral processing, agriculture, pharmaceutical and geotechnical engineering. His main research areas include: (i) heat transfer and chemical reactions in gas-solid flows, (ii) multiphase flows in water treatment, (iii) granular flow stability pertinent to segregation and mixing, and (iv) development of numerical techniques and virtual process models. Dr Hou has published 60+ articles, and attracted over A$2M research funds. Dr Hou has also received various awards in the past, reflecting the recognition at different stages, and been invited to give talks at different international conferences. He has also involved in the co-supervision of 4 PhD candidates (one graduated in 2018) and undergraduate teaching at UNSW and Monash University.

Three-dimensional Modelling of Blast Furnace with Layered Cohesive Zone

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Abstract

In the Blast Furnace (BF) ironmaking process, the burden materials consisting of coke, ore, and flux particles are charged into the furnace, in most cases, layer by layer. The resulting layered structures play a crucial role for the cohesive zone behaviours that largely determine BF performance. Moreover, BFs present three-dimensional (3D) characteristics in terms of flow and thermochemical behaviours, especially when the top and bottom operations are not uniform along the circumference. To describe these complicated characteristics, we have developed a steady-state 3D parallel comprehensive BF process model, based on our existing axisymmetric model. This model, solved by Computational Fluid Dynamics (CFD), is integrated with our recent developments in modelling the layered burden structures, the stockline variation, and the liquid flow in the dripping zone. It also considers the redistribution of reducing gas by raceways. The applicability of the model is examined by comparing the predicted and measured results under various experimental and industrial BF conditions. Also, the commonly used CFD BF process models, namely, slot, axisymmetric, and 3D models are quantitatively compared against the in-furnace states and performance indicators. The result highlights the influences of different treatments related to burden and raceway in these models. The 3D model can offer a convenient way to predict in-furnace states and global performance of BF under realistic conditions.

Brief Biography

Dr. Shibo Kuang is currently a research fellow in ARC Research Hub for Computational Particle Technology at Monash University. His research has been focused on the development and application of numerical models at different time and length scales, with the support of physical experiments, for the fundamental and applied research on particle-fluid flow and granular dynamics. The specific topics include particle transportation, particle separation, and reacting multiphase flows in the process engineering. In this area, he has published over 70 papers including 50 (40 in the past five years) journal papers collected in Web of Science. The number of citations from these publications is > 980 (H-index=18) according to Google Scholar.

Simulation Study on the Mixing of Granular Materials in a Screw Conveyor

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Abstract

In contrast to physical experiments, the discrete element method (DEM) can readily reveal the details of granular flows at the particle level, and thus has been extensively employed in both fundamental research and engineering practice. Nevertheless, most applications are restricted to small scale problems due to its high computational cost. Based on previous work and collaboration, a parallel simulation method and software is developed, coupling GPU (Graphics Processing Unit) and CPU (Central Processing Unit) computing for non-linear DEM models on a multi-scale heterogeneous supercomputing system. With this method and software, the mixing mechanisms of an industrial scale screw conveyor are investigated systematically. The influence of geometry and operating conditions on mixing performance is evaluated with respect to the Lacey mixing index. It is found that the mixing properties of the screw conveyor depend strongly on operating conditions and structural dimensions. The screw speed and feeding rate have dominant effects on the mixing extent, while the sizes of the granular materials and the screw pitch of the mixing region have a secondary effect. According to these findings, reasonable selection of technical parameters can effectively avoid equipment defects and guarantee good mixing performance to a certain extent.

Brief Biography

Dr. Qi is a research fellow in Institute of Process Modeling and Optimization of Jiangsu Industrial Technology Research Institute. He has received his Doctoral degree of chemical engineering from Institute of Process Engineering, Chinese Academic of Sciences. His research interests relates to discrete element models for the simulation of particle systems and high performance computation, in particular the application of GPU-based discrete simulation to the study of mixing, heat transfer and pyrolysis of granular materials

Flow Simulation and Performance Analysis of a Cyclone–Granular Bed Filter

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Abstract

It is a common challenge and key issue to remove the flying char particles from high temperature pyrolysis vapors in thermal conversion processing such as biomass, coal or oil shale. In this work, an integrated dust removal technology of cyclone-granular bed filter (C-GBF) which utilizes the separation potential in cyclonic motion and avoids stagnant zones in granular moving was designed. The flow pattern of C-GBF was numerically simulated on the platform of ANSYS-FLUENT. The Reynolds stress model (RSM) was used to predict the anisotropic turbulence and the strong swirling flow in cyclonic motion space of the C-GBF. The tangential velocity, axial velocity and pressure drop under different inlet gas velocity and filtration velocity were investigated. The free vertex of flow pattern in C-GBF was observed and the maximum tangential velocity was about 1.2 times greater than the inlet gas velocity. The pressure drop of C-GBF was mainly due to the effect of granular bed and little affected by the outer vertex space. The verification of simulation results was conducted by comparing with the experiments of separation performance.

Brief Biography

Dr. Minshu Zhan is a research fellow in Institute of Process Modeling and Optimization of Jiangsu Industrial Technology Research Institute. He received a PhD in 2015 from China University of Petroleum, Beijing. Dr. Zhan mainly works on the gas-solid multiphase flow and separation technology R&D in coal or biomass thermochemical conversion, especially high temperature pyrolysis vapors filtration with granular bed filter and two-phase flow analysis in cyclone.

Investigation of Burden Matrix Effects on Gas Flow in a Blast Furnace

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Abstract

Burden matrix is the feeding mechanism of burden materials into blast furnace throat; thus the burden distribution depends on the burden matrix. Further, the burden distribution makes a direct impact on the gas distribution thus ironmaking process in a blast furnace, and hence adjusting the burden matrix is one of the most important methods to take control of a blast furnace. In present study, the burden distributions in different conditions are simulated by combining Discrete Element Method (DEM) with Computational Fluid Dynamics (CFD). The variables are including, for example, particle size, cohesive zone and multi-layer effects. Further, the shifting of burden profile, porosity distribution, gas velocity distribution and pressure distribution are presented and analysed. The results showed that burden profiles vary with time due to the later-dumped materials during descending. Burden matrix determines the burden profiles but its effect gradually decreases in the descending process. Porosity distribution corresponds with coke and ore distributions in the burden layers, and thus determines the gas velocity distribution.

Brief Biography

Dr. Sida Liu obtained his bachelor's degree in 2008 from Dalian Jiaotong University, and then started his master study in University of New South Wales under the supervision of Prof. Aibing Yu and Dr. Zongyan Zhou. He completed his master's degree and continued to pursuit a PhD in 2011. He transferred to Monash University in 2014 and completed his PhD program in 2015. In 2016, Dr. Sida Liu went to China and joined the Institute for Industrial Progress Simulation and Optimization as a program manager. Dr. Sida Liu's research area is mainly related to blast furnace burden distribution. The major duty for Dr. Sida Liu in China is commercialization/industrialization and marketing management for SIMPAS research outcomes.

Key notice & instructions: DEM, CFD, Blast Furnace, Burden Distribution

Discharging of Ellipsoidal Particles in a Rectangular Hopper

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Abstract

Hoppers are widely used in many industries such as mining, metallurgy, and food industries. It is the essential feeding mechanic for blast furnace, thus fundamental study is required in this area. To develop a comprehensive understanding of the dynamic behavior of granular flow in a hopper, extensive studies have been carried out by means of analytical, experimental and numerical approaches. In particular Discrete Element Method (DEM) plays an important role. A major concern in plant applications of hopper flow is wall stress distribution. Ellipsoid is an ideal shape that can represent a wide range of shapes varying from disk like to cylinder like particles, thus it has been increasingly used to examine the effect of particle shape on different behavior. In present study, ellipsoidal particles with various shapes are simulated by DEM to investigate the particle shape effects on silo wall stress. The results indicate that the particle shape changes the internal properties thus bulk material properties hence make impact on wall stress. The simulation results show that the wall stress in the stagnant area is not suitable to use theoretical calculations, especially for ellipsoidal particles. The silo wall experiences smaller stress when compared with spheres. One interesting phenomena is fluctuation of discharge rate at the starting stage of the hopper flow which is related to force archer formed above the orifice. The wall stress shifts simultaneously with the opening of orifice, and will reach a steady state when the force archer is completely formed above the orifice. The maximum value of wall stress is not significantly changes for a specific shape of solids, until the loading in the hopper drops to a lower level.

Brief Biography

Dr. Sida Liu obtained his bachelor's degree in 2008 from Dalian Jiaotong University, and then started his master study in University of New South Wales under the supervision of Prof. Aibing Yu and Dr. Zongyan Zhou. He completed his master's degree and continued to pursuit a PhD in 2011. He transferred to Monash University in 2014 and completed his PhD program in 2015. In 2016, Dr. Sida Liu went to China and joined the Institute for Industrial Progress Simulation and Optimization as a program manager. Dr. Sida Liu's research area is mainly related to blast furnace burden distribution. The major duty for Dr. Sida Liu in China is commercialization/industrialization and marketing management for SIMPAS research outcomes.

Modeling of complex liquid-solid flow of particle swelling in slurry loop reactors

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Abstract

A swelling-dependent two-fluid model (STFM) is developed for the liquid-solid flows of swelling particles in polyethylene reactors. The model integrates the two-fluid model (TFM) with a species transport equation (STE) to account for the diffusion of alkane molecules from the liquid bulk to the amorphous region of particles, and a population balance equation (PBE) to consider the aggregation of swelling particles. Simulations show that only the TFM fails to capture the main features of swelling systems. By contrast, the STFM captures the gradual increase of power consumption due to particle swelling and aggregation, which agrees with the experiments in a stirred tank. The STFM predicts also the slug formation and a sharp increase of power consumption in a slurry loop reactor as well as the solid accumulation behind pump. The difference of model prediction for stirred tanks and loop reactors suggests the potential of reactor optimization by enhancing local mixing while still keeping high solid concentration for productivity.

Mesoscale modeling of emulsification in rotor-stator devices Part II: A model framework integrating emulsifier adsorption

Ning Yang[a,*], Chao Chen[a,b], Xiaoping Guan[a], Ying Ren[a], Jinghai Li[a], Christian Kunkelmann[c], Eduard Schreiner[c], Christian Holtze[c], Kerstin Mülheims[c], Bernd Sachweh[d]

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Abstract

Precise and rational control of droplet size distribution (DSD) is important in emulsification for target-oriented product design. To develop a complete DSD model, crossing the two mesoscales of two different levels is of great significance, viz., the emulsifier adsorption at interfacial level (Mesoscale 1) and the droplet breakage and coalescence in turbulence in rotor-stator device level (Mesoscale 2). While the first mesoscale can be simulated by coarse-grained molecular dynamic (CGMD), the second has been investigated in computational fluid dynamics and population balance model (CFD-PBM) simulation through the Energy-Minimization Multi-Scale (EMMS) approach in Part I. We then developed a model framework in Part II, coupling CGMD and CFD-PBM simulation through surfactant transport equations in bulk phase and at interface, with source terms taking account of emulsifier adsorption parameters. The parameters including maximal adsorption amount, diffusion coefficient and adsorption/desorption kinetic constants are acquired from CGMD. The coalescence efficiency is then corrected by the interfacial area fraction not occupied by surfactant and fed into the coalescence kernel functions in PBM. Compared to traditional CFD-PBM simulation, the coupled model can greatly improve the simulation of DSD, Sauter mean diameter, median diameter and span for high dispersed phase amount (DPA), and correctly reflect the influence of DPA, surfactant concentration and rotational speed of rotor-stator (RS) devices. While the simulation cases validate and demonstrate the advantage of this new model framework, it is also promising to incorporate different types of surfactant in future.

Mesoscale modeling of emulsification in rotor-stator devices Part I: A population balance model based on EMMS concept

Ning Yang[a,*], Chao Chen[a,b], Xiaoping Guan[a], Ying Ren[a], Jinghai Li[a], Christian Kunkelmann[c], Eduard Schreiner[c], Christian Holtze[c], Kerstin Mülheims[c], Bernd Sachweh[d]

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Abstract

Droplet size distribution represents one of the key parameters of emulsification products and emulsification efficiency. While there is a large number of computational fluid dynamics and population balance model (CFD-PBM) simulation for droplet size distribution in various emulsification devices, fitting parameters or empirical correlations were always involved to generate the reasonable simulation. In this study, we applied the Energy-Minimization Multi-scale (EMMS) approach for the liquid-liquid flow in rotor-stator (RS) mixing devices. The so-called mesoscale energy dissipation for droplet breakage was derived to close the population balance equations through a breakage rate corrector. The correction factor was then integrated into the fully-coupled CFD-PBM simulation for a surfactant-free MCT-oil/water system. Compared to the original Alopaeus breakage model or the combination of Alopaeus model and Prince coalescence model, this new model could greatly improve the prediction of droplet size distribution, Sauter mean diameter, median diameter and span of size distribution for both the dilute and the dense systems of dispersed oil phase.

Understand Solids Loading Effects in Dense Medium Cyclone

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Abstract

Industrial cyclones, such as gas, hydro and dense medium, are widely used in chemical, mineral and process industries to separate particles from fluids or classify particles by size, density or other solid properties. It is well known that the loading of particles can significantly affect fluid flow in such cyclones but the specific effect can be confusing due to a limited fundamental understanding of the working mechanisms involved. In this work, the effect of solids loading effect in dense medium cyclone (DMC) is discussed by mainly analyzing the simulation data obtained from a combined approach of Computational Fluid Dynamics (CFD) and Discrete Element Method (DEM) (CFD-DEM). It suggests that the effect of solids loading rate heavily depends on particle properties (which includes coal particle size and density distributions and other solids properties such as particle shape and particle surface roughness). The most notable finding is that particles of different density/size have different trajectories in the cyclone (e.g., Figure 1), leading to different spatial distributions of solid particles and thus different spatial distribution of volumetric particle-fluid interaction forces which cause different effects on the fluid flow. A universal rule to describe the specific effect of solids loading rate in DMCs is very difficult to develop. This is because, even for given/constant solids loading rate, the flow and DMC performance can still vary significantly with properties of particles. In other words, the specific effect of solids loading rate depends on particle material properties. In the future, the effect of solids loading rate for different particle properties can be better defined with the CFD-DEM approach as the major tool and the support of physical experiments. The findings should be useful for developing a better understanding the working mechanisms of solids loading effects in DMCs and also in other similar swirling multiphase flow systems.

Brief Biography

Dr Kaiwei (Kevin) Chu is specialized in the modelling and simulation of complex particle-fluid flows that are ubiquitous in nature and industries. He carried out extensive pioneering work to elucidate the fundamentals of complex particle-fluid flows by developing and applying combined approach of computational fluid dynamics and discrete element method (CFD-DEM), leading to >80 publications, with total citation times of 1955 and H-index of 21 (as at 8 Nov. 2018 via google scholar). He has 3 first-authored articles belonging to “Most Cited Articles” and 7 first-authored articles belonging to “Top25 Hottest Articles” in their respective journals. He obtained his PhD degree from UNSW Australia in 2010 and is current a Research Fellow at Monash University of Australia.

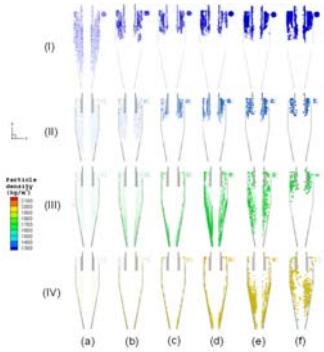

Figure 1. Spatial distribution of particles of different size and density: (I) 1200 kg/m^3, (II) 1400 kg/m^3, (III) 1700 kg/m^3 and (IV) 2000 kg/m^3; and (a) d = 0.25 mm, (b) d = 1 mm, (c) d = 5 mm, (d) d = 20 mm, (e) d = 40 mm, and (f) d = 60 mm (Chu et al., 2017).

Evaluation of effective thermal conductivity of random packed bed: heat conduction through fluid voids and effect of packing structure

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Abstract

Effective thermal conductivity (ETC) is an important parameter in packed-bed systems and is affected significantly by packing structure. Heat flow through a packed bed can be divided into three parallel paths: the solid-fluid-solid path, the solid-solid path and the fluid path. The models to evaluate ETC in packed beds for the first two paths were previously developed. In the present work, a comprehensive model to consider the conduction heat transfer through the voids of a randomly-packed spherical particle beds was further developed using the Delaunay tessellation. The results shows that heat conduction through the fluid-filled voids becomes significant when the solid-to-fluid conductivity ratio decreases (<5). The effect of microstructure on the ETC of packed beds is then investigated using the discrete element method (DEM). Four modes of heat transfer (solid path conduction, fluid path conduction, radiation between particles, and all combined mode) were considered. Generally, the probability density distribution of heat flow is dependent on the packing structure, although the difference is not very significant for some types of heat transfer mechanisms. With an increase in porosity, the heat conduction and radiation via the solid path decreased, while the heat conduction via the fluid-filled voids increased.

Computational Fluid Dynamics of Regenerator-Downer for CO_2 Sorbent Regeneration

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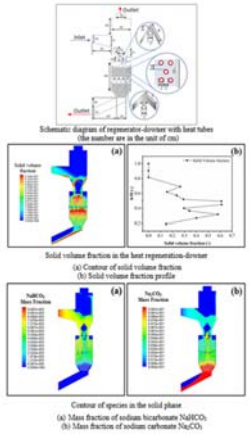
Abstract

Regenerator-downer is an important part for a compact continuous carbon dioxide capture unit using solid sorbent. The primary design of regenerator-downer which includes both cyclone and downer sections of a fluidized bed reactor is expected to be less than 3.5 meters tall. Computational fluid dynamics has been used to study an appropriate system dimension to regenerate the solid sorbent. The simulation shows that two sizes of baffle are required for well solid sorbent distribution. The size, space and the alignment of heat exchange tubes are crucial design parameters to handle the solid sorbent entrainment. The number of tubes highly depend on their surface temperatures which are maintained at 60 °C and 130 °C for the upper and the lower cluster tube sections, respectively. The designed regenerator-downer clearly demonstrates that the spent solid sorbent is fully regenerated and its temperature is exactly the same as the suggested temperature for the CO2 sorption. Therefore, the regenerated sorbent is ready for being utilized in the riser for next cycle without the need of temperature correction in the CO2 capture unit.

Brief Biography

Dr. Sutthichai Boonprasop is a post doctor fellowship of Department of Chemical Technology at Faculty of Science, Chulalongkorn University. He holds a Bachelor and master of Science degree in chemical technology from Chulalongkorn university and Doctor of Philosophy degree in chemical technology from Chulalongkorn university. His research interest relates to computational fluid dynamics simulation, experimental design and analysis, carbon dioxide capture and circulating fluidized bed technology. He has published 5 articles in professional journals.



CFD Simulation of Heat and Mass Transfer, Decomposition Rate Field in Lime Shaft Kilns

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Abstract

A gas-solid reaction model has been developed to understand the heat and mass transfer related to the flue gas and chemical reaction. The transport of mass, momentum and energy in the gas phase is modeled by computational fluid dynamics (CFD),while the numerical of solid temperature and decomposition rate are modeled by a shrinking core approach. Limestone granules pass through preheating zone, calcined zone, cooling zone. Novel part addressed in this study is the side wall effect of the granule packed bed. This work contain convective heat transfer between gas phase and granules, radiation and contact heat transfer between particles as well as decomposition reaction. Uneven decomposition rate problem is solved by the proposal from this study. Simulations of a shaft kiln including fuel combustion calculations demonstrate the suitability of the proposed approach for the modelling of industrial scale systems.

Brief Biography

Zhengzhe Fang, Postgraduate, study at the School of Metallurgy, Northeastern University, Shenyang, Liaoning, China. Researches focus on enhanced heat transfer technology, numerical simulation of shaft kiln, combustion technology and fluid power engineering.

Numerical Simulation of A Top Injection Two-Phase Flow

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Abstract

Molten slag is pneumatically stirred by N_2/O_2 gas injected through a top-submerged lance during a slag treatment process. In order to understand the flow field characteristics, a scaled-down physical model was designed and the corresponding numerical simulations were performed with a combined VOF-LES model. The numerical results were validated by TR-PIV experiments. The results obtained from two different sub-grid scale models (namely, the Dynamic Smagorinsky-Lilly (DSL) model and the Wall-Adapting Local Eddy-Viscosity (WALE) model) satisfactorily represent the mean features and fluctuating behavior of the flow. The DSL model slightly outperforms the WALE model, especially at a deep submergence level case (h/H = 0.52) where turbulence is more intensive. Additionally, a better mixing effect is achieved for a deep lance submergence level.

Keywords: top-submerged injection; combined VOF-LES; sub-grid scale models; submergence level; PIV experiment.

Brief Biography

Yannan Wang is a PhD candidate in the Department of Materials Engineering, KU Leuven, Belgium. His main research interests are experimental and numerical modelling of multiphase flows (*e.g.*, gas-liquid or gas-liquid-solid flows), droplet breakage and coalescence in a continuous liquid phase, and metal recycling by high temperature experiment.

Yannan Wang first studied Metallurgical Engineering at North China University of Science and Technology, China, and obtained his bachelor degree in 2012. He then studied vanadium extraction from vanadium-bearing slags using high temperature experiment and hydrometallurgical techniques at University of Science and Technology Beijing, where he completed his Master degree in 2015. For the past three years, he has been involved in physical modelling of droplet breakage and coalescence, numerical simulation of multiphase flows in a slag treatment process at high temperature, and metal recycling from metallurgical residues at KU Leuven.

CFD modelling of bubble-particle collision efficiency in froth flotation

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Abstract

In order to improve understanding of the interaction between bubbles and particles during the flotation process, the interaction between the various factors that affect the collision efficiency has been analyzed. In this paper, four kinds of mineral particles (quartz, chalcopyrite, copper sulfide and galena) were investigated. Particle-bubble collisions between bubbles with size ranging from 0.6μm to 2.0μm and particles with diameter from 31μm to 150μm were examined. The results of the CFD model are compared with the existing mathematical model to analyze the advantages and disadvantages of the existing mathematical model, as a description of the collision process of the flotation process. The results show that the GSE model fits the CFD predictions well in the particle size range below 74 microns. The Schulze model exhibits a good fit to the CFD predictions when the particle density is greater than 4200 kg/m3 (especially 4200–5600 kg/m3). It would be expected that the CFD model would be more exact than either semi-theoretical model, given that it involves fewer assumptions. In this paper, the influence of bubble diameter on particle– bubble interaction is analyzed in detail from the theoretical point of view, and a computational fluid dynamics model, which is expected to be applicable over a wide range of parameters, is established.

Brief Biography

Shuofu Li is currently a doctoral candidate at University of Science and Technology Beijing, Faculty of minerals processing, and a visiting student at CSRIO. His current research focuses on the bubble-particle collision in froth floatation.

Electrochemical Reduction of CO_2 Under Seawater as Electrolyte

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ABSTRACT

Electrochemical CO_2 reduction reactions, as a potential path towards reusing CO_2 to prepare fuel, is of great significance for alleviating the shortage of fossil fuels and combatting global climate change. Within electrochemical CO_2 reduction reactions, the electrolyte has been proved by reported studies to be an important factor affecting the Faraday efficiency and products selectivity of CO_2 reduction. The optimized electrolyte surface reaction at present has the neutral pH and low-concentration electrolyte, which owns a high solution resistance overvoltage, and thus caused a significant proportion of energy loss. In addition, the local environment of the electrolyte can significantly affect the products selectivity. In the previous reports, the researchers mainly used single electrolyte aqueous solution as supporting electrolyte solution, which was prepared based on deionized water. However, the manufacturing cost of deionized water is still high, limiting the practical application and large-scale industrial production of this technology. In fact, seawater is the majority of the earth's water resources. In this case, the research on seawater based electrolyte is extremely necessary and important. There are a variety of inorganic ions and organics in seawater. The interaction mechanism between various species was not clear yet, as well the complexity of using seawater as supporting electrolyte was still difficult to control. Here, the effects of various ions in seawater on the mechanism of electrochemical CO_2 reduction and the suppression of H_2 evolution on the Cu electrode were investigated comprehensively. The electrochemical CO_2 reduction measurements displayed that the Faradaic efficiency of CO, CH_4, and format was increased successively while the H_2 Faradaic efficiency was decreased in 0.1 mol/L CO_2-saturated Na^+, Mg^{2+}, K^+, Ca^{2+} bicarbonate aqueous solution and KBr, KCl, K_2SO_4, $KHCO_3$ aqueous solution, at a applied potential of -2.0 V_{RHE}. The influence mechanism of cations on the electrochemical reduction was due to the effects of the cation size on hydrolysis and the coupling effects between cations and H_2O. The effects from anions were attributed to the effect of buffer action of anions on pH in reaction system. The influence mechanism of various ions in seawater solution on the reaction Faraday efficiency and the selectivity of reaction products were investigated by simulated seawater as an electrolyte for the first time. Based on these results, an optimum scheme for electrochemical reduction of CO_2 in seawater has been proposed and the feasibility of large-scale electrochemical reaction for preparing renewable energy in seawater system is analyzed.

BRIEF BIOGRAPHY

Shengjie Bai is currently a Ph.D. student in State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University(Xi'an, Shaanxi, China), as well as International Research Center for Renewable Energy Xi'an Jiaotong University(Xi'an, Shaanxi, China). His research interests focus on designing and fabricating novel photocatalysts with high selectivity, high stability for photoelectrochemical carbon dioxide reduction. His supervisor is Prof. Liejin Guo, who is an Academician of CAS. He earned his Master's degree from Fuzhou University (Fuzhou, Fujian province, China). He had nearly four years' research experience in labs. During these years, he engaged in several aspects of theoretical and industrial research under her tutor's guidance, mainly included: (a) concentration and deodorization of waste leachate, (b) fluorinated acrylate copolymers and its applications; (c) biomass-based composites, (d) partly involved the preparation and application of photocatalytic materials. The close cooperation with enterprise industrialization project has given him important opportunities to know about the transformation of scientific and technological achievements. Meanwhile, he applied for several patents, of which four have been authorized, and published three papers as the first author. Besides, he had attended several conferences in related research fields and given oral presentations. At present, his main research focus on: (a) the effect of electrolyte on photo-electrochemical reduction of carbon dioxide, (b) the synergistic effect of various ions on the reaction potential of electrochemical reduction of carbon dioxide, (c) application of gas chromatography and liquid chromatography in detection of products from electrochemical reduction of carbon dioxide, (d) designing and optimization of electrochemical carbon dioxide reduction reactor.

GPU Parallel Multiphase solver to simulate flow in cyclones operating at high solids concentration

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Abstract

The development of GPU parallelized unstructured multiphase solver and its application in predicting turbulent swirling flow of slurries inside cyclones is presented. Algebraic slip mixture model (ASM) is modified with additional shear lift forces and slurry rheology is corrected with fines fraction. The flow inside hydrocyclones are highly turbulent and predicting the anisotropic nature of the turbulent flow structures is limited while using RANS based turbulence model. This may affect the cyclone performance prediction as the instantaneous flow rates through the overflow and the underflow are not correctly predicted using RANS based turbulence models. LES can accurately resolve flow structures that are few times the Kolmogorov scale at an increased computational cost due to finer mesh requirement. Hence this solver has been parallelized using general purpose graphics processing units (GPGPUs). In the current solver, the Pressure Poisson equation has been parallelized on GPU architecture along with Algebraic multigrid method using CUDA programming language for unstructured grids. The coupled LES-ASM model is used to simulate the dynamics of slurry inside the hydrocyclone and study the particle classification. The simulated results are validated against experimental findings.

The effect of turbulent dispersion forces on particle segregation for cyclones operating with high solid concentration is studied by modifying the slip velocity calculations to incorporate the effect of turbulent fluctuation on the particle motion given by the formulae

$$u_{Cp} = u_{Cp0} + K_{pc}.\frac{D_{st}}{\alpha_p}\nabla\alpha_p$$

$$Where, u_{Cp0} = \frac{d_p^2(\rho_p - \rho_m)}{18\, f_{Rep}\mu_c}(g_i - \frac{\partial}{\partial t}u_{mi} - u_{mj}\frac{\partial}{\partial x_j}u_{mi} + 0.75\frac{\rho_c}{\rho_p - \rho_m}C_{lp}\epsilon_{ijk}\omega_{mj}u_{pck}$$

The term K_{pc} is the drag coefficient, and the turbulent diffusion coefficient is given by

$$D_{st} = \sigma(\kappa\alpha_c v_c' + (1-\alpha_c)v_p'$$

The effect of these additional forces on the particle separation efficiency of the hydrocyclone is simulated using the parallel solver and the change compared to the model with no turbulent diffusion is reported. Further, the parallel efficiency of the solver compared to the serial version is also reported.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

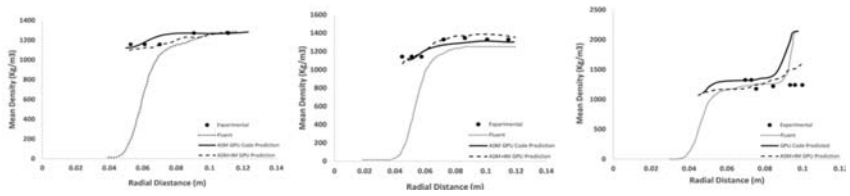

Figure 1. Comparison of predicted density using Maninnen model GPU code, Ishii Mishima viscosity corrected, Fluent and experimentally reported values in Subramaniam et.al 2001 at 0.23m (left), 0.47m (middle) and 0.65m (right)

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Brief Biography

Kumar Mayank is a Ph.D. research scholar in the department of Chemical Engineering, Indian Institute of Technology Hyderabad, India under the guidance of Dr. Narasimha Mangadoddy. He completed his masters from the same institute in the year 2014. Mayank's area of interest include CFD multiphase modeling, Euler-Lagrangian coupling and parallel/GPU computing. He has 3 referred conference papers and is the recipient of the 2016 IIME Khare best paper award in MPT Pune.

Fabrication and Characterization of Sulfur Modified Copper Catalyst for Selective Formate Production from CO_2 Reduction

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ABSTRACT

Fossil fuels are non-renewable, which play a very important role in the energy demand and supply. Nonetheless, the use of this finite and exhaustible source is invariably linked with carbon dioxide emission. Electrochemical reduction of carbon dioxide (CO_2 Reduction Reaction, CO2RR) to hydrocarbons provides a great technique for CO_2 utilization. With this technology, sustainable energy can be stored in green chemical fuels, enabling an easier way to utilize renewable energy. In addition, it has been gaining increasing attention due to its immense potential to establish a more sustainable energy cycle. The electrochemical reaction at the catalyst interface is especially important for the process of carbon dioxide reduction, which will affect the distribution of products and the energy loss of the overpotential. The catalytic reaction is very sensitive to the surface of the electrodes. And numerous works show that the oxygen modified copper, such as an Oxide-Derived copper electrode, can significantly change the catalytic performance. Similarly, due to the similar chemical properties of the sulfur and oxygen elements, the sulfur-modified copper catalyst will also influence the catalytic performance of CO2RR. Here, sulfur modified copper catalyst was fabricated by a simple surface drip method. We tried to use sulfide ion to change the surface of the copper electrode, and studied the surface structures of sulfur- modified copper catalyst. The goals of this work is to improve the selectivity and faradic efficiency of products by the sulfur-modified copper catalyst. Compared with pure copper, the catalytic activity of sulfur-modified copper catalyst with a simple surface drip method was obviously enhanced, and the reason for the characterization of sulfur-modified copper catalyst was demonstrated by XRD, SEM, X-ray photoelectron spectroscopy, cycle voltammetry, electroactive surface area measurements. The gas and liquid products of electrocatalytic carbon oxide reduction using the sulfur-modified copper electrode will be qualitatively and quantitatively analyzed by GC and HPLC method. In addition, the electrochemical performances of catalysts were studied under a series of applied potentials. The results of the products in CO2RR showed that the C1-C3 hydrocarbons and carbohydrates were produced here. Moreover, we found that the CO2RR on sulfur modified copper catalyst prefer to produce formate. Finally, the mechanism of high selective formate production was also analyzed by first principle calculations. For future work on the sulfur-modified copper catalyst for CO2RR, we suggest that the surface structures and the interface reaction may be a key factor in determining the selectivity of products in CO2RR, and the addition work is required to determine the effect of energylevel barrier on the selectivity of products in CO2RR. Moreover, more preparation methods of copper catalysts for CO2RR need study.

BRIEF BIOGRAPHY

Feng Wang is a Ph.D. candidate in International Research Center for Renewable Energy, as well as the State Key Laboratory of Multiphase Flow in Power Engineering from Xi'an Jiaotong University, China. His major is power engineering and engineering thermophysics. From September 2007 to July 2011, as a Bachelor of Science in the applied chemistry, studied at Nanchang University, China. And the main research field during his bachelor degree is solar photocatalytic water splitting to produce hydrogen especially in the photocatalysis of ternary ZnS-In_2S_3-CdS solid solution photocatalysts. In this research, ZnS-In_2S_3-CdS solid solution photocatalysts were prepared by a hydrothermal method. The results showed the ZnS-0.25In_2S_3-0.1CdS solid solution had the highest photoactivity and amount of hydrogen evolution of 0.10 g catalyst loaded with 0.50 wt% Pt under visible light for 2h irradiation was 242.1 μmol. After graduation, he joined a pharmaceuticals company, in where he is engaged in research on the organic chemical synthesis, including optimization of the synthesis process, small organic synthesis reaction, the pilot scale reaction, and the industrial synthesis reaction. In September 2015, he joined Xi'an Jiaotong University and started a successive postgraduate and doctoral program. During the graduate period, his research were mainly focus on photo- electrochemical carbon oxide reduction to produce carbon fuels. He also devoted himself to the fabrication and characterization of electrode, as well as the mechanism analysis of the surface states of the electrode.

An SPH Investigation of Wear Due to Impact of a Spherical Granule

Dhairya Vyas[1*], Sharen Cummins[2], Murray Rudman[3], Gary Delaney[2], Devang Khakhar[4]

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Abstract

Erosion is a major concern in many industrial applications involving dry granular flows and slurry transport. The control and prediction of erosive wear can result in significant extensions to the useful life of machinery, reduction in down-time and associated cost savings. Previous methods used for analyzing erosive wear have mainly been limited to experimental techniques (analyzing wear after it has occurred) and wear models based on either simple experimental setups or on theories involving significant assumptions.

In this work we employ Smooth Particle Hydrodynamics (SPH) to investigate wear in ductile materials by performing impact studies for a broad range of impact conditions. In contrast to numerical methods like the Finite Element Method (FEM) which have been used in studies to analyze erosion, SPH offers advantages in avoiding issues of mesh entanglement for large deformations and difficulties in modelling the fracture and detachment of material from the eroding surface. We investigate the effect of impact velocity on wear by varying the velocity in the range of 10 m/s to 100 m/s and quantify the corresponding wear observed in terms of plastic deformation.

Figure 1 shows the plastic strains observed in simulations of an oblique impact of a spherical granule with a stationary substrate at impact velocities ranging from 10 m/s to 100 m/s. The deformation of both the impacting granule and the substrate is calculated using the using the Johnson-Cook model, with increasing surface deformation visible for higher impact velocities

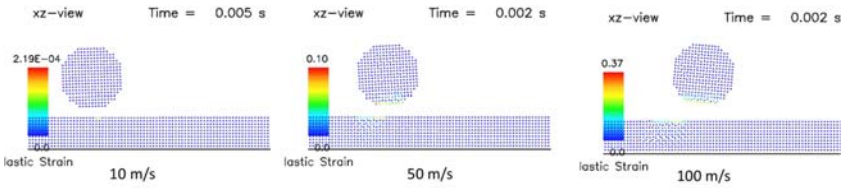

Fig. 1: Effect of velocity on plastic strain.

Brief Biography

Dhairya Vyas is a doctoral student in IITB-Monash research academy. His project is sponsored by CSIRO's Data61 where he is analyzing wear in industrial granular flow applications using Smooth Particle Hydrodynamics.

Sharen Cummins is a Senior Research Scientist in Data61's Computational Modelling (CM) Group at CSIRO. She is a software and algorithm developer for the CM group's particle-based modelling capability where her work contributes to the accurate, efficient and robust simulation of industrial, biological and geophysical applications. Her career interests are in the development of particle and grid-based methods; in particular their coupling to model multi-physics and multi-scale applications and their efficient implementation in large commercial codes.

Murray Rudman is a Professor in the Department of Mechanical and Aerospace Engineering with nearly 30 years experience in the development and application of computational models to problems of fundamental and practical importance. His current research interests are in the areas of wave-structure interaction, mixing and particle-laden flow.

Dr. Gary Delaney leads Data61's Computational Modelling Group at the Commonwealth Scientific and Industrial Research Organisation (CSIRO) in Melbourne. His primary research interests are in computational modelling and structural characterization of granular systems, and applications of Machine Learning in understanding and optimizing natural and industrial processes.

Prof. Devang Khakhar is Professor of Chemical Engineering at the Indian Institute of Technology Bombay. His research interests include dynamics of particulate systems and fluid mixing. He is a fellow of the Indian National Academy of Engineering and the Indian National Science Academy.

Analysis of Multi-Field Coupling In The Steel Belt Sintering Process

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Abstract

The main objective of this paper is to analyze the kinetics of the drying and oxidation of pellets in the steel belt sintering furnace. The two-stage drying thought and shrinking core model are used to investigate the flow field, the temperature field of gas-solid two-phase, moisture content of raw pellets, combustion of carbon powder and the oxidation of iron ore pellet in the moving pellet bed synchronously. A mathematical model of the multi-field coupling transfer process of the bed has been developed in the steel belt sintering process. The reliability of the drying and oxidation kinetic of pellets is validated against empirical data in field conditions by comparing the modelling results against measurements at key positions. The results show that the model can be successfully used for predicting the steel belt sintering process. It also provides an analysis system of accurate control and optimization for iron ore pellet drying and oxidation process which has practical significance.

Brief Biography

Changjun Wang, born in 1995, is getting a degree of Master of Science in Engineering at Northeastern University (China). I have gotten Bachelor of Engineering degree at School of Metallurgy, Northeastern University. My major academic interests include the heat and mass transfer in the process of sintering process, and I have made some deep researches on the kinetics of drying and oxidation of pellets in the material layer as a beginner. I have participated in the project of the technological process study of the manufacturing of high carbon ferrochrome, in charge of the simulation of steel belt sintering.

Bubble-induced Light Refraction and Marangoni Convection during Photoelectrochemical Conversion

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Abstract

Photoelectrochemical (PEC) water splitting is a promising way to produce hydrogen from solar energy. Its conversion involves complicated physicochemical processes, operating through successive stages including photogeneration of charge carriers, separation of photogenerated carriers, surface reaction and evolution of gas products. Comparatively, the evolution of gas products in the form of bubbles proceeds at a time scale of seconds, acting as the rate-limiting step and a crucial aspect of the PEC system. Modestino et al. [1] emphasized the bubble effects during the mass transport analysis of solar-hydrogen generation. On the one hand, bubble-induced mixing near the electrode surface can reduce the transport losses. On the other hand, if bubble cannot be released from surface rapidly, the increased reaction kinetic losses, undesirable scattering and reflection will affect PEC performance detrimentally.

This research focuses on the bubble evolution process and its effects on photoelectrochemical conversion, including light and the species transportation. Through COMSOL Multiphysics, the incident light transportation during bubble evolution, induced local temperature distribution at photoelectrode and the temperature gradient Marangoni convection were investigated. The results demonstrate the optical refraction of incident light and the result-in local optical concentrating effect at the edge of bubble-photoelectrode contact area, whichs implies an unwanted nonuniform generation of electron-hole pairs and subsequent nonuniform current density distribution will arise, and will finally cause the ohmic and kinetic losses. While Marangoni effect causes a negative pressure area at bubble foot near the electrode and forms a recirculation, which will accelerate the species transportation and bubble evolution. The above points provide convincing evidence to our former experimental results on bubble growth characteristics.

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Brief Biography

Yechun Wang received his B.S. degree in 2004 from School of Energy and Power Engineering and M.S. degree in 2008 from State Key Lab of Multihphase Flow in Engineering, Xi'an Jiaotong University, China. After that, he became an Engineer in State Key Lab of Multihphase Flow in Engineering mainly engaging in the measurement and analysis of multiphase flow and interfacial characteristics. He is now a Ph.D. student (supervised by Professor Liejin Guo) with research area of multiphase thermophsyics in photoelectrochemical conversion.

Large Eddy Simulation of Non-premixed Pulverized-coal Combustion in Foursquare Tangential Furnace at Various Atmosphere

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Abstract

Numerical simulations were carried out to study coal combustion in a simplified foursquare tangentially-fired furnace. The LES for turbulent gas coupled with DPM for coal particles trajectories was considered, as well as non-premixed combustion model for pulverized-coal combustion, two-competing-rates model for devolatilization, kinetics/diffusion-limited model for combustion process and the P-1 model for radiation. The analysis focused on the effects of the excess air coefficient on pulverized-coal combustion. More specifically, the oxygen-rich and fuel-rich atmospheres were set to simulate the horizontal bias burner in practical applications. The fuel and thermal NO_x pollutant formation were greatly influenced by the excess air coefficient. Moreover, turbulence, char and volatile combustion and the pollutants' emissions were compared qualitatively and quantitatively. These findings may provide insight into strategies to design and monitor tangentially-fired pulverize-coal boilers.

Brief Biography

Wenjing Sun, female, is a fourth-year PhD candidate in Thermal Engineering, Southeast University. Dr. Wenqi Zhong, a professor at Southeast University, is specialized in multiphase flows, computational fluid dynamics, clean coal combustion technologies and biomass thermal transformation. Dr. Tarek Echekki, a professor at the department of Mechanical and Aerospace Engineering at North Carolina State University, is currently developing multi-scale models for turbulent combustion and improving methods for direct numerical simulation of turbulent combustion.

DEM Study of the Effects of Particle Shape and DRI-flap Shape on Burden Distribution in COREX Melter Gasifier

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Abstract

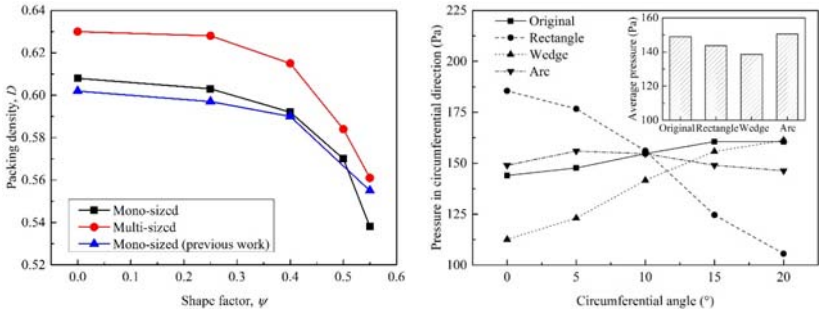
Burden distribution plays a crucial role in controlling gas flow distribution and achieving the stability operation of the melter gasifier in COREX. It has been observed that the structures of burden pile are affected by the shape of coke or coal particles and flaps. However, previous studies on the COREX process based on the discrete element method (DEM) mainly used spherical particles, resulting bed density and voidage significantly different from the experimental results [1].

In this work, a non-spherical DEM-CFD model was used to model the irregular coke particles. To validate the DEM model, the packing simulation was carried out at first. Mono-sized or multi-sized (ternary) particles were poured into a rectangular container to form a random packing, the gas was then injected from the bottom of the container. The effects of non-convexity shape factor and size were investigated, and the results were validated by comparing packing properties with those obtained by previous researchers. Then, a one-eighth COREX melter gasifier furnace stack model with the periodical boundary conditions in the circumferential direction was established to model the burden distribution and gas flow distribution.

In the packing process, the packing density decreases with the shape factor increasing, and the packing density of multi-sized particles bed is significantly larger than that of mono-sized particle bed (Fig. 1a). This is because of the surface of the non-spherical particle with a large shape factor is rougher, resulting in more bridges between the particles. Besides, the mono-sized particle packing density is similar to the previous work [2]. The mean coordination number increases with the increase of the shape factor. Although the variation range of coordination number of multi-sized particle bed is larger than that of mono-sized bed, the mean coordination number of the former is slightly smaller than that of the latter, which is consistent with previous work [3]. In addition, the results show that the simulated pressure drop over the packed bed is comparable to the theoretical calculation results based on Ergun equation. The pressure of larger shape factor (0.5-0.6) non-spherical particle bed is significantly smaller than that of spherical particle bed (shape factor 0), indicating that there will be a notable error when modelling the pressure drop in the irregular shaped particles packed bed by using spherical particles.

After validating the model, the work was extended to the burden distribution simulation in the COREX melter gasifier. The effects of particle shape and DRI-flap shape were investigated.

The results show that the particles were unevenly distributed in the circumferential directions with the Original flap shape, i.e. more DRI particles were accumulated at the region between two charging points. To reduce the uneven distribution of particles, four types flap shapes were investigated. The results show that the burden pile thickness below the charging point was proportional to the cross-sectional area of the flap. The uneven burden distribution directly affects the gas flow distribution, as shown in Figure 1b. The pressure of Original and Wedge flap increases along the circumferential direction, while that of Rectangle flap decreases gradually, only the pressure of Arc flap is almost constant and fluctuates around 150 Pa. Finally, it can be concluded that the Arc-shape flap, with a medium size of cross-sectional area, was able to control the uniform distribution of DRI particle and formed a uniform pressure distribution in the circumferential direction.



(a) (b)

Figure 1. (a) Variations of packing density with the non-convexity shape factor, and (b) Average pressure at inlet in different flap shapes.

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Brief Biography

Yang You is a PhD student at the School of Metallurgy, Northeastern University, China. He is also currently a visiting PhD student at the School of Materials Science and Engineering, University of New South Wales supervised by A/Professor Runyu Yang. He received his B.E. (2013) and M.E. (2015) from Northeastern University, China. He is currently doing research on the charging process in the COREX melter gasifier. The main work includes burden distribution, particle segregation and gas-solid flow under different operation conditions through experimental and numerical (DEM, DEM-CFD) method.

FEA Investigation of Structure and Strength of Compacts

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Abstract

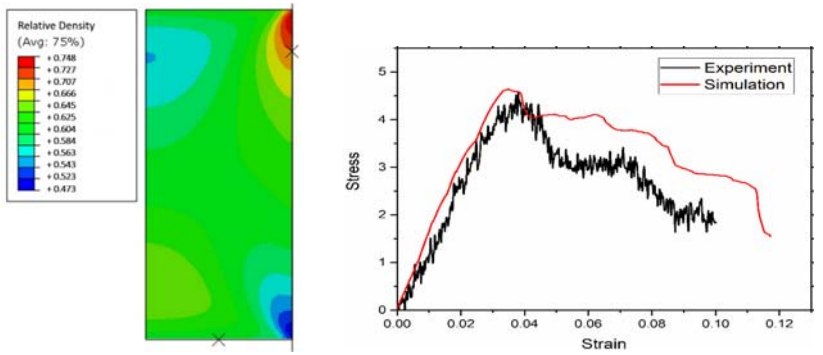
Compaction is a technique to consolidate loose particles which carries the fundamental importance of many industrial purposes. Structure and stress change diversely depending on particle properties after being compacted under external loading condition. Characterization of compact structure and strength is important and different particles exhibit different responses.

In this work, the behaviour of the die compaction of iron ore particles and strength of the compact are analyzed by Finite Element Method (FEM) opting the Drucker-Prager Cap (DPC) model as a constitutive model. To calibrate the elastic and plastic parameter for functionating the DPC model, experimental tests have been conducted similar to previous work [1, 2]. The die compaction is characterized by two stages such as compression and decompression. structural states of the formed compact change at each stage. Density along with different states are utilized to define behaviour of the compact iron. Figure 1a illustrates that a higher density located on the top corner revealing that the compact bed is very loose on lower corner with lower density. This top area can easily be changed after the unloading stage due to some elastic response.

The compact strength is characterized by its tensile strength. The diametrical compression is conducted to identify the tensile strength of a formed compact of iron ore particles. A tensile dominated failure criterion which travels through the centre area of the compact is gained. A little crack may be positioned at the loading area which is the because of loading force. Figure 1b shows the comparison of stress-strain curve for both simulation and experimental test of iron ore particles which is utilized to identify the compact strength. The curve exhibits a linear elastic behaviour before being fluctuated continuously. The fluctuation after the peak value implies the reduction of cohesion among the particles. The overall comparison for both cases is compatible with experimental work on DPC and MCC powder [3].

In summary, the FEM Model can predict the iron ore particles behaviour and failure criteria such as capping, cracking both for die compaction and diametrical compression. For die

compaction, structural states along with density were determined and compared with experimental results. In diametrical compression, the crack intents more concentration towards the centre line.



(a) (b)

Figure 1 (a) Density distribution of die compact bed; (b) Stress-strain relation of diametrical compression

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Brief Biography

I, Md Tariqul Hasan, received my BSc degree in Mechanical Engineering from Chittagong University of Engineering & Technology (CUET), Bangladesh, and MSc at University of Ulsan, South Korea. I also worked as an Assistant Director in one of the most renowned Engineering company in Bangladesh. Now, I am currently pursuing my PhD supervised by Associate Professor Runyu Yang at the University of New South Wales, Sydney Australia. I am working on Finite Element Modeling of Briquetting of Iron-ore coal particles.

From Discrete to Continuum Properties of the Flow of Cohesive Particles in Gas Fluidization

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Abstract

The discrete solid-like granular materials can exhibit continuum fluid-like properties in gas fluidization. Such transition becomes especially complicated for cohesive particles with the significant interparticle force. This work numerically investigates the flow of cohesive particles in gas fluidization through the combined approach of computational fluid dynamics and discrete element method (CFD-DEM), and facilitated by a time-volume averaging method for linking the discrete to continuum properties. First, it is shown the discrete particle flow patterns and pressure drop are significantly affected when particle cohesion becomes large; the particle velocity distributions becomes inhomogeneous and deviates from the Maxwellian distribution with increasing particle cohesion. Then, a proper averaging method is employed to obtain the continuum properties (including solid fraction, velocity and pressure) which indicate the circulation of solids in the bed is deteriorated with increasing cohesion and the bed walls are important for the distribution of bulk properties. Finally, it is shown the solid pressure of cohesive particles is underestimated by the widely used kinetic theory, even when solid fraction is smaller than 0.49. Accordingly, a modified equation for predicting the solid pressure of cohesive particles considering the particle contact and granular temperature is proposed based on the averaged CFD-DEM results.

Brief Biography

Yongli Wu is a PhD student in SIMPAS group (ARC Research Hub for Computational Particle Technology) of Monash University. He obtained his Bachelor's and Master's degrees in Northeastern University of China in 2013 and 2015, respectively. His research work is mainly focused on numerical simulation of particle-fluid flows at different scales.

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Pore Scale Study of Fluid Flows and Drag Forces in Packed Beds of Different Porosities

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Abstract

Understanding the relationship between bed structures and fluid flows is not only of fundamental importance for developing reliable correlations for modelling particle-fluid flows, but also beneficial for industrial applications. This work presents a pore scale study of fluid flows through random packed beds by a network model. The effects of bed structures with a wide range of porosities on the pore scale fluid flows and drag forces are discussed. The results show in addition to local porosity, the connections of pores are also important in determining the local fluid flows. The normalized fluid velocity distribution is exponential with a single peak regardless of bed porosity at the pore scale, whereas there is a transition from the two-peak to single-peak distribution of normalized flow flux when the porosity increases. The distribution of normalized drag forces for individual particles is Gaussian, which is related to the joint distribution of normalized throat diameter and throat length of the pore structure. The mean drag force of a bed by the pore scale model largely agrees with a previous drag model, but deviations will increase when Reynold number or the bed porosity becomes high. Further consideration of the inertial effect in the present model is necessary for the potential application to the simulation of dynamic particle-fluid flows with particle dynamics solved at a particle scale (DEM) and the fluid dynamics solved at a pore scale.

Brief Biography

Yongli Wu is a PhD student in SIMPAS group (ARC Research Hub for Computational Particle Technology) of Monash University. He obtained his Bachelor's and Master's degrees in Northeastern University of China in 2013 and 2015, respectively. His research work is mainly focused on numerical simulation of particle-fluid flows at different scales.

Numerical Study of Gas-solid Flow Behaviour in the Air Reactor of Coal-direct Chemical Looping Combustion with Geldart D Particles

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Abstract

Chemical Looping Combustion (CLC) is a promising combustion technology alternative to conventional oxy-combustion because of its economic and technical feasibility to achieve intrinsic separation of CO_2. In a typical Coal-Direct Chemical Looping process (CDLC), iron-based oxygen carriers are used which belong to Geldart D particles. Previous studies of typical CLC units was almost limited to hydrodynamic behaviour of fine and cohesive powders belonging to Geldart A, B or C particles. There is a need to understand the hydrodynamic behaviour of Geldart D particles in the CLC system. In this work, an Eulerian-Eulerian two-fluid model is developed for describing gas and granular flow in a bottom-enlarged air reactor of CDCL process and considers Geldart D oxygen carrier particles. The simulation results indicate oxygen carrier particles show a slugging flow in the bottom section of air reactor, and the whole air reactor show a periodic fluctuation in both bottom combustor and upper riser. The formation, growth, rising and bursting of slugs can be captured. The influence of superficial gas velocity, wall boundary condition and different drag models on pressure fluctuation, rising velocities and frequency of slugs are investigated. This model provides a cost effective tool for better understanding of flows in the air reactor of CLC.

Brief Biography

Shuyue Li is a PhD student in the School of Chemical Engineering of University of New South Wales. She received her BS of Process Equipment and Control Engineering from China University of Petroleum, Beijing and MS of Chemical Engineering as a joint student from China University of Petroleum, Beijing and Institute of Process Engineering, Chinese Academy of Sciences. Her major research interests are clean coal technology, multiphase flow and reacting flow.

Simulation of Desulphurization Wastewater Evaporation through Flue Gas

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Abstract

Spray evaporation technology is an advanced processing method for desulphurization wastewater. The desulfurization wastewater is sprayed into the flue gas in the end part of the boiler, and the residual solid particles after the evaporation process are captured by electrostatic precipitator, thus eliminating liquid discharge of desulfurization wastewater [1,2]. It has advantages of simpler process, less investment and space. To effectively reveal the evaporation mechanism of desulphurization wastewater, many numerical simulations on the process of desulphurization wastewater evaporation were carried out [3,4]. In the process of setting up the droplet evaporation model, most researchers simplified droplets of desulphurization wastewater as droplets of pure water, ignoring the particular property of desulphurization wastewater with high-salt concentration, which leads to unreliable simulation results under highly idealized assumptions.

Under this background, Eulerian method with the k-ε turbulence model is adopted to calculate the steady-state gas flow in current work. The flow of droplets is calculated by Lagrangian particle tracking method. The wastewater is assumed as aqueous solution of $CaCl_2$. In order to make the simulation results consistent with the reality, the evaporation model of droplets with different salinity is used.

Compared to alternated arrangement of nozzles, the droplets hardly collide with the flue pipe-wall under symmetrical arrangement, reducing the occurrence of sculling and corrosion of flue, as shown in Fig. 1. One can find that the temperature distribution in the flue under symmetrical arrangement of nozzles is more uniform.

The evaporation rate of droplets with uniform diameter is much faster than that of droplets with non-uniform diameter, indicating that the more uniform the diameter is, the shorter is the evaporation time. By comparing the mean distance and time needed for evaporation process of droplets with different uniform diameters, the most optimal diameter of droplets, in terms of minimum mean distance and time of evaporation, is found to be 54μm under BMCR condition, as shown in Fig. 2.

By simulating droplet evaporation process under different temperatures (110℃, 120℃, 130℃, 140℃, 150℃), it is found that 130℃ is the most appropriate temperature under BMCR

condition. At this temperature, the droplet evaporation process can be completed quickly, and the negative impact on the heat exchanger and dust collector will be within acceptable limits.

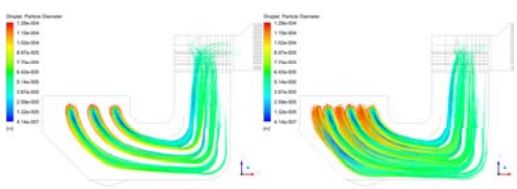

Fig. 1 Droplet motion trajectories under symmetrical nozzle arrangement (a) and alternative nozzle arrangement (b)

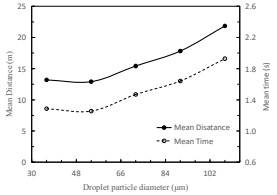

Fig. 2 Mean distance and mean time of evaporation process of droplets with different diameters

Through studying the evolution curve of evaporation rate of droplets for different salt contents (0%, 2%, 4%, 6%, 8%, 10%), with respect to the mean distance, one can see that the evaporation rate of pure water is faster than that of salt containing wastewater. When the droplet evaporation rate is less than 82%, the effect of salt content of droplets on the evaporation rate can be ignored. With the increase of salt content of droplets, the maximum evaporation rate of droplets decreases and the distance of transition stage of evaporation process increases.

After comparing the droplet trajectories under different THA conditions, it is found that when the flue gas evaporation equipment is opened under 75% THA work condition, there is risk of corrosion in the heat exchange tube.

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[4]Z. Liang, L. Zhang, Z. Yang, et al., The effect of solid particles on the evaporation and crystallization processes of the desulfurization wastewater droplet, Applied Thermal Engineering 134 (2018) 141-151.

Brief Biography

The author graduated from the Physics Department of South China University of Technology in 2015 with a Bachelor of Science degree, currently studying for a master's degree in particle simulation research group at the School of Metallurgy, Northeastern University. The author's main research interest is the discrete element method (DEM) and finite element method (FEM) numerical modelling and physical experiment on elemental and composite powders in PM production.

Three-Dimensional MPFEM Modelling on Isostatic Pressing and Sintering of Tungsten Powders

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Abstract

Among all methods used in PM (Powder metallurgy) forming process to produce tungsten metal or alloy, cold isostatic pressing (CIP) method has been widely applied due to its unique advantages such as high relative density, uniform density and stress distributions. Hence, many previous numerical and physical studies had been carried out to obtain high performance tungsten metal or alloy. However, although physical experiments could investigate the effects of different factors on the forming process and sintering process of PM from macroscopic scale, they were unable to intuitively and effectively characterize the powder behavior during compaction and sintering from particulate scale, like particle rearrangement and deformation, stress distributions and transfer, and densification dynamics and mechanisms. The disadvantages in physical experiments can be conquered by computer simulations. While most numerical work was based on macro continuous scale, and the forming stage and sintering stage were considered separately and independently rather than in a unified model; in addition, they failed to characterize the microscopic properties such as stress distribution, force structure and transmission, particle rearrangement and deformation, void filling behavior, as well as the densification dynamics and mechanisms during forming and sintering.

In this study, the CIP and subsequent solid-state sintering of tungsten powders were simulated by continuum FEM as well as MPFEM (Multi-particle finite element method) from both macroscopic and particulate scale. The effects of initial packing structures, pressing pressure and sintering temperature on the properties of tungsten component including evolution of overall relative density, local relative density and stress distributions, particle rearrangement and deformation, as well as the densification dynamics and mechanisms, were systematically investigated and discussed.

This simulation contains two models, a DEM coupled continuum FEM model to study the macroscopic properties such as total stress distribution, distribution and evolution of overall relative density during CIP, and a DEM coupled MPFEM model to study the microscopic properties of the component like stress distribution, force structure and transmission, particle rearrangement and deformation during CIP and sintering from particulate scale.

In the first model, the initial packing structure generated by DEM and corresponding continuum model utilized in FEM are shown in Fig. 1. The mold used in CIP is define as rubber with Mooney Model, each element face of its surface is subjected to the same pressure to simulate the condition in liquid pressure medium. Tungsten powder is considered as a compressible continuum defined by Shima-Oyane model, where its Young's modulus and Poisson's ratio are functions of its relative density. The model is shown in Fig. 2(a). In the second model, a random initial packing structure of tungsten powder is generated in DEM and then imported to FEM. In this model, the definition of the rubber mold is the same as the previous model, but in this case, each tungsten particle is set to be an independent elasto-plastic deformable body defined by Johnson-cook model. The model is shown in Fig. 2(b).

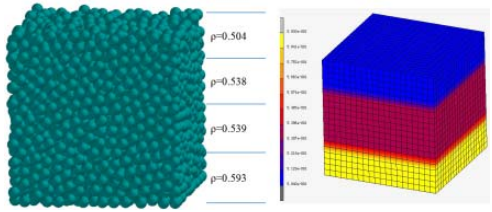
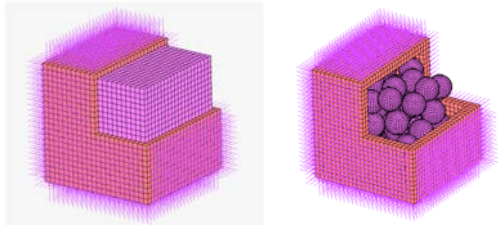


Fig. 1 Initial packing structure and relative density distribution in compact



(a) (b)

Fig. 2 (a) Continuum FEM model (b) multi-particle FEM model

This study provide a new approach when similar problems are concerned. Unlike previous studies that simulated the forming and sintering process of tungsten metal or alloy separately, this study uses a unified model to simulate the forming and sintering process from particulate scale, which can reduce the assumptions in the modeling and make the simulation results more accurate and closer to reality. Microscopic properties such as stress distribution, force structure and transmission, particle rearrangement and deformation, void filling behavior, as well as the densification dynamics can be systematically characterized. Also, a continuum model is established to make up for the shortcomings of MPFEM by studying the overall macroscopic properties of the entire compact. By coupling continuum FEM method and discrete MPFEM method, the details of forming and sintering processes in PM and the factors that affect them can be learnt from two different scales. Recent results indicate that the model is consistent with experimental data, and previous research by our team has already shown that MPFEM is an effective method to simulate the whole PM process for tungsten powders in a two-dimensional scale.

Brief Biography

The author graduated from the Physics Department of South China University of Technology in 2015 with a Bachelor of Science degree, currently studying for a master's degree in particle simulation research group at the School of Metallurgy, Northeastern University. The author's main research interest is the discrete element method (DEM) and finite element method (FEM) numerical modelling and physical experiment on elemental and composite powders in PM production.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

Understanding the Mutual Influence of Simultaneous Vapour Absorption and Droplet Evaporation during Antisolvent Vapour Precipitation

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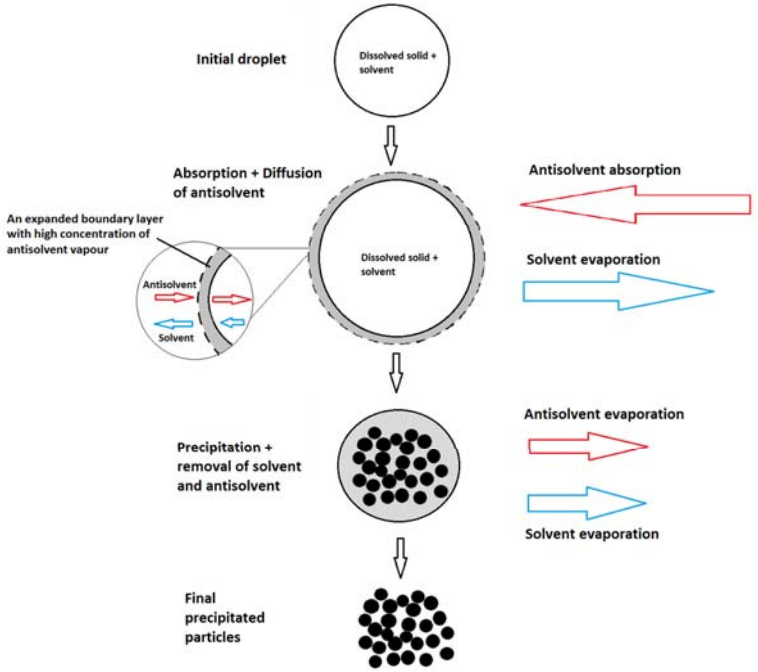
Abstract



Antisolvent vapour precipitation (AVP) is a new spray drying technique which involves a simultaneous absorption-dehydration and antisolvent precipitation of uniform particles in micrometer range. Conventional spray drying focuses on dehydrating individual droplets to form particles while AVP approach has been shown to produce multiple ultrafine particles from each single aqueous droplet at atmospheric pressure. The mechanism of AVP has been well described qualitatively. AVP process is undertaken by exposing aqueous droplet

containing dissolved solids to an ethanol-nitrogen environment, where ethanol vapour is used as an antisolvent. This involves the simultaneous absorption of ethanol and droplet evaporation. Previous work had been tried to model this phenomena using the conventional gradient driven heat and mass transfer model. However, it was found that this model was not capable for capturing the mass transfer depression effect due to high mass flux at the droplet interface. In order to quantitatively understand the effect of the simultaneous transfer of ethanol and water across the droplet surface on the particle precipitation, we will investigate numerically the mutual effect of heat and mass transfer during vapour absorption and removal on the surface of a single droplet exposing to the inert stream containing ethanol vapour. An AVP drying model will be developed based on the fundamental heat and mass conservations of a droplet with the incorporation of heat and mass transfer correlations. We will use the modified correlations which considers the mass transfer depression effect across the droplet surface, since we expect vapour flux at the droplet surface will be high as well as the 'shielding effect' due to the absorption of ethanol vapour in counter direction during AVP process. Several drying kinetics properties will be studied, namely droplet mass change, droplet temperature and droplet size. The reliability of modelling will be validated with the experimental result obtained via a single droplet drying (SDD) method for investigating the drying profile under a controlled environment. Through the modelling, analysis of ethanol vapour absorption to aqueous droplets accompanied by evaporation of the aqueous droplet can be used in determination of minimum ethanol concentration in the droplet required for particle precipitation, and hence ethanol humidity in convective stream can be controlled. This will help in the understanding of drying kinetics during AVP process for scaling-up purpose in future application and subsequently improve the quality of final products.

Keywords: Antisolvent vapour precipitation, drying kinetics, mass transfer depression

Brief Biography

Kian Siang Lim is a PhD candidate of Chemical Engineering in Monash University, Australia. He is also a member of ARC Research Hub for Computational Particle Technology. His research focus is on single droplet drying behavior under the mutual influence of heat and mass transfer during vapour absorption and droplet evaporation.

DEM Simulation on the Packing Densification of Binary Tetrahedral Particle Mixtures Subjected to 3D Vibration

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Abstract

The transition from random loose packing (RLP) to random close packing (RCP) of binary regular tetrahedral particle mixtures under 3D mechanical vibration was modeled by using discrete element method. The effects of vibration conditions, particle size ratio (volume of large particles versus small particles), and composition of the binary mixtures (volume fraction of large particles) on the packing densification were systematically studied, and the micro properties such as coordination number (CN), particle contact type, radial distribution function (RDF) were characterized and analyzed. The results show that for each fixed composition and size ratio, the packing density of the binary mixture first increases with vibration frequency or amplitude and then decreases, high packing density can be obtained by properly controlling the vibration parameters. Under the optimum operating condition, the packing density increases gradually with the increase of particle size ratio. The packing density remains constant when the size ratio exceeds 5. With the increase of the volume fraction of large particles in the binary mixtures, the packing density first increases to a maximum value and then decreases. Appropriate composition (e.g. 70 vol.%, volume fraction of large tetrahedral particles in this work) with large size ratio can contribute to the high packing density. The micro property characterization shows that the packing densification of binary regular tetrahedral particle mixtures is mainly due to the relative movement of small particles.

Fig.1 (a) shows the multi-sphere model for representing the tetrahedral particle in this work. Fig.1 (b) shows the whole process of pour packing of binary regular tetrahedral particle mixtures. At the beginning of the simulation, the particles are generated at the top of the container with periodic boundary. The particles will firstly collide with the bottom of the container and then bounce back and forth. At the same time, the interaction between particles occurs, which leads to the change of the relative position of the particles in the process of packing. After the stable static packing is formed, the container begins to vibrate, and the periodic sinusoidal vibration is used in three mutually perpendicular directions to realize the densification of the packing structure.

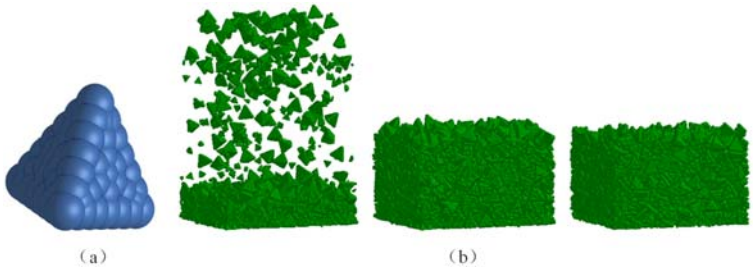

Fig.1 (a) Multi-sphere model used in the simulation; (b) Snapshots showing the formation of the packing of binary regular tetrahedral particle mixtures.

Fig. 2 shows the packing density of the binary mixtures with size ratio $r = 2$ as a function of the composition when vibration amplitude $A = 2.0$ mm and frequency $f = 31.85$ Hz. It can be observed that the packing density increases with the volume fraction of large particles to a maximum value and then decreases. It indicates that there is an optimal volume fraction of large particles (X_L^*) to realize the highest packing density. For size ratio $r = 2$, X_L^* is about 70 vol.%, which is much comparable with the results on the packing densificaiton of binary sphere mixtures and binary sphere/cube mixtures.

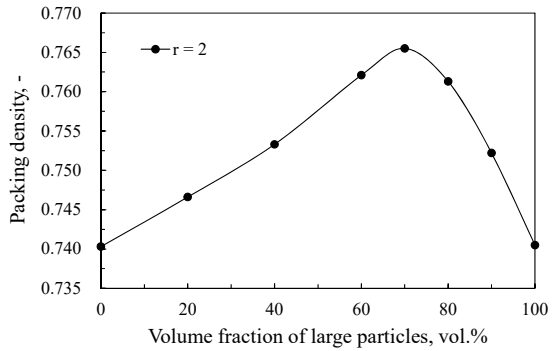

Fig. 2 Evolution of packing density with the volume fraction of large particles for the binary tetrahedral mixutres with the size ratio of $r = 2$ when $A = 2.0$ mm and $f = 31.85$ Hz.

Brief Biography

Bo Zhao, PhD candidate of materials science in the school of Materials Science and Engineering since 2016 in Northeastern University (NEU), got the Master Degree from NEU with the major of Metallurgy Engineering. Until now, 4 paper has been published. Mr. Zhao's research interest is numerical and physical studies on the packing densification of non-spherical particles, especially the packing of tetrahedral particles.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

Three-Dimensional Modeling of the Flow and Thermo Behavior of High-turbulence Zone in Slowly Moving Bed Slagging Coal Gasifier

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Abstract

A novel slowly-moving bed coal gasifier is developed for utilizing the largely-reserved coals high in ash (Ad > 40%) and high at ash fusion temperature (>1400℃) in China. The high-turbulence zone plays an important role during the gasification process, which is greatly affecting the airflow, the activity of hearth charge falling and heat energy needed for production. In this paper, a three-dimensional (3D) CFD-based mathematical model is developed for describing the state of high-turbulence zone in terms of the flow pattern and the related thermo behavior. The model is based on the solution of conservation equations of both gas and solid phases as interpenetrating continua on a Eularian-Eularian framework. A modified k-ε model is adopted for gas phase turbulence. The solid phase constitutive equation is characterized by the solid pressure, bulk viscosity and shear viscosity, which are evaluated from the kinetic theory of random motions of granular materials in a fluid flow. The thermo behavior of the high-turbulence zone is also reflected by considering the heat and mass transfer of key chemical reactions. The results show that the 3D boundary surface of high turbulence zone can be characterized by Reynolds number and volume fraction of solid phase with the critical value 250 and 0.6, respectively. And the influences of gasifying agent velocity and coal particle size distribution on the shape and size of high-turbulence zone are investigated. The simulation results of thermochemical reactions shows that the combustion reactions are mainly concentrated in Z=0~0.5m, which accounts for about 1/6 of the whole bed. And the oxygen/steam ratio effects on the gas and solid temperature and the components of the gas phase obviously.

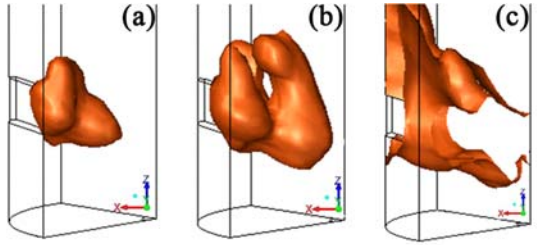

Fig.1 3D boundary surface of high-turbulence zone under different gasification agent velocities (a) 150m/s (b) 200m/s (c) 250m/s

Fig.1 illustrate the 3D shapes of high-turbulence zone under different gasification agent velocities. In the practice of slowly moving bed coal gasifier, the gasifying agent is blown into the coal-packed bed at high velocity through tuyere, resulting in a cavity, termed high-

turbulence zone in front of the tuyere. In present work, the boundary of the high-turbulence zone is characterized by volume fraction of solid phase (αs = 0.6) and Reynolds number of 250. As show in Fig. 1, an increase in the size and a change in the shape of the high-turbulence zone are noted with the increase of the gasifying agent velocity. Especially, a slugging occurred in the bed when the velocity reaches over 250 m/s, and the complete and stable shape of high –turbulence zone cannot be maintained anymore.

Fig. 2 shows the temperature profiles of gas and solid phase at the clip surface of Y=0. It is observed that the both the solid phase and gas phase are generally lower near the center axis of the tuyere, because of the coal particles are blow away by the low temperature preheated gasification agent at high velocity and no intense exothermic chemical reactions occurred subsequently. However, the gas and solid phase temperature are increased rapidly by the fully chemical reaction and distributed circumferentially over the boundary of high-turbulence zone. It is noted in Fig. 2(b), the highest temperature of the solid phase is around 1400℃, which is indicated that the ash component of coal particles is above the melting point temperature and can be discharged smoothly.

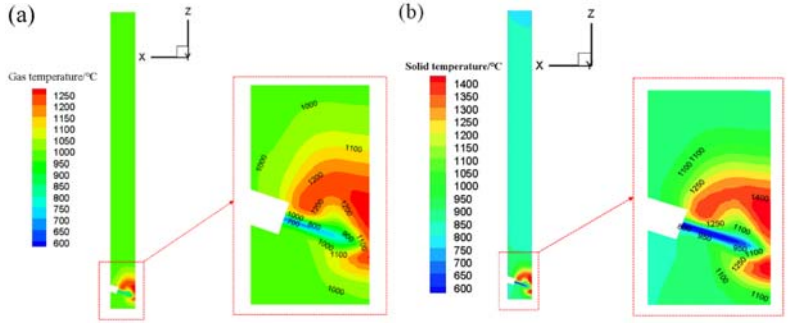

Fig.2 Temperature profiles of gas phase (a) and solid phase (b) of the high-turbulence zone under the gasification agent velocity of 150m/s and $O_2/H_2O_{(g)}$=0.4/0.6

Brief Biography

Jin Xu is currently a PhD student under the supervision of Prof. Nan Wang at School of Metallurgy, Northeastern University, P.R. China. He received his B.S. degree in Metallurgical Engineering at Anhui University of Technology (2014) and M.S. degree in Ferrous Metallurgy at Northeastern University (2016). His on-going research is centered on the experimental and numerical simulation research of reduction behavior of blast furnace dust particles during in-flight process. And he is also interested in modelling of moving bed slagging coal gasification process. He has three related peer-reviewed papers published in Industrial & Engineering Chemistry Research, Powder Technology and Journal of Iron and Steel Research, International.

Study On Equivalent Stiffness Of Elastic Particle Materials

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Abstract

This paper mainly studies the contact pressure of granular materials. The finite element software was used to simulate two disks in contact with each other. By changing the elastic modulus, dimension and contact displacement of the disk material, the change of contact pressure was observed. The average displacement between the extrusion displacement and the contact pressure curve is equivalent to the stiffness of the disk group. It is found that the contact pressure between two disks increases with the increase of contact displacement, and the equivalent stiffness of the disk group increases approximately linearly with the increase of elastic modulus of the disk. This study can provide reference for the constitutive simulation study of granular media materials.

Brief Biography

My name is Wang Dianrui, 21 years old, and I 'm going to be a graduate student of Beijing university of aeronautics and astronautics, Beijing, P.R.China.My major is civil engineering. My mentor is Zhengguo Gao, and he is an associate professor of Beijing university of aeronautics and astronautics. Under the guidance of my t mentor, I often use finite element software to simulate some problems.

Numerical Study on Flow Behavior of Multi-component Particles in a Fluidized Bed Using a TFM-DEM Hybrid Model

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Abstract

Fluidized beds are widely used in chemical, petroleum, and power generation industries. The complex hydrodynamics of gas-solids fluidized beds have been studied by computational fluid dynamics (CFD). The mono-component particle flow is a simplified method in the numerical simulation, which ignores the different interactions of particles species, and lost complicated flow structure details. In general, the bed materials consist of multi-type particles with different sizes and densities, thus it is necessary to conduct researched on the flow behavior of multi-type particles.

In this paper, flow behaviors of multi-type particles are investigated by TFM-DEM hybrid model coupled with kinetic theory of granular flow in a gas-solids bubbling fluidized bed. The flow behaviors of different discrete particles and continuum solids phase are analyzed. The effects of drag models, coefficient of restitution and friction coefficient on the flow behavior are predicted. Simulated results reveal that the higher restitution coefficient and friction coefficient give rise to higher velocities and lower solids volume fractions. The Huilin-Gidaspow drag model provides a better correspondence with the experiments. The influence of Coulomb friction coefficient on hydrodynamics is considered to simulate the flow of discrete particles, and the simulated results with Coulomb friction coefficient are in better agreement with experiments, comparing to results without this consideration.

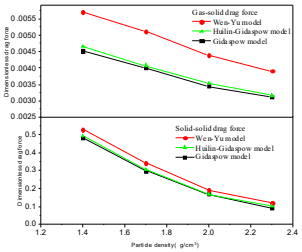

Fig. 1 Drag forces of discrete particles with different drag force models

Key words: Hybrid model; multi-component particles; drag force model; restitution coefficient; friction coefficient

Brief Biography

Xu Wang, a PhD student coming from the Northeast Petroleum University in China. Recently, she is study in the University of Sheffield in UK as a visiting student for one year. She was concentrated on the flow behavior of particles in a fluidized bed and she also interested in the flow behavior of oil and gas in a pipeline.

Simulation of Electrostatic Precipitator Considering Particle Space Charge

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Abstract

Electrostatic Precipitators (ESP) have been widely used to separate fine particles from large scale industrial exhaust gases, particularly in coal fired power generation plants. In-depth knowledge and careful design optimization are critical to meeting the $PM_{2.5}$ discharging limit, e.g., 5-10 mg/Nm^3. Due to the complex nature in the interaction among electric field, gas-particle flow and particle charging, there are a number of phenomena yet to be well understood. In the present work, coupled electric field, gas-particle flow and particle charging processes are simulated using Eulerian-Lagrangian method in Computational Fluid Dynamics (CFD), for an electrostatic precipitator with four-wire electrodes. For other dimensions, the wire diameter is 3.5 mm, wire-to-wire spacing 0.24m, wire-to-plate 0.2m. The effect of particle charging on the electric field distribution, IV characteristics and particle collection efficiency are investigated, as the entry particle loading/concentration varies from 0 up to 50 g/Nm^3 for a particle size of 1.5-5.0 μm under fixed gas velocity of 1.0 Nm/s and applied voltage Va=60 kV.

The results show that the electric field can be distorted significantly by the secondary electric field generated by the space charges on the floating particles, which mostly reduces particle collection efficiency, except at very low loading. A maximum collection efficiency exists at a particle loading that depends on particle size. Under fixed voltage the corona current decreases as particle loading/concentration increases. As particle loading increases to some point, the corona current from the downstream wires can be extinguished completely (corona quenching). At high particle loadings, corona ion charges may fail to reach the plate due to the absorption of passing particles. The electric streamlines in a small zone around the last wire reverse direction locally. A charged particle, once falls accidently within the zone, could be trapped and be attracted to the same wire. Thus this wire is subject to heavier dust deposition. The significance of ion transfer and space charge of fine dust particles is clarified systematically.

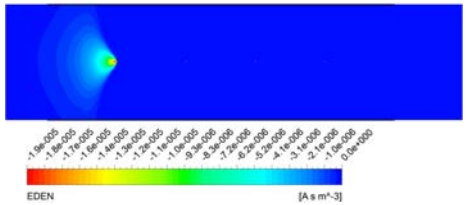

Figure 10. Distribution of corona ion charge density (Loading=10 g/Nm^3, Va=60kV).

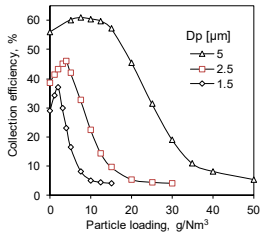

Figure 11. Collection efficiency as function of particle loading (Va=60kV).

Brief Biography

The 1st author, Ding Yang, (Bachelor degree from Chang'an University, Master degree from Xi'an University of Architecture and Technology, Email: yblued@139.com), currently studying towards PhD degree in Northeastern University in China. He is a Registered Engineer specialised in Air pollution control technology. He is Director of Experiment Centre in Longking Co. Ltd. Since 2011, as a project leader or a chief investigator, he has participated in 3 significant applied research projects sponsored respectively by Chinese state and Fujian province. and received 8 authorised patents (with 6 the 1st author). He has also authored /co-authored several SCI/EI academic articles.

Dynamic Behavior of Solid Particles in Rotating Drum with Inclined Axis

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Abstract

Particle flow in rotating drums exhibits a range of complex phenomena, such as avalanche, segregation and convection. This has generated considerable interests among researchers. Many numerical studies have been carried out to evaluate various properties and behavior of particles in horizontally rotating drums in the past, but little effort has been made to investigate the dynamic behavior of particles in rotating drum with inclined axis of rotation, though such drums also exist in mining, food processing, biochemical and pharmaceutical industries. To overcome this gap, in this work, the discrete element method was used to simulate flow of ellipsoidal particles in a rotating drum with variable inclined axis of rotation. Three critical aspects of the gyro-dynamics were examined: axial dispersion, thickness of the active and passive layer and the particle velocity. The results show that these properties are affected by the angle of inclination. In particular, with the increase in angle of inclination, axial dispersion and active region decreases. Further study will be conducted to fully understand the influence of the inclination on the dynamical behavior of various shaped particles in rotating drums with inclined axis.

Brief Biography

Mr. Parag Widhate is currently a PhD student in School of Computing, Engineering and Mathematics, Western Sydney University (WSU). Before joined WUS, he was an Assistant Professor in Department of Mechanical Engineering at Genba Sopanrao Moze College of Engineering, Balewadi Pune, Maharashtra in India affiliate to Shrimati Savitribai Phule Pune University from 2015 to 2018. He had a progressively responsible education with De Montfort University, Leicester UK in 2015 and MIT College of Engineering, Pune in 2013, and awarded MSc with Merit and BE First class respectively in Mechanical Engineering. His current key research areas are Granular Mechanics, Discrete Element Method, Finite Element Analysis and Mechanical Vibrations.

Interactions between Gold Nanoparticles and Their Forces Derived from Molecular Dynamics Simulation

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Abstract

Understanding of the interactions between gold nanoparticles will allow us to explore their potential for a range of applications. In this work, the interactions of gold nanoparticles are investigated by molecular dynamics simulation and their interaction forces are derived. During the simulation, an external force is applied to the pair of nanoparticles, which allows them to approach each other. Some interesting behaviours have been observed in their interactions. In addition, the effects of such external force, nanoparticle size and approaching direction have been examined.

Brief Biography

Mr Pany Yang is currently a PhD student in School of Computing, Engineering and Mathematics, Western Sydney University (WSU). Mr Yang has completed his Master of Philosophy at WSU in 2018 and a Bachelor degree in Metallurgical Engineering in China. Before joined WUS, he was an engineer in rare-earth metallic metallurgy in China. His current research focuses on interactions forces between nanoparticles, self-assembly of nanoparticles, and molecular dynamics simulation.

Gas Bubble Nucleation on TiO_2 Nanotube Surface

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Abstract

Photoelectrochemical water splitting has been considered as one of the most efficient approaches to produce renewable energy. The gas bubble evolution is a significant characteristic of interfacial mass transfer and energy conversion during photoelectrochemical water splitting. Despite tremendous progress in the development of high-efficiency photocatalysts, the evolution of gas bubbles produced on the catalyst surface has been rather poorly understood. The bubble nucleation on photocatalyst, especially, has been rarely detailed, because of the lack of a reliable analysis of the free energy for concentration-driven bubble nucleation and effective measurement method for bubble nucleation threshold.

Herein, a thermodynamics approach was performed for the heterogeneous concentration-driven gas bubble nucleation inside the nanotube, and an analytical expression of the critical energy of nucleation was evaluated considering a spherical gas bubble nucleus nucleating inside the nanotube. The influential factors of bubble nucleation were discussed respectively. It was found that the critical nucleation free energy gradually increased with the increase of the size of the nanotube and the decrease of the contact angle, as shown in **Figure 1**. A combined method of electrochemical measurement and visualization imaging method was used to determine the bubble nucleation critical concentration at nanotube TiO_2 of different nanoscale size. The self-organized TiO_2 nanotube arrays were prepared by an anodization process of Ti foil, whose morphologic structure is illustrated in **Figure 2a**. As shown in **Figure 2b-c**, the experimental results indicate that the bubble nucleation on the surface of the larger diameter of nanotube needs higher dissolved gas concentration, coincided with the theoretical analysis. It is suggested by this work that the nanometer scale stucture has an important role in gas bubble nucleation, which should be consider in optimizing the geometric construction of photocatalyst.

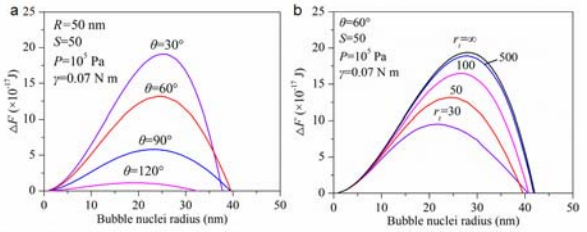

Figure 1. The free energy of bubble nucleation versus (a) the contact angle and (b) the radius of nanotubes

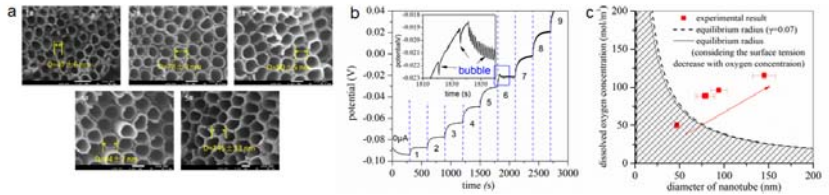

Figure 2. (a) The morphologic structure of nanotube array TiO_2. (b)The potential-current curve for critical nucleation saturation test. The arrow indicates the fluctuation caused by the bubble evolution. (c) The relation of critical concentration and the diameter of the nanotube.

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Brief Biography

Juanwen Chen

Juanwen Chen has been studying in State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University under the direction of Prof. Liejin Guo as a Ph. D student. Her research interests include multiphase flow and mass transfer process, especially bubble dynamics in photocatalysis system.

Liejin Guo

Prof. Liejin Guo is an academician of the Chinese Academy of Sciences, a scientist of engineering thermophysics and energy utilization in State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University. His current research concentrates on multiphase flow and heat and mass transfer, high efficient clean energy-power system and thermal power conversion process, multiphase flow thermophysics and key technologies of in exploitation and mixed transportation of oil and gas, high efficient conversion and utilization of renewable energy such as solar energy, biomass energy, and the mass production and use of hydrogen energy.

Zhenshan Cao

Zhenshan Cao is now a Ph.D. student in State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University (supervised by Prof. Liejin Guo). He is mainly engaged in the research of photocatalysis water splitting and multiphase flow, especially in bubble dynamics.

Yechun Wang

Yechun Wang is now an engineer as well as a Ph.D. student in State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University (supervised by Prof. Liejin Guo) with research area of multiphase thermophsyics in photoelectrochemical conversion.

Numerical and Experimental Investigation of Aerosolisation and Deposition Process in the Mouth-Throat Models with Handihaler®

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[b]*Department of Chemical Engineering, Monash University, Clayton, Vic 3800, Australia*
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Abstract

The inhaled drugs are generated as aerosol in dry powder inhalers (DPIs) and then transported into respiratory tract. The deposition in the target sites mainly depends on a number of factors related to anatomical structure variation, particle characteristics and inhalation conditions (inhaled angle and breathing pattern e.g.). This project aims to numerically and experimentally investigate the inhalation parameters affecting fine particle deposition in the US pharmacopeia throat (USP), idealized mouth-throat (IMT) and realistic mouth-throat (RMT) models with a commercial inhaler (Handihaler®). In the numerical model, the flow-field equations are solved by computational fluid dynamics (CFD). The monodispersed and Rosin-Rammler distributed particles in the size range of 1-30 μm are tracked with discrete phase method (DPM). Corresponding physical experiment under the same inhalation conditions are designed to quantitatively characterize particle deposition in realistic mouth-throat as well as validate the numerical models. The results indicate that the deposition fraction and spatial distribution are highly sensitive to the geometrical variation and respiratory conditions such as the inhalation airflow rate, particle size and inhalation angle. Moreover, the effect of geometrical variation on the particle deposition pattern is more dominant. In the RMT model, inhalation angle creates quite obvious effect on the aerosol delivery, especially for particles depositing in oral cavity on the tongue. This study could be used to develop an in vitro method which aims to better predict in vivo lung deposition mechanisms of pharmaceutical aerosol.

Keywords: computational fluid dynamics, aerosolisation, dry powder inhalers, mouth-throat geometry, deposition efficiency.

Biography

Fen Huang is a PhD candidate from Southeast University-Monash University Joint Research Institute, and supervised by Prof. Aibing Yu and Zhenbo Tong at Southeast University, Dr. Zongyan Zhou at Monash University. She received her BSc and MSc degrees from Northeastern University, Shenyang, P. R. China. Her research interest is focused on numerical and experimental investigation of aerosolisation and deposition process in the commercial dry powder inhalers and realistic respiratory tract.

Numerical Modelling and Design of a Hydrogen Storage Tank

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School of Chemical Engineering, University of New South Wales, Sydney, Australia

Email: ys.shen@unsw.edu.au

Abstract

Hydrogen is a promising eco-friendly fuel and renewable energy. Effective hydrogen storage has constantly been a major challenge in hydrogen industry and attracted significant attention in recent years. In this study, a three-dimensional CFD model is developed to simulate the hydrogen absorption and desorption process in a storage tank where $LaNi_5$ is used as metal hydride. The typical thermo-chemical phenomena during hydrogen desorption and absorption within the tank are simulated. A new design is proposed by introducing an internal heating tube covered by aluminum foam for improving heat transfer efficiency between metal hydride and heating source and tested using the model. The simulation results indicate that the design distinctly favors the absorption and desorption efficiency. This model can be used as a cost-effective tool to investigate hydrogen storage and process optimization with respect to operating conditions and design.

Brief Biography

Mr Siwoo Jung is an undergraduate student in the School of Chemical Engineering, University of New South Wales. He will receive his Bachelor degree at the end of 2018.

CFD Study and Plant Test of Semicoke-coal Co-injection in an Ironmaking Blast Furnace

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2 Ironmaking plant, Baoshan Iron&Steel Co Ltd, Shanghai 201900, China

3 School of Chemical Engineering, University of New South Wales, Sydney, New South Wales 2052, Australia

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Abstract

Low rank coals can be upgraded and used to produce semicoke. Semicoke has a potential to partly replace high grade metallurgical coals in pulverized coal injection (PCI) in ironmaking blast furnace (BF) under increasingly constrained environmental conditions. In this paper, a three-dimensional Computational Fluid Dynamics (CFD) model is used to simulate the flow and thermochemical behaviours related to the PCI operation of co-injecting typical PCI coal and semicoke under full-scale BF conditions. The typical phenomena of in-furnace aerodynamics and physicochemical behaviours relevant to the co-injection are simulated for both overall performance of the blend and the individual behaviours of the components - PCI coal and semicoke, in terms of flow, temperature, gas composition and combustion characteristics. Moreover, the co-injection of coal and semicoke are tested in a commerical BF, ranging from 10% to 20% blending fraction of semicoke. The numerical and plant test results indicate that the co-injection of PCI coal and semicoke have demonstrated the similar combustion profiles with the conventional PCI operation, confirming the feasibility of replacing PCI coal with semicoke partly. The study provide a combined views of co-injecting PCI coal and semicoke in terms of fundamental combustion profiles and plant performance in a commerical BF.

Brief Biography

Mr ZJ Hu is a PhD student in the School of Metallurgical and Ecological Engineering, University of Science and Technology Beijing, China.

A Numerical Study on Shear Thinning due to Breakup of a Particle Aggregate

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[2]*Central Research Institute of Electric Power Industry, 2-11-1 Iwadokita, Komae-shi, Tokyo, Japan*

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Abstract

Suspended aggregates of colloidal particles substantially affect the rheological aspect of suspensions. This study proposes an effective way of detecting the aggregate microstructure by studying the shear thinning behaviour of sheared suspensions, which is a rheological manifestation of shear-induced deformation of the aggregate structure [1,2].

Previous studies have placed a major emphasis on qualitative and quantitative analysis of the structural characterization of aggregates that varies with time and applied shear rates [3,4]. However, the effects of the deforming aggregate microstructure on the macroscopic rheological behaviour of the suspensions have been less studied.

Rheological information of suspensions can be better correlated with the qualitative evaluation of the aggregate microstructure by means of a numerical approach. Simulation of the shear-induced deformation of a particle aggregate should properly account for the particle-particle (PP) and particle-fluid (PF) interactions as well as motion of individual particles. However, no proper numerical models exist in the literature for simulation of the shear-induced deformation of aggregates: limitation in low Reynolds regimes [1,2], complex two-way evaluation of PF interactions of constituent particles of an aggregate [4].

The objective of this study is to investigate the effects of the microstructure of particle aggregates on the macroscopic rheology of suspensions. Herein, we consider two types of aggregate: the spherical aggregate ('cluster') and the hollowed-out shell ('shell'). To do this, we also propose an effective numerical model that can simultaneously deal with PP/PF interactions in a straightforward manner.

Multi-phase dynamics of suspensions were simulated by the DEM-DNS method [5]. This method simultaneously simulates (i) the PP interactions using Discrete Element Method (DEM) [6] and (ii) the PF interactions with Immersed Boundary Method (IBM) [7]. This coupling with DNS can achieve effective two-way evaluation of PF interactions of constituent particles with the surrounding flow fields.

We found that, on increasing shear rates, the shell type showed higher degree of shear thinning than the cluster type. This is because the shell with structural strength more susceptible to shear-induced deformation was more likely to break up under hydrodynamic stress. Under fairly high shear rate regimes, where both the shell as well as the cluster completely dissolves into individual particles freely streaming in the flow direction, the steady-state viscosity disparity can be explained by Krieger-Dougherty model for concentration dependence of the macroscopic viscosity increase of dispersions. Once the complete break-up is achieved, the steady-state viscosity matches that of dispersions with corresponding solid volume fraction. Thus, the ratio of the resulting viscosities of the two types of aggregate is comparable to an increase in viscosity of a dispersion with concentration corresponding to the shell upon addition of particle loading equivalent to the interior void region of the shell. By demonstrating that the difference in the aggregate microstructure significantly affects the macroscopic rheology of the suspensions, we propose a new way of structural determination of suspended aggregates using numerical simulation.

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Brief Biography

Hirotake Udono (Mr.) is a PhD candidate from the University of Tokyo, Japan. He works on physics of micro-scale multi-phase flows by the Direct Numerical Simulation (DNS).

A Study of the Impact of Swirler Design on Dry Powder Inhaler Behaviour

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Abstract

Introduction: Use of dry powder inhalers (DPI) is attracting interest as an alternative therapeutic method of drug delivery over metered dose inhalers or nebulizer. DPIs in conjunction with targeted deposition have advantages over other drug delivery method to treat respiratory diseases, such as asthma, COPD and bronchitis. As a result, many CFD simulations on various DPIs for design modifications have been made to investigate device efficiency, performance and aerosol dispersion [1-2]. Furthermore, the CFD-DEM coupling method is employed to observe the de-agglomeration mechanism, particularly for carrier-based devices [3-5].

Problem and scope of study: Despite many recent CFD modelling studies of various DPIs and the influence of parameters have been performed, less effort has been expended on studying the influence of turbulence by the cyclonic flow generated in the device chamber in relation to the particle transportation, de-agglomeration and aerosol dispersion. The current study presents comparison of swirling flow, as well as dispersion as a function of the number of tangential inlets to see how the cyclone flow field influences the flow, swirl pattern and production of turbulence. The effect of the turbulence modelling approach used is also studied.

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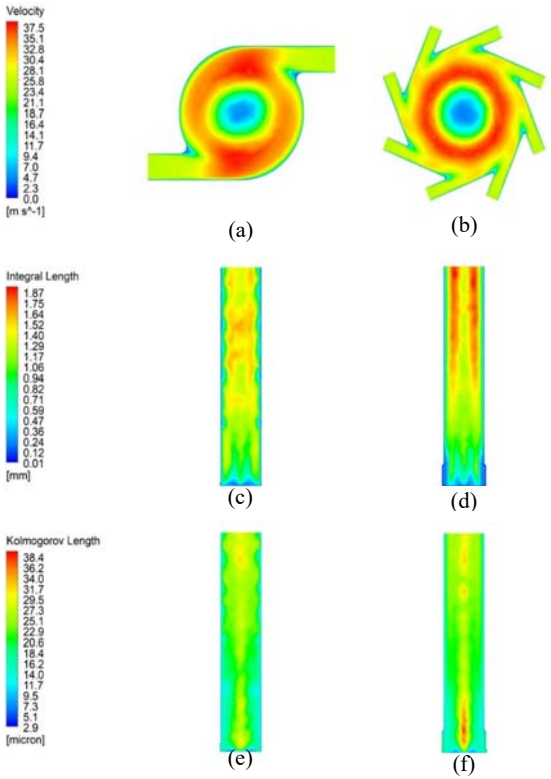

Fig 1. The impact of the number of inlets. Contour plots for 2 inlets (left) and 8 inlets (right): (a), (b) velocity at outlet; (c), (d) integral length scale of turbulence; and (e), (f) Kolmogorov length scale of turbulence.

Brief Biography

Yun Hwan Kim (Joshua) is currently a Ph.D. candidate at the School of Chemical and Biomolecular Engineering in the University of Sydney. He has earned his B.E. in Aerospace (2014) and M.Phil. in Materials Science (2016) from the UNSW Sydney and has worked as an analyst at Hyundai Motor Group prior to pursuing the research degree at UNSW Sydney in 2015. His research has been focused on the CFD modelling of fine powders in the respiratory tract and CFD-DEM modelling of the dry powder inhalers using advanced turbulence models.

A coupled VOF-DEM framework for the particle-bubble interaction

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Introduction

Despite that separation of valuable minerals using flotation has been utilized over a century, it is still of significant research interest due to complex physio-chemical interactions involved in the process. Particle recovery in flotation is often modelled by a first order kinetics rate equation wherein the rate constant is expressed as a product of the probabilities of three sub-processes namely bubble-particle collision, particle attachment and detachment. The effects of flow field on these sub-steps and interactions at the interface are known to be critical for process performance. Although, in recent time, macro-scale multiphase CFD models have been successfully applied in flotation [1] to understand these effects, treatment of gas-liquid interface in a resolved manner remain largely unexplored. This study aims to address this knowledge gap by developing a coupled Volume of Fluid (interface behaviour) and Discrete Element Method (particle motion) model to investigate the effect of bubble surface hydrodynamics and particle surface properties on bubble-particle interactions.

Method

The volume-averaged Navier-Stokes equations including the contribution of surface tension force were used to describe the fluid

$$\frac{\partial(\varepsilon\rho\mathbf{u})}{\partial t}+\nabla\cdot(\varepsilon\rho\mathbf{u}\mathbf{u})=-\varepsilon\nabla p+\nabla\cdot(\varepsilon\boldsymbol{\tau})+\mathbf{f}_s+\mathbf{f}_{pf}+\varepsilon\rho\mathbf{g}\,, \tag{1}$$

$$\frac{\partial\varepsilon}{\partial t}+\nabla\cdot(\varepsilon\mathbf{u})=0\,, \tag{2}$$

The volume fraction of liquid (α_1) is transported as a scalar and can be written

as

$$\frac{\partial(\varepsilon\alpha_1)}{\partial t}+\nabla\cdot(\varepsilon\alpha_1\mathbf{u}_f)+\nabla\cdot(\varepsilon\alpha_1(1-\alpha_1)\mathbf{u}_r)=0\,. \tag{3}$$

The particle-bubble surface interaction was modelled as a combination of the maximum capillary force [2] and a Hookean spring like force [3] as a function of the liquid volume fraction (α_1) .

$$F_{\text{int}erface}=\pi\sigma R_p(1-\cos\theta)+k\Delta\alpha_1\,, \tag{4}$$

Results and discussion

The proposed model showed good mass conservation of the gas phase during rising process in the presence or absence of particles. The bubble rising velocity agreed well with the correlation and experimental measurements from the literature. In order to validate the implementation of the interaction between the particle and the interface, the trajectory of a particle falling onto a stationary droplet was compared to experimental observations from the literature [4]. Effect of particle hydrophobicity and forces on the capture of particles were further analysed at different particle surface properties. Finally, settling particles captured by a rising bubble were simulated to demonstrate the capability of the model in a more practical condition. The particle-bubble collection efficiency predicted from simulations were compared to the existing theoretical models [5].

Brief Biography

Linhan Ge obtained his Master of Engineer degree in mineral processing Engineering from China University of Ming and Technology (CUMT) in 2015. Afterwards, he began his PhD study at the Discipline of Chemical Engineering, School of Engineering of the University of Newcastle under the supervision of Prof. Geoffrey Evans and Dr. Roberto Moreno-Atanasio. His PhD research project is to model the particle-bubble interaction under different hydrodynamic environments as applied to many industrial processes especially to the froth flotation in mineral processing field. The major methods he applied include unresolved CFD-DEM coupling, interface resolved Volume of Fluid (VOF)-DEM coupling and fictitious domain methods to resolve the dynamics at different length and time scales.

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CFD-DEM MODEL OF GAS-SOLID REACTING FLOWS IN THE BLAST-OFF OPERATION OF IRONMAKING BLAST FURNACES

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Abstract

Gas-solid reacting flow in a packed bed subjected to a lateral gas inlet is commonly used in many industrial applications such as blast furnace ironmaking, catalyst regeneration, granular drying, and coal gasification and combustion. In this paper, a CFD-DEM model is used to describe the gas-solid reacting flow in the blast-off operation of an ironmaking blast furnace, including gas-solid multiphase flow, heat and mass transfers related to coke particles combustion chemical reaction. The typical flow, temperature and composition fields are captured including force chain distribution. Then the effects of gas inlet velocity, particle size, and bed height on gas-solid flow pattern including void shape and size, temperature distribution and species distribution are investigated. The quantitative results indicate that a larger gas inlet velocity, finer particles and lower bed heights will lead to a larger void and stronger chemical reaction. The study provides a cost-effective tool to understand and optimize the blast-off operation in blast furnaces.

Keywords: Gas-solid flow, Thermo-chemical behavior, Raceway, CFD-DEM, Blast furnace

Brief Biography

Jiaxin Cui is a PhD student in the School of Chemical Engineering, The University of New South Wales. She received MEng in Materials Engineering from University of Science and Technology Beijing, and BS in Materials Chemistry from University of Science and Technology Liaoning.

DEM Modelling of the Segregation of a Binary-sized Mixtures During Formation of Stockpiles

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Abstract

Stockpiles are commonly observed for the storage of bulk materials in various industries, such as mining and refining industries. One of the main issues in the formation of stockpiles is the segregation of materials due to different properties, e.g. size and shape. There has been intensive studies on size segregation of spheres on stockpiles in the literature. However, the particle shape can have an influence on the extent and configuration of size segregation. Makse et al.[1-3] have ever considered the effects of a faceted shape type on the segregation of a binary-sized stockpile. It was argued that the large-cubic particles tend to size segregate to the bottom of the pile, whereas shape segregate at the top of the pile. It leads to stratification, i.e. moderate segregation, in the pile.

In this work, DEM is employed to study the particle shape effects on the segregation phenomenon of a binary-sized stockpile. In the binary mixtures, large particles are non-spherical, with aspect ratio varying from the unity to produce ellipsoidal shapes, and small particles are kept spherical. It has been reported that segregation can be developed for binary-sized stockpiles with large particles at the bottom of the pile[4]. The results reveal that the stockpiles of ellipsoids could end up with similar segregation configuration. It is also found that as aspect ratio of large particles deviates from 1.0, the segregation becomes moderate. For both the mixtures of ellipsoids and spheres, increasing the size difference could deepen the segregation. Additionally, the increase of damping coefficient lowers the segregation extent.

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Experimental Study and DEM Simulation of Wet Cohesive Particles with Liquid Bridge Model

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Abstract

Wet cohesive particles are often encountered in many chemical engineering processes, such as fluidized bed, screw conveyor and coating. Due to the liquid bridge between particles or particle-wall, the wet granular system is more complicated than that of a dry system. Most researchers studied the liquid bridge forces by the Laplace-Young equation, in which the contours of bridges are concave. But once the radius of particle is too small, or the amount of liquid is too much, the shapes of liquid bridge would change into a convex one. The existing models (Mikami and Lian) are no longer suitable for this situation. In this paper, the liquid bridge force is studied experimentally. Comparing the experimental results with Mikami's model, there is a large deviation in the range between the convex and the transition point. The liquid bridge force is stable at a lower level when the bridge contour is convex. According to the experimental data and existing model, the liquid bridge model is modified by regression analysis and validated in the repose angle and hopper discharging experiments. It is shown that the modified model can accurately predict the kinetics behavior of the wet cohesive particles.

Brief Biography

Fei Xiao, Doctor Candidate of Southwest Petroleum University majoring in Oil & Gas Storage and Transportation Engineering in School of Petroleum & Nature Gas Engineering. I mainly focus on the particle kinetics by means of the discrete element method, especially for wet cohesive and bonding particles. I am also interested in the gas-solid multiphase flow and the corresponding the erosion characteristics.

The Computational Fluid Dynamics Study on the Law of Proppant Placement in Wedge Fracture

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Abstract

The Fracturing treatment, in conventional gas and tight reservoir, is a key technology. For production increased, the effective proppant placement requires the understanding of shape of fracture and the law of proppant transportation and settling in fracture. However, the law of proppant transport and settle in wedge fracture is unclear to the researchers. Most of the fracture model simulates using the uniform width of fracture and using the Euler-Euler multiphase to study the law of proppant transportation and settling in single fracture.

In this study, the non-uniform width fracture(wedge fracture) case was first simulated and using the CFD-DPM(3D) model to track the movement of proppant. Besides, using a series variables which include proppants size, laboratory scale pump rate and proppants concentration to simulate proppants transport in wedge fracture. Meanwhile, we do some simulation about proppant transportation in rectangular fracture and wedge fracture which can distinguish the difference law of proppant movement in different style of fracutures.

Finally comparing the result of proppant movement in wedge fracture and rectangular fracture, based on the Velocity simulation analyze, we will find that the distance of proppant in wedge fracture are greater than the rectangular fracture. Due to the more narrow width of wedge fracture, the higher velocity of proppant will have in wedge fracture. What's more, using the method of dimensionless variables ,we also find that the pump rate is the most important factors of three lab variables. Meanwhile, it also explain that the velocity plays an important role in the proppant movement in the wedge fracture.

Brief Biography

Jun Li will be a PHD student at Monash university. His reserach interests are hydraulic fracturing.Li has authorized or coauthorized three technical papers,and he hold ten chinese patents. He was the chairman of the SPE student chapter at Southwest petroleum university. Li holds master degrees at Southwest petroleum university and University of Regina .

Pingli Liu is a Professor in Southwest petroleum university. His reserach interests are hydraulic fracturing and acidizing.He is famous about acidizing area in China .He have published a lot of technical papers and patents.

Research on the Effects of Silt Mean Diameters and Silt Concentrations on the Cavitation Flow in a Two-Dimensional Nozzle

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Abstract

Effects of silt mean diameters and silt concentrations on cavitation flow are researched in a two-dimensional nozzle. Silt mean diameters are 0.02mm, 0.04mm, 0.06mm, 0.07mm and 0.08mm and silt concentrations are 0.02, 0.04, 0.06, 0.07 and 0.08. When silt mean diameters are invariant, silt concentrations are changed to consider the effects on cavitation flow and when silt concentrations are the constants, silt mean diameters are varied to consider the effects on cavitation flow. Results show that cavitation occurs at the beginning parts of the jet orifice and distributions of static pressure, vapor and silt particles are axial symmetrical. Cavitation number variations with silt concentrations or with silt mean diameters reflect the effect degree of silt particles towards cavitation flow. With silt mean diameters being 0.06mm, 0.07mm and 0.08mm, fluctuations of cavitation number with the increase of silt concentrations are much more remarkable than it with silt mean diameters being 0.02mm and 0.04mm. During silt concentrations are fixed, all fluctuations of cavitation number with the increase of silt mean diameters are remarkable, demonstrating that silt mean diameters have a more intense effect on cavitation flow. Reasons why silt particles promote the development of cavitation are analyzed. Effects of properties of silt particles, cavitation nuclei, virtual mass force, velocity slip, Saffman lift force and turbulent kinetic energy are considered and studied.

Brief Biography

Xiangdong Han was born in 1989. Now, he is one Ph.D candidate of Key Laboratory of Hydraulic Machinery Transients, Ministry of Education of Wuhan University. He received his bachelor degree in 2014. He received his master degree in 2017. His major is fluid machinery and engineering. His main research field is effects of silt particles on the development of cavitation flow via numerical simulations and experimental measurements.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

Numerical study of sandpile segregation with ellipsoidal particles

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Abstract

A better understanding of particles segregation is of great significance for both research purpose and practical concern. Sandpile as a fundamental granular system has been a major research focus for years. Previous researches have put great efforts on explaining the effects of various factors on sandpile segregation both simulations and physical experiments. But a comprehensive study of shape effects is still needed. Here we used a discrete element method to study the behaviour of ellipsoids in sandpiles. The shapes of ellipsoid ranges from prolate to oblate by adjusting its aspect ratio (AR). It was found that for a binary mixture of spheres and ellipsoids, the mechanism of shape effects is based on the repose angle of the pile. For 0.5<AR<2.0, mixing index increases while angle of repose decreases, which means lower particle sphericity can induce worse mixing property. But for extreme shapes while AR<0.5 or AR>2.0, the relationship between repose angle and mixing index shows opposite patterns. Considering the time needed to reach the steady mixing point, it was concluded that mixture with larger aspect ratio will result in faster mixing. In order to further obtain the details of these behaviours, velocity and force profiles were also investigated which rather supports the previous conclusions.

Brief Biography

Dizhe Zhang is a full time Ph.D student affiliated with the Department of Chemical Engineering at Monash University, Australia. His study focus on the numerical study of particle behaviors in segregation systems. Dizhe Zhang earned his BSc from School of Energy and Power Engineering at Beihang University, China.

Particle Scale Modelling to Study the Effect of Cohesive Inter-particle force on Bubble Dynamics

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Abstract

Gas-solid fluidized beds are widely encountered in many industrial applications due to their excellent mixing and heat and mass transfer characteristics. In gas-solid fluidized beds, the inter-particle forces can alter the fludization behavior. In this study, CFD-DEM was used to study the properties of bubble and bed microstructure when an inter-particle force was externally imposed in a single jet fluidized bed of different particle shape. The inter-particle force used in this study is van der Waals force which was varied from 0.5, 1, 2, 5, 10, 15, and 20 times the Hamaker constant. The particle shape used in the study are spheroids which varies from aspect ratio of 0.5 to 2, ranging from disc-like to needle shaped particles. The investigation is carried out for two different jet velocities of 0.2 and 0.3 m/s. The results shows that the bubble formation time and bubble properties are sensitive to inter-particle forces. With the increase of van der Waals force bubble detachment time increases while the bubble size decreases for all kinds of particles. The bubble size distribution was found to be narrower and the bubble frequency decreased with the increase of van der Waals force.

Brief Biography

Siddhartha Shrestha is a PhD student at Monash University since 2016 under the supervision of Dr. Zongyan Zhou. He is working on the project titled "Particle scale study of bubble dynamics in gas-solid fluidization". The simulation technique used in the study is CFD-DEM and the particles used in the simulations are fine non-spherical particles. He completed his undergraduate degree in Chemical Engineering from Bangladesh University of Engineering & Technology in 2011. He obtained his Master's degree in Engineering (Chemical Engineering) by research from University of Malaya in 2015.

CFD-DEM Investigation of Flow Regimes in Horizontal Hydraulic Conveying

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Abstract

Hydraulic conveying is widely used in many industries, such as mining, chemical, ocean and petroleum industries. During this process, the flow regimes and their transition play a critical role, but are not fully understood yet. This paper presents a numerical study of hydraulic conveying by the approach of combing Computational Fluid Dynamics (CFD) for the fluid phase and Discrete Element Method (DEM) for particles. The validity of the CFD-DEM model is confirmed by the reasonable agreement between the predicted and measured pressure drop at different superficial fluid velocities and delivered solid concentrations. It is then used to study the liquid-solid flow behaviors in horizontal hydraulic conveying. The numerical result shows that in the dense-phase conveying, the pressure drop decreases with the increasing superficial fluid velocity at a fixed delivered solid concentration, where in turn stationary flow, moving-bed flow, and sheared flow occur. Conversely, in the dilute-phase transportation, the increasing superficial fluid velocity leads to the increase of the pressure drop, where particles are partially or fully suspended throughout the pipe. In addition, the flow regimes and transition are analyzed in details in terms of force and flow structures on a particle scale, which reveals the relative importance of various forces on particles in different flow regimes.

Brief Biography

Miss Mengmeng Zhou obtained her BSc in Mechanical Engineering on June 2014 at University of Sussex, and MSc in International Management on December 2015 at University of Southampton. In 2017, she as a PhD candidate joined ARC Research Hub for Computational Particle Technology, Department of Chemical Engineering at Monash University, Australia. Her PhD project is focused on the development and application of CFD-DEM model to hydraulic conveying.

Large Eddy Simulation of Particle Flow during Liquid A356 Alloy Transported by screw Pump with Discrete Phase Model-Volume of Fluid Coupled Model.

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Abstract

Screw pumps are mainly used to transport liquid metal with high density and high temperature in metallurgical industry. The liquid A356 alloy contains many particles. For the particle liquid flow, particle movement plays a significant role in the phase structure and causes the unsteady complex turbulent flow. A 3D gas-fluid-solid three phase model with large eddy simulation (LES) is developed to probe the particle movement. The Eulerian volume of fluid(VOF) model is used for tracking the liquid-air free surfaces and the Lagrangian discrete phase model(DPM) is used for describing the particle movement. The turbulent liquid flow is induced by particle-liquid interactions and is solved by LES. Numerical predictions are validated against pump head in an industrial test. According to the results, a new pump was designed to enhance the quality of the A356 alloy.

Brief Biography

Zhuan Ge, Master, study in the School of Metallurgy, Northeastern University, Shenyang, Liaoning, China. Researches focus on rotating machinery, multiphase flow and Deep learning in CFD.

Numerical Study on Flow and Heat Transfer Characteristics of Coal Particle in Supercritical Water Fluidized Bed Reactor

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Abstract

Supercritical water gasification (SCWG) of coal is a promising technology to convert coal into hydrogen rich gas. However, due to the extreme operation condition in reactor, there exists many barriers to directly measure the details of physical field. The information is essential to understand the flow and heat transfer characteristics of SCWG of coal and optimize the gasification process. This study develops a comprehensive 3D numerical model based on Eulerian-Lagrangian approach to simulate the fluid-particle flow, heat transfer and coal gasification process in a supercritical water fluidized bed (SCWFB) reactor. In this model, the inter-particle interaction is evaluated by the kinetic theory of granular flow (KTGF), the radiative transfer in fluid and particle phase is solved by discrete ordinate (DO) method, and the chemical reaction rate is computed by Arrhenius equation.

The temperature field, velocity field, distribution of gasification products and particle trajectory are predicted, and simulation results are verified against experimental data. Results show that cold feed slurry flows downward after injecting into reactor, due to the buoyancy force, a strong swirling flow is formed below feed inlet and increases the particle residence time obviously. According to the spatial distribution of particles, there presents core-annular flow structure in radial direction, particle concentration is relatively uniform in the core region, while increases rapidly with the increase of radius near the wall. In this paper, the heat transfer characteristics in the reactor are also quantitatively analyzed. Convection dominates the inter-phase heat transfer: the convective heat transfer coefficient (HTC) at particle surface is approximately 9 times higher than the radiative HTC. Moreover, gas radiation largely overwhelms the particle radiation in the SCWFB reactor, which is noticeably different from the phenomenon of coal combustion in the chamber. In addition, this study investigates the effect of particle size on coal gasification efficiency in supercritical water (SCW). Results indicate the HTC and temperature of particle decrease with the increase of particle diameter, which results in a proportionate increase on time for complete conversion of coal. This study gives a deep insight into the flow and heat transfer behaviors of particle inside the SCWFB reactor, and the results may be useful for optimizing operation and design of the reactor.

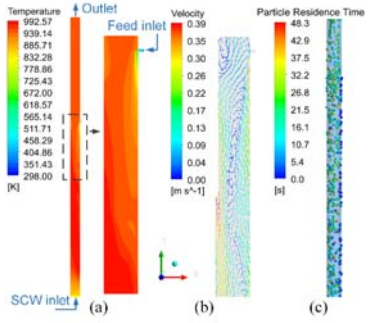

Fig. 1 (a) Contour map of fluid temperature and (b) vector diagram of fluid velocity below feed inlet at central cross-section, and (c) particle distribution inside the reactor.

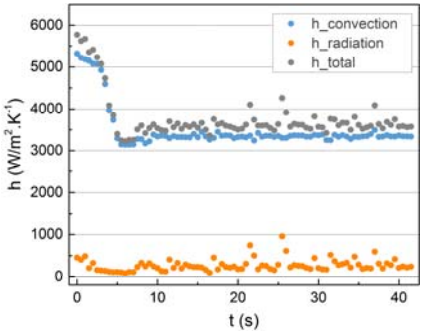

Fig. 2 The change of coal particle (75 um) heat transfer coefficient (h) (consists of convective and radiative components) with residence time (t).

Brief Biography

Zhenhua Ren, was born in a poor rural family in China, in 1993. He received his bachelor degree in thermal and power engineering from University of Shanghai for Science and Technology (USST) in 2015. In the same year, he was admitted to school of energy and power engineering of Xi'an Jiaotong University for postgraduate degree. Now, he is a Ph.D. candidate under supervision of Prof. Liejin Guo in State Key Laboratory of Multiphase Flow in Power Engineering (SKLMF), Xi'an Jiaotong University, in China, committed to the research and development of supercritical water gasification (SCWG) technology.

His main research interests lie in the flow and heat transfer behaviors in the supercritical water fluidized bed (SCWFB) reactor, involving the complex fluid-particle flow dynamics, radiative heat transfer in participating gas and particle, and heterogeneous multicomponent chemical transport. So far, he has completed the exploratory research on radiation property of supercritical water (SCW) based on line-by-line calculations, and has developed a comprehensive 3D numerical model of hydrodynamics to accurately predict the flow and thermal fields in a SCWFB reactor.

In the course of studies, he has won several national encouragement scholarships and excellent student scholarships, and has received two national invention patents till now.

2nd International Symposium on Computational Particle Technology & 13th International Conference on CFD in the Minerals and Process Industries, 4-8 December 2018, Melbourne, Australia

A Methodology for Predicting Marine Icing

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Abstract

Advances in technology have led to an increasing interest in petroleum exploration in the Arctic area. This poses special operational challenges such as sea spray icing on supply vessels and offshore drilling units. Sea spray icing occurs in subfreezing air temperatures by the impact of waves on vessels and fixed structures and leads to severe safety hazards and operational issues in offshore operations. Developing scientific knowledge and prediction capabilities in this area is needed to support technology for prevention of well incidents, and improve intervention as well as oil spill response capabilities.

The icing process can naturally be divided into three stages: 1) Impact of waves onto the construction and the formation of a water spray, 2) Transport of water droplets by wind onto the construction and 3) Ice formation on the construction as the water is cooled below the freezing point.

There exist a number of empirical engineering correlations for the liquid water content in the spray cloud. However, the correlations differ from experimental data by an order of magnitude, and thus need to be improved.

In this paper we describe a methodology for predicting marine icing by combining different CFD methods and deriving engineering correlations and engineering lookup tables from simulations. By running systematic computer experiments, simulation data for fitting engineering relations can be generated.

From a practical point of view, there is currently no single CFD model that covers the entire process from wind wave formation, wave slamming on constructions, spray formation, spray transport by wind onto the construction and cooling and ice formation. Thus, we use a pragmatic approach: 1) The wave statistics are assumed known from meteorological data, 2) The waves approaching the construction are simulated by a Volume-Of-Fluid method (VOF) method, including slamming onto the construction and formation of a high-velocity liquid film, but not the actual formation of the spray. 3) The droplet and velocities in the spray resulting from the slamming are estimated from engineering relations based on droplet Weber numbers and liquid film Reynolds number. 4) The transport of droplets from the spray onto the construction is calculated using Lagrangian tracking of droplet trajectories.

We illustrate the methodology on an idealized 2D test case shown in Fig. 1 where an incoming wave hits a solid object.

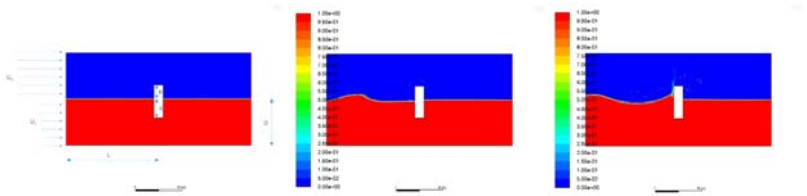

Figure 1. a) Geometry, b) Incoming wave, c) Slamming on object

Stages in the simulation approach are:

1. Definition of geometry and variables (wind, current, wave length and height, water depth, wave model (e.g. 3rd order Stokes), object dimension, densities, viscosities, surface tension, mesh resolution, time step).
2. Screening simulations using VOF: a) Select a high and low value for N selected variables, b) Run a systematic fractional 2^k factorial computer experiment in 2N runs. An illustrative factorial design in three variables are shown in Table 1, c) Analysis of effects of the variables.
3. Computer experiments. Variables are selected based on a latin hypercube design and the water flux to generate spray is fitted to a universal kriging model.
4. An engineering spray model based on Weber and Reynolds numbers is formulated.
5. Droplet trajectories and deposition are simulated using Lagrangian tracking of droplets. This will enable to perform a higher level of parametric studies, expanding a latin hypercube for the effects of wind, wave, object speed, and geometrical configuration. This will be future work.

Table-1. Example experimental design with 2N=6 runs in N=3 variables. Note that only one variable changes from one row to the next. Each variable changes value twice, and the two changes occur at complementary values of other variables

CFD run	Variable 1	Variable 2	Variable 3
run 1	high	low	high
run 2	low	low	high
run 3	low	high	high
run 4	low	high	low
run 5	high	high	low
run 6	high	low	low

Brief Biography

John Morud received his doctorate degree in Process Systems Engineering at the Norwegian Institute of Technology (NTH, now NTNU) in 1996. His Masters degree (1987) was in Applied Fluid Dynamics from the Department of Aero- and Gas Dynamics, NTH, and from the von Karman Institute for Fluid Dynamics in Brussels. He has been working with applied fluid dynamics in Norsk Hydro (1988-1991); with Process Control in Norske Skog (1996-1999); within Chemical Engineering and Fluid Dynamics in SINTEF (1999-present). He is currently Chief Scientist in the Fluid Flow department in SINTEF Industry. His main research areas is within modelling and simulation of fluid flow, mass- and heat transfer.

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Linear Stability Analysis of Rotating Horizontal Convection with a Moving Heated Surface

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Abstract

Rotating flows subjected to differential shear find practical engineering applications within rotating machinery, as well as providing physical insights into models of wind-driven ocean circulations. The key question is how does the surface shear stress, such as moving blade within machinery or wind stress on the ocean, the affect heat transfer characteristics and flow stability of the system? Previous studies (Barkan *et. al.,* 2015, Vreugdenhil *et. al*., 2017) investigated rotating shear flow in a rectangular enclosure. However, to the best of the authors' knowledge, no research has been done to systematically investigate a coupled horizontal convection and surface shear stress on a rotating cylindrical setup. In this study, the nonlinear dynamics of a moving heated surface on the three-dimensional instability of a rotating horizontal convection flow in a cylindrical enclosure driven by a radially increasing temperature over the base is numerically investigated using a linear stability analysis. The instability modes are classified based on energetics of the perturbation flow fields.

The control parameters used in this investigation are rotation parameter, Q, which quantifies the importance of rotation, and the Rossby number, Ro, which represents the differential rotation rate between the moving bottom base and the main rotating tank. The results demonstrate two distinct unsteady regimes within the rotation parameter Q and the Rossby (Ro) parameter space separated by a region of time independent flow. Based on linear stability and energetics analysis, the steady region is further divided into four linearly unstable regions: (R) rotation affected zero Rossby number, (L-) low Q negative Rossby number, (H-) high Q negative Rossby number and (H+) high Q positive Rossby number as depicted in figure 1.

In the low Q negative Rossby number regime, instability is localized near the buoyant end of the cylinder, whereas the high Q negative Rossby number regime has disturbance features toward centre of the tank which extends deep into the enclosure. On the other hand, the high Q positive Rossby number instability is confined near the edge of the cylinder due to vertical shear induced by the moving heated surface.

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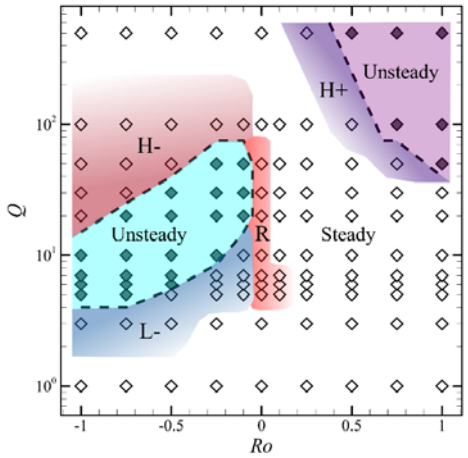

Figure 1. Flow regime map in the rotation parameter (Q) and Rossby number (Ro) space. The plot identifies time-dependent regimes shaded with light blue and light purple. The linearly unstable regions are shaded with colour gradient, each with a label as described in the text.

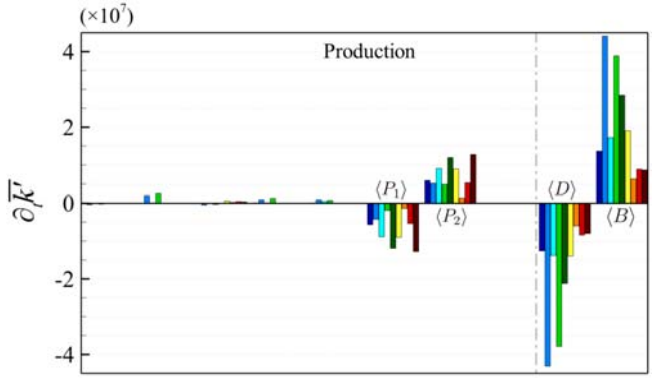

Figure 2. Contributions to rate of change of the perturbation kinetic energy from eight production terms due to velocity shear with two dominant terms labelled as $\langle P_1 \rangle$ and $\langle P_2 \rangle$, viscous dissipation, $\langle D \rangle$, and contribution from buoyancy flux $\langle B \rangle$. The parameters (Q, Ro, wavenumber) for each of the nine columns are as follow: (6, -0.1, 12), (6, -0.1, 26), (6, -0.25, 12), (6, -0.25, 21), (10, -0.1, 23), (20, -1, 9), (50, -0.5, 23), (50, -0.75, 21) and (50, -1, 15).

Brief Biography

TzeKih Tsai is a PhD researcher from the Department of Mechanical and Aerospace Engineering, Monash University, with research interests in understanding the fundamental dynamics of horizontal convection under the influence of buoyancy forcing and the effect of rotation through idealised numerical modelling.

Modeling an Effect of Water on Asphaltene Deposition in a Turbulent Production Pipeline Flow

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Abstract

Asphaltenes are molecular substances, which together with resins, aromatic hydrocarbons, and saturates compose crude oil. Asphaltene deposition in production pipelines is an important problem of flow assurance because an asphaltene deposit layer, if formed, may significantly obstruct pipe cross-section leading to a large production rate drop. In majority of practical cases, asphaltene particles precipitate from oil due to a thermodynamic destabilization induced by a pressure decrease; therefore, an intense asphaltene deposition can occur only in a vertical well where a substantial pressure reduction is caused by hydrostatic pressure gradient. The deposition process needs to be modeled to make decision on necessity of preventing deposit formation by an asphaltene inhibitor injection. Usually, deposition modeling is reduced to calculation of a flux of asphaltene particles to the pipe wall. A number of asphaltene deposition models, known from open literature, are based on different approaches to calculation of this flux. For example, in 2011-2012 Eskin with co-authors suggested a comprehensive asphaltene deposition model, according to which the deposition flux is mainly determined by Brownian motion of asphaltene particles whose size distribution, varying along a pipe due to agglomeration, is calculated by a population balance equation. These authors identified deposition model parameters by experiments conducted in a laboratory Couette device.

Production of oil is almost always accompanied with a production of water; therefore, an effect of water on asphaltene deposition has to be also modeled. Two major physical effects, which may lead to a reduction of the deposition flux due to presence of water in oil are: 1) reduction of concentration of asphaltene particles in a hydrocarbon fluid due to absorption of precipitated asphaltene nanoparticles on water droplets dispersed in oil; 2) reduction of a pipe wall area, available for deposition, due to a dynamic wall coating with droplets bombarding its surface in a turbulent flow.

Both the mentioned effects are to a significant extend determined by droplet size distribution. To characterize this distribution, in the present work we employed the droplet Sauter diameter calculated by known semi-empirical correlations.

The first water effect has been evaluated as follows. It is known that asphaltene nano-agglomerates, being absorbed by surface of water droplets, form a monolayer. A rather simple estimation showed that an amount of asphaltenes absorbed by droplets is small to significantly affect the deposition flux to the pipe wall through a reduction of asphaltene concentration in oil.

An evaluation of the effect of dynamic wall coating on deposition has been done by an analysis of collisions of droplets with the wall. A pipe surface area, dynamically coated with droplets, is determined by both the frequency of pipe-wall interactions and a droplet-wall contact area changing during interaction of a deforming droplet with the wall. According to experimental data, available in open literature, distribution of the droplet

fluctuation velocity is nearly Maxwellian that allows straightforwardly calculating the frequency of droplet – wall collisions. Evolution of the droplet-wall contact area during a collision event is determined by an approximate momentum equation derived assuming a small droplet deformation. An initial droplet velocity at the moment of interaction with the wall was assumed to be equal to the corresponding fluctuation fluid velocity calculated by an empirical correlation available in literature. The developed model of droplets-wall interactions allows determining a fraction of the pipe wall area dynamically coated with dispersed droplets. This fraction is equal to the sought factor of a deposit flux reduction due to presence of water in oil. Numerous calculations showed that this reduction factor rapidly increases with an increase in both the water volume fraction and the mean flow velocity through a pipe. However, even at the highest water volume fraction considered (40 %), the reduction factor does not exceed one percent.

Thus, the major finding of the present research is a smallness of an effect of water on the asphaltene deposition process; therefore, this phenomenon can be ignored in engineering calculations.

Brief Biography

Dmitry Eskin is a Professor at Skolkovo Institute of Science and Technology in Moscow, Russia. Previously, he was a Scientific Advisor at Schlumberger-Doll Research Center in Cambridge, MA. Eskin's current research interests are in the area of multiphase flows in application to flow assurance, hydraulic fracturing and other areas of petroleum engineering. He has authored and co-authored over 70 journal papers. Eskin holds Ph.D. degree in Chemical Engineering from Mendeleyev University of Chemical Technology of Russia.

Design and Optimization of steam jet ejector using Computational Fluid Dynamics and Genetic Algorithm.

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Abstract

Steam jet ejectors are vacuum producing device used in refrigeration cycle. The aim of this study to find out the flow structure and mixing process inside steam jet ejector using Computational Fluid Dynamics. Since the flow inside the steam jet ejectors is compressible in nature hence density based solver is used for the simulation and water vapor as a working fluid. Further the design optimization of steam jet ejector using genetic algorithm the aim of optimization is to maximization of entrainment ratio which is function of primary stream pressure, secondary stream pressure, exit pressure, secondary stream temperature while keeping geometric parameter nozzle inlet diameter 67.2 mm, nozzle throat diameter 39.5mm, nozzle outlet diameter 53 mm, nozzle length 295 mm, diameter of diffuser chamber 144 mm, length of diffuser chamber 176.4 mm kept fixed.

Brief Biography

1. Harshwradhan Kulkarni is research scholar from Institute Of Chemical Technology, Mumbai. He completed his bachelors degree in petrochemical engineering and masters degree in Modeling and Simulation. His research area is application of Computational Fluid Dynamics, Artificial Intelligence in process industries for the simulation of different pipe fittings.

A MULTI-SCALE MODELLING OF OSCILLATORY BLOOD FLOW AND MASS TRANSPORTATION IN A HUMAN CORONARY ARTERY

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ABSTRACT

Oscillatory flow is intrinsic to the cardiovascular system and is driven by the rhythmic beating of the heart. As a system for mass transport, the cardiovascular system hosts a variety of biochemical and cellular species, whose transport is subjected to the flow oscillations. The influence is most prevalent near the heart and particularly within arteries, where pressure fluctuations are most significant.

This makes modelling of long-term mass transport and resulting potential development of atherosclerosis difficult to evaluate, since intermediate oscillations need be explicitly resolved. By applying Reynolds averaging of the governing mass transport equations on a representative period of oscillation, this problem may be alleviated. However, doing so introduces extra terms akin to the
Reynolds stresses in the flow equations as well as perturbed-flux terms in the mass transport equations. These terms are investigated in the present study and their distributions assessed. A human right coronary artery is used as the subject geometry, wherein the oscillatory transport behaviour of low density lipoprotein is studied.

Keywords: coronary artery, oscillation, period-average, pulsatile, flow, species transport.

BRIEF BIOGRAPHY

Dr Yuqing Feng (B Eng, 1992; M Eng, 1995; Ph D, 2004, UNSW, Australia) is a principal research scientist at CSIRO Mineral Resources, leads in the development and application of advanced computational fluid dynamics (CFD) models for complex multiphase flow systems involving bubbles, particles and droplets, with a focus on their applications in process industries, including light metal production, mineral processing & extractive metallurgy, chemical and petroleum engineering. In addition to provide practical advice for reliable scale-up, design and control/optimization of different multi-phase complex flow systems, he has been co-supervising over 10 PhD students in conjunction with several universities and published 3 book chapters, over 130 scientific papers and 31 industrial reports.

Numerical simulation on non-equilibrium condensation using wet-steam model in steam ejector

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Abstract: Non-equilibrium condensation of steam occurs in the steam catapult. In the present paper, a numerical model for the simulation of wet steam flow has been used within a commercial CFD code (ANSYS Fluent) to investigate the non-equilibrium condensation process. The effects of inlet pressure and vapor temperature on the liquid distribution and flow field were studied. The result shows that liquid mass fraction of the outlet decreasing with the increased inlet vapor temperature whereas temperature and velocity of the outlet increasing with the increased temperature. However inlet vapor temperature has little influence on the average pressure of the outlet. The average velocity of outlet decrease as the injection pressure increasing and the liquid mass fraction and temperature of outlet increase with the increased injection pressure. Injection pressure has a great influence on the average pressure of the outlet.

Key words: wet steam; steam catapult; non-equilibrium condensation; high pressure; CFD

1. Introduction

The steam from the steam catapult has a great influence on the airplane engine. It may cause temperature distortion at the engine [1]. The vapor was saved in a cylinder at a high pressure and released from the cylinder to push the airplane accelerating. The pressure of the cylinder keeps constant. In order to reduce the calculation, the cylinder was instead by seven pressure inlets. The equipment is shown in the **Fig.1**. During this process, non-equilibrium condensation of steam occurs. The ingestion of vapor and water liquid by the engine inlet can be seen visually during a catapult launch stroke. The leakage vapor and water liquid can reach the engine inlet and produce an engine inlet temperature distortion. It is important to investigate the distribution and the mass fraction of the water liquid.

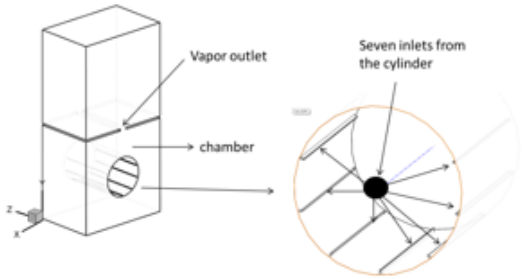


Fig.1 The steam ejector

In the present paper, a numerical model for the simulation of the wet steam flow has been developed to investigate the distribution and the mass fraction of the water liquid at the outlet of the cylinder when the vapor was released. There are two main wet steam models. One is the single-fluid model which is a kind of no-slip model and another one is the two-fluid model which takes into account the velocity slip between the vapor and the liquid phase. Investigations of wet steam model have been made by many authors for many years now. The first numerical predictions of the condensing steam flow were focused on one dimensional flow in the Laval nozzle using linearized equations by Puzyrewski[2]. In the present paper a single-fluid wet steam model implemented by commercial software ANSYS Fluent which has been used by several research teams[3][4][5] was used to simulate the non-equilibrium condensation of steam.

2. Model Description

2.1 Turbulence model

The standard k- ε model was used to simulate the flow field. The main governing equations for this model are described by B. E. Launder[6]:

$$\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x_i}(\rho k u_i)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]+G_k+G_b-\rho\varepsilon-Y_M+S_k$$

$$\frac{\partial}{\partial t}(\rho\varepsilon)+\frac{\partial}{\partial x_i}(\rho\varepsilon u_i)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right]+C_{1\varepsilon}\frac{\varepsilon}{k}(G_k+C_{3\varepsilon}G_b)-C_{2\varepsilon}\frac{\varepsilon^2}{k}+S_\varepsilon \quad (1)$$

In these equations, G_k represents the generation of turbulence kinetic energy due to the mean velocity gradients which is calculated as:

$$G_k=-\rho\overline{u_i'u_j'}\frac{\partial u_j}{\partial x_i}$$
$$G_k=\mu_t S^2$$
$$S\equiv\sqrt{2S_{ij}S_{ij}} \quad (2)$$

where S is the modulus of the mean rate-of-strain tensor. G_b is the generation of turbulence kinetic energy due to buoyancy which is calculated as:

$$G_b\equiv\beta g_i\frac{\mu_t}{\mathrm{Pr}_t}\frac{\partial T}{\partial x_i}$$
$$\beta=-\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_p \quad (3)$$

where $\mathrm{Pr}_t=0.85$ is the turbulent Prandtl number for energy in the present work and g_i is the component of the gravitational vector in the i th direction. β is the coefficient of thermal expansion.

2.2 Wet steam model

The wet steam is a two phase mixture which contains water-liquid and vapor. Steam with high velocity in low-pressure site achieves the non-equilibrium condensation. The following relationships between the liquid and the vapor phase:

$$\alpha=\frac{V_v}{V_m}$$
$$\rho_m=(1-\alpha)\rho_v+\alpha\rho_l$$
$$h_m=(1-y)h_v+yh_l \quad (4)$$
$$y=\alpha\frac{\rho_l}{\rho_m}$$

where α is the volume fraction and y is the mass fraction of the liquid phase.

The conversation equations for mass, momentum and energy equations for a vapor/liquid mixture are then written:

$$\frac{\partial \rho_m}{\partial t}+\frac{\partial(\rho_m u_m)}{\partial x_j}=0$$
$$\frac{\partial(\rho_m u_{mi})}{\partial t}+\frac{\partial(\rho_m u_{mi}u_{mj}+p\delta_{ij})}{\partial x_j}-\frac{\partial \tau_{ij}}{\partial x_j}=0 \quad (5)$$
$$\frac{\partial(\rho_m E_m)}{\partial t}+\frac{\partial(\rho_m u_{mj}H_m)}{\partial x_j}+\frac{\partial(q_i-u_{mi}\tau_{ij})}{\partial x_j}=0$$

where E_m is the total internal energy.

$$E_m=H_m-\frac{p}{\rho_m}+\frac{1}{2}u_{mj}u_{mj} \quad (6)$$

Two other equations are needed to describe the formation and growth of the liquid phase which are:

$$\frac{\partial(\rho_m y)}{\partial t}+\frac{\partial(\rho_m u_{mj}y)}{\partial x_j}=\Gamma_1+\Gamma_2$$
$$\frac{\partial(\rho_m n)}{\partial t}+\frac{\partial(\rho_m u_{mj}n)}{\partial x_j}=J \quad (7)$$

where "n" is the number of droplets per unit mass of the mixture which is assumed that no slip exists between phases. Γ_1 is the mass source of critical droplets of the mass m_l^* created due to the nucleation process, and Γ_2 is the mass condensation rate of all droplets per unit volume of the two-phase mixture.

$$\Gamma_1 = m_l^* J = \frac{4}{3}\pi\rho_l r^{*3} J$$
$$\Gamma_2 = \rho_l \overline{a_r} n \rho_m \frac{dr}{dt} = 4\pi\rho_l \rho_m n r^2 \frac{dr}{dt} \quad (8)$$

where J is the rate of nucleation of new generated droplets per unit volume of vapor and is expressed here:

$$J = C\sqrt{\frac{2\sigma}{\pi}} m_l^{-3/2} \frac{\rho_v^2}{\rho_l} \exp\left(-\beta \frac{4\pi r^{*2}\sigma}{3kT_v}\right) \quad (9)$$

where coefficient C is calculated from the relation:

$$C = \left[1 + 2\frac{\gamma - 1}{\gamma + 1}\frac{h_v - h_l}{RT_v}\left(\frac{h_v - h}{RT_v} - \frac{1}{2}\right)\right]^{-1} \quad (10)$$

and σ is the surface tension, m_l is the mass of a water molecule, and $\beta = 1$ is the correction factor in the presented calculations. r^* is the critical radius a stable liquid cluster.

$$r^* = \frac{2\sigma}{\rho_l RT_v \cdot \ln \varphi_{ss}} \quad (11)$$

where φ_{ss} is the supersaturation ratio:

$$\varphi_{ss} = \frac{P_v}{P_{sat}(T_v)} \quad (12)$$

Gyarmathy's droplet growth model[7] was used in the present work. This model takes into account the diffusion of vapor molecules through the surrounding vapor as well as the heat and mass transfer, and the influence of capillarity:

$$\frac{dr_d}{dt} = \frac{p_v}{\rho_l h_{lv}\sqrt{2\pi RT_v}} \frac{c_p + c_v}{2} \cdot \left(T_s(p_v) - T_v\right) \quad (13)$$

There are many forms of real gas equations of state for steam known from literature. In the present work, the real gas state equation was used in a form which described by Young[8].

$$p = \rho_v RT_v \cdot \left(1 + B\rho_v + C\rho_v^2\right) \quad (14)$$

where B and C are the second and third virial coefficients. Equations from (1) to (12) form a closed system of equations that can be solved as long as the vapor and liquid equations of state and thermodynamic properties are provided.

2.3 Numerical details

The computation is performed using the commercial computational fluid dynamic package Fluent v18.0, which is based on a finite volume approach. The details about the geometric parameters for the present simulation are

summarized in **table 1**. The model is used structured quadrilateral elements which the mesh density is approximately 300W elements and the 3D all-hexahedral element mesh is determined as follows: the mesh size in vertical direction of the equipment is set to 2mm and the mesh size of the inlet is set to 0.3mm. The maximum mesh size of 10 mm and a stretching ratio of 1.1 is used. **Fig.2** shows the computational element configuration with a magnified view of the mesh elements near the inlet and the boundary conditions. Pressure inlet and pressure outlet boundaries were selected in the present work. The calculation is carried out by the transient density-based solver. The time step size is set to 1×10^{-7}s.

Table1

geometric parameters

Parameters	Values
Cylinder diameter	210mm
Inlet width	1.9mm
Inlet length	5mm
Outlet width	37.7mm
Outlet length	10mm
Chamber length	500mm
Thickness	322mm

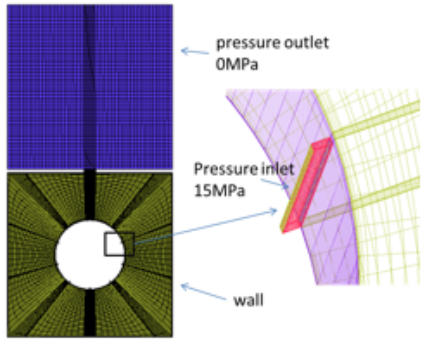


Fig.2 Computational mesh and boundary conditions

3. Results of numerical simulation and discussion

3.1 Influence of inlet vapor temperature on the performance of the catapult

In this paper, the injection pressure was set at 1.5MPa. The variation of outlet velocity distribution, outlet temperature distribution and outlet liquid mass fraction was studied at inlet vapor temperatures of 473, 523 and 573K. **Fig.3** shows the contours of liquid mass fraction profiles at different locations and times. Most liquid was generated at the outlet and spread to both sides of the outlet. **Fig.4** shows the contours of velocity that the velocity

is nearly 1000m/s along axis of the outlet but the velocity of both sides are nearly 0m/s. This might account for the liquid distribution. As can be seen from the **Fig.5(a)(b)(c)**, liquid mass fraction of the outlet decreasing with the increased inlet vapor temperature whereas temperature and velocity of the outlet increasing with the increased temperature. **Fig.5(d)** shows that inlet vapor temperature have few influence on the average pressure of the outlet,

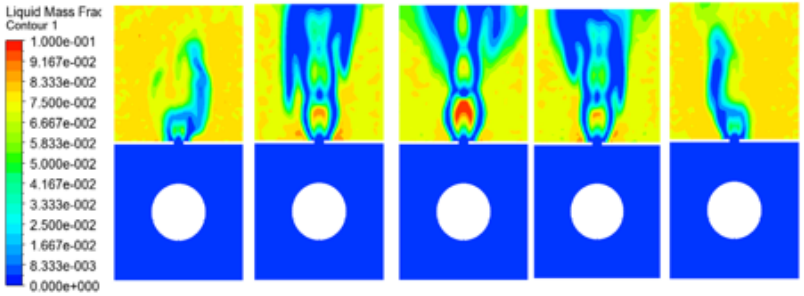


Fig.3 Contours of liquid mass fraction profiles at different locations

(The planes was cut along the z-axis at which z=-0.02, -0.08, -0.16, -0.24, -0.3.)

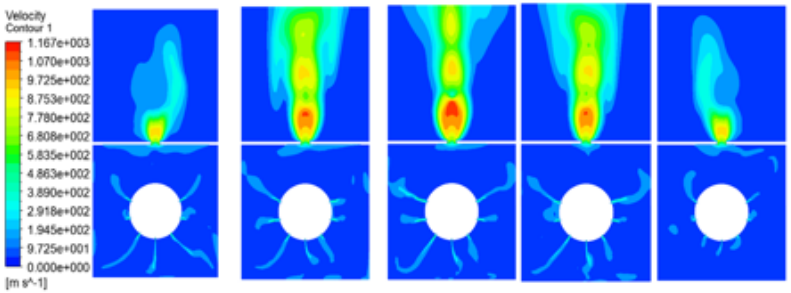
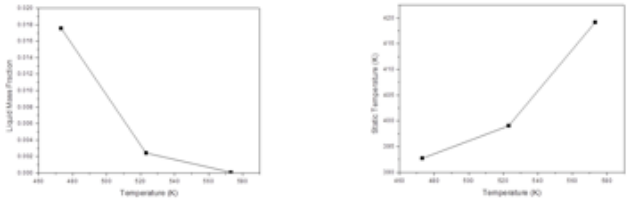
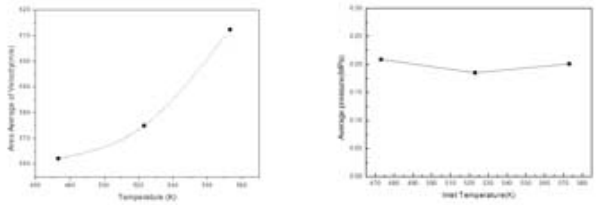


Fig.4 Contours of velocity profiles at different locations

(The planes was cut along the z-axis at which z=-0.02, -0.08, -0.16, -0.24, -0.3.)



(a) (b)



(c) (d)

Fig.5 (a) liquid mass fraction of the outlet with different inlet vapor temperature

(b) static temperature of the outlet with different inlet vapor temperature

(c) Average velocity of the outlet with different inlet vapor temperature

(d)Average pressure of the outlet with different inlet vapor temperature

3.2 Effect of inlet pressure to the performance of the catapult

The inlet vapor temperature was set at 523K. The variation of outlet velocity distribution, outlet temperature distribution and outlet liquid mass fraction was studied at injection pressure of 1.5, 2 and 3MPa. **Fig.6** shows the contours of liquid mass fraction profiles at different locations with different injection pressure. From the figure, the liquid distribution is larger as the injection pressure increasing. As can be seen in the **Fig.7(a)(b)**(c), the average velocity of the outlet decreasing with the injection pressure increasing and the liquid mass fraction and temperature of the outlet increasing with the increased injection pressure. **Fig.7(d)** shows that the average pressure of the outlet increase as inlet pressure increasing, it means airplane could get more energy by increasing the inlet pressure.

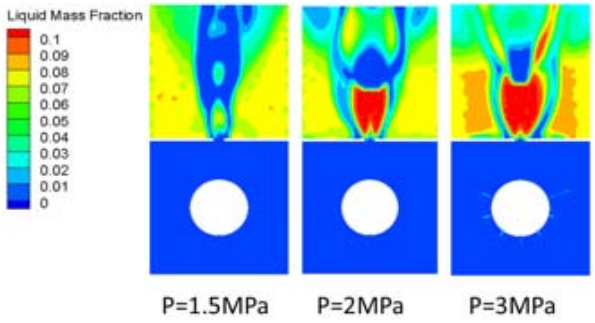
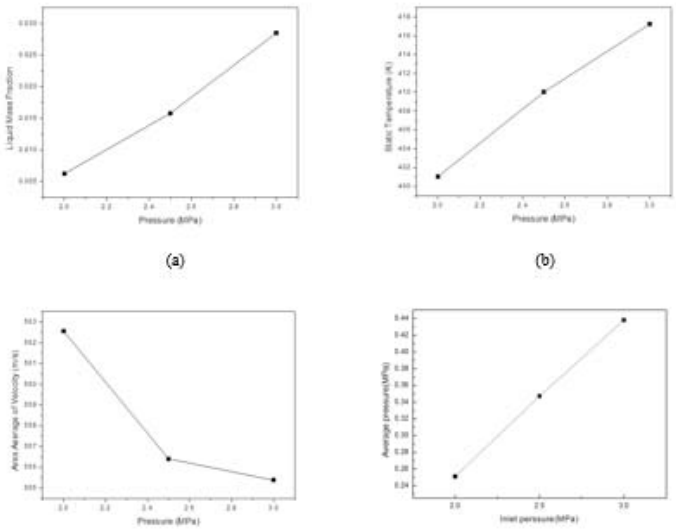


Fig.6 Contours of liquid mass fraction of the outlet with different injection pressure



(a) (b)

(b) (d)

Fig.7(a) Liquid mass fraction of the outlet with different injection pressure
(b) Static temperature of the outlet with different injection pressure
(c) Average velocity of the outlet with different injection pressure
(d) Average pressure of the outlet with different injection pressure

4. Conclusion

In this paper, we investigate the effect of the injection pressure and inlet vapor temperature on the liquid mass fraction, temperature average pressure and velocity distribution near the outlet using numerical simulations. The following conclusions were obtained:

(1) Liquid mass fraction of the outlet decrease with the increased inlet vapor temperature whereas temperature and velocity of the outlet increase with the increased temperature.

(2) The average velocity of the outlet decrease with the injection pressure increasing and the liquid mass fraction and temperature of the outlet increase with the increased injection pressure.

(3) Inlet vapor temperature have few influence on the average pressure of the outlet, however the average pressure of the outlet increase as inlet pressure increasing.

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