CFD MODEL DEVELOPMENT FOR FLUID-PARTICLE FLOWS

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ABSTRACT

This presentation will give an overview of the work in my research group at Purdue University in the development of improved CFD models for simulation of fluid-particle flows. The development and validation of numerical models for fluid-solid flow phenomena is an interdisciplinary research area of both great technological and commercial importance. Particle flow processes pervade the pharmaceutical, chemical, mining, agricultural, food processing and petroleum industries. Hence the applications for this research are very diverse, as well as are the fundamental problems that need to be addressed.

Model development for dilute and dense-phase flows, including the effects of particle size distribution and particle clustering will be discussed. Discrete element method (DEM) simulations, which can give insight into improved constitutive models for the particle-phase stress in these situations, will be presented. Finally, comparison of model predictions to experimental measurements, some performed in our laboratory using laser Doppler velocimetry, will be shown.

In order to simulate fluid-particle flow in practical systems, two-fluid models for dilute and dense-phase fluid-particle conveying have been developed. One of the most notable successes for my research group has been the adoption of our multiphase flow models by two key commercial computational fluid dynamics software companies - Fluent and AEA Technology. Such two-fluid models treat the particle phase as a continuum, rather than tracking the motion of each individual particle (Anderson and Jackson, 1967). Models which are able to treat systems that are not extremely dilute typically employ a kinetic theory treatment for describing the stress associated with particle-particle interactions (Lun et al, 1984). These models have been extremely successful in predicting the flow patterns in dilute-phase conveying and flow patterns in fluidized beds, for example. Specific successes will be shown (Bolio et al, 1995). Particle segregation, pressure drop, detailed gas and solids velocity and gas turbulence modulation can be fairly accurately predicted for certain classes of particles. In fluidized beds, bubble size, rise velocity and shape can be accurately predicted as a function of bed height and fluidization velocity. We have also developed a CFD model which describes a bimodal mixture of particles (van Wachem et al. 2001). In fluidized beds, such a model is capable of describing particle segregation by size and the phenomenon of layer inversion in fluidized beds. The model is able to capture differences in bed expansion and minimum fluidization when the flow behaviour of a bimodal particle mixture is compared to the flow behaviour of a mono-dispersed particle mixture at the same Sauter mean diameter.

These models, however, still have many restrictive assumptions such as the assumption of fairly spherical particles and the assumption of a fixed mono-dispersed or binary particle mixture that does not change with time. In addition, particle-phase turbulence or particle clustering, a flow phenomenon characteristic of dense-phase conveying, is presently treated in an ad-hoc fashion via analogy to eddies in a single-phase turbulent fluid (Hrenya and Sinclair, 1997). Finally, particle interactions in these models are assumed to be inertia-dominated and the effect of the interstitial fluid on particle collisions is neglected.

For particles larger than approximately 100 microns, an assumption which neglects the effect of the interstitial fluid is a reasonable one. However, many particulate flows occurring in the mining, chemical and process industries frequently contain particulate materials that are smaller, and the interstitial fluid does play a role in particle-particle interactions and the resulting particlephase stress. Recent experimental measurements in my research group using laser Doppler velocimetry in a dilute turbulent jet have shown where the standard kinetic theory concepts fall short in adequately describing the fluctuating motion of smaller particles in a gas where interstitial fluid effects are important. The same result holds true for particle flow in a liquid.

We have recently proposed a new continuum-based model (Hadinoto and Curtis, 2003) for fluid-particle flow applications with smaller particles that builds on concepts put forth by Lun and Savage (Lun and Savage, 1987; Lun and Savage, 2003). This new model employs kinetic theory of dense gas concepts in describing momentum and kinetic energy transfer between colliding particles and incorporates the influence of the interstitial fluid on the random motions of the particles by introducing two distinct particle coefficients of restitutions, ef and es, to characterize the inelasticity of particles colliding in a fluid and in a vacuum, respectively. These coefficients of restitution are measurable properties of particles, and we have previously conducted research which involved measurement of e_f in conditions that approached that of a vacuum (Massah et al., 1995). Other measurements of ef in viscous fluids have been conducted by Gondret et al. (2002), for example. These measurements reveal that when two particles collide in a fluid, a fraction of the particle's fluctuating kinetic energy is dissipated into thermal heat as a result of inelastic collisions and another fraction is dissipated into the fluid, as the particles must exert work on the fluid to displace the interstitial fluid between the two particle surfaces. This fraction of kinetic energy dissipated into the fluid is described in our model and is dependent on the ratio of the particle inertia to the viscous force in the fluid.

As also mentioned, flowing particulate systems often involve particle clustering. In riser flow, clusters appear as the particle concentration increases: in systems involving fine or cohesive particles, clusters are also present. Laser Doppler velocimetry measurements in pneumatic conveying show that the onset of particle clustering is associated with a transition from a Gaussian distribution of the particle velocity fluctuations to a bimodal distribution. In addition, the solids loading at the onset of clustering is highly dependent on particle size and size distribution. Large-scale, three-dimensional DEM simulations of shearing particulate flow (involving up to 300,000 particles) reveal the presence of particle clusters or banding even for slightly inelastic systems (Lasinski et al, 2003). However, the simulated system must be of sufficient size in order to manifest clustering; the more elastic and the denser the particulate system, the larger the system size that is required to observe clustering. The presence of the particle-phase microstructure is associated with an increase in the particle-phase stress. In continuum-based CFD models, this additional stress is often described as a contribution due to 'particle-phase turbulence'. DEM simulation also enables us to efficiently describe, optimize and better understand such processes as particle mixing in blenders and particle discharge from hoppers. These are areas of current and future research work and interest.

One of the next key hurdles in multiphase CFD development is the treatment of an evolving particle size distribution such as is found in particle systems involving attrition, agglomeration or reaction. Current research is aimed at coupling the general dynamic equation with multiphase flow dynamics to describe such systems (Hamilton et al, 2003). The first problem we are analysing is gas-solids flow in a conveying line where particles undergo breakage by collisions with the wall. In this model, the local variables of particle velocity and particle volume fraction affect the rate of particle attrition. Particle breakage then modifies the average size of the particles and, in turn, affects the characteristics of the multiphase flow. Such a model would find application in cyclone design, for example, where knowledge of the amount and size of fines produced from attrition is critical. Also, prediction of energy consumption from particle breakage is needed to ensure that pneumatic conveying lines continue to operate in the desired flow regime.

REFERENCES

ANDERSON, T., and JACKSON, R. (1967), "A Fluid Mechanical Description of Fluidized Beds", *I. & E. C. Fund.*, **6**, 527

BOLIO, E.J., YASUNA, J.A., SINCLAIR, J., (1995), "Dilute Turbulent Gas-Solid Flow in Risers with Particle-Particle Interactions". *AICHE J.*, **41**, 1375

GONDRET, P., LANCE, M., PETIT, L., (2002), "Bouncing Motion of Spherical Particles in Fluids", *Phys. Fluids*, **14**, 643 HADINOTO, K. and CURTIS, J., (2003), "Effect of Interstitial Fluid on Particle-Particle Interactions in Kinetic Theory Approach of Dilute Turbulent Fluid-Particle Flow Simulation", *I & EC Research*, in press.

HAMILTON, R., CURTIS, J., and RAMKRISHNA, D., (2003), "Investigation of Particle Attrition in Pneumatic Conveying via Population Balances", *Proceedings of the Topical Conference on Engineered Particle Systems: Synthesis, Processes and Applications*, 2003 Annual AIChE Meeting, San Francisco, CA, in press.

HRENYA, C., and SINCLAIR, J., (1997), "Effects of Particle-Phase Turbulence in Gas-Solid Flows", *AIChE J.*, **43**, 853

LASINSKI, M., CURTIS, J.S., and PEKNY, J., (2003), "Effect of System Size on Particle-Phase Stress and Microstructure Formation", *Phys. Fluids*, accepted.

LUN, C.K.K., SAVAGE, S.B., JEFFREY, D.J., CHEPURNIY, N., (1984), "Kinetic Theory for Granular Flow: Inelastic Particles in Couette Flow and Slightly Inelastic Particles in a General Flowfield", *J. Fluid Mech.*, **140**, 223.

LUN, C.K.K. and SAVAGE, S., (1987), "Kinetic Theory for Rapid Flow", unpublished manuscript; Department of Civil Engineering and Applied Mechanics, McGill University: Canada.

LUN, C.K.K., and SAVAGE, S., (2003), "Kinetic Theory for Inertia Flows of Dilute Turbulent Gas-Solids Mixtures", *Lecture Notes in Physics: Theory of Granular Gases*; Springer: Berlin, New York, in press.

MASSAH, H., SHAFFER, F., SHAHNAM, M., and SINCLAIR, J., (1995), "Measurements of Specular and Diffuse Particle-Wall Collision Properties", Fluidization VIII, C. Laguerie and J.F. Large, eds., Engineering Foundation, NY, 641

VAN WACHEM, B., SCHOUTEN, J., KRISHNA, R., VAN DEN BLEEK, C., and SINCLAIR, J, (2000), "CFD Modelling of Gas-Fluidized Beds with Bimodal Particle Distribution", *AIChE J.*, **47**, 1292