Third International Conference on CFD in the Minerals and Process Industries
CSIRO, Melbourne, Australia
10-12 December 2003

Future Trends for Computational Fluid Dynamics in the Process Industry

Ahmad H. HAIDARI[1] and Brent MATTHEWS[2]

[1] Fluent Inc. 10 Cavendish Court Lebanon, New Hampshire, 03766, U.S.
[2] Leap Australia, Sydney, AUSTRALIA.

ABSTRACT

This paper provides an overview of how CFD technology is currently being used in the process industry, and reviews the current technology trends and research initiatives that will make CFD an even more useful tool to process engineers in the near future. The overview is achieved by taking a brief look at six influencing factors: 1) effect of computing technology, 2) model building and mesh generation, 3) mathematical methods and numerics, 4) relevant physical models, 5) validation, and 6) post-processing and data extraction.

INTRODUCTION

Rapid progress in three influencing technologies over the past two decades has brought CFD to the forefront of process engineering. Advances in computational technology, a sustained effort by CFD providers to implement comprehensive physical models, and advances in numerical methods have combined to make it possible for engineering and R&D groups to use CFD routinely in many process industry companies. As evidence of this growth, Figure 1 shows the explosion of published scientific papers using CFD in the later part of 1990s.

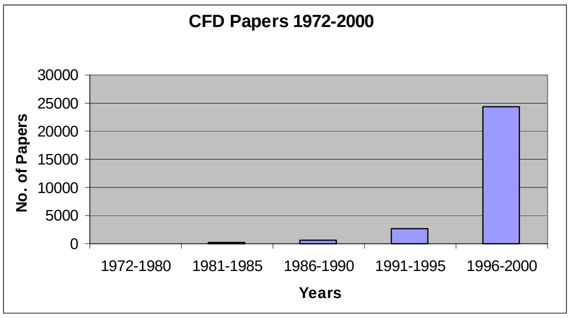


Figure 1: Number of Scientific publications using CFD between 1972 and 2000

Despite substantial gains in the use of CFD and the fact that CFD has become a discipline in its own right, it still is not fully integrated in the engineering workflow of many process engineers. Today, CFD is being used in a range of process engineering applications from analysis of process industry equipments such as: rotating kilns, particle separators, mixers, to biomedical, electronic, and food processing applications. The underlying need for CFD in the process industry is as strong as it is in all other industries. Engineers everywhere are faced with the need for better equipment performance, faster time to market, and lower design and production costs. CFD can help meet these needs by providing useful insight into the working of new and existing equipment. While CFD may have its traditional roots in the aerospace industry, the trends over the past few years have been to add more process industry enhancements, more complex physical models, better integration to other process engineering tools, and customized interfaces for process engineering applications. These trends suggest that CFD will continue to have more to offer to, and a broader base of acceptance by process engineers. In this paper, a perspective is given on how key developments and influencing factors will enhance the value of CFD in the process industry in the years to come.

EFFECT OF COMPUTING TECHNOLOGY

One of the main reasons for the growth of CFD is the dramatic reduction in-turn-around time required for most CFD simulations. In recent years, there have been tremendous improvements in computer technology, and microprocessor speed is expected to continue to follow Moor's law for the foreseeable future. Interestingly, computer technology is not the only reason for gains in computational speed in CFD over the past few years. Compared with 1996 for example, it is possible to run the same sample problem over 100 times faster. Gains in processor speed account for speed up of a factor of 30 (double every 18 months). The remaining gains are due to enhancements in numerical methods and faster solver algorithms. This is without taking into account what parallel processing can offer. Considering that it is now possible to run large calculations on a network of Linux and PC cluster, something that previously was not available, it becomes clear that the trends are toward faster time to solution for many typical CFD problems.

Broad accessibility of large or massively parallel computers to many CFD users and improvements in parallel computing algorithms, such as dynamics load balancing, day/night resource sharing, remote computing, and recovery from computer and network crashes will further enhance CFD computing time. As a result, the trend is to continue solving large problems (increased mesh size, refined geometry), using refined physics (in the form of turbulence models, increased turbulence chemistry interaction, multiphase) and new multi-physics applications (such as fluid structure interaction, detailed particle motion such as DEM models, or new applications such as aerodynamic induced acoustics.)

Generally, parallel efficiency and scaling are problem dependent, however, for appropriate gains in what parallel processing can offer attention must be given to the benefits of parallel processing during the initial stages of code development. Figure 2 illustrates the potential speed gains for a sample problem using a large number of compute nodes. The figure illustrates how well the calculations scale compared with theoretical limits. Up to forty-eight CPU nodes were evaluated in this example.

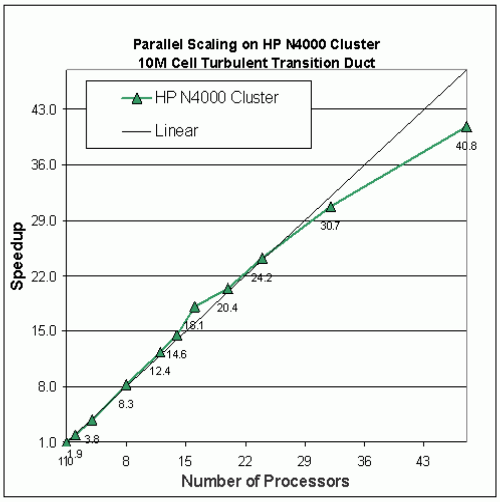


Figure 2: Parallel efficiency and scaling on a calculation speed up for a cluster of CPUs**.**

MODEL BUILDING/MESH GENERATION

Process industry applications of CFD often require that the flow be resolved both in a complex geometry and with complex physics. With increased CFD capabilities, there is a continuous demand for more reliable and accurate simulations. This demand drives the need for better geometry resolution, more mesh flexibility, and improved model building tools within the same environment. Figure 3 is an example of an Eulerian multiphase calculation in a static mixer, a simulation that needs both complex geometry and advanced physical models.

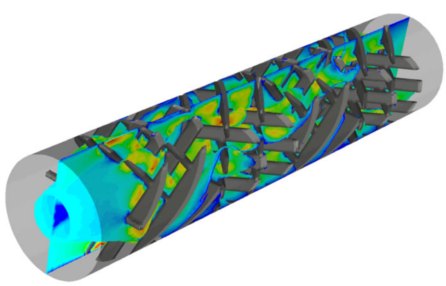


Figure 3: Contours of velocity magnitude in a multiphase calculation of kerosene mixing in oil in a SMX static mixer.

Today many CFD practitioners want control over their mesh generation and do not just pass the task of geometry and mesh generation to their in-house CAD experts. Many CFD users also believe the meshes needed for CFD calculations are of different quality than the meshes generated by some CAD packages for structural analysis. Furthermore, in certain CFD applications where the underlying geometry is needed to perform a fluid structure interaction calculation, or perform a geometry base optimization the CFD solvers need direct access to the CAD and mesh files. This means that model building software should include geometry generation, and the ability to handle mesh flexibility, mesh motion, mesh adaption, and geometry-based mesh refinement while maintaining mesh quality.

One example of such coupling between the geometry and flow field, i.e. the need for geometry information in the CFD calculation, is illustrated in the blow molding animation of which a snapshot is presented in Figure 4. In this example, the parison is first extruded as a tube and is then “pinched-off”. The next step in the process is for the mold to close and air be blown into the mold to inflate the parison until it makes contact with the mold walls. The last step is for the mold to open. To optimize the mold design and the flow of material in the mold, the designer needs to make geometry changes and control the flow of material throughout the mold.

Figure 4: A snapshot of a 3d simulation of blow molding example to make a plastic milk bottle.

MATHEMATICAL METHODS/NUMERICS

The standard PDE methods based on the Navier-Stokes will continue to dominate, however, there are other mathematical models that may be used for certain applications in the process industry. Some of these are the Euler-Lagrange, Lattice Boltzmann, Direct Simulation Monte Carlo (DSMC), PDF transport, discrete element model (DEM), and vortex methods. These methods have the potential to be used in certain gas-dynamic, multiphase flows, particle-laden flows, and/or combustion and reaction. These methods open further capabilities to solve very large problems in the coming years. For example the DEM methods will be able to provide information about individual particles accounting for particle shape, particle kinematics, and particle-particle interaction. Figure 5 is a still picture of an animation sequence from work done using DEM by researchers at CSIRO in Australia (Cleary & Sawley 1999). This animation shows the effect of particle size and the segregation of individual particles as the result of a vertical oscillation of the supporting screen. In the animation posted on CSIRO's web site it is possible to see that finer particles fall through the screen as the screen moves upward.

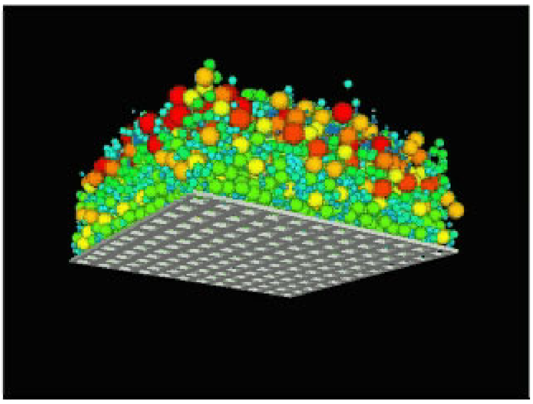


Figure 5: A snapshot of a 3d simulation of a vibrating screen with different particle size (colored by diameter). (Cleary & Sawley 1999).

In Navier-Stokes solver development, the future trends are toward "smart solvers" which means the necessary numeric will be added to for example, account for mesh sensitivity and automatic error reduction, and estimation of uncertainty in the results.

In the area of solution sensitivity, and optimization the area of research appears to be on sensitivity of results to boundary conditions, influence of mesh and mesh adaption strategies, as well as geometric and parameter optimization. An example of design optimization is shown in Figure 6, for extrusion of rubber in a die design problem. With an uneven flow of material (Figure 6a), the resulting extruded piece is highly deformed. The material deformation is caused by the shear resulting from velocity differences between layers of the extruded rubber as it leaves the die. From the perspective of the die designer, it is desired to have the CFD tool be able to automatically optimize the geometry so that the flow is uniformed and the material can be extruded to the desired shape. In most extrusion processes the final shape depends on more than just the flow. Other factors include: the material property,

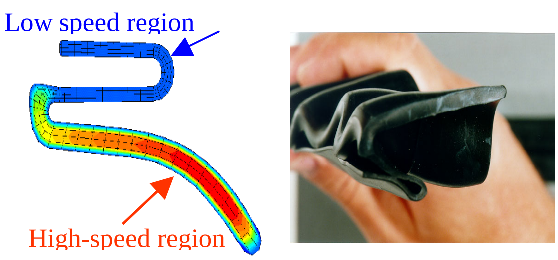
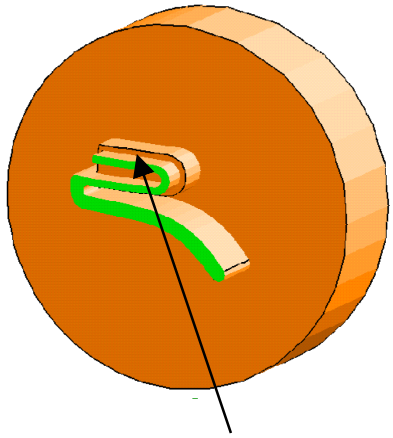


Figure 6a: Initial non-uniform flow distribution through a die result in a highly deformed extruded piece.

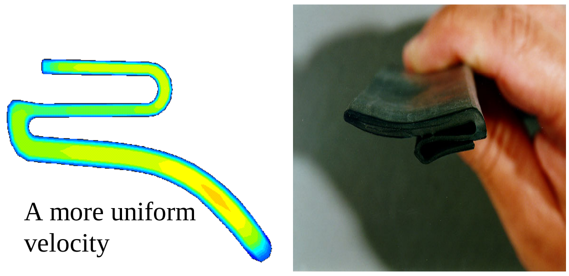
the extruder pressure, the complexity of the extrusion profile, and possible thermal effects.

Despite these complexities, it is possible to "balance" the flow using an iterative method in which the geometry and the mesh are adjusted semi automatically. In this example, as is shown in Figure 6b it is possible to widen the upper lip of the die until a uniform flow is achieved throughout the die cross section. For this example, the resulting optimized flow, and therefore the desired extrusion shape is then achieved (Figure 6c). (This work is courtesy of *Hutchinson s.a.)*



The feeding section is opened in order to bring more rubber where the speed is too low.

Figure 6b: Proposed geometry changes to the die.



Courtesy of Hutchinson s.a.

Figure 6c: Optimized geometry yield a uniform flow distribution resulting in successfully extruded product

A very important area of numerics that has historically been given sporadic attention is the solution of population balance equations within CFD to track a range of droplet, bubble, or particle sizes. Initial efforts have focused on sectional methods for gas-liquid systems, but work has also been done using the method of moments for applications such as crystallization, and aerosols flows using fine particle models (FPM). These methods have their own advantages and areas of applicability; however, there has not been a systematic approach in applying population balance to a large class of process industry applications so that size distribution can be accounted for (some industrial examples include: bubble column flows, crystallizers, decanters, and liquid separators). The attractive feature of the population balance is in its ability to deal with dispersed phase growth and decay, a feature that make this methodology very useful to process industry applications.

The population equation can be written equation (1):

$$\frac{\partial n(v;\mathbf{x},t)}{\partial t}+\langle u_i\rangle\frac{\partial n(v;\mathbf{x},t)}{\partial x_i}-\frac{\partial}{\partial x_i}\left[\Gamma_t\frac{\partial n(v;\mathbf{x},t)}{\partial x_i}\right]=$$

$$-\frac{\partial}{\partial L}\left[G(v).n(v;\mathbf{x},t)\right]+B(v;\mathbf{x},t)-D(v;\mathbf{x},t) \qquad (1)$$

Where n(v; **x**, t) is the number density function expressed with “v” as the internal co-ordinate that could represent particle volume, particle size, or any other suitable variable. **x** is the position vector, and t, the time. The terms on the right hand side represent growth, birth and death functions in that order. There are various ways to represent the birth and death expressions, but they are inherently a collection of break up and coalescence terms. The rate of breakage and aggregation depends on the type of dispersed phase, and varies for example from gas-liquid systems to liquid-liquid systems. Because of space limitations the expressions for coalescence and break up are not presented here.

The population balance equations can be solved using different techniques. A common method is the sectional method, which divides the dispersed phase into a pre-selected set of particle sizes or bins (or diameter classes). Figure 7 illustrates the gas-bubble distribution in a mixing tank using coalescence and break up kernels developed by Luo, and Svendsen (1996), and Luo (1993).

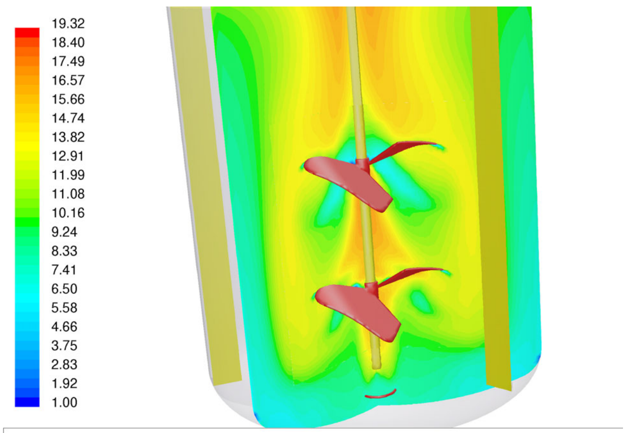


Figure 7: Contours of bubble size distribution (bubble diameter) in a gas-sparged stirred tank.

Another technique of solving population balance equations makes use of the Quadrature Method of Moments (QMOM) is used by Rodney Fox and his colleagues at Iowa State University (AICHE to be published) for particle size distribution in crystallization and polymerisation problems. This method is a variation on method of moments and tracks subsets of particle sizes by solving the transport equation of the particle size distribution. The method has the advantage of not having to track large class of sizes, so has the potential to be more computationally efficient for certain type of flow problems.

PHYSICAL MODELS

Fluid mechanics applications in the process industry cover almost all aspects of thermo-fluid sciences. There are many applications that require understanding of single phase flow parameters, for example, the flow maldistribution, pressure drop, or the extent of flow mixing and separation. However, there always will be a demand for complex physical models to deal with the diverse flow modeling needs within the process industry. The high end modeling requirements to solve complex problems in the process industry goes beyond multiphase and reacting flows. Independent of the original development purpose of a given physical model in CFD, it appears that there is always a problem in the process industry that can benefit from it. Large Eddy Simulation (LES) and aerodynamic generated noise are two examples. CFD engineers in the process industry use these models for calculations in mixing tank and fan noise prediction respectively. Three major physical model developments are reviewed in this section.

Turbulence modelling

Over the past few years, turbulence modeling has become very sophisticated in CFD software. In RANS calculations there is a focus on the improved capturing of near wall physics. There is also an increased use of LES and hybrid methods like the Detached Eddy Simulation (DES) model, which allows the flow near the wall to be solved using an average method, while the reminder of the solution domain is solved using a transient eddy simulation method. The advantage of DES is that it saves the expense of solving LES throughout the entire solution domain.

LES models are playing an integral role in other calculations and are bases in which one can develop new capabilities in CFD, for example modelling acoustics. In this case engineers are able to account for equipment noise and perform calculation of acoustics within the CFD package. In Figure 8 the far field noise calculated using the Ffowcs Williams-Hawkings approach for an object is shown. The results of the computation include the sound pressure level, power spectral density at observer’s location and surface source strength.

Modeling combustion and reaction

With increased computational efficiency there is a natural tendency to include more of the desired physics. One example is the effect of including more chemistry and turbulence-chemistry interaction in combustion and reacting flow calculations. Emphasis is often on unsteady, turbulent, reacting problems both for gaseous combustion and multiphase reaction systems. Solving these types of problems requires efficient solvers, an understanding of the kinetics, and the possible need for reaction reduction algorithms. These algorithms also need to handle stiff and laminar chemistry, micro-mixing, and competing reactions. An increased need for modelling catalytic reactions, surface reactions, and pollutant formation further increases the utility of stiff chemistry solvers, and the need to develop techniques that help increase the efficiency of the computations.

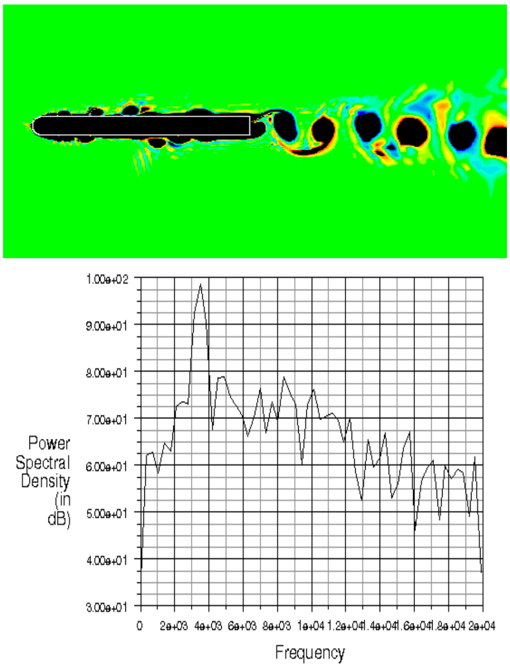


Figure 8: Contours of vorticity Magnitude (top), and power spectral density (bottom) caused by aerodynamically generated noise passed a bluff body

Models to solve finite rate chemistry will be used more often. One such model using particle methods is composition PDF transport model. The method is used to incorporate finite rate chemistry in turbulent flames, and accounts for complex chemistry with arbitrary chemical mechanisms. Monte-Carlo method is used to solve the PDF equation, and the mean reaction rate is calculated from expression (2):

$$\overline{\dot{w}_k} = \int_0^\infty \int_0^1 \cdots \int_0^1 \dot{w}_k \; P \; dY_N \cdots dY_1 \; dT \qquad (2)$$

The stiff reaction rate is integrated many times. While it is possible to create a table that stores the rates, compiling such a table for a typical reaction problem is impractical. The alternative is to create a table made of only local values. There is also a need to accelerate the chemistry calculations. ISAT (In-Situ Adaptive Tabulation), perfected by Steve Pope (1996) can achieve both of these tasks. The table is created during the simulation, and allows the rates to be tabulated locally. Initial iterations are typically slow as the table is built, but at convergence, iterations are rapid as mappings are retrieved from the table. Validated against Sandia Flame D experiments (Skeletal CHE4 (41 reaction, 16 species)), the method does a reasonable job of picking up the mean flame temperature and the mass fraction of the species. Figure 9 shows PDF particle traces colored by particle temperature for a methane flame solved using this technique.

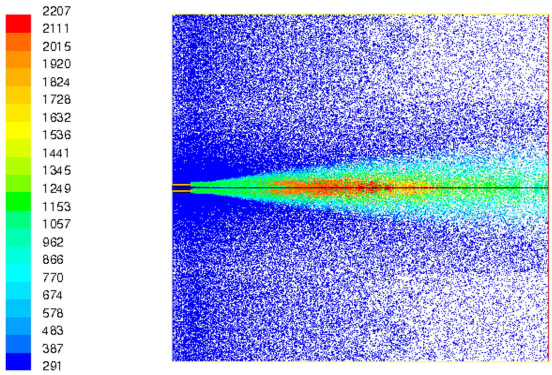


Figure 9: Piloted jet flame combustion example using PDF transport method (particles colored by temperature)

Multiphase flows

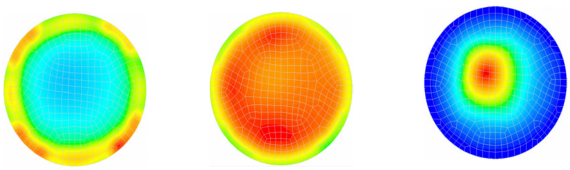
The discrete phase model (DPM) historically has been the workhorse for solving many multiphase flow calculations where the second phase is dispersed and consists of particles, droplets, or bubbles. This method, which is an Eulerian-Lagrangian approach when applicable gives the analyst a lot of control over the description and fate of individual particles. It is therefore possible to account for a wide range of physics for the second phase, such as size distribution, body forces, evaporation, agglomeration, and break-up using DPM. Recent trends in DPM modeling include performing the particle track calculations in parallel, using a large number of particles, and accounting for time dependent particle injection. These developments have enabled simulations of problems such as spray atomization.

Other notable advances in multiphase flows models are developments in the volume of fluid (VOF) technique used to model free surface flows. The trend has been to develop VOF models with the capability to solve for a thin (a sharp) interface. The VOF model has a broad range of applicability from ship hydrodynamics to ink jets, from tank sloshing to water treatment applications.

For interpenetrating fluids, there has been a steady development of two equation models, which solves a separate set of fluid equations for each phase. In these flows, interfacial drag plays a critical role in the accuracy of the calculations. Information about the flow regime and the appropriate choice of drag coefficient is needed prior to the start of the CFD calculation. Another common consideration is the influence of size distribution in some multiphase flows. Although the formulations are available for n-number of interpenetrating phases, it may become necessary to neglect size distribution and perform the calculations for a single size. This simplification is need to make the simulation more computationally tractable.

Another approach simplifies the numerics to help reduce the solution time. This approach called the mixture model (formulated by Manninen, M. 1996), solves a single set of fluid equations and a separate equation for the slip velocity between the phases. It is applicable to problems with small dispersed phase relaxation times. The trend for solving interpenetrating fluids, however, is to solve Eulerian model for gas-liquid and liquid-liquid flows, and Eulerian granular for gas-solid, and liquid-solid flows. Work is also progressing on models for three phase systems, such as slurry bubble columns, hydrogenation processes, and some fluidized bed reactors where liquid, solid, and gas phases are present.

The historical use of CFD in gas-liquid flows has been in nuclear industry, but more applications such as gas sparged in mixing tanks, gas-lift reactors, and bubble columns are being simulated with CFD. The trends for gas-liquid applications are to include bubble size distribution and interfacial mass and heat transfer. The trends also has been to account for the effect of bubble coalescence and break-up in gas-liquid systems. Figure 10 illustrates contours of time averaged gas hold up in a bubble column for different bubble diameters. The calculations were performed with nine different bubble classes using Eulerian multiphase model in conjunction with population balance equation. (Dudukovic and Peng, 2003).



1.6 mm　　6.3 mm　　32 mm

Figure 10: Contour plots of time averaged gas hold-up in a bubble column for three different bubble sizes. The results are plotted at the same axial location.

The trend for particle laden multiphase flow has been to account for more of the physics involved in particle dynamics. The development focus has been to include effect of "solids pressure" in the solids phase momentum equation, and to use the "granular temperature" concept to calculate the solid viscosity. Current applications of these models include simulations of: fluidization, riser flows, solid suspension, particle transport, sedimentation, and separation. Figure 11 is a snapshot from an animation sequence of an Eulerian-granular calculation showing contours of the volume fraction of solids in a fluidized bed containing transverse tube bundles (but solved using an isothermal assumption). The animation shows the initial lifting of the bed and subsequent formation of bubbles, and the motion of solids in the bed.

The range of industrial applications of multiphase flows involving solids requires continuous improvement to both the numerics and the physics offered in CFD. Other development areas include the effects of: turbulence, particles collision, particle shape, and cohesion forces.

The Eulerian-granular model assumes that the solids are a continuous phase in the presence of another fluid (a liquid or a gas). Thus information about individual particles, such as attrition, rotation and particle-particle interaction cannot be directly accounted for. The Discrete Element Method (DEM) appears to provide additional capabilities for solid handling applications. The method keeps track of each particle so its fates, along with deformation, contact with other particles or objects, and displacement can be followed. DEM calculations currently may not be applicable to problems with large number of particles, or systems with large particle size or particle shape variation. The next step of development in this area is to combine DEM and Eulerian models or use DEM to develop particle related models that can be used in Eulerian calculations.

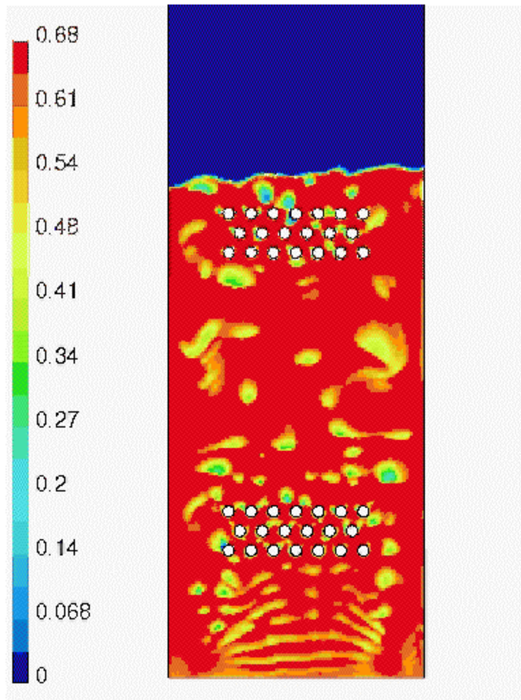
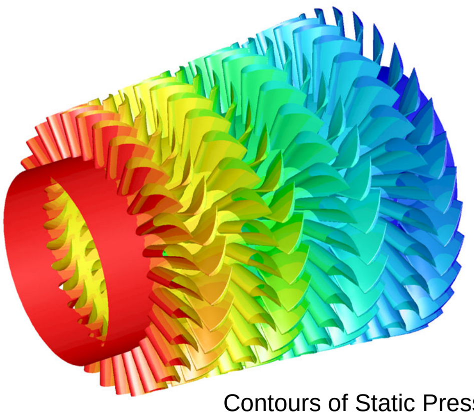


Figure 11: Contour of volume fraction of solids in an Eulerian-granular calculation.

VALIDATION

As for other engineering tools, CFD has a range of applicability. The numerics, the models used, and the user's error tolerance influence the accuracy of CFD results. CFD practitioners in the process industry continuously benchmark their calculations, especially when they want to use a physical model or a combination of physical models and numerics (e.g. sliding mesh and multiphase) for the first time. As the use of CFD in the process industry moves from research and development and specialized engineering to be one of the process engineer's every day tools, out-of-the-box reliability is needed. This requires rigorous testing and quality control during the development phase. The validation is generally performed in various stages of code development and model implementation. The CFD results for benchmark problems are routinely checked against known analytical results, and experimental data. Use of industrial scale application testing is a final check to ensure the interoperability of the various functionalities, and the overall quality of the CFD code.

Figure 12 illustrates a sample industrial application test case used to validate some of the rotating capabilities of a CFD code. Industrial scale tests such as this must be used to help access the capability and the range of applicability of certain models. The intended benefit is to work toward reducing the cost of code validation and Q& A by the CFD end users.



Contours of Static Pressure

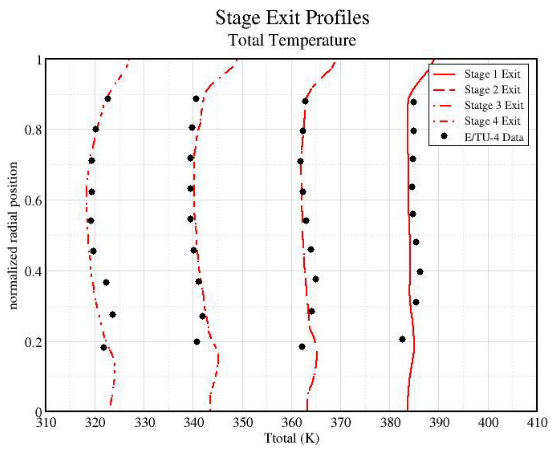


Figure 12: Validation results of profiles of the total pressure at exit stages of 4 stage turbine.

POST PROCESSING AND DATA EXTRACTION

The visualization of results provided by CFD has long been considered one of the leading benefits of this technology. Full 3-dimensional post-processing with the ability to monitor flow variables at any point in the domain, create animation, and follow particle trajectories, are only some of the useful tools that are available. Figure 13 illustrates the flow and thermal results for a tube and shell heat exchangers. In this simulation all geometric details including nearly 100 tubes were modeled. The trends are to create more innovative post-processing that yield information more relevant to design goals and can help with design optimization. Other areas of interest are in data mining, feature detection and data extraction, especially for time dependent calculations and large complex models with large amounts of data. Other trends toward more effective post-processing are effective data management, real time post processing, virtual reality, impressive 3D feature highlights and graphics, and investigative tools (e.g. auto, and cross-correlations using FFT).

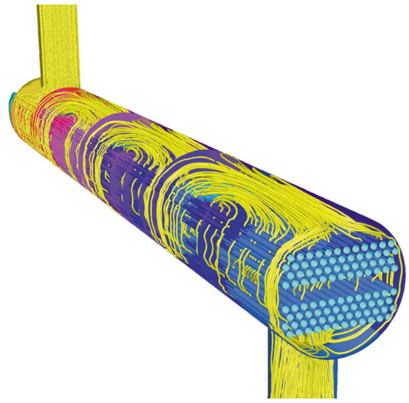


Figure 13: Fluid pathlines (yellow) and temperature contours on the tube and baffles of a shell and tube heat exchanger (Courtesy of Heat Transfer Research, Inc.)

CONCLUSIONS

During the past two decades, CFD has steadily moved from its traditional roots in the aerospace industry to be a valuable analysis tool for engineers in many disciplines. The combination of influencing factors, including computational speed, ease of use through automated mesh and model creation and availability of appropriate physical models has and will continue to bring CFD to the forefront of engineering in the process industry. The next level of development and capabilities will make it possible for process engineers to use CFD on a routine basis and with a higher degree of confidence when they need to understand problems involving fluid mechanics.

ACKNOWLEDGEMENTS

The authors wish to acknowledge the efforts of doctors D. Choudhury and S. Subbiah at Fluent Inc. Their work in presenting their vision on the future technology direction on CFD forms the bases of this presentation. A sincere thanks also goes to the engineers at Fluent Inc. who have directly or indirectly helped with preparation of the material used in this manuscript.

REFERENCES

CLEARY, P.W. and SAWLEY, M.L., (1999), "Three dimensional modeling of industrial granular flows", *Proc. 2nd International Conference on CFD in the Minerals and Processing Industries*, Melbourne, Australia 95-100 (1999)

DUDUKOVIC, M.P. and PENG, Y. (2003) "bubble column flows experiments and modeling", CFD *in Chemical Reaction Engineering III Davos Switzerland*, Oral presentation

LUO, H. and SVENDSEN, H. F. (1996). "Theoretical Model for Drop and Bubble Breakup in Turbulent Dispersions". *AIChE J.*, **42**, 1225-1233.

LUO, H. (1993). “Coalescence, Breakup and Liquid Circulation in Bubble Column Reactors.” D.Sc. Thesis, Norwegian Institute of Technology.

MARCHISIO, D.L. PIKTURNA, J.T., FOX, R.O., VIGIL, R.D. and BARESI, A.A. , “Quadrature method of moments for population*balances with nucleation, growth and aggregation”, AIChE Journal (to appear).*

MANNINEN, M. TAIVASSALO, V., AND KALLIO, S. “On the mixture model for multiphase flow.” *VTT Publications 288, Technical Research Centre of Finland*, 1996.

POPE, S.B. (1996) " Reducing the tabulation dimension in the in situ adaptive tabulation (ISAT) method," *Cornell University Report FDA 96-04*.

ANIMATIONS

Animation file for Figure 4. Blow Molding of a plastic milk bottle. Simulations were performed by Polyflow.
Animation file name: CFD03-114Hai-BlowModling.avi

Animation File for Figure 11. Contour of volume fraction of solids in an Euler-granular calculation.
Animation file name: CFD03-114Hai-3d-fluidized-bed.avi