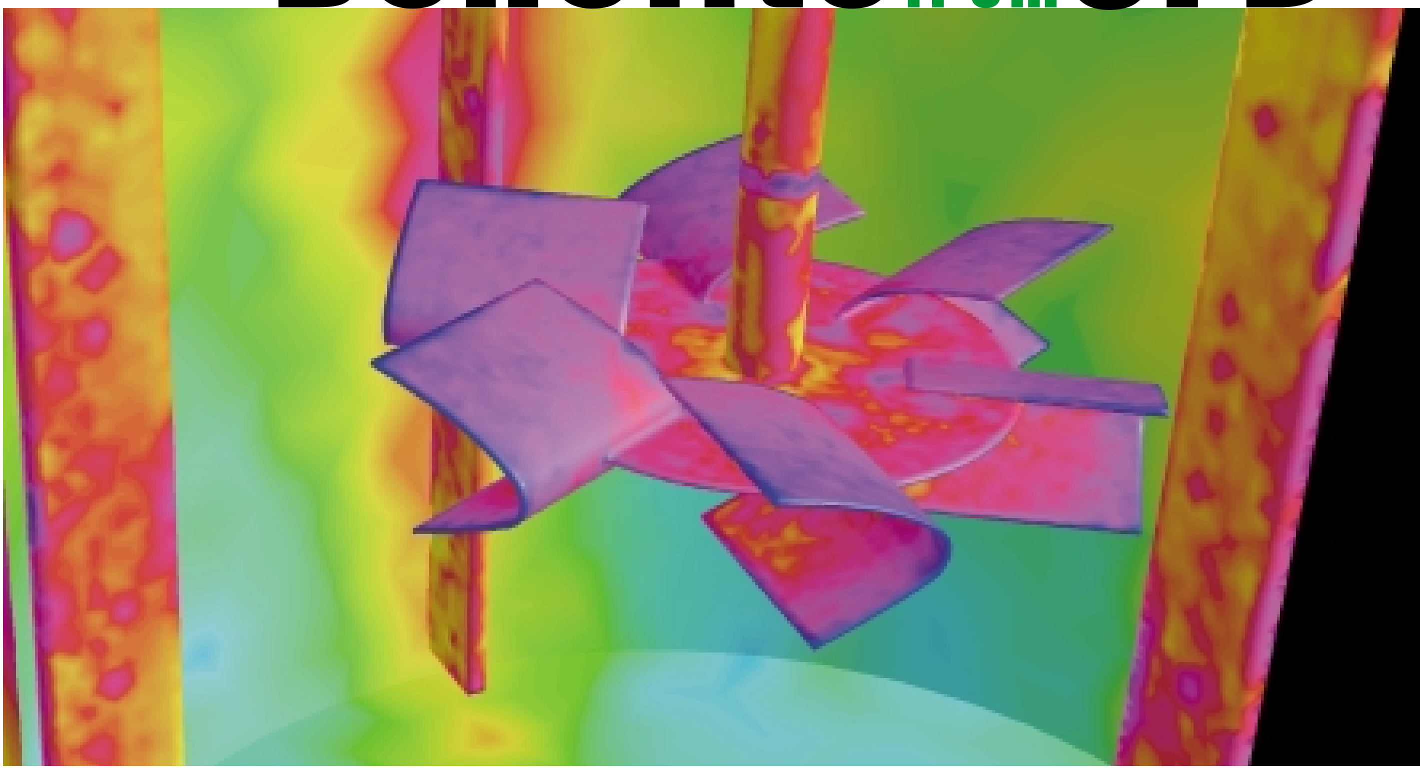
Realize Greater Benefits from CFD



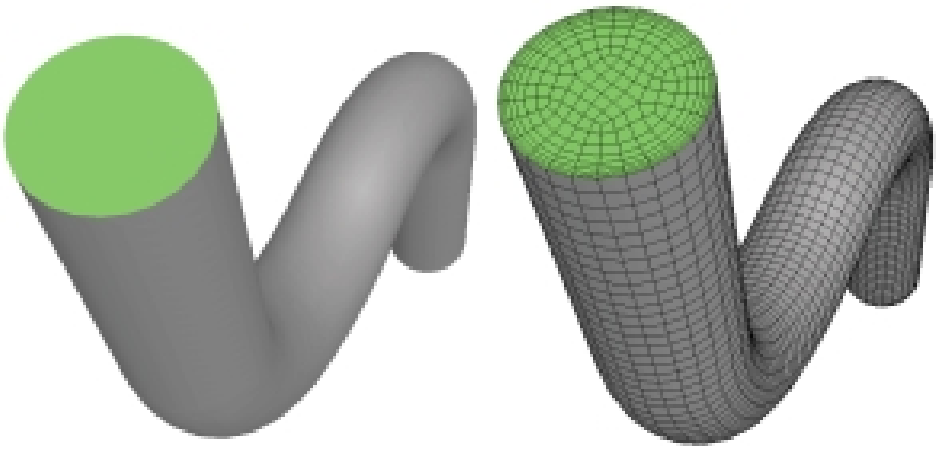
André Bakker and Ahmad H. Haidari,
Fluent Inc.
Lanre M. Oshinowo,
Hatch

Computational fluid dynamics has moved from mainframes to PCs and laptops. Newer and better software lets you conduct analyses not possible before. Regular engineers, not just experts, can now carry out CFD.

The design, scale-up, and running of unit operations in the chemical process industries (CPI) rely heavily upon empiricism and correlations of overall parameters for nonideal or nonequilibrium conditions. Many equipment designs in use are based on the experience of experts applying rules of thumb, resembling art more than science. Processes that are sensitive to local phenomena and reactant concentrations are often difficult to design or scale up, because the design correlations do not take local effects into account. Nonidealities introduced by scaling up of lab or pilot-scale equipment are difficult, if not impossible, to predict empirically.

Researchers, equipment designers, and process engineers are increasingly using computational fluid dynamics (CFD) to analyze the flow and performance of process equipment, such as chemical reactors, stirred tanks, fluidized beds, cyclones, combustion systems, spray dryers, pipeline arrays, heat exchangers, and other equipment. CFD allows for an in-depth analysis of the fluid mechanics and local effects in these types of equipment. In many cases, this results in improved performance, better reliability, more confident scale-up, improved product consistency, and higher plant productivity.

The first CFD programs were developed in the 1960s, but were severely limited because of the restrictions of computers in those days. It was not until the early 1980s that commercial codes became available. The aerospace, automotive, and nuclear industries were early adopters, since the complicated physics behind many unit operations, including multi-



■ Figure 1. A section of pipe is represented as computational cells.

phase flows and chemical reactions, limited the application of CFD in the CPI. The continual and exponential increase in computer power, improved physical models in many CFD codes, and better user interfaces now enables nonexperts to use CFD as a design tool on a day-to-day basis. As a consequence, CFD has progressed from the domain of the mainframe to the high-end engineering workstation, and even to laptop PCs.

In this article we will first discuss the technology behind CFD, and then illustrate today's possibilities with a number of practical design applications. We'll conclude with a discussion of expected future developments.

What is CFD?

CFD is the science of predicting fluid flow, heat transfer, mass transfer, chemical reactions, and related phenomena by solving the mathematical equations that govern these processes using a numerical algorithm (that is, on a computer). The results of CFD analyses are relevant engineering data used in conceptual studies of new designs, detailed product development, troubleshooting, and redesign.

To apply CFD, the geometry of interest is first divided, or discretized, into a number of computational cells. Discretization is the method of approximating the differential equations by a system of algebraic equations for the variables at some set of discrete locations in space and time. The discrete locations are referred to as the grid or the mesh.

Figure 1 shows the continuous physical domain of the pipe on the left. The pipe is spatially discretized into a number of computational cells, shown by the grid on the right.

The continuous information from the exact solution of the Navier-Stokes partial differential equations is now replaced with discrete values. The number of cells can vary from a few thousand for a simple problem to millions for very large and complicated ones.

Codes and cells

Cells can have a variety of shapes. Triangular and quadrilateral cells are generally used for two-dimensional (2-D) problems, in which the flow depends only on two spatial coordinates: for example, an axisymmetric stirred tank without baffles. For 3-D problems, where the flow depends on all three spatial coordinates (as in a stirred tank with baffles), hexahedral, tetrahedral, pyramidal, and prismatic shaped cells can be used.

In the past, CFD codes required the use of structured grids containing one cell type, such as brick-shaped hexahedral elements, in which the cells were positioned in a regular pattern. Current codes allow cells to be located in an irregular, unstructured pattern, giving much greater geometric flexibility. Additionally, good CFD codes can accept grids consisting of a combination of different cell types, or hybrid grids, to address complex geometries, providing flexibility to the CFD analyst. Geometries are often created using computer aided design (CAD) software. The geometry, either a wireframe or solid model, is exported to the grid-generation software program to create the CFD-quality grid. A few packages have combined both functions of CAD geometry creation and mesh generation into a single interface. This phase of the CFD analysis is referred to as preprocessing.

Boundary conditions

Once the grid has been created, boundary conditions need to be applied. Pressures, velocities, mass flows, and scalars such as temperature may be specified at inlets; temperature, wall shear rates, or heat fluxes may be set at walls; and pressure or flow-rate splits may be fixed at outlets. The component material transport properties, such as density, viscosity, and heat capacity, need to be prescribed as constant or selected from a database. These can be functions of temperature, pressure, or any other variable of state. Fluids can be modeled as either incompressible or compressible. The viscosity of the fluid can be either Newtonian, or non-Newtonian, using the power law, Herschel-Bulkley, Carreau, or viscoelastic models. In mass- or heat-transfer applications, binary diffusivities and thermal properties need to be defined as well.

With the grid created, the boundary conditions and physical properties defined, the calculations can start. The code will solve the appropriate conservation equations for all grid cells using an iterative procedure. Typical CPI process problems involve solving for:

• Mass conservation (using a continuity equation);

• Momentum (using the Navier-Stokes equations);
• Enthalpy;
• Turbulent kinetic energy;
• Turbulent energy dissipation rate;
• Chemical species concentrations;
• Local reaction rates; and
• Local volume fractions for multiphase problems.

Current codes allow cells to be located in an irregular, unstructured pattern, giving much greater geometric flexibility.

Turbulence modeling

Special attention needs to be paid to accurate modeling of turbulence. The presence of turbulent fluctuations, which are functions of time and position, contribute a mean momentum flux or Reynolds stress for which analytical solutions are nonexistent. These Reynolds stresses govern the transport of momentum due to turbulence and are described by additional terms in the Reynolds-averaged Navier-Stokes equations. The purpose of a turbulence model is to provide numerical values for the Reynolds stresses at each point in the flow. The objective is to represent the Reynolds stresses as realistically as possible, while maintaining a low level of complexity.

The turbulence model chosen should be best suited to the particular flow problem. A wide range of models is available, and understanding the limitations and advantages of the selected one is required if the best answer is to be obtained with the minimum computation. The type of model that is chosen must be done so with care. Some of the most widely used ones are listed in Table 1. It is understood that these models are not used when modeling laminar flows.

For chemically reacting systems, special reacting flow models need to be employed. Chemical reactants may seem well mixed on the scale of the grid cells, but may not yet be so on the molecular level. As a result, reactions may proceed slower than at kinetic rates. Much progress has been made in this area of micromixing and models are available.

The final result of the flow, turbulence, reaction, heat transfer, and multiphase calculations will be a detailed map of the local liquid velocities, temperatures, chemical reactant concentrations, reaction rates, and volume fractions of the various phases. These outcomes can be analyzed in detail using graphical visualization, calculation of overall parameters and integral volume or surface averages, and comparison with experimental or plant data. This analysis phase is referred to as postprocessing.

Because of improvements in computer power and enhanced graphics software, it is now much easier for CFD analysts to create animations of their data. These often help in understanding complex flow phenomena that are sometimes difficult to see from static plots. Examples of the flow in various types of CPI process equipment are available on the Web *(1, 2)*.

What do I need?

Many commercial, and even some freeware or shareware CFD codes, are available, each with different capa-

Table 1. Overview of Turbulance Models

Turbulence Models	Description, Advantages, and Disadvantages
k-ε (standard)	The most widely used model. Its main advantages are short computation time, stable calculations, and reasonable results for many flows. Not recommended for highly swirling flows, round jets, and in areas with strong flow separation.
k-ε RNG	A modified version of the k-ε model, with improved results for swirling flows and flow separation. Not suited for round jets. Not as stable as the standard k-ε model.
k-ε Realizable	Another modified version of the k-ε model. Solves the flow in round jets correctly, and provides much improved results for swirling flows and flows involving separation when compared to the standard k-ε model. More stable than the k-ε RNG model.
RSM	The full Reynolds stress model provides good predictions for all types of flows, including swirl, separation, and round and planar jets. Longer calculation times than the k-ε models.
LES	Large eddy simulation (LES) provides excellent results for all flow systems. LES solves the Navier-Stokes equations for large-scale motions of the flow and models only the small-scale motions. The main disadvantage is that the required computational resources are considerably larger (often 10 to 100 times) than with the RSM and k-ε style models, mainly because all calculations are conducted in a time-dependent fashion, since steady-state flow is not assumed, and a finer grid is needed to allow for accurate modeling of the turbulence at the subgrid small-scale level.

bilities, special physical models, numerical methods, geometric flexibility, and user interfaces. Specialized pre- and postprocessing programs are also offered. Excellent overviews can be found on the Web *(3, 4, 5)*. The increased use of CFD in the CPI has led to the formation of a dedicated CPI CFD user group *(6)* that is another excellent resource.

In the past, CFD was the realm of high-powered computer systems. But, much of today's modeling work can be accomplished on low-end Unix workstations or high-end PCs. A typical configuration might be a one- or two-processor Intel Pentium or Compaq Alpha system, running Windows NT or Linux, and having between one-half and one gigabyte of memory. Unix workstations with one or two or more processors are also commonly used. These are more than adequate for the typical steady-state analysis.

For complicated models and problems requiring time-dependent calculations, multiprocessor workstations are often set up. Although supercomputers are still employed for high-end research and development work, they are not commonly needed for typical engineering design applications. A recent trend is also the clustering of multiple, inexpensive PCs running Windows NT or Linux in a parallel-computing network. Such systems provide supercomputing power at a fraction of the cost of a supercomputer.

The user-friendliness of CFD software has also increased significantly. In the past, the software was characterized by text- or command file-based "interfaces" and it was difficult to configure solvers. This made fluid-flow analysis the exclusive domain of highly trained experts. However, the latest generation of commercial CFD software has been developed specifically to be used through graphical user interfaces, to have much more stable and robust solvers, and to allow an easy geometry exchange between CAD programs and the CFD solver.

This has permitted engineers who are not experts in fluid dynamics to make efficient use of this methodology and use it on a day-to-day basis in their design and optimization work. Most commercial CFD companies will provide training and continual technical support with their software licenses. The average engineer typically requires one week of training to get started using one of the modern, graphical CFD packages.

> Much of today's modeling work can be accomplished on low-end Unix workstations or high-end PCs.

Caveats and benefits

Despite the increased user-friendliness of modern CFD software, there are still a number of potential pitfalls to watch out for. From experience, we can say that the most commonly made mistakes are:

• *Using a low-quality, coarse grid.* One cannot resolve details that are smaller than the grid's cell size. Often, small flow features in one region need to be determined in great detail to accurately predict large flow features in other regions. This may lead to the need for a much finer grid than initially thought.

• *Using unconverged results.* CFD solvers are iterative and it is often tempting to cut a calculation short when deadlines are approaching or the coffee break is over. However, one should always ensure that proper convergence has been obtained before using the results from the solver.

• *Using the wrong physical property data.* This sounds trivial, but it is not. For example, viscosity curves may have been determined at one temperature and shear rate range, but if the actual values in the flow domain are outside of this range, then the curves may no longer be valid and incorrect results may be obtained.

Fortunately, none of these problems is fundamental to CFD technology itself. A coarse grid may be refined, unconverged calculations continued, and accurate physical constants may be measured. These easily avoided pitfalls are far outweighed by the following benefits:

• CFD can be used when design correlations or experimental data are not available.

• It provides comprehensive data that are not easily obtainable from experimental tests.

• This method reduces scale-up problems, because the models are based on fundamental physics and are scale-independent.

• When evaluating plant problems, CFD highlights the root cause, not just the effect.

• This technique can be used to complement physical modeling. Some design engineers actually use it to analyze new systems before deciding which and how many validation tests need to be performed.

• Many "what if" scenarios can often be analyzed in a short time.

To illustrate the successful application to many types of process equipment, we will discuss a number of examples here: a stirred tank reactor, a fluidized bed, a cyclone, a bubble column, and a twin-screw extruder. Unless otherwise noted, these simulations were performed with software from Fluent Inc. *(7)*.

Stirred tank reactors (STRs)

Stirred tanks are one of the most widely used pieces of processing equipment. Traditionally, their design is performed based on correlations of overall parameters, such as power draw and impeller pumping capacity. Mixing time correlations are available, but these are often difficult to extend outside of the experimentally studied parameter range. Further, it is known that for certain chemical reaction processes, specifically those involving multiple competing reactions, the location of the feed pipe relative to the impeller affects not only the mixing time, but also the final product composition. Many examples are available for single-phase flow, solids suspension, chemical reaction, and gas dispersion *(1)*. STRs are a prime example of a hydrodynamically controlled process operation and have been the focus of extensive CFD modeling in recent years.

From a numerical perspective, the rotation of the impeller relative to the baffles poses a special problem when modeling stirred tanks. A variety of methods has been devised to address this issue. The simplest is to use a black box, where the actual geometry of the impeller is not modeled, but the velocity profile of the impeller discharge, determined experimentally, is prescribed. The experimental data are usually obtained from laser Doppler velocimetry experiments. Data for a variety of impeller styles are available from a number of sources *(8)*.

More advanced ways to model the impeller geometry explicitly include the multiple reference frame (MRF) and the sliding mesh methods. With both of these, the flow around the impeller blades is modeled in detail, and no prescribed experimental data are required. With MRF, one "snapshot" of the flow field at one point in time during the impeller rotation is calculated. Using sliding mesh, the flow field is calculated as a function of time with the impeller actually rotating. The rotating grid in the impeller region "slides" past the stationary grid in the baffle region.

Mixing time calculations can be performed by one of two different methods. The first uses the unsteady tracking of a number of neutrally buoyant particles. After release, the turbulent dispersion of the particles can be tracked, and the particle concentration can be sampled at various instances. The second method follows the transport of a tracer liquid, similar to a dye injection. The tracer can be added and concentrations monitored throughout the vessel as a function of time. This approach is similar to the most common experimental methods. It makes use of a key advantage of CFD — that multiple locations can be sampled simultaneously to show concentration changes in many locations in the tank.

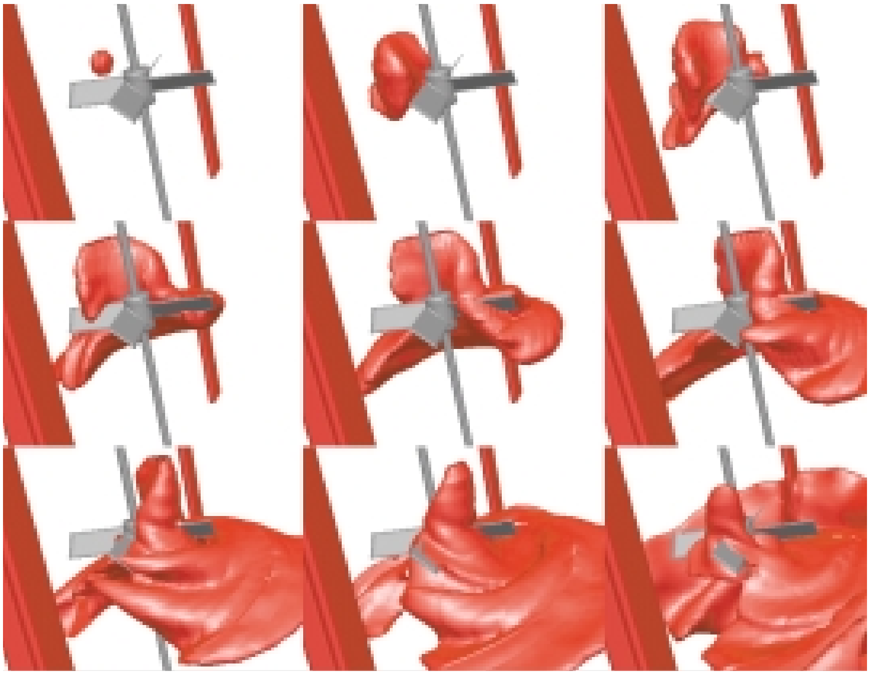


Figure 2. The dispersion of a tracer in a stirred tank as the impeller turns.

The results of these models typically compare well with experimental data *(9)*, for example, that from the dispersion of a chemical tracer in a stirred tank. In this example, a standard pitched-blade turbine was used to mix two water-like materials. A neutrally buoyant tracer was injected at time 0 as a blob above the impeller, as shown on the top left in Figure 2. The blob's dispersion is shown after ¼, ½, ¾, 1, 1¼, 1½, 1¾, and 2 impeller revolutions, respectively.

The flow field was calculated via the sliding mesh model, and the dispersion of the tracer was derived from the flow field. For this particular example, the LES turbulence model was used, although good results have also been obtained with other ones.

The blob is stretched and the chemical is mixed with the rest of the fluid over time. Despite that there are four impeller blades and four baffles, the concentration field is not symmetrical, because of the off-axis injection. This requires that the full tank be modeled, instead of just a 90-deg. section. CFD can be used to model blending time, power requirements, circulation time, and uniformity of mixing in STRs, in addition to modeling the residence time distribution (RTD) in CSTRs (continuous STRs) and backmixing in multistage columns.

Fluidized beds

Fluidization is effective for handling solids during transport, drying, heating, mixing, coating, and chemical reaction. As a result of fluidization, solids behave like fluids, so that efficient continuous processing is more easily achieved. Understanding the hydrodynamics of the process is essential for good fluidization process design.

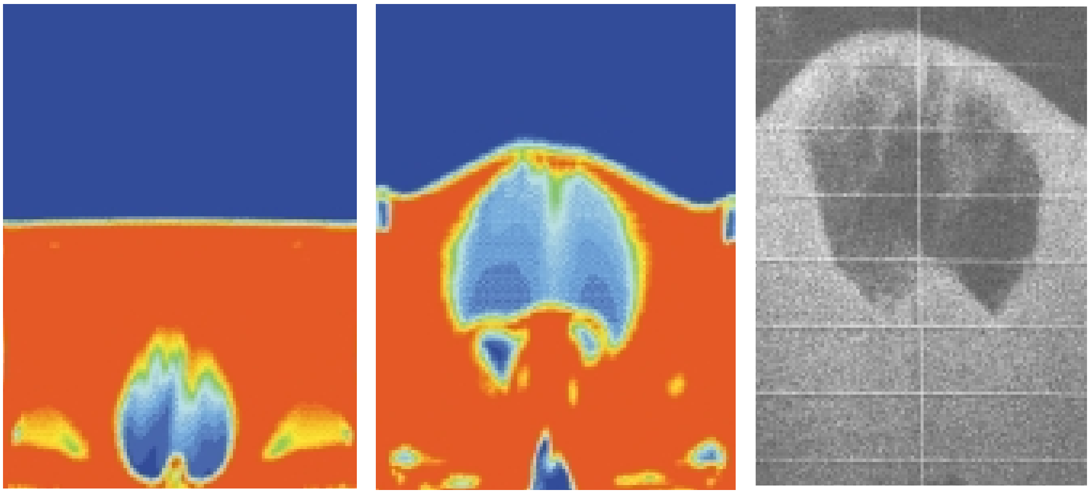


Figure 3. Solids concentration in a fluidized bed after 0.2 and 0.4 s, and compared with an actual photo.

Laboratory measurements of gas/solid flow interaction are difficult, if not impossible, especially in dense gas/solid flows. However, CFD generates comprehensive information on the details of the flow at all points in space and time.

Eulerian granular multiphase (EGM) models can be used to calculate the flow field in fluidized beds. The EGM model is a multifluid modeling approach, where both gas and solids are presented as interpenetrating continua. The model provides a detailed prediction over a wide range of solids concentrations. It calculates the formation, evolution, and coalescence of gas bubbles in time and space; predicts the rise velocity of bubbles and relative velocity of gas within the emulsion; and calculates the average, minimum, maximum, and standard deviation of variables such as velocity, temperature, or volume fraction of solids in a selected region.

Figure 3 shows the results of a calculation for a two-dimensional fluidized bed with a uniform fluidization velocity and an additional central jet. The simulation begins with the tank filled halfway at packing density and halfway with air. In the figure, the volume fraction of solids is shown after 0.2 and 0.4 s from the start of the simulation. Red corresponds to a solids volume fraction of 0.6, which was assigned as the packing limit. Blue represents pure air. The experimental photo shows the bubble at 0.44 s *(10)*.

Particle-to-particle interactions are important in determining the hydrodynamics in gas/solid flows. The EGM model uses kinetic theory formulations that take particle-to-particle interaction into account to formulate constitutive equations for viscosity, solids pressure, thermal conductivity, and other properties of interest. The interaction between gas and solids is prescribed by drag formulae.

EGM models provide an efficient framework for studying fluidization. They can model other operations, such as pneumatic-transport lines, hoppers, risers, or any application involving fluid/solid mixing, separation, or transport.

Cyclones

The conventional cyclone is a well-established process tool used for separation and classification. The unit works by inducing a spiral rotation on the fluid, thereby enhancing the radial acceleration on any suspended secondary phase. The absence of moving parts and a simple compact construction combined with a high material throughput make the cyclone a convenient, practical, and extensively used tool in the CPI.

Figure 4 shows a model of a typical cyclone of Stairmand design *(11)*. An unstructured, hexahedral mesh was used in modeling. The swirling flow in the cyclone is shown by particle traces. When the flow patterns are used to calculate the flow of particles through the cyclone, separation efficiencies can be determined, and areas that may be subject to erosion can be made visible.

In these simulations, a time-averaged flow field was calculated. The results of these simulations compared well with experimental data presented in the literature *(12)*, provided that the Reynolds stress turbulence model was used. However, under certain conditions, the vortex in the cyclone may not be steady and can actually be subject to a precessing motion. Such situations can also be modeled, but require the use of the LES model in Table 1, which is computationally more intensive. This is an area that is still under investigation.

Bubble columns

Bubble columns are contactors in which a discontinuous gas phase as bubbles moves relative to the continuous liquid phase. As reactors, they are used in a variety of CPI processes, such as Fischer-Tropsch synthesis, manufacture of fine chemicals, oxidation and alkylation

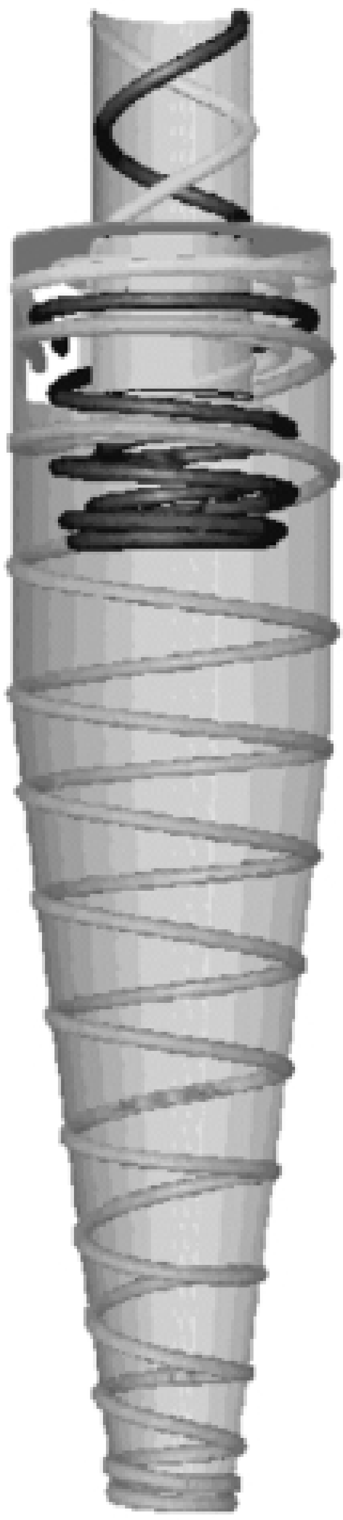


Figure 4. Model of a cyclone using an unstructured, hexahedral mesh.

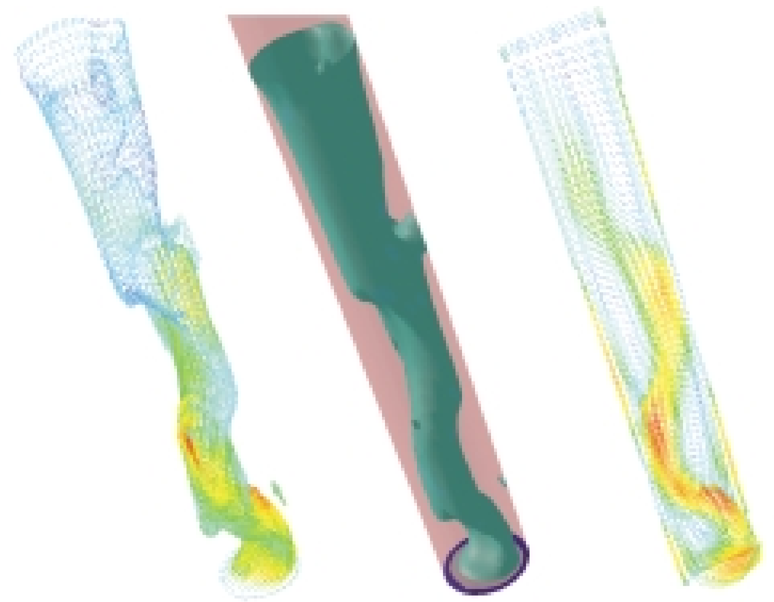


Figure 5. Simulation of the time-dependent velocity field and gas holdup profile in a bubble column.

reactions, effluent treatment, coal liquefaction, fermentation, and in cell cultures and the production of single-cell protein. Their principal advantages are the absence of moving parts, leading to easier maintenance; high interfacial areas and transport rates between the gas and liquid phases; good heat-transfer characteristics; and large liquid holdup, which is favorable for slow liquid-phase reactions. The complex fluid dynamics in these reactors affects their operation and performance. The complex two-phase flow and turbulence determine the transient and time-averaged values of gas holdup distribution, extent of liquid-phase backmixing, gas/liquid interfacial area, gas/liquid mass- and heat-transfer coefficients, bubble-size distributions, bubble coalescence and redispersion rates, and bubble-rise velocities. The lack of complete understanding of the fluid dynamics makes it difficult to improve the performance by judicious selection and control of the operating parameters.

CFD is being used to interpret of the interaction of the above-mentioned fluid dynamic variables. Both bubbly and churn-turbulent bubble-column flows can be simulated *(13)*. Figure 5 shows the results of a time-dependent simulation of the velocity field and gas-holdup profile. The plot on the right represents the liquid velocity vectors in a plane through the center of the column. The plot in the center shows a surface at which the volume fraction of gas is 30%. Inside the surface, the volume fraction of gas is higher. The plot on the left is of the velocity vectors at this surface.

The CFD results have been validated against experimental data in a number of studies, *e.g.,* Ref. 14. Good agreement is obtained when the comparison is made with data obtained via the noninvasive, computer-automated radioactive-particle tracking experimental technique (CARPT).

Simulations can be used to predict gas holdup, mass-transfer and mixing rates, and process performance. One of the advantages of CFD over the use of traditional bubble column design-correlations is that its models also apply outside of the range where experimental data were obtained.

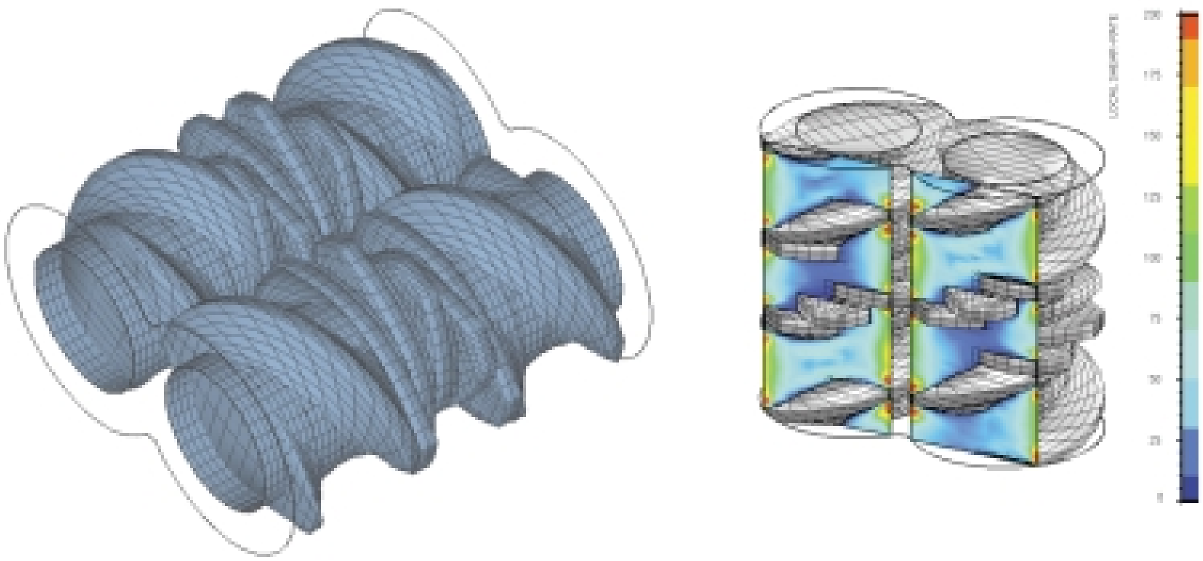


Figure 6. The flow of polystyrene is analyzed via a combination of conveying and kneading block elements.

Twin-screw extruders

The twin-screw extruder is a widely used tool, not only in the plastics and rubber industry, but also in other operations such as food processing. Single and twin-screw units melt, convey, compress, and mix different compounds, and these steps can considerably affect the quality of a process. This explains the large interest in screw analysis and, more specifically, the numerous attempts to model twin-screw machines through numerical simulations. But, the challenges here (with moving parts, thermal behavior, difficult meshing and remeshing tasks, and partial filling, for example) often lead to many simplifications of the actual problem.

To ease the setup of a 3-D unsteady twin-screw unit, a technique referred to as mesh superposition has been implemented by Polyflow s.a. *(15)*. The firm's eponymous software employs this robust technique because it greatly simplifies the meshing of geometric entities and does not present the complexities and limitations of other commonly used simulation methods. Polyflow is available for 2-D and 3-D nonisothermal, generalized Newtonian fluids.

Polyflow generates a finite-element mesh for each part of the flow simulation: one for the flow domain, the other for each screw. The screws are assumed to be rigid, and their motion is a combination of translation and rotation. At each timestep, the screw meshes are moved to their new position, overlapping the flow mesh. For each node of this new domain that lies within a given screw, a special formulation is used for imposing the proper velocity to match the rotational speed of that screw. Hence, the flow is calculated for a set of successive screw positions at constant angular displacement. The history of the flow pattern is thus obtained and stored for further analysis.

Figure 6 shows the shear rate in a plane in the extruder. The mesh superposition technique allows this complex, time-dependent flow to be modeled. The figure shows the local shear rate in the extruder, with red denoting regions of high shear rate and blue denoting regions of a low rate.

High shear rates are found near the tips of the extruder elements, as expected. This is relevant when dealing with shear-sensitive materials. However, other quantities of interest, such as residence-time distributions, material thermal history, stretching rates, and many other quantities, can be obtained. This allows for a detailed comparison between alternative designs. For example, using this technique, it was found that the extruder shown in the figure, in which conveying elements were alternated with kneading elements, provides a 25% better mixing per unit length vs. a standard unit that contains only conveying elements *(16)*. However, the residence-time distribution was narrower with the latter. Being able to obtain such detailed performance information without experimentation allows process engineers to design advanced and more efficient equipment with confidence.

To sum up

In the past decade, the applicability of CFD in the CPI has grown considerably. CFD is an analysis tool capable of providing extensive and detailed information about flow-related phenomena in many different types of processing equipment that cannot be obtained any other way. A broad range of newer and better models now exists, including some for turbulence, multiphase/multicomponent flows, and chemical reactions. The technology is still improving and what was once the exclusive domain of highly specialized experts is now accessible to most engineers in the CPI through increased computational power of common desktop computers and better interfaces to the CFD codes.

Flowsheet modeling is a necessity in the plant. Improvements in process simulation technology nowadays make the simulation of entire plants commonplace. However, current CFD simulations typically model a single unit operation or piece of equipment and provide much more accurate and detailed information than the simpler, lumped models used in process simulation software. Future developments will not only include further enhancement of the available physical models and code usability, but will also focus on a tighter integration between CFD and process simulation software. Efforts are underway to create an integrated software system capable of linking hierarchy models to allow seamless blending of flowsheet models with more detailed CFD ones *(17)*. This opens the prospect of a future in which entire plants are simulated based on fundamental principles, further reducing process problems and improving efficiency. CEP

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A. BAKKER is the regional consulting manager at Fluent Inc. in Lebanon, NH ((603) 643-2600; Fax: (603) 643-3967; E-mail: ab@fluent.com). Bakker is an internationally recognized expert in the field of industrial mixing and CFD modeling of chemical engineering applications. His specialization includes experimental and computational fluid mixing. He holds engineering and doctorate degrees from Delft University of Technology in the Netherlands, both in applied physics. He has coauthored more than 50 technical articles and presentations on fluid dynamics and mixing, and is a member of AIChE

A. H. HAIDARI is the chemical team leader at Fluent Inc. in Lebanon, NH ((603) 643-2600; Fax: (603) 643-3967; E-mail: ah@fluent.com). Haidari has 15 years of experience in the application of flow modeling in addressing industrial process equipment design, process troubleshooting, analysis, and scale-up. He holds a PhD in mechanical engineering from Lehigh University, is a member of AIChE, and has made numerous presentations and written publications on modeling chemical process equipment.

L. M. OSHINOWO is a senior engineer at Hatch in Ontario, Canada ((905) 403-4239; Fax: (905) 855-8270; E-mail: loshinowo@hatch.ca). Prior to joining Hatch, he was MixSim product manager at Fluent Inc. Oshinowo solves industrial problems related to the CPI including momentum, heat and mass transfer, multiphase and reacting flows, and has co-authored numerous technical and scientific publications in these areas. His specialization includes computational fluid mixing, and he has experimental and numerical experience in gas/liquid flows and turbulence. He holds a PhD in chemical engineering from the University of Toronto, Canada, and is a member of AIChE and CSChE.

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