Advanced Gas-Solid Multiphase Flow Models Offer Significant Process Improvements

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Major advancements in the area of gas-solid multiphase flow modeling offer substantial process improvements that have the potential to significantly improve process plant operations. Prediction of gas-solid flow fields, in processes such as pneumatic transport lines, risers, fluidized bed reactors, hoppers and precipitators, are crucial to the operation of most process plants. Up to now, the inability to accurately model these interactions has limited the role that simulation could play in improving operations. In recent years, computational fluid dynamics (CFD) software developers have focused on this area to develop new modeling methods that can simulate gas-solid flows to a much higher level of reliability. As a result, process industry engineers are beginning to utilize these methods to make major improvements by evaluating alternatives that would be, if not impossible, too expensive or time-consuming to trial on the plant floor.

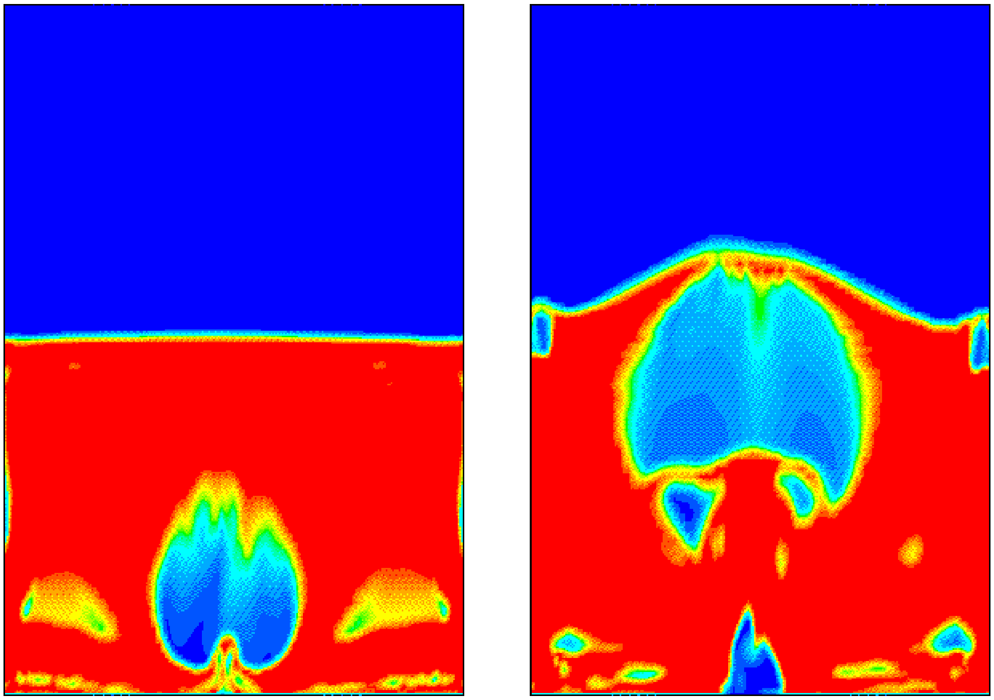

Figure 1: An initially stationary bed of solids is fluidized by the action of a central jet. Red indicates regions of maximum solids volume fraction(~0.6), and blue indicates regions of maximum air volume fraction (1.0).

Over the past few decades, CFD has been used to improve process design by allowing engineers to simulate the performance of alternative configurations, eliminating guesswork that would normally be used to establish equipment geometry and process conditions. The use of CFD enables engineers to obtain solutions for problems with complex geometry and boundary conditions. A CFD analysis yields values for pressure, fluid velocity, temperature, and species or phase concentration on a computational grid throughout the solution domain. The key advantages of CFD are:

1. It provides the flexibility to change design parameters without the expense of hardware changes. It therefore costs less than laboratory or field experiments, allowing engineers to try more alternative designs than would be feasible otherwise.
2. It has a faster turnaround time than experiments.
3. It guides the engineer to the root of problems, and is therefore well suited for trouble-shooting.
4. It provides comprehensive information about a flow field, especially in regions where measurements are either difficult or impossible to obtain.

Modeling approach:

CFD involves the solution of the governing equations for fluid flow, heat and mass transfer, radiation, and chemical reaction. These equations are solved at several thousand discrete points (called a computational grid) in the defined flow domain. When the process involves the flow of more than one phase, i.e. gas and solids, one approach is to model this process by solving one set of Navier-Stokes equations for each phase. This modeling technique, called the two-fluid, multi-fluid, or Eulerian-Eulerian technique, assumes that phases are interpenetrating continua. The Eulerian-Eulerian approach is especially useful and computationally cost effective when the volume fractions of the phases are comparable, or when body forces (such as gravity) act to separate the phases, or when the interaction within and between the phases plays a significant role in determining the hydrodynamcis of the system. When the volume fraction of one phase is low (roughly less than 10%), an alternative method is available in which the minor phase is treated as a set of discrete particles or droplets which are tracked individually. This Lagrangian technique is appropriate for spray dryers, but breaks down for fluidized beds and risers, where the volume fraction of the minor phase exceeds the 10% limit.

The multi-fluid or Eulerian-Eulerian approach has been applied to both fluid-fluid flows (water and oil, or gas and liquid, for example) and fluid-solid flows (liquid and particles or gas and particles). When it is used for fluid-solid flows, analogies to kinetic theory for dense gases have been made to develop constituent relations for the pressure and viscosity of the solid phase. These theories are based on a direct analogy between the fluctuation of individual solid particles, or granules, and the fluctuation of gas molecules due to the local temperature. Hence, the term "granular temperature " has been used to describe the fluctuating energy of individual solid particles. Granular temperature is an essential ingredient in the solids pressure and solids viscosity formulation and hence needs to be computed as a part of the CFD calculation. By incorporating the granular temperature in the "Eulerian-Granular" Model, or EGM, the treatment of the solids pressure and viscosity is more realistic, and this leads to a more realistic prediction of other hydrodynamic features of fluid-solid systems, such as the distribution of solids in the domain when the packing limit is approached.

Modeling difficulties

Most processes involve solids with irregular shapes and a distribution of sizes. These features affect the mean and turbulent flow interactions between the solids and fluid. The shape and size distributions, as well as the cohesion of particles that sometimes occurs, also affect frictional stresses within the solids phase. The interaction between the solids and fluid along with the stresses within the solid assembly combine to affect many flow field features, such as solids distribution, pressure drop, and the velocity fields of both phases.

Several limitations exist that prohibit the accurate modeling of the phase interactions. The kinetic theories that describe the constituent relations for solids viscosity and pressure are based on binary collisions of smooth and spherical particles, and do not account for deviations in shape or size distribution. The interaction between the mean flow fields of the phases is described by drag formulas, which are derived experimentally. Proposed by various authors, they are primarily a function of solids volume fraction, and do not include particle size distribution or particle shape. They do not include turbulent interactions either, since there is very little known about the interaction between the turbulent fields of solids and fluid phases, especially when the solids concentration is high. The formulas that describe cohesion and frictional stresses within the solids assembly are also not well established.

Despite the many difficulties in modeling gas-solid flows, engineers have used the current capabilities to gain insight about their processes and make crucial changes that have helped the company bottom line. Some of the shortcomings can be circumvented numerically. For instance, at the expense of more CPU time, multiple solid phases can be used to simulate multiple particle sizes. A discrete set of 2 or 3 particle-size phases can provide a rough approximation for a continuous particle size distribution. Drag formulas can be modified to take into account the effect of particle size distribution on other problem variables, such as pressure drop or minimum fluidization velocity. By making adjustments to the EGM in this manner, or by using the model as is, a large number of applications can be successfully simulated. Details of some of these applications follow.

Fluidized bed

Fluidization is an effective technique for handling solids for processes such as chemical reaction, transportation, drying, heating, and cooling. The solid phase is fluidized in order to achieve efficient continuous processing, nearly isothermal operation, and effective heat and mass transfer between gas and solids. Understanding the hydrodynamics of fluidized beds is essential for proper gas-solid contacting, and hence a good fluidization process design. The challenge is capturing the gas flow patterns, including the volume, size and velocity of bubbles that rise through the fluidized bed. To achieve a high rate of conversion, uniform gas distribution throughout the reactor with a large interfacial surface area between the gas and solids is desirable. To achieve a high rate of production, higher gas velocity needs to be used. These two contradict each other. Baffling and staging is sometimes used to bring these two needs to a compromising point. The existence of internals such as heat exchangers adds to the complexity of the problem by creating potential dead spots. An example of a fluidized bed is shown in Figure 1, where fluidization is due to the action of a weak uniform airflow and a central high speed flow in a bed of solids.

In the past, researchers have attempted to understand the hydrodynamics of fluidized-bed reactors by performing laboratory-scale experiments. Unfortunately, the laboratory-scale data does not necessarily scale up accurately. To best understand the hydrodynamics in a commercial-scale fluidized bed reactor, it is necessary to study a vessel of that size. However, the capital cost of such a program can be prohibitive. Alternatively, the EGM can be used to calculate the flow field in a typical fluidized bed. Using the EGM, CFD software can calculate the formation, evolution and coalescence of gas bubbles in time and space, predict the rise velocity of bubbles and relative velocity of gas within the promotion phase. It can calculate the average, minimum, maximum and standard deviation of variables such as velocity, temperature or volume fraction of solids in a selected region. More importantly, it can be used to study the effect of internals on the gas-solid flow patterns.

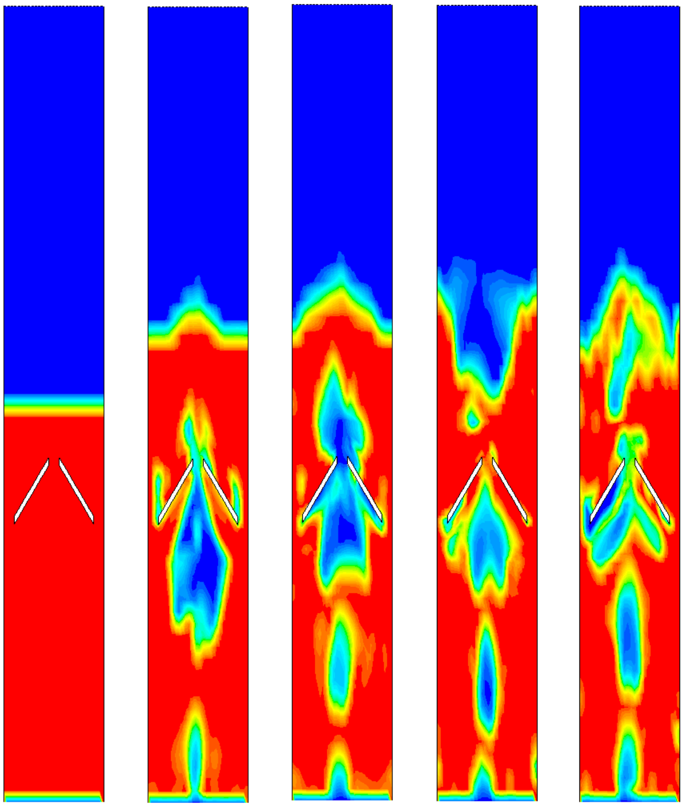

Figure 2: Volume fraction during the transient fluidization of a bed of solids. Red indicates regions of maximum solids volume fraction(~0.6), and blue indicates regions of maximum air volume fraction (1.0). ***Courtesy Dow Chemical***

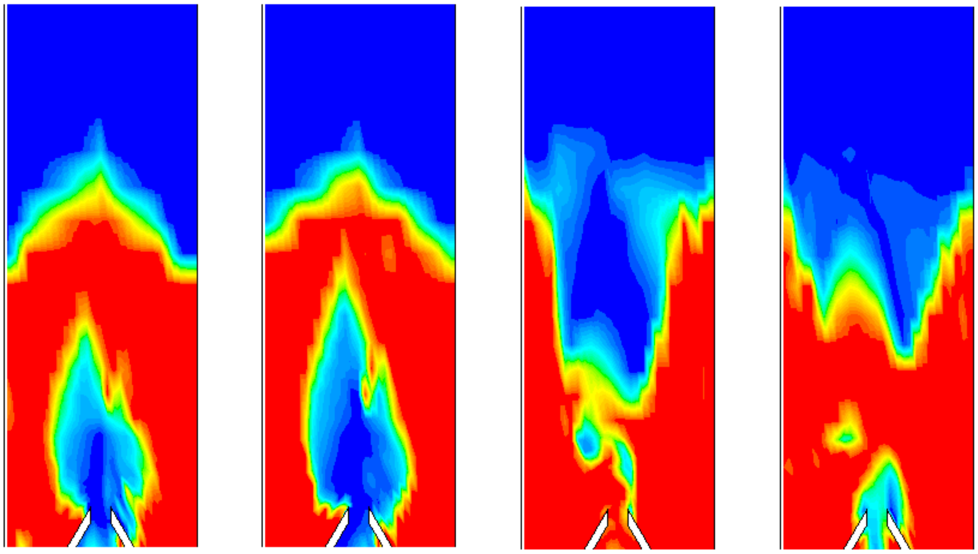

Figure 3: The top surface of the fluidized bed is examined closely. The bubble of air rises and breaks through the surface during a period of about 0.5 seconds from left to right.
Courtesy Dow Chemical

In another example, a two-dimensional fluidized bed with uniform fluidization velocity, a central jet, and a pair of internal baffles was studied. The simulation begins with the tank filled halfway with solids at the packing limit volume fraction of 0.6. In Figure 2, the volume fraction of solids is shown during the first few seconds of operation. Red corresponds to a solids volume fraction at the packing limit. Blue corresponds to pure air.

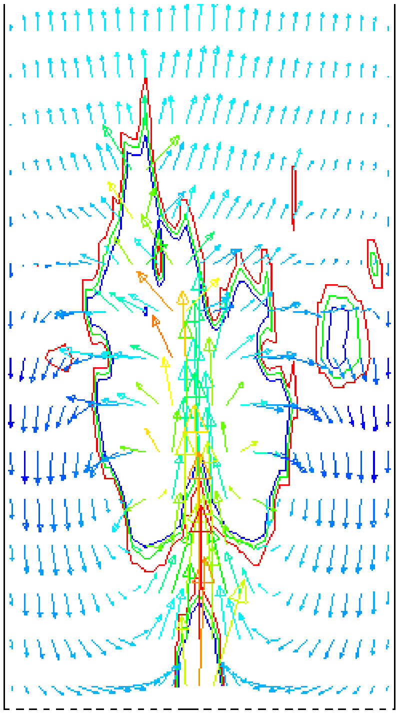

Figure 4: The dynamics of a bubble are examined using contour lines to mark the surface of the bubble and vectors to show the motion of the gas inside the bubble and in the remainder of the bed.
Courtesy Dow Chemical

A close-up view of the surface is shown in Figure 3, spanning times from 0.7 seconds through 1.2 seconds. The bubble rises from the baffle gap (left), rises, and breaks through the surface of the solids. In Figure 4, the dynamics of the gas flow in the bubble are examined. Along with line contours to mark the edge of the bubble, velocity vectors for the gas phase are shown. The vectors show the expansion and rising motion of the bubble. Also shown is how the bubble pushes the air in the solids region out of the way as it moves.

Particle-particle interactions are very important in determining the hydrodynamics in dense gas-solid flows, such as those in fluidized beds. The EGM is used with kinetic theory formulations that take particle-particle interaction into account to formulate constitutive equations. In the above example, the Gravity Downward Gidaspow model is used for viscosity and solids pressure. The Arastoopour formulation is used to calculate the drag between the solids and air. Solids are treated as laminar, while air is treated as turbulent.

Risers

Risers (Figure 5), frequently used in petroleum refineries, present another challenging gas-solids modeling problem. In FCC units, high molecular weight gas and catalyst is normally injected into the bottom of the riser. During the transit through the riser, the catalyst, in the form of solid particles, acts to break down the gas molecules into smaller components. The primary design goal is to spread the catalyst evenly throughout the riser in order to increase the efficiency of the reactions taking place. The primary problem in riser operation is usually that the solid material distribution is either unknown, or is known to be non-uniform. . Additionally,

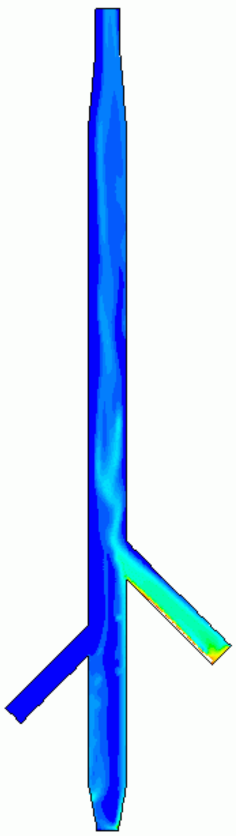

Figure 5: Transient flow in a riser shows the unsteady flow pattern that is typical of these units.

at higher production rates, which require a higher solids flux, the down-flow of solids near the wall occurs, and causes back mixing. These are further complicated by the effects of the inlet and outlet configurations. Prediction of solids distribution, gas velocity, and residence time presents a challenge to optimize the design of a riser reactor. The EGM in FLUENT can be used to study the overall flow pattern of both gas and solids while studying the effect of inlet and outlet configurations. Formation, coalescence and the breakup of clusters and streamers are revealed by the EGM if there is sufficient resolution in the computational model.

Dilute pneumatic transport lines

Pneumatic transport lines are another process industry application where gas-solid interaction plays an important role. In this application, gas under pressure is used to transfer a solid material at high-speed. Line diameters typically range from 6 to 12 inches and the volume fraction of the solid is normally quite low. The objective is to transfer the material with the lowest possible pressure drop to save cost. The major contributor to pressure drop is the friction generated between the material and the wall. The primary advantage of the EGM in this application is the ability to calibrate friction factors for the solids phase based on small-scale laboratory experiments and complementary CFD calculations. These friction factors can then be used to simulate larger transport lines, or sections of transport lines with complex shapes, such as elbows or bends.

Flow through a hopper

Hoppers are used as storage and feeding devices in the chemical, food, pharmaceutical and petrochemical industries. Engineers involved in implementing and maintaining the emptying process want to design the hopper for a predictable, uniform flow rate. The challenge to CFD analysts is that factors such as particle size distribution, and cohesion and friction between the particles and hopper walls affect the emptying behavior. This can lead to arching or choking, flooding, piping, segregation and a nonuniform flow rate. In the past, the only way to deal with this issue was to build models and perform physical experiments. In many cases it was necessary to build expensive full-scale models because of scaling difficulties.

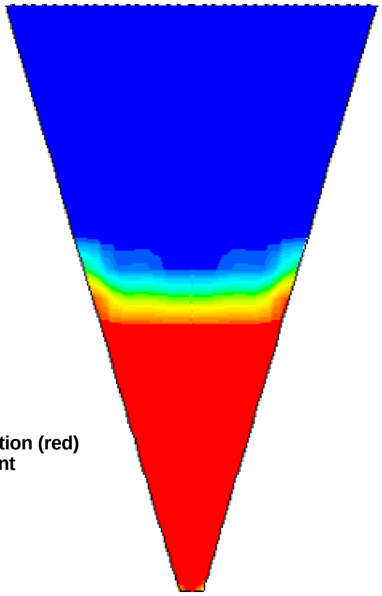

Figure 6: Solids volume fraction (red) are shown during the transient emptying of a hopper

The EGM can effectively predict comparative flow characteristics as a function of material properties in a hopper. Consider the example of a two-dimensional axisymmetric hopper that is filled partially with 100 grams of solid particles with a volume fraction of 0.57. The packing limit is set at 0.62, which means that the particles are not tightly packed at the start of the problem. Atmospheric pressure is applied to the top and bottom openings. Figure 6 shows the volume fraction of the solids (with red the maximum) during the emptying process. Figure 7 shows the mass flow rate calculated by FLUENT as a function of time. This plot is typical of the trend usually observed in the

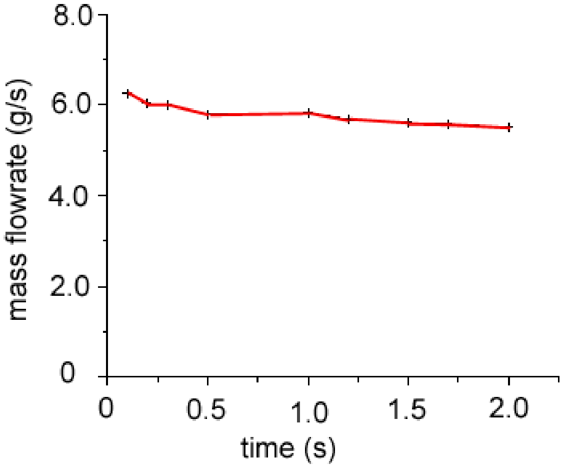

Figure 7: The mass flow rate of solids during the emptying of a hopper is nearly constant in time for this example, consistent with field observations.

field, namely, one of constant mass flow rate. When this occurs, the flow rate does not reduce with the height of solids in the hopper. The EGM can be used to evaluate the relative performance of different hoppers with different internals, wall angles, etc. Hopper flows were compared for hoppers filled with different materials: one with 600-micron particles and another with 50-micron particles. In both simulations, a no-slip boundary condition was applied for both the gas and solids phases at the walls. The CFD results showed that the 600-micron particles took longer to discharge than the 50-micron particles. In the 50-micron particle case, a constant mass flow pattern was demonstrated: all particles moved simultaneously during the discharge process with no areas of stagnation. In the 600-micron case, on the other hand, the behavior was closer to a funnel flow, where the particles in the center discharged quickly, with stagnation regions developing along the sides. Comparison of these cases illustrates that the EGM is capable of predicting both flow regimes: constant mass flow as well as funnel flow. The EGM can also be used to study aerated hoppers and can grossly simulate vibrational effects.

Precipitators

CFD predictions of flow distribution and solids accumulation has been used to reduce physical testing, optimize filtration efficiency, and extend the operating range of electrostatic precipitators. In Figure 8, dust loaded airflow enters a precipitator at the upper left and is distributed to the separator plates. An important design goal is to distribute the flow across the entire separator plate, avoiding regions of high dust loading where particle sedimentation could occur.

The two-dimensional CFD model uses the EGM to include both dust and air flow. The porous media model is used to represent the resistance of the filter plates. Based on the CFD results, the filter manufacturer found that dust accumulation upstream of the filter was causing a problem and an adjustable device was designed to minimize it. The resulting design operated with improved efficiency by using the full precipitator flow area, and operated over a wider range of dust loading.

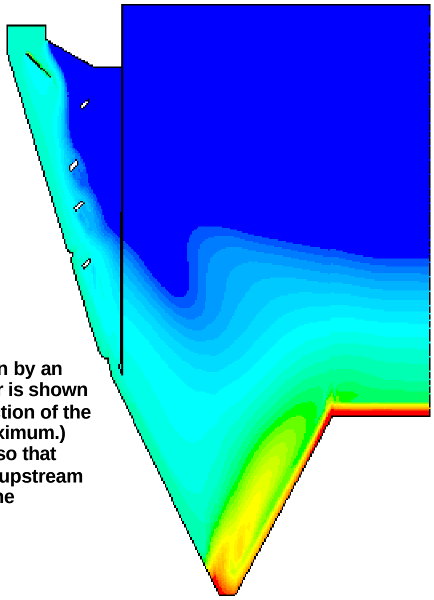

Figure 8: Dust collection by an electrostatic precipitator is shown through the volume fraction of the dust phase. (Red is maximum.) The design was altered so that less dust was collected upstream of the filter, improving the efficiency of the device.

Traditionally, the filter manufacturer qualified their designs using a combination of scaled 2D water tunnel studies and scaled 3D testing with air. Unlike the scaled tests, the CFD models correctly include density variations, full-scale effects, and the impact of variable dust loading. Using CFD, the manufacturer has replaced part of their test program with CFD modeling that is 3 to 5 times less costly than testing.

Summary

Recent advances in modeling methods have dramatically improved process design capabilities involving gas-solid interaction for a wide range of industrial applications. Until recently, these applications required the construction and testing of physical prototypes, a difficult, expensive, and time-consuming process. The need to perform this task has been reduced by the development and integration of new modeling methods such as the EGM with its customizable options. By making it possible to analyze gas-solid problems, engineers can bring the advantages of CFD to an entirely new class of problems.