COMPUTATION-BASED ENGINEERING OF MULTIPHASE PROCESSES USING COMPUTATIONAL FLUID DYNAMICS

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Abstract— *Computer-based engineering tools such as computational fluid dynamics (CFD) provide tremendous insight into flow details that are inaccessible using simpler approaches. Used in conjunction with a well-founded verification and validation (V&V) process, these details enable improved engineering designs with tighter margins and reduced costs. Wherever the potential for high risk/exposure exists and design uncertainty must be reduced, CFD is an enabling technology.*

This paper presents three illustrations of how CFD models can be applied to gas-solid, gas-liquid, and solid-liquid multiphase flow problems. Two cases show how CFD can be applied to engineering projects and how validation data is used to add confidence to the model predictions. The third case specifically illustrates how validation is used to improve the process of building a CFD model. Together, these illustrations are indicative of how Bechtel is at the cutting edge of bringing multiphase CFD into mainstream engineering.

Keywords— *computational fluid dynamics (CFD), gas-liquid, gas-solid, mixing, modeling, multiphase, numerical, scrubbing, simulation, slurry, solid-liquid, verification and validation (V&V)*

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INTRODUCTION

The use of computational fluid dynamics (CFD) to model multiphase transport phenomenon is becoming a commonplace engineering practice. Many processes that Bechtel encounters in its engineering projects include multiphase flows. For example, gas-liquid flows are encountered when a liquid flashes into vapor behind a valve. Solid-liquid mixing occurs in tanks when a radioactive slurry is processed for vitrification. Gas-solid flows involving particulate injection, mixing, and transport occur in many mining operations.

Syamlal et al. [1] present an excellent review of the importance and future of computational science and the significant role it can play in furthering technology development. The authors point out four pathways along which computational science, including CFD, can contribute:

- Identifying the most promising concepts
- Getting the design right the first time at any scale
- Reducing the amount of building and testing at intermediate scales
- Learning and disseminating information when deploying a technology from the first plant to subsequent plants

The broad range of examples this review uses to demonstrate these four pathways is very relevant to Bechtel projects.

Applying CFD to an engineering problem begins by choosing a domain of interest and representing this domain with a computational mesh. It is upon this mesh that the equations representing conservation of mass, momentum, and energy are discretized and solved numerically. Along with these conservation equations, there may be additional equations such as those representing the time-evolution of certain turbulence quantities or those representing different chemical species concentrations or material phase quantities.

Associated with each equation being solved are numerous other mathematical relationships that capture the specific details of fluid and particle behavior. Examples of these constitutive relations and submodels are expressions for stress tensor, heat flux vector, chemical reaction rate, momentum exchange between phases, and production and dissipation of turbulence quantities. The CFD approach has the benefit of maximizing the application of first principle relations and minimizing empirical relations. Combined with a numerical procedure that solves all coupled, nonlinear equations

ABBREVIATIONS, ACRONYMS, AND TERMS

AOA	angle of attack
ASME	American Society of Mechanical Engineers
atm	standard atmosphere
CFD	computational fluid dynamics
DDT	deflagration-to-detonation transition
FEA	finite element analysis
FFT	fast Fourier transform
LNG	liquefied natural gas
TUI	text-user interface
UDF	user-defined function
V&V	verification and validation
VOF	volume of fluid

> *Using commercially available CFD codes, engineering workstations and clusters are sufficiently powerful to simulate very complex flow phenomena, often with reasonable turnaround times.*

simultaneously, CFD is remarkably general and broadly applicable.

Using commercially available CFD codes, today's engineering workstations and clusters are sufficiently powerful to simulate very complex flow phenomena, and can often do so with reasonable turnaround times. Further, available commercial codes such as ANSYS® FLUENT® and CD-adapco STAR-CCM+® include the necessary models for the complex physics present in multiphase problems. Current customer focus on the enhanced performance of new and existing technologies, coupled with tighter industry requirements to meet stricter codes and standards, makes it inevitable that verified CFD models with validated solutions in parameter ranges of interest will be integrated into the design process.

Verifying CFD models and validating their solutions are nontrivial tasks. In 2009, the American Society of Mechanical Engineers (ASME) released its verification and validation (V&V) standard for CFD codes (ASME V&V 20: Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer). Bechtel has already begun a V&V effort to qualify FLUENT for gas-solid-liquid mixing systems.

This paper presents three illustrations of how CFD models can be applied to gas-solid, gas-liquid, and solid-liquid multiphase flow problems. Two cases show how CFD can be applied to Bechtel projects and how validation data is used to add confidence to the model predictions. The third case specifically illustrates how validation is used to improve the process of building a CFD model.

MULTIPHASE FLOW MODELING STRATEGIES

Bechtel National, Inc.'s, Advanced Simulation and Analysis group primarily uses two commercial solvers for multiphase simulations—the FLUENT and STAR-CCM+ software programs. These industry-leading CFD packages offer several different modeling approaches to multiphase flow. No one approach is optimal for all situations. The user must review the solution strategies and, based on the particular problem being confronted and the questions being asked, select the one that makes the most sense. A brief overview of the modeling strategies follows.

Eulerian-Lagrangian Approaches

When a multiphase system consists mainly of a single continuous phase carrying a relatively small volume of discrete particles, droplets, or bubbles, a Eulerian-Lagrangian model can be used. The carrier phase is modeled from a Eulerian point of view, solving the mass, momentum, and energy transport equations on a mesh. Particle trajectories are modeled with ballistic equations that use properties extracted from the carrier phase solution to compute the local forces acting on the transported particles. By randomizing the injection location on the particle inflow boundary and adding a stochastic component to emulate turbulent diffusion, a large number of unique particle trajectories can be calculated that are all equally likely. A statistical assessment of the expected particle distributions allows particle effects to be impressed onto the carrier phase (for a two-way coupled solution).

FLUENT and STAR-CCM+ offer Eulerian-Lagrangian modeling strategies with extensions that allow relatively high-volume fractions. Details of these Eulerian-Lagrangian formulations are documented in the FLUENT and STAR-CCM+ user manuals.

At Bechtel, Eulerian-Lagrangian models have been used to simulate alumina injection and transport in dry scrubbing systems for handling the off-gas stream from aluminum smelting, which is the example presented in this paper. Other examples from the literature where Eulerian-Lagrangian models have been applied are cyclone dust separators, vehicle soiling, spray coating, aerosol dispersion, spray cooling, and liquid fuel combustion.

Eulerian-Eulerian Approaches

FLUENT and STAR-CCM+ also offer Eulerian-Eulerian multiphase modeling options. For example, FLUENT has three Eulerian-Eulerian strategies for solving multiphase flows with interpenetrating continua. The first strategy is the volume-of-fluid (VOF) model, a front-tracking method for the volume fraction of the immiscible phase that uses a single momentum equation. The second strategy, the mixture model, solves mixture momentum equations and uses relative velocities to describe the dispersed phases. The third strategy, the Eulerian model, is the most detailed of the three, solving continuity and momentum equations for each phase present. When particle volume fractions routinely approach the packing limit, only the Eulerian model is appropriate. Details of these three strategies may be found in the FLUENT *Theory Guide*. [2] The Eulerian-Eulerian approach is used in the gas-liquid and solid-liquid simulations presented in this paper.

GAS-SOLID FLOWS

Introduction

Gas-solid flows are common in Bechtel projects. Recent simulations have modeled the incursion of sand into buildings, the transport of flyash in power plant ducts, and the suspension of alumina within dry scrubbing units at aluminum smelting facilities. Although different in scope, these applications engage the same underlying mathematical models.

In the gas-solid simulation example presented here, a Eulerian-Lagrangian multiphase model is applied to a dry scrubbing unit for a notional aluminum smelting facility. This application demonstrates how computation can enable a system to be optimized for performance and risk mitigation before equipment choices are narrowed and purchases made. Performance metrics are:

- Pressure losses across the stages of the unit (limiting the number of scrubbers that can be attached to an exhaust manifold with a fixed available vacuum capacity)
- Development of a well-mixed region of alumina and smelter off-gases for multiple alumina recycle rates (ensuring optimum toxin adsorption for removal)
- Distribution of alumina by particle size in the hopper (limiting scale formation on the bag filters and affecting bag filter pulse rate)

Each metric affects the production capacity of the smelting facility and thus the bottom line.

The Mathematical Model

The Eulerian-Lagrangian multiphase model solves the set of Reynolds-averaged equations for mass, momentum, and energy conservation and a two-equation model for turbulence for the carrier phase. If an option for two-way coupling with transported solids is selected, a drag model for interphase momentum (and energy) transfer is enabled.

Individual particle trajectories are computed using a ballistic equation coupled with the carrier phase fields for the expected local flow conditions. If a model option for turbulence dispersion is selected, a stochastic submodel is implemented to jitter the particle direction. This submodel depends on the integral time, determined from the carrier phase turbulence model parameters. If an option for two-way coupling is selected, particle statistics are computed to facilitate momentum interchange with the carrier phase.

FLUENT's detailed Eulerian model solves continuity and momentum equations for each flow phase present.

A Notional Dry Scrubbing System

Because the features of specific dry scrubbing units simulated by Bechtel are client-confidential and cannot be published, a generic dry scrubbing unit has been modeled for this paper that has the salient features of real systems. STAR-CCM+ was used to discretize the flow volume and provide the multiphase solution. An image of the notional scrubbing unit with a visualization of the computational surface mesh is presented in the left image of **Figure 1**.

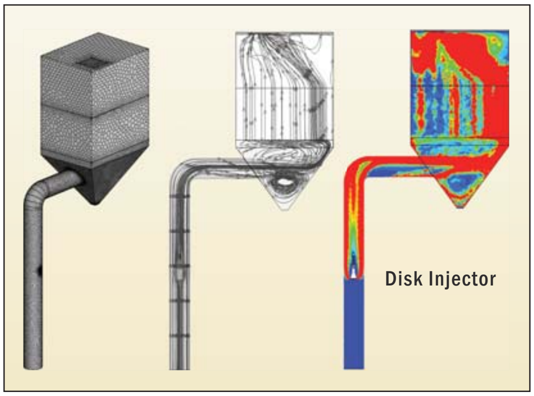

Figure 1. Notional Dry Scrubbing Unit: Surface Mesh (left), Streamlines (middle), and Total Solids Distribution (right)

The dry scrubber consists of an off-gas duct from a supply manifold from the smelter. This duct routes toxin-laden gas to a reaction zone, where virgin alumina mixed with recycled alumina is injected into the duct. There are many injection schemes. This injector produces a downward spray of alumina into the upward flow of gas. The intent is to have the gas-solid mixture homogenize across the duct within the reaction zone to ensure adequate gas-solid contact for adsorption. The solid-laden flow is then directed into a hopper where an abrupt expansion reduces the flow velocity, allowing larger particles to settle out for removal. Smaller particles remain suspended to follow the flow and deposit on the bag filters, providing a final opportunity for toxin adsorption. The bag filters are pulsed periodically to remove deactivated solids and scale, allowing fresh material to deposit. The cleansed gas stream passes through the bag filters and leaves the scrubber for venting to the environment.

CFD enables injector geometry to be optimized to improve solids distribution and, thus, quality of gas-solid contact.

The computational mesh shown in Figure 1 uses a generalized polyhedral element meshing approach. The mesh was generated using the STAR-CCM+ development suite. Approximately 400,000 polyhedral cells resolve the flow and the viscous boundary layers. The bag filters were modeled as a porous zone that enforces the experimentally observed pressure drop. The turnaround time from submission to converged solution using 20 processors on a Cray® CX-1® supercomputer was approximately 5 hours. Approximately 8 hours of preprocessing was required to set up the initial case. The first solution can be turned around in less than 1 day.

Examples from the flow solution showing streamlines and total solids distribution are provided in the middle and right images, respectively, of Figure 1. The streamlines show significant swirl in the duct after the elbow and in the hopper, features difficult to predict with simpler design codes. The injected solids mix within the reactor, where high quality contact between the gas and the injected alumina is desired. CFD enables the injector geometry to be optimized to improve the solids distribution and, thus, the quality of the gas-solid contact. The alumina recycle rate for this computation is six parts used alumina to one part new alumina, leading to a relatively high solids loading. The gas-solid mixture exhausts to a hopper. Without any turning vanes to redirect the flow, the alumina-laden jet impinges on the opposite wall. CFD could be used to optimize a set of turning vanes to improve the distribution of alumina in the hopper.

Figure 2 shows alumina distributions by particle size. The 20 µm particles disperse throughout the hopper. The larger particles deflect upward to impinge on the filter bags. This notional configuration would be expected to form scale on the filter bags, to have significant wear on the filter bags, and to exhibit poor performance.

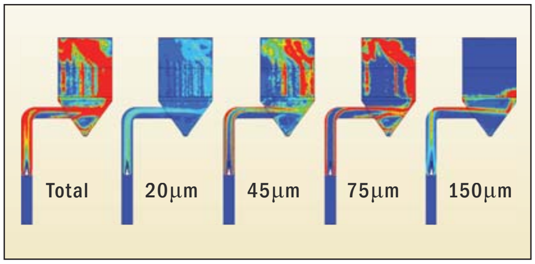

Figure 2. Alumina Distribution, by Particle Size, in the Dry Scrubbing Unit

Benchmarking

There is only limited CFD model benchmarking for dry scrubber simulations. Those comparisons show that CFD can accurately predict the total pressure drop across the dry scrubbing unit and the velocity distribution across the duct.

GAS-LIQUID FLOWS

Introduction

An example of a gas-liquid flow may be considered by picturing a mischievous child with a glass of water containing a drinking straw. At some instant, the curious child takes a deep breath and blows as hard as possible into the straw. Initially, the water inside the straw accelerates until all water is expelled from the straw into the glass. Subsequently, air is released into the glass. Bubbles form rapidly and rise toward the free surface.

Moving from the kitchen to a large industrial production facility, consider a large liquid-filled process vessel containing a small pipe used to remove the liquid from the vessel. Due to the vertical extent of the pipe, any gases generated or released within the liquid tend to collect at the highest local point within the pipe network. If these gases are combustible, a small ignition source could initiate a deflagration. Because the flame would be propagating within a confined space, if the gas mixture is detonable, a sufficiently long gas pocket could provide the flame enough run-up distance for it to transition to a detonation.

The gas-liquid flow illustrated here begins with a gas-phase detonation inside a submerged pipe. Sitting within a large liquid-filled vessel, the pipe contains both a detonable gas mixture of hydrogen and oxygen and the liquid. **Figure 3** shows two piping configurations, one fitted with a vertical pipe and one fitted with a compound, semi-horizontal pipe. The detonation is presumed to have initiated on the far side of the semi-horizontal pipe network where the reactive gas mixture resides. The detonation propagates toward the pipe end submerged within the large vessel, whereupon it collides with the stationary liquid. Upon colliding with the liquid, the reflected detonation causes an extremely large, short-term pressure peak at the gas-liquid interface that begins to accelerate the liquid into the vessel.

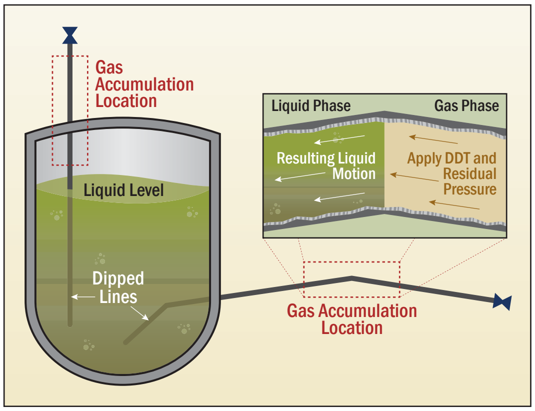

Figure 3. Straight and Bent Routing Configurations

Subsequent to this peak pressure and a rapid exponential decay, longer-term sustained pressures associated with the high temperature of the combustion products continue to accelerate the liquid from the pipe. High-velocity liquid ejected from the pipe acts as an impinging jet on the vessel bottom. Immediately after the liquid is ejected, the high-pressure combusted gases that accelerated the liquid are themselves vented into the vessel. A gas-phase, radial-wall jet is momentarily formed at the vessel bottom. As the velocity of the radially propagating gases decay, buoyancy takes over and causes a brief but strong bubble plume.

Loads are applied to the piping, supports, and vessel internals not only by the high pressures generated by the detonation, but also by the stagnation pressures associated with high velocity liquid impacting structures and high amplitude acoustic waves caused by the gas motion within the vessel. Additional forces, not included in this discussion, are generated by the drag and added mass associated with the local flow velocities and accelerations adjacent to internal items such as piping. Given the potential for peak detonation reflection pressures of hundreds of atmospheres, the destructive potential from gas-phase detonation events in liquid-filled piping networks is enormous.

This example demonstrates the importance and utility of using multiphase CFD models to help understand the forces caused by a potential detonation. The hydrodynamic loading mechanisms discussed here are of interest as an aid to piping system and pressure vessel designers in designing support structures, vessel internal structures, and vessels that can safely and adequately sustain the loads produced in the event of a gas-phase detonation inside the piping system.

Immediately after the liquid is ejected, the high-pressure combusted gases that accelerated it are vented into the vessel. A gas-phase, radial-wall jet is momentarily formed.

CFD Model

For the example under consideration, rather than computing the deflagration-to-detonation transition (DDT) event, the application of the CFD model begins with a time-dependent static pressure boundary condition at the gas-liquid interface within the pipe. The simulation is accomplished using the VOF models in FLUENT v6.3, coupled with a user-defined function (UDF) containing an equation-of-state that permits sound transmission through liquids. Based on these configurations, two CFD geometries are created, as shown in **Figure 4**.

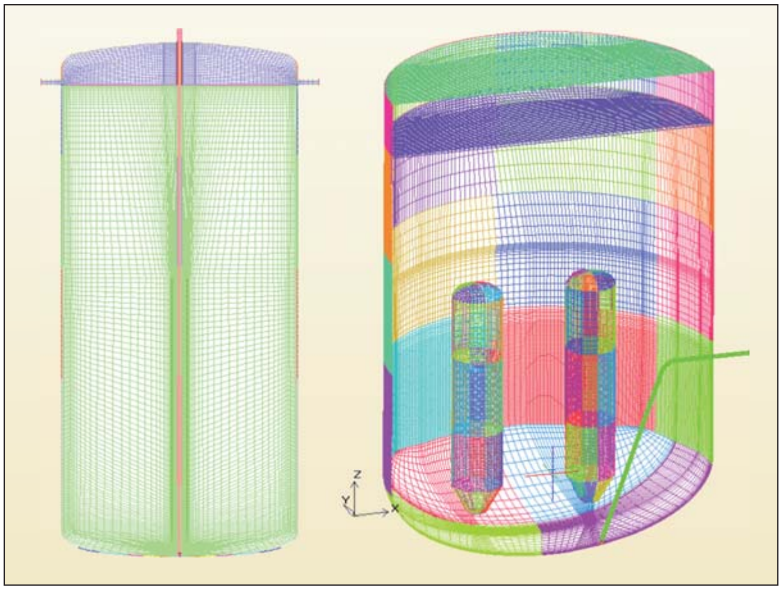

Figure 4. CFD Grid Used in a Study of a Detonation Aftermath in Straight Routing and Bent Routing

To avoid computing the detonation itself, the pressure–time-history curve representing the static pressure seen at the gas-liquid interface during and subsequent to the detonation reflection is found for an initial gas pressure of 2.38 atmospheres (atm) absolute and gas pocket length of 408 inches (34 feet). The static pressure is prescribed as a very brief period where an extremely large pressure is felt by the liquid, followed immediately by an exponential decay toward the system's deflagration pressure. This static pressure profile is imposed as a boundary condition in the CFD model.

For the liquid ejection example under consideration, there is reasonable agreement between the Mathematica integration results and CFD simulations.

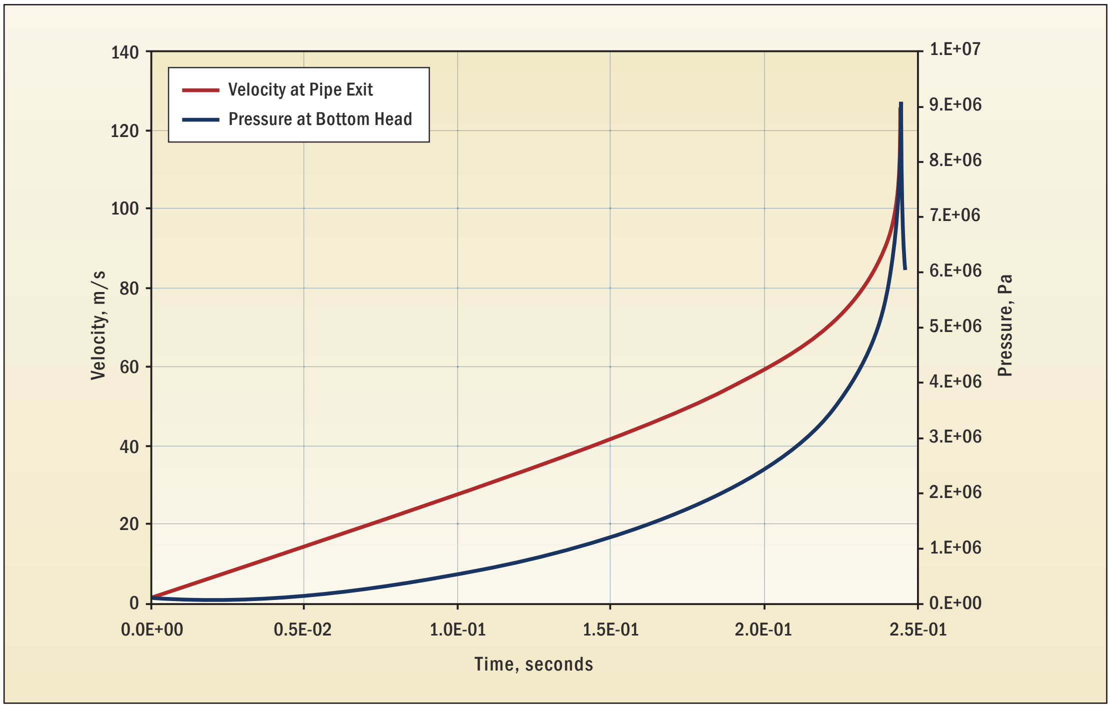

Figure 5. Pipe Exit Velocity and Stagnation Point Pressure on Vessel Bottom from CFD

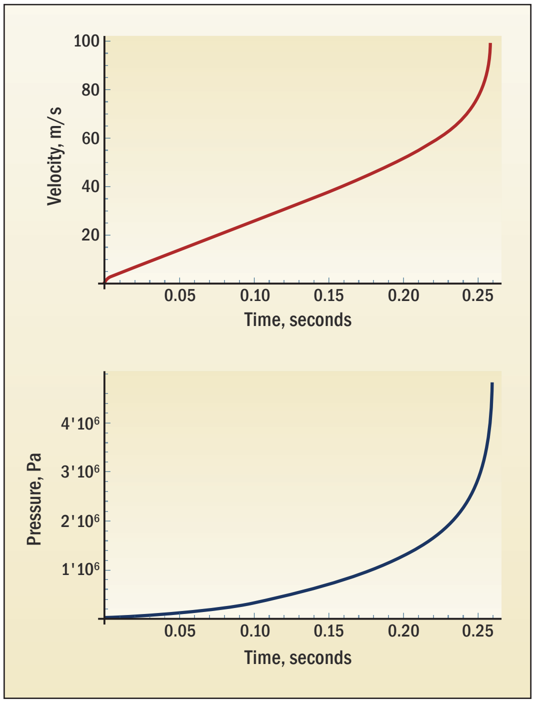

Figure 6. Solution of One-Dimensional Equations Using Mathematica: Pipe Exit Velocity (top) and Stagnation Point Pressure (bottom)

Liquid Ejection

Based on the specified gas-liquid interface pressure boundary condition above, the liquid inside the pipe is rapidly accelerated until all liquid is ejected from the pipe. **Figure 5** shows both the pipe exit velocity and the stagnation point pressure seen on the impingement wall, as derived from the CFD calculations.

Wolfram Research Inc.'s computational application, Mathematica® (v5.2), is used to validate the time-dependent pipe exit velocity and stagnation point pressure results, using an integration of the one-dimensional momentum equation in time. The main parameters for comparison are the pipe exit velocity and the stagnation point pressure at the bottom of the pressure vessel. **Figure 6** shows both velocity and stagnation point pressure from the Mathematica runs as a function of time. It is observed that there is reasonable agreement between the Mathematica integration results and the CFD simulations shown in Figure 5.

Gas Ejection

Stagnation Point and Bubble Plume Characterization

The exiting gas from the nozzle creates a bubble that rapidly floats to the surface after the deflagration event. Upon final ejection of the gas-liquid interface across the plane of the pipe exit, the gas-phase ejection begins. Due to the high gas pressures, the gas-phase initially vents into the vessel with a choked condition at the pipe exit. To better understand the frequency content of the stagnation point pressure field, a fast Fourier transform (FFT) is performed on the pressure field at the stagnation point. The dominant stagnation point frequency is observed at about 425 Hz (**Figure 7**). The frequency of the bubble plume is obtained by performing an FFT of pressure forces on an internal object at a later moment, after the gases have fully vented from the pipe. The FFT of the bubble plume gives a frequency of about 40 Hz (not shown).

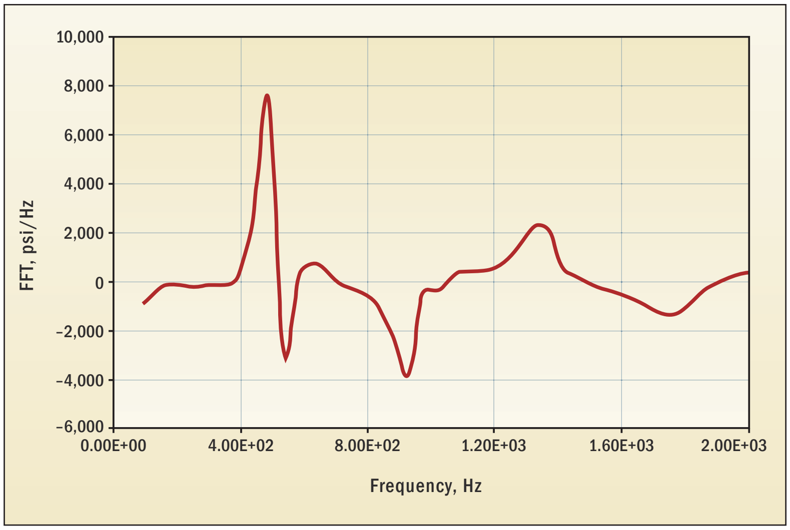

Figure 7. FFT of Stagnation Point Pressure Signal

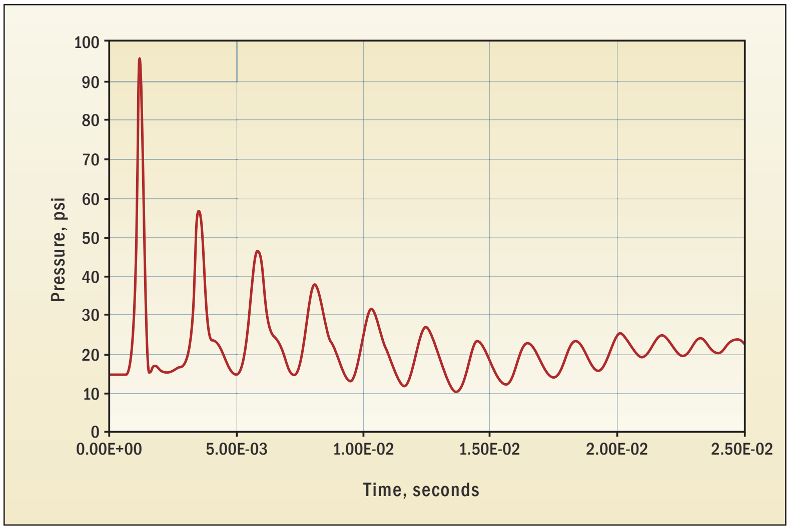

Figure 8. Acoustic Pressure Waves in the Vessel Emanating from the Explosion in the Nozzle

To validate these results, a CFD simulation was performed on a substantially different vessel configuration where a large, high-pressure gas venting event occurred. Because pressure sensor data was available for this event, CFD results could be compared to the experimental values. Omitting details of the event, CFD matched pressure frequencies quite well but appeared to over-predict pressure amplitudes by ~20%.

To validate FFT stagnation point and bubble plume characterizations, a CFD simulation was performed on a substantially different vessel configuration where a large, high-pressure gas venting event occurred.

Peak Loading

To get realistic estimates of the net loading to internal components during this rapid transient event, the peak pressure gradient magnitude is considered as well as the peak spatial differences in pressure. Each can be expressed in both a spatially and temporally varying manner. The acoustic waves emanating from the pipe exit in a series of diminishing pressure wave amplitudes is seen in **Figure 8**.

Subsequently, pressure differences on an internal object experience up to Δp_{max} = 1.5 psi during the bubble plume phase of the event. Acoustic forces applied to internal components within the vessel by the initial 425 Hz gas venting are computed using

$$F_{Acoustic} = S_{Factor} * A_{X\text{-}Section} * L_{Thickness} * |\nabla p|_{max},$$

where S_{Factor} is a safety factor, $A_{X\text{-}Section}$ is a cross-sectional area of an internal component relative to the incoming disturbance, and $L_{Thickness}$ is the component's thickness. Values of the maximum pressure gradient are significantly higher inside the venting gas than in the liquid. Once in the liquid, the maximum pressure gradient is seen to decay as approximately $r^{-5/3}$. This implies that this loading mechanism is more relevant to objects at the bottom of the vessel.

Forces imposed on vessel internals during the 40 Hz bubble plume phase of the event are given by

$$F_{Bubble\ Plume} = S_{Factor} * A_{X\text{-}Section} * \Delta p_{max},$$

where the force is taken to depend on the maximum observed pressure change on the surface of an internal object. These forces are largest in the upper portions of the vessel.

Using this approach, a realistic and standardized load-time curve was obtained that was implemented for all pressure vessels having internal items in finite-element stress calculations.

The approach used to determine peak loading yielded realistic and standardized load-time curve that was implemented for pressure vessels having internal items in finite-element stress calculations.

SOLID-LIQUID FLOWS

Introduction

Particle-laden liquids are a common occurrence in nature and in engineering systems. Sediment transport in rivers and unwanted soil erosion are important contexts where particle-laden liquids are of concern. In the chemical process industries, slurry flows are common. However, from the point of view of CFD, they have received considerably less attention than particle-laden gas flows. Consequently, there are fewer validation data sets available with which to calibrate CFD models. Among the many differences between particle-laden liquid and gas flows is the significance of freestream turbulence effects on the ultimate flow behavior. To investigate this, a stirred vessel is considered where freestream turbulence levels are extremely high and several experimental datasets are available.

Stirred Vessel with Solids

This section presents the results of a study that compares CFD simulations to experiments for solid-liquid flows in a lightly loaded pitch-bladed turbine test case described in [3 and 4].

Experiment Description

In this study, a 0.48-meter-diameter by 1.44-meter-high cylinder served as the testing medium for the acquisition of experimental data. The flow in the experiment was fully turbulent and was lightly loaded with a value of 4% average volume fraction. Tests were was conducted in a laboratory by the Mixing Research Group in the Chemical Engineering Department at the University of Bologna in Italy using 327 µm spherical glass beads with a specific gravity of 2.45. The test vessel, seen in **Figure 9**, consisted of four baffles and incorporated three pitch-bladed turbines to provide mixing energy to the system. Water was used for the working fluid in this experiment.

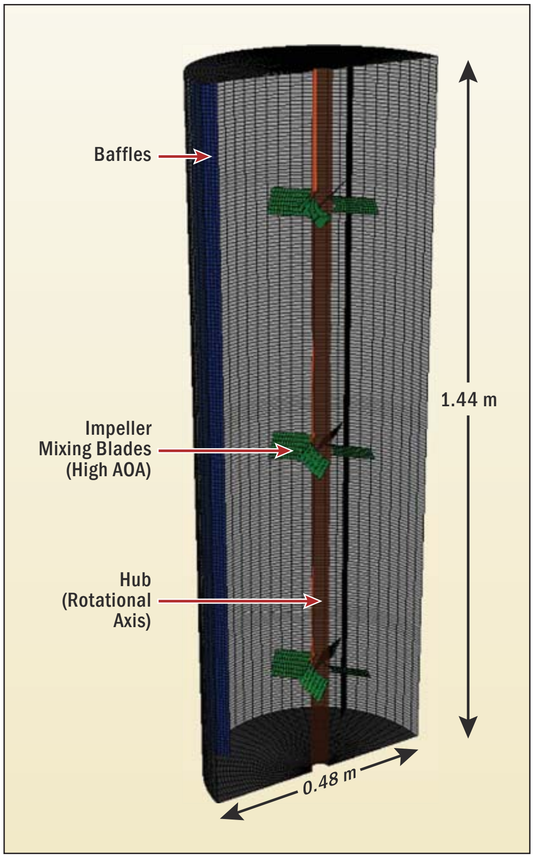

Figure 9. CFD Model

The experiment was conducted with an impeller rotational speed of 475 rotations per minute, which corresponded to the just-suspended velocity of the particles being studied. This speed essentially defined the lowest power input at which the system could operate without solids settling at the bottom of the vessel. Particle concentrations were measured using an optical technique that employed a laser diode coupling to measure the attenuation in light as it traversed the vessel cross-section.

CFD Model

A series of parametric studies that varied the CFD model settings were conducted to determine which settings in FLUENT v12.1 yielded results closest to experimental data. To summarize, it was shown that the virtual mass term had virtually no impact on the solution and that choosing between cell- and node-based spatial discretization of the gradient had minimal effect on the final concentration profile. Moderate sensitivity in the overall concentration profile was observed by changing the turbulence model and the spatial derivative operator. The greatest sensitivity with regard to solution outcome was dependent on the interphase momentum transfer treatment. In terms of physical models, the standard k-ε turbulence model with nonequilibrium wall functions yielded results closest to the experimental data.

Further Studies on Interphase Momentum Transfer

FLUENT v12.1 offers three choices for the interphase momentum exchange term in solid-liquid flows. These are described in [2]. While each includes a Reynolds number and a particle volume-fraction dependence on particle drag, none accounts for particles traversing freestream turbulence. To include this effect, two corrections are needed. The first effectively corrects the particle slip velocity, while the second accounts for modifications to the boundary layer and wake of the local particle flow field that are caused by the freestream turbulence.

Using the text-user interface (TUI) in FLUENT v12.1, the momentum dispersion force is invoked to address the particle slip velocity problem. [4] This term is only appropriate at low particle volume fractions where the turbulence is unaffected by the particles. To correct for modifications to the drag coefficient caused by freestream turbulence, the Gidaspow drag model (including an improved stitching function) is coded into a UDF and supplemented with a model by Fajner et al. [5] Freestream turbulence corrections in this model are conditioned on the ratio of the particle diameter to the local Kolmogorov length scale of the fluid turbulence. When the Kolmogorov length scale is larger than the particle, no correction is made to the particle drag coefficient. As the Kolmogorov length scale becomes smaller than the particle, the drag coefficient is reduced initially. When the Kolmogorov length scale becomes an order of magnitude smaller than the particle, the drag increases (following [5]).

Figure 10 compares particle concentrations in the stirred vessel measured experimentally as a function of normalized height to those computed by FLUENT for several different model choices. The first step was to test the UDF implementation of the Gidaspow model relative to the one internally coded into FLUENT. At higher particle volume fractions, the effect of the improved stitching function may be seen. While it appears that the UDF implementation of the Gidaspow model matches the one in FLUENT, the comparisons to the experimental results are quite poor. This can be seen not only from visual inspection but also by realizing that the area under each curve should be the same. Even after

The greatest sensitivity with regard to solid-liquid flow solution outcomes was dependent on the interphase momentum transfer treatment.

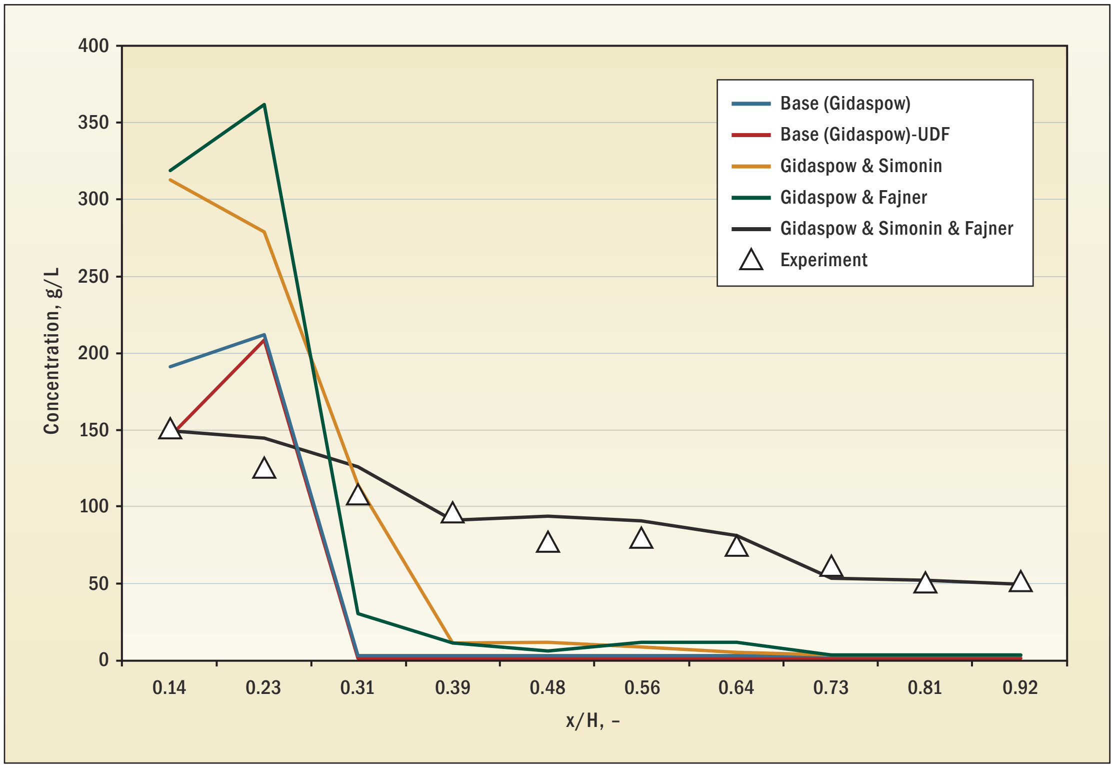

Figure 10. Particle Concentrations as a Function of Normalized Vessel Height for Experiment and CFD Depending on the CFD Treatment of Freestream Turbulence in the Interphase Momentum Transfer Term

correcting the particle slip velocity or the particle drag coefficient while using the Gidaspow model, the comparisons to the experimental results are still poor, but the respective areas under the curve are now closer to the experimental. Finally, by using the Gidaspow model in conjunction with both the slip velocity and particle drag coefficient corrections, the CFD model compares very well to the experimental.

Computer-based engineering tools such as CFD provide tremendous insight into flow details that are inaccessible using simpler approaches.

CONCLUSIONS

Multiphase processes span many different industry applications. In 2010, Bechtel National Inc.'s Advanced Simulation and Analysis group used multiphase simulation to service projects for four of Bechtel's five global business units: Bechtel Systems & Infrastructure, Inc.; Mining & Metals; Power; and Oil, Gas & Chemicals. Those projects spanned gas-solid, gas-liquid, and gas-solid-liquid systems. The simulations were conducted within project schedule and budget, showing that state-of-the-art multiphase flow CFD is a viable engineering design and forensics tool.

The three examples presented in this paper represent three types of multiphase flows: solid-gas, gas-liquid, and solid-liquid. The first example demonstrates how CFD can be used to learn how particles of differing size follow different flow paths in the same geometry—very important to process requirements—and indicates where CFD could be applied to design improvement. The second example shows CFD's utility in difficult environments with numerous unknowns that would overwhelm many other methods. The rapid expansion and bubble rise of a gas in a liquid, where both the gas and the liquid need to be simulated as compressible flow fields, is ideally suited for CFD. The third example, where solids mix in a liquid, demonstrates the importance of knowing the relevant physics among the many modeling choices available. The comparison to experimental data confirms the knowledge and experience of, and the need for, the technical specialist.

Computer-based engineering tools such as CFD provide tremendous insight into flow details that are inaccessible using simpler approaches. Used in conjunction with a well-founded V&V process, these details enable improved engineering designs with tighter margins and reduced costs. One company reports a sixfold return on investment as a result of using CFD throughout various design phases. [6] Wherever the potential for high risk/exposure exists and design uncertainty must be reduced, CFD is an enabling technology. Bechtel is at the cutting edge of bringing multiphase CFD into mainstream engineering. ■

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ADDITIONAL READING

The following additional information source was used to develop this paper:

- O. Simonin, E. Deutsch, and J.P. Minier, "Eulerian Prediction of the Fluid/Particle Correlated Motion In Turbulent Two-Phase Flows," *Applied Scientific Research*, Vol. 51, 1993, pp. 275–283, purchasable at http://www.springerlink.com/content/m178j517v8452624/.

BIOGRAPHIES

Christopher Kennedy, PhD, is a senior engineering specialist whose focus is computational fluid dynamics. He works with the CFD team in Bechtel National, Inc.'s Advanced Simulation and Analysis group. Most of his nearly 5 years at Bechtel have been concentrated on the topics of gas-phase detonations and multiphase mixing at the Waste Treatment Plant being built in Richland, Washington, to clean up one of the world's largest concentrations of radioactive waste, a legacy of Cold War nuclear weapons production.

Chris holds a PhD and an MS, both in Applied Mechanics, from The University of California, San Diego. His BA, in Natural Sciences, is from the Johns Hopkins University, Baltimore, Maryland.

Philip Diwakar is a senior engineering specialist for Bechtel National, Inc.'s, Advanced Simulation and Analysis group. He employs state-of-the-art technology to resolve a wide range of complex engineering problems on large-scale projects. Philip has more than 15 years of experience in CFD and finite element analysis for structural mechanics. His more recent experience includes work on projects involving fluid-solid interaction.

During his 9-year tenure with Bechtel, Philip has received two full technical grants and a mini-grant. One full grant was used to determine the effects of blast pressure on structures at LNG plants, for designing less costly, safer, and more blast-resistant buildings. The other was used to study transient thermal fatigue stresses using fluid-structure interaction in molecular sieve dehydrators, with applicability to other components that may be subject to fatigue failure. Philip has also received four Bechtel Outstanding Technical Paper awards, as well as two awards for his exhibit on the applications of fluid-solid interaction technology at the 2006 Engineering Leadership Conference in Frederick, Maryland. This paper is his third contribution to the *Bechtel Technology Journal*.

Before joining Bechtel, Philip was a project engineer with Caterpillar, Inc., where he was part of a Six Sigma team. He applied his CFD expertise to determine the best approach for solving issues involving the cooling of Caterpillar heavy machinery.

Philip holds an MTech in Aerospace Engineering from the Indian Institute of Science, Bengalaru; a BTech in Aeronautics from the Madras Institute of Technology, India; and a BS in Mathematics from Loyola College, Baltimore, Maryland. He is a licensed Professional Mechanical Engineer and is a Six Sigma Yellow Belt. His current focus is on LEED and sustainable development.

Leonard (Joel) Peltier, PhD, is a principal engineer in Bechtel's Advanced Simulation and Analysis Group and an adjunct assistant professor of mechanical engineering at the Pennsylvania State University. He has 19 years of experience in applied fluid mechanics, computational fluid mechanics, and numerical heat transfer. At Bechtel, Joel has worked on projects for BSII, M&M, and Power and has been elected to the ASME V&V 20 code committee (Verification and Validation in Computational Modeling and Simulation) as a contributing member.

Before joining Bechtel, Joel worked at the Pennsylvania State University's Applied Research Laboratory, a university-affiliated research center for the US Navy, performing simulations and analyses of turbomachinery and undersea vehicle flows. His research work extended to passive heating of architectural spaces, simulation of arterial stenoses and glottal aerodynamics, and modeling of atmospheric transport and dispersion. His expertise includes steady and unsteady Reynolds-averaged, Navier-Stokes (RANS) modeling; large-eddy simulation (LES); and hybrid RANS/LES techniques, including detached-eddy simulation (DES) and its zonal (ZDES) and delayed (DDES) variants. At Pennsylvania State University, he taught fluid mechanics at the undergraduate and graduate levels, specializing in turbulence theory and turbulence modeling.

Joel holds PhD and MS degrees, both in Aerospace Engineering, from the University of Colorado at Boulder and a BS degree in Chemical Engineering from Princeton University, New Jersey. He spent 3 years as a post-doctoral research associate in the Department of Meteorology at Pennsylvania State University.

Brigette Rosendall, PhD, is a principal engineer and the lead computational fluid dynamics specialist in Bechtel National, Inc.'s, Advanced Simulation and Analysis group. She specializes in multiphase transport phenomenon, heat transfer, and reaction kinetics. For the past 10 years, her focus has been on modeling mixing within vessels for the Waste Treatment Plant being built in Richland, Washington, to clean up one of the world's largest concentrations of radioactive waste, a legacy of Cold War nuclear weapons production.

Brigette has been with Bechtel for 13 years and has supported projects in the Power; Mining & Metals; and Oil, Gas & Chemicals global business units, in addition to Bechtel National. Some key projects include National Missile Defense, the Tacoma Narrows Bridge, Darwin LNG, Atlantic LNG, and Cerro Matoso. She also participated in a technical grant to determine the ability of CFD to model pump intake flow. Brigette has received two Bechtel Outstanding Technical Paper awards, as well as an award for the best exhibit on the application of advanced simulation at Bechtel's 2002 Engineering Leadership Conference in Frederick, Maryland.

Brigette is a member of the board for the Computer Aids for Chemical Engineering (CAChE) Corporation and co-chair of the CAChE CFD Task Force, and has been the industrial director of the National Science Foundation-funded Industry & University Cooperative Research Program (I/UCRC) on Multiphase Transport Phenomenon. She is an adjunct assistant professor of chemical engineering and material science at Michigan State University.

Brigette holds a PhD and an MS in Chemical Engineering from the University of Washington and a BS in Chemical Engineering from Michigan State University.