WHITE PAPER

Enabling Innovation in the Chemical Industry: A Novel Approach

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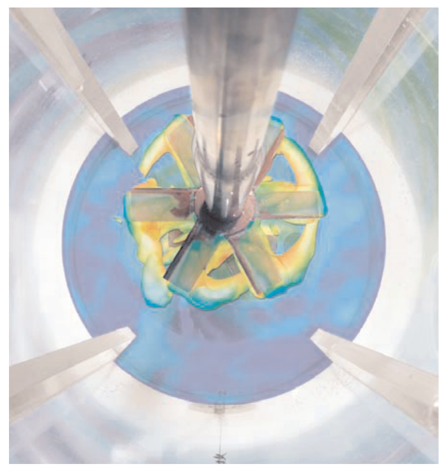
ABSTRACT

As markets expand due to globalization, chemical manufacturers are faced with the challenge of meeting the rapidly growing global demand for production at a time when production costs are increasing due to rising feedstock prices. One way for chemical manufacturers to ensure profitability in the current environment is to foster innovation through the use of advanced modeling techniques. The Chemical Industry Vision2020 Technology Partnership[1] highlights opportunities to address several challenges in the chemical industry through shared pre-competitive research and development activities in many technology areas, and offers a special focus on high-end modeling. In this paper we examine the available technologies in the chemical industry and highlight several areas where major advances have been achieved through innovation fostered by advanced modeling of industrial processes.



Courtesy of Prague Institute of Chemical Technology

INTRODUCTION

The chemical industry is critically important to economies around the world. It touches every aspect of humanity, from clean drinking water to space travel. The chemical industry contributes to more than 2% of the US gross domestic product (GDP) and provides a million domestic jobs. This essential sector of the US economy[2] (see Table 1) is under constant threat from foreign competition, economic fluctuations, and rising feedstock prices. Growth, not to mention survival, in the chemical industry demands a significant stimulus for innovation utilizing technology tools across the board. Under Vision2020, the challenges and opportunities in the chemical industry are being addressed through shared pre-competitive research and development activities in many technology areas. This effort has helped to build shared knowledge through network-

Table 1: Industry Snapshot	
Value of Shipments	$435.40 billion
Employment	$1.04 million
Capital Expenditures	$14.80 billion
Net Trade Balance	$8.28 billion
Net Energy Consumption	6.30 quads

Source: American Chemistry Council

ing among industry, academia and government. A core technology identified by this initiative is computational fluid dynamics (CFD). CFD is a strategic innovation tool that the chemical industry has come to rely on to maintain and foster technology to meet economic challenges. In this paper we highlight some of the ways that CFD is being used by the industry leaders to innovate. The broad range of applications where CFD is accepted as an essential engineering and innovation tool include batch and in-line mixers, bubble column reactors, fluidized bed reactors, trickle-bed reactors, packed beds, crystallizers, solids dissolution and suspension equipment, all separation processes, pneumatic conveyors, classifiers, desolventizers, sprays, spray dryers, scrubbers, fuel cells, crackers, furnaces, heat exchangers and emission control devices.

CHEMICAL INDUSTRY LANDSCAPE

In general, the chemical industry trades on two broad classes of products: bulk and specialty chemicals. The bulk chemicals market is characterized by low margins and high volumes, whereas specialty chemicals are generally produced in lower volumes and command higher prices. Most chemical companies have refocused their R&D efforts and sustainable growth strategies over the past few years to keep pace with the changing business landscape. For example, in 2001, while referring to the chemical industry in general, then chairman of the Dow Chemical Company, William S. Stavropoulos, was quoted on acs.org3 calling for revitalizing R&D as an engine for growth. In 2005, Dow had a record growth in net income of 61% over 20044. In 2002, DuPont reorganized their R&D activities. DuPont's revenues resulting from new products increased from 20% in 2000 to 30% in 2004. Over this time period DuPont's R&D expenses remained steady at $1.3 billion5. The key to such successes was the increased focus on innovation in R&D.

In addition to benefiting from R&D, the chemical industry continues to invest in and benefit from technology solutions in the areas of energy optimization, production efficiency, reduction of downtime, reactor scale-up and troubleshooting[2].

CFD-based strategies allow chemical & process companies to improve revenue growth (top line) while lowering costs (improve bottom line) through:

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- Enhanced operating performance
- Better unit operation reliability
- More confident process scale-up
- Enhanced product consistency
- Increased plant productivity
- Deeper technical knowledge and understanding of unit processes
- Lower equipment downtime for maintenance
- Compliance with health, safety and environmental regulations

THE ROLE OF CFD IN THE INNOVATION PROCESS

Whether it is tuning of solvents in an ink-jet printing technology, mixing of miscible fluids, scaling up reactors, or any of the dozens of other areas where CFD is applied, innovation is influenced and facilitated by flow modeling. Technical advances contributing to the wider use of simulation tools have progressed in two distinct directions. Firstly, more complex and reliable physical models have evolved rapidly in recent years. Secondly, CFD analysis has been extended to non-expert users through the deployment of custom desktop and enterprise software tools that are based on CFD. The latter trend has permitted smaller chemical companies to make use of flow modeling and larger entities to take full advantage of the power of the technology by deploying its use throughout the organization.

"Engineers who scoffed at CFD analysis a year and a half ago now prefer that design changes be evaluated using CFD before being tried in the field. Computer simulation using Fluent's CFD software made it possible to triple the efficiency of equipment design engineers while improving the quality of our product."
– Phil Staples, DuPont, 2000

GAS-SOLIDS AND PARTICULATE FLOWS

CFD methods that account for the presence of secondary phases are well established. Recent advances in such methods now enable simulation of flows with very high solid loading such as hoppers, chutes, and particle milling, and also gas-solid flows with particle size and number density variations such as polymerization reactors.

The effect of particle shapes and particle mechanics can be accurately captured in CFD models. It is now possible to gain insight into the fates of individual particles. Calculation of particle motion, particle size, bed porosity, particle-particle interaction, and other hydrodynamic concerns is currently tractable. More advanced models can account for particle cohesion, attrition, and other prescribed phenomenological attributes.

Gas-solid reactors commonly include an internal tube bank to control the flow and add heat and/or gas to the bed. The presence of the internal tube banks alters the flow patterns and can cause the bubbles in the bed to collide, leading to coalescence or break-up. Three-dimensional simulations of reactor beds are desired to achieve a good understanding of the effects of the internals and assess possible erosion rates on the walls and components.

Insight into reactor performance through such models significantly improves reactor performance and efficiency, and therefore improves a company's bottom line. For example, reactor designs can be modified to reduce erosion, and thus improve equipment safety. Improving equipment safety reduces the possibility of the economic penalties that might be incurred through lawsuits and bad publicity associated with accidents. Additionally, extending the life of equipment allows higher product volumes without having to replace the equipment as often, saving considerable cost.

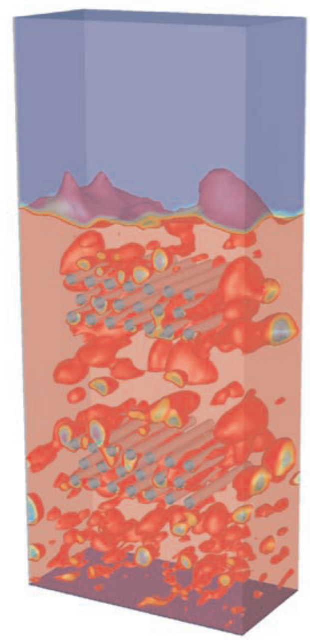


Figure 1: Iso-surfaces of gas volume fraction in a fluidized bed reactor

Figure 1 shows a snapshot of a time-dependent simulation of a rectangular crosssection fluidized bed including two sets of tube banks. Iso-surfaces of gas-volume fraction (shown in red) illustrate that gas bubbles formed within the bed are broken up as they pass through the tube banks, but not where they pass around the sides. With increased confidence in models for dense bed fluidization, the knowledge gained about the distribution of the gas-solid volume fractions helps in debottlenecking design and operation issues. A recent publication by Derek Colman from British Petroleum addresses many of these issues like fluidization, variation in drag, bed effective viscosity, solids pressure and heterogeneous chemical reactions[6].

DESIGNING SIZE DISTRIBUTION IN MICRO-EMULSIONS

Tailoring real-life complex fluids such as emulsions to achieve specified target properties is an active business driver in the chemical industry. The properties of such emulsions are based on the droplet size distribution (DSD) of the dispersed phase. Because they are often thermodynamically metastable, there is a persistent threat that the texture of the emulsion will be altered during the course of preparation or packaging, or during the subsequent shelf life. Many processes over widely varying length scales could cause the DSD to change, and it is important that they be well understood so that the emulsion quality can be maintained.

As an example, one ongoing project involves studying several aspects of droplet behavior using the volume of fluid (VOF) model in CFD software. Some of the results have been compared to experiments carried out on microfluidic

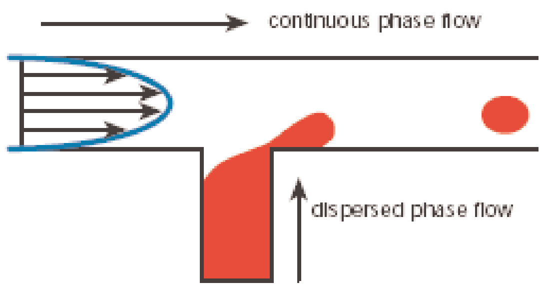


Figure 2: Schematic of the experimental setup7

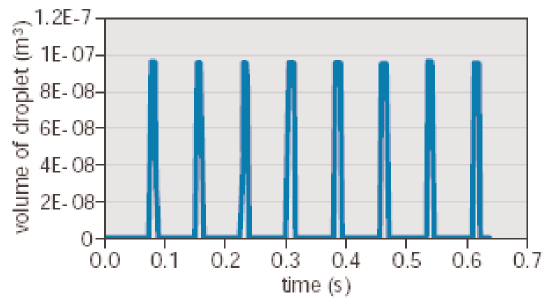
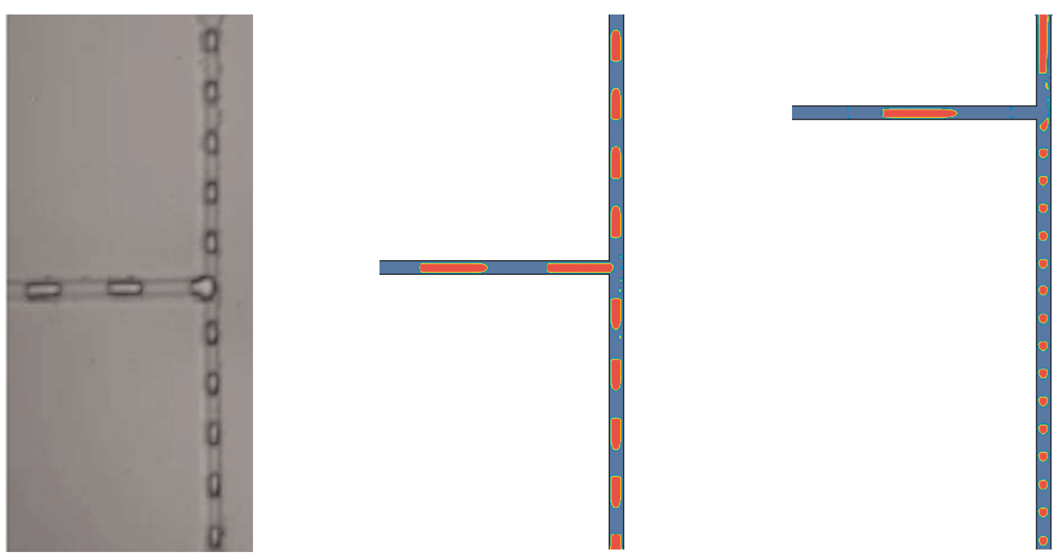


Figure 3: Volume of droplets produced at the T as a function of time

devices capable of generating a precise droplet size distribution. Figure 2 shows an example where the generation of droplets at a T-junction using two streams of immiscible liquids has been simulated. Figure 3 illustrates that droplets of uniform size were rapidly produced at the junction in a consistently repeatable manner as a result of the surface tension and the shearing motion of the fluid in the main channel, in agreement with measurements.

In another study, the geometrically mediated breakup of droplets in a microfluidic device8 was simulated. By changing the position of the arms of the T-junctions shown in Figure 4, the droplet can be split into daughter droplets of unequal size. By using a network of asymmetric T-junctions, emulsions of a given DSD can be produced. Both 2D and 3D simulations matched the qualitative and quantitative aspects of the experiments, such as the size of the daughter droplets for a given T-junction and the critical parameters required for droplet breakup as a function of capillary number.

The ability to ensure droplet size uniformity leads to improved products and increased customer satisfaction. Additionally, the ability to predict droplet size formation reduces development costs and time to market compared to physical experiments, providing a competitive advantage to those who employ CFD.



a) b) c)

Figure 4: Experimental validation of droplets breakup: a) symmetric experiments[7]; b) symmetric FLUENT simulation, and c) asymmetric simulation showing different droplet sizing through the T-junctions[9]

CRYSTALLIZATION IN STIRRED TANKS

One of the main challenges in industrial crystallizers is to control the crystal size distribution (CSD). CSD control is important to ensure product quality and purity and the successful operation of the crystallizer. It often affects downstream processing such as filtration, centrifugation, and milling. In spite of its importance, CSD is not well understood. Part of the difficulty is that the size distribution varies in space and time in a crystallizer due to non-ideal flow patterns and heat transfer. Solution thermodynamics and crystallization phenomena also play a role.

Process time scale, reactor opacity, and the inconvenience and intrusive nature of in-situ experimental assessments are some of the formidable obstacles that prevent full understanding of the process dynamics within the crystallizer stirred tanks. CFD is an attractive alternative approach to understanding the hydrodynamics. However, it requires additional capabilities to account for the coupled effects of fluid mechanics and crystallization phenomena in order to analyze the crystal population balance in the tank. The crystal population balance alters the local fluid properties and hence the hydrodynamics, which in turn influence the CSD. Population balance models that quantitatively monitor nucleation, growth, dissolution, aggregation and breakage make it possible to account for the coupling between the CSD and hydrodynamics.

Fluent, Dow Chemical, and the University of Utah worked together to model a pilot scale crystallizer at Dow's Ludington facility, shown in Figures 5 and 6. The physical process is the enrichment and purification of a stream that is rich in chlorides of calcium ($CaCl_2$), sodium (NaCl) and potassium (KCl) by crystallization of NaCl and KCl, which are considered impurities. The inlet stream is a mixture of 20% $CaCl_2$, 45% KCl, and 1% NaCl. It also contains 2.7% NaCl particles with a Sauter mean diameter of 122 microns. The objective was to further reduce the NaCl in the solution to about 0.42%. The jacketed reactor is cooled to 300 K with the inlet stream at approximately 325 K. The solubility curve of NaCl, which is linear with temperature in this range, was obtained using Stream Analyzer from OLI Systems, Inc.

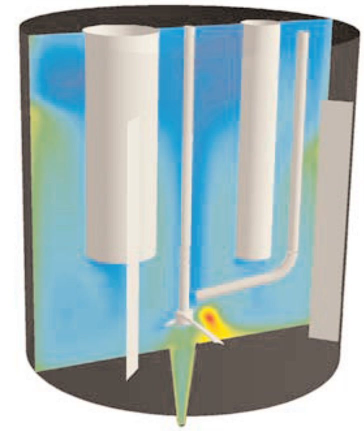


Figure 5: Super-saturation profile shows high degree near the solute inlet where there is ample supply of solute

Figure 6: NaCl crystal volume fraction isosurface superimposed on the liquid phase velocity field in the tank

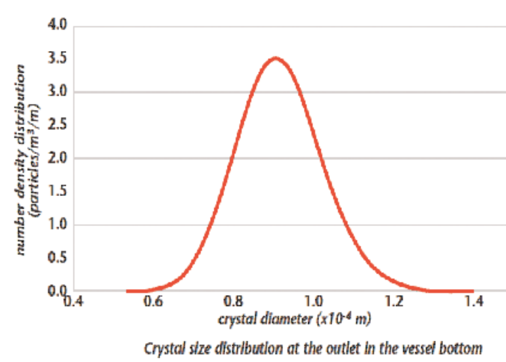


Figure 7: Outlet crystal size distribution at the tank bottom

The Eulerian granular multiphase model in the CFD software was used in conjunction with the population balance solver. The rotation of the impeller was simulated using the multiple reference frames (MRF) approach. The constituents NaCl, $CaCl_2$, and KCl in water were each modeled as a species in the primary phase. The vessel had a curved feed tube, baffles on the walls, and two dip filter cartridges where clarified liquor was removed by collecting crystals on their surfaces. Results showed that as the NaCl solute entered the cooler reactor, it was quickly consumed to form crystals. At the outlet, the mass fraction of NaCl in solution was 0.37%, compared to 1% at the inlet, indicating a purification of the solution. The solids volume fraction showed some settling and collection at the outlet filter. At the bottom of the crystallizer, the amount of solids was 3% and the Sauter mean diameter of the crystals was 133.8 microns, almost 10% larger that the size at the inlet. Results show that the region containing the maximum number density of the crystals is located close to the inlet where there is ample supply of solute and a high supersaturation ratio. The crystal size distribution at the outlet is in good qualitative agreement with observations.

The ability to predict crystal size distribution through flow modeling provides insight into the processes occurring in the crystallizer and can lead to improved crystallizer performance. Improved performance leads to higher revenues through increased production, and improved product quality and consistency through control of the CSD.

CUSTOM TOOLS FOR PROCESS ENGINEERS

The basic requirement of custom analysis and visualization tools for process engineers is to ensure that these tools are able to provide reliable, predictive answers to various "what-if" scenarios for design and operational changes of equipment or processes. The most important benefit of using these tools, aside from their ability to provide answers to a specified problem, is that they eliminate user errors. This allows process engineers with their focused domain knowledge to handle these tools flawlessly without needing to learn the intricacies of flow modeling, thus eliminating any formal CFD learning curve. The end result is increased equipment uptime, reduced time to market, and reduced development costs.

Some of the application areas that have benefited from custom tools with extremely high return on investment have been die design templates, mixing analysis tools, spray dryer simulators, cyclone separator design tools, a continuous fiber module, and a host of custom engineering analyses involving free surfaces, multiple phases, phase change, suspensions, emulsification and phase inversion, and flow balancing in complex polymer die flows.

Figure 8 shows an example of a custom mixing tool developed for glass-lined stirred tanks. This tool allows the user to quickly select from a long list of tank internals only those specific impellers, shafts, tanks, baffles and dip tubes of interest. It also allows the user to modify the location and geometric dimensions of all these components. The engineer then inputs the

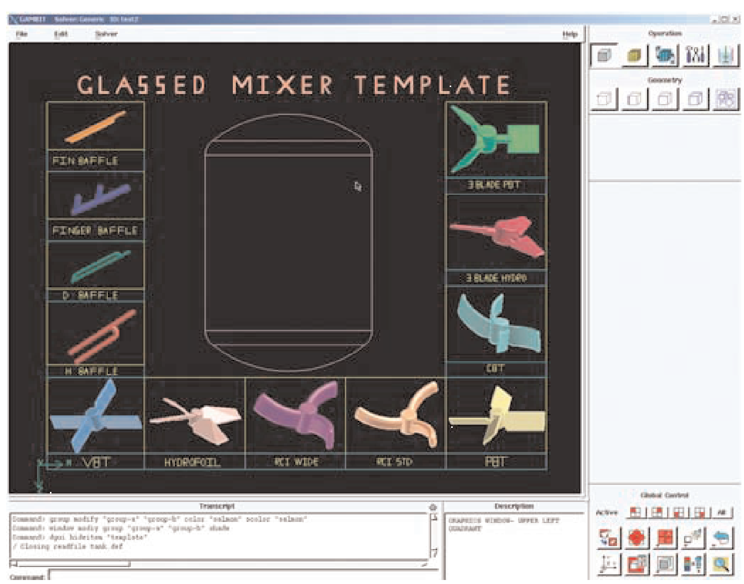


Figure 8: Mixing analysis template for glass lined stirred tanks

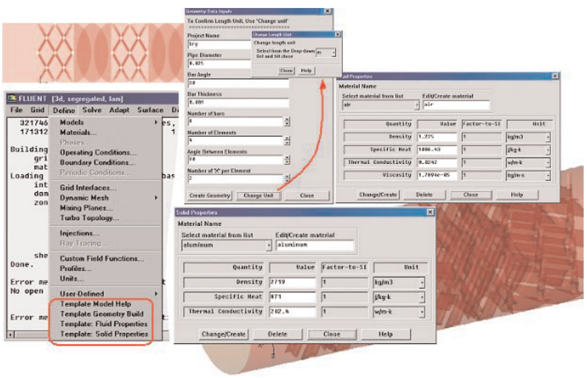


Figure 9: Custom tool to analyze static mixer performance

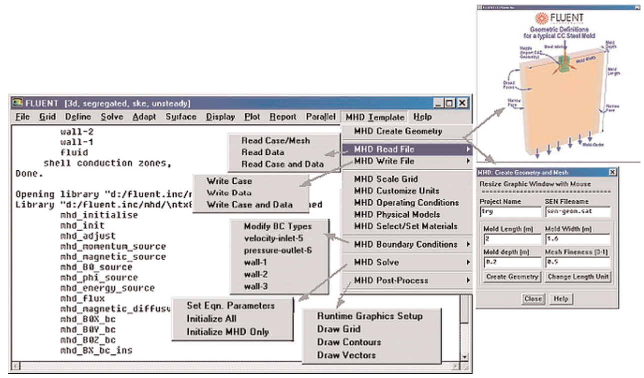


Figure 10: Simulator for magneto-hydrodynamics induced flow in continuous casting of steel

fluid properties, rotational speeds for the impeller and the type of analysis intended. The tool automatically creates the entire geometry, sets up and solves the flow analysis problem, and generates a set of graphics as well as an HTML report with a pre-specified format containing the analysis inputs and results.

Figures 9 and 10 show two other similar custom tools for in-line mixers and magneto-hydrodynamic simulators, respectively.

SUMMARY

Progress in both software and hardware has now enabled CFD tools to reach throughout the chemical industry for both developmental and troubleshooting applications. There are numerous business benefits to using flow modeling technology, including:

profitability through improved operating efficiency;

- increased revenue through higher process throughput;
- increased profitability and revenue through reduction of planned and unplanned maintenance costs;
- faster time to market through more effective scale-up of new process prototypes, leading to competitive advantage and increased revenues; and
- timely and cost-effective troubleshooting of flow-related problems leading to reduced operating costs, increased operational uptime and, ultimately, increased revenues.

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