

First 3D Simulation of Bubble Column Hydrodynamics Paves Way for Commercial Gas-to-Liquid Conversion in Slurry Reactor

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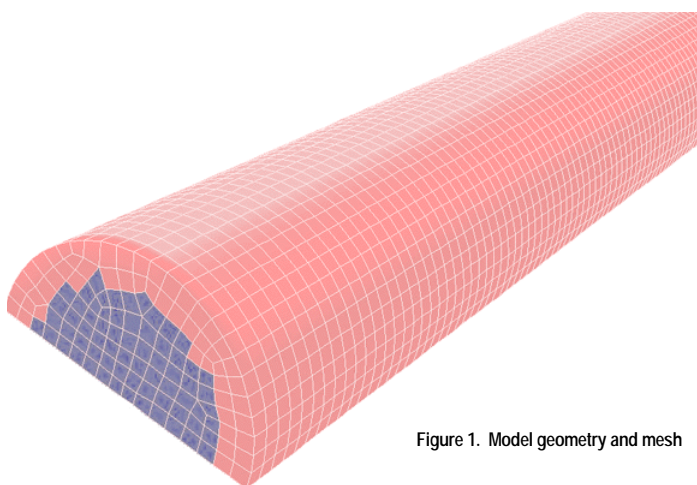


Figure 1. Model geometry and mesh

By achieving 3D simulation of hydrodynamics in a bubble column reactor, engineers at Rentech Inc. have taken an important step towards designing an efficient slurry reactor for large-scale conversion of synthesis gas to liquid hydrocarbons. The simulation allows us to determine gas holdup, a key variable affecting the reaction rate of gas-to-liquid (GTL) conversion using Fischer-Tropsch (FT) chemistry. This information is important because there is the potential for the wide application of FT for conversion of refinery residues, an ever-increasing problem on a world-wide basis. A slurry reactor offers one such method, but detailed knowledge of the hydrodynamics of commercial-size reactors is required. Validated three-dimensional computational

fluid dynamics modeling allows us to simulate a commercial reactor.

Rentech Inc. is an 18-year-old corporation that owns, licenses, and markets a proprietary and patented process that converts syngas, a mixture of hydrogen and carbon monoxide produced from any carbon containing material, into valuable liquid hydrocarbons including diesel fuel, naphthas, and waxes. The Rentech process utilizes an iron-based catalyst in a slurry reactor to affect the GTL conversion. Rentech is one of only four companies in the world that have operated a commercial-scale GTL facility.

One of our goals is to expand the commercial application of GTL technology. The economic benefits of doing this are compelling. For example, petroleum coke, a residual material from the refinery process, contains a concentration of metals and sulfur. The high sulfur and metals in this petroleum coke typically results in a refiner assigning a zero or even negative value to the material. A refinery producing 1500 tons per day of petroleum coke can use gasification of the coke to produce syngas and GTL technology to create about 3000 barrels per day of clean, low sulfur, low aromatics synthesis liquids, including gasoline and diesel. Depending on the

price of petroleum coke and the price of the synthesis liquids a refiner might expect \$20 million additional revenue each year, assuming a petroleum coke value of \$5/ton and synthesis liquids at \$25.00/barrel.

Other important feedstocks for conversion plants using the Rentech technology include natural gas from wells that are not producing due to their remote location, natural gas unsuitable for commercial sale because it contains diluents such as carbon dioxide or nitrogen, oil wells that flare associated gas, and industrial off-gas. These feedstocks are in abundant supply worldwide.

Optimizing a slurry reactor

GTL is a two-step process that begins with the conversion of the feedstock into syngas. The second step is a Fischer-Tropsch reaction, a process invented in Germany in 1923. The Fischer-Tropsch reaction converts the carbon monoxide and hydrogen into a wide range of hydrocarbons from methane to heavy waxes. The Fischer-Tropsch reaction can be carried out in different kinds of reactor vessels. Currently, there is much interest in using a slurry reactor for this process because a slurry reactor is relatively inexpensive to build and operate and they give excellent heat and mass transfer which promote high reaction rates.

A slurry reactor is a vessel containing the catalyst suspended in liquid hydrocarbon. The synthesis gas is brought in at the bottom of the vessel and bubbled up through the reactor. As the bubbles contact the catalyst, the Fischer-Tropsch reaction takes place. The hydrodynamics in the reactor are complicated but understanding them is important to achieving the high reaction rate needed for commercial GTL conversion. To achieve a high mass transfer rate, the goal is to have good gas bubble distribution throughout the reactor with a large interfacial surface area between bubbles and the liquid hydrocarbon media.

In the past, researchers have attempted to understand the hydrodynamics of slurry reactors by performing laboratory-scale experiments. A slurry reactor has the synthesis gas coming in at the bottom and bubbling

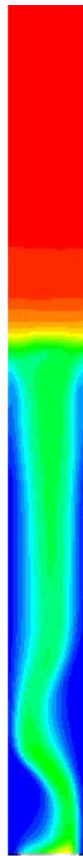


Figure 2. Results showing contours of air volume fraction

up through the slurry. The drawback to using laboratory-scale reactors to understand hydrodynamics is that the results don't necessarily scale up accurately. For example, small diameter reactors are known to have an effect on bubble movement, bubble coalescence, and bubble breakup through wall effects. Most researchers assume that bubble movement will be somewhat different in the larger reactor, but they don't know the extent of the difference. To get accurate information about hydrodynamics in a commercial-scale slurry reactor, it is necessary to study a vessel of that size. However, the capital cost of such a physical model is prohibitive.

Computer simulation of bubble column dynamics

Computational fluid dynamics (CFD) software offers a promising option for the study of large slurry reactor hydrodynamics because a validated model of a small reactor can be easily scaled up.

Until recently, CFD had not been used to study bubble movement. But in August 1999, researchers from Washington University, St. Louis, Missouri, and Fluent Inc., a Lebanon, New Hampshire-based a supplier of CFD software, presented a 2D simulation of gas-liquid dynamics in a bubble column reactor at GLS '99: 4th International Conference on Gas-Liquid and Gas-Liquid-Solid Engineering. Concurrently, we began to develop a 3D CFD model for simulating bubble column dynamics using FLUENT. As our first step, we used computer simulations to calculate bed expansion and gas holdup. Gas holdup is an important factor in the reaction rate because holdup determines interfacial surface area and therefore reaction rate. Gas holdup is one of the variables that need to be maximized to have a high reaction rates. A computer simulation of gas holdup is a complicated problem because it requires tracking the transient movement of each bubble in three dimensions and because the flow is generally turbulent.

The first step in developing the computer simulation was to create a 3D model of the reactor. For this, we used GAMBIT, FLUENT's preprocessor that permits both geometry creation and meshing. The geometry

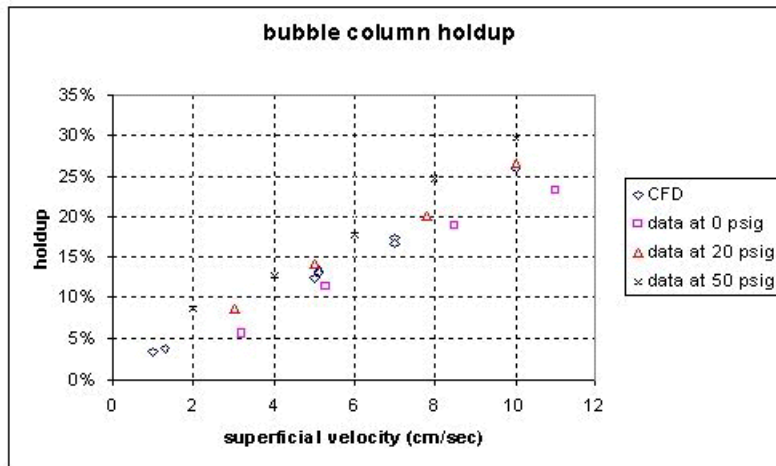


Figure 3. Comparison of CFD model and experimental data

of the column was simple to create. It was basically a vertical cylinder with an inlet at the bottom and an outlet at the top. Figure 1 shows a view of the cylinder looking up towards the inlet. Once the model had been developed, the next step was supplying the software with the boundary conditions for the problem. These included the fact that the sides of the cylinder were walls, that the inlet at the bottom was a velocity inlet, and the outlet on top was a pressure outlet. Since the model was symmetrical and the boundary conditions were the same for each side, we then sliced the model vertically, making a one-half symmetry plane. This was done to reduce solution time. Next we had GAMBIT create the mesh. The outer surface of the mesh is also visible in Figure 1.

After importing the mesh into FLUENT, the next step was to supply some additional information about the problem. We selected the k-epsilon turbulence model provided by the software. We also needed to specify the diameter of the bubbles. Based on our experimental work and also on data reported in the literature, we chose three millimeters. We specified a time step of 1 millisecond for each analysis iteration. Finally we specified the properties of the liquid (water) and the gas (air). We ran the simulation on a Dell 410 workstation with dual 600-MHz Pentium III processors running Windows NT. Dual processors allowed two simulations to be run simultaneously with little loss of computational efficiency.

At that point, we ran the transient simulation. The software required a few dozen iterations to converge at each time step. Figure 2 shows a snapshot of the

distribution of gas and liquid in the symmetry plane after 5.6 seconds. Lateral distortion of the gas jet is easily seen in the contour plot as is the location of the gas/liquid interface. Vector plots, not shown, allowed us to see the backmixing caused by bubble movement up the center of column and the liquid returning on outside.

We calculated gas holdup by plotting the distribution of gas volume fraction versus column height. The plot showed a point where the concentration of gas increased rapidly, which is the liquid-gas interface. This is the same method we use when measuring interface height experimentally. The next step was to compare the height of the liquid-gas interface to the original height of the liquid-gas interface. The expansion, or the amount the liquid-gas interface rose, showed how much gas was held up in the reactor, from which gas holdup is easily calculated.

Correlation with experimental data

Since we were interested in correlating gas holdup with gas inlet velocity, we ran the simulation with several inlet velocities and determined holdup for each. We compared our findings from the computer simulation with results of experimental work, Figure 3, and found that there was a good agreement.

This work is an important step toward understanding the hydrodynamics of large-diameter slurry reactors. Once Rentech has validated a computer model that can simulate all aspects of bubble column hydrodynamics, the size of the model can be increased to answer similar questions about larger reactors. When the hydrodynamics of these vessels can be simulated on the computer, it will be possible to use the computer to optimize the process, ultimately achieving a transfer rate that is high enough to bring this technology into widespread commercial use. With potential savings in the millions of dollars for a single refinery, the technology offers great promise.