Ninth International Conference on CFD in the Minerals and Process Industries
CSIRO, Melbourne, Australia
10-12 December 2012

PREDICTING UNEXPECTED BEHAVIOUR IN INDUSTRIAL DEEP-BED FLUIDIZATION REACTORS AND DEVELOPING ENGINEERED SOLUTIONS WITH CFD

Kenneth A. WILLIAMS* and **Scott THIBAULT***
CPFD Software, LLC, 10899 Montgomery Blvd., Albuquerque, NM 87111, USA
*Corresponding author, E-mail address: ken@cpfd-software.com

EXTENDED ABSTRACT

Many important consumer and industrial products are produced in a highly efficient fluidized bed reactor (FBR) including oil refining for gasoline and diesel, plastics, polypropylene, acrylonitrile, specialty chemicals, as well as the gasification and combustion of coals. These valuable products are often producing in so-called "deep-bed" reactors that promote highly efficient contact between gases and particles (e.g. a catalyst), resulting in high heat transfer, chemical reaction rates, and product yields. These industrial units vary in physical size somewhat, but typically have a diameter from 1 to 10 meters and a bed height between 2 and 5 times the diameter, resulting in a "deep bed". As an example, consider the ubiquitous refinery unit, the fluidized catalytic cracking (FCC) unit, many of which have been in near-continuous commercial operation for over 70 years. The regenerator in FCC units can be 12 meters in diameter, with a bed depth of 10 to 15 meters. The catalyst particles typically have an average diameter of 70 microns, making the solids a Geldart Group A material. Gas superficial velocities are typically 0.4 to over 1.0 m/s, which means the particles are subjected to a gas velocity that is well over 10 times their terminal velocity.

It had long been thought that at such gas velocities the solids in the bed would always be 'well fluidized', with a turbulent, churning motion that promotes excellent mixing and hence product yields. However, within just the past few years it has been discovered experimentally that an unexpected behavior could easily occur – the bed may not be well mixed, and very poor gas-solids contact would result, dramatically reducing product yields and having many other undesirable impacts on the fluid bed operation and on-stream reliability. One of the early experimental reports of this effect was by PSRI (Karri, et al. at Fluidization XI), whose experiments recreated conditions typical of FCC units. The PSRI work revealed that the bed could in fact actually begin in a well-fluidized turbulent mode, as-expected, but could subsequently transition into an unexpected mode subsequently labeled "gas bypassing."

The PSRI data covered a range of conditions for gas velocity, bed depth and fines content ('fines content' in this case being defined as the percentage of the particles with diameter below 44 microns). For example, data showed that a bed operating at 0.6 m/s gas flow with a bed height of 4 meters was well fluidized at 12% fines content. However, if the bed loses fines as it is operated, which is very often the case, the fines content drops and the bed undergoes a transition to gas-bypassing mode. Indeed, the data show that at conditions of 4% fines any bed with a depth of greater than 1 meter would operate in a gas-bypassing mode. The depletion of fines through elutriation in commercial units is a normal occurrence, so it is easy to imagine an FBR could begin operation showing as-designed product yield and then suddenly start to show a reduction in yield, eventually to levels at which the process becomes uneconomical or the operation cannot continue reliably.

Very importantly, the experiments showed that the bed's differential pressure was essentially unchanged before and after this transition to bypassing. Consequently, differential pressure measurements across the bed would not change from one fluidization mode to the next. Operators of the unit would have no clear indicator of why yields, emissions, or other key operational parameters were degrading over time.

It is desirable to determine whether or not this otherwise-unexpected gas bypassing phenomenon, and other potentially unexpected fluidization behaviors, can be predicted computationally using CFD. CPFD Software, LLC (CPFD), is the publisher of the commercial multiphase CFD package Barracuda Virtual Reactor™, which is based on a numerical method called MP-PIC, or multiphase particle-in-cell. CPFD has been a Member of PSRI for over 5 years and uses PSRI's large-scale data for validation of this commercial software. The Barracuda VR™ package is used worldwide by a wide range of commercial clients to simulate exactly this type of process: deep-bed reactors. As a result, CPFD was extremely interested in determining if this unexpected behavior of gas bypassing could be predicted by the method.

The Barracuda VR software was used to simulate a wide range of conditions covered by the PSRI experiments, namely bed heights of 4 feet, 8 feet, and 12 feet, with a range of gas velocities and fines content from 3% to 12%. This validation work compared PSRI data and Barracuda VR calculations to show that this unique CFD technology can be used to predict reliably the onset of gas bypassing. Even more importantly, the detailed CFD data from the calculation helps to better understand the underlying physics and phenomena causing this deleterious behavior to occur and has since routinely been used to suggest corrective actions to the design or operation of fluidized beds.

Analysis of the Barracuda results, which covered flow regimes with both 'good' fluidization and those in a bypass mode, reveals the root cause of the bypassing behavior. First, it must be again noted that the bed is operating at a gas velocity that is well above (10X) the typical 70-micron particle's terminal velocity, yet the particles are not "blown out" and the bed's solids remains in a churning, turbulent mode.

This 'high' gas velocity mode of operation with Group A particles does not occur in a smaller-diameter vessel as the particles will indeed be ejected. However, in larger-diameter vessels more typical of those in actual industrial applications, the gas penetrates through the bed's emulsion phase as streamers or jets. Stated another way, the upwards volumetric flux of gas is nowhere near the idealized one-dimensional motion through the solids (i.e. never is the average gas velocity occurring uniformly). Rather, several very high-speed gas streamers jet through the bed. These streamers form randomly and can penetrate the entire bed height but then collapse due to instabilities and new streamers form, resulting in the observed 'quasi-steady' turbulent motion.

In a well fluidized bed, this stochastic process results in very effective fluidization and mixing, leading to excellent gas-particle contact, relatively uniform gas temperature distribution, and reliable/steady operation. However, even when operating the bed well below the well-fluidized limit in superficial velocity, it is clear the fluidization phenomena are 3D in nature. In fact, they MUST be 3D or else the particles would be blown out of the vessel. If the bed's fines content drops as a result of the (slow) elutriation process, a point is reached wherein streamers cannot penetrate the bed as readily and then gas streams frequently become attached to walls or vertical surfaces, such as cyclone diplegs. Gas streamers remain mostly stable in this mode, and hence steady bypassing occurs that results in regions of the bed with excessive gas passing through, while other regions are poorly fluidized or even defluidized entirely. While the streams of gas may move to different vertical surfaces, the effective gas-solids contact is dramatically reduced – the bed is 'bypassed".

Barracuda VR validation simulations are shown for different combinations of bed height, gas velocity and fines content spanning the range from well fluidized to stable gas bypassing. CPFD's own research and analysis has concluded that the elements of CFD numerical models required to reliably predict these complex phenomena include:

(1) A model for discrete particles, as opposed to various multiple-continua methods (in effect, this means an Eulerian-Lagrangian formulation);

(2) The maintaining of detailed, true particle size distributions across a wide range of sizes (e.g.,1 to 300 microns) for every solid species present in the bed, including the ability for each PSD to change as a result of fines losses or changing of particle sizes from ongoing chemical reactions or combustion;

(3) A numerical approach that is capable of simulating the behavior of beds with very large physical particle counts, on the order of 1014-1016 particles, in a practical time frame;

(4) A fully three-dimensional and compressible gas flow formulation that also includes homogeneous and heterogeneous chemical reaction modeling as these impact particle PSD and hence the fluidization behavior;

(5) A tight 'two-way' coupled drag between the gas phase and the particles;

(6) The ability to calculate results reliably for solids loadings that range from dilute to dense-phase simultaneously and without apriori knowledge of what the loading will be; and

(7) The speed required to simulate, at full scale, industrial-size units in a practical run time so as to achieve meaningful time averaged values across, for example, 200 to 300 seconds of simulation.

[The comparisons shown, plus the industrial examples cited below, show that the MP-PIC method employed in the Barracuda VR software package satisfies these requirements.]

Simulations of commercial FCC regenerators, CFB combustors, and others application have shown that this unexpected gas bypassing behavior does occur, usually with severe penalties to the operating unit. In just one example, an FCC regenerator at a large U.S. refinery (proprietary and not shown), a large streamer penetrated the catalyst bed on only one side of the vessel. The resulting high velocity jet of particle-laden gas was later determined as the root cause of severe damage to the regenerator cyclones and cyclone support structures. This damage was so severe that it necessitated total replacement of much of the internals on one side of the vessel after less than one year in operation. The Barracuda software was subsequently employed as part of the engineering process to devise a remedial redesign, which has since been implemented with the unit in operation for over a year so far. This project demonstrated the value of this CFD technology for development of engineered solutions to fluidization unit problems, whether the issues arise from the fundamental design of the equipment or changes to the operation from that for which it was originally designed, which was the case for the FCC unit cited above.

Several other examples are shown of full-scale industrial fluidized bed applications, as follows, all of which demonstrate different engineered solutions that arose from having an accurate and reliable model of the detailed, 3D fluidization (and in most cases chemistry/combustion as well) inside these units.

- A 40MW biomass-fired CFB boiler in Strongoli, Italy was studied to determine engineered solutions to excessive erosion at multiple points in the CFB loop, including the cyclone inlet region, fluidized-bed heat exchanger, and suspension tube assembly downstream of the cyclone. Modest modifications were devised that were predicted to reduce erosion by more than 50% and service life by significantly more than 50%, since erosion is a non-linear process. The plant has already operated to longer than ever previously achieved, though it remains in operation and the full operational life improvement has therefore not yet been determined.

- An FCC regenerator at a U.S. refinery was studied to determine the root cause of afterburning (temperature rise between the top of the bed and the cyclone inlets) that had been observed in the operating unit for its entire 70-year operating life to date. The CFD calculation was performed at full-scale and included the coke combustion kinetics with the intent of predicting afterburn, NOx and SOx generation, CO & CO2 production, and both temperature and mass loading distributions to the cyclones. Simulations clearly show the afterburn that is observed in the actual unit while results from the temperature and mass loading distributions to the cyclones agreed with observed operational data and emissions followed trends considered reasonable. The simulations suggest that gas bypassing of combustion air results in excessive excess oxygen in the freeboard, which would lead to the afterburn observed. Meanwhile, an oxygen-poor, catalyst-rich region forms in the bed center. Design changes were suggested based on these findings but have not yet been implemented.

- A 140MW coal-fired CFB furnace at a municipal power plant in Duisburg, Germany, was modeled to determine the impact of co-firing the unit with 25% biomass. The results of the 3D, fully reacting calculations indicated that the unit would be oxygen starved in the upper regions and that additional secondary air would be required to achieve full combustion when co-firing, even though it was not needed when 100% coal feed is employed.

- A unique sorbent-based warm syngas clean-up system being developed for IGCC (Integrated Gasification Combined Cycle) applications was modeled, including both hydrodynamic effects and chemistry. Findings resulted in important design changes in the unit prior to the actual commercial deployment, almost certainly resulting in savings of millions of USD.

- An FCC reactor was modeled to determine the likely erosion reduction from design changes proposed by the equipment licensor. Erosion patterns and magnitude were compared for two proposed design changes versus the original baseline design, which had been exhibiting unacceptably high erosion levels. The unit is now in operation and the actual results of the erosion reduction effort are not yet known.

- Other examples may be shown if time allows and permission is granted by those with the rights to the subject simulations or other proprietary technology.

Having the ability to simulate, understand, and optimize industrial-scale FBRs with CFD provides tremendous value to commercial clients designing or operating FBRs. Both the comparison to the PSRI gas bypassing experiments and the cited industrial examples illustrate that the technology to model even otherwise-unexpected fluidization behavior in full-scale industrial fluid beds is available right now. The result of using this CFD technology in this way is that designers and operators of fluidization equipment can now put real science behind critical decisions regarding unit design and operation that can and do have profound impacts on the safe, reliable, and profitable operation of all manner of fluidized systems.

REFERENCES

REDDY KARRI, S.B., ISSANGYA, A., and KNOWLTON, T.M. Gas Bypassing in Deep Fluidized Beds, *Proceedings of the 11th International Conference on Fluidization*, pp. 515-521, (2004).

BLASER, P. and CORINA, G. Validation and Application of Computational Modeling to Reduce Erosion in a Circulating Fluidized Bed Boiler, *International Journal of Chemical Reactor Engineering*, **10**, A51 (2012).

FLETCHER, R. and CLARK, S. CFD Regenerator Case Study: Fluid Dynamics with Coke Combustion Kinetics, presented at *American Fuel and Petrochemical Manufacturers' Cat Cracker Seminar and Exhibition*, Houston, TX, (2012).

WENG, M., NIES, M., and PLACKMEYER, J. Computer-aided Optimization of Gas-Particle Flow and Combustion at the Duisburg Circulating Fluidized Bed Furnace, *VGB PowerTech*, pp64-69 (2011).

BLASER, P., and SEXTON, J. CFD Reactor Case Study: Comparison of Cyclone Erosion Characteristics for Proposed Redesigns for the Marathon Petroleum Catlettsburg Refinery FCC Reactor, presented at *American Fuel and Petrochemical Manufacturers' Cat Cracker Seminar and Exhibition*, Houston, TX, (2012).

ANDREWS, M.J., and O'ROURKE, P.J. The Multiphase Particle-in-cell (MP-PIC) Method for Dense Particle Flow, *International Journal of Multiphase Flow*, **22**, 379-402, (1996).

SNIDER, D.M. An Incompressible Three-Dimensional Multiphase Particle-in-Cell Model for Dense Particle Flows. *Journal of Computational Physics*, **170**, 523-549, (2001).

SNIDER, D.M., and O'ROURKE, P.J. Multiphase Particle-in-Cell Method for Dense Particle Flow, Computational Gas-Solids Flows and Reacting Systems: Theory, Methods and Practice, Chapter 9. Eds. Pannala, S., Madhava, S., and O'Brien, T.J., IGI Global, (2010).