Multiphase Simulation of a Commercial Fluidized Catalytic Cracking Regenerator

Samuel M. Clark, CPFD Software, LLC, Albuquerque, NM, USA
Dale M. Snider, CPFD Software, LLC, Albuquerque, NM, USA
Ray P. Fletcher, INTERCAT$_{JM}$, Utrecht, NL

Abstract

A multiphase, thermal, and chemically reacting simulation of a commercial Fluidized Catalytic Cracking (FCC) regenerator was conducted. The simulation was full-scale, 3-dimensional, and included complex internal structures. The regenerator is 70 ft tall, with a diameter of 47 ft. The particle inventory in the system is about 400 tons. The computational method used was an Eulerian-Lagrangian approach called MP-PIC (multi-phase particle-in-cell). Barracuda® VR™, a commercially available CFD software package, was used to perform the simulation. Discrete particle-level chemistry was applied for the chemical reactions of coke burn-off from the catalyst particles.

The simulation had several goals, including: (1) gain insight into the performance of the unit regarding effectiveness of coke combustion from the spent catalyst particles; (2) predict the severity of afterburn in the freeboard, and understand its causes; (3) predict the production rates of pollutants such as SOx from the regenerator; and (4) identify any maldistribution of particles or gas from the highly complex spent catalyst distributor.

Results of the simulation are presented, including particle-fluid flow behavior, thermal profiles throughout the vessel, and gas compositions exiting the system. A comparison of actual operations with the simulation results will be presented to demonstrate the predictive capability of the computational model.

FCC Regenerator As-Built System Geometry

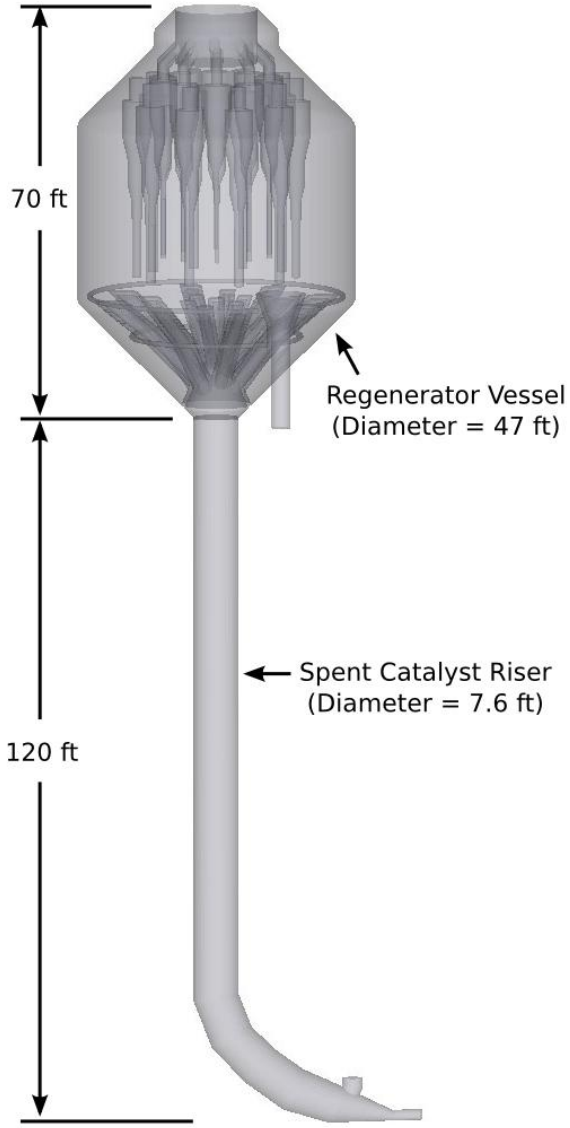

Figure 1: FCC regenerator system geometry

The portions of the FCC regenerator which were modeled included the spent catalyst return riser, the spent catalyst distributor, and the inside of the regenerator vessel. Figure 1 shows a CAD model of the regenerator system considered. The spent catalyst riser was modeled starting at the entrance of lift air, and a short portion of the spent catalyst feed pipe was included. The interior flow region of the regenerator vessel was modeled, with internal structures such as the spent catalyst distributor, combustion air rings, and 12 pairs of internal cyclones. A portion of the regenerated catalyst standpipe was included, allowing particles and gas to exit the regenerator.

Computational Method

Barracuda VR, a commercially available CFD software package, was used to perform the simulation. Barracuda VR uses a proprietary implementation of the MP-PIC method, known as the Computational Particle Fluid Dynamics (CPFD®) method. The MP-PIC method has been described previously (Andrews and O'Rourke, 1996), and several specific aspects of the method as applied in Barracuda VR have also been published (O'Rourke, Zhao, and Snider, 2009; Snider, 2001; Snider, Clark, and O'Rourke, 2011). The CPFD method solves the fluid and particle momentum equations in three dimensions, treating the fluid field(s) as Eulerian and the particles as Lagrangian. There is strong coupling between the fluid and the particles, i.e. the fluid drags the particles, and the particles displace the fluid. Thermal and chemistry calculations are also available, with the fluid and particle phases coupled for energy and reaction purposes. The reader is referred to the papers listed above for details of the CPFD method.

Additional studies of applications of Barracuda VR, with comparisons against operational experience and/or experimental data, have also been conducted (Parker, 2011; Snider, 1998; Snider, 2007; Snider and Banerjee, 2009; Snider, Guenther, Dalton, and Williams, 2010; Zhao, Snider, and Williams, 2006).

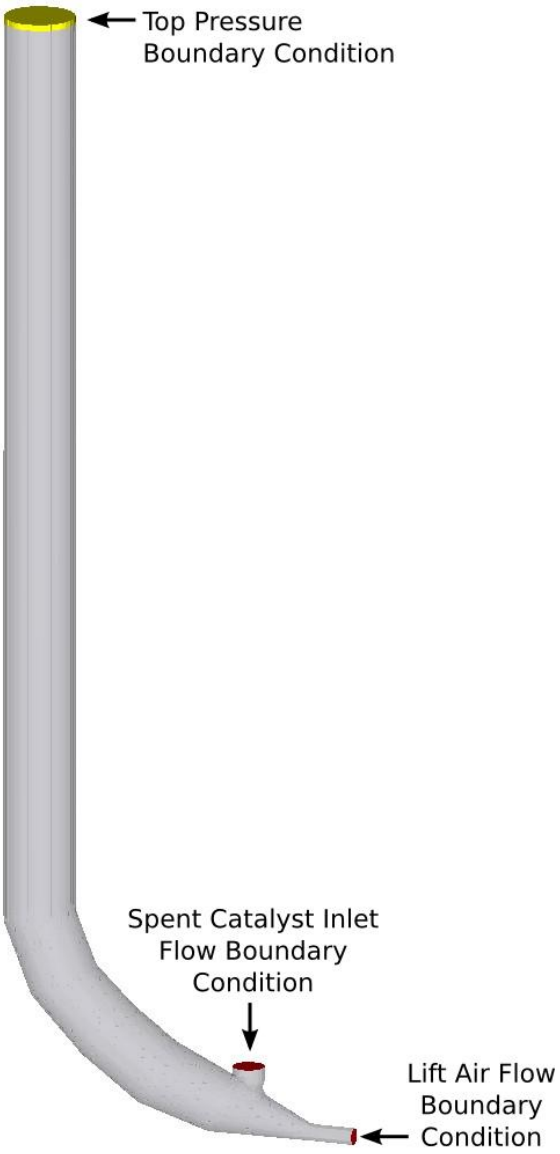

Figure 2: Spent catalyst riser simulation boundary conditions

Multiple-Simulation Strategy for the Regenerator System

For a system as complex as the commercial FCC regenerator considered in this paper, a simulation of the entire geometry, and also including thermal and chemical reaction calculations, would result in a long calculation time. Rather than simulating the entire system with a single calculation, three distinct computational models were constructed and run. The first model was an isothermal, non-reacting simulation of the spent catalyst return line. The second model was a thermal, chemically reacting simulation of the spent catalyst distributor. The third model was a thermal, chemically reacting simulation of the inside of the regenerator vessel. Each of these models is discussed in turn in the following sections.

Spent Catalyst Riser Simulation

Computational Grid and Particles

The computational grid used for the spent catalyst riser simulation was specified with simulation speed in mind. Since the results from this simulation were primarily intended to provide inlet conditions to the subsequent spent catalyst distributor simulation, it was important that the simulation run quickly so as not to delay the overall schedule of the three simulations. The grid consisted of 30,360 real cells, with a typical cell side-length of about

6 inches (0.15 m).

At steady operating conditions, from 100 s to 150 s of simulation time, the spent catalyst riser had an average of about 550,000 computational particles. The average particle mass in the system during this time-period was about 46 tons (42,000 kg).

Boundary Conditions

The spent catalyst riser had three boundary conditions, as shown in Figure 2: (1) a flow boundary condition to bring spent catalyst and carrier gas into the system; (2) a flow boundary condition to bring lift air into the riser; and (3) a pressure boundary condition at the top exit of the riser. The flow rates and pressures were specified to match typical operating conditions of the unit.

Simulation Results

The main purpose of the spent catalyst riser simulation was to determine the distribution of particles and gas exiting the top of the riser. This information would then be used to define boundary conditions in the spent catalyst distributor simulation. Flux planes, as shown in Figure 3, were used to measure the particle and gas flow rates across several regions defined near the outlet. The measured fluxes are given in Table 1.

Table 1: Spent catalyst riser simulation mass fluxes from flux planes

Flux Plane	Fluid Mass Flux ($kg/s/m^2$)	Particle Mass Flux ($kg/s/m^2$)
A	9.40	254
B	9.80	275
C	12.52	184
D	9.80	275
E	10.34	214
F	16.75	165
G	10.34	214
H	11.13	283
I	17.03	170
J	11.13	283

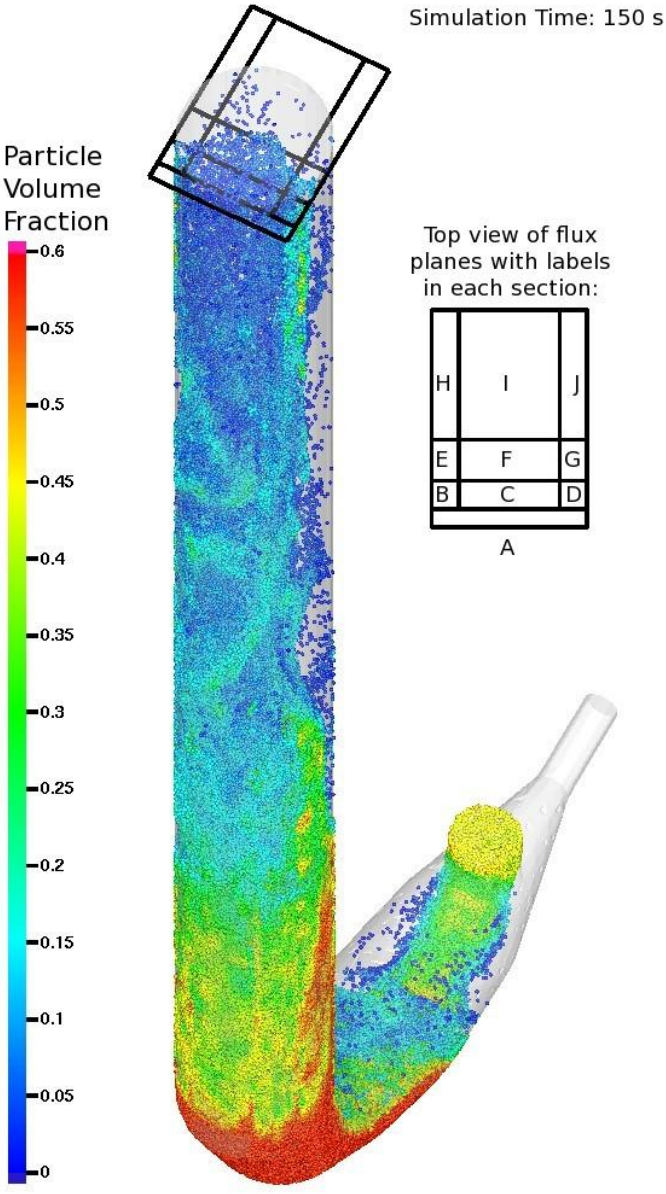

Figure 3: Spent catalyst riser simulation results with flux planes shown and labeled

Potential Improvements

The spent catalyst riser simulation was successful in providing a good estimate of the distribution of particles and gas as they exited the riser. In hindsight, it might have been useful to run the simulation with thermal and chemical reaction calculations. This could have provided better gas and particle composition information for use in the subsequent regenerator vessel simulations, especially if reactions were occurring as particles travelled through the riser.

Spent Catalyst Distributor Simulation

Computational Grid and Particles

The computational grid used for the spent catalyst distributor simulation was designed to capture individual nozzles in the spent catalyst distributor arms. There were 192 nozzles, and particles and gas passed through the nozzles from the insides of the arms into the regenerator vessel. The computational grid consisted of 407,200 real cells.

The computational particles used in the spent catalyst distributor simulation were composed of multiple materials, including catalyst, carbon, hydrogen, sulfur, and nitrogen. The multi-material particle specification was chosen because chemistry and thermal calculations were included in the simulation. Particle composition and size distribution information was based on operating conditions at the refinery.

Boundary Conditions

The results of the spent catalyst riser simulation were used to specify the flow rates of gas and particles at the bottom flow boundary condition in the spent catalyst distributor simulation. Flow and

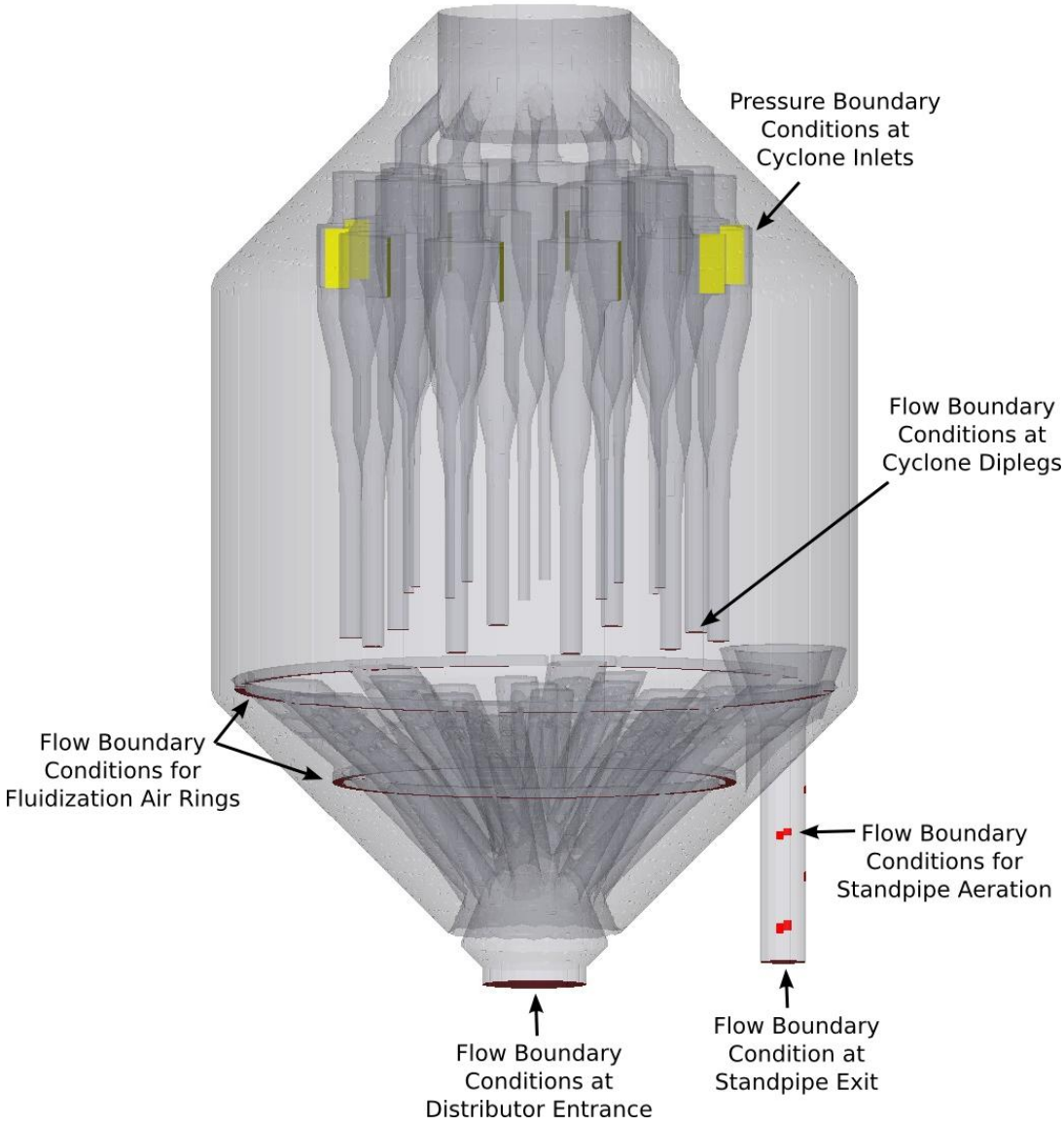

Figure 4: Spent catalyst distributor simulation boundary conditions

pressure boundary conditions were defined as shown in Figure 4, with parameters set to match actual regenerator operating conditions as closely as possible.

Simulation Results

The main purpose of the spent catalyst distributor simulation was to provide particle and gas flow rate information for the individual distributor arms. The flux planes use to measure the particle and gas flow rates are shown in Figure 5, and the numerical flux plane results are presented in Table 2. This information was ultimately used to define flow boundary conditions on the distributor arm surfaces in the final model of the entire regenerator vessel.

Table 2: Spent catalyst distributor simulation gas and particle flow rates.

Arm	Gas (kg/s)	Particles (kg/s)	Arm	Gas (kg/s)	Particles (kg/s)	Arm	Gas (kg/s)	Particles (kg/s)
1	3.78	69.1	7	5.87	57.8	13	1.26	23.6
2	5.14	77.6	8	6.34	65.7	14	1.31	22.2
3	3.86	75.2	9	3.60	40.1	15	1.36	23.6
4	5.06	78.2	10	3.45	40.6	16	1.35	22.9
5	3.56	70.0	11	3.71	37.8	17	0.53	17.4
6	6.34	66.4	12	3.50	42.2			

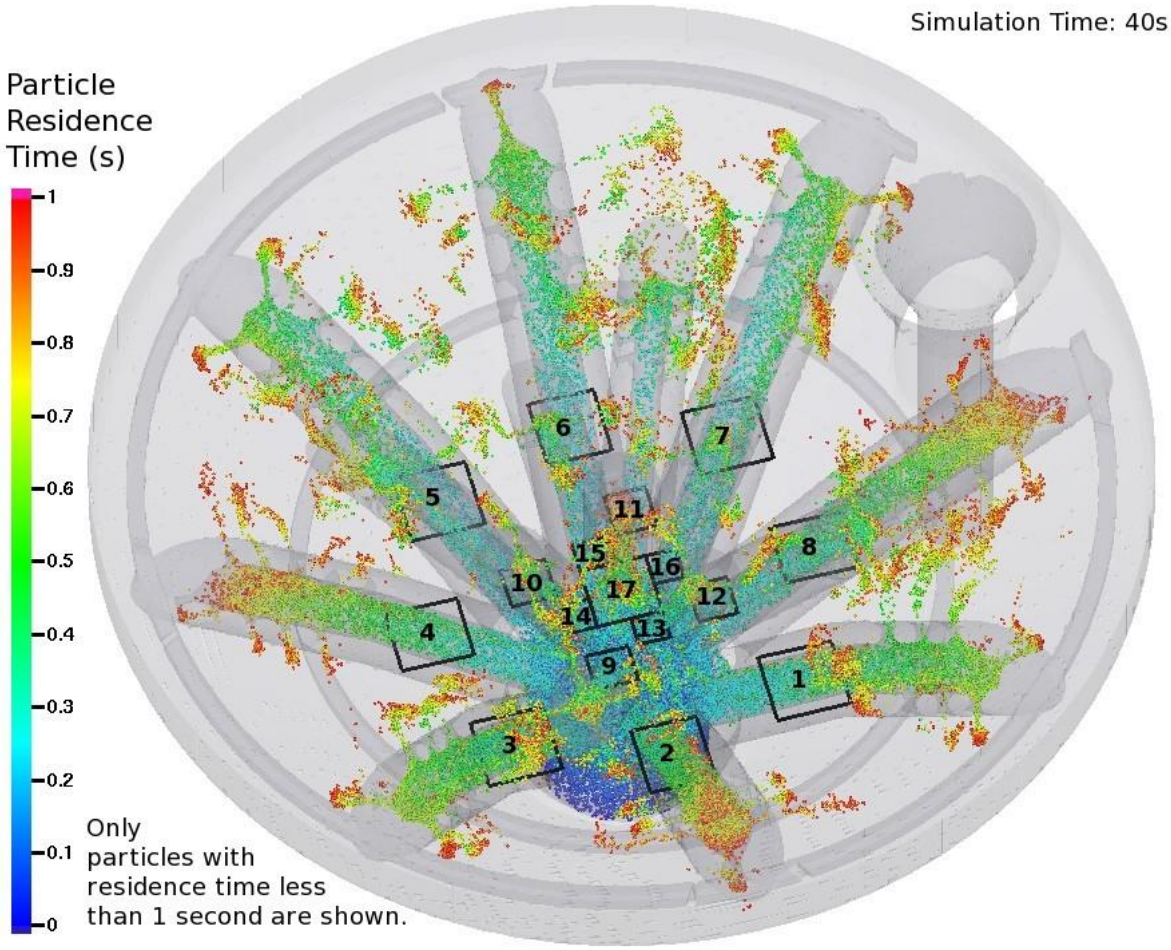

Figure 5: Spent catalyst distributor simulation flux planes with labels.

Regenerator Vessel Simulation

Computational Grid and Particles

The computational grid for the regenerator vessel simulation was coarser than that used for the spent catalyst distributor simulation. The flow of particles and gas through the individual holes in the distributor arm was not modeled, allowing for larger grid spacing and resulting in 237,999 real cells. This reduced number of cells resulted in a faster-running model, while still maintaining acceptable accuracy and resolution of the system geometry. A typical cell side-length was about 7 inches (0.18 m).

Multi-material particles, as described above for the spent catalyst distributor simulation, were used in the regenerator vessel simulation. An equilibrium particle species was defined for the initial catalyst bed, and a coked catalyst species (equilibrium catalyst containing carbon, hydrogen, sulfur & nitrogen) was defined for spent catalyst particles fed from the distributor. At steady operating conditions, from 200 s to 250 s, the simulation had 2.5 million computational particles, representing 507 tons (460,000 kg) of catalyst.

Boundary Conditions

Flow boundary conditions were defined at 196 distinct locations on the surfaces of the spent catalyst distributor arms, with particle and gas flow rates based on results of the spent catalyst distributor

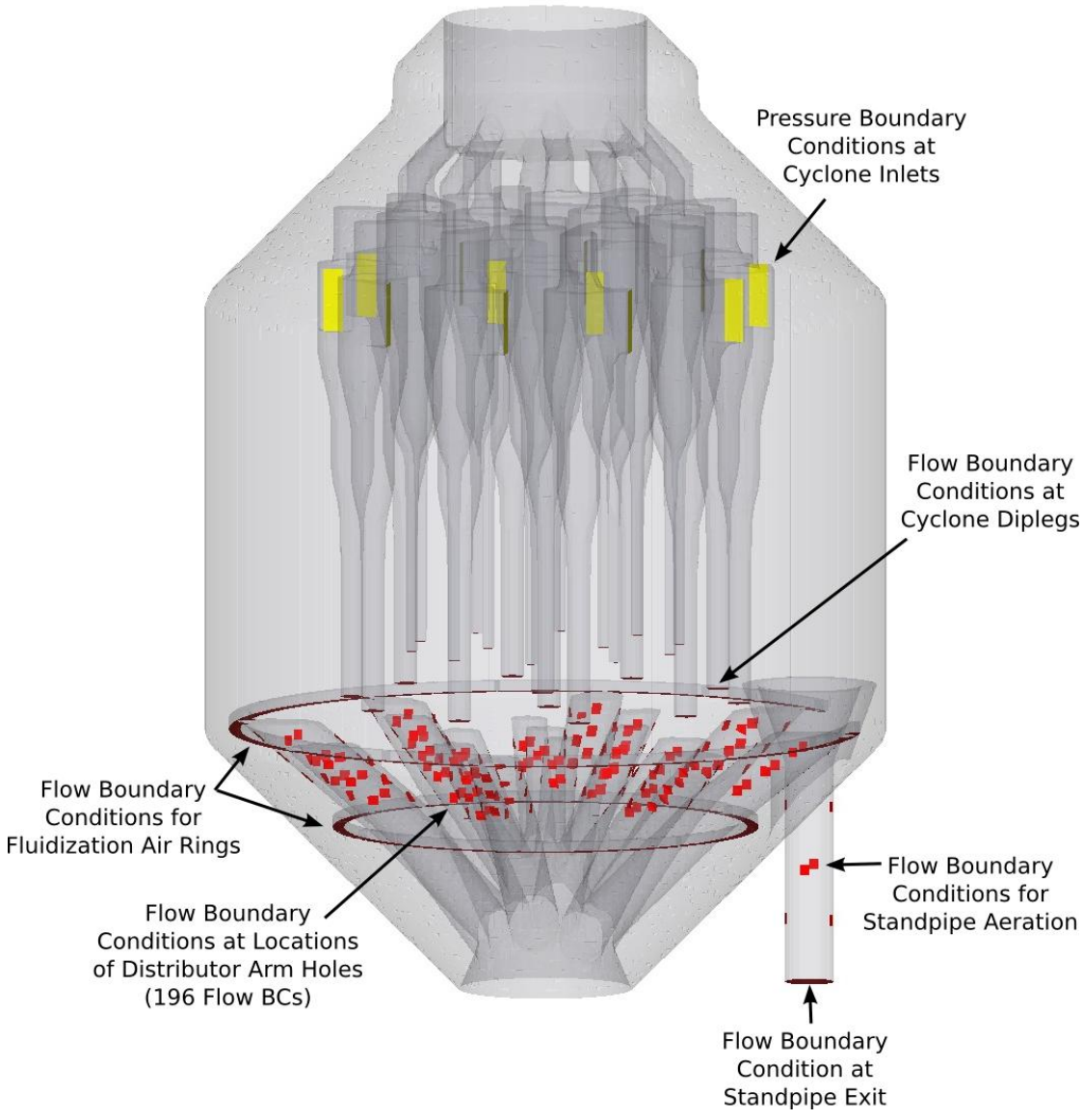

Figure 6: Regenerator vessel simulation boundary conditions

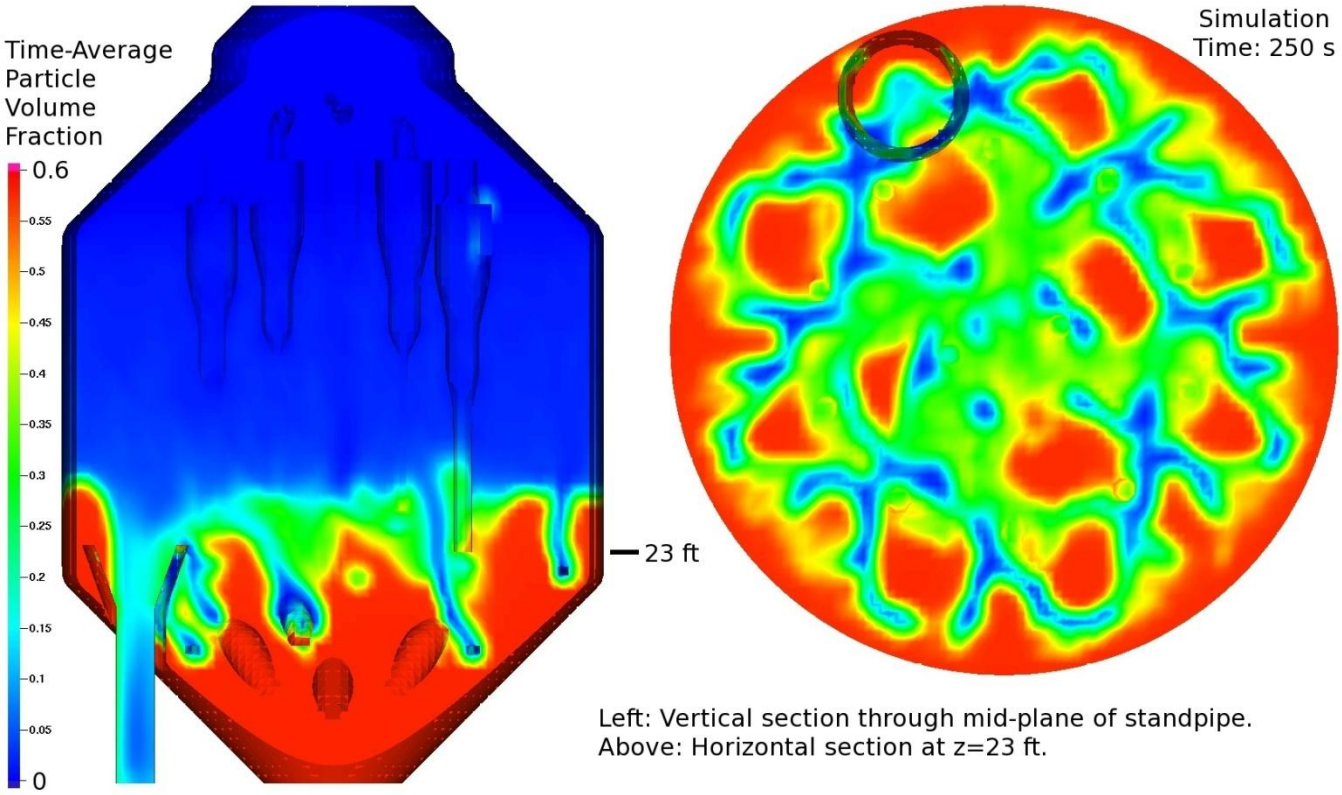

Figure 7: Regenerator vessel time-average particle volume fraction plots

simulation. Other boundary conditions were similar to those used in the spent catalyst distributor simulation, with parameters set to match actual operating conditions as closely as possible. Figure 6 shows the boundary conditions for the regenerator vessel simulation.

Simulation Results

The simulation of the regenerator vessel provided many interesting results, and was studied in greater detail than either of the preceding simulations. In this paper, we will highlight several specific results, namely: (1) general fluidization and particle flow behavior; (2) thermal behavior, particularly as it pertains to afterburn; and (3) gas species compositions throughout the system, including outlet gas compositions through the cyclones. Many other aspects of the system could be studied extensively and further insight into the operation of the regenerator would surely be gained.

The fluidization behavior of the system was studied with effectiveness of mixing in mind. Figure 7 shows the time-average particle volume fraction on vertical and horizontal cross-sections. Time-averaging was started at 220 s, once a pseudo-steady state was reached in the simulation, and was continously calculated up to 250 s. The bottom portion of the regenerator, i.e. below the level of the lower air ring, was found to be non-fluidized with stationary particles at close-pack. Gas from the air rings and distributor arms formed persistent paths of low-particle volume fraction. From the top view, numerous areas of high-volume fraction particles were present throughout the fluidized bed. Altogether, these results indicated less than optimal mixing behavior, and the gas-particle contact time in the simulation was likely impacted by the gas bypassing behavior observed.

Afterburn, which is a large temperature increase in the dilute phase (freeboard) above the fluidized bed, is a known issue for the regenerator simulated in this paper. The time-average fluid temperature predicted in the simulation is plotted in the upper-left hand corner of Figure 8. A 100 °F temperature difference was expected based on operational experience, and the simulation is showing a temperature difference of about this magnitude from the lower to the upper regions of the vessel.

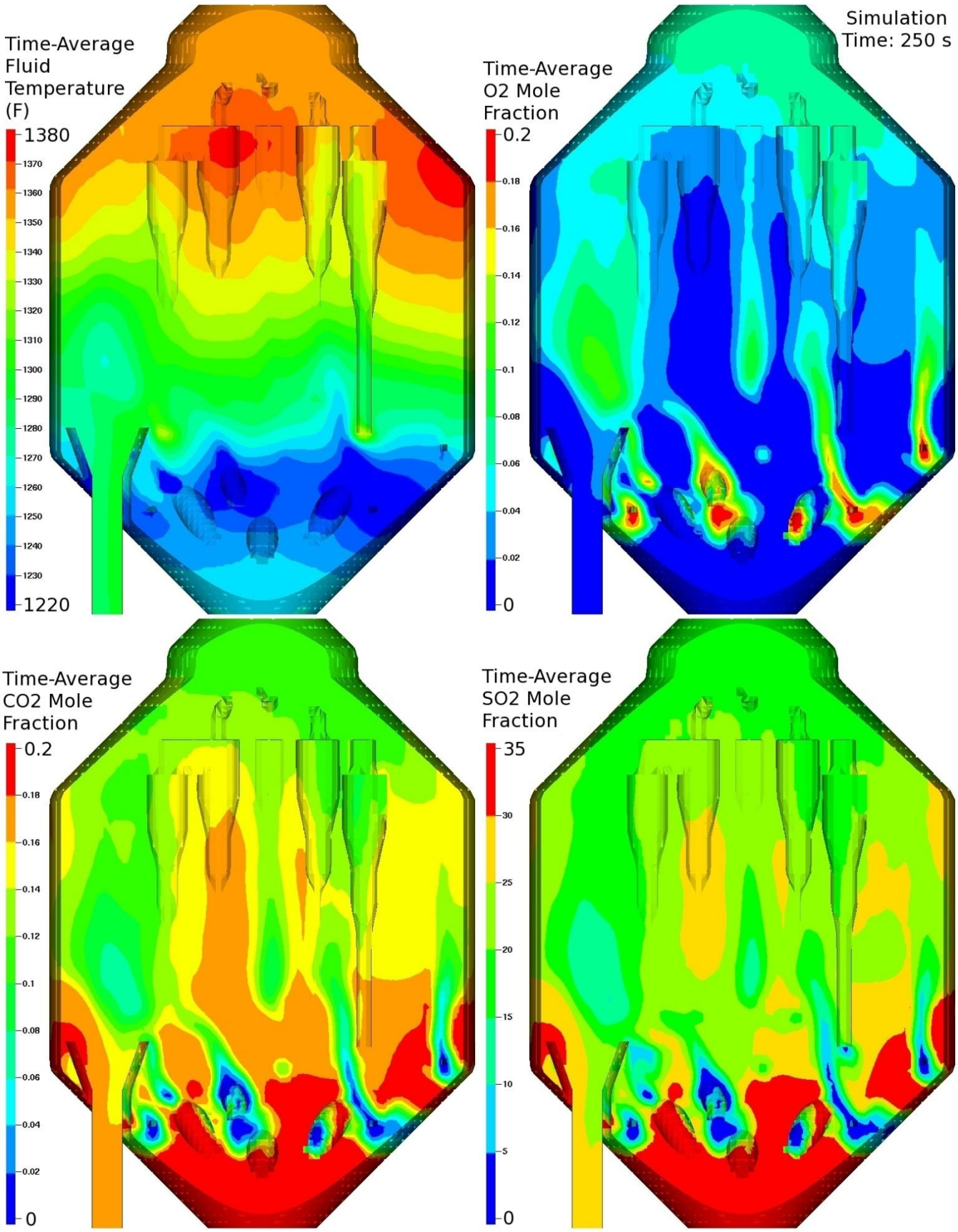

Figure 8: Regenerator vessel simulation thermal and chemistry results

Afterburn is undesirable because it negatively impacts the FCC catalyst deactivation rate and limits operating flexibility due to metallurgical constraints. Future simulations of this system could include analyses of proposed design changes to reduce afterburn. The current simulation gives a baseline against which future results can be compared.

The gas composition at the outlet of the regenerator was analyzed and compared with typical gas composition data from the regenerator. Vertical slices of time-averaged gas composition are shown in Figure 8 for O_2, CO_2, and SO_2. For O_2, a typical mole fraction value during unit operation is about 0.02. The simulation predicted higher concentrations than this in a significant portion of the upper half of the regenerator. It is suspected that the regions of high O_2 concentration were due to either: (1) bypassing of the gas exiting the distributor, or (2) the fact that combustion was neglected in the spent catalyst riser simulation. The CO_2 mole fraction near the cyclone inlet horns was near the expected value of 17. The SO_2 concentration, in parts per million, was also close to the expected outlet SO_2 concentration of 30 ppm.

Conclusions

The simulations of the commercial FCC regenerator provided many insights into the operation of the system. The thermal and chemistry results of the regenerator vessel simulation showed good agreement with real-world operating experience from the commercial regenerator. The multiple-simulation strategy used to analyze the overall regenerator system was successful in allowing an analysis of the entire system, while at the same time meeting project schedule goals. A single large simulation of the entire system would likely have taken much longer to yield the same amount of useful engineering information.

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