Computational Particle-Fluid Dynamics Simulations of a Commercial-Scale Turbulent Fluidized Bed Reactor

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Abstract

The three-dimensional gas-solid flows inside a dense-phase fluidized bed with a diameter close to 5 meters, and running in the turbulent to fast fluidization mode, is numerically simulated and analyzed. The solids are FCC-type material, the superficial gas velocity is 43 cm/s, and all key internals are modeled, such as ganged cyclones, spargers, and air injectors. The commercial Barracuda-CPFD^{TM} software package was used to simulate the reactor's behavior for over 187 s in order to obtain meaningful time-averages for solids concentrations, gas and solids velocities, and pressures. The new Barracuda commercial software is an advanced math-based computational particle-fluid dynamics (CPFD^{TM}) tool developed for efficient simulation of dense-phase fluidization in industry-scale units. The software's numerical methodology uses a direct element method wherein solids are modeled as discrete particles with proper size and density distributions, and the fluid is modeled as a continuum. The actual solid particles numbering on the order of 10^{13} are modeled with 5×10^5 ~ 5×10^6 numerical particles, each of which groups the physical particles with the same properties (size, shape, density, etc.) as a single entity. The fluid (gas) flow is compressible and isothermal. The model includes complex internal structures such as cyclones and diplegs inside the bed. The elutriated particles exit the bed through the cyclones, and then particles feed back into the bed through the diplegs in various elevations. The simulation is the first of its kind in terms of efficiency, accuracy, run-time, and the geometrical scale (commercial size bed) of the model.

The deep turbulent fluidized bed does not behave as an idealized plug flow fluidized-unit, and its complex solids-fluid dynamics differ from the traditional bubbling fluidized bed. Specifically, gas streaming occurs in certain regions, resulting in poor gas-solids contact and reduced product yields. The occurrence of gas streaming behavior in large, deep beds is supported by experimental data. The fluidization properties such as solid concentration distribution, particle size distribution (PSD), particle species distribution, particle residence time distribution(RTD), pressure distribution, and gas and solid flow patterns are analyzed. The simulation provides a unique insight into the complex behavior of a commercial-scale turbulent fluidized bed reactor with internals.

1. Model Geometry

A full three-dimensional reactor model with major internals is shown in Figure 1. The reactor is a cylindrical vessel, which is 16.31 m (53.5 ft) high and 4.57 m (15 ft) in diameter, and has a dome on the top-end. Internals include three 2-stage (primary and secondary) cyclones with diplegs, cooling coils in the reaction zone and gas spargers near the bottom of the reactor. Air and gaseous chemicals feed the reactor through gas spargers. Heat generated by the chemical reaction is taken away by the coolant running through the cooling coils. The entrained solids are separated from the gas by the cyclones and return to the reactor at different elevations through the primary- and secondary-stage diplegs.

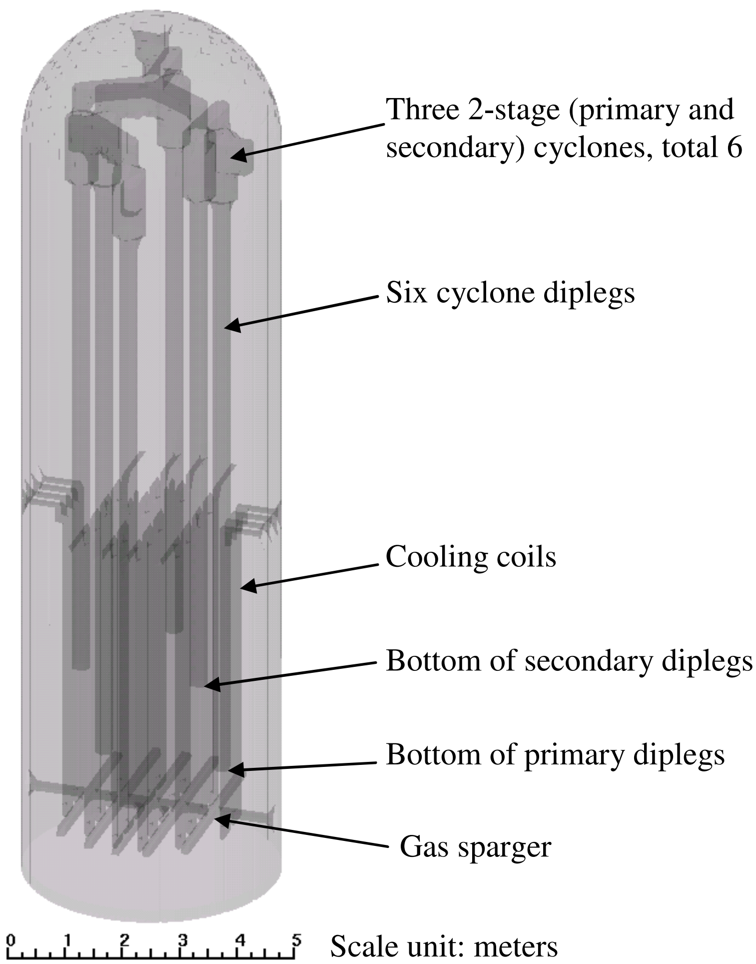


Figure 1. Three-dimensional large-scale reactor model with internals. The turbulent gas-solid flow inside the reactor was numerically simulated with the commercial Barracuda CPFD™ software package.

2. Simulation Conditions

The reactor is initially loaded with near close-packed FCC-type particles with a user specified particle size distribution. Fluidizing gas, which is air in this case, flows in from the bottom and from the gas spargers. Gas and solids exit the reactor through cyclones , and particles return to the bed through diplegs. Flow boundary conditions are applied at the bottom, the gas spargers, the cyclone inlets and the diplegs bottom. Figure 2 shows the boundary locations in the model. Table 1 lists the simulations conditions. The simulation was run to 187 s and averaging of calculated properties started at 90 s, which is after the initial transient stage.

Table 1. Simulation conditions

Number of particles	~688,500
Particle radius (FCC-type)	9.2 to 96 μm
Fines content (radius < 22 μm)	11.5 %
Particle density	1275 kg/m^3
Close-pack particle volume fraction	0.55
Particle mass in reactor	32,390 kg
Static bed height	3.3 m
Fluidizing gas	Air at 2 atm
Type of flow	Compressible and isothermal
Superficial gas velocity	0.43 m/s
Number of grid cells	~54,000

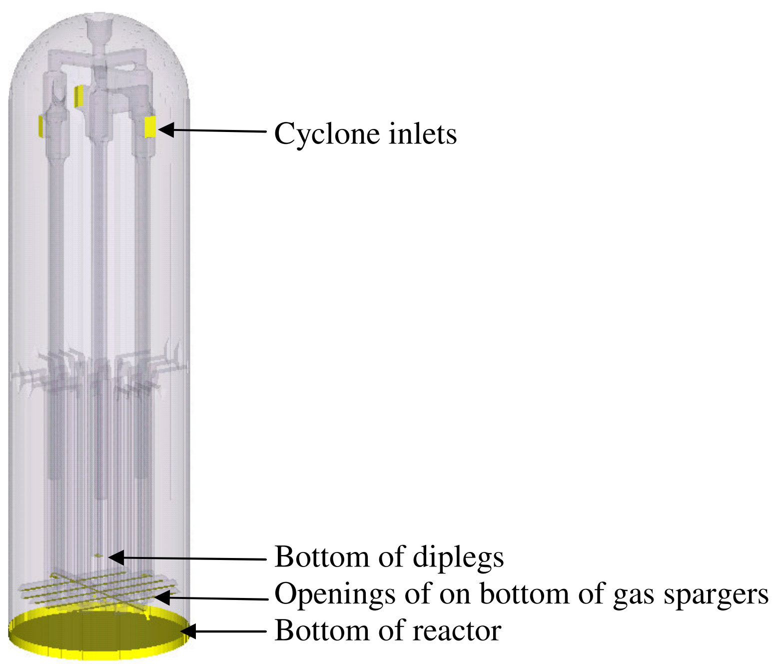
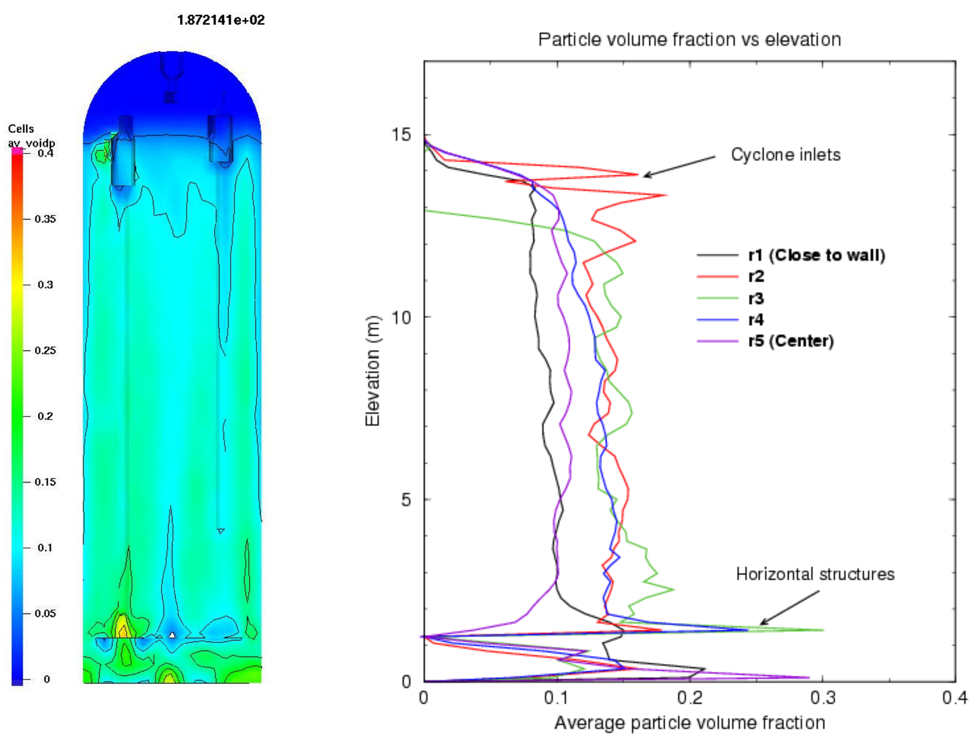


Figure 2. Flow boundaries shown as yellow. The pressure boundary conditions are applied at the cyclone inlets and the flow velocity boundary conditions are applied at the bottom of diplegs, the gas sparger openings and the reactor bottom.

3. Results and Discussion

3.1. *Solid distribution in the reactor*

The average solid volume fraction at the end of the simulation is shown in Figures 3(a) and (b), where (a) shows the profile of the volume fraction in a vertical plane across the center line and (b) shows the volume fraction versus elevation at different radial positions. In the dense bed section, which extends from the vessel-bottom to the static bed height, the solid volume fraction is very non-uniform, ranging from 0.1 to 0.3. Since particles are pushed down by the downward-directed sparger gas flow , the solid volume fraction immediately below the sparger is near zero. Higher solid concentration is seen above the sparger because some solids sit on the top of horizontal structures, which block the flow. In the freeboard, which extends from the dense-bed surface to the cyclone inlets, the solid volume fraction is close to 0.1 and almost constant vertically. The solid concentration is lower near the outer wall and in the center. There is no distinct dense-dilute interface in the solid concentration profile, indicating a fast fluidization regime in this case. This is because the particle density is low (1275 kg/m^3) and particles are small (radius from 9.2 to 96 μm). Across the height of the cyclone inlets, the solid volume fraction drops from approximately 0.1 to zero. There are virtually no solids in the dome region above the cyclone inlets.



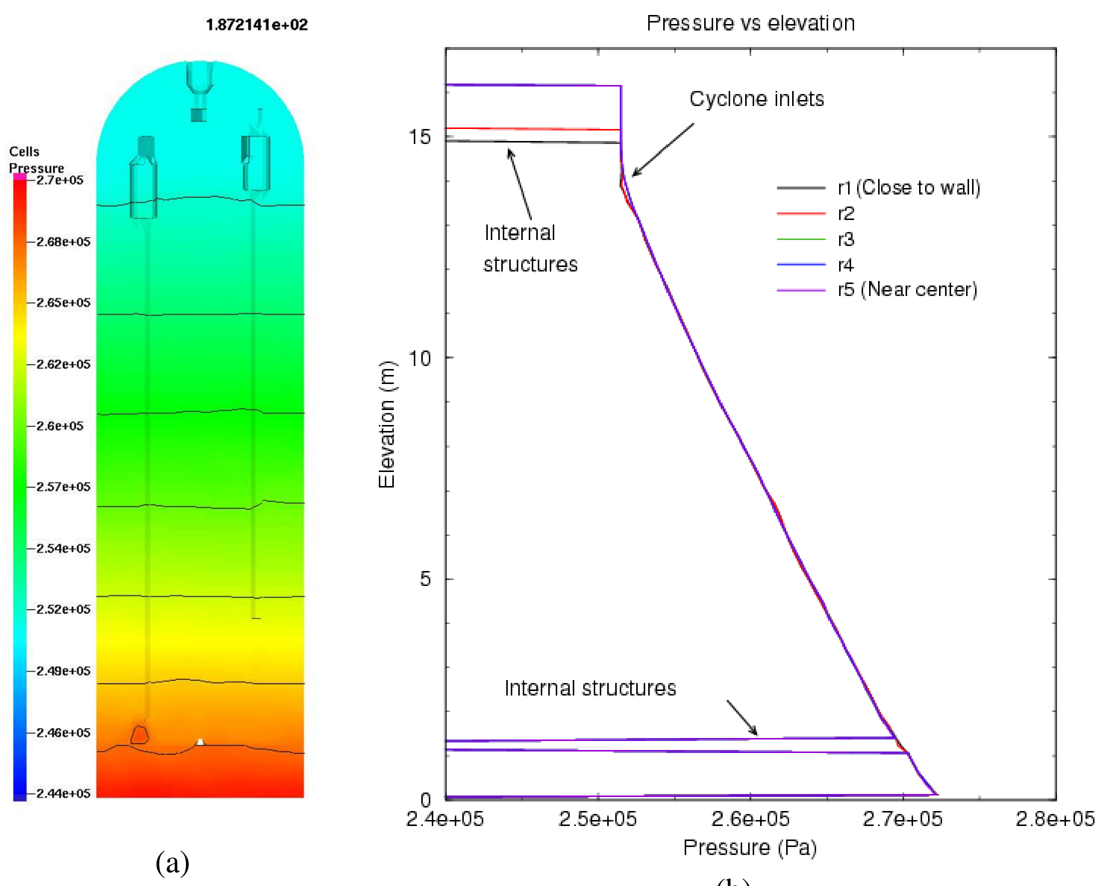
(a) (b)

Figure 3. Average solid volume fraction profile in a vertical plane cut through the center line (a) and versus elevation at different radial positions across the plane.

3.2. *Pressure distribution*

Figure 4 shows the pressure distribution in the reactor. The pressure is almost uniform in the radial direction and almost linearly decreases with elevation up to the cyclone inlets, above which the pressure is constant. This is consistent with the solid concentration distribution presented in the previous section. A linear pressure distribution corresponds to a constant solid volume fraction, and a constant pressure distribution corresponds to a zero solid volume fraction. The horizontal lines in Figure 4(b) indicate vertical positions of the horizontal structures which are not in the computational domain and the pressure is given a value of zero inside the structures.

The pressure drop across the reactor height is 2.05×10^4 Pa. By a simple force balance, where pressure drop balances the bed weight of the solids, the pressure drop is $\Delta p = m_p g / A = 1.93\times10^4$ Pa, where m_p, g and A are the solid mass, the gravity and the reactor cross section area, respectively. The Barracuda calculated pressure drop is very close to that by the simple force balance.



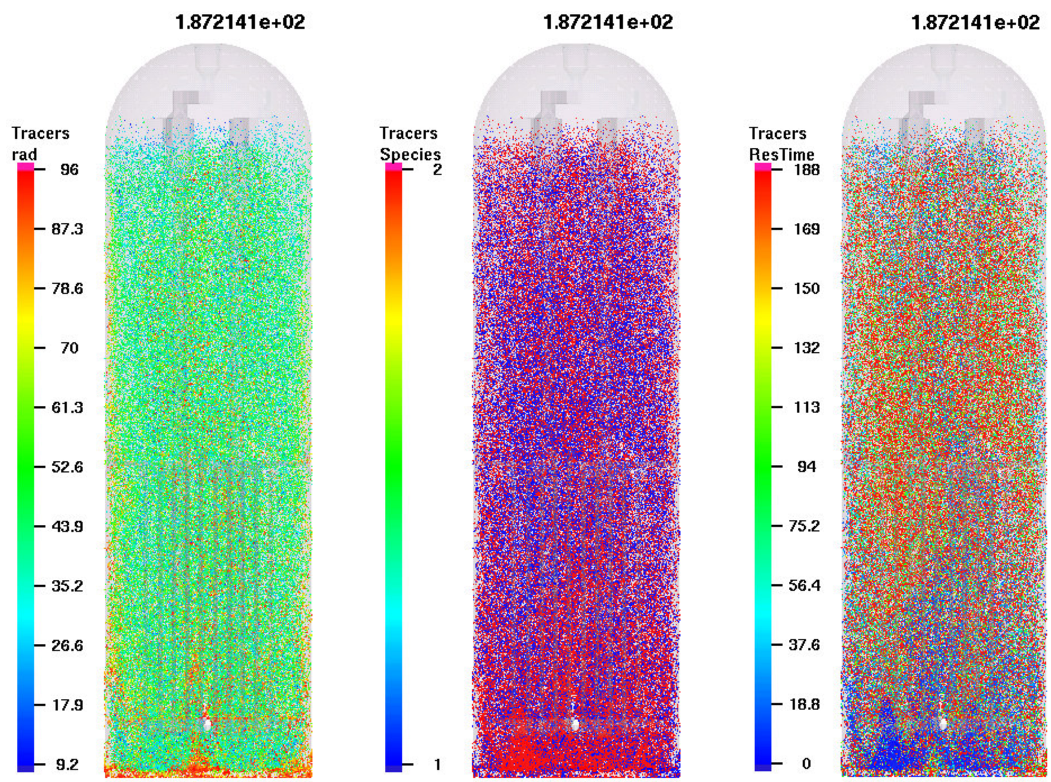
(a)

(b)

Figure 4. Pressure distribution in the reactor at the end of simulation. (a) Pressure profile in a vertical plane across the center line. (b) Pressure versus elevation at different radial positions.

3.3. *Particle size, species and residence time distribution*

Figure 5(a) shows particles colored by their radius. Most larger solids (in red) are at the bottom of the reactor. While in the freeboard, different sizes of solids are nearly uniformly distributed. At the elevation of cyclone inlets, i.e., the top of the fluidized bed, there are less larger solids. Larger particles are also seen in vertical channels near the outer wall of the reactor where gas velocity is high (see next section on flow pattern). Figure 5(b) shows solids colored by their species. Solids initially loaded in the bed are species 1, those returning to the bed from the diplegs are species 2. Overall the species are well mixed except near the bottom of the bed where there are more solids of species 2. Figures 5(c) shows the particle residence time distribution (RTD). Solids in blue color are newly fed particles from the diplegs, and most of the "new" solids are near the bottom of the diplegs. The freeboard contains solids with a wide range of residence times from a few seconds to the current simulation time (187.2 s). In the cyclone inlet region, there are some solids with residence times short than 30 s. These particles quickly flowed up from the dipleg discharge near the bottom of the vessel.



(a) (b) (c)

Figure 5. Particle size distribution (a), particle species distribution (b) and particle residence time distribution (c) shown in a vertical centerline plane with the front half of the reactor cut off. In (b), species 1 are the initially loaded particles and species 2 are particles feeding from the diplegs. Color bar unit is μm in (a) and s in (c).

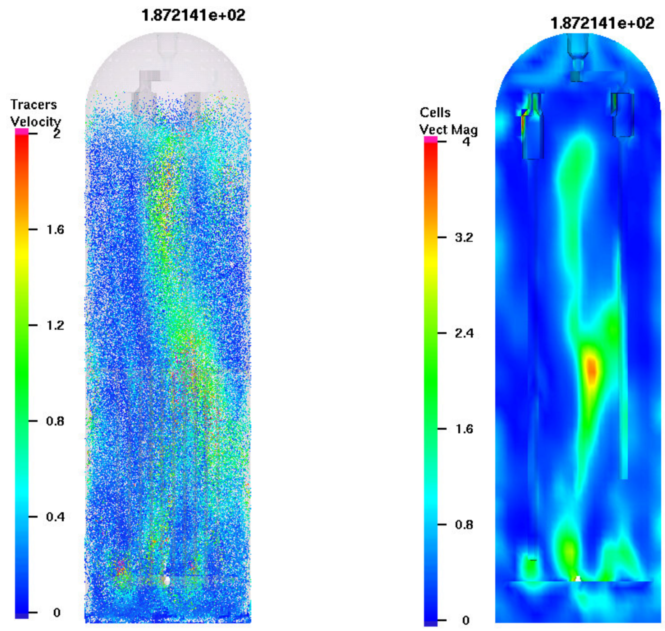
3.4. *Gas and solid flow pattern*

Figures 6(a) and (b) show the instantaneous solid and gas velocities, respectively, in a vertical plane across the center line of the reactor, where the color shows the velocity magnitude. The solid and gas velocity profiles are similar, both showing a long high-velocity channel in the freeboard near the center of the reactor. Gas velocity inside the channel is up to 3.5 m/s, which is 8 times of the superficial (average) gas velocity. The highest solid velocity in the channel is close to 2 m/s. The velocity distribution is far from uniform even though the reactor runs in a fast fluidization mode and the flow is highly turbulent.

Figure 7 shows the horizontal profiles of the instantaneous and average vertical components of gas and solid velocities at two elevations, one of which is in the bed section and the other in the freeboard. The three blue circular areas in the profiles at the 1.83 m (6-ft) elevation show the radial locations of the three first stage diplegs. Due to the downward flow of solids from the diplegs, the vertical components of both the solid and gas velocity are negative near the bottom of feeding diplegs. The influence of the downward diplegs feeding on the gas and solid flow pattern decreases with elevation. This is reflected in the profiles at elevation 7.62 m (25 ft), where the downward gas and solid flows are significantly reduced.

The instantaneous gas velocity profile at elevation 1.83 m (6 ft) from the vessel-bottom shows a number of small areas (red spots) where velocity is much higher than the average flow velocity, and the latter is close to the superficial gas velocity. These areas are the locations of gas streamers or long bubbles, which are shown at the outer wall of the reactor and inside the reactor between the diplegs. Gas streamers and long bubbles tend to form in regions away from the bottoms of the feeding diplegs, where the solid and gas flows are downward. The average gas velocity profiles show much weaker streamers with different locations than those in the instantaneous profiles. This indicates that the instantaneous streamers are not stationary but are unstable, and they either change horizontal positions with time or collapse and reform. The average profiles show streamers move between the feeding diplegs and circumferentially along the outer wall of the reactor. Streamers become more unstable as elevation increases, at elevation 7.62 m (25 ft) (in the freeboard) the average gas velocity becomes more uniform, but even in the freeboard, there are a number of strong streamers in the instantaneous profile.

The gas and solid flows are far from uniform as shown in the average gas and solid velocity profiles. Gas and solid vertical-circulations occur in the dense-bed section and in the freeboard. Overall the upward gas flow occurs in the center of the vessel, encircled by the diplegs, and in a thin layer along the outer wall with downward flow of solids in an annulus in between. The solid flow pattern is similar to the gas flow except that the overall downward solid flow region is larger. This disparity between gas and solids flow patterns results from regions of slow upward flow gas not being able to support the solids. The Barracuda CPFD predicted gas and solid flow pattern in this large-scale reactor differs from that observed in a small lab-scale fluidizing unit where solids were observed to flow down the vessel wall. The difference in the flow pattern is partly due to size difference of the units, and partly from complex internal structures with the solids return to the dense bed from the diplegs, which were absent in the lab-scale units.



(a) (b)

Figure 6. Instantaneous particle velocity (a) and gas velocity (b) distribution in a vertical plane across the center line with the front half of the reactor cut off, at simulation time 187.2 s. The unit of the color-bar legend is m/s.

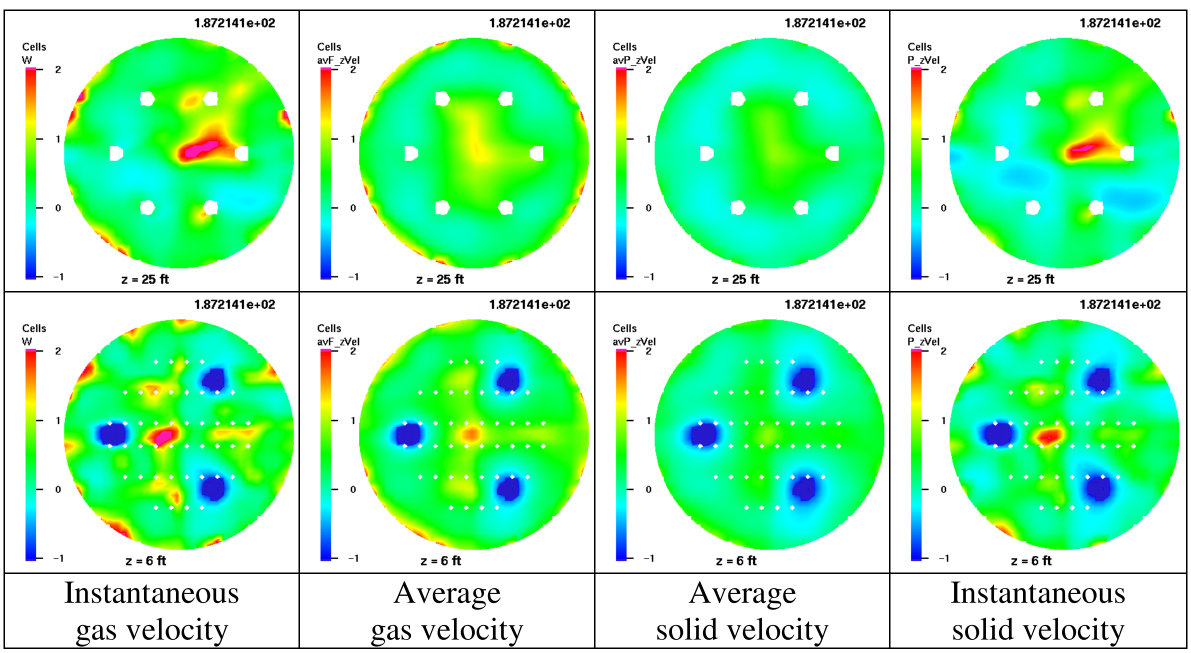


Figure 7. Radial distribution of instantaneous and average vertical components of gas and solid velocities at elevations 6 ft and 25 ft.

4. Conclusion

The fluidization behavior of a large commercial-scale reactor has been numerically simulated with the Barracuda CPFD^{TM} software package. The software has been extensively validated against available theoretical and experimental data, which are not presented here. The simulation presented in this work is three dimensional with all major complex internal structures included in the model. The FCC-type particles, with a user specified size distribution, are properly handled by the software. Particles are entrained to leave the reactor and enter the cyclones and return to the reactor through diplegs. The simulation provides data on the solid distribution, pressure distribution, particle size distribution, particle species distribution, particle residence time distribution (RTD), fluid and solid flow patterns, and other fluidization characteristics. The calculated pressure drop over the reactor height matches well with the solid weight force balance.

Simulation results reveal that, under the applied conditions, the gas and solid flows in the reactor are far from uniform. Strong instantaneous gas streamers form which channels gas through the bed at 5 to 10 times the average superficial gas velocity. Gas streaming results in extremely non-uniform gas and solid flows and poor gas-solid mixing, which reduces reactor performance. The gas streamers appear in the reactor between the diplegs and along the outer wall. The time averaged gas streamers are weaker than the instantaneous streamers indicating the streamers are unstable and change horizontal positions with time. The average gas and solid velocities are upward in the center region of the vessel and in a layer along the outer wall. Downward gas and solid flows occur in the annulus region defined by the circular-ring of the diplegs. The gas and solid flow patterns are different than those observed in small-scale laboratory units which exhibit upward flow in a center core and downward flow along the wall. The difference is attributed to the size difference of the units and the absence of internal structures and solids return to the dense bed from the diplegs in the lab-scale units.