MFIX-Exa simulation of the baby CFB

William D. Fullmer
National Energy Technology Laboratory, Morgantown, WV, USA
william.fullmer@netl.doe.gov

Overview

The "baby CFB" is a small-scale, prototypical circulating fluidized bed that was generated as a test case for MFIX-Exa. The simulation case was designed to run on 12 GPUs with a one-to-one MPI rank to fluid grid mapping. Although substantially smaller in size and run with reduced chemistry and physics (non-reacting and cold flow), the CFB geometry and the operating conditions test the code by producing some of the complex flow hydrodynamics expected in NETL's 50kW chemical looping reactor.

Material Properties

The working fluid is assumed to be incompressible with a constant density and viscosity of ρ_g = 1.2 kg/m^3 and μ_g = 1.8·10^{-5} kg/m-s, respectively. The idealized particles are d_p = 1 mm diameter with a density of ρ_p = 1000 kg/m^3 having restitution and friction coefficients of $e_{pp} = e_{pw}$ = 0.9 and $\mu_{pp} = \mu_{pw}$ = 0.3, respectively. The solids spring constant is set to k_n = 1000 N/m which corresponds to a collision time of approximately τ_{coll} = 5·10^{-5} s. The solids time step used by the discrete element method is set to $dt_{\mathrm{DEM}} \leq \tau_{coll}/20$, and the maximum fluid timestep is set to $dt_{\mathrm{CFD}} \leq 20\,\tau_{coll}$. Note that the fluid time step is Courant-limited below the upper bound dynamically by satisfying CFL ≤ 0.9.

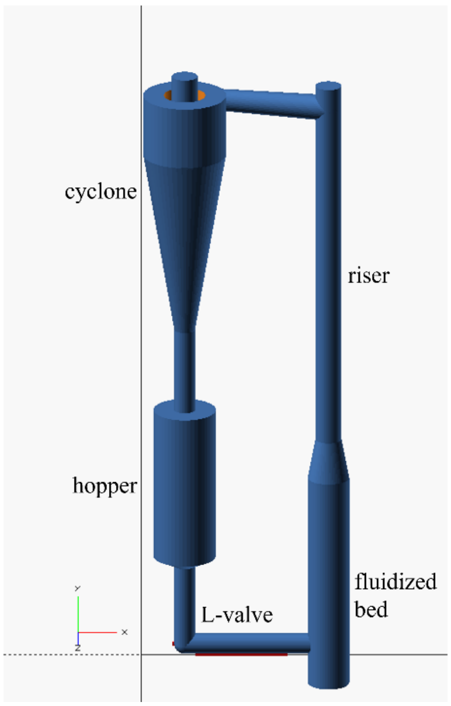

Figure 1. Geometry of the baby CFB with the five major components labeled.

Geometry and Boundary Conditions

A uniform fluid mesh of dx = 4 mm (dx/d_p = 4) is applied with a base grid of 64^3, giving an edge length of L = 0.256 m. The domain is then set at $L_x = 2L$, $L_y = 6L$, and $L_z = L$, yielding 12 grids, each managed by one MPI rank during the simulation. As identified in Fig. 1, the major components of the baby CFB are the cyclone, hopper, fluidized bed, riser and L-valve which are composed of 8-, 6-, 4-, 2.5-, and 2-inch inside diameter piping, respectively. The exact geometrical configuration can be found in the associated openSCAD file. The Wen and Yu (1966) minimum fluidization correlation predicts $U_{mf} \approx 0.26$ m/s for the given particle properties. The flow rate is set to U = 1.5 m/s at the inlet (y = 0) of the fluidized bed, which should violently fluidize the particles at approximately $5U_{mf}$. As the 4-inch fluidized bed is constricted to the 2.5-inch riser, the superficial gas velocity increases to 3.84 m/s which is near the particle terminal velocity and should be sufficient to transport most of the particles that reach the riser. The riser extends to within 1dx of the top of the domain forming the top of a blinded T-junction. A cross-over connects the riser to the cyclone and introduces particles tangentially into the back side of the top of the cyclone. Gas flow and any entrained particles exit the cyclone through a pressure outlet at the top of the domain ($y = L_y$) and the remaining solids material drops into the hopper. The L-valve at the bottom of the hopper returns particles to the fluidized bed, completing the loop. There are two gas flow boundary condition regions to help move particles through the tight 90° elbow of the L-valve. A jet is placed on the back side, aligned with the center of the cross-over directing particles towards the fluidized bed and a simplified sparger region is placed on the bottom of the cross-over to fluidize the particles. The jet is square with an edge length of 2dx; the modeled sparger is rectangular with a depth of 2dx and is 56dx in length. The jet and sparger regions are shown in red in Fig. 1 and their exact placement can also be found in the openSCAD file. Note that these regions are not rendered as part of the complex solid geometry (CSG) but prescribed as boundary conditions on the embedded boundary (EB) defined by the CSG. The jet and sparger velocities are set to 4.0 and 1.0 m/s, respectively. These flow conditions were determined by trial and error to provide good movement of the particles through the L-valve.

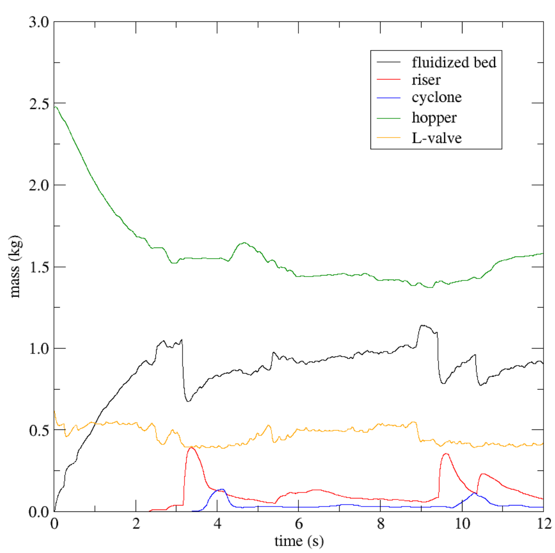

Figure 2. Particle mass in the primary components of the baby CFB up to a simulated time of 12 s.

Initial Conditions

The fluid is initialized with zero velocity everywhere. Particles are placed throughout the L-valve, extending 8 inches up into the hopper. The particles are generated in a hexagonal close packed lattice with a solids concentration of 64%. This results in approximately 5.9 million particles.

Results

The baby CFB is simulated with MFIX-Exa on NETL's Joule2 HPC. The hypre linear algebra software library is used for the bottom solve of the nodal and MAC projection, specifically the GMRES solver and the BoomerAMG preconditioner. The Godunov advection scheme is used and the drag force is included in the approximation to the right hand side of the momentum equation when extrapolating from cell centers to face centers. The state redistribution algorithm is applied and a maximum solids packing of 0.75 is set, above which mass is distributed to surrounding cells. Ascent *in situ* visualization package is used to save images of the particles colored by velocity magnitude. In addition, user averaging regions are placed throughout the domain to monitor the movement of particles within the five major components of the baby CFB. The instantaneous solids mass in each component is shown in Fig. 2. For the first three seconds, particles drain out of the hopper, through the L-valve and into the fluidized bed. As particles accumulate in the bed, the bubbling/slugging becomes more violent until a slug rapidly ascends through the riser, around the cyclone and back down into the hopper. A quasi-steady flow of particles remains in the riser after the initial slugging event until a second slug forms at approximately ten seconds. It is expected that the most challenging aspects of the circulating flow dynamics have been achieved by $t = 12$ s and that the developed quasi-steady flow pattern will continue in time.

Acknowledgement

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References

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