PARTICLE-X: THREE-DIMENSIONAL EULERIAN-LAGRANGIAN SIMULATIONS OF FLUIDIZED BEDS

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ABSTRACT

There have been several approaches for developing computer simulations of fluid-particle systems. One is the *Eulerian-Lagrangian* approach, also known as *Computational Fluid Dynamics-Discrete Particle Method*. In this type of computer simulations, the discrete phase is handled by calculating position and velocity of each individual particle using Newtonian physics. The continuous phase is treated as flowing through a porous region, in which the voidage is determined by the distribution of particles.

Two-dimensional simulations have been largely successful in representing fluidized-bed systems, but cannot accurately model the packing of particles at low fluid velocities. They also present difficulties with particle size distributions. Three-dimensional models, on the other hand, can overcome these difficulties, but demand much more computational power.

Particle-X is a proprietary Fortran code that has been developed primarily at Oregon State University. It is a fully three-dimensional Eulerian-Lagrangian simulation of fluidized beds. Fluid motion is calculated using the SIMPLE algorithm, particle collisions are resolved using the soft-sphere model, and motion of the particles is obtained by integrating the equation of motion of each particle, either using the explicit Euler or second-order Adams-Bashforth method. Aside from particle motion and fluid dynamics, Particle-X also features basic models for heat and mass transfer and magnetic forces acting on particles. Simulation data is saved to a set of binary files and visualized (post-processed) using Bolitas 2.

The simulation code has been validated by comparison with experimental evidence. Several examples of the use of the code are shown., including some cases of experimental conditions not readily reproducible such as micro- and zero-gravity fluidization. Future capabilities of the simulation code are examined as well.

INTRODUCTION

There are several unit operations that involve the contact of a solid (particulate) phase and a continuous (liquid or gas) phase. Among the many approaches for modeling these systems, the *Eulerian-Lagrangian* or *Computational Fluid Dynamics-Discrete Particle Method* (CFD-DPM) has been subject of extensive development in the last 15 years, partly because the rapid increase in computational power.

The CFD-DPM model (Figure 1) treats each individual particle as a sphere obeying Newtonian physics. The spatial distribution of the particles is used to calculate an average voidage for the discretized domain. The fluid phase is then simulated as a continuous flow through a porous region of prescribed voidage. The interactions between the fluid and the particles are calculated between this average flow and each particle.

| Particle distribution | Average cell vodage | Fluid velocity and pressure |
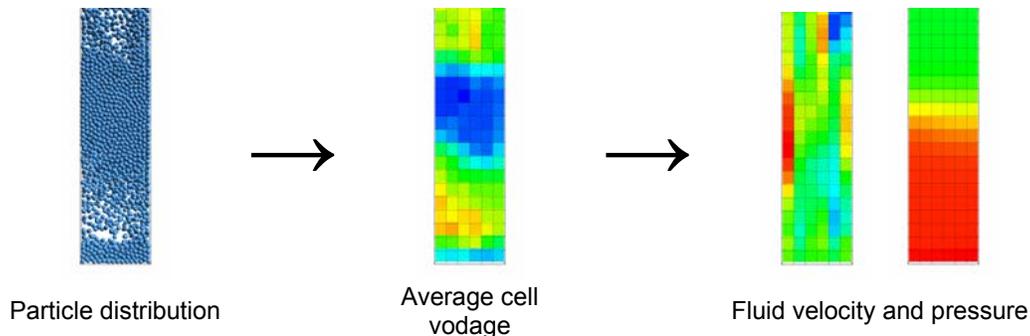
Figure 1. CFD-DPM approach for simulating fluid-particle systems.

The main advantage of this model is that the interactions between particles, including interparticle forces, can be adequately modeled and studied independently of one another. It is also possible to replicate conditions not readily available in the lab, such as the expected behavior of a fluidized system in micro- and zero-gravity (Pinto-Espinoza, 2002; Sornchamni, 2004; Reed, 2006).

Due to the limited computational power available in the past, most computer simulations of fluidized beds were two-dimensional models in which the bed was assumed to be exactly one particle diameter thick, and the particles were constrained between frictionless surfaces. Unfortunately, the voidage of a packed bed of spheres cannot be accurately represented because particles are constrained to a vertical plane, and it is difficult (or at least inaccurate) to model systems with particle size distributions.

A fully three-dimensional model would not suffer these constrains, and it would be capable of a more accurate representation of the actual conditons of the fluidized bed. However, the computational requirements scale very rapidly with the number of particles. With the computational resources as of 2006, simulations with $O(10^6)$ particles can be done with desktop computers at an approximate rate of 24 hours of computation time for 1 second of simulation time (Reed, 2006).

The simulation code presented in this document, *Particle-X* is a fully 3D CFD-DPM simulation code developed mainly at the School of Chemical, Biochemical, and Environmental Engineering (formerly the Chemical Engineering Department) of Oregon State University.

THEORETICAL BACKGROUND

The governing equations of the continuous phase are the mass conservation equation (or continuity equation, Equation 1), and the momentum conservation equation (or Navier-Stokes equation, Equation 2) with a Newtonian viscous stress tensor (Equation 3).

$$\frac{\partial \varepsilon}{\partial t} + \tilde{N} \times (\varepsilon \mathbf{u}) = 0 \tag{1}$$

$$\rho_f \frac{\partial}{\partial t}(\varepsilon \mathbf{u}) + \rho_f \tilde{N} \times (\varepsilon \mathbf{uu}) + \varepsilon \tilde{N} P + \tilde{N} \times (\varepsilon \tau) - \varepsilon \rho_f \mathbf{g} - \mathbf{f} = 0 \tag{2}$$

$$\tau = - \mu_f \acute{e} (\tilde{N}\mathbf{u}) + (\tilde{N}\mathbf{u})^T \grave{u} \tag{3}$$

The governing equations of the discrete phase, given by Newton's second law, are the linear momentum equation (Equation 4) and the angular momentum equation (Equation 5)

$$m_P \frac{d\mathbf{v}_i}{dt} = \overset{\circ}{a} \ \mathbf{F}_i \tag{4}$$

$$I_P \frac{d\vec{\omega}_i}{dt} = \overset{\circ}{a} \ \mathbf{T}_i \tag{5}$$

The collisions (particle-particle or particle-wall) are modeled using the soft sphere model originally proposed by Cundall and Strak (1979). The colliding system is represented by normal and tangential spring-dashpot systems. The particles are assumed to overlap a short distance, and the normal component of the force is assumed to be proportional to this overlap.

EXPERIMENTAL VALIDATION

Particle-X code has been validated by direct comparison with fluidization data obtained at the laboratory scale, including phenomena at the particle level and overall bed-scale properties and behavior (Cruz-Fierro, 2005; Reed, 2006). Figures 2 through 5 show several examples of qualitative and quantitative comparisons between experimental data and simulations. In each case, the simulation replicates as much as possible the experimental conditions of geometry, dimensions, particle characteristics, and flow conditions.
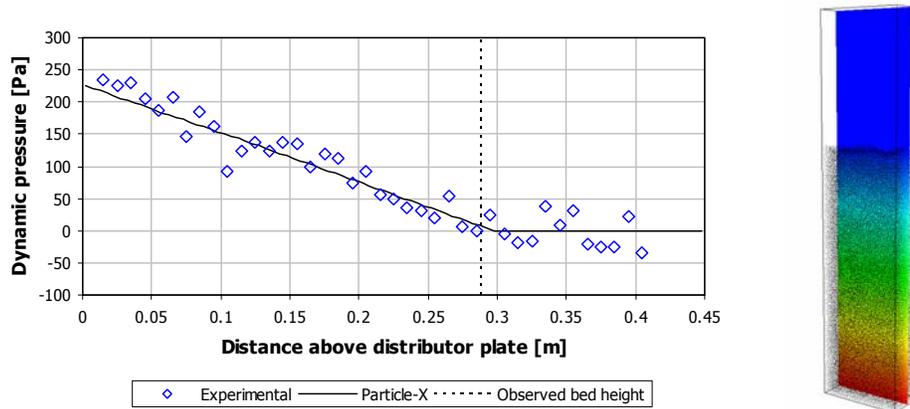

Figure 2. Pressure drop validation using a liquid-solid system, u_0 = 0.017 m/s, d_p = 2.63 mm, ρ_p = 1181 kg/m³. Experimental data from Cruz-Fierro (2005).
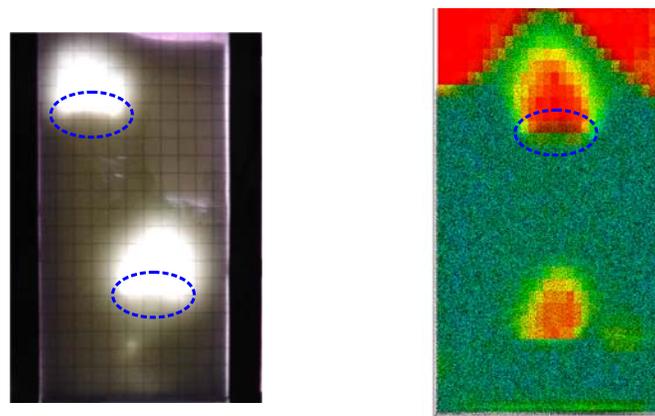
Figure 3. Bubble formation and dynamic behavior in gas-solid fluidized bed, d_p = 720 µm, ρ_p = 2700 kg/m³, u_0 = 0.340 m/s. **Left**: Experiment. **Right**: Particle-X simulation. Color plane represents voidage. Adapted from Reed (2006).

t = 0 s	t = 1s	t = 2s	t = 3s	t = 4s	t = 5s	t = 6 s	t = 7 s	t = 8 s	t = 9 s
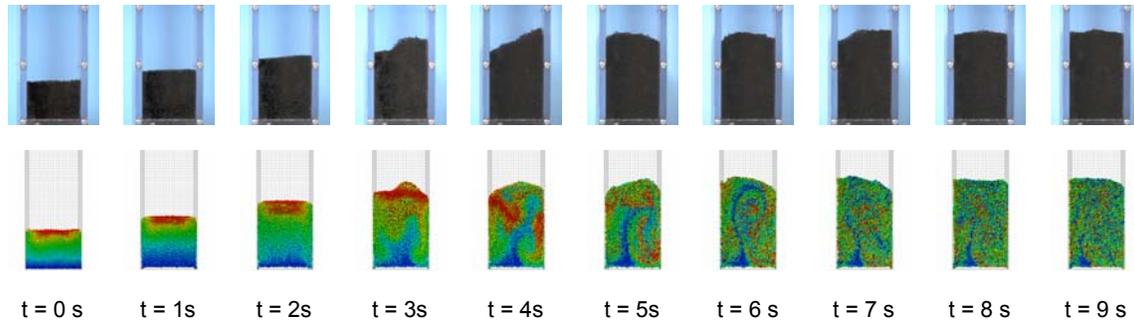
Figure 4. Bed expansion at startup of a liquid-solid fluidization. Fluid velocity is suddenly increased from zero to 0.037 m/s. d_p = 2.63 mm, ρ_p = 1181 kg/m³. **Top**: Experiment. **Bottom**: Simulation. Adapted from Cruz-Fierro (2005)
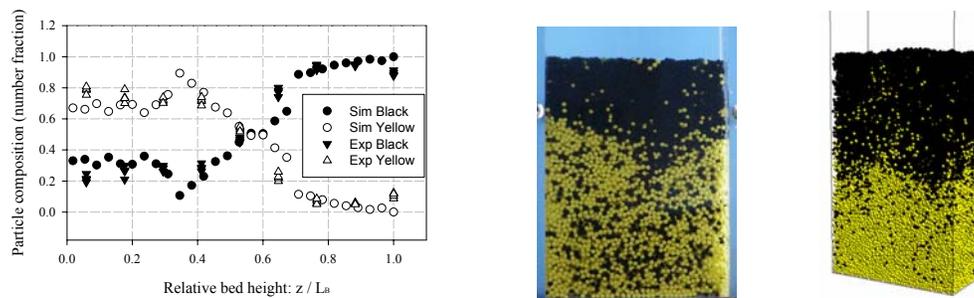
Figure 5. Segregation of particles in binary solid-liquid system.
Left: Experiment and simulation comparison. **Middle**: Experiment. **Right**: Simulation.
Yellow particles: d_p = 2.21 mm, ρ_p = 1160 kg/m³. *Black particles*: d_p = 2.30 mm, ρ_p = 1114 kg/m³. Adapted from Reed (2006).

CONCLUSION

Most simulation results agree within ±5 ~ 15% of the corresponding experimental data, showing that the code is reliable and captures the key features of the studied fluidized beds. As of the time of this writing (2007), the Particle-X code implements the following key features:

- Rectangular computational domain, with inlet at the bottom and outlet at the top, and walls with no-slip condition.
- Constant number of particles, all contained within the column.
- Particles of uniform or distributed size, and uniform or distributed density.
- Soft-sphere model for particle-particle and particle-wall collisions.

- Motion of the particles determined by twice-integrating the Newtonian equation of motion. Available integration schemes are explicit (forward) Euler and second-order Adams-Bashforth.

- Voidage calculated with equivalent-volume cube approximation (Reed, 2006).

- Fluid flow calculated in a rectangular grid, using the Semi-Implicit Pressure Linked Equation (SIMPLE) method (Patankar, 1977). The discretized equations of motion and pressure correction equation are solved using the over-relaxed Gauss-Seidel method.

- Fluid properties (density, viscosity) can be assumed constant or be variable.

- Drag force calculated using DiFelice (1994) correction for voidage.

- Basic models for fluid-particle heat and mass transfer.

- For magnetically susceptible particles, calculation of external magnetic force and interparticle magnetic forces (non-interacting dipoles model).

- Parameters for simulation (including optionally the initial position of particles) provided through a text input file. Especification of several variables such as inlet flow and gravity as functions of time, by means of another text input file.

- Simulation results recorded in the FLU/FLX file format suitable for visualization and post-processing using Bolitas 2 (Cruz-Fierro *et al.*, 2005)

Future extensions of this simulation code should include non-rectangular geometry, variable number of particles, non-spherical particles, compressibility continuous phase, and models for turbulent flow in the system.

REFERENCES

Cruz-Fierro (2005). "Hydrodynamic Effects of Particle Chaining in Liquid-Solid Magnetofluidized Beds: Theory, Experiment, and Simulation". *PhD Thesis*, Oregon State University, 196 p.

Cruz-Fierro, Reed, and Pinto-Espinoza (2005). "Bolitas 2: Viewer for Fluidization Simulation Data". Electronic resource available at http://cruzfierro.com/academic/bolitas.htm

Cundall, P.A. and O.D.L. Strack (1979). "A discrete numerical model for granular assemblies." Géotechnique **29**(1): 47-65.

Di Felice (1994). "The voidage function for fluid-particle interaction systems". International Journal of Multiphase Flow **20**(1): 153-159.

Patankar (1977). "Numerical heat transfer and fluid flow". McGraw-Hill, 197 p.

Pinto-Espinoza (2003). "Dynamic Behavior of Ferromagnetic Particles in a Liquid-Solid Magnetically Assisted Fluidized Bed (MAFB): Theory, Experiment, and CFD-DPM Simulation". *PhD Thesis*, Oregon State University, 271 p.

Reed (2006). "Development and Experimental Validation of a Discrete Particle Simulation for Fluidized Beds with External and Inter-particle Forces". *PhD Thesis*, Oregon State University, 313 p.

Sornchamni (2004). "Magnetically assisted liquid-solid fluidization in a gradient magnetic field: Theory and application". *PhD Thesis*, Oregon State University: 121 pp.

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