Particulate modeling in ANSYS CFD

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Agenda

- Summarize and illustrate approaches for modeling particulate media in ANSYS CFD products
- Highlight aspects that help in customizing and extending the models available in Fluent and CFX
Introduction

- Rheology of a collection of particles or grains
- Complex mechanical behavior
  - Fluid like – pneumatic transport, fluidized beds
  - Solid like – heaps, foundations
- Main factors governing behavior
  - Volume fraction
  - Shear rates
  - Influence of fluid
Overview of modeling approaches

Lagrangian models

Trajectories of individual particles

Flow around individual particles or local averaging

Eulerian Granular

Continuum model (multidimensional)

Local averaging

Concept illustration borrowed from Prof. Tsuji Presentation at WCPT5, April 2006
Granular models available in ANSYS

- **Two fluid models**
  - Euler-granular
  - Euler-granular with frictional viscosity for dense phase

- **Particle models**
  - DPM for dilute phase (steady and time dependent)
  - Particle tracking model with a probabilistic collision model
  - Dense phase DPM (DP-DPM) for dense flows with large size distributions (UDF)
  - Macroscopic Particle Model (MPM) for large particles (UDF)
<table>
<thead>
<tr>
<th>Method</th>
<th>Particle to particle interactions</th>
<th>Coupling with cont. phase</th>
<th>Additional physics &amp; chemistry</th>
<th>Particle shape, size distribution</th>
<th>Order of # of particles</th>
<th>Computation speed &amp; parallelization</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM</td>
<td>Direct contact and other forces implementation</td>
<td>None or through ext. CFD code</td>
<td>Not implemented</td>
<td>Arbitrary (clustered spheres) shape &amp; distribution</td>
<td>~10^5</td>
<td>Strongly dependent on # of particles, not parallelized, Rel. slow</td>
</tr>
<tr>
<td>DPM</td>
<td>Collisions &amp; breakup indirectly; packing limit not accounted</td>
<td>Correlation-based drag force</td>
<td>Coupled with all std. Fluent models, easy to customize</td>
<td>Spherical and ellipsoidal</td>
<td>~10^6</td>
<td>Very fast, parallelized</td>
</tr>
<tr>
<td>MP-PIC</td>
<td>Particles are represented by clusters, packing limit is maintained</td>
<td>Correlation-based drag force</td>
<td>Coupled with all std. Fluent models, easy to customize</td>
<td>Spherical, arbitrary size distribution available</td>
<td>No limit on part/ clusters (tested up to ~2.5x10^5)</td>
<td>Rel. fast, affected by mesh size &amp; # of particles, parallelized</td>
</tr>
<tr>
<td>MPM</td>
<td>Direct contact and other forces implementation</td>
<td>Drag &amp; torque resolved</td>
<td>Further customization possible</td>
<td>Spherical*, arbitrary distribution</td>
<td>~10^5</td>
<td>Slow, parallel tracking (interactions not parallel)</td>
</tr>
<tr>
<td>Euler Granular</td>
<td>Indirect: solid pressure &amp; radial distr., other forces implemented indirectly</td>
<td>Cell-avg. drag, lift &amp; other inter-ph. terms</td>
<td>Coupled with all std. Fluent models; easier to customize</td>
<td>Spherical; Size dist. through population balance</td>
<td>Practically unlimited</td>
<td>Fast, depends on the mesh size &amp; physics only, parallelized</td>
</tr>
</tbody>
</table>
Euler-Granular models
For best results …

- Run the simulations transient
- Calibrate the drag law
  - Governs the minimum fluidization velocity
  - Minimum fluidization velocity should be matched with the experimental value
- For the maximum packing limit
  - Set to the volume fraction at minimum fluidization
- Time step ~ 0.001s
  - May need to use lower time steps if additional physics is added
Segregation

• Differences in particle sizes and density could cause segregation

• In liquid fluidized beds
  – At low superficial velocities smaller and denser particles are at the bottom and lighter and bigger particles are on top
  – At high superficial velocities smaller and denser particles are at top and lighter particles are at the bottom

• Simulation setup to reproduce experimental data of Moritomi et al (1982)
Prediction of solid inversion

Char and glass beads are well mixed at the low liquid velocity of 2.5mm/s.

Inversion of char and glass beads at a high liquid velocity of 9mm/s.
Quantitative comparison with experiments of Moritomi et al.
Lagrangian information from Eulerian simulations

- Is it possible to recover any particle level information from the Eulerian solution?
- Do particles released from the same position at different instants, spend the same time in the reactor?
- What is the distribution of the residence times at various zones in the equipment?
  - Time spent in the spray zone of a Wurster bed determines coating thickness
Tracking particles with the secondary phase

- We need a mechanism to convect particles based on the Eulerian velocity.
- By default, DPM particles convect with the primary phase.
- We can customize Fluent into convecting particles by the secondary phase by:
  - Copying secondary phase velocities to the primary phase just before particle position update.
  - Restore primary phase velocities after the particle update.
- UDF to do this available.
Some results
Lagrangian models
Lagrangian models

- Particle/parcels are tracked in the Lagrangian phase
- Economical way of accounting for particle size distributions
  - Generally do not account for particle-particle collisions
  - Restricted to low volume fraction of solids (< 10%)
- We will highlight models that relax these restrictions
  - Particle tracking with the Sommerfield collision model in CFX
  - Dense phase DPM model in Fluent (UDF)
A particulate model for slightly dense flows

- For highly loaded gas-solid flows, particle collisions cannot be neglected
  - Calculating collisions between all particles can be computationally expensive
- CFX’s particle tracking model allows for slightly dense gas-solid flows where a stochastic model for particle-particle collisions is available
  - High mass loading
  - Moderate volumetric concentration (<~ 20%)
  - Can be run with the steady state solver as well
Experiment of Fohanno & Oesterlé
Particle trajectories without / with collision model

without collision model

with collision model
A particulate model for fluidized beds

• Advantages of a particulate model
  – Account for particle size distribution
  – Ability to include more complicated particle level physics
    • Friction, electrostatic, cohesion etc.
• Simple treatment of collisions/contact is not suitable for dense regimes of granular flow
  – Fluidized beds, pneumatic transport, risers
The Dense phase DPM model

- A custom model has been developed to account for all dense phase effects
  - Uses the framework of DPM model in FLUENT
  - Allows access to all DPM models and numerics
- The DP-DPM model accounts for
  - Particle-particle and particle-wall collisions
  - Reduced area available for fluid flow
  - Drag laws for dense fluidized beds
Validation of the DP-DPM model

- Prediction of the minimum fluidization velocity for the *static* bed
  - For fluidization experiments, the bed will behave like a *stationary* bed for gas velocities below the minimum fluidization velocity
  - Beyond the minimum fluidization velocity the pressure drop balances the buoyant weight of the bed and is a constant
Structure of the bed for various gas velocities

Particle Traces Colored by User Value 4 (Time=6.2500e-02)  Feb 07, 2007
FLUENT 6.3 (3d, dp, pbns, lam, unsteady)

Pressure at the inlet

V = 0.30m/s, T = 0.082500
The fluidization curve

![Fluidization curve graph]

- **Gas superficial velocity (m/s)** vs **Pressure drop (Pa)**
- **Weight of bed** and **DPDPM predictions**

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Flow in a cyclone

- Mass loading of 10 at inlet
- Rossin-Ramler distribution of particles
  - Mean = 3e-5m
  - Min = 2e-6m
  - Max = 1e-4m
  - Spread = 0.806
- RSM model for turbulence
- 200,000 particles at steady state
Dense particle flow in a cyclone
Flow of solids in a riser

- 16 m tall and ID of 0.35 m
- FCC particles are of 175 microns diameter
- At “steady state” about 1.5 million parcels are handled
- Approximately 0.2s of flow time simulated in a day in a single processor
- Each parcel represents 20000 particles
Formation of clusters, strands and structures clearly captured, as is the downflow near the walls
Pressure profiles compared

"#3 Riser pressures with height"

- Dilute region in the middle
- Dense accelerating region at the bottom

Graph showing pressure profiles with height for #3 riser, comparing experimental (Exp.) and DPDPM results.
Summary

• Wealth of options available for modeling particulate flow in Fluent and CFX
• Review of particulate flow regimes and models appropriate for each of them
• Examples of successful application and validation of the models
• Examples of extensions made to the standard models to increase range of applicability

• Acknowledgements: Kartik Mahalatkar, John Stokes