Particulate Modeling with ANSYS CFD

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Agenda

Introduction
Review models for particulate flows
Models for dense particulate flows
Example applications
Questions
Introduction
Particulate Flows: Issues and Physics

Spans wide range of
• Length scales
• Time scales

Physics
• Particulate physics
• Fluid particle interaction
• Particle size distribution
• Homogenous and heterogeneous reaction
• Particle structure interaction

From: Fundamental of Multiphase Flow, C. E. Brennen
A Platform for Modeling Particulate Flows
Fluid Solid Interactions

From: E Loth, 
Particles, drops and bubbles 
Fluid dynamics and numerical methods
Effect of particle volume on gas phase

- Excluded volume
Fluid phase
• Almost always Eulerian!

Particle phase
• Eulerian or Lagrangian

Size of particles with respect to fluid grid
• Sub-grid or super grid
• Particle fluid interaction
  – Modeled or resolved

Particle-particle interactions
• Modeled or resolved
For Example ...
Particle phase
- Treated in a multi-fluid framework
  - Ensemble and time averaged over particles to arrive at PDE
  - Maximum packing
- Cell based
  - Volume fraction, velocity, temperature

Particle-particle interactions
- Modeled. Kinetic theory, frictional models
- Granular pressure, granular viscosity

Particle fluid interactions
- Empirical models
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
Catalytic Oxidation of Methane

Conversion of methane to synthesis gas is an important chemical process

Modeling of partial oxidation of methane in presence of Ni-alpha-alumina catalyst is carried out in a bubbling fluidized bed reactor.

Simulation results were compared to experimental data obtained from literature.
Figure 3 Effect of feed composition on methane conversion

Figure 4 Variation of species concentration with height above the gas distributor
NETL Fluidization Challenge

Contours of Volume fraction (coarse) (Time=5.6160e+01)  Nov 05, 2010
ANSYS FLUENT 13.0 (3d, dp, pbns, eulerian, lam, transient)
Framework to track a dispersed phase in a Lagrangian framework
• Account for the presence of the dispersed phase in the equations of motion for the primary phase
• Treat fluid-particle interactions in an efficient manner

Particle-particle interactions
• Collision breakup model for droplets
• Expression for solid pressure – KTGF
• Explicit particle interaction – DEM
• Other models ...

Particle fluid interactions
• Empirical models
NETL Challenge: Effect of Depth on Fluidization

- Deeper bed has a tendency to exhibit gas streaming (larger fluctuations in DP) compared to shallow bed (Issangya et. al. 2007). DDPM model qualitatively predicts the trend as observed in experiments.
Effect of Fines on Fluidization

Axial Pressure Gradient Profile

Case 3:
- 3% fines - Experiment
- DDPM

Case 4:
- Experiment - 12% fines
- DDPM
Particle-particle interactions – DEM

- Resolved using a spring dashpot model
- Can model size dependent phenomenon
  - Brazil nut effect
- Model Particles as parcels or individual particles
- Accurate modeling of particle-particle interaction
- Independent of fluid mesh!
Macroscopic Particle Model
Available as a UDF

Hard sphere analogy

Particle phase
• Lagrangian representation of BIG particles
• Particles ideally span several cells

Particle-particle interactions
• Resolved

Particle fluid interactions
• Determined as part of the solution
### Summary: Models for Particulate Flows

<table>
<thead>
<tr>
<th>Model</th>
<th>Numerical approach</th>
<th>Particle fluid interaction</th>
<th>Particle-Particle interaction</th>
<th>Particle size distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>DPM</td>
<td>Fluid – Eulerian</td>
<td>Empirical models for sub-grid particles</td>
<td>Particles are treated as points</td>
<td>Easy to include PSD because of Lagrangian description</td>
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<td>Particles – Lagrangian</td>
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<tr>
<td>DDPM - KTGF</td>
<td>Fluid – Eulerian</td>
<td>Empirical; sub-grid particles</td>
<td>Approximate P-P interactions determined by granular models</td>
<td>Easy to include PSD because of Lagrangian description</td>
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<td>DDPM - DEM</td>
<td>Fluid – Eulerian</td>
<td>Empirical; sub-grid particles</td>
<td>Accurate determination of P-P interactions.</td>
<td>Can account for all PSD physics accurately including geometric effects</td>
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<td>Particles – Lagrangian</td>
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<tr>
<td>Euler Granular model</td>
<td>Fluid – Eulerian</td>
<td>Empirical; sub-grid particles</td>
<td>P-P interactions modeled by fluid properties, such as granular pressure, viscosity, drag etc.</td>
<td>Different phases to account for a PSD; when size change operations happen use population balance models</td>
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<tr>
<td>Macroscopic Particle Model</td>
<td>Fluid – Eulerian</td>
<td>Interactions determined as part of solution; particles span many fluid cells</td>
<td>Accurate determination of P-P interactions.</td>
<td>Easy to include PSD; if particles become smaller than the mesh, uses an empirical model</td>
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