Towards a comprehensive strategy for modeling gas-solid flows

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Overview

• Introduction/motivation
• Applications of gas-solid flows
• Modeling particulate flow approaches
  – Two fluid models
  – Eulerian–Lagrangian
  – Hybrid methods
• Modeling Dense phase flow using Lagrangian models
  – Volume fraction of particles
  – Particle-particle interaction
  – Particle collision
• Recap and conclusions
Motivation

- Develop a modeling platform for a range of industrial applications using multiple modeling approaches:
  - for multi-physics,
  - multi-component
  - multi-scale requirements for a range of industrial applications

- Applications include
  - Particle Products
    - Powders, granules
    - Crystals
    - Flakes, pellets
    - Pastes, emulsions
  - Matrix material
    - Filled fibers
    - Filled polymers
    - Building materials
  - Non-particulate
    - Droplets and bubbles
Focus on Particulate flows

- Modeling Gas–solid systems can include:
  - Particle flows
  - Particle size distribution
  - Particle mechanics
  - Surface and morphology
  - Particle-particle interaction
  - Turbulence and dispersion
  - Geometry effects
  - Particle attrition
  - Homogenous and hydrogenous reaction
  - Fluid forces and drag
  - Cohesion
  - Electrostatic
Modeling Multiphase Flows

- Ability to model Multiphase flows expanding
Gas-solid flows

Group A: small size and density like FCC powder

Group B: Most common Material Like Sand

Group C: Cohesive powder

Group D: Large and/or very dense particles

Courtesy: Prof. Martin Rhodes, Monash University, Australia.
Classification of granular flows

- **Kinetic regime** *(diluted flow)*
  - grains randomly fluctuate and translate, these forms of viscous dissipation and stress is named kinetic effect.

- **Collisional regime** *(higher concentration)*
  - in addition to dissipation, grains can collide shortly, enhancing dissipation and stress, named collisional effect

- **Frictional regime** *(typically ε >50%)*
  - grains starts to endure long, sliding and rubbing contacts, which gives rise to a totally different from kinetic and collisional, named frictional effect.
Dilute vs. Dense Flows

- **Average time between particle collisions:**

  \[ \tau_C = \frac{1}{f_C} = \frac{1}{n \pi d_P^2 v_r} \]

- **Particle response time:**

  \[ \tau_P = \frac{\rho_P d_P^2}{18 \mu_C} \]

- **Inter-particle spacing:**

  \[ \frac{L}{d_P} = \frac{3 \sqrt{\pi}}{6 \alpha_P} \]

- **Dilute flow:**

  \[ \frac{\tau_P}{\tau_C} < 1 \]

- **Dense flow:**

  \[ \frac{\tau_P}{\tau_C} > 1 \]
Dilute vs. Dense Flows

Inter-particle spacing

100 10 1

Dilute disperse

Dense disperse

One-Way Coupling

Two-Way Coupling

Four-Way Coupling

Volume fraction $\alpha$

$10^{-8}$  $10^{-6}$  $10^{-4}$  $10^{-1}$
Common Multiphase Models

- Modeling particulate flows has been of long-standing interest and commonly used models include:
  
  - **Lagrangian Models**
    - DPM for dilute phase (steady and time dependent)
    - Macroscopic Particle Model (MPM) for large particles.
  
  - **Eulerian Models**
    - Euler-Granular with constitutive relations for particle stresses
  
  - **Hybrid Methods**
    - Dense Phase DPM for dense flows with large size distributions.
      - Stress modeled on GKT
      - Explicit contact
Hybrid Models

- A general framework in which the continuous phase is solved on an Eulerian grid and the particulate phase in a Lagrangian frame.
- Accounts for the volume fraction of the particulate phase and particle size distribution.
- Provides cell-averaged information from Lagrangian to Eulerian frame.
- Accounts for particle-particle and particle-wall interactions (GKT or explicitly).
Transport equations for Eulerian granular flow

Continuity

\[
\frac{\partial}{\partial t} (\alpha_s \rho_s) + \nabla \cdot (\alpha_s \rho_s \vec{u}_s) = \dot{m}_{fs}
\]

Momentum

\[
\frac{\partial}{\partial t} (\alpha_s \rho_s \vec{u}_s) + \nabla \cdot (\alpha_s \rho_s \vec{u}_s \vec{u}_s) = -\alpha_s \nabla p_f + \nabla \cdot \vec{\tau}_s + \sum_{s=1}^{n} \left( \vec{R}_f + \dot{m}_{fs} \vec{u}_{fs} \right) + \vec{F}_s
\]

Note
Transport equations for fluid-fluid system and fluid-solid system differ only in the treatment of stress tensor and inter-phase terms
Solids stress tensor

- Constitutive equations needed to account for interphase and intraphase interaction:
  - Solids stress \( \nabla \cdot \bar{\tau}_s \)
  - Accounts for interaction within solid phase. Derived from granular kinetic theory

\[
\bar{\tau}_s = -P_s \bar{I} + 2\alpha_s \mu_s \bar{S} + \alpha_s (\lambda_s - \frac{2}{3} \mu_s) \nabla \cdot \bar{u}_s \bar{I}
\]

where,

\[
\bar{S} = \frac{1}{2} \left( \nabla \bar{u}_s + (\nabla \bar{u}_s)^T \right)
\]

strain rate

\( P_s \) \hspace{1cm} solids pressure

\( g_o \) \hspace{1cm} radial distribution function

\( \lambda_s, \mu_s \) \hspace{1cm} solids bulk and shear viscosity
Algorithm of the Dense Discrete Phase Model

Particle equation of motion, Collision force

\[
\frac{d\vec{u}_s}{dt} = F_D (\vec{u}_f - \vec{u}_s) - \frac{1}{\rho_p} \nabla p + \vec{g} \left( \frac{\rho_p - \rho_f}{\rho_p} \right) + \vec{a}_{other} + \vec{a}_{col}
\]

Cell based averaging

\[
< \phi > = \frac{\sum_i n_i \phi_i}{\sum_i n_i}
\]

\[
< \alpha_s \rho_s \vec{u}_s > \quad \text{mass flux}
\]

\[
< \alpha_s > \quad \text{vol. fraction}
\]

Kinetic theory

\[
\frac{3}{2} \left( \frac{\partial}{\partial t} (\langle \rho_s \alpha_s \rangle \theta + \nabla \cdot (\langle \rho_s \alpha_s \vec{u}_s \rangle \theta)) \right) = \\
= \tau_s : \nabla < \vec{u}_s > + \nabla (k_\theta \nabla \theta) - \gamma_\theta + \phi_{ls}
\]

Cell based averaging

\[
\frac{\sum_i n_i \phi_i}{\sum_i n_i}
\]

\[
< \alpha_s \rho_s \vec{u}_s > \quad \text{mass flux}
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= \tau_s : \nabla < \vec{u}_s > + \nabla (k_\theta \nabla \theta) - \gamma_\theta + \phi_{ls}
\]
Circulating Fluidized Bed
Investigation of Particle Segregation

Particles
\[ \rho_p = 2400 \frac{kg}{m^3} \]
\[ \alpha_p \leq \alpha_{max} \]

Gas
\[ \rho_g = 1.225 \frac{kg}{m^3} \]
\[ u_g \approx 1, 1.1 \frac{m}{s} \]

Circulating Fluidized Bed
Investigation of Particle Segregation

<table>
<thead>
<tr>
<th>Settings</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Model</strong></td>
<td>Dense Discrete Phase, Multi Fluid</td>
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<tr>
<td><strong>Drag</strong></td>
<td>Morsi-Alexander</td>
</tr>
<tr>
<td><strong>Grids</strong></td>
<td>2d: 64k cells</td>
</tr>
<tr>
<td></td>
<td>3d: 20k, 114k, 264k cells</td>
</tr>
<tr>
<td><strong>Number particles</strong></td>
<td>2d: 523k in steady state</td>
</tr>
<tr>
<td></td>
<td>3d: 314k, 1.57 mio, 3.14 mio</td>
</tr>
<tr>
<td><strong>Time</strong></td>
<td>60s</td>
</tr>
<tr>
<td><strong>Time step</strong></td>
<td>0.001s</td>
</tr>
<tr>
<td><strong>Computing time for 1000</strong></td>
<td>160 min on 40 CPUs for fine mesh</td>
</tr>
<tr>
<td></td>
<td>time steps</td>
</tr>
</tbody>
</table>
Circulating Fluidized Bed Setup

Mesh

PDA measurement planes
Circulating Fluidized Bed Mesh

- Hexahedral mesh in riser
- Tet mesh for transition
- Hexahedral mesh at exit

Top of CFB
Circulating Fluidized Bed
Results Averaged for 30 Seconds

- axial particle velocity
- particle volume fraction
- d10 diameter
Circulating Fluidized Bed Flow at Exit

particle velocity

gas velocity

particle volume fraction
Circulating Fluidized Bed
Particle Accumulation at Bottom

particle volume fraction
Circulating Fluidized Bed
Influence of the Mesh Resolution

- z/H = 0.95
- z/H = 0.5

Axial particle velocity vs y/d for different mesh resolutions:
- Fine mesh
- Medium mesh
- Coarse mesh

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Circulating Fluidized Bed
Axial/Transverse Velocity $z/H = 0.5$

- Traversal particle velocity
- Axial particle velocity

- 3d simulation
- 2d simulation
- Experiment

$z/H = 0.5$

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Circulating Fluidized Bed
Axial Velocity at z/H = 0.6/0.95
Summary of results

• Riser simulation:
  – Validation of particle segregation effects in circulating fluidized bed.
  – DDPM predicts proper distribution of velocity profiles.
  – Results clearly show 3-dimensional effects.

• Further studies needed to investigate
  – drag models,
  – turbulence models,
  – averaging procedures

• DDPM highly efficient for particle size distributions at all volume fractions.
Modeling contacts explicitly

- An extension of the DDPM takes into account the explicit contacting of particles through collision detection.
- Soft sphere based models
  - Soil mechanics: Cundall and Strack (1979)
  - Fluidized beds: Tsuji, Hoomans (1998*)
  - Pneumatic conveying: Tsuji, Herrmann (1999*)
  - Parcel based approach: Joseph (2001)
Current implementation

- Accounts for explicit contact of parcels
  - The forces at contact are determined by using a soft-particle spring dashpot model
  - The contact law is customizable
  - Ability to include more complicated physics
- The framework is extendable to include heat transfer, reactions and is parallelizable
Structure of the bed for various gas velocities

Pressure at the inlet

V = 0.30 m/s, T = 0.062500
The fluidization curve

![Fluidization curve graph]

- **Pressure drop (Pa)**
- **Gas superficial velocity (m/s)**

- **Lines**:
  - Magenta line: Weight of bed
  - Blue line: DPDPM
- **Gasification UDF for Euler-Granular model**
  - Developed under funding from NETL
  - Based on the work reported by Syamlal and Bissett (1992) and Wen et. al. (1982)
  - H₂ and CO combustion reactions also included
  - Used heterogeneous stiff chemistry solver of Fluent12 to take care of the stiffness of these reactions
NETL partnership – Carbon capture

- 5 m tall cylindrical domain
  - Fluid bed height = 0.5 m
- Flue gas (12% CO2, 10% H2O, rest N2) moves upward through the limestone bed (all size distributions under one secondary phase).
- **Particle Surface reaction takes place** (gas temperatures 600-850 C)
  - CO2(g) + CaO (s) = CaCO3(s)
- Last picture shows start of limestone conversion to CaCO3 at the bottom.
Conclusion

• ANSYS is committed to providing “best in class” technology for modeling dilute to dense granular flows.
• Continue to improve speed and fidelity through experimental validation of results.