Dispersed Multiphase Flow Modeling using Lagrange Particle Tracking Methods

Dr. Markus Braun
Ansys Germany GmbH
Overview

• The Euler/Lagrange concept
• Breaking the barrier of mass points
• Breaking the barrier of dilute flow limitation
• Summary
Particles:
• Move arbitrarily
• Heat up
• Cool down
• Loose mass
• Change composition

Particles see only surrounding fields
Forces Acting on a Particle

\[ \vec{F}_{\text{drag}} \]

\[ \frac{d(m_p \vec{\ddot{u}_p})}{dt} \]

\[ \vec{F}_{\text{gravitation}} \]
Basic Equations

- **Dispersed flow: Particle acceleration**
  \[
  \frac{d(m_p \ddot{u}_p)}{dt} = \vec{F}_{\text{drag}} + \vec{F}_{\text{pressure}} + \vec{F}_{\text{virtual mass}} + \vec{F}_{\text{gravitation}} + \vec{F}_{\text{other}}
  \]

- **Location**
  \[
  \frac{d\vec{x}_p}{dt} = \ddot{\vec{u}}_p
  \]

- **Fluid flow: Navier/Stokes equations**
  \[
  \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_{c,dp} \\
  \frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\vec{T}) + \rho \vec{g} + \vec{F} + \vec{S}_{m,dp}
  \]
What else is needed?

- Starting Conditions (primary breakup)
- Boundary Conditions (reflection, erosion, wall films)
- Numerical solvers for ODE sets (yes, there is numerics different to CFD)
- Coupling to flow solver (particle source terms)
- Extensions of numerical algorithms of flow solver

- Models for heat/mass exchange (evaporation/combustion/drying/devolatization)
- Models for breakup, collision, combustion, etc.
Simplifying Assumptions

- Moving particle $\rightarrow$ moving mass point
  - Abstractions for particle shape and volume
- Details of flow around particle neglected:
  - Spherical shape
  - No resolution of Vortex shedding, Flow separation, boundary layers, ...
    (modeled in drag)
- Tracking of reference particle
- Distance between particles is “large”
  - No inter-particle collisions
• Impractical to predict tracks of all particles
  → particle DNS
• Consider a cube of 1 m$^3$ with 0.1% particle volume fraction

<table>
<thead>
<tr>
<th>$d_p$, mm</th>
<th>$N_p$/m$^3$</th>
<th>$\alpha_p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.0</td>
<td>30,000</td>
<td>0.001</td>
</tr>
<tr>
<td>1.0</td>
<td>~2 mio</td>
<td>0.001</td>
</tr>
<tr>
<td>0.1</td>
<td>~2 bio</td>
<td>0.001</td>
</tr>
</tbody>
</table>

• Particle equations are solved for representative particle trajectories
What can we do with this?

Address main application areas:

• Sprays
  – Piston Engines
  – Gas turbine combustion chambers
  – Process/chemical industries, dryers
  – Spray paint devices

• Particulate flows
  – Coal combustion furnaces
  – Particle transport in tubes
  – Particle separation as in cyclones

• Huge amount of other applications
Spray: Gasoline Injector
Spray Penetration and Atomization

ΔP=4.76 MPa

Pre and Main Spray tip penetrations

Sauter Mean Diameter @ Plane 39 mm downstream of Injector

ΔP=4.76 MPa
Why is this useful?

- Sometimes particle extend over several cells near boundary layers, due to meshing of geometric details needed for the flow
- Consideration of particle/wall collision at the particle radius sometimes necessary
- Direct particle/particle collisions based on real particle diameters

Two solutions: MPM + DEM
Parcels Based Discrete Element Method

- Forces acting on a particle

\[
\frac{d(m_{p,1}\vec{u}_{p,1})}{dt} = \vec{F}_{\text{drag}} + \vec{F}_{\text{pressure}} + \vec{F}_{\text{virtual mass}} + \vec{F}_{\text{gravitation}} + \vec{F}_{\delta} + \vec{F}_{\text{friction}}
\]

- Soft Sphere Approach
- Spring dashpot law

\[
\vec{F}_{\delta} = (K\delta + \gamma((\vec{v}_1 - \vec{v}_2) \cdot \vec{n})\vec{n}
\]

- Friction law

\[
\vec{F}_{\text{friction}} = \mu \vec{F}_{\text{normal}}
\]
What are Parcels in the Context of DEM?

- For real applications, cannot afford to track all particles individually.
  - Put several particles of same properties into one parcel.
  - Track this parcel by a representative particle.

DEM can make use of the same concept, but:
- The mass used in collisions is that of the _entire_ parcel.
- Parcels are treated as massive spheres.
  - Note: This way, close packing of parcels gives the correct volume fraction for sphere packing.
Discharger Flow in Silo

Total discharge-time \[ T \] = 30.2 s

Experiments from: Chemical Engineering Science 66 (2011) 5116–5126
Breaking the Barrier of Dilute Flow Limitation

Why is this needed?
• to extend application range of Lagrangian models to large volume fractions.
• to add appropriate physics for dense flows like
  – collision and coalescence
  – frictional flows

Solution:
• Statistical models to consider particle/particle interactions
• DDPM plus various extensions
Multiphase Flow Models

- **Euler-Euler Multiphase**
  - Interpenetrating continua
  - Full N-phase framework
  - Phase indicator function
  - Phase weighted averaging
  - Additional unknowns → consequence of averaging
  - Empirical closure
  - PDE transport eq.’s for unknowns

- **Hybrid Models (DDPM)**
  - Solve disperse phase using Lagrange Technique
  - Provide averages to Euler-Euler context
  - Solve Euler/Euler
  - Particle/particle interaction can be considered during tracking using DEM or statistical collision models

- **Lagrange Particle Tracking**
  - Continuous, carrier phase → Euler
  - Tracking of single particles or particle groups
  - Interaction with carrier phase → 2-way coupling
  - Allows for broad size distributions
  - ODE’s for particle properties
Equation of motion for particles, „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

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

\(< \alpha_s \rho_s \vec{u}_s >\) mass flux

\(< \alpha_s >\) vol. fraction

Navier Stokes: primary phase

\[
\frac{\partial \alpha_q}{\partial t} + \nabla \cdot (\alpha_q \vec{u}_q) = \frac{1}{\rho_q} \left( \sum_{p=1}^{n} m_{pq} - \alpha_q \frac{d\rho_q}{dt} \right)
\]

\[
\frac{\partial}{\partial t} (\alpha_q \rho_q \vec{u}_q) + \nabla \cdot (\alpha_q \rho_q \vec{u}_q \vec{u}_q) = -\alpha_q \nabla p + \nabla \cdot \tau_q + \alpha_q \rho_q \vec{g} + \alpha_q \rho_q \left( \vec{F}_q + \vec{F}_{lift,q} + \vec{F}_{vm,q} \right) + \sum_{p=1}^{n} \left( K_{pq} (\vec{u}_p - \vec{u}_q) + m_{pq} \rho_{eq} \vec{u}_{pq} \right)
\]

\(\vec{a}_{col}\) from DEM or ktgf
How the Averaging is Done

- Two step approach:
- 1\textsuperscript{st} accumulate variables on nodes

2\textsuperscript{nd} distribute to cell centers of finite volume method

using kernel like

\[ w(\vec{x}_p^k - \vec{x}_{node}) = \exp \left( - a \frac{\left| \vec{x}_p^k - \vec{x}_{node} \right|^2}{\Delta x^2} \right) \]
Segregation with Coupled CFD-DEM

- Bed dimensions: 15 x 1.5 x 70 cm
- Particle mixture:
  - 50% 1.5 mm
  - 50% 2.5 mm
- Particle density: 2500 kg/m³
- Initial bed height: 7.5 cm
- Minimum fluidization velocities
  - 1.5 mm particles – 0.8 m/s
  - 2.5 mm particles – 1.25 m/s
- Segregation studied with superficial velocity of 1.1 m/s
Segregation results

Center points of particle size collective

experiment

small particles

large particles
Summary and Conclusion

- Overview to modeling multiphase flows using Lagrangian Models, showing applications of
  - dilute flows
  - dense flows
- Introduction parcel based DEM approach usable with
  - single phase flow models
  - in DDPM context
- Lagrangian models can be used efficiently in particular when size distributions of the dispersed flow is important
- Comparison with experimental data show good agreement for
  - Sprays,
  - Discharger flows in silos,
  - Segregation of bi-disperse particle mixtures