A fully coupled CFD-DEM method for solid-liquid mixing in stirred vessels

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Outline

髃 Lassaigne mixer

 squid DEM
• CFD-DEM coupling
• Gidaspow drag force
• 2-way coupling with source smoothing

ջ Results
• Tracking suspended particles
• Comparison with experiment
• 2-way vs. 1-way coupling

ዓ Summary and discussion
Typical solid-liquid mixing data (& correlations):
- Light loading of small diameter particles in turbulent low viscosity liquid.

Lassaigne’s study:
- Laminar – transition regime (Re < 350)
- Particle loading (10 - 35 wt%)
- Particle diameter: 0.5 and 3 mm
- Viscous Newtonian (1 - 4 Pa.s)

Lassaigne’s results:
- Zwietering correlation over-estimates $N_{js}$ in cases of impeller diameter $D=T/3$ and larger particle diameter 3mm.

Mechanisms of particle lifting:
- Turbulent – burst of turbulent eddies.
- Laminar – shear and pressure distribution on particles (ideally represented by DEM).
Lassaigne solid-liquid mixer

Tank diameter: \( T = 0.365 \text{ m} \)
Tank height: \( H = T \)
Impeller: PBT
Impeller diameter: \( D = T/3 \)
Off-bottom clearance: \( C = T/4 \)
Blade width: \( W = D/5 \)
Baffle: None

Liquid phase and particles

Liquid: Glucose Solution
- Density 1400 kg/m³
- Dynamic viscosity 1 Pa-s

Solid: Glass beads

<table>
<thead>
<tr>
<th>Material</th>
<th>Diameter</th>
<th>Density</th>
<th>Young’s M</th>
</tr>
</thead>
<tbody>
<tr>
<td>Glass beads</td>
<td>3 mm</td>
<td>2500 kg/m³</td>
<td>100 MPa</td>
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</table>

Impeller’s speed: between 30 and 550 rpm
DEM (Discrete Element Method)

Linear momentum of particle:

\[ m_i \frac{d \vec{v}_i}{dt} = \vec{F}_{\text{Drag}} + \vec{F}_{\text{Contact}} + \vec{F}_{\text{Other}} \]

Angular momentum:

\[ I_i \frac{d \vec{\omega}_i}{dt} = \sum_{j=1}^{k} \left[ \vec{\tau}_{ij} + \vec{M}_{ij} \right] \]

\[ \vec{M}_{ij} = -\mu_{\text{roll}} \left| \vec{F}_{\text{Contact}} \right| \vec{\omega}_i \]

\( \vec{M}_{ij} \) = rolling torque

\( \mu_{\text{roll}} \) = rolling friction coefficient
Drag force on glass beads is based on a combination of Wen-Yu model and Ergun based model

- Known as Gidaspow model

\[ F_{\text{drag}} = \frac{1}{2} \rho_f C_d A_d \pi r^2 |u - v|(u - v) \]

\[ C_d \text{ is a function of } Re_p = \frac{\rho_f |u - v| d}{\mu} \]

\[ C_d = \begin{cases} 
\frac{4}{3} \left( \frac{150(1 - \alpha_p)}{\alpha_p Re_p} + 1.75 \right) & \text{if } \alpha_p < \alpha_{\text{min}}; \text{Ergun} \\
24 + 3.6 Re_p^{0.687} Re_p^{-3.65} & \text{if } \alpha_p \geq \alpha_{\text{min}}; \text{Wen Yu} 
\end{cases} \]

\( \alpha_{\text{min}} \) is the cutoff void fraction (=0.8)

Buoyancy force (pressure gradient force) accounted

Contact force

<table>
<thead>
<tr>
<th>Contacts</th>
<th>Friction</th>
<th>Restitution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle-Particle</td>
<td>0.6</td>
<td>0.1</td>
</tr>
<tr>
<td>Particle-Wall</td>
<td>0.1</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Solid: Glass beads

- 150,000 DEM particles (10 wt%) as in experiment
- At time zero particles injected in packed state resting motionless at bottom of the vessel
Number of cells used in flow calculation: 517,070
- Smallest cell size = 0.324 mm is less than particles size

For particle calculation cells are grouped into
43,357 clusters
- Of approximately equal volume

In “packed clusters” we have about 35 particles per cluster
- Void fraction calculation is using clusters
- Resulting momentum sources to CFD solution due to particles are smooth
- Convergence of the solution is greatly improved
Global behavior of the mixing system

- Fig 11 in Lassaigne et. al. paper shows particle states for the range of rpm below and above fluidization

- $N_0$ is the onset of erosion speed
- $N_{js}$ is “just suspended” speed
- $N_H$ is homogenization speed

Results

30 (rpm)  

31.4 (rpm)  

101 (rpm)  

Particle Velocity: Magnitude (m/s)

Solution Time 0.02 (s)

Solution Time 10.02 (s)

Solution Time 11.02 (s)
Results

200 RPM

Solution Time 10.02 (s)

Particle Velocity: Magnitude (m/s)

250 RPM

Solution Time 11.02 (s)

Particle Velocity: Magnitude (m/s)

300 RPM

Solution Time 10.02 (s)

Particle Velocity: Magnitude (m/s)
Results

250 (rpm)  

351 (rpm)  

401 (rpm)  

350 RPM  

400 RPM  

450 RPM
Results

451 (rpm)

501 (rpm)

500 RPM

550 RPM
Connected components and suspended particles

- Connected components size 2
- Connected components size 3
- Connected components size 1
- Connected components size 11.

Size >= 10 : particles not suspended

size < 10: Particles are suspended
Number of suspended particles as a function of time
Results for suspended particles

Both simulations and experiment show transition from settled to fluidized state at rpm range between 250 and 400
- Experiments use “pressure gauge technique”

Connected component method for counting suspended particles provides better agreement with experiment
Experiment measures pressure to estimate number of suspended particles.

Simulation results are close to experimental data:
- More noisy at high rpm.
Comparison between 1-way and 2-way coupling (200 rpm)

1-way

2-way
Computing time

Performance:
• around 2 hours to simulate 1 second on 24 cores

Computing time:
• 30 seconds to reach steady cloud height (see slide 15), hence typical simulation requires 60 hours (2.5 days) on 24 cores
Conclusions

- 2-way coupled CFD-DEM model for stirring solid particles in glucose solution
  - Used novel Source Smoothing with Cell Clustering coupling algorithm

- Predicted fluidization of particles occurs at the same range of rpm as in experiment

- Introduced “connected components” method of counting suspended particles in DEM simulations
  - Reasonable agreement with experimental data for suspended particles