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CFD-DEM simulation of nanoparticle agglomerates fluidization with a micro-jet

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*This work was performed at Delft University of Technology
1. Nanoparticle fluidized bed

Application: Atomic layer deposition (ALD) in a fluid bed is a new way of coating nanoparticles at a large scale

Valdesueiro et al., Materials 8 (2015) 1249
2. Strategy

Nanoparticles are agglomerated with a multi-stage structure

de Martín et al.. Langmuir 30 (2014) 12696.

In case of too strong agglomeration: microjet

~20% gas, high velocity

~80% gas, low velocity

The simple agglomerates are represented by DEM particles with cohesive and plastic properties.
2. Strategy

**Step 1**
Adhesive CFD-DEM model

- Modify conventional CFD-DEM model for nanoparticle agglomerate fluidized bed; Test/validate model

**Adhesive CFD-DEM model**

= conventional CFD-DEM + adhesive contacts + drag force scaling


**Step 2**
Agglomerate analysis method

- Develop method to identify agglomerates;
- Characterize agglomerates (probability distribution of size, density, packing, fractal dimension et al.)

**Step 3**
Application micro-jet FB

- Use the above methods to analyze effect of micro-jet on agglomerate dynamics
3. **Adhesive contact model**: predict contact behavior curve

\[
Bo_{vdw} = \frac{F_{vdw0}}{mg}
\]

Normal impact

\[d_p = 40 \mu m, Bo_{vdw} = 100, V_0 = 2 cm/s\]

**stick case**

\[V_0 = 4 cm/s\]

**bounce case**

It can predict the stick and bounce collision behavior, giving the particle properties (size, density, stiffness, plastic, cohesive force, et al.) and impact velocity.
3. Test of adhesive DEM model

**Angle of repose**

- $Bo_{vdw} = 0$
- $Bo_{vdw} = 10$
- $Bo_{vdw} = 20$
- $Bo_{vdw} = 50$

$(Bo_{vdw} = F_{vdw0}/mg)$

**Agglomerate formation**

- $Bo_{vdw} = 0$
- $Bo_{vdw} = 20$
- $Bo_{vdw} = 40$
- $Bo_{vdw} = 100$
3. Test of adhesive CFD-DEM model: fluidized bed

Particle flow pattern under different $Bo_{vdw} = F_{vdw0}/mg$

$Bo_{vdw} = 0$

$Bo_{vdw} = 20$

$Bo_{vdw} = 50$

$Bo_{vdw} = 100$

Averaged pressure gradient along the bed height

\(d_p = 40\mu m, \rho = 250kg/m^3\)

\(k_{n,unload} = 2\ N/m, \psi_p = 0.2\)

\(F_{vdw0}/mg\)

- 0
- 20
- 50
- 100
4. Visualization of (complex) agglomerate breakage
4. Visualization of agglomerate breakage

SiO₂; Bo = 20; Ug = 2 cm/s

TiO₂; Bo = 20; Ug = 2 cm/s

TiO₂; Bo = 20; Ug = 4 cm/s

TiO₂; Bo = 5; Ug = 4 cm/s
4. Statistics of agglomerates

For (complex) agglomerates: statistics show that the averaged coordination number of agglomerates is around 3.0, packing fraction around 0.2~0.3, and fractal dimension around 1.9~2.3.
5. Effect of micro-jet: general flow pattern

schematic of micro-jet in fluidized bed

<table>
<thead>
<tr>
<th></th>
<th>$F_{vdw,0}/mg=20$</th>
<th>$F_{vdw,0}/mg=50$</th>
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<tr>
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<td>jet ON</td>
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<tr>
<td>vdw50jet36</td>
<td>0.00 s</td>
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</tbody>
</table>
5. Effect of micro-jet: agglomerate

Agglomerate breakage with time for different cases

The jet can promote agglomerate breakage.

- The statistics of the agglomerate properties, e.g., diameter, fractal dimension, packing density, can be obtained directly from the agglomerate analysis.
- The fraction of larger agglomerates is decreased when the jet is turned ON.
Conclusions

(1) Adhesive CFD-DEM model developed for simulating nanoparticle agglomerate fluidization.

(2) Model tested against: normal impact, repose of angle, fluidization.

(3) Agglomerate breakage/reunion is visualized.

(4) Preliminary study on effect of micro-jet on fluidization: The micro-jet can promote overall solid mixing, as well as complex-agglomerate breakage.

(5) This is an on-going study on “micro-jet”. Comments welcome!