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

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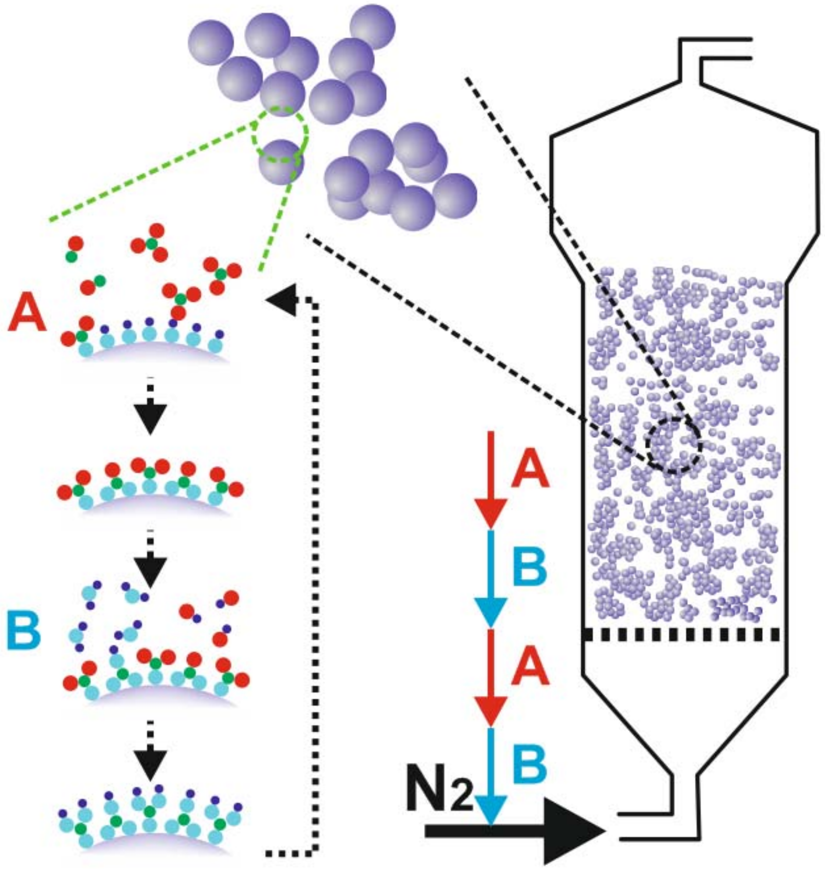
*This work was performed at Delft University of Technology

1. Nanoparticle fluidized bed

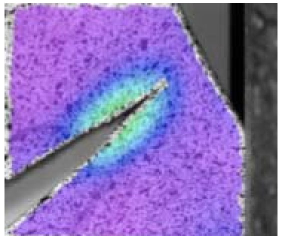
[Application: Atomic layer deposition (ALD) in a fluid bed is a new way of coating nanoparticles at a large scale]



Valdesueiro et al., Materials 8 (2015) 1249

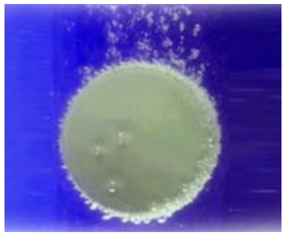
Catalysts

Q-dots for PV



Self-healing mat.

Li-ion batteries



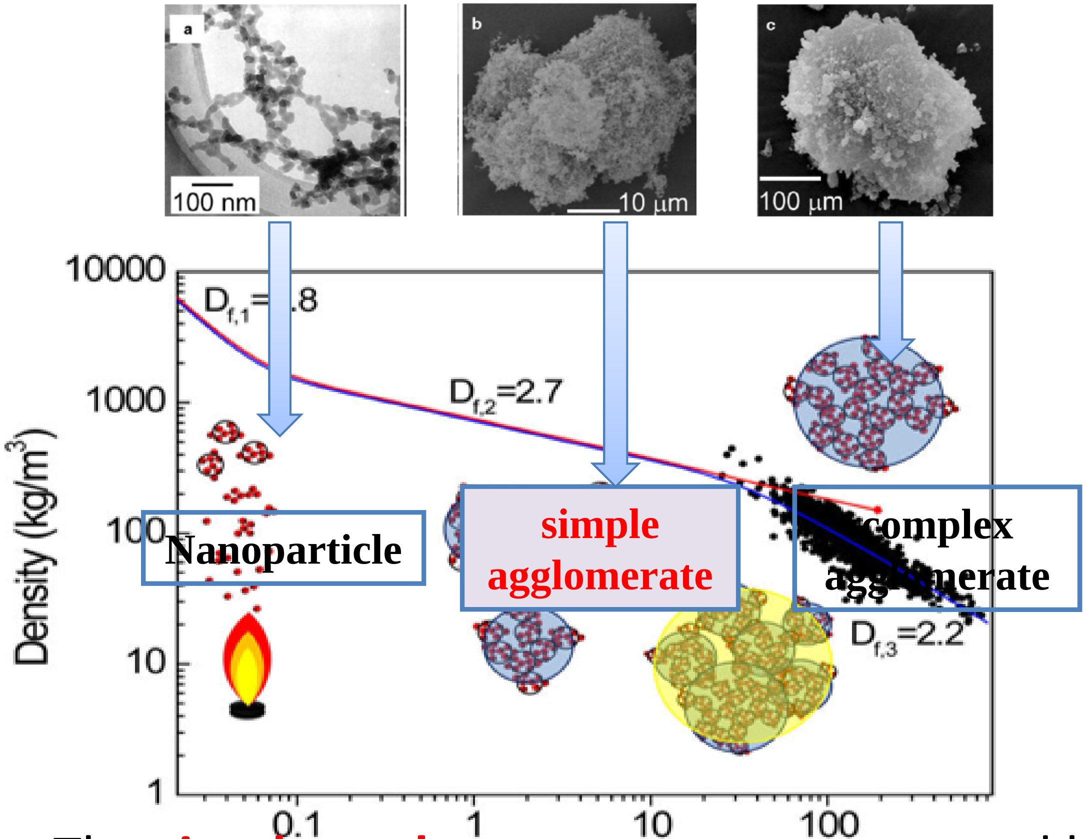
Controlled release

Nuclear medicine

2. Strategy

Nanoparticles are agglomerated with a multi-stage structure

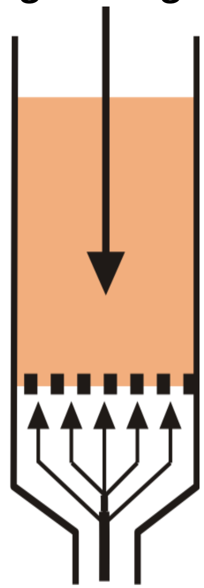
de Martín et al.. Langmuir 30 (2014) 12696.



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

In case of too strong agglomeration: microjet

~20% gas, high velocity



~80% gas, low velocity

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

Liu D, et al., AIChE J. 2016; DOI: 10.1002/aic.15219. In press.

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

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

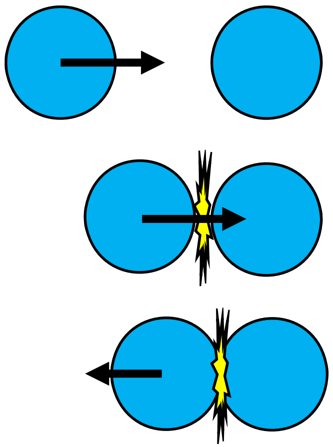
Normal impact

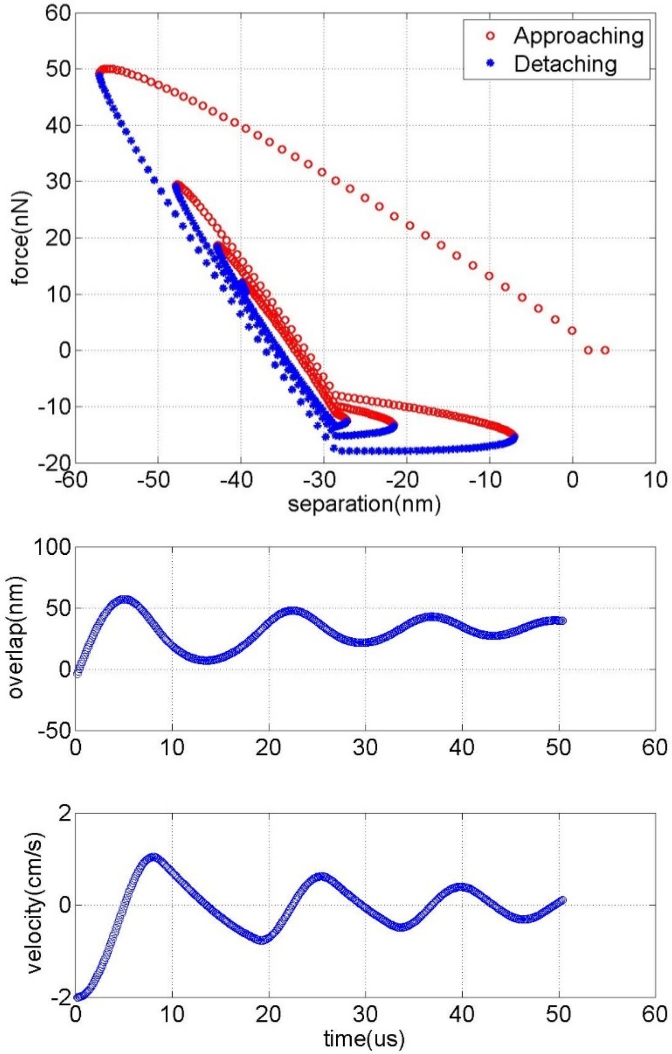
$dp = 40\mu m$, Bo_{vdw}=100, V_0=2cm/s

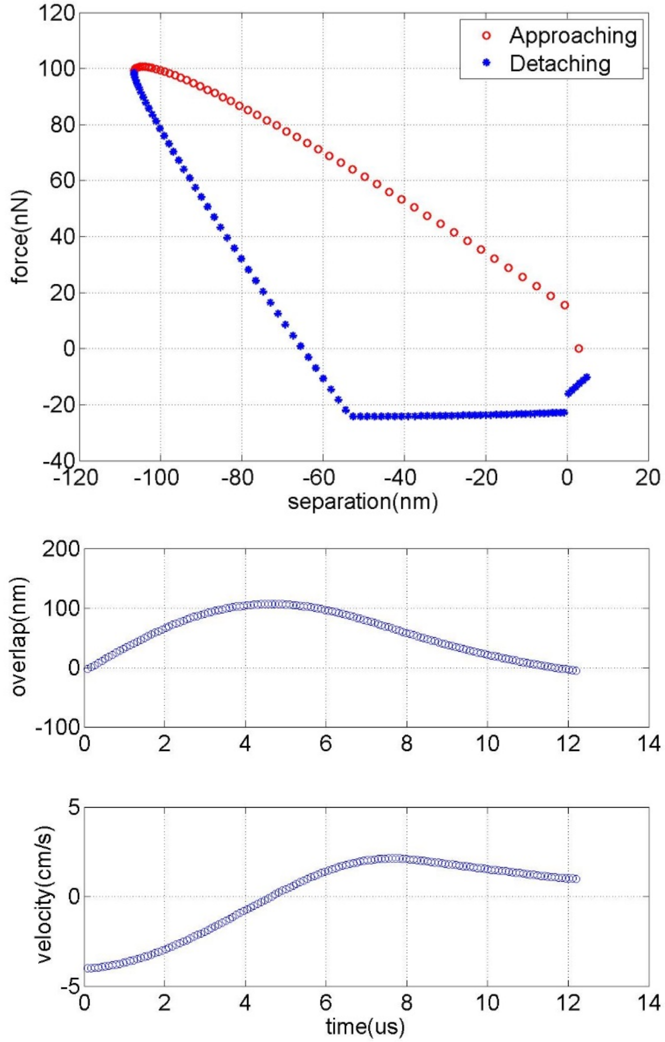
V_0=4cm/s

stick case

bounce case



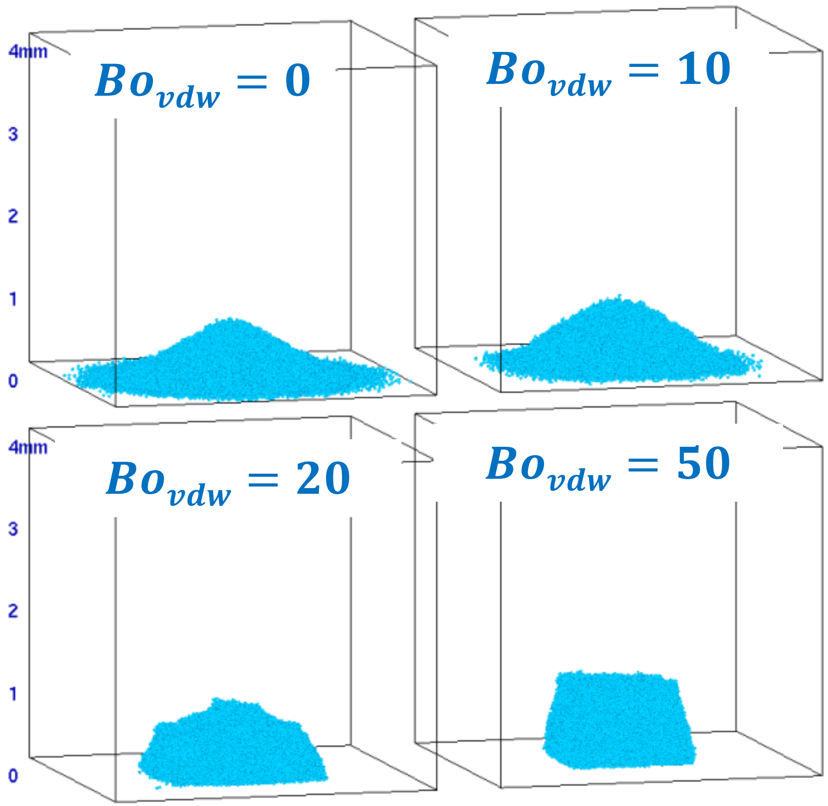




It can predict the stick and bounce collision behavior, giving the particle properties (size, density, stiffness, plastic, cohesive force, et al.) and impact velocity.

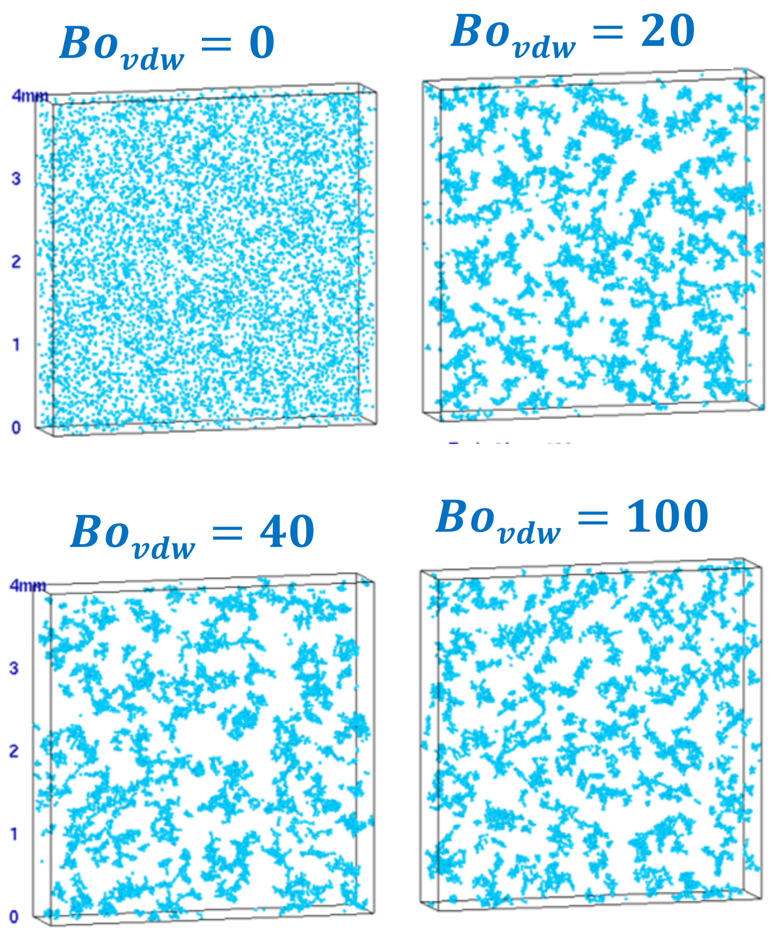
3. Test of adhesive DEM model

Angle of repose



$(Bo_{vdw} = F_{vdw0}/mg)$ ↑

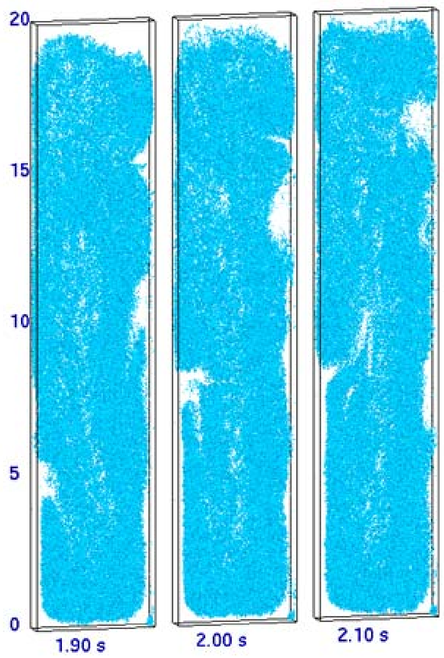
Agglomerate formation



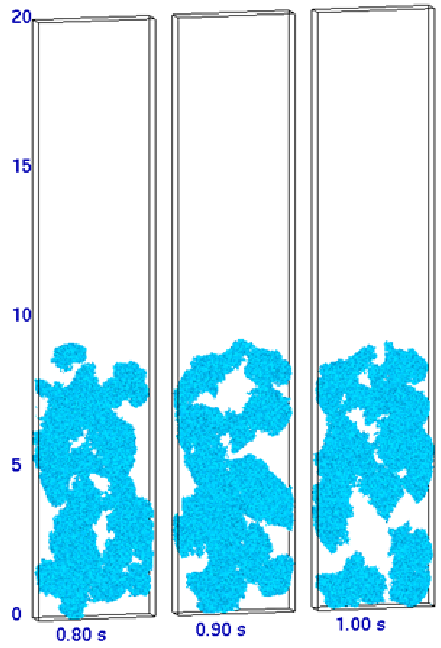
3. Test of adhesive CFD-DEM model: fluidized bed

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

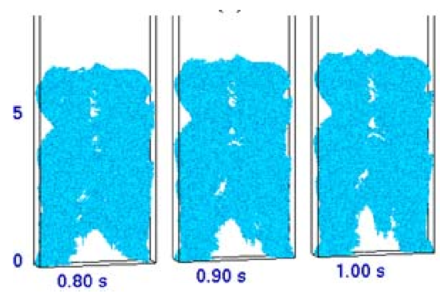
$Bo_{vdw} = 0$



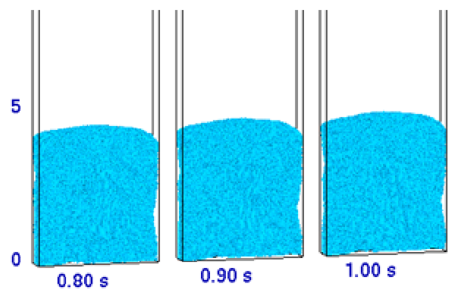
$Bo_{vdw} = 20$



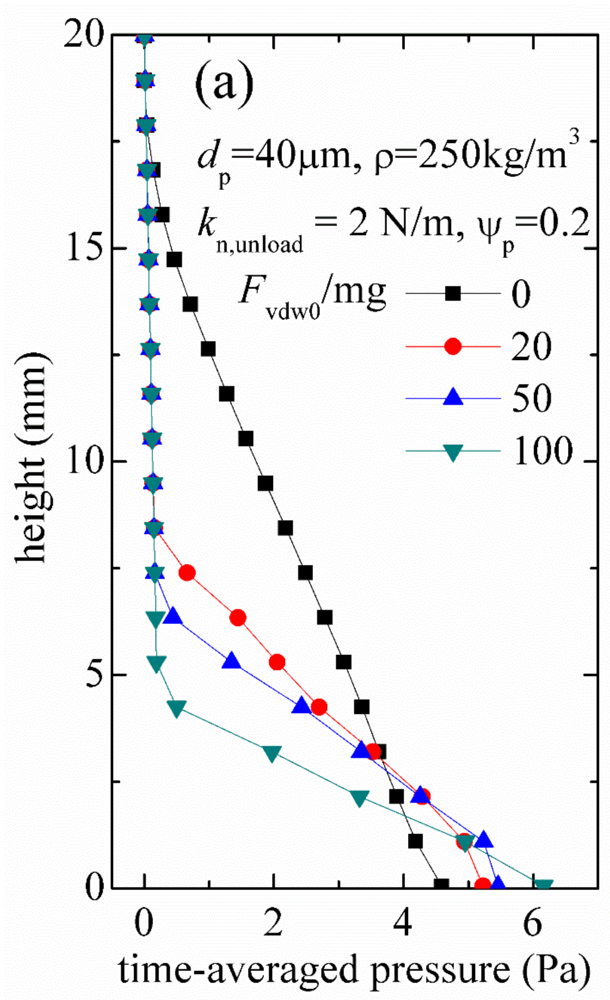
$Bo_{vdw} = 50$



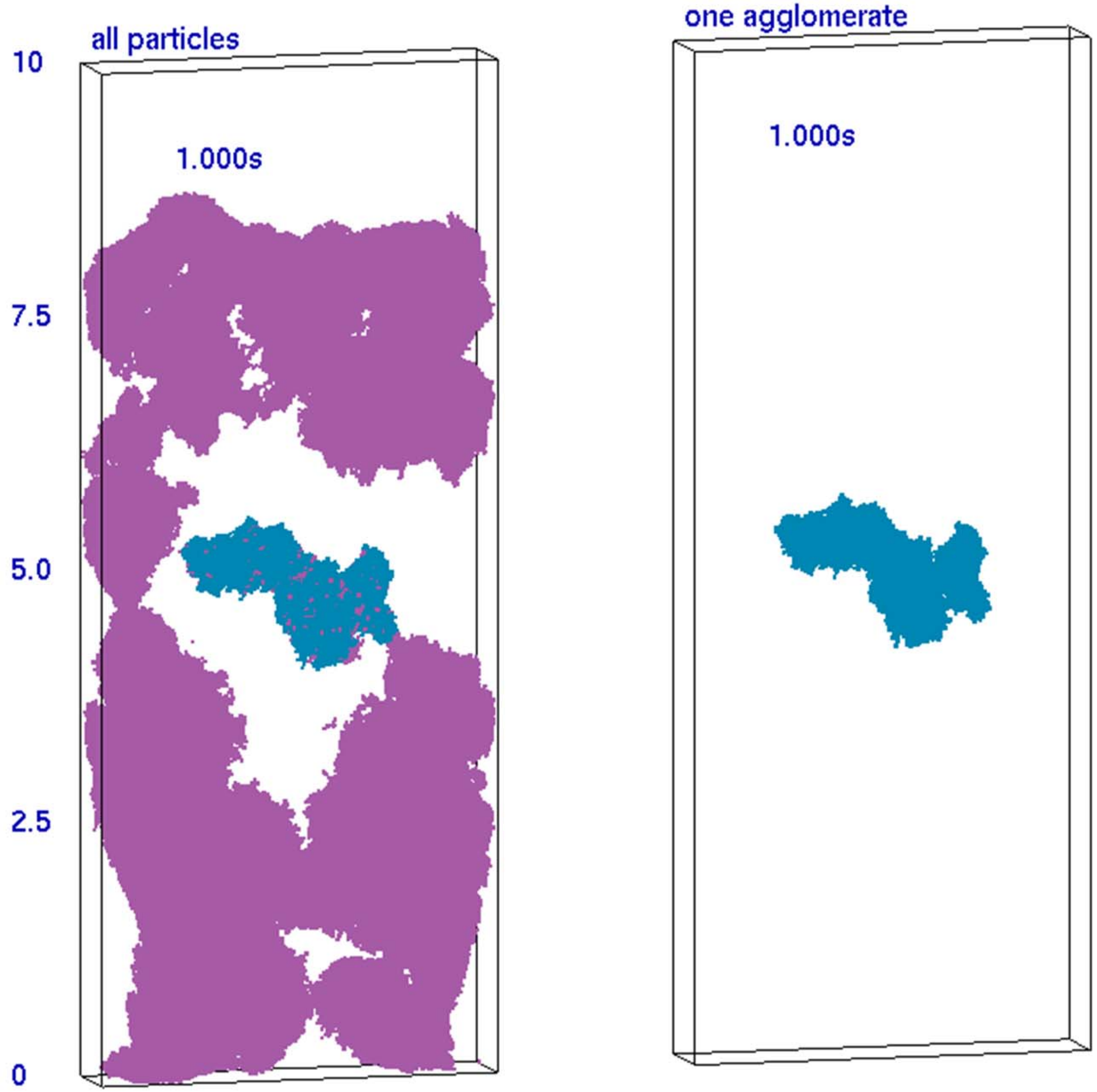
$Bo_{vdw} = 100$



Averaged pressure gradient along the bed height

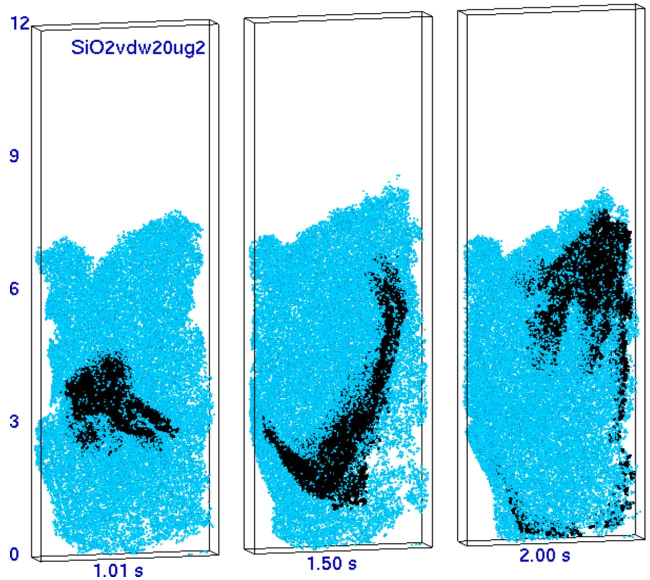


4. Visualization of (complex) agglomerate breakage

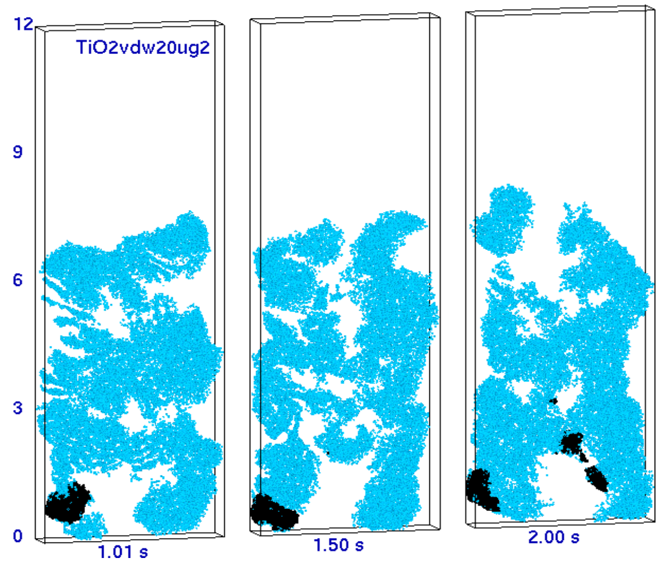


4. Visualization of agglomerate breakage

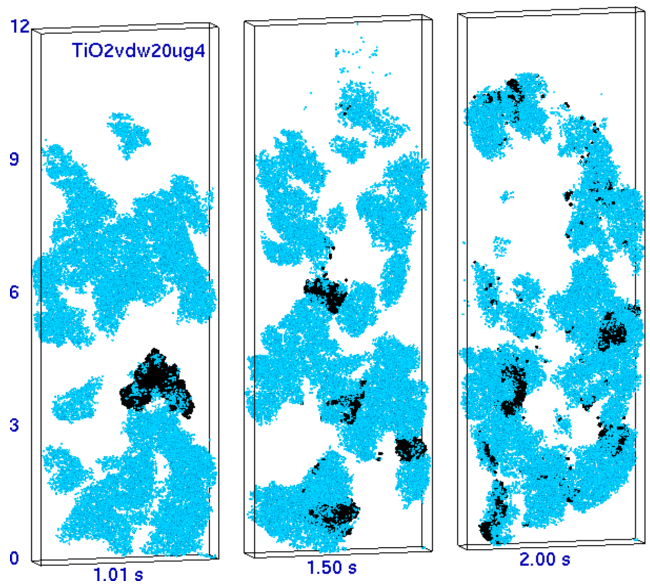
$SiO2$; Bo = 20; Ug = 2cm/s



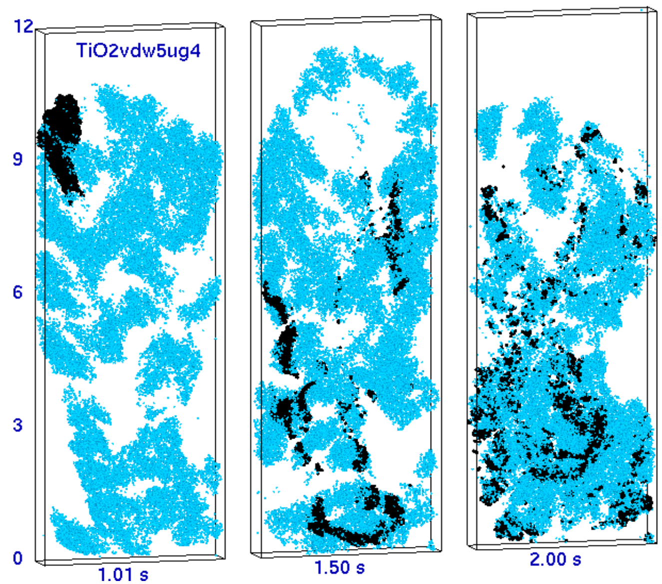
$TiO2$; Bo = 20; Ug = 2cm/s



$TiO2$; Bo = 20; Ug = 4cm/s

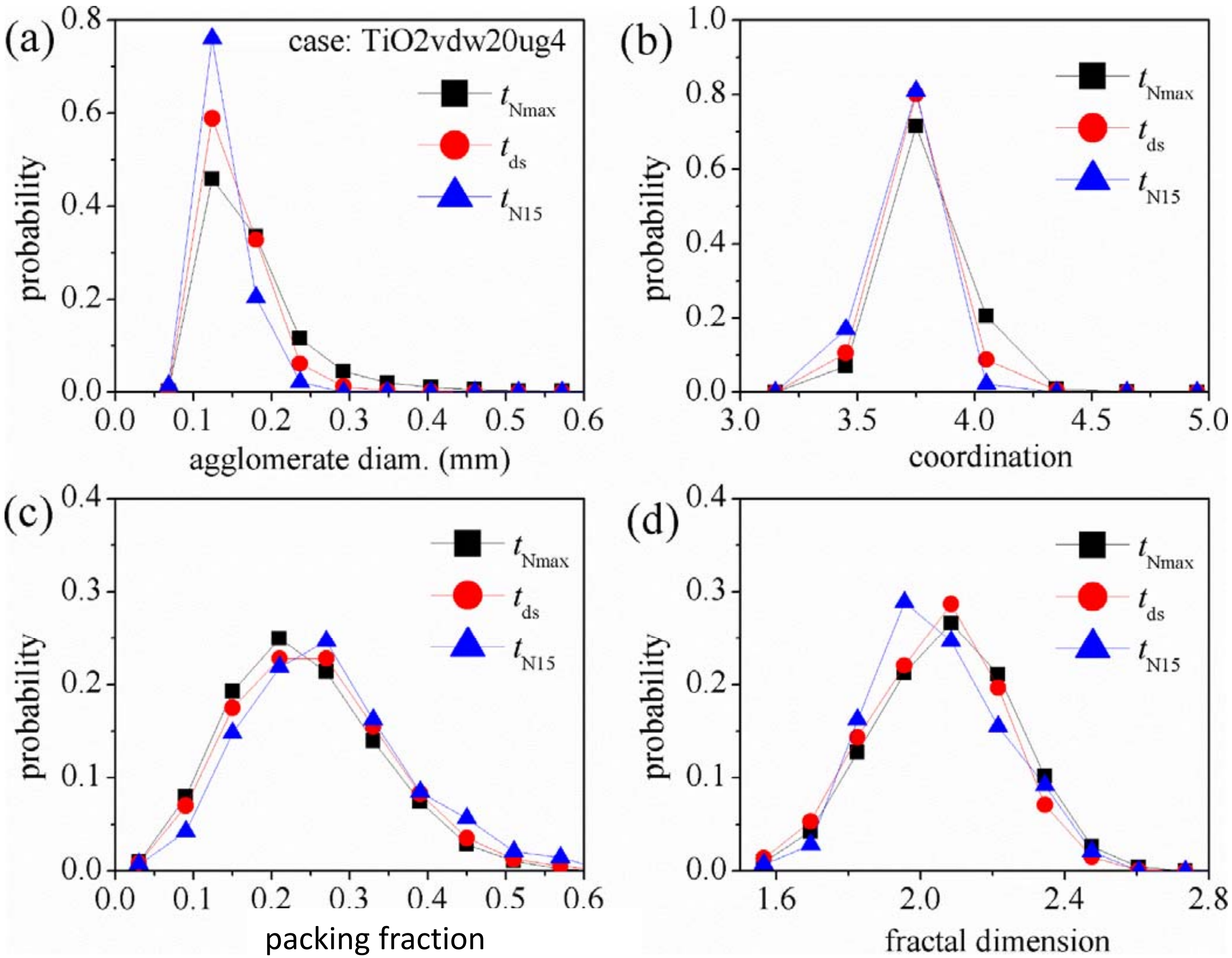


$TiO2$; Bo = 5; Ug = 4cm/s



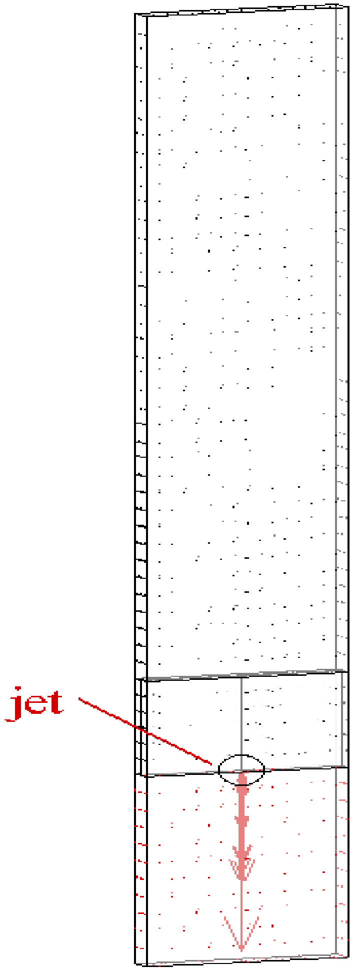
4. Statistics of agglomerates

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.

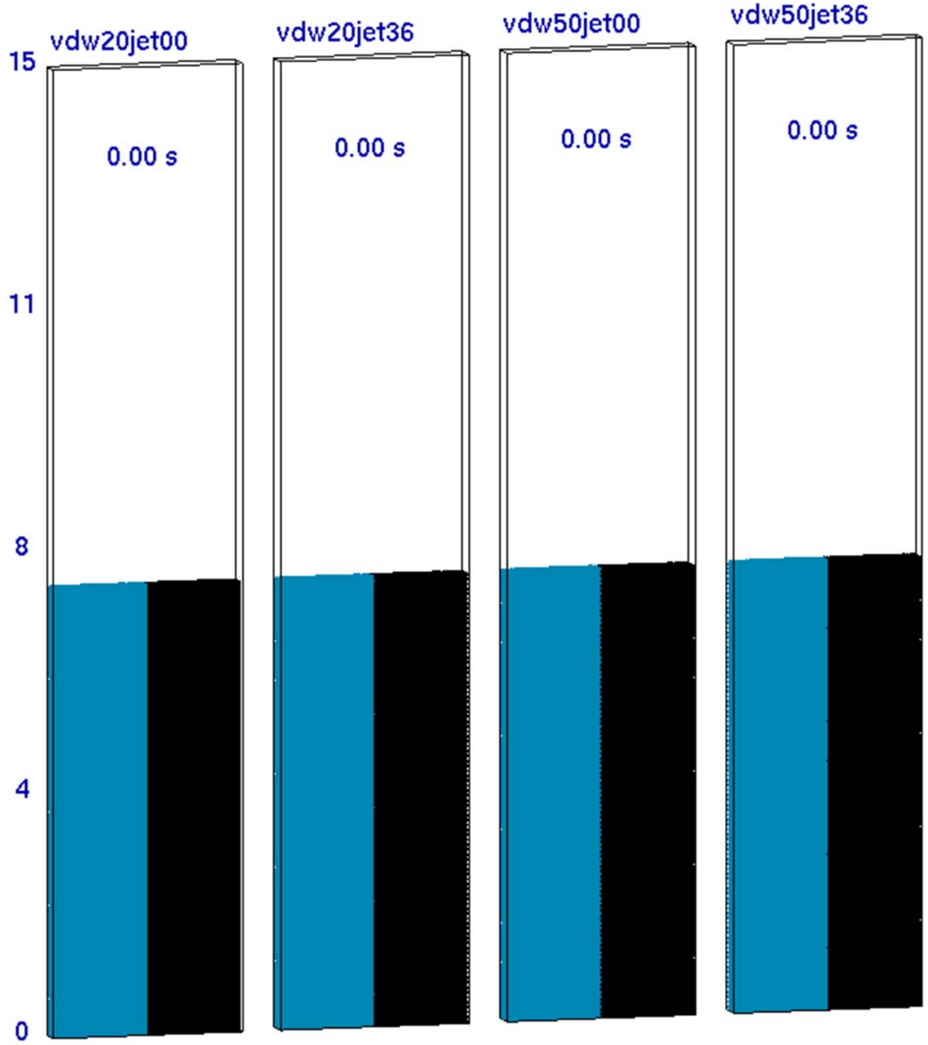


5. Effect of micro-jet: general flow pattern

schematic of micro-jet
in fluidized bed

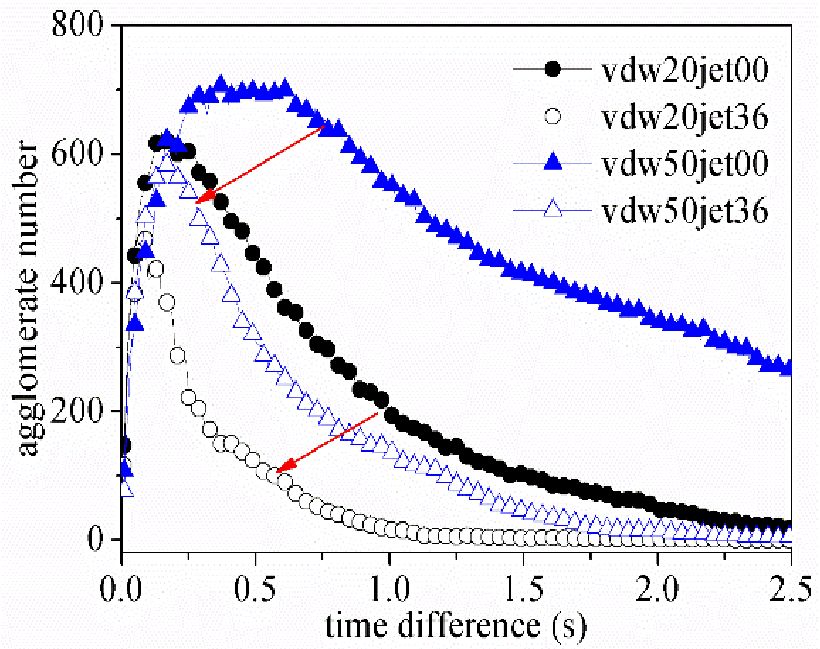


$F_{vdw,0}$/mg=20		$F_{vdw,0}$/mg=50	
jet OFF	jet ON	jet OFF	jet ON



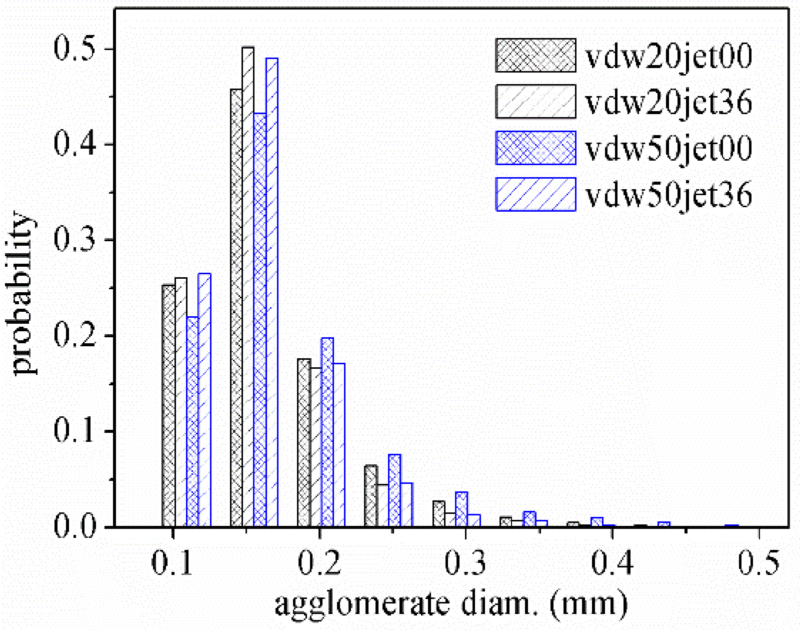
5. Effect of micro-jet: agglomerate

Agglomerate breakage with time for different cases



The jet can promote agglomerate breakage.

e.g. Histogram of agglomerate diameter



- ✓ 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!