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NETL 2021 Virtual Workshop On Multiphase Flow Science

A method to predict fluidized bed particle collision speeds and their propensity to agglomerate

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Fluidized beds: Random and correlated particle motion

The Science and Beauty of Fluidization: High Speed Imaging of Particle Flow Fields
Frank Shaffer and Balaji Gopalan
USDOE/NETL

https://youtu.be/lFhrpSJZzck?t=53

Note:

- Random particle motion
- Collective/correlated particle motion
- The circulating fluidized bed video is technically not of a fluidized bed. The video is of a riser (which *transports* particles). Nonetheless, it beautifully illustrates both random and correlated particle motion.

Background: Particle agglomeration

http://www.balajiminerals.in/silica-sand.htm

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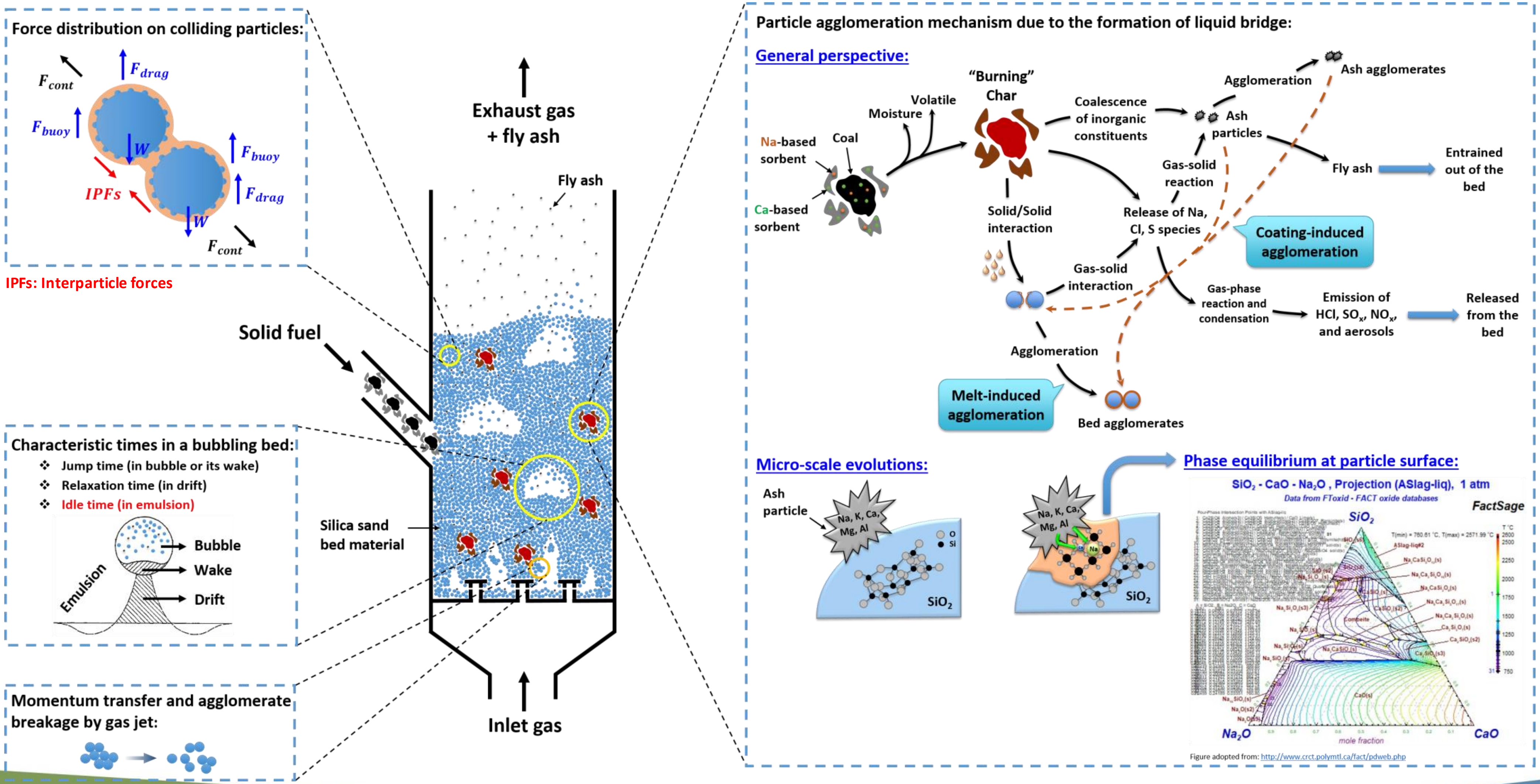
Shabanian et al., *Energy Fuels* 33 (2019) 1603-1621.

Background: *Wet* particle agglomeration overview

Prepared by Jaber Shabanian



Force distribution on colliding particles:

IPFs: Interparticle forces

Characteristic times in a bubbling bed:

- Jump time (in bubble or its wake)
- Relaxation time (in drift)
- Idle time (in emulsion)

Momentum transfer and agglomerate breakage by gas jet:

Particle agglomeration mechanism due to the formation of liquid bridge:

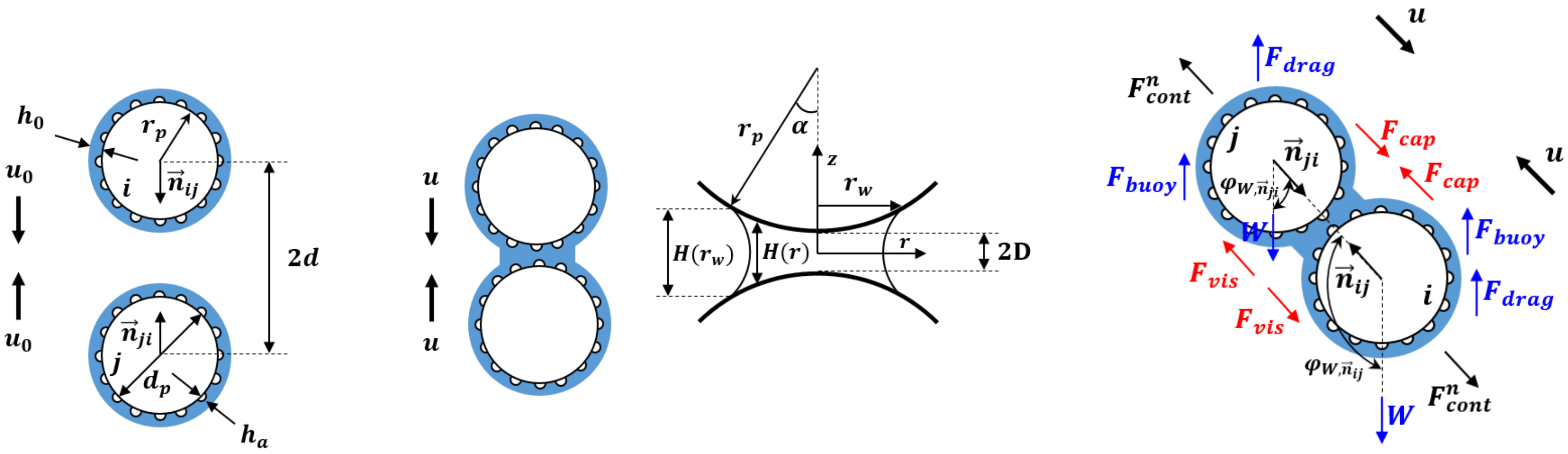
General perspective:

Micro-scale evolutions:

Phase equilibrium at particle surface:

Figure adopted from: http://www.crct.polymtl.ca/fact/pdweb.php

Background: Wet particle collision dynamics

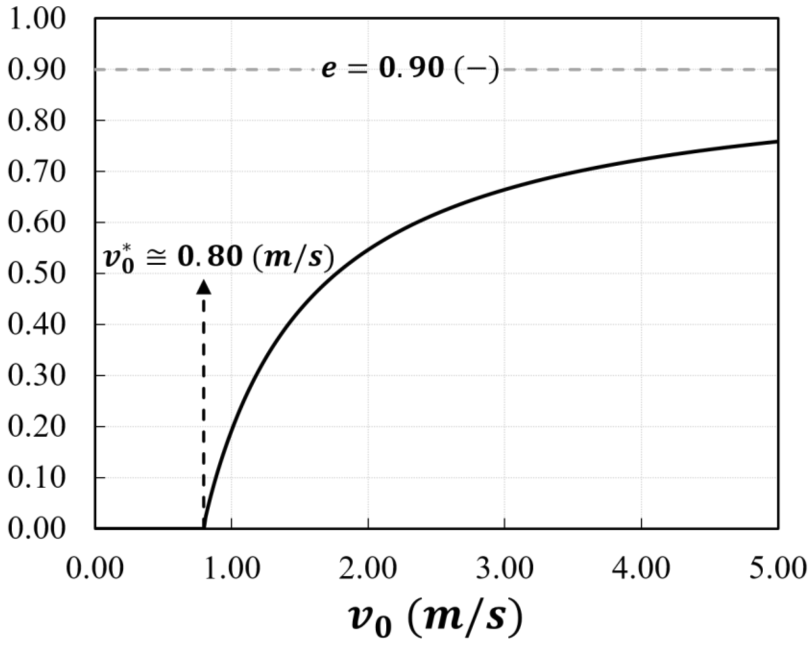


Includes viscous flow and capillary effects. Restitution coefficient expressed as a closed-form equation.

Has since been extended to non-identical particles.

Jaber Shabanian, Marc A. Duchesne, Allan Runstedtler, Madhava Syamlal, Robin W. Hughes, Improved analytical energy balance model for evaluating agglomeration from a binary collision of identical wet particles, Chemical Engineering Science, Volume 223, 2020.

Background: Wet particle collision dynamics



Restitution coefficient

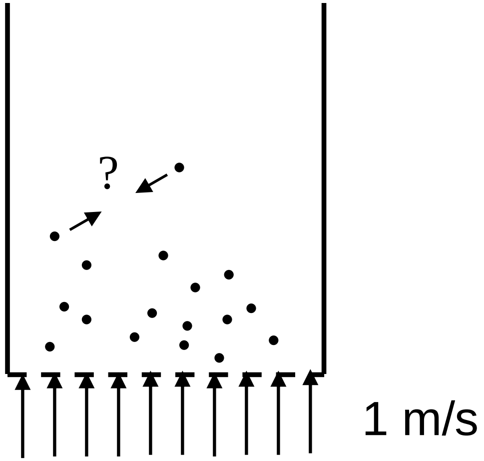
Collision speed

Jaber Shabanian, Marc A. Duchesne, Allan Runstedtler, Madhava Syamlal, Robin W. Hughes, Improved analytical energy balance model for evaluating agglomeration from a binary collision of identical wet particles, Chemical Engineering Science, Volume 223, 2020.

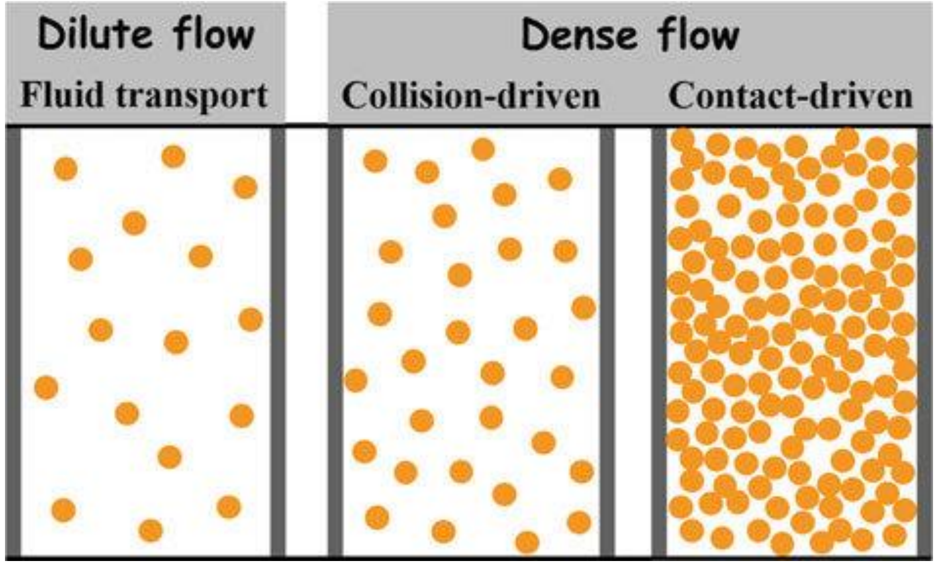
Restitution coefficient depends on collision speed. In fact, below a critical speed, the particles fail to rebound at all. If we could predict collision speed, we could advise on the tolerable coating layer thickness.

Key Questions

1. What is the average particle-particle collision speed?
2. Is there a rapid way to predict it?
3. Will the result be any surprise (*i.e.*, how will it compare to the superficial gas velocity supporting the bed)?



Applicability of the new method: Collision-driven, dense particle flow



e.g., pulverized fuel furnace | fluidized bed | tablet coater

Sommerfeld, Martin. (2017). Chapter: Numerical Methods for Dispersed Multiphase Flows. Particles in Flows, eds. Tomáš Bodnár, Giovanni P. Galdi, Šárka Nečasová

Dilute flow: Particle collisions are infrequent and, therefore, do not dissipate much kinetic energy.
Contact-driven: Particles are nearly always in contact. The fluid flow has little impact on particle motion.
Collision-driven: Fluid flow drives particle motion. Kinetic energy dissipation in the system is dominated by inelastic particle-particle collisions.

Elements of the new method:
Particle experiences repeated inelastic collisions

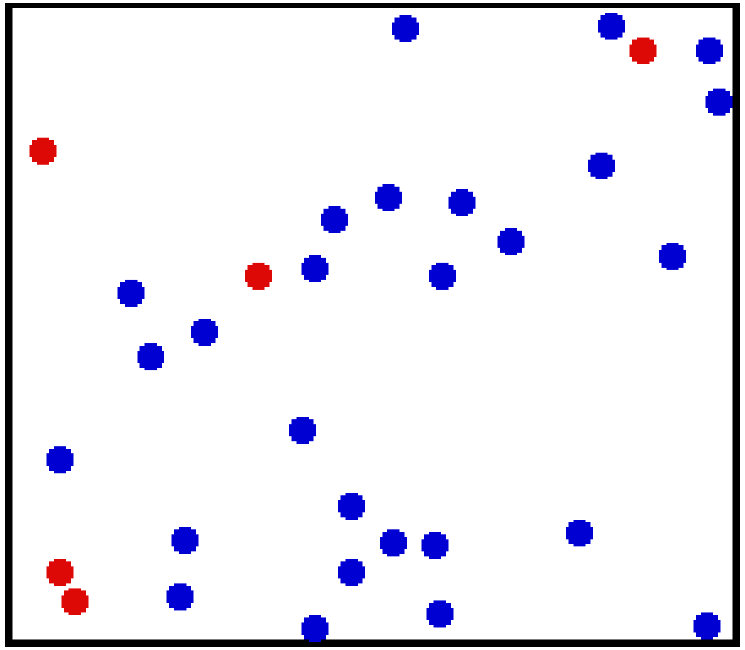
Wikipedia: “Bouncing ball”

Elements of the new method:

Particle is accelerated by the flow after each collision

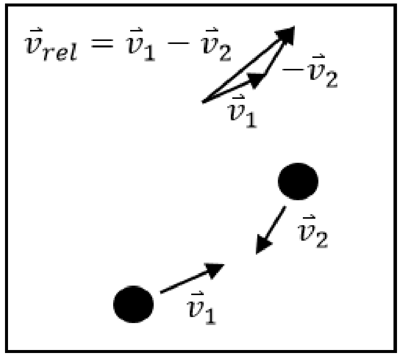
Wikipedia: “Lazy river”

Elements of the new method:
Random particle motion, time between collisions



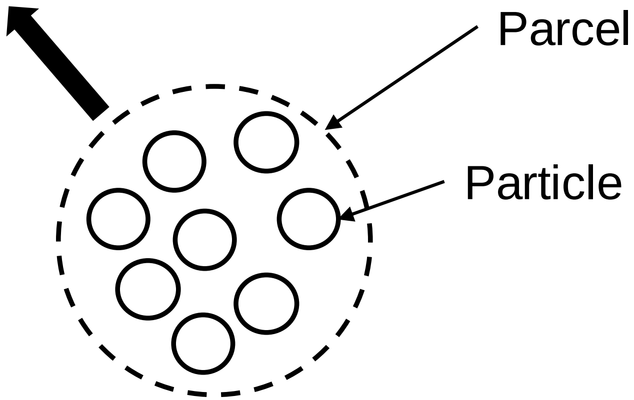
Animation: Wikipedia: “Kinetic theory of gases”

Elements of the new method: Collective/correlated particle motion



Parcel concept and definition borrowed from DEM

e.g., Liqiang Lu, Balaji Gopalan, Sofiane Benyahia, Assessment of Different Discrete Particle Methods Ability To Predict Gas-Particle Flow in a Small-Scale Fluidized Bed, Ind. Eng. Chem. Res. 2017, 56, 27, 7865–7876



W particles per parcel

Average relative particle velocity, $v_{rel} = c\sqrt{2}\,v$

where $0 < c \leq 1$ is “randomness coefficient”

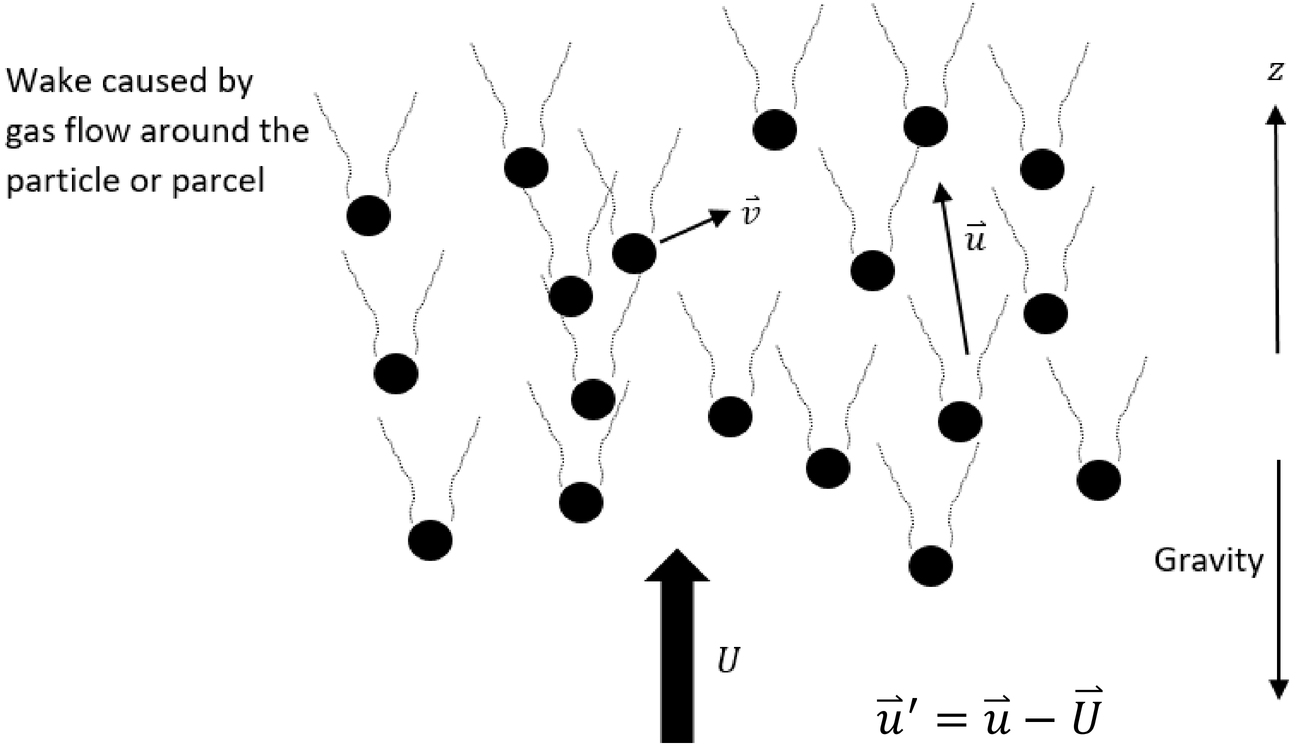
Using the DEM definition of a parcel, we find that

$$c = W^{-1/3}$$

Then the mean free time between collisions is given by

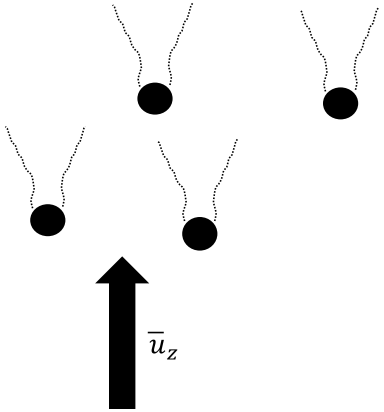
$$\tau = \frac{1}{\pi\, d^2\, n_V\, \left(c\sqrt{2}\,v\right) g_0}$$

Elements of the new method: Dominant upward flow suspending the bed



$$\vec{u}' = \vec{u} - \vec{U}$$

Effect of the dominant upward flow on drag



Equation of motion for particle

$$m\frac{d\vec{v}}{dt} = \vec{F}_D + \vec{F}_g$$

Essence of the effect of the dominant upward flow on drag

$$\frac{\vec{F}_D}{m} \propto |\vec{u} - \vec{v}|^2 \, \frac{\vec{u} - \vec{v}}{|\vec{u} - \vec{v}|} = (\vec{u} - \vec{v})\,|\vec{u} - \vec{v}| \approx (\vec{u} - \vec{v})\sqrt{\bar{u}_z^{\,2}} = \bar{u}_z(\vec{u} - \vec{v})$$

Result is a viscous flow equation where the dominant, mean velocity augments the drag force in all directions

Steady fluid bed is isotropic

$$\left\{\begin{aligned}
\frac{dv_x}{dt} &= \frac{\pi\,\mu\,d}{8\,m\,\epsilon^{2.65}}\left(0.3969\frac{\rho\,\epsilon\,d\,\bar{u}_z}{\mu}+6.048\left(\frac{\rho\,\epsilon\,d\,\bar{u}_z}{\mu}\right)^{0.5}+23.04\right)(u'_x-v_x) \qquad + \\
\frac{dv_y}{dt} &= \frac{\pi\,\mu\,d}{8\,m\,\epsilon^{2.65}}\left(0.3969\frac{\rho\,\epsilon\,d\,\bar{u}_z}{\mu}+6.048\left(\frac{\rho\,\epsilon\,d\,\bar{u}_z}{\mu}\right)^{0.5}+23.04\right)(u'_y-v_y) \qquad + \\
\frac{dv_z}{dt} &= \frac{\pi\,\mu\,d}{8\,m\,\epsilon^{2.65}}\left(0.3969\frac{\rho\,\epsilon\,d\,\bar{u}_z}{\mu}+6.048\left(\frac{\rho\,\epsilon\,d\,\bar{u}_z}{\mu}\right)^{0.5}+23.04\right)(\cancel{\bar{u}_z}+u'_z-v_z)-\cancel{g}
\end{aligned}\right.$$

$$\frac{dv}{dt} = \frac{\pi\,\mu\,d}{8\,m\,\epsilon^{2.65}}\left(0.3969\frac{\rho\,\epsilon\,d\,U}{\mu}+6.048\left(\frac{\rho\,\epsilon\,d\,U}{\mu}\right)^{0.5}+23.04\right)(u-v)$$

Note: Norouzi et al. and DiFelice drag models have been used here

Incorporate mean free time between collisions

Particles suffer speed reduction after collision according to restitution coefficient, R.
Solve for the particle speed versus time after the collision.

$$\frac{v}{u} = 1 - (1 - R)\, e^{-\frac{\pi\, \mu\, d}{8\, m\, \epsilon^{2.65}}\left(0.3969\frac{\rho\, \epsilon\, d\, U}{\mu} + 6.048\left(\frac{\rho\, \epsilon\, d\, U}{\mu}\right)^{0.5} + 23.04\right)t}$$

Note the particle never recovers all its speed due to the exponential dependence.
A cut-off value will need to be chosen.

Substitute the mean free time, τ, which depends on the particle speed.

$$\frac{v}{u} = 1 - (1 - R)\, e^{-\frac{\pi\, \mu\, d}{8\, m\, \epsilon^{2.65}}\left(0.3969\frac{\rho\, \epsilon\, d\, U}{\mu} + 6.048\left(\frac{\rho\, \epsilon\, d\, U}{\mu}\right)^{0.5} + 23.04\right)\left(\frac{1}{\pi\, d^2\, n_V\, c\, \sqrt{2}\, v\, g_0}\right)}$$

Result

$$\frac{v/u - R}{1 - R} = 1 - e^{-\left(\frac{0.3969\, Re_U + 6.048 (Re_U)^{0.5} + 23.04}{8\sqrt{2}\, c\, g_0\, \epsilon^{1.65}\, (1-\epsilon)}\right)\frac{1}{St_v}} \qquad (\epsilon > 0.8)$$

$$\frac{v/u - R}{1 - R} = 1 - e^{-\left(\frac{25}{\sqrt{2}\, c\, g_0} + \frac{7\, Re_U}{24\sqrt{2}\, c\, g_0\, (1-\epsilon)}\right)\frac{1}{St_v}} \qquad (\epsilon \leq 0.8)$$

where

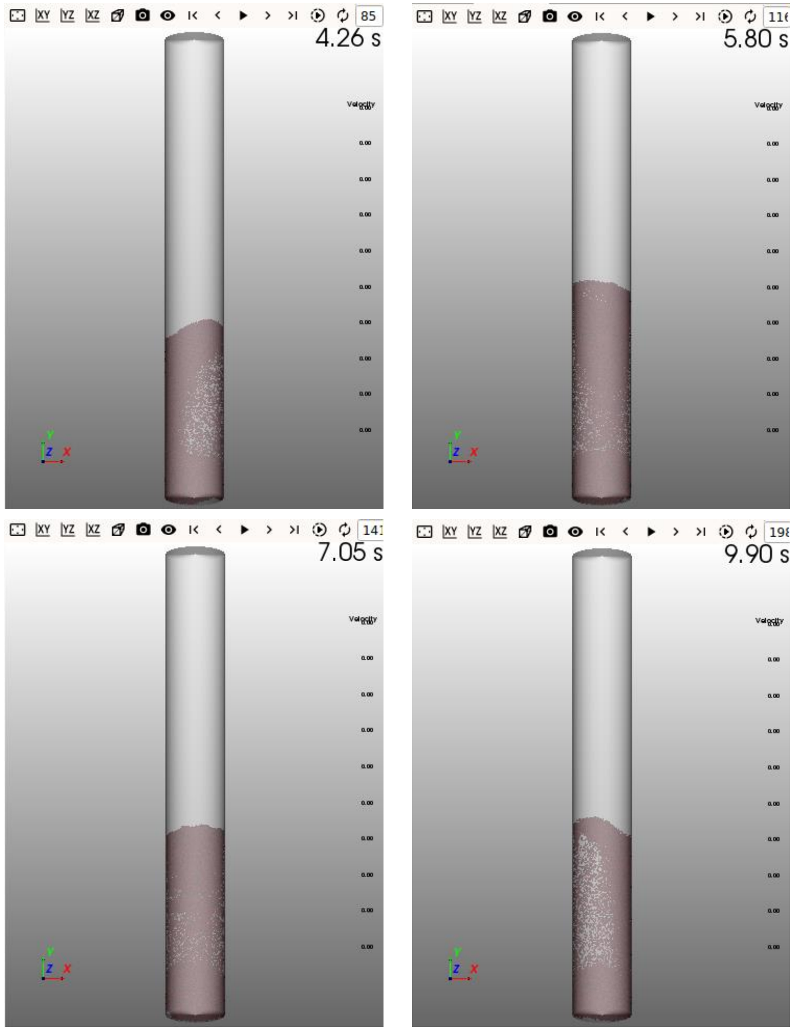
$Re_U = \dfrac{\rho\, d\, \epsilon\, U}{\mu}$ and $St_v = \dfrac{\rho_s\, d\, \epsilon\, v}{\mu}$

Choose cut-off, $\frac{v/u-R}{1-R}$, the fraction of speed the particle must recover prior to next collision. Then solve for particle speed, v.

1-inch bed, bubbling regime

- Simulations performed by Jaber Shabanian using MFiX-DEM. This was intended to be a small, rapid test case.
- Description: bed diameter 0.0254 m, particle density 2650 kg/m^3, particle diameter 0.8 mm, particle restitution coefficient 0.9, 28 thousand particles, ambient pressure, air temperature 850°C, superficial gas velocity 1.5 m/s
- Therefore, $u/u_{mf} \approx 7.9\ \left(u_{mf} \approx 0.19\ m/s\right)$. This case is expected to have significant collective particle motion.

1-inch bed, bubbling regime



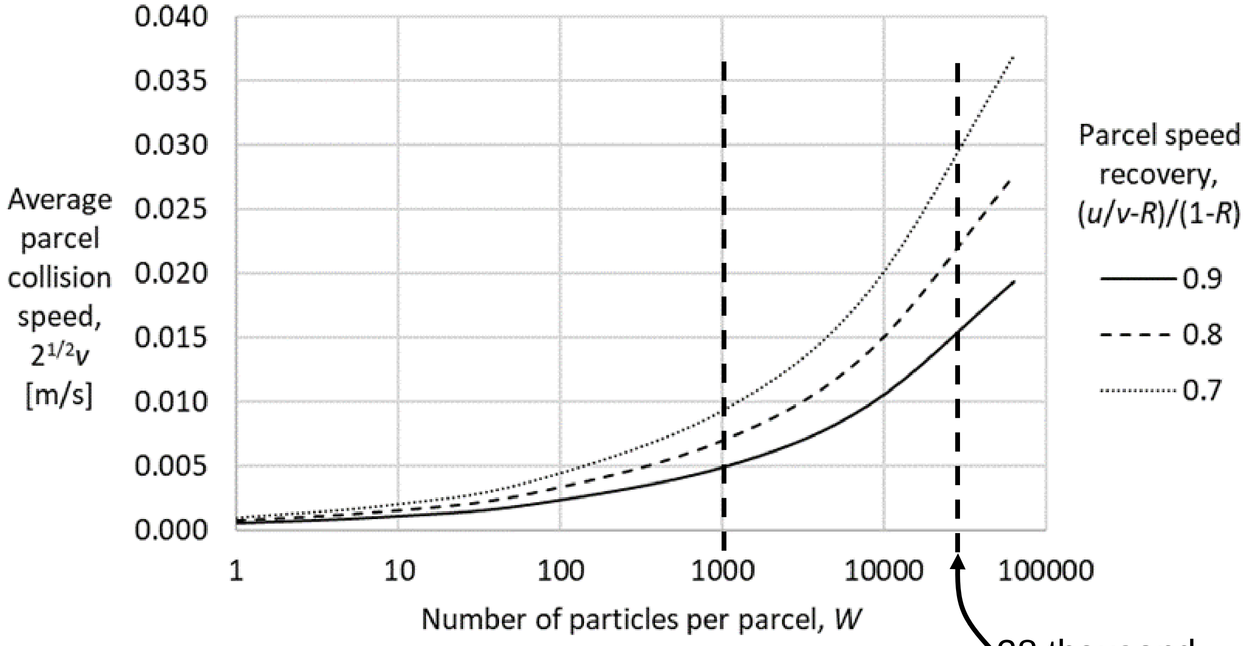
- Wall effects are significant due to the small (1-inch) diameter of the bed.

- Result was a “bouncing” bed. Would probably have been a “bubbling” bed were it not for its small diameter.

- According to MFiX-DEM, the average void fraction for this case was 0.61.

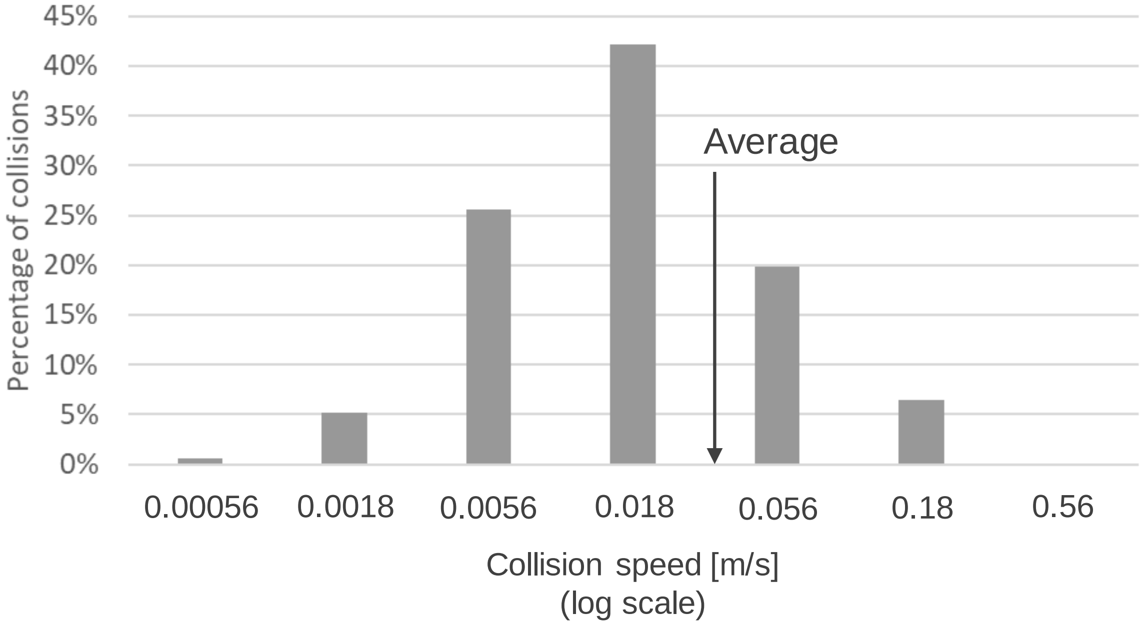
1-inch bed, bubbling regime

The present method



28 thousand particles

MFiX-DEM

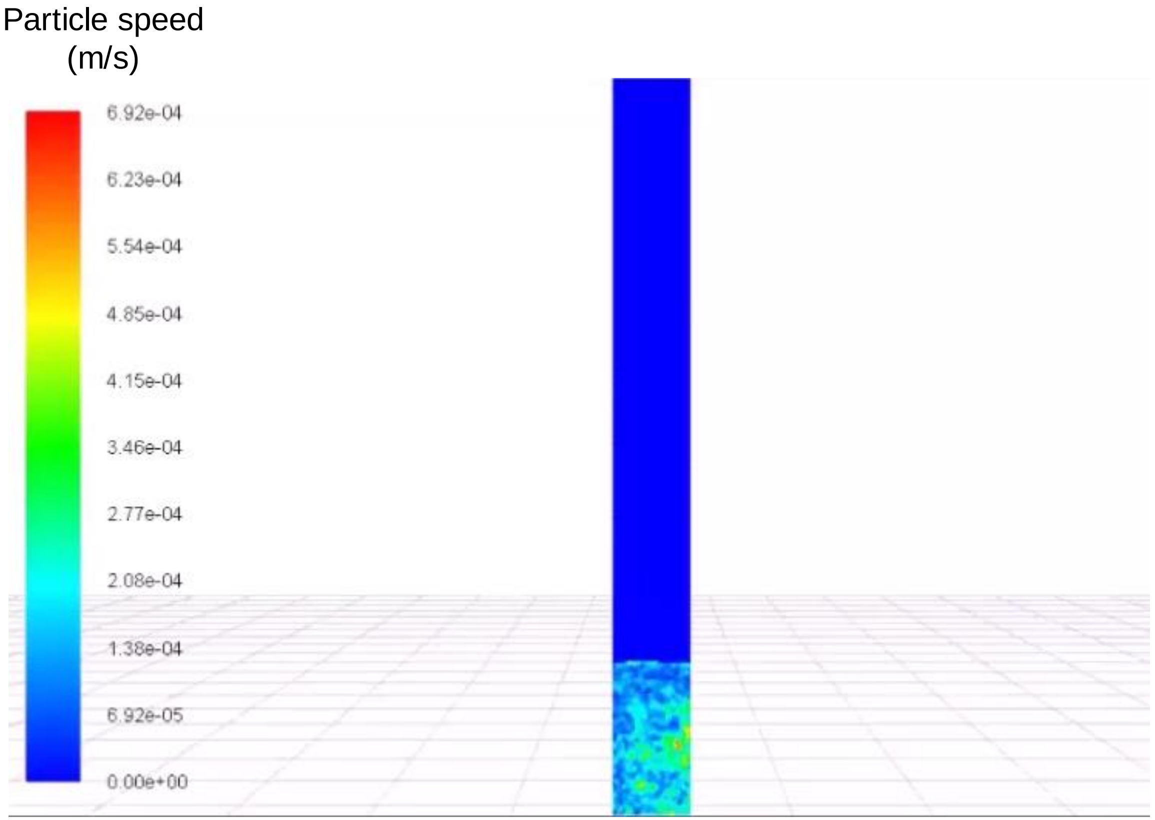


Particle collision speed divided by superficial gas velocity is approximately 1%

2-inch bed, smooth regime

- Simulations performed by Haining Gao using Fluent-DEM. This case represents upcoming experimental runs.
- Description: bed diameter 0.053 m, particle density 2445 kg/m^3, particle diameter 0.55 mm, particle restitution coefficient 0.9, 1.6 million particles, ambient pressure, air temperature 1000°C, superficial gas velocity 0.0942 m/s
- Therefore, $u/u_{mf} \approx 1.2 \ (u_{mf} \approx 0.0785 \ m/s)$. Average void fraction estimated to be 0.345. Predominantly random particle motion expected for this case.
- Note: 35 days using 18 cores to simulate 3 seconds of operation!

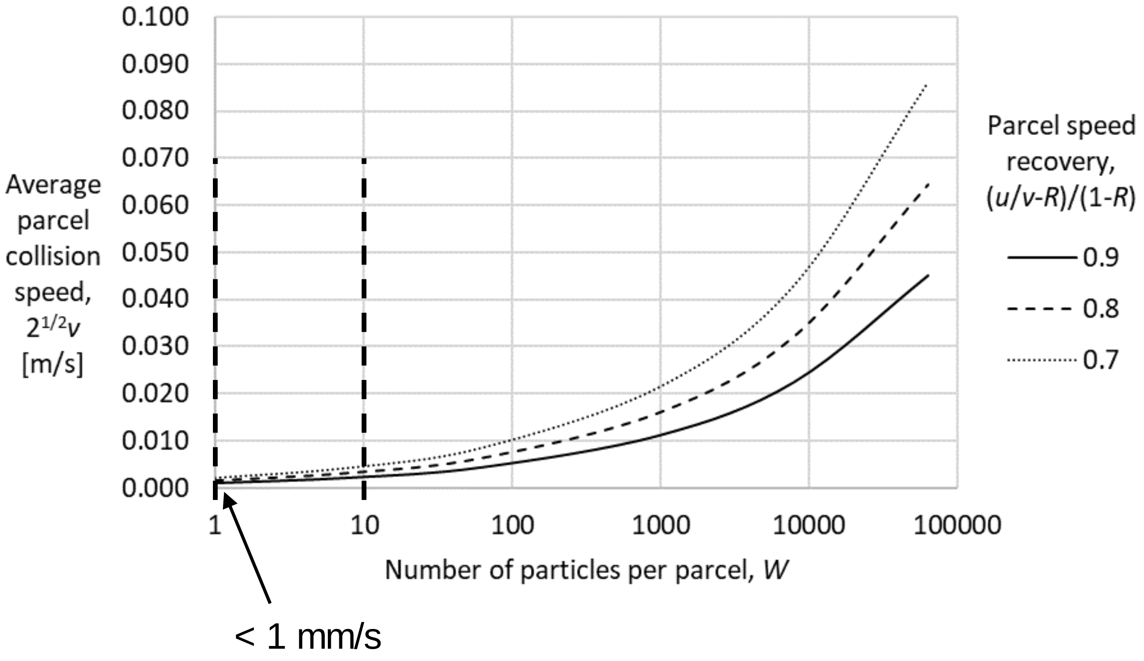
2-inch bed, smooth regime



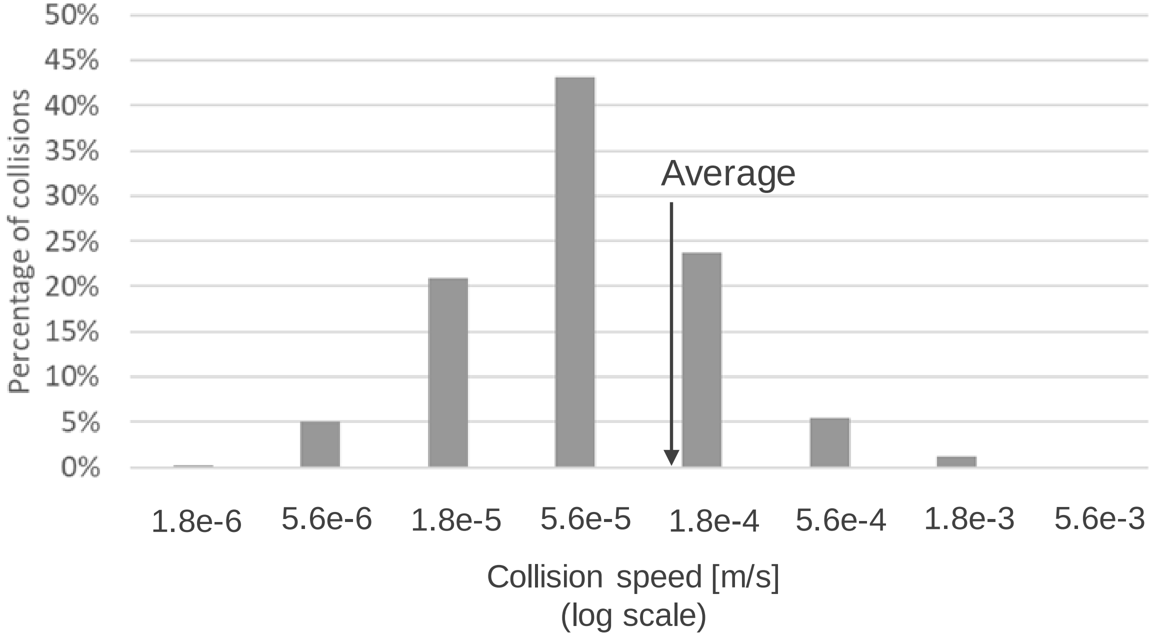
Fluent-DEM animation: 2 seconds of operation

2-inch bed, smooth regime

The present method

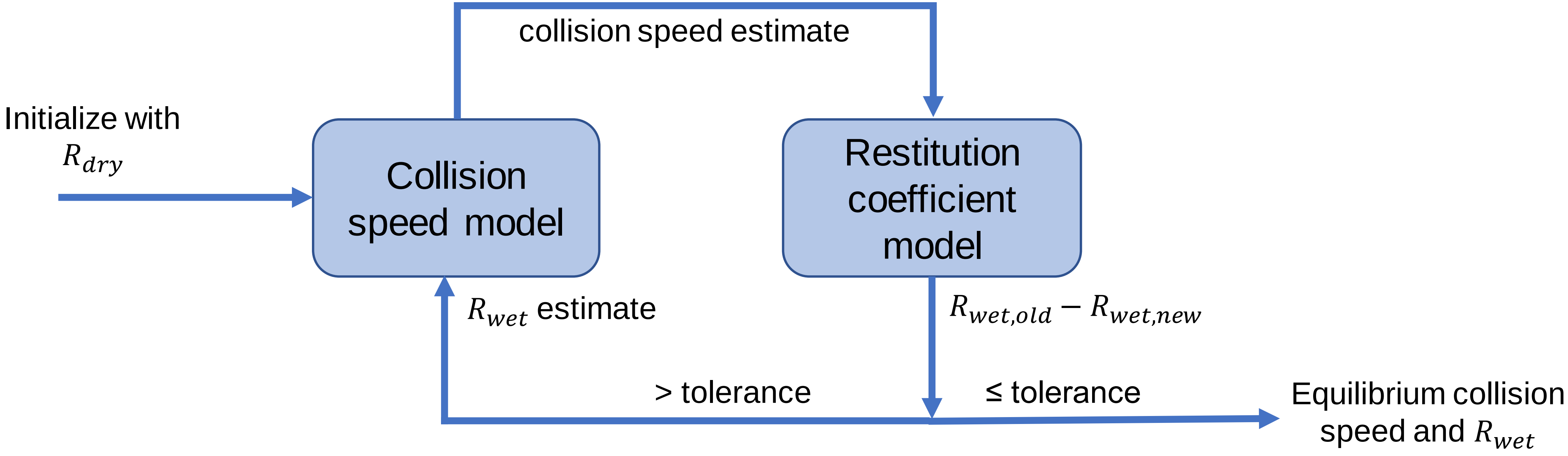


Fluent-DEM



Particle collision speed divided by superficial gas velocity is approximately 0.5%

Coupling the collision speed and restitution coefficient models



Result: The tolerable coating layer thickness was found to be very small (<1 micrometer), suggesting significant vulnerability to particle agglomeration.

Conclusion

- A new, rapid analysis method was developed to predict the average particle collision speed in fluidized beds whose kinetic energy dissipation is dominated by collisions (the “collision-driven” regime).
- The method accommodates collective particle motion.
- The results agreed with two CFD-DEM cases, one of a smooth fluidization regime and the other of a bubbling regime.
- The average particle collision speed was found to be two orders of magnitude lower than the superficial gas velocity that suspends the bed.
- The tolerable liquid coating thickness was found to be less than 1 micrometer, which suggests high sensitivity of fluid bed operation to particle stickiness.