Prediction of Particle Agglomeration and Deposition by Reduced Particle Stiffness Discrete Element Simulations
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Introduction

- The collisions of small particles ($d_p < 10\ \mu m$) in dry air are typically dominated by van der Waals attractive forces.
- Discrete element method (DEM) simulations combined with the analytical JKR adhesive model [1] is a promising mechanistic-based approach to accurately predict agglomeration and deposition of micron-sized particles [2].
- The general applicability and relevance in scientific fields ranging from particle fouling and deposition, micromechanisms in details.
- However, resolving collisions of micron-sizes particles typically requires time step sizes in the order of nano seconds ($10^{-9}\ \text{s}$).

Main conclusions

- Simulation time can be reduced several orders of magnitude by reducing Young’s modulus from $E$ to $E_{\text{mod}}$ while modifying the surface energy density $\gamma$ as:

$$\gamma_{\text{mod}} = \gamma \left( \frac{E_{\text{mod}}}{E} \right)^{2/5}.$$  (1)

- Simulations that would take years can now be done in hours or days.

Overview of modified model

- Figure gives an overview of the force-overlap relation of the JKR model and modified model based on eq. (1):

  - Original JKR model
  - Modified model using (1)

- Where $F_0 = 3\pi\gamma R$ is the critical pull-off force to separate particles and $\delta_{0,0,\text{mod}} = \left(\frac{3\pi^2\gamma R^2}{E^5}\right)^{1/7}$ is the equilibrium normal overlap. Graphical overview of DEM forces:

Agglomerated formed by van der Waals attractive forces

Validation cases

Initial position

Final possible states

Coupling to turbulent flow

- Coupling DEM to large eddy simulations (LES) is a promising approach to investigate particle agglomeration and deposition mechanisms in details.
- Information is passed between fluid and particle phase by momentum exchange terms. Fluid drag takes local particle volume fraction into account.
- Example of pipe flow at $Re_d = 10,000$ in a periodic domain with length $L/D = 4$.

Outlook

- Particle fouling in heat exchanger pipes is a major problem with high associated costs. The particulate fouling process can be decomposed up into the following sub-processes:

- Full-scale simulation using OpenFOAM and LIGGGHTS shows early stages of particulate fouling. Larger agglomerates are being formed in the centre of the pipe.

Collaborating partners

References