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

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

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Introduction

- The collisions of small particles ($d_p < 10$ µm) 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 prediction [3] to early stages of planet formation in outer space [4] make the JKR model increasingly popular [5].
- However, resolving collisions of micron-sizes particles typically requires time step sizes in the order of nano seconds (10^{-9} s).

Purpose of study

- To provide a criterion on how to introduce softer particles with the same adhesive behaviour in DEM.
- Using softer particles (lower Young's modulus) allows for an increased time step size and thereby lower computational cost.

Main conclusions

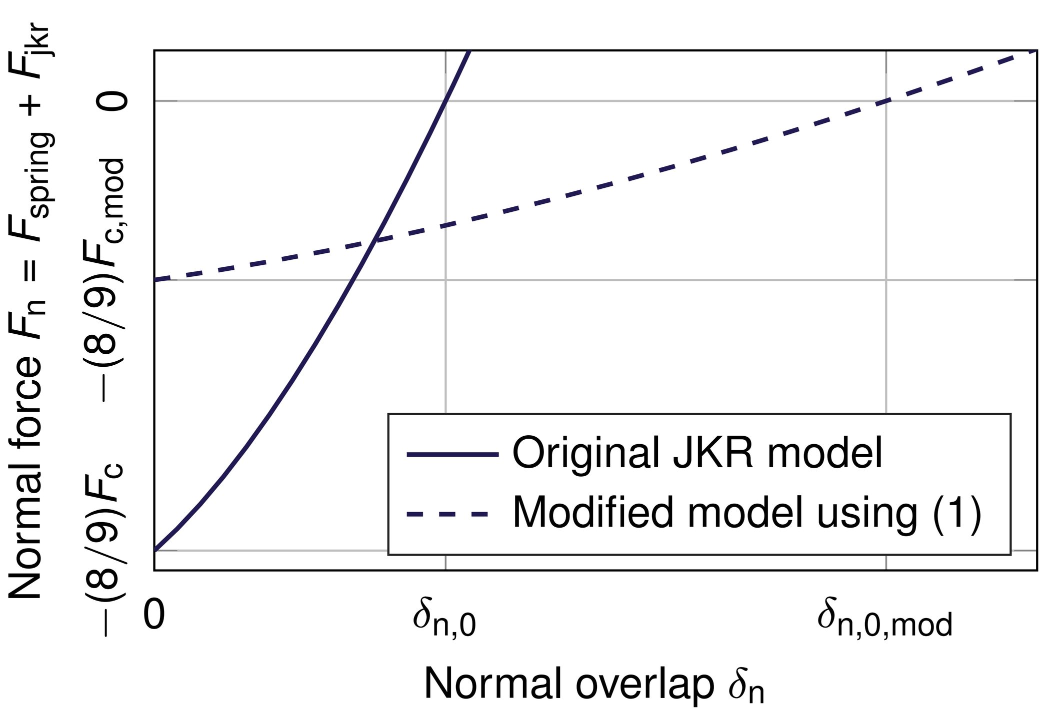
- Simulation time can be reduced several orders of magnitude by reducing Young's modulus from E to E_{mod} while modifying the surface energy density γ as:

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

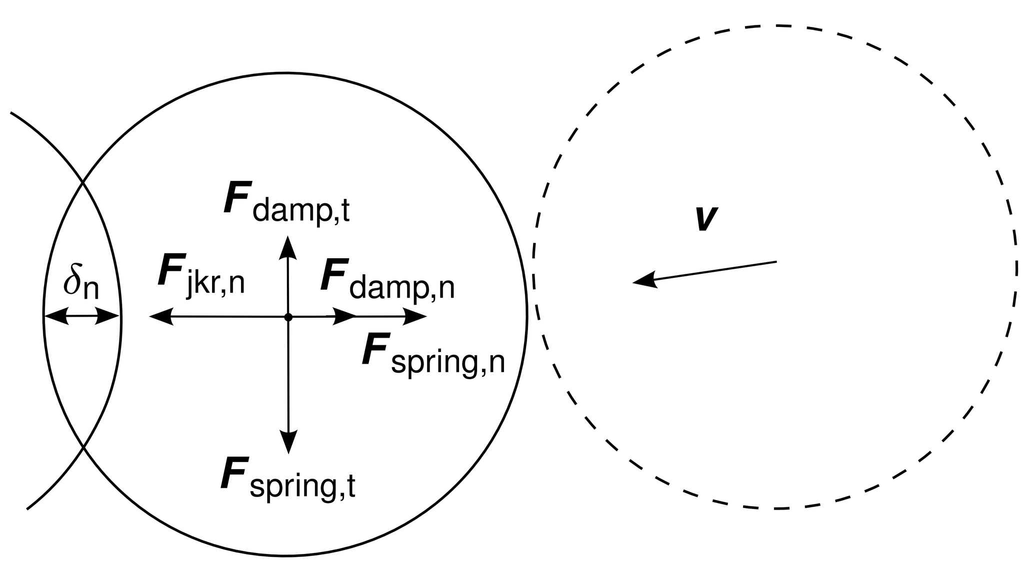
- Simulations that would take **years** can now be done in **hours** or **days**.

Overview of modified model

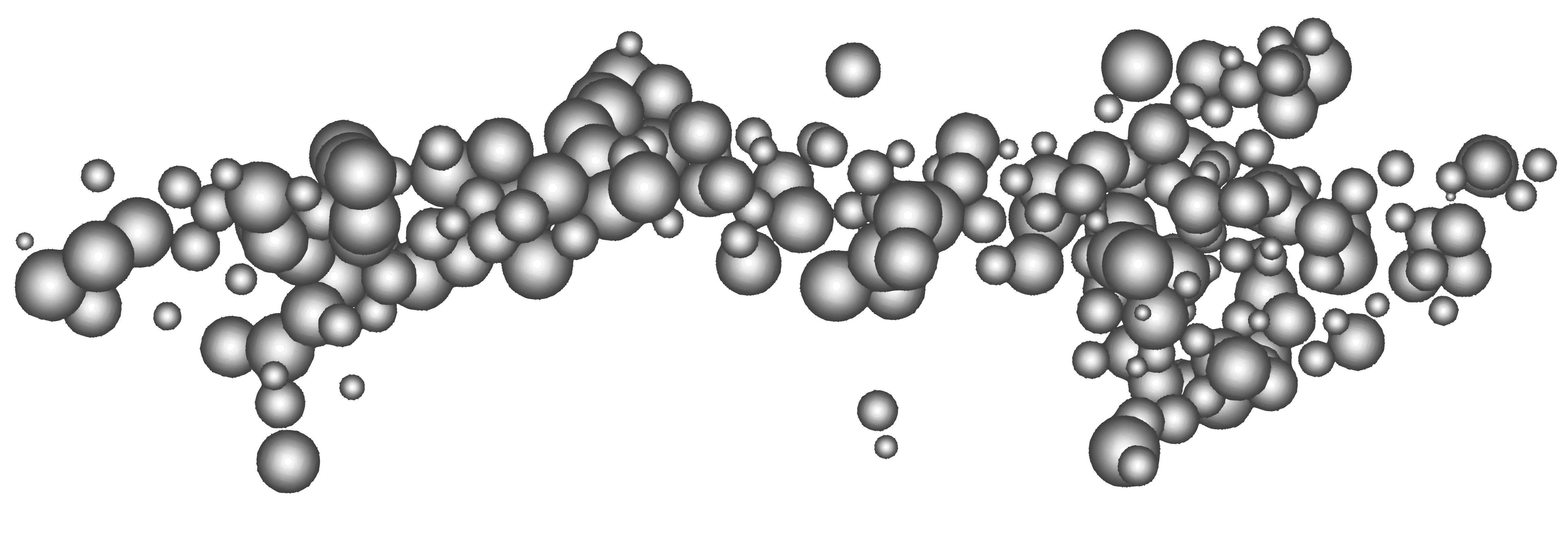
- Figure gives an overview of the force-overlap relation of the JKR model and modified model based on eq. (1):



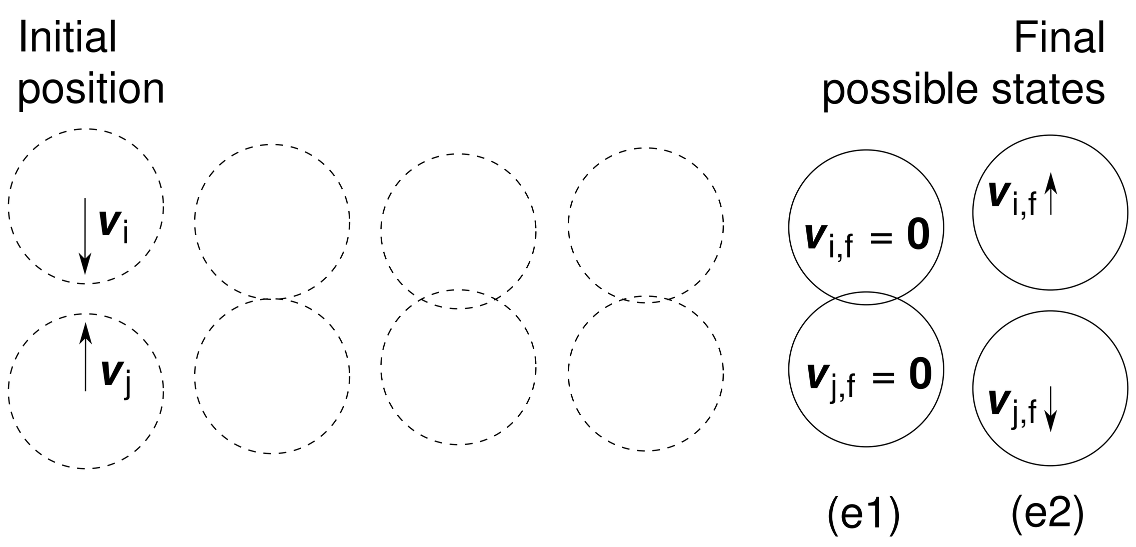
- Where $F_c = 3\pi\gamma R$ is the critical pull-off force to separate particles and $\delta_{n,0} = \left(3\pi^2\gamma^2 R/E^2\right)^{1/3}$ is the equilibrium normal overlap. Graphical overview of DEM forces:

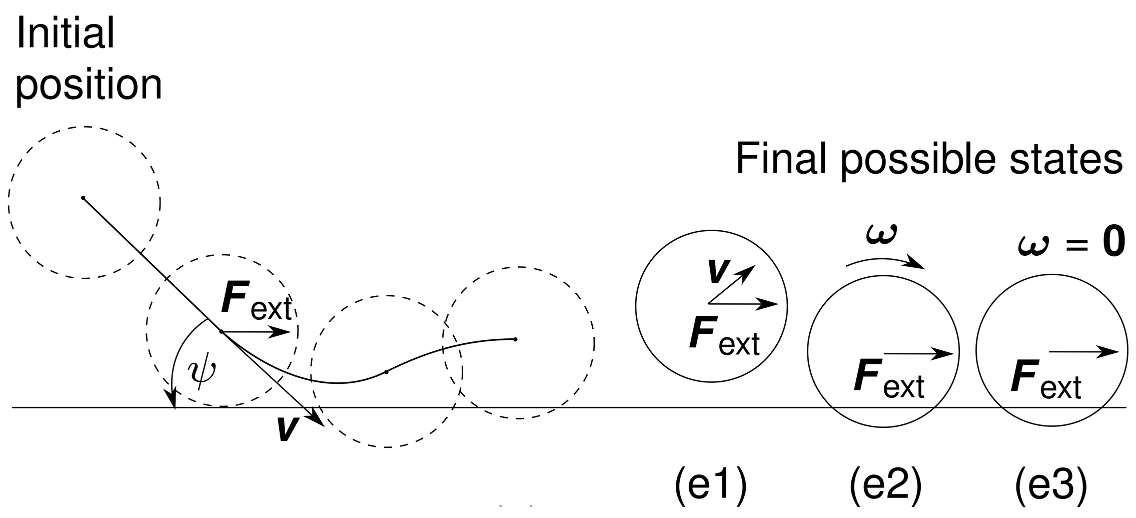


Agglomerate formed by van der Waals attractive forces



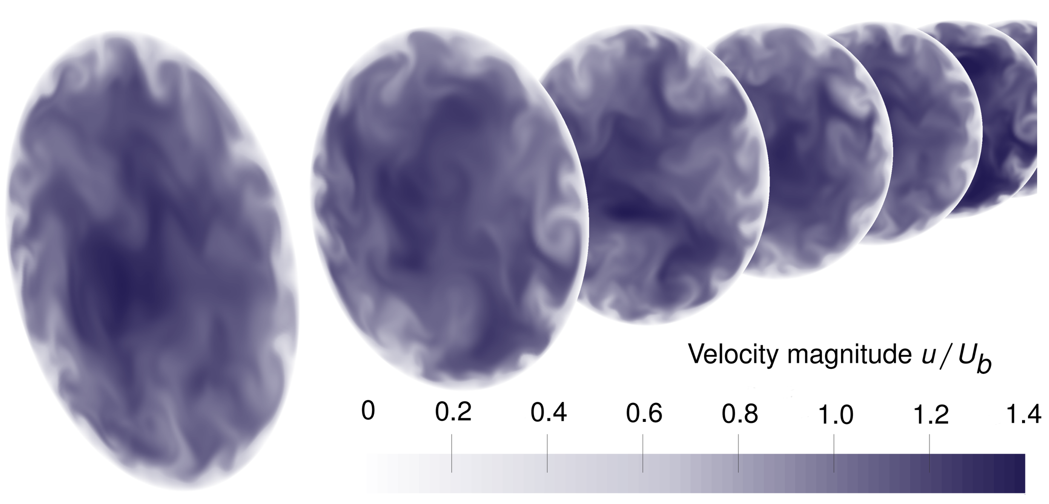
Validation cases





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.



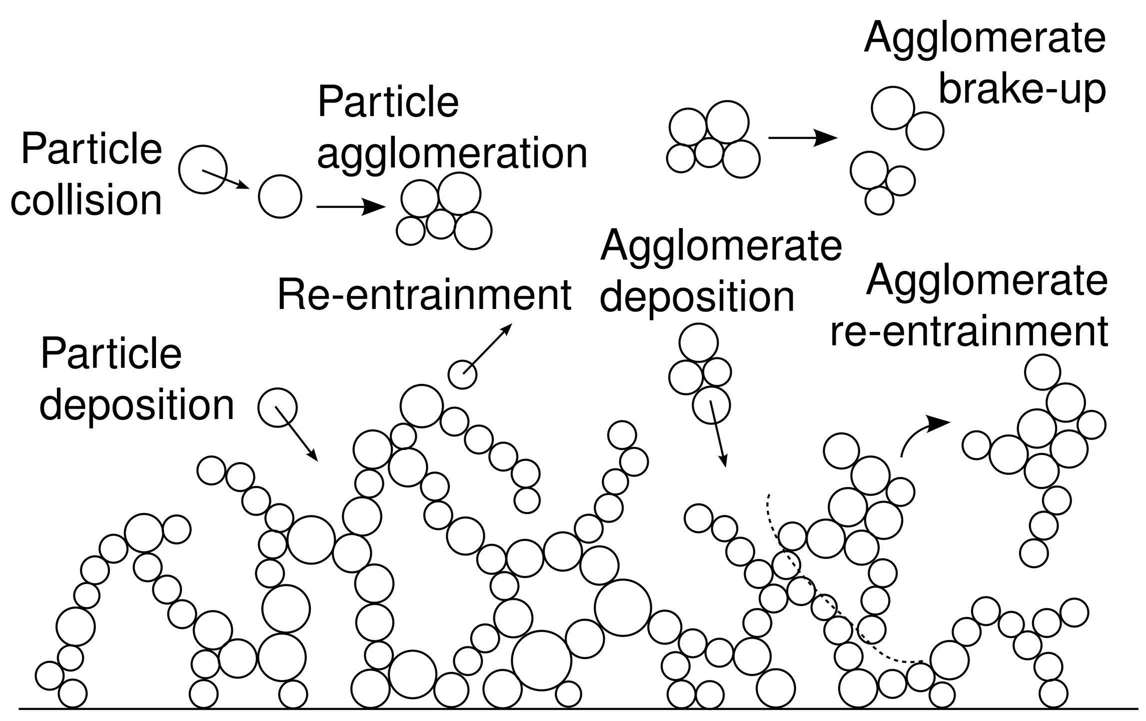
- Example of pipe flow at $\mathrm{Re}_b = 10{,}000$ in a periodic domain with length $L/D = 4$.

Collaborating partners

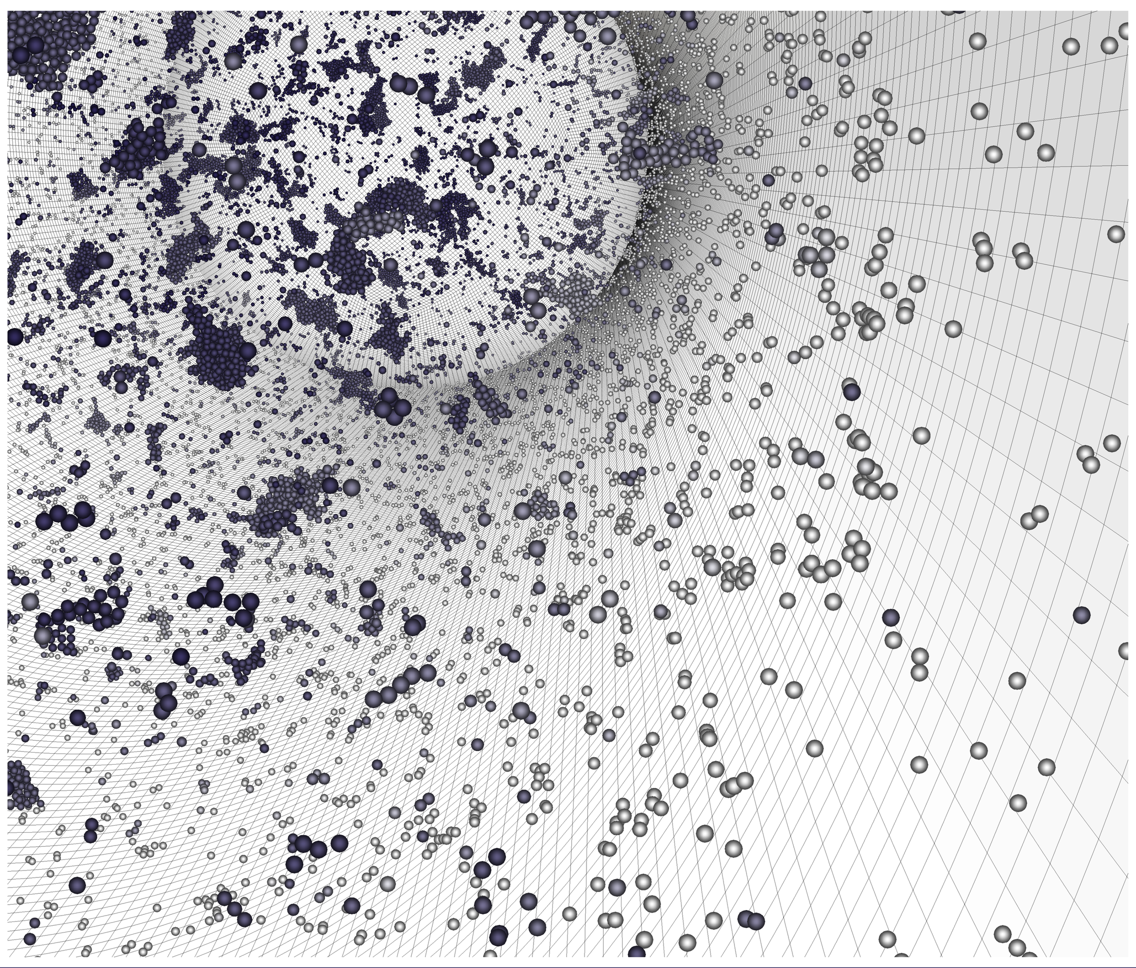
TUM Technische Universität München, TUDelft Delft University of Technology, DTU Technical University of Denmark, Aalborg University Denmark, Alfa Laval, MAN, MAERSK, Danfoss, Arla, Danish Technological Institute, viegand maagøe energy people

Outlook

- Particulate 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:



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