Simplified Coagulation Dynamics of Agglomerates at Self-Preservation

Swiss Federal Institute of Technology Zürich

M. R. Kholghy, G.A. Kelesidis, and S.E. Pratsinis

Particle Technology Laboratory, ETH Zürich, CH-8092 Zürich, Switzerland

mkholghy@ethz.ch

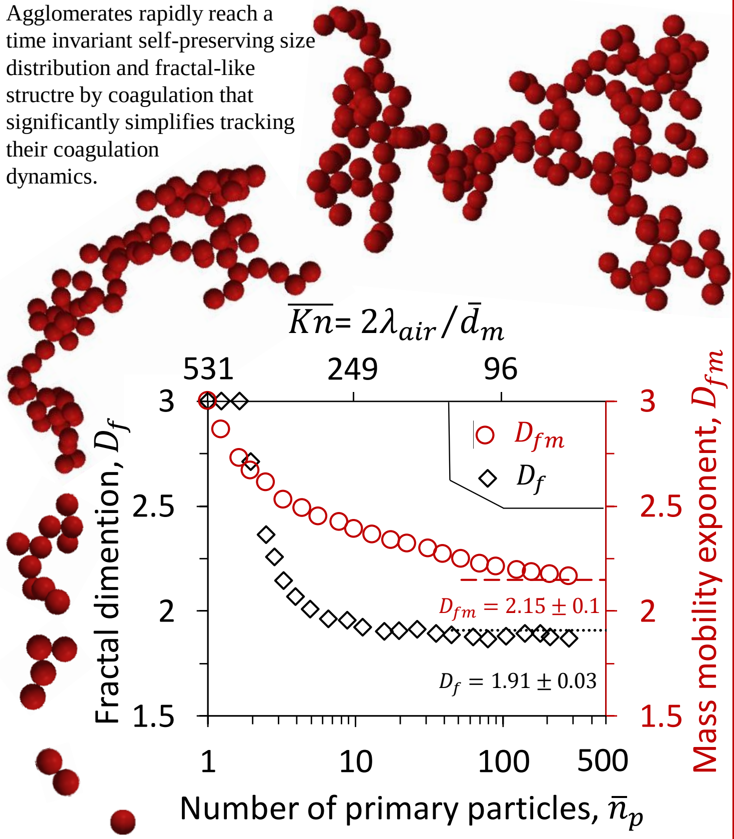
www.ptl.ethz.ch

Motivation

Nanoparticle morphology and concentration are important for emission control. Monodisperse population balance models (MPBM) are computationally affordable and easy to use to predict particle dynamics when particles have attained their self-preserving size distribution and asymptotic fractal-like structure. This is typically the case when high concentrations of nanoparticles are involved such as for engine emissions. Here, a monodisperse model for particle dynamics by agglomeration is introduced that uses scaling laws from Discrete Element Modeling (DEM) simulations to accurately predict particle morphology and collision frequency. The model accurately predicts the evolution of particle concentration, mobility and gyration diameters as well as the effective density with a single equation.

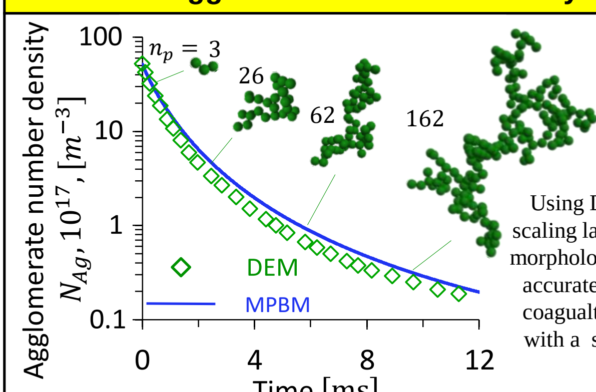
Evolving Fractal-Like Structre by Coagulation

Agglomerates rapidly reach a time invariant self-preserving size distribution and fractal-like structre by coagulation that significantly simplifies tracking their coagulation dynamics.



DEM-derived fractal dimension, D_f and mass mobility exponent, D_{fm} of agglomerates reach their asymptotic fractal-like structure with $D_f = 1.91 \pm 0.03$ (dotted line) [1] within 1.8 ms when $\bar{n}_p = 10$ ($\bar{d}_m/d_p = 2.35$) and with $D_{fm} = 2.15 \pm 0.1$ (dashed line) [1] within 4.77 ms when $\bar{n}_p = 50$ ($\bar{d}_m/d_p = 4.79$) .

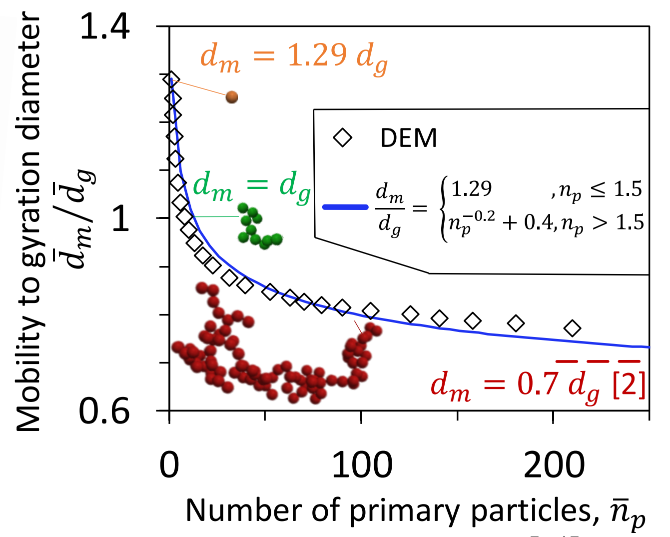
Agglomerate Number Density



Using DEM derived scaling laws for particle morphology and enables accurate prediction of coagualtion dynamics with a simple model.

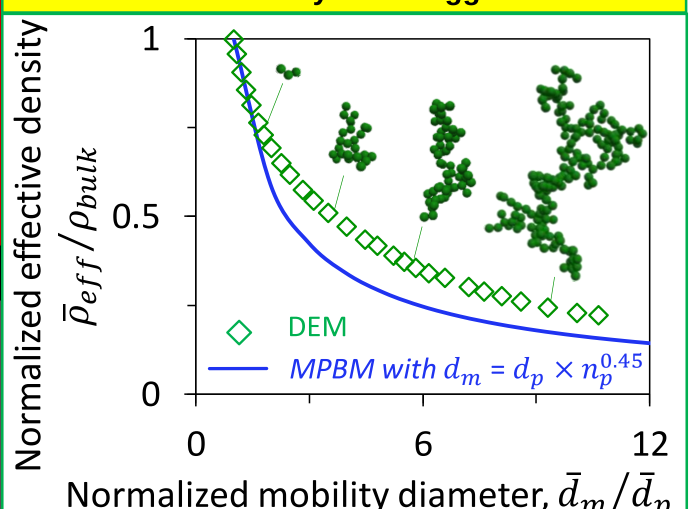
Evolution of a) N_{Ag} and b) $\bar{n}_p$ as a function of time during agglomeration in the free molecular regime derived by DEM (diamonds) and MPBM (lines) simulations.

Evolution of Mobility and Gyration Diameters



The ratio of mean mobility diameter over that of gyration, $\bar{d}_m/\bar{d}_g$, evolves from 1.29 for single spheres, but rapidly decreases to 1 for agglomerates with $n_p \sim 10$ and asymptotically reaches 0.7 (dashed line) for large agglomerates with $\bar{n}_p \geq 700$ [2]. The DEM-derived relation [3] (solid line) quantifies the evolution of $\bar{d}_m/\bar{d}_g$ within 4% of DEM simulations.

Effective Density of the Agglomerates



Normalized effective density, $\bar{\rho}_{eff}/\rho_{bulk}$, (diamonds) as a function of normalized mobility diameters during agglomeration rapidly decreases from 1 to 0.2 for $\bar{d}_m/d_p = 12$. With $\bar{d}_m/d_p = n_p^{0.45}$ [3] normalized effective denisty can be calculated within 28.5% of DEM-derived values.

Conclusions

1. Accurate scaling laws to describe particle morphology can be obtained with Discreate Element Modeling simulations.

2. Using such scaling laws in population balance modeling enables accurate prediction of the dynamics of particle coagulation.

3. These simple models can be used to accurately predict mobility size and number concentration of engine emissions after exhaust.

References

[1] Ball, R. and R. Jullien, Journal de Physique Lettres, 1984. **45**. 1031.

[2] Wang, G. and C. Sorensen, Physical Review E, 1999. **60**. 3036.

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