Settling rate of nanosized fractal-like agglomerates by Brownian Dynamics simulations

Swiss Federal Institute of Technology Zurich

A. Spyrogianni,[1] K.S. Karadima,[2,3] E. Goudeli,[4] V.G. Mavrantzas[1,2,3] and S.E. Pratsinis[1]

[1] Dept. of Mechanical and Process Engineering, ETH Zurich, Switzerland; [2] Dept. of Chemical Engineering, University of Patras, Patras, Greece; [3] Inst. of Chemical Engineering Sciences, FORTH/ICE-HT, Patras, Greece; [4] Dept. of Mechanical Engineering, University of Minnesota, USA

PTL Particle Technology Laboratory

Introduction

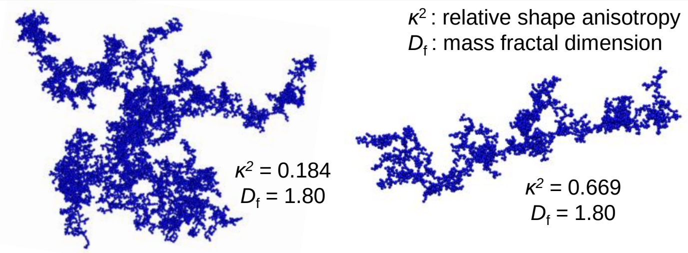
The precipitation of agglomerates impacts water cleaning, nanotoxicology, nanomedicine as well as the stability of engineered nanofluids. Here, the settling rate, u_s, of fractal-like SiO_2 agglomerates[1] is calculated by Brownian Dynamics (BD)[2] tracking their translational and rotational[3] motion under gravity in water.

The agglomerate mobility diameter is calculated from the translational diffusion coefficient[4] and compared to scaling laws from the literature.[5,6] The effect of constituent primary particle (PP) geometric mean diameter, $d_{p,g}$, and standard deviation, $\sigma_{p,g}$, (polydispersity) on agglomerate u_s is investigated.

An analytical expression for u_s is derived and compared to deposition rate measurements by UV-vis spectroscopy of fumed SiO_2 agglomerates in water.

Agglomerate structure

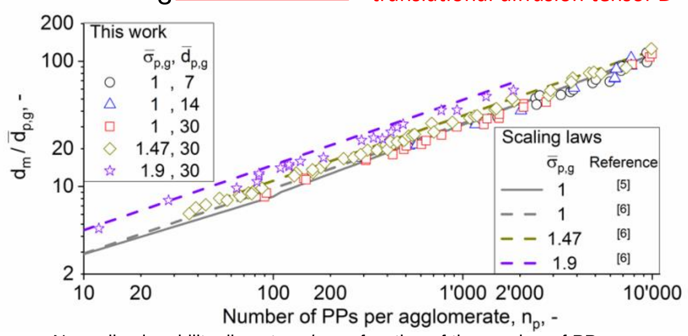
κ^2 : relative shape anisotropy
D_f : mass fractal dimension



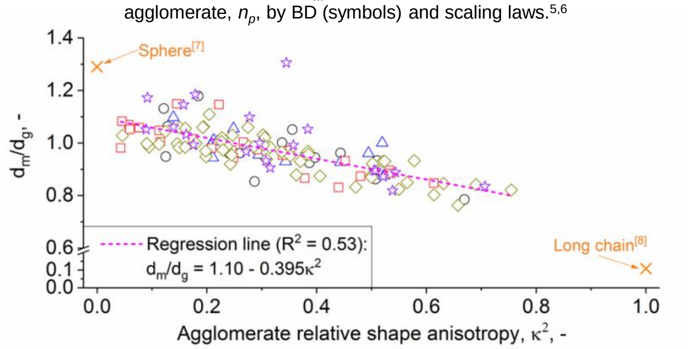
Mobility diameter, d_m

Stokes-Einstein equation: $$d_m = \frac{k_B T}{3\pi\mu D^{tt}}$$

with[4] $$D^{tt} = \frac{1}{3}\left(D_x^{tt} + D_y^{tt} + D_z^{tt}\right)$$ Diagonal elements of translational diffusion tensor $\boldsymbol{D}^{tt}$

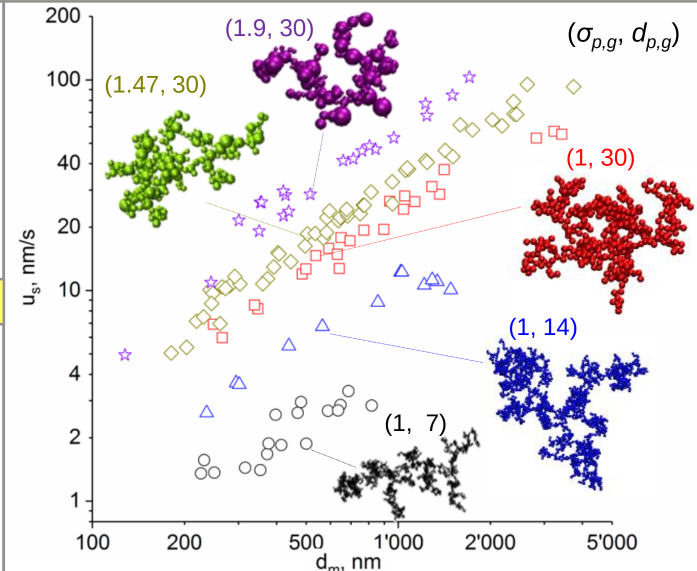


Normalized mobility diameter, d_m, as function of the number of PPs per agglomerate, n_p, by BD (symbols) and scaling laws.[5,6]



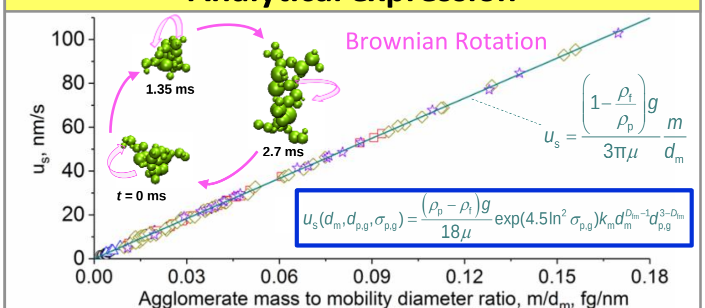
Mobility diameter over diameter of gyration, d_m/d_g, as function of κ^2 for agglomerates with D_f = 1.8 (open symbols), spheres[7] and long chains[8].

BD-obtained settling rate, u_s



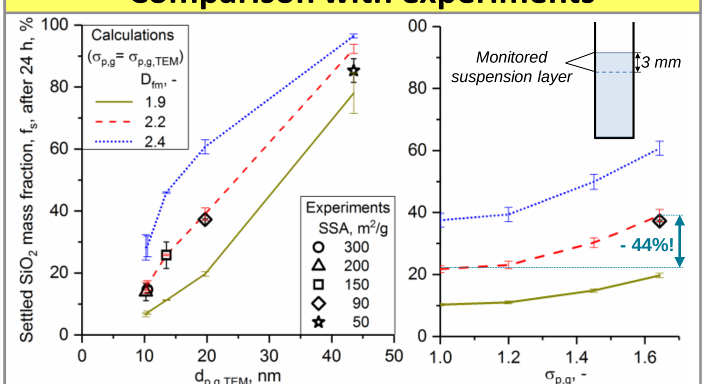
Agglomerate settling rate, u_s, as function of their mobility diameter by BD simulations.

Analytical expression



Agglomerate settling rate, u_s, as function of their mass to mobility size ratio. The BD-obtained data are fitted to an analytical expression. k_m, D_{fm}: mass-mobility prefactor & exponent; ρ_p, ρ_f: density of PPs and fluid; μ: fluid viscosity; g: gravitational acceleration.

Comparison with experiments



Mass fraction of settled SiO_2 agglomerates after 24 hr as function of the PP size (left) and polydispersity (right).

Conclusions

- The d_m is in agreement with scaling laws[5,6] & the d_m/d_g decreases with increasing κ^2
- For constant d_m, the agglomerate u_s increases with increasing $d_{p,g}$ and $\sigma_{p,g}$
- Linear relationship of u_s with m/d_m is revealed, due to fast Brownian rotation
- Comparison with experiments indicates D_m of 2.2 for fumed SiO_2 in water, consistent with aerosol measurements of other flame -made agglomerates[10]
- If monodisperse PPs are assumed, the agglomerate u_s is underestimated considerably

References

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