Settling rate of agglomerates consisting of polydisperse primary particles by Brownian Dynamics

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Abstract

The dynamics and settling rate of nanoparticles dispersed in aqueous solutions is important for *in vitro* dosimetry in nanotoxicology, nanomedicine and stability of nanofluids. Settling rate measurements of sub-micrometer agglomerates are not trivial, contrary to millimeter-sized ones that can be easily tracked in a settling column.

Here, the mobility of such nanosized fractal-like SiO_2 agglomerates (Goudeli et al., 2016) in dilute suspensions is investigated and their settling rate is calculated by Brownian Dynamics (BD) simulations. The BD method is thoroughly validated and the agglomerate mobility diameter is calculated *ab initio* and compared with that obtained by well-known scaling laws for fractal-like agglomerates and settling rate experiments (Kasper et al., 1985). The effect of the constituent primary particle mean diameter and geometric standard deviation (polydispersity) as well as the agglomerate shape anisotropy on their settling rate is elucidated for the first time. For constant agglomerate mobility diameter, the BD-obtained settling rate increases with increasing primary particle size for agglomerates consisting of monodisperse primary particles as well as with increasing primary particle polydispersity when agglomerates consist of polydisperse spheres, but is hardly affected by the particle shape anisotropy due to their fast rotation and small mass.

Furthermore, an analytical expression for the settling rate of agglomerates consisting of lognormally distributed primary particles is derived. The common assumption of monodisperse constituent primary particles leads to underestimation of the agglomerate settling rate compared to the settling rate calculated from analytical expressions. This underestimation depends on the primary particle polydispersity and agglomerate mass mobility exponent D_{fm} (an indicator of the agglomerate structure).

The proposed expression is compared also with experiments for the deposition rate of fumed SiO_2 agglomerates in aqueous suspensions (Spyrogianni et al., 2017).

Keywords: settling rate, mobility diameter, nanosized agglomerates, Brownian Dynamics.

References:

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