The Effect of Primary Particle Polydispersity in the Evolving Agglomerate Structure and Size Distribution

E. Goudeli[1], M.L. Eggersdorfer[2] and S.E. Pratsinis[1]

[1]Department of Mechanical and Process Engineering, ETH Zurich, Zurich, 8092, Switzerland
[2]Novartis Pharma AG, Basel, 4002, Switzerland
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Presenting author email: goudeli@ptl.mavt.ethz.ch

Gas-phase processes offer a proven scalable route for the large scale production of commodities like fumed silica, carbon black and pigmentary titania (Buesser and Pratsinis, 2012). Modeling the particle growth is of utmost importance for the design of aerosol reactors. There particle dynamics span 10 and 15 orders of magnitude in length and time, respectively. Also they determine particle structure influencing the electrical conductivity and mechanical stability of product films and powders (Buesser and Pratsinis, 2012).

Agglomeration (i.e. particle formation with loosely attached primary particles) occurs both in environmental and industrial processes, especially in low temperature regions where sintering or coalescence are rather slow. The dominant coagulation mechanism is cluster-cluster agglomeration leading largely to formation of filamentary structures that are attractive in nanocomposites, particle suspensions (paints or polishing slurries), catalysis and lightguide preforms. Fractal-like agglomerates typically consist of polydisperse primary particles that affect the clusters' optical, dispersion and transport properties. Understanding agglomeration is essential for optimal process design for manufacture of nanomaterials as their fractal structure affects their handling and processing and eventually their performance.

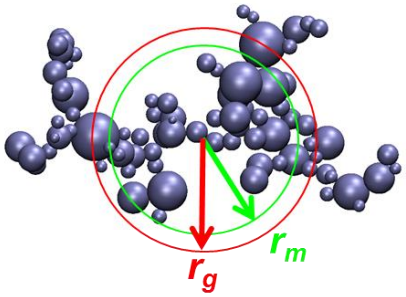

Figure 1: A ballistic cluster-cluster agglomerate consisting of polydisperse PPs having a log-normal size distribution, $\sigma_{g,PP}$ = 1.5. The radius of gyration, r_g, scales with the PP number to the fractal dimension, D_f, and is larger than its mobility radius, r_m.

The growth and detailed structure of fractal-like aerosol particles undergoing agglomeration is investigated here in the free molecular regime by discrete element modeling (Goudeli et al., 2015) accounting for the polydispersity of constituent primary particles (Fig. 1). The evolution of particle structure (fractal dimension, D_f, and mass mobility exponent, D_{fm}) from spheres to fractal-like agglomerates is elucidated. Increasing the polydispersity of the constituent PPs from geometric standard deviation $\sigma_{g,PP}$ = 1 to 3 delays the attainment of the asymptotic D_f and D_{fm} of the resulting agglomerates.

Figure 2 shows the D_{fm} evolution (line) of agglomerates consisting of polydisperse PPs ($\sigma_{g,PP}$ = 1.5; insets) from spheres (ρ_{eff}/ρ_b = 1) to fractal-like agglomerates (ρ_{eff}/ρ_b = 0). When agglomerates are fully evolved D_{fm} attains its asymptotic value of 2.2, consistent with Sorensen (2011). The simulations are in good agreement with experimental measurements of Ag (Kim et al., 2009), ZrO_2 (Eggersdorfer et al., 2012) and Cu (Stein et al., 2013).

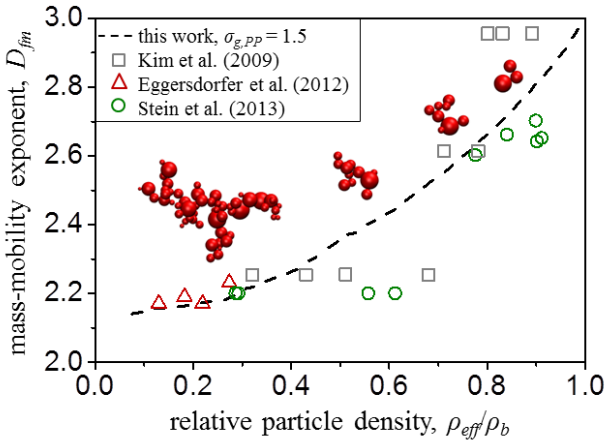

Figure 2: The D_{fm} for agglomerates consisting of polydisperse PPs with $\sigma_{g,PP}$ = 1.5 (line), as obtained by simulations. The D_{fm} obtained by experimental measurements (symbols) increases with increasing relative particle density, ρ_{eff}/ρ_b.

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