Multiscale design of aerosol synthesis of materials: Effect of evolving structure (D_f) on TiO_2 & SiO_2 diameters

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Motivation

- The effect of evolving agglomerate structure (D_f) on product primary particle and hard-agglomerate diameter is important in aerosol synthesis of materials and monitoring of ambient aerosols.
- It is explored here by interfacing continuum, mesoscale and molecular dynamics models.

Aerosol Dynamics

Number Concentration, N: $\frac{dN}{dt} = -\frac{1}{2}\beta N^2 \rho_g$

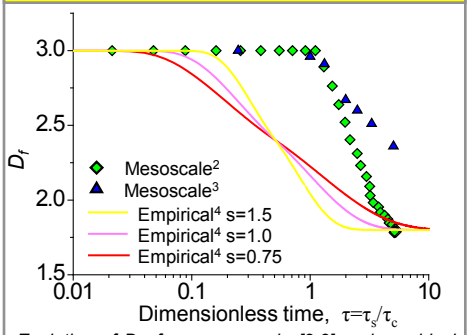
Agglomerate Area Concentration, A: $\frac{dA}{dt} = -\frac{1}{\tau_s}(A - Na_s)$ (τ_s from TiO_2 molecular dynamics[1])

Agglomerate Volume Concentration, V: $\frac{dV}{dt} = 0$

Primary Particle Diameter: $d_p = \frac{6V}{A}$

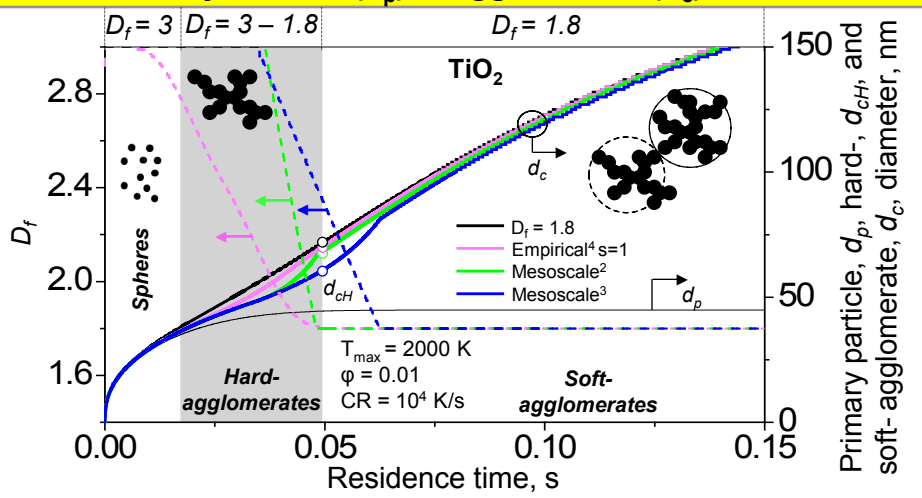
Collision Diameter: $d_c = d_p \left(\frac{A^3}{36\pi N V^2}\right)^{1/D_f}$

Structure Evolution

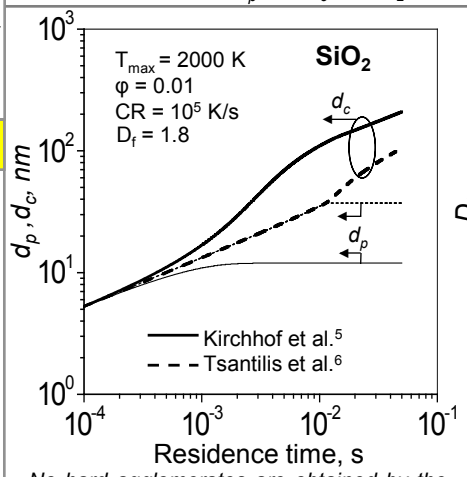


Evolution of D_f from mesoscale [2,3] and empirical [4] models.

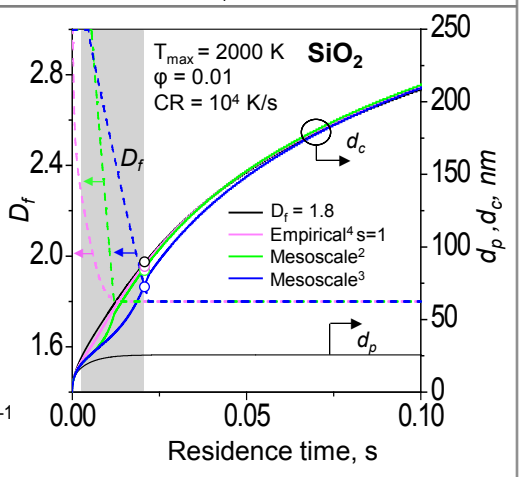
Primary Particle (d_p) & Agglomerate (d_c) Growth



Evolution of d_p and d_c of TiO_2 at constant and varying D_f from three models.

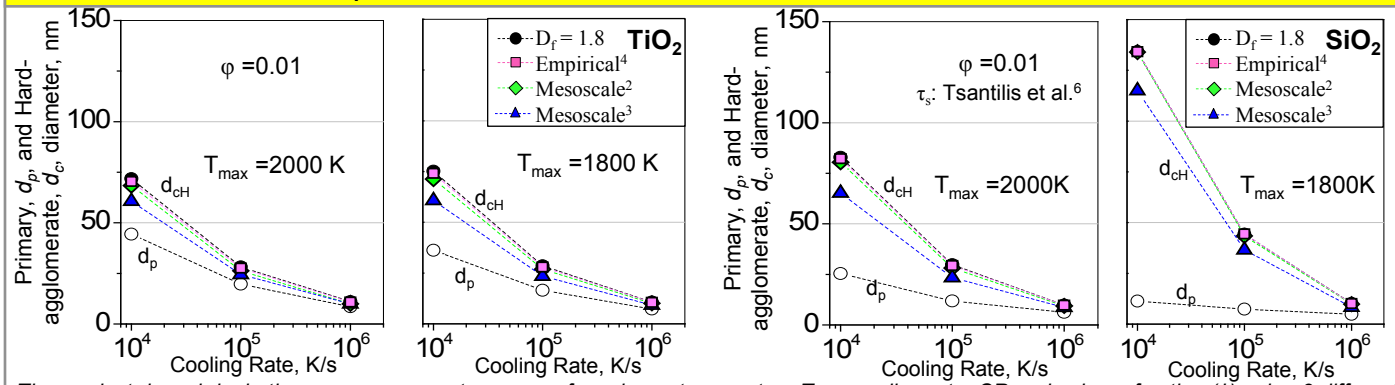


No hard agglomerates are obtained by the τ_s of Kirchhof et al.[5] for T_{max}=1800 – 2400 K, φ=0.001 – 0.1 and CR=10^4 – 10^6.



Evolution of SiO_2 d_p and d_c with varying and constant D_f using the τ_s of Tsantilis et al.[6]

Effect of Structure (D_f) Evolution Mode on Primary Particle & Hard-agglomerate Diameters



The product d_p and d_{cH} in the process parameter space of maximum temperature T_{max}, cooling rate, CR and volume fraction (ϕ) using 3 different models for the evolution of agglomerate D_f. The primary particle diameter is not affected by D_f.

References

[1] Buesser et al. (2011) *J. Phys. Chem. C* **115**, 11030.
[2] Eggersdorfer et al. (2012) *J. Aerosol Sci.* **46**, 7.
[3] Schmid et al. (2006) *Chem. Eng. Sci.* **61**, 293.
[4] Artelt et al. (2003) *J. Aerosol Sci.* **34**, 511.
[5] Kirchhof et al. (2012) *J. Aerosol Sci.* **45**, 26.
[6] Tsantilis et al. (2001) *Aerosol Sci. Tech.* **20**, 237.

Conclusions

- Varying D_f does not affect d_p and d_c even though it alters the transient evolution of d_c during the hard- to soft-agglomerate transition.
- The hard-agglomerate diameter, d_{cH}, from detailed structural models (accounting for variable D_f) deviates up to 25% for TiO_2 and 20% for SiO_2 compared to d_{cH} obtained at constant D_f =1.8. For all D_f models, this deviation decreases with increasing CR and T_{max} and even with precursor loading according to a mesoscale model[3].