

Calculation of dynamic properties of fractal aggregates in the transition regime.

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The dynamic properties of spherical particles depend on the relation between their primary particles size (R_1) and the gas mean free path (λ). In the transition regime, when R_1 is comparable to the gas mean free path λ , the friction coefficient can be calculated from the creeping-flow Stokes expression divided with a correction factor called Cunningham factor ($C(Kn)$).

$$f_N = \frac{6\pi\mu R_h(0)}{C(Kn)} = 6\pi\mu R_h(Kn). \quad (1)$$

where μ is the dynamic fluid viscosity, R_h the hydrodynamic radius, and Kn the Knudsen number ($Kn = \lambda/R_1$). The calculation of $C(Kn)$ can be done by the following empirical expression $C(Kn) = 1 + AKn$, where $A = \alpha + \beta \exp(-\gamma/Kn)$. The values of α, β, γ depend on the fraction of molecules diffusely reflected and the size of the monomers used to fit experimental data. While for a monomer the calculation of the Cunningham factor is trivial, for more complicated structures few results are reported in the literature. The reason is that in general the Knudsen number maybe defined in term of characteristic length scale L ; for a monomer $L = R_1$, while for a more complex structure it is difficult to specify it. Dahneke (1982) suggested the use of an adjusted sphere radius which has the same $C(Kn)$ as the non-spherical structure would have had. He provides values of Kn_a for straight chains with the fraction of molecules diffusely reflected 0.93. The calculation of Kn_a is very important as it allows the calculation of many parameters in the transition regime like the mobility radius (R_m), the dynamic shape factor (χ_N) and the effective density (ρ_{eff}).

Isella and Drossinos (2010) introduced an approximate method for friction coefficient calculations in the continuum regime, where it is related to the ratio of molecular collision rates of a N -particle structure (K_N) to a monomer's. In the continuum regime by solving a diffusion equation with the appropriate boundary conditions (Dirichlet boundary conditions) we can calculate the R_h and the f_N . We extend this method in the transition regime by solving the steady-state molecular diffusion equation with a Robin boundary condition. Far away from the aggregate we have $\rho = 1$ while on the aggregate surface $\rho(R_1) = \alpha(Kn)(d\rho/dr)|_{R_1}$. Our basic claim is that

$$C_1(Kn_a) = C_N(Kn) = \frac{f_N(0)}{f_N(Kn)} = \frac{K_N(0)}{K_N(Kn)}. \quad (2)$$

The factor α defines a virtual boundary inside a monomer in the transition regime where the collision rate equals the one in the continuum regime. Hence, from the analytical solution of the diffusion equation, we obtain $\alpha(Kn)/R_1 = C(Kn) - 1$. From the above $\alpha(Kn)$ depends only on the flow regime and the fraction of gas molecules diffusely reflected.

An alternative method that we used for the Kn_a calculation is the interpolation between the two limiting cases, the continuum regime ($Kn = 0$) and the free molecular regime ($Kn = \infty$). The calculation of Kn_a is done by (Zhang et al. 2012),

$$Kn_a = \frac{\lambda \pi R_m(0)}{PA} \quad (3)$$

where PA is the projected area of an aggregate. In the free molecular regime it equals the mobility radius squared times π .

We use both methods for the friction calculations in the transition regime. We validate the methods by calculating $C(Kn_a)$ of straight chains and by comparing them with the results of Dahneke. The good agreement suggests that both methods can be used for friction calculations of structures with $d_f \neq 1$ in the transition regime.

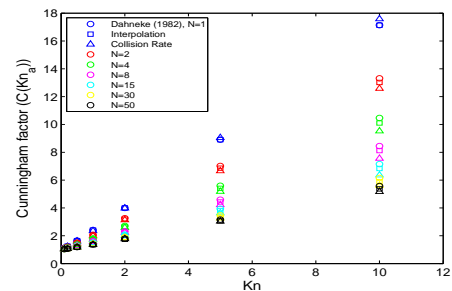


Figure 1: Comparison between $C(Kn_a)$ calculated by Dahneke and by our two different methods.

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B. Dahneke (1982), *Aerosol Sci. Technol.* **1**, 179.

L. Isella, Y. Drossinos (2011), *J. Colloid Interface Sci.* **356**, 505.

C. Zhang, T. Thajudeen, C. Larriba, T. E. Schwartzentruber, C. J. Hogan, *Aerosol Sci. Technol.* **46** (2012) 1065.