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A methodology to calculate the friction coefficient in the transition regime: Application to straight chains

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ABSTRACT

A methodology is introduced, the Collision Rate Method (CRM), to calculate the friction coefficient of power-law aggregates across the entire momentum-transfer regime. The friction coefficient is calculated via the ratio of two fictitious particle-aggregate collision rates evaluated in the continuum and slip-flow regimes. The effective collision rates are obtained from the numerical solution of the Laplace equation with Robin boundary condition. The methodology was justified by comparing the slip correction factor of straight-chains composed of up to 50 spherical monomers with literature results. We determined the validity of the CRM to lie in an extended slip-flow regime, the maximum monomer Knudsen number being 2. We calculated the adjusted-sphere radius, the radius of a sphere with the same slip correction factor as the chain, in slip flow. We found it to be weakly dependent on flow conditions, as specified by the carrier-gas mean free path, a dependence that leads to a weak effect on calculated slip correction factors. The CRM was combined with the Adjusted-Sphere Method to extend its validity to all Knudsen numbers. Excellent agreement of calculated, straight-chain, slip correction factors with literature values was obtained for monomer Knudsen numbers up to 100. Various characteristic length scales, geometric (equivalent volume radius, radius of gyration) and dynamic (equivalent hydrodynamic and mobility radii), were calculated.

1. Introduction

The drag force a fluid exerts on a particle influences its transport properties, being important in dynamical processes, such as particle sedimentation, respiratory deposition, agglomeration, and in industrial processes like combustion, filtration, gas-phase particle synthesis, performance of air cleaners (Friedlander, 2000). The drag force $\mathbf{F}_D$ and the friction coefficient f, defined by $\mathbf{F}_D = f\mathbf{v}_p$ where $\mathbf{v}_p$ is the particle velocity, depend on the nature of the fluid around the particle, and, consequently, on the mechanisms of momentum transfer between the particle and the carrier-gas molecules. These mechanisms are specified by the relative magnitude of the carrier-gas mean free path λ and a characteristic particle length

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scale L. Their ratio, the Knudsen number $\mathrm{Kn} = \lambda/L$, is the natural parameter to characterize the degree of rarefaction of a gas (Ivchenko, Loyalka, & Tompson, 2007).

Different Knudsen numbers specify different flow (or momentum transfer) regimes, as described, for example, in Crowe & Michaelides (2006). In the small Knudsen number limit, $\mathrm{Kn} < 0.001$, the fluid behaves as a continuum. In the slip-flow regime, $0.001 < \mathrm{Kn} < 0.25$, a velocity slip develops between the fluid velocity at the surface of the particle and the velocity on the side of the fluid closest to the surface. The fluid flow is considered to be transitional for $0.25 < \mathrm{Kn} < 10$. In the free molecular limit, $\mathrm{Kn} > 10$, the velocity distribution of fluid molecules is unaffected by the presence of the particle. Transfer processes for colloidal particles dispersed in a liquid are mainly in the continuum regime, while for spherical aerosol particles they may lie in any mass/momentum transfer regime.

The friction coefficient $f_N(\mathrm{Kn})$ of a power-law aggregate composed of N monomers over the entire (momentum-transfer) transition regime is usually expressed in terms of the empirical relation (Friedlander, 2000):

$$f_N(\mathrm{Kn}) \equiv \frac{f_N(0)}{C_N(\mathrm{Kn})}, \tag{1}$$

where $f_N(0)$ is the aggregate friction coefficient in the continuum regime, and $C_N(\mathrm{Kn})$ is the slip correction factor (hereafter referred to as the slip factor).

The slip factor is difficult to calculate for non-spherical structures. Instead, their mobility is usually analyzed via *virtual* spherical particles that have desired properties. Two such spheres are commonly used: the mobility equivalent sphere of radius R_m (see, for example, Rogak & Flagan, 1992), and the adjusted sphere of radius R_{adj} (Dahneke, 1973). In addition, the equivalent hydrodynamic sphere of radius R_h (Filippov, 2000) is occasionally used to describe aggregate mobility in near-continuum flows. The mapping of an aggregate to a virtual sphere of characteristic length (radius) L allows the use of the single-sphere slip factor $C_1(\mathrm{Kn}(L))$ to correct the continuum friction coefficient in the transition regime.

Dahneke (1973) introduced the adjusted-sphere method that allows the calculation of an aggregate's friction coefficient over the entire momentum transfer regime. The adjusted sphere is defined as a sphere of radius R_{adj} that has the same *slip* factor as the aggregate over the entire transition regime:

$$f_N(\mathrm{Kn}) \equiv \frac{f_N(0)}{C_1(\mathrm{Kn}_{\mathrm{adj}})}, \tag{2}$$

where the adjusted-sphere Knudsen number is $\mathrm{Kn}_{\mathrm{adj}} \equiv \lambda/R_{\mathrm{adj}}$. It is assumed to be constant, independent of the Knudsen number (i.e., independent of the flow regime as specified by λ), in contrast to the mobility radius. The adjusted-sphere model has been used in the analyses of numerous experiments (Cheng, Allen, Gallegos, Yeh, & Peterson, 1988; Rogak, Baltensperger, & Flagan, 1991; Shapiro et al., 2012; Thajudeen, Jeon, & Hogan, 2015) and in numerical simulations (Rogak & Flagan, 1992). More recently, Zhang, Thajudeen, Larriba, Schwartzentruber, and Hogan (2012) ascertained its validity via direct simulation Monte Carlo (DSMC). The direct simulation Monte Carlo method solves the Boltzmann equation at finite Knudsen number via stochastic simulations of virtual particles that represent groups of physical particles. As such, it provides accurate results for the friction coefficient of complex structures, despite its numerical complexity. They found excellent agreement of the mobility radii calculated via DSMC and via the adjusted-sphere method at varying Knudsen numbers. Thus, there is considerable evidence, both numerical and experimental, that the adjusted-sphere model provides accurate estimates of the friction coefficient of non-spherical objects in the transition regime.

The adjusted-sphere Knudsen number is constructed such that it gives the expected limits in the continuum and free molecular regimes. Its determination requires the calculation of the mobility radii in these two regimes. An accurate, but approximate, methodology to calculate the (orientationally averaged) continuum-regime mobility radius of arbitrarily shaped Brownian particles was proposed by Hubbard & Douglas (1993). They argued that it may be obtained from the solution of the Laplace equation. Independently, Isella & Drossinos (2011) used a heuristic argument, based on the collision rate of fictitious Brownian particles with a straight chain, to argue that the solution of the Laplace equation may be used to obtain their continuum-regime mobility radius. Gopalakrishnan, Thajudeen, and Hogan (2011) used the Langevin equation for point mass particles, an alternative way to solve the diffusion equation, to calculate the mobility radius. These analytical and numerical results, in addition to the previously mentioned experiments, suggest that the mass-transfer equivalent radius is approximately equal to the mobility radius in the continuum regime. In fact, Gopalakrishnan et al. (2011) referred to the mass-transfer radius in the continuum regime as the Smoluchowski radius, and the related approximation as the Hubbard–Douglas approximation.

In the free molecular limit, it is expected that the mobility radius be proportional to the square root of the orientationally averaged projected area of an aggregate (the probability of gas-aggregate collision being proportional to the projected area), see, for example, Sorensen (2011). Experimental measurements (Cai & Sorensen, 1994; Rogak, Flagan, & Nguen, 1993) and gas-molecule scattering calculations (Larriba & Hogan, 2013; Zhang et al., 2012) support this proportionality. The approximate equality of the mobility radius to the mass-transfer radius in the free molecular regime has been referred to as the projected-area approximation (Zhang et al., 2012).

The question our work addresses is whether the approximate equality of the mass-transfer radius to the mobility radius holds in the entire transition regime. To do so, we extend the continuum-regime methodology introduced by Isella & Drossinos (2011), a methodology used to calculate the hydrodynamic radius of power-law aggregates (Melas, Isella, Konstandopoulos, & Drossinos, 2014a), to the slip-flow regime. The methodology may be applied to calculate the friction