

Calculation of Aggregate Friction Coefficient from Active Surface

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The hydrodynamic behaviour of fractal-like soot aggregates suspended in a viscous fluid is of considerable importance for their transport and depositional properties. The calculation of the drag force on a fractal aggregate consisting of n primary spherules, henceforth called monomers, involves solving numerically Stokes equation for a low Reynolds number steady flow past the aggregate (Filippov, 2000). Analytical treatments usually require simplifying assumptions like aggregate spherical symmetry.

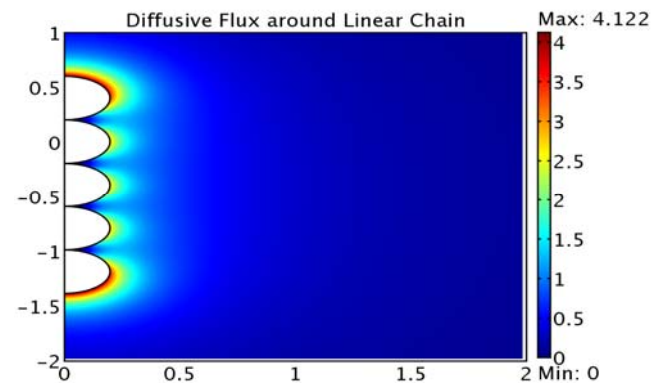
In this study we suggest an agile, albeit approximate, method to determine the aggregate friction coefficient β_n in the continuum regime relying on aggregate active surface A , defined as the fraction of aggregate geometrical surface available for gas absorption. Experimentally, A can be measured by evaluating the fluid-molecule-to-aggregate integral collision cross section.

Experimental findings (Siegmann & Siegmann, 2000) show that the product of aggregate mobility (inversely proportional to aggregate friction coefficient) times active surface is constant over a wide range of mobilities. This is not unexpected since the drag force (fixing aggregate mobility) felt by an aggregate in a viscous fluid is also due to collisions with the carrier flow.

The approach we follow tracks closely the experimental method. We solve the steady-state diffusion equation for fluid molecules surrounding the aggregate assuming molecule concentration $\rho = 0$ on aggregate geometrical surface (absorption of colliding molecules) and $\rho = \rho_\infty$ far away from aggregate surface. This amounts to neglecting the possibility of multiple scattering of fluid molecules by the aggregate. The calculated diffusive flux can then be integrated along the aggregate geometrical surface, to determine the overall fluid-molecule-to-aggregate collision rate, proportional to the active surface and hence to the aggregate friction coefficient. Though the proportionally constant is still unknown, one can take the ratio of the aggregate collision rate to n times the collision rate on an isolated monomer, where n is the number of monomers in the aggregate. This yields the ratio between the aggregate and the monomer friction coefficients. The method neglects that momentum transferred to the aggregate by the fluid is only approximately proportional to the number of collisions underwent by fluid molecules, since the velocities of molecules approaching the aggregate are

in general position-dependent, hence not all the collisions transfer the same momentum.

In order to test the goodness of the approximation, we calculated the friction coefficients of linear chains, for which there are theoretical and experimental results in literature. The simulations were performed in cylindrical coordinates with the finite element software Comsol Multiphysics. We calculated also the friction coefficients along the direction parallel and orthogonal to the symmetry axis, β_n^\uparrow and β_n^\rightarrow , by integrating on the aggregate surface the projected diffusive flux along the axial and radial direction, respectively.



The calculated friction coefficients for different values of n are in within a few percents from the findings illustrated in other studies, a few of which are reported in the table below.

	Filippov	Happel & Brenner	Diffusion
$\beta_2^\uparrow / \beta_1^\uparrow$		0.645	0.633
$\beta_2^\rightarrow / \beta_1^\rightarrow$		0.716	0.725
$\beta_8^\rightarrow / \beta_1^\rightarrow$	0.435		0.428

Although validated on linear chains, the method can be applied to aggregates of arbitrary shape. This means e.g. that whenever high-resolution images of an aggregate are available, it is possible to estimate its active area and friction coefficient, thus gaining valuable insight on aggregate catalytic activity and diffusional properties.

Filippov, A. V. (2000). *J. Colloid and Interface Science*, 229, 184-195.

Siegmann, K. & Siegmann, H.C. (2000). *Society of Automotive Engineers*, 2000-01-1995.

Happel, J. & Brenner, H. (1983). *Low Reynolds number hydrodynamics*. Dordrecht, Holland: Kluwer Academic Publishers.