On the relation between aerodynamic and mobility diameter distributions for aggregates consisting of few monomers

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Combined measurements of electrical-mobility-based (measured by Scanning Mobility Particle Sizer, SMPS) aerodynamic-diameter-based (measured and by Electrical Low Pressure Impactor, ELPI) distributions are typically employed to study the morphology of soot aggregates produced by diesel engines. This approach is used to calculate the aggregate's effective density, $\rho_{\rm eff}$ (Virtanen *et al.*, 2004). The effective density can be correlated to the particle morphology assuming specific morphology descriptors. For well-defined isotropic fractal aggregates the appropriate descriptor is the fractal dimension. In this way the size-dependence of the fractal dimension be estimated can (Konstandopoulos et al., 2004, Baltzopoulou et al., 2012).

In some cases, such as diesel soot and flame soot (Di Stasio *et al.*, 2002), the aggregates consist of a relatively small number of monomers or exhibit specific (non-random) anisotropic structures. In these cases the concept of effective density is under question and the exploitation of the aerodynamic and the mobility diameter distributions cannot be made without incorporating knowledge on the structure of the aggregates.

From a fundamental point of view, ELPI gives the aggregate distribution with respect to the variable f/m (where f is the friction factor and m is the particle mass). The mobility analyzer (SMPS) gives the distribution with respect to f. The inverse problem of determining the structure of the aggregates for these distributions is difficult to be solved. Therefore, the direct problem of determining the two distributions for given structures is evaluated. In particular, the cases of the well-defined structures (e.g. linear aggregates) and of oligomers (3-5mers) are studied.

For given distributions of these particles the mobility and aerodynamic radius distributions were constructed and compared. The mobility radius (R_m) in the continuum regime was calculated as suggested by Isella and Drossinos (2011) who related it to the molecule-aggregate collision rate. By calculating the steady-state molecular diffusive flux over the aggregate surface we determine the collision rate. This method is expanded to the transition regime by changing the boundary conditions. While in the continuum regime the fluid density on the surface is zero, in the transition regime it depends on a constant $\alpha(Kn)$ which depends on the Knudsen number. The aerodynamic radius is

related to the mobility via the effective density, $R_{ac}^2 = \rho_{eff} R_m^2 / \rho_o$, where ρ_o is the unit density (1g/cm³).

Figure 1 presents the mobility and the aerodynamic radii of trimers in the continuum regime against the trimer angle, a morphological descriptor of the spatial arrangement of the three monomers. The trimer angle (θ_{213}) is specified by two intersecting lines passing through the center of the central monomer (2) and the center of the two (1, 3) monomers pairwise touching it. These results combined with similar calculations in the transition regime provide a complete approach for the extraction of information on particle size and morphology.



Figure 1. The mobility (R_m) and the aerodynamic radius (R_{ae}) of 3-mers against the trimer angle in the continuum regime.

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