The role of the scaling-law prefactor in the morphology of fractal aggregates

A.D. Melas[1 2], A.G. Konstandopoulos[1 3], L. Isella[4] and Y. Drossinos[2]
[1]Department of Chemical Engineering, Aristotle University, 50006 Thessaloniki, Greece
[2]European Commission, Joint Research Centre, 21027 Ispra (VA), Italy
[3]Aerosol & Particle Technology Laboratory, CERTH/CPERI, P.O. Box 60361, 57001 Thessaloniki, Greece
[4]European Commission, DG Energy, 2530, Luxemburg
Keywords: fractal prefactor, shape anisotropy, fractal dimension.
Presenting author email: Anastasios.Melas@jrc.ec.europa.eu

Fractal-like aggregates created via agglomeration (aerosols) or flocculation (colloids), obey a scaling law, $N = k(R/R_1)^{d_f}$ where N is the number of primary particles, R_1 the primary particle radius, and d_f the fractal dimension. The factor R is a characteristic length scale which can be either the radius of gyration (R_g), or the geometric radius (R_{geo}) which is the radius of the largest sphere encompassing the cluster centered at its center of mass, or the maximum distance in a fractal aggregate (L). A generalized prefactor corresponds to each characteristic length scale: these prefactors are the fractal prefactor (k_f), the inverse of the filling factor ($1/f$) and the packing fraction (ϕ) respectively. The physical meaning of these prefactors and more specifically the importance of k_f has been stressed recently (Wu and Friedlander, 1993). In this study, we relate large and small-scale structure properties to N, d_f and k_f changes.

For the needs of our study we created fractal aggregates with a mimic cluster-cluster algorithm (Filippov et al., 2000). The use of this algorithm gives us the advantage to create very fast fractal aggregates that have precisely prescribed number of primary particles, fractal dimension and fractal prefactor. We study the effect of N, d_f and k_f on shape anisotropy (A_{13}), mean angles (θ_{ijk}) and average number of near neighbors (c_N). Anisotropy is a large-scale indicator, a measure of the cluster stringiness. It is calculated from the principal radii of gyration R_i ($i = 1,2,3$) by diagonalizing the aggregate's inertial tensor. An indicator of a cluster's small-scale structure is the probability distribution of the angles formed by three monomers. The angles are specified by two intersecting lines passing through a central monomer i and two (j,k) monomers pairwise touching it. For every monomer i we calculated the number of its neighbors k, to which we associated $k(k-1)/2$ angles (possible pairwise combinations). In Fig. 1 we present distributions of angles for different N, d_f and k_f.

An alternative indicator of local compactness is the mean number of nearest neighbors, or coordination number, defined as the average number of contacts of a particle in a fractal aggregate. The synthetic fractals analyzed herein have coordination number close to 2, a consequence of our algorithm that requires that two clusters have only one sticking point. Since the coordination number is approximately constant we calculated the average number of near neighbors (c_N) at a fixed distance $5R_1/2$. The parameter choices are summarized in Table 1. The results are averaged over 5000 fractal aggregates.

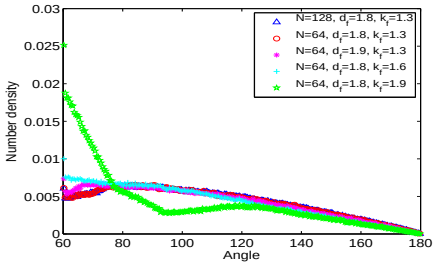

Figure 1: Ensemble-averaged probability distributions of three-monomer cluster angles.

Table 1: Mean characteristic structural parameters: shape anisotropy $< A_{13} >$, three-monomer angle $< \theta_{ijk} >$, and number of neighbors c_N.

	N	(d_f, k_f)	R_g/R_1	$\langle A_{13} \rangle$	$\langle \theta_{ijk} \rangle$	c_N
1	128	(1.8, 1.3)	12.8	3.78	105.8	2.63
2	64	(1.8, 1.3)	8.7	3.76	105.6	2.60
3	64	(1.9, 1.3)	7.8	3.30	104.0	2.73
4	64	(1.8, 1.6)	7.8	3.61	101.1	2.96

The effect of d_f is shown by comparison of rows 2 and 3, whereas k_f from the rows 2 and 4. These effects may be considered comparable as clusters (1.9, 1.3), row 3, and (1.8, 1.6), row 4, have the same radius of gyration. These comparisons indicate that changes of d_f produce larger changes of A_{13}, and a change of k_f large changes in the mean three-monomer angles and c_N. Hence, in general, the fractal dimension is an indicator of the overall aggregate's shape (large-scale aggregate morphology), while the prefactor becomes an indicator of local structure (small-scale morphology).

This work was supported by a European Commission Doctoral Fellowship (ADM).

M. Wu, S.K. Friedlander, J. Colloid Int. Sci. 159 (1993) 246.

A.V. Filippov, M. Zurita, D.E. Rosner, J. Colloid Interface Sci. 229 (2000) 261.