Fractal-like aggregates created via agglomeration (aerosols) or flocculation (colloids), obey a scaling law, $N = k(R/R_1)^{df}$ where $N$ is the number of primary particles, $R_1$ the primary particle radius, and $df$ 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 ($\phi$) 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 $N$, $df$, 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 $N$, $df$, and $k_f$ on shape anisotropy ($A_{13}$), mean angles ($\theta_{ijk}$) 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 $N$, $df$ 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.](image)

The effect of $df$ 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 $df$ 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).

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