Study on the fractal structure of carbon nanomaterials’ smokescreen

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Abstract. In the diffusion of carbon nanomaterials’ smokescreen, the condensates generated by the collision of particles have fractal structures. In order to research this process, this paper is based on DLA condensation model programmed by MATLAB. Using DLA model, the geometrical structure of agglomerate formed by spherical nanoparticles is simulated and the fractal dimensions of agglomerates were computed by using the cyclotron radius method. Large numbers of simulations indicated the fractal dimension of agglomerates on two-dimensional plane distributed between 1.4 and 1.7. And with the increasing number of the particles, the fractal dimension displayed in intensive range. The research in this paper has laid a foundation for the study of the aerodynamic characteristics of condensed particles in the next stage.

1. Introduction

In the diffusion of carbon nanomaterials’ smokescreen, particles are condensed into larger particles through continuous collisions. This aggregation process and the formation of non-spherical structure have an important impact on aerodynamic characteristics. Previous experiments and researches showed that the aggregates produced by particle aggregation process have fractal structure. The fractal properties of the structure react on the aggregation in the next step, which is usually called the fractal aggregation process. Fractal dimension is an important parameter to characterize fractal features. Fractal graphs and their dimensions are often quite different under different growth conditions. Fractal particles floating in the air, even particles with the same volume, will suffer different viscous resistance if their fractal dimension is different. In other words, the viscous resistance of particles in the process of falling is related to the fractal structure. Based on this, this paper studies the fractal shape of particles formed by the collision condensation of tiny spherical particles in the smokescreen diffusion process through numerical simulation, and calculates its fractal dimension. This paper lays a foundation for the further study of its aerodynamic characteristics.

2. Fractal structure and fractal dimension

Fractal was proposed by B. B. Mandelbrot in 1975 [1,2]. The original meaning of fractal refers to the concept of "extremely irregular" and "fragmented" objects. As a geometric object, fractal is firstly broken and irregular. But not all broken and irregular shapes are fractals as fractals generally have self-similarity. The complex morphology of condensates can be described by fractal dimension. Fractal dimension is an important parameter to describe fractal features. In addition, the fractal dimension of particles affects their dynamic behavior, which can be inferred according to the fractal dimension.
Due to the complexity of fractal sets, there are many definitions of fractal dimension. The most representative one is Hausdorff dimension, which was defined by Felix Hausdorff, a mathematician at the University of Bonn, in 1919 from the perspective of measure. He believed that the dimension of space could be continuous, which could be an integer or a fraction. We call this dimension Hausdorff dimension, or fractal dimension. For a geometric body with a definite dimension, if it is measured with a "ruler" lower than its dimension, the result will be infinite; if it is measured with a "ruler" higher than its dimension, the result will be zero; if it is measured with a "ruler" of the same dimension, the value will be determined. Then Hausdorff dimension is defined as [3]:

$$D_f = \lim_{\eta \to 0} \frac{\ln N(\delta)}{\ln(1/\delta)}$$  \hspace{1cm} (1)$$

Hausdorff dimension can be an integer or a fraction. The fractal shapes and dimensions under different growth conditions are often quite different. Air floating fractal particles, even particles with the same volume, will suffer different viscous resistance if their morphological complexity is different.

3. The fractal structure of condensed particles

3.1. Simulation of condensed particle structure

The simulation of agglomerate growth process must involve the dynamic growth model of agglomerate fractal structure. The gradual maturity of fractal theory provides theoretical support for the study of the kinetic properties of condensed particles. According to the theoretical model, the aggregation process and fractal structure can be simulated by computer. While these models are far from perfect compared to real processes and structures, and can only be viewed as simplified, extreme cases, they are nevertheless an effective way to understand real processes and structures. With the development of the research on the fractal growth process, various dynamic growth models are proposed, which can be divided into those categories: diffusion limited aggregation [4] (DLA), ballistic aggregation (BA)[5], and reaction limited aggregation (RLA), CCA[6,7]. Each kind of model is divided into monomer agglomeration and group agglomeration.

The condensation model is a monomer condensation model based on random fractals appearing in the growth process. It was proposed by Witten and Sander in 1981. According to this model, a disordered, irreversible growth process can produce a special fractal dimension shape. The model is simulated on a computer and its generation process is: A particle (called a seed) is placed at the center of a two-dimensional lattice, and then a particle is introduced at the edge of the lattice, and let it walk randomly on the two-dimensional lattice. When the particle travels to the center of the lattice, it will combine with the seed at the center point and then stop moving. Or if the particle gets to the edge of the lattice, it will disappear. In either case, once the wandering particle is lost, a new wandering particle needs to be introduced from the edge of the lattice. When the new particle moves upstream of the lattice, the above two situations will occur: go to the center of the lattice and combine with the stationary particles, or go to the edge of the lattice and disappear, and then introduce a new particle from the edge. With this constant introduction of particles from the edges, a coherent group of particles will gradually appear in the center of the lattice. Since the new particle diffuses to the condensate through random walk before polymerization, the amplitude and direction of each step are random in the process of random walk, which is the origin of the name of diffusion finite condensation model. In the three-dimensional Euclidean space, the fractal dimension of the condensate is less than that of the Euclidean space. This is because the trajectory of the randomly moving particles is tortuous, and the probability of particle condensation is larger at the forked tip end extending outside the group. The particles are not easy to penetrate the deep part of the group and have a shielding effect, so they form a more open fractal structure.
3.2. Simulation of the shape of carbon nanoparticles aggregates

Comparatively, DLA condensation model is easy to simulate and calculate. The simple kinematics and dynamics equations can generate self-similar fractal structures and become one of the most important growth models. DLA models can be used to describe urban sprawl, electrolytic deposition, dendritic crystal growth, metal particle aggregation, aerosol aggregation, etc. In view of this, DLA model was used to simulate the complex fractal structure of nanoaggregates in two-dimensional space. The original particle was taken as a sphere, and the geometric structure of the condensate formed by 49 original particles was simulated through MATLAB programming. Several typical simulation results are shown in Figure 1.

![Figure 1. Several structures of the condensate with N=49.](image)

4. The fractal dimension of condensed particles

4.1. Fractal dimension calculation of condensed particles

For the condensates obtained by the DLA model, the fractal dimension of the condensates is calculated by the radius method. The method is based on the following analysis and calculation: one-dimensional chain condensed particles composed of monomer particles with radius $R_0$. In the chain with length $L=2R$, the number of monomers is: $N=(R/R_0)^1$. For two-dimensional plane condensation, the number of monomer is: $N=\rho (R/R_0)^2, \rho = \pi / 2\sqrt{3}$ is the surface of the accumulation of ball density. Therefore, the relation between the number $N$ of the condensed particle system and the minimum sphere radius (radius of gyration) $R_g$ surrounding the condensate can be expressed in the following general form:

$$N \sim R_g^{D_f}$$

(2)

Where $D_f$ is the fractal dimension of condensed particles.

If each particle in the system is assumed to have the same mass, the formula for calculating the cyclotron radius is:

$$R_g^2 = \frac{1}{N} \sum_{i=1}^{N} r_i^2$$

(3)

Where $r_i$ is the distance from the center of the sphere of monomer $i$ to the center of the system.
Plotting the relation curve of \( \ln N - \ln R_g \) and find the slope to get the value of \( D_f \). The relationship curve and fractal dimension obtained through calculation for several structures shown in Figure 1 are shown in Figure 2.

![Figure 2](image)

**Figure 2.** The fractal dimension calculation curve and dimension of condensed particles.

4.2. Fractal dimension statistics of condensates

In the case of using the average field, M. Muthukumar[8] theoretically derived the expression of fractal dimension:

\[
D_f = \frac{d^2 + 1}{d^2 - 1}
\]  

(4)

Where \( D_f \) is the fractal dimension of the condensed particle, \( d \) is the Euclidean dimension.

Under the condition of using the average field, Hentschel[9] also derived another expression of fractal dimension through some assumptions:

\[
D_f = \frac{8 + 5d^2}{6 + 5d}
\]  

(5)

In the two-dimensional plane, the fractal dimension of the condensates calculated by the expression of M. Muthukumar and the expression of Hentschel were 1.67 and 1.75, respectively. According to a large number of simulation statistics, the fractal dimension of non-spherical particles condensed from 49 small particles is mainly distributed between 1.4 and 1.7. The reason for the wide distribution is that the number of particles forming aggregates is small. If the number of condensed particles is increased, the fractal dimension is concentrated in a small range. For example, the fractal dimension of
the condensate formed by 1000 small particles is distributed between 1.64 and 1.76. Figure 3 shows the condensate formed by 1000 small particles, and the fractal dimension is 1.6836.

Figure 3. A fractal structure composed of 1000 small particles.

5. Conclusions
In this paper, the shape of the condensate formed by particles is simulated on a two-dimensional plane with a DLA model, and the fractal dimension of the condensate is calculated. A large number of simulations show that the fractal dimensions of the condensates on a two-dimensional plane are distributed between 1.4 and 1.7. And the more particles form the aggregates, the more concentrated the fractal dimension distribution is. The viscous resistance of particles in the process of falling is related to the fractal structure. Moreover, particles with fractal structure will be subject to greater resistance than spherical particles of the same volume. As smokescreen particles, this property will help keep them suspended in the air.

References
[1] Mandelbrot B B 1979 Fractals: Form, chance and dimension[J] San Francisco (CA, USA): WH Freeman & Co.
[2] Mandelbrot B B 1982 The Fractal Geometry of Nature[M] New York: WH freeman
[3] Mattila P 2015 Fourier Analysis and Hausdorff Dimension[M] Cambridge University Press
[4] Witten Jr T A, Sander L M 1981 Diffusion-limited aggregation, a kinetic critical phenomenon[J] Physical review letters 47(19) 1400
[5] Brilliantov N V, Bodrova A S, Krapivsky P L. A model of ballistic aggregation and fragmentation[J]. Journal of Statistical Mechanics: Theory and Experiment, 2009, 2009(6): P06011
[6] Meakin P 1983 Formation of fractal clusters and networks by irreversible diffusion-limited aggregation[J] Physical Review Letters 51(13) 1119
[7] Kolb M, Botet R, Jullien R 1983 Scaling of kinetically growing clusters[J] Physical Review Letters 51(13) 1123
[8] Muthukumar M 1983 Mean-field theory for diffusion-limited cluster formation [J] Phys. Rev. Leve. Let. 14 839–842
[9] Hentschel H G E 1984 Fractal dimension of diffusion-limited aggregates [J] Phys. Rev. Leve. Let.
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