Dealing with the Computer Simulation Models on Dynamic Growth

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Abstract

Particle aggregation and growth have drawn immense attention in recent years for a various reasons, for example aerosol pollution, dust protection. Various experiments and simulations are used to model its dynamic process and aggregation/growth mechanism, but these studies mostly limited in the certain particle type and cannot describe the multi-type particle coexistence system. In the general atmosphere/water pollution, the inter-aggregation between different type particles widely occurs in this coexistence system. Based on this viewpoint, this paper developed the traditional models to simulate this phenomenon by adding the type constraint and used the fractal dimension to describe the aggregation structure. The simulation results shows that type constraint has less influence on the aggregation structure and its fractal dimension in the coexistence system. This can be explained that type constraint can be seen as the stickiness possibility.
Keyword: Particle aggregation growth, DLA, RLA, Stickiness possibility

1. Introduction

In recent years, there have been significant advances in our understanding of the process of particle aggregation and growth. Many studies of this area, including experiments and theory, have been used to investigate the aggregation/growth process [1, 2]. Although the reasons for aggregation/growth are complex and vary from one system to another due to different physical or chemical origins, it is now generally accepted that there are two limiting regimes of aggregation/growth: 1) diffusion limited aggregation (DLA), in which every collision between particles leads to the formation of a permanent aggregation structure, and 2) reaction limited aggregation (RLA), in which only a small fraction of particle collisions leads to the formation of an aggregation structure. A fast aggregation process, in which particles stick to each other upon aggregation as a result of diffusion, results in a loosen, ramified structure. On the other hand, a slow aggregation process, in which more than one collision is required for particles to form permanent aggregations, yields a more dense structure. Although these two models are similar in essential, the morphologies of the aggregation growth are different and lead to the different scaling behavior (Fractal dimension). The difference of these two models is given in detailed in this study. Based on the results of these two models, a new model is developed to solve the aggregation growth of many kinds of particles. Generally speaking, in the water or atmosphere environmental system, it is rather common that many kinds of particles are to aggregate and growth. The aggregation mechanism in this coexistence system may be more complex than one of single-type system because of various physical and chemical reasons. There have so far been few studies on the aggregation dynamics in this coexistence system. The objective of this paper is to study its aggregation growth behavior. The highly disordered structure of particle aggregation and growth is quantitatively characterized by fractal dimension.

2 Simulation of Particle Aggregation Growth

2.1 Methodology

The particle random walk is applied in this paper. The aggregation structure is analyzed by fractal method. There exist various definitions of fractal dimension. Here, we applied the box counting method, which is the most straightforward method at present, to calculate the scaling behavior of aggregation structure [3]. In this study, box dimension was determined by counting the number (N) of particles around the center particle, as a function of distance away from the seed particle. The concrete formula is obtained below:

$$N(s) \propto s^{D} \quad (1)$$

where s is distance away from the seed particle and D is fractal dimension. Then the fractal dimension can be obtained:

$$D = \frac{\lg(N(s))}{\lg(s)} + k \quad (2)$$

where k is a constant.

Fractal dimension is determined by the least square fitting as Eqn. (2) in the simulation program.

2, Simulation Detail

A two dimensional squared lattice, L by L with L^2 sites, is set to model the region of particle aggregation growth. In the simulation images, one pixel is behaved of one particle. Starting with a single particle, we fix this particle at the center of the squared lattice as the stationary seed particle. A second moving particle is 'created' in a random position where not particle sites at some distance from the stationary seed particle. There are eight sites encircle this particle, marked from 1 to 8 (shown in the Fig.1). Then the particle will judge whether there are particles encircle it. If yes, this particle will immobilize instantly and stick with that particle to become part of the growing aggregate; if not, it will perform the random walk (Brownian motion). It can walk pass only one pixel grid on each step of walking. For example, in each step, this particle can only walk to one of the eight sites randomly. After each step of walking, this particle will judge whether there are particles encircle it. If yes, this particle will immobilize instantly and become part of the growing aggregate; if not, it will go on the random walking until it reaches a grid adjacent the growing aggregate. In the particle random walking course, if the particle walks out of the squared lattice, it will escape and disappear. A third moving particle is then generated like the second particle and allows wandering randomly. The particle will stick it finds itself adjacent to any stuck particles. The procedure is repeated many times until all the particles complete the whole process. This is a schematic description of DLA process. Similar to DLA, the stickiness possibility between particles, which can be regarded as the energy barrier between particles, is only introduced.

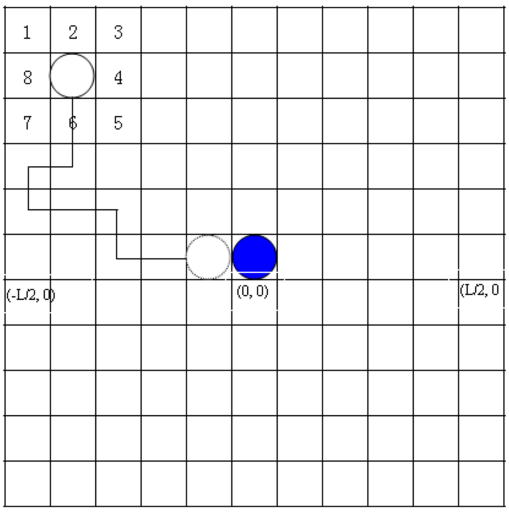

Fig.1 Schematic Description of DLA

Based on the diffusion limited aggregation, the Multi-types DLA model with a 'type' constraint is developed. This type constraint is used to control the growth of the aggregation structure. For example, the aggregation between the same-type particles is not allowed. The two approaching particles will aggregate together once they collide if they satisfy this type constraint. Otherwise, the collision cannot lead to aggregate.

The type of the seed particle is generated randomly and fixed on the center of the simulation lattice. Each released particle is generated with the random position and type in the simulation program. In this study, the particle type is randomly selected with uniform distribution. This uniform distribution represents that the concentration fractions of various type particles are the same. In fact, this uniform distribution can be modified as the practical condition in the natural or industrial systems.

Multi-types RLA model with stickiness possibility is also developed.

The simulation programs are executed in the Matlab 7.1. Because the particle is randomly released in the simulation program, we investigated the influence of simulation times on the fractal dimension of the aggregation structure. Fig.2 shows that simulation times has less influence on fractal dimension. Hence, all simulation programs are executed for 15 times to obtain the average the fractal dimension.

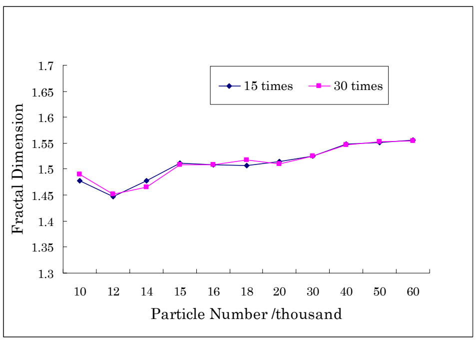

Fig 2 Relationship between simulation times and fractal dimension

3 Results and Discussion

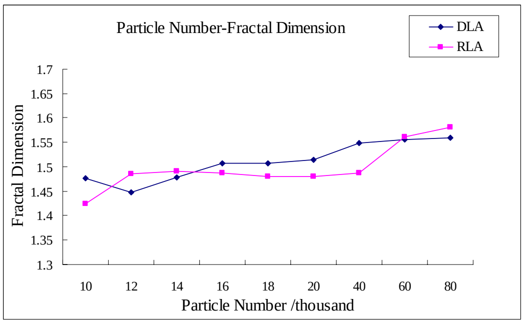

Fig.3 Fractal dimensions of DLA and RLA changes with the total released particle number (the stickiness possibility is 0.5)

Fig. 3 shows that fractal dimensions have no obvious difference between DLA and RLA. Hence, we tried to compare the total number of the aggregation structure between them and found that the particle number of RLA aggregation structure is much more than DLA one at the same distance away from the seed particle. This seems to present that the total number of released particles is not enough to eliminate the random effect.

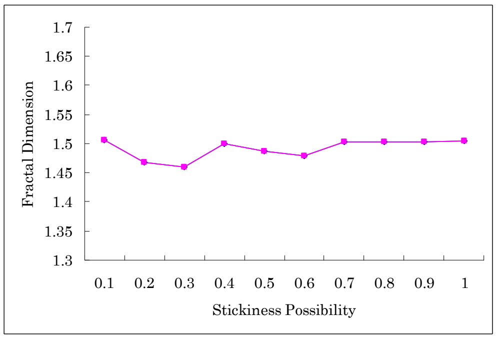

Fig.4 Fractal dimension change with stickiness possibility in the RLA process (20,000 released particles)

From Fig.4, fractal dimension of RLA aggregation structure has somewhat change with increasing the stickiness possibility. The bigger stickiness possibility leads to the bigger fractal dimension. If the stickiness possibility is equal to one, RLA will change to DLA. From this aspect, the aggregation structure will become more and more ramified and open with the stickiness possibility increasing.

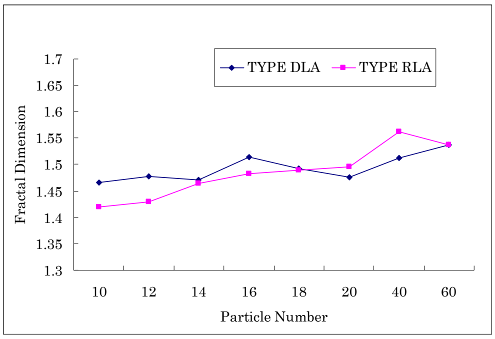

Fig.5 Fractal dimensions of TYPE DLA and TYPE RLA changes with the total released particle number (0.5 stickiness possibility and 5 particle types)

The values of fractal dimension between two curves change irregularly and do not approach to stable value. Hence, all the fractal dimension values in Fig.5 are summed to obtain the average value. The average values of fractal dimension are 1.4933 and 1.5263 for TYPE DLA and TYPE RLA respectively.

Compared Fig.3 and Fig.5, we found that fractal dimensions are the same for TYPE DLA and RLA and have somewhat difference between TYPE RLA and DLA. This result can be well explained as the simulation conditions. Type constraint can be seen as the stickiness possibility. The TYPE DLA with the high stickiness possibility is similar to RLA with the low stickiness possibility. Hence, their fractal dimension values have little difference.

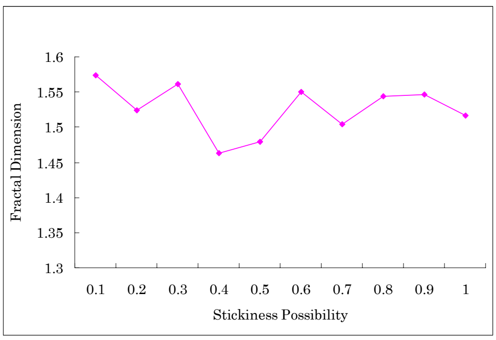

Fig.6 Relationship between the stickiness possibility and fractal dimension in the Type RLA model

Compared Fig.6 and Fig.4, fractal dimension of TYPE-RLA is shifted bigger around 1.5, and it is almost stable in the RLA case.

Conclusion

Various models of particle aggregation growth are simulated in this study. The simulation results indicated that the fractal dimension of DLA is similar to RLA one, but the particle number in the aggregation structures has the big difference. This seems to present that the total number of released particles is not enough to eliminate the random effect. This phenomenon will be investigated in future work. For multiply-Type DLA and RLA, the simulation results indicated that type constraint has less influence on the fractal dimension of aggregation structure. It can be explained that type constraint can be seen as the stickiness possibility.

This approach to deal with models seems to be too simple to simulate the complex physical or chemical interactions in the aggregation/growth process, but practical enough to get essential features of the aggregation and dynamic growth process as the first step. Future developments on these models will consider these factors with fine granularities of physicochemical mechanisms and larger systems to get an insight on the scalability.

Reference

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