The growth simulation of diffusion limited aggregation floc and its characterization of fractal structure

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Abstract. Basing on analyzing the principle of real coagulation reaction and studying the mechanism of growth of flocculation, to write programs of DLA (short for "Diffusion-Limited Aggregation") model in the MATLAB platform, and using high-performance computer to display processes of the Brownian motion, collision and coagulation of particles visually, thus obtaining fractal simulated flocculation. In addition, introducing fractal dimension and porosity to characterize morphological structure of flocculation, and quantitatively studied the effects of DLA model main parameters on microstructure of flocculation through method of statistical analysis, that is to impact on values of fractal dimension and porosity specifically, the differences of forming mechanism and fractal structural characteristics of two dimensional and three dimensional simulated flocculation was also discussed to supplement some theory research for problems of observing and analyzing real three dimensional flocculation, which were still can't be solved so far.

1. Introduction

Coagulation reaction is complex process with microscopic motion characteristics, diffuse in the fluid solid suspended particles and colloidal particles constantly for the spread of the random movement, which under the action of coagulant, particle surface and internal chemical reaction happens, and by the coagulation mechanism of the existing research known particles near each other or collide between condensed into flocculation body with different spatial form, dense degree of flocculation body are controlled the sedimentation performance, thus determines the final water treatment effect [1]. In many past coagulation studies, mainly on the merits of coagulation final removal from wastewater each index, which can only begin to study the complexity of the entire process from a macroscopic coagulation reaction results ,in recent years, people have tried the coagulation reaction was studied from the new way, through a detailed study by means of the advanced computer simulation technology, in the process of coagulation on the basis of the fractal theory [2], the computer simulation technology for the tool, establish the corresponding flocculation body growth model, not only the coagulation reaction process of chaos can be presented in the form of visualization, but also can study from the Angle of the micro flocculation body space form structure, establishment of diffusion-limited agglomeration model (DLA) model for people with new ideas and methods for further research of flocculation morphology problem [3] ~ [7], through the observation of the formation process of flocculation body and its microscopic quantitative analysis of the fractal structure of for practical factors in the coagulation control, improve the coagulation effect and provide effective research on the basis of rapid solid-liquid separation.

2. Test equipment and methods

A. The primary equipment and software

1)DELL desktop computer

2)MATLAB software

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B. Experimental methods

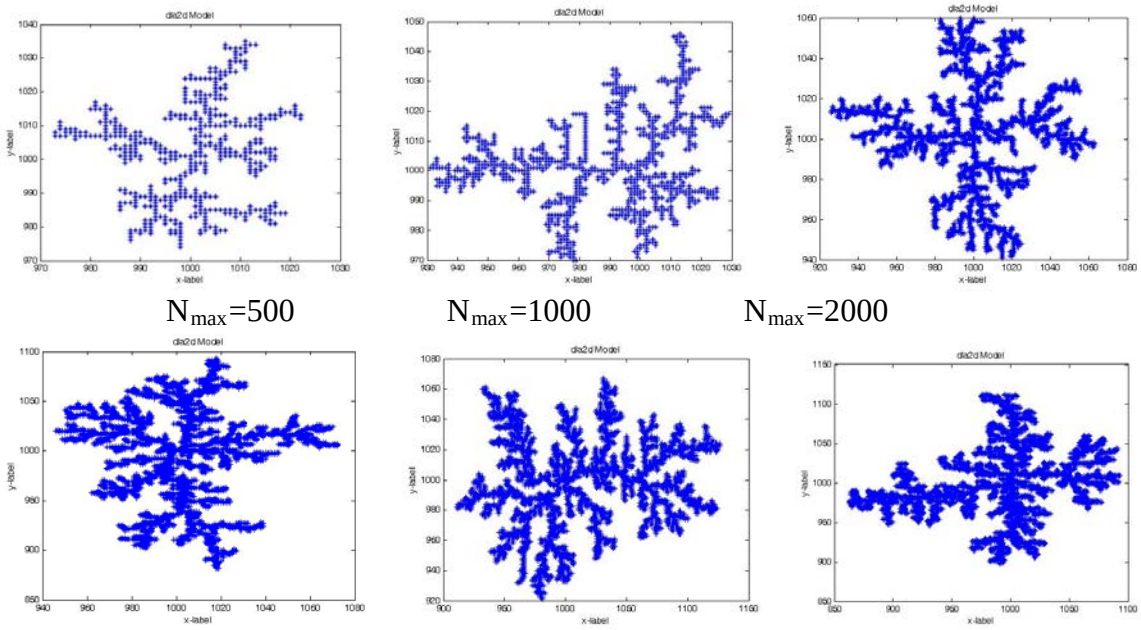
Based on MATLAB platform to build 2 d and 3 d DLA model, and write the corresponding program, with the help of computer simulation of swim out of the spread of the particles and the condensation process and get the final flocculation body, in the form of programming and the radius of gyration method to calculate the flocculation body of fractal dimension, porosity calculation formula to calculate the flocculation body of porosity, and statistical analysis of fractal dimension of important parameters in the model, the quantitative influence of the size of the porosity.

3. DLA simulation results

A.2d DLA simulation results

Flocculation body generated by moving particles gradually attached, the total number of particles directly affects the flocculation "size" of the body, the total number of particles respectively 500, 1000, 2000, 1000, 4000, 5000, the simulation results are shown in Fig.1.

It is easy to find the flocculation body branch, branch structure is obvious. At the same time, also found that the flocculation body shape is different, but also has a certain phase is like sex, namely has obvious geometric center, comparing the flocculation of the total number of particles is obvious, with the increase of the total number of particles make flocculation body "physique" gradually increases.



N_{max}=500 N_{max}=1000 N_{max}=2000

N_{max}=3000 N_{max}=4000 N_{max}=5000

Fig.1 Different particle flocculation body figure of the total

The total number of particles and the relationship between the fractal dimension

To statistic the total number of particles and the relationship between the fractal dimension, conducted from 500 to 19000 different particle simulation test of the total, the total number of each particle simulation eight times, select eight fractal dimension values of intermediate value, statistical results as shown in Fig.2.

As can be seen from the statistical results in Fig.2, the fractal dimension of statistics on the local not strictly obey a rule, which show some random features, but as you can see on the whole it with the total number of particles and the change of a downward trend.

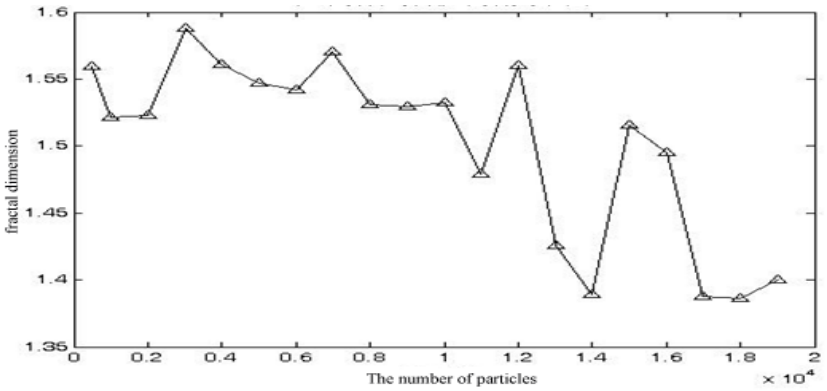
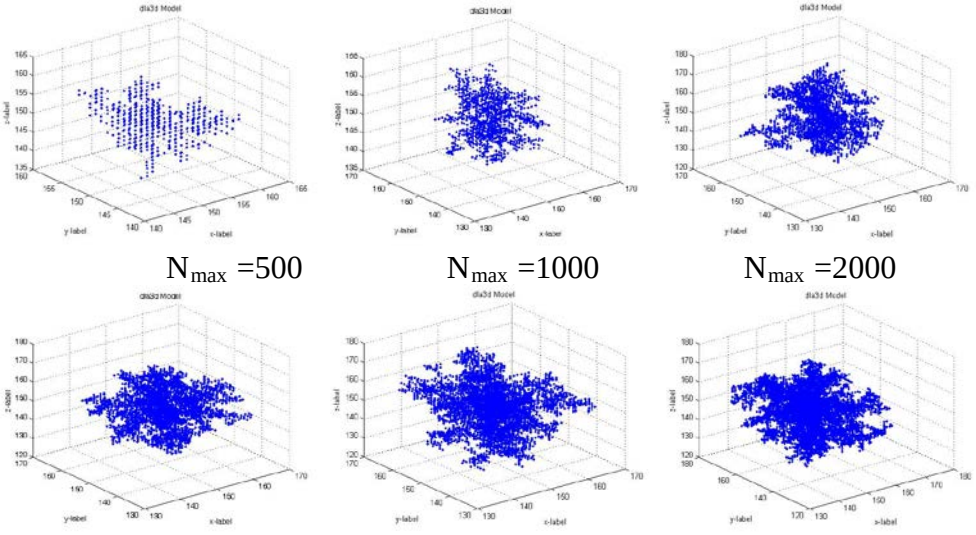


Fig.2 Two dimensional DLA fractal dimension and the relationship between the total number of particles

B.3d DLA simulation results

Total number of particles respectively 500, 1000, 2000, 3000, 4000, 5000, the three dimensional DLA simulation result is shown in Fig.3.

The three-dimensional structure of DLA floc Fig.4 shows the dense at its center and has larger particles fill rate, and gradually grow from the inside out, open branches fork height, overall floc fractal structure very clear comparison of different particle the total number of floc particles found that as the total increase in floc size increased along with the longer "branches" and more irregular tentacles, then increasing the porosity, in addition to the series floc have a distinct geometric center.



N_{max} =500 N_{max} =1000 N_{max} =2000

N_{max} =3000 N_{max} =4000 N_{max} =5000

Fig.3 The simulation results of the total number of different particles

The total number of particles and the relationship between the fractal dimension

For the relationship between the total number of particles and the fractal dimension D statistics between DLA floc, make the total number 500-10000 different particle simulation, statistical results obtained in Fig.4.

Fig.4 shows that when the total number of particles of less than about 4000, the fractal dimension was significantly increased with the total number of particles increases, and the total number of particles in 4000, the fractal dimension is greater than 1.96, continue to increase the total number of particles to 10,000, the fractal dimension was at 1.96 fluctuations in the vicinity, did not continue to increase in the overall signs may be due when the total number of particles reaches a

certain value outside floc fractal structure has basically reached the maximum, detailed enough branches fork has been very difficult to significantly thinner.

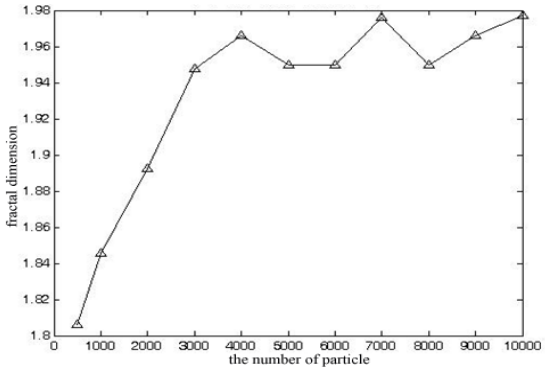


Fig.4 3D DLA fractal dimension and the total number of particles

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