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修士論文

Dealing with Computer Simulation Models on Dynamic Growth

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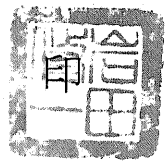

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Dealing with Computer Simulation Models on Dynamic Growth

by

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Thesis submitted to Human Environmental Studies,

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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 the 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, Fractal, Fractal Dimension

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Chapter 1

Introduction

Particle aggregating growth process plays the important role in the natural environmental systems, scientific and engineering fields, such as coatings, electronic inks, photonic crystals, drug delivery, and biosensors, polymer polymerization, secondary oil recovery, etc.

In the past decades, a large number of simulation models and experiments have been devoted to understand the dynamic growth of the aggregate structure and the aggregation mechanism. In this chapter, we will introduce the importance of particle aggregation, some main models and the objective of this research.

1.1 Importance of Particle Aggregation Growth

Particle aggregation processes have long been observed and used in many areas of both natural and engineered systems. This aggregation process is particularly widely seen in applications related to chemical, electrical and environmental engineering. For example, it is a common process used in water and wastewater treatment plants [1]. Particles found in water come from many different sources, and the sizes of these particles range from submicron to more than 1 cm for some oceanic aggregates (Jackson and Lochmann, 1933) [2]. Several mechanisms cause these particles to constantly collide with each other and form aggregates. Not only do they influence the rheological properties of suspensions, but they play important roles in handlings of solid particle such as the liquid–solid separation, the coating of particles on a surface and the formation of the crystalline assemblies. It also affects the behavior of particles in natural systems. The prediction and the control of aggregate size in fluid having various static

and dynamic properties are required for a lot of processes in which nano- and micro-particles are treated [3].

Industry has become progressively more interested in controlling the microscopic properties of particles, such as composition, shape, surface roughness, surface characteristics, and porosity. It has been estimated that 70% of all industrial processes involve dealing with fine particles at some point in the process (Bushell 1998) [4]. Characterization of these particles helps us to understand and predict or control their behavior in many processes. In industry, the properties of particles determine whether or not a dust is a respiration hazard, whether granular materials will mix or segregate when agitated, and whether material in a hopper will flow in a controllable fashion, behave like a liquid, or not flow at all. In most industrial applications, the shape, structure, and strength of aggregation play an important role, since many characteristics of the suspensions (such as the electrical, optical, magnetic, and adsorptive properties) are mostly dependent upon the morphology, size distribution, and strength of the aggregates [5].

Although particle aggregation growth is so important in the scientific and engineering fields, the aggregation mechanism is often rather complex and vary from one system to another due to different physical or chemical origins. Until, the aggregation mechanism is far away from complete understanding.

1.2 The objective of this research

Because of the important roles of the particle aggregating growth process in natural, scientific and engineering systems, such as coatings, dust protection, water pollution, and so on, many studies of this area, including experiments and simulations have been considered to get an insight on growth process and mechanism.

The earliest simulation model of the aggregate growth process was gotten by Vold using the computer simulation in 1963 [6] which model has a three layers' structure. In

1966, Sutherland criticized this random characteristic in the particle coagulating process of the Vold aggregation model and believed that the main mechanism of the aggregation growth is not the only particle collisions but also the clusters aggregation [9]. In the above research, the particles and clusters follow the linear movement but did not include the Brownian motion which is inconsistent with the actual situation in the natural systems. Witten and Sander had made the modification about this [8]. After these early simulations and experiments, there are also many special experiments have been done and various models have been proposed.

Although the reasons for aggregation/growth are complex and vary from one system to another due to different physical and chemical reasons, 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.

So as not to miss underlying essential mechanisms in the process of particle aggregation and dynamic growth, morphological features are at first to be simulated by a set of simple models.

These two models, DLA model and RLA model are so simple and universe that they can easily give some explanations for some complex aggregation process. In fact, there exists the weak or strong interactions between particles when particles have the possibility to attract each other and stick together. For particles which carry some

electrical charge (ions) the forces are typically very strong and thus there is a gain in energy when they build aggregates. So aggregates are a preferred state compared to spread ions. Usually such aggregates are well ordered, they form crystals. The ordering force is the shape and charge of the ions, you will (almost) always get the same shape with a distinct set of ions (NaCl typically forms a cube). And with crystals formed by charged particles the forces may work on comparable long distances. In ideal situations the crystals are very compact and regularly shaped. This situation can be explained by RLA model and energy gain can be understood as stickiness possibility in RLA model. Without an electrical charge the forces are much weaker. So, it may happen that particles stick together for a while but at distinct opportunities they travel around again. Without the ordering force of the electrical field of charged particles, the aggregates have no distinct shape. Each aggregate is unique. Such a building is also named a cluster. Often the aggregates are quite fluffy, not compact, but maybe tree like. This situation can be explained by DLA.

Based on the description above, we can find that the explanations for aggregation growth from DLA and RLA are limited and simple because they simplify many necessary considerations.

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 due to various physical and chemical reasons. For example, there are many different types of pollutant particles contained in the waste water, such as various kinds of metal particles, latex particles, organic and inorganic colloids, cohesive sediment, and so on. Utilizing the developed model to simulate such multi-type particle aggregation and dynamic growth process can help us to get insights on the growth behavior and mechanism. This plays important roles in understanding and improving the more effective and economical treatment techniques.

But the present studies and simulations mostly limited in the certain particle type and there have so far been few studies on the aggregation dynamics in this coexistence system. Based on the results of these two models, the new extended models will be developed to solve the aggregation growth of many kinds of particles, in which the 'type' constrain condition will be added to each particle to control the particles sticking behavior when they collide.

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.

Chapter 2

Aggregation Growth Model

In this chapter, the development of aggregation growth model is reviewed. With the deeply researching about the fractal growth, a variety of dynamic growth models had been founded, which basically can be divided into three kinds:

1. Diffusion-Limited Aggregation model (DLA model);
2. Ballistic Aggregation model (BA model);
3. Reaction-Limited Aggregation model (RLA model).

Each of these three models has two different forms: monomer aggregation and cluster aggregation. For the DLA model, the monomer aggregation is named Witten-Stander model, while the cluster aggregation is named Diffusion-Limited Cluster Aggregation model. For the BA model, the monomer aggregation is named Vold model, while the cluster aggregation is named Sutherland model. For the RLA model, the monomer aggregation is named Eden model, while the cluster aggregation is named Reaction-Limited Cluster Aggregation model [9].

In the Diffusion-Limited Aggregation model and Reaction-Limited Aggregation, the particles perform random walk due to Brownian motion; these two models can be useful for the study of fractal structure growth, such as colloid collision and deposition, flocculation growth, and so on. While in the Ballistic Aggregation model, the particle will follow the random ballistic (linear) trajectory and stick to the surface of the structure when it comes close to a previously added particle in the growing aggregate. This aggregation results in the formation of a fanlike structure if the initial seed is a structureless point. This simplified BA model can be useful for the study of surface

growth processed, such as physical vapor deposition on a cold substrate under high vacuum.

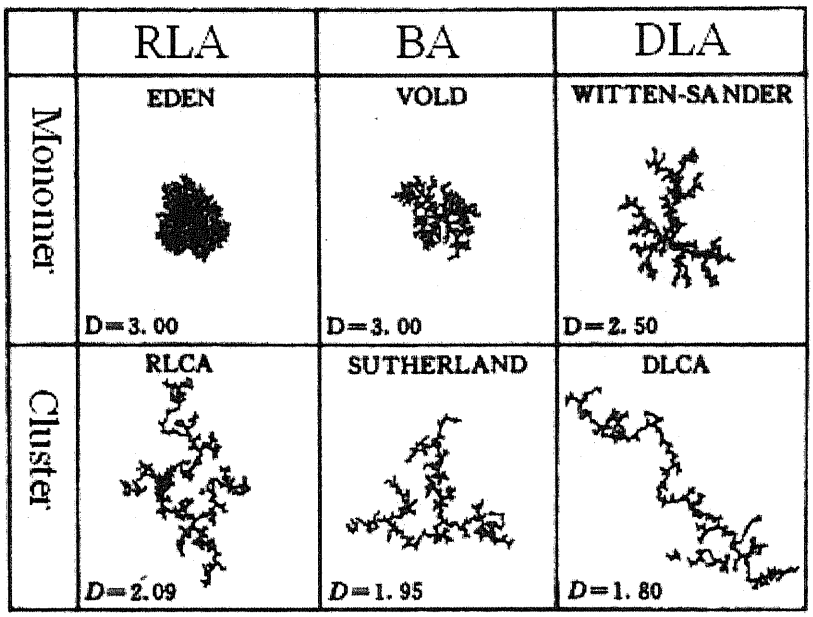

Fig. 2.1 The three basic fractal growth models

Figure 2.1 shows the above three kinds of models' diagram in the two-dimensional plane. These diagrams are obtained by computer simulation by P. Meakin [7]. The fractal dimension values (D) listed on the diagrams are obtained in the three-dimensional space.

2.1 Diffusion-Limited Aggregation

2.1.1 Diffusion

Diffusion is a random motion. Although the motion of individual particles is totally random with respect to the direction, it may happen that particles walk somewhat far relative to a starting point. But, in contrary to a normal flow, where all particles under investigation move more or less into the same direction, the average of walked distance of all particles within a random walk (Brownian motion) is zero. While one particle

moves into this direction, another moves into another direction.

In diffusion there might be a net transport of material, when the starting situation is not a uniform distribution. As you might imagine, when you open a container with dye within an aquarium, after a while you will find the dye spread around all available water. When you do this experiment, you will see, that it takes a lot of time until you have a uniform color. This is typical for the underlying random mechanism. The dye particles move forth, back, back, forth, back, forth, forth, forth, back.... and this way it takes its time. This slowliness is typical for diffusion. Diffusion is not only a phenomenon in fluid systems, but also in solid phases. It just takes much more time.

2.1.2 DLA Model Theory

Diffusion-limited aggregation (DLA) is the process whereby particles undergoing a random walk due to Brownian motion and stick together to form aggregates. This theory was proposed by two physicists T.A. Witten and L.M. Sander [8] in 1981 who try to use it to explain the observed fractal aggregation of the dust particles. This theory can be applicable to aggregation in any system where diffusion is the primary means of transport in the system. Diffusion-limited aggregation can be observed in many systems such as electrodeposition, Hele-Shaw flow, mineral deposits and dielectric breakdown.

Basically, a DLA is a model of irreversible growth process whereby individual particles stick to one another to form clusters or aggregates. It was found to be very useful for a wide range of growth processes in which diffusion (some kind of random motions) is the important limiting step and rearrangement of the material within a cluster is not allowed. The DLA is one of the most important models of fractal growth.

The growth rule is remarkably simple. We start with an immobile seed particle fixed in a central lattice site of the plane. A walker is then launched from a random position far away the seed and is allowed to diffuse. The released particle moves following a Brownian trajectory. If it touches the seed, it is immobilized instantly and becomes part

of the aggregate. Next we launch similar walkers one-by-one and each of them stops upon hitting the cluster. After launching a few hundred particles, a cluster with intricate branch structures results [8].

The structure of this aggregate has the characteristics: dendritic and complex structure with the changeless scaling that occurs in the diffusion limited products. In 3 D space, the fractal dimension of this aggregate is about 2.50.

2.1.3 Model simulation

The simulation procedure for the DLA is quite straightforward: Imagine a computer screen is the 'ground' for the fractal cluster to grow and the screen is made of tiny grids called pixels. Only one particle can occupy a pixel. Starting with a single-seed, fixed particle at the center of the screen, a second moving particle is 'created' randomly at some distance from the origin and move randomly on the pixel grids until it reaches a grid adjacent to the seed and becomes part of growing cluster. A third moving particle is then generated like the second particle and allows wandering randomly. The particle will stick if it finds itself adjacent to any stuck particles. The procedure is repeated many times and the end result, instead a lump as one may expect, is (surprise) a fractal.

Diagram (Figure 2.2) below shows a typical Witten-Sander (WS) cluster model grown on two dimensional square lattices (grids) which consists of 3000 particles (or pixels as are generated on the computer screen).

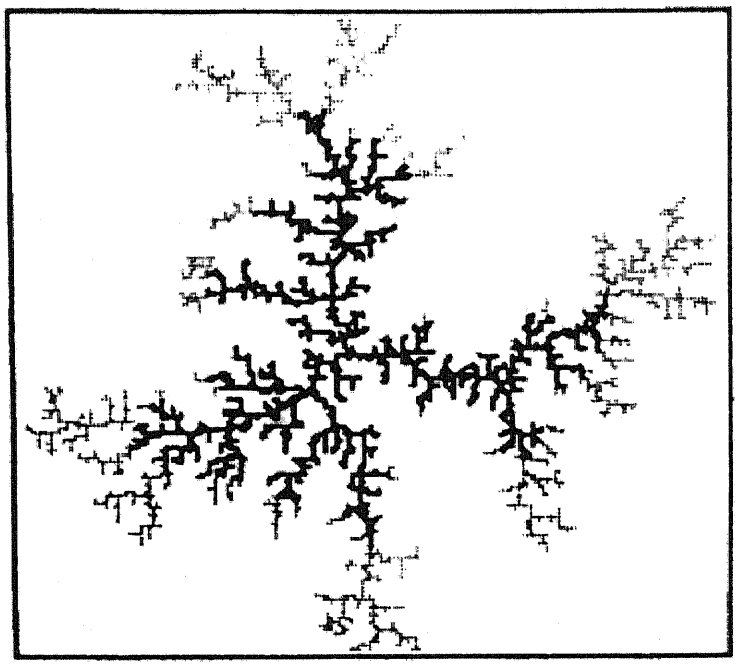

Fig.2.2 DLA aggregate consists of 3000 particles

The aggregate has randomized crossover, open structure and obvious self-similarity that can be seen from the above diagram. The characteristics of the aggregate indicate that the aggregate structure has shielding effect. This shielding effect is very obvious that the top of the branches have the most chances to effectively capture the diffusing particles.

In the Figure 2.2, in order to show the shielding effect clearly, show the previous 1500 particles in the aggregate as small circles which have deep color that form the internal organization of the aggregate; and show the latter 1500 particles as small point. Because of the shielding effect, these latter 1500 particles are basically located on the periphery position of the aggregate and only a few particles can enter the inside [9].

2.1.4 Application

The aggregation process leading to the DLA cluster is widespread in nature. Branched structures reminiscent of DLA have been observed in viscous fingering, electrodeposition, dielectric breakdown, dendritic and snowflake growth, chemical

dissolution, thin film crystallization, geological phenomena such as disequilibrium silicate mineral textures, and even biological phenomena such as bacterial growth, neuronal growth, and fingering of HCl across the mucus lining of the stomach.

2.2 Reaction-Limited Aggregation

The aggregation phenomenon is usually classified in two regimes: diffusion-limited aggregation (DLA) and reaction-limited aggregation (RLA). DLA occurs when collision efficiency of two clusters is relatively high or close to unity, while RLA prevails at very low collision efficiencies. Because of differences in hydrodynamics of particle/cluster interactions, the kinetics of aggregation is dissimilar in the two regimes. DLA follows power-law growth kinetics (Figure 2.3a) while RLA kinetics conforms to an exponential growth law (Figure 2.3b) [10].

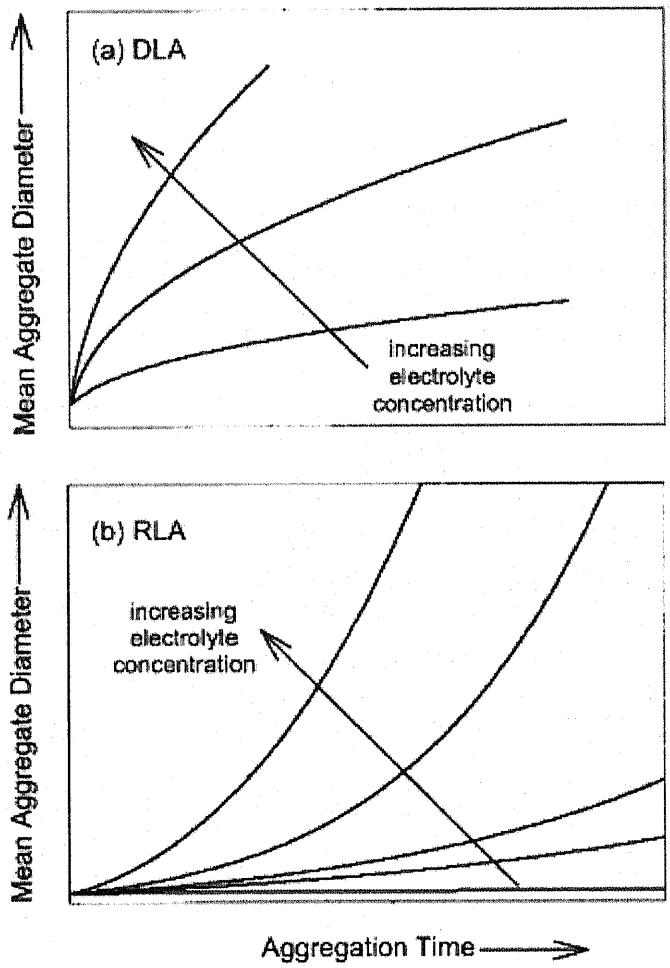

Fig. 2.3 Representative aggregate growth curves (a) diffusion-limited aggregation - power law growth, and (b) reaction-limited aggregation - exponential growth

The Reaction-Limited Aggregation model is also known as Chemically-Limited Aggregation model, which includes two basic types: Eden model for monomer growth and RLCA model for cluster growth (Fig. 2.1). The phenomena and process of the silicon dioxide aggregation on the water solution can explain the basic characteristic of this reaction-limited aggregation model.

2.2.1 Model theory

Reaction-limited cluster aggregation models were first introduced by Jullien and Kolb [11, 12].

In reaction-limited aggregation model, particles also perform Brownian motion, but a small repulsive energy barrier must be crossed before the particles can contact each other and become irreversibly joined. This means that on average many encounters between clusters must take place before a bonding event occurs and the clusters are able to explore all possible bonding possibilities (or at least a representative sample of them) before a new bond is formed. That is when one particle collide with other particles or clusters, if they can overcome the energy barrier between the two approaching particles they will stick together and form the new cluster, if not they will walk apart respectively and take the next collision. So one particle must take many times of collision with other particles to overcome the energy barrier before it sticks with other particle or cluster. The potential energy diagram was shown in the Figure 2.4 [13]. This idea provides the basis for most models for reaction-limited aggregation. While it is possible to simulate RLA using the diffusion-limited aggregation with a very small stickiness possibility (σ), this is not a practical procedure for carrying out large scale simulations near to the $\sigma \rightarrow 0$ limit.

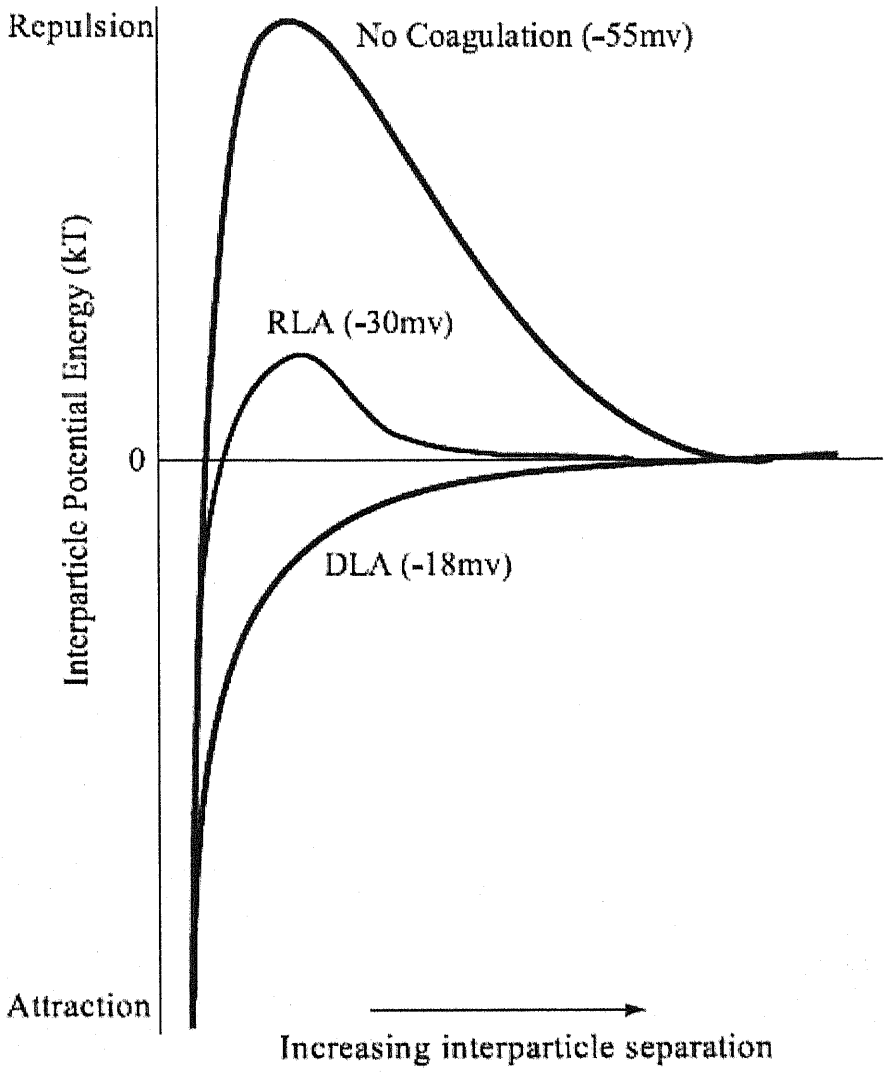

Fig. 2.4 Interparticle potential energy diagram showing the high repulsive energy barrier when no coagulation takes place, the low barrier for reaction limited aggregation, and the lack of a barrier for diffusion limited aggregation

2.2.2 Comparison of DLA and RLA model

Coagulation of latex particles is most often carried out in the diffusion limited aggregation regime where the time for coagulation to take place is on the millisecond timescale. This process produces aggregates of low density, irregular shape, and a broad particle size distribution. When the coagulation is carried out in the reaction limited

aggregation regime, a coagulation time of about 1-120 seconds, the system can be controlled by mixing to yield dense, spheroidal aggregates with a very narrow particle size distribution (shown as Fig. 2.5). Controlled coagulation in the RLA regime yields much narrower particle size distributions than are achievable with DLA. Figure 2.5 is a comparison of representative distributions both having an average size of about 200 μm in diameter [13]. Note the large amount of oversized and undersized particles in the DLA curve compared to the RLA curve. Aggregate morphology also differs significantly.

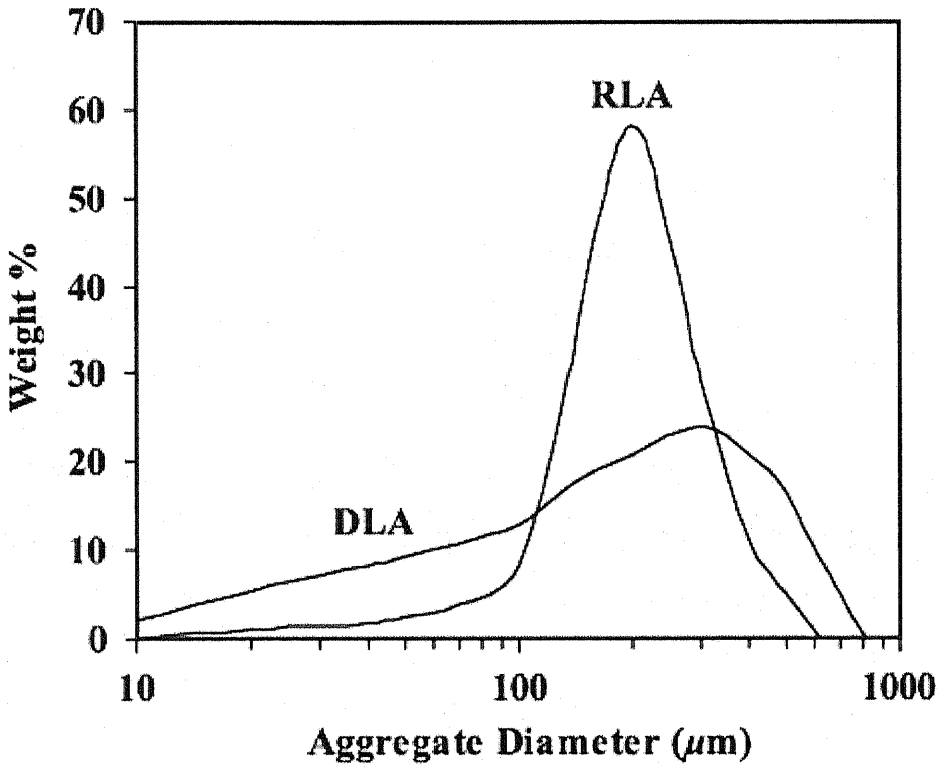

Fig. 2.5 RLA produces a much narrower aggregate size distribution than DLA

In this experiment, the latexes used in this study were produced by redox initiated seeded emulsion polymerization run under monomer-starved conditions to ensure that the composition remained constant throughout preparation. The surfactant was 1% sodium dodecyl sulfate based on monomer included butyl acrylate (BA) and methyl

methacrylate (MMA). All latexes were coagulated at 10% polymer solids with CaCl2 solution at pH=4.

Conventional coagulation involves adding a coagulant (e.g., Ca^{2+} ions) to the latex in excess of the critical coagulation concentration (CCC). This causes coagulation of the latex particles in a matter of milliseconds and is termed diffusion limited aggregation (DLA). In DLA latex particles form aggregates as quickly as they can diffuse together and collide [14]. Each collision results in the particles "sticking" together. If slightly less coagulant than the CCC is used, then the coagulation rate is slowed to the timescale of seconds instead of milliseconds and mixing can be used to control aggregate size and shape. This is termed reaction limited aggregation (RLA) and the latex particles may collide several times before "sticking" together. The result is a denser, more uniform aggregate than is formed in the DLA process. RLA usually occurs in the region between 5–20% volume solids and is quite unexpected and unique. Below about 5% solids there is incomplete coalescence and above about 20% solids the viscosity during coagulation becomes prohibitively high [13].

The differences between DLA and RLA can best be explained using the DLVO theory of particle interaction energies [15, 16]. In DLVO theory, the total interparticle potential energy for two particles approaching one another, V_{tot} , is expressed as

$$V_{tot} = V_{vdw} + V_{ele} \tag{2.1}$$

where V_{vdw} is the van der Waals attractive energy and V_{elec} is the electrical repulsive energy. V_{vdw} is a function of the polymer composition (i.e., its Hamaker constant) and the interparticle distance. V_{elec} is a function of the interparticle distance and the particle size and its surface potential, usually approximated by the zeta potential. By carefully adjusting the amount of coagulant in the process, the zeta potential is affected and consequently the potential energy barrier height, V_{max}, is thereby adjusted to yield a slow, controlled coagulation rate. Figure 2.8 shows the interparticle potential energy

curves for a 100 nm diameter latex with no coagulant (–55 mv), enough coagulant to be in the RLA regime (–30 mv), and enough coagulant to exceed the CCC and reach the DLA regime (–18 mv). In this example, for RLA, V_{max} is 11 kT, whereas it is 0 kT for the DLA regime and 57 kT for the system without any added coagulant.

Chapter 3

Fractal

In the previous chapters, we introduced some dynamic growth models about particle aggregation. Computer simulations for such models, which are in close relation to many practical process (such as solidification of alloys, secondary oil recovery etc), play an important role for us to understand aggregation growth processes and aggregation structure. However, the general mathematics cannot give a quantitative description for aggregation structures due to its extra complexity and fractal concept is introduced to describe the aggregation structure. In this chapter, we will introduce the concept of the fractal geometry and the fractal dimension. In addition, we will also introduce some numerical methods for how to calculate the fractal dimension.

3.1 Introduction of the fractal geometry

During the last 30 years it has widely been recognized that many structures possess a rather special kind of geometrical complexity. The particular geometrical properties of these structures have been shown to be related to fractal, in which objects have non-integer dimensions. In general, a fractal is "a rough or fragmented geometrical shape that can be subdivided into parts, each of which is (at least approximately) a reduced-size copy of the whole [17]." In this definition, fractal has self-similar characteristics. However, this definition has undergone many refinements, but the precise definition for fractal is not submitted until now. Benoit Mandelbrot first defined that fractal is a set with fractional (no-integer) Hausdorff dimension. However, this definition has a lot of drawbacks (for example, it says nothing about self-similarity even though the most commonly known fractals are indeed self-similar). The present common definition can be understood as the following set [18]:

1) It has a fine structure at arbitrarily small scales;

2) It is too irregular to be easily described in traditional Euclidean geometric language;

3) It is self-similar (at least approximately or stochastically);

4) It has a Hausdorff dimension which is greater than its topological dimension (although this requirement is not met by space-filling curves such as the Hilbert curve);

5) It has a simple and recursive definition.

Self-similarity is the most important feature of fractals. In general, fractal must satisfy the scale invariance if it is self-similar. Descriptive formulated self-similarity means that if you enlarge a part or section of a similar fractal this enlargement 'resembles' the original fractal. Or: In different 'zones' the basic structure of the total object is preserved, these fractals are scale invariance. One could call this characteristics or self-similar fractals the 'structure preservation'. In mathematic, this is called dilation symmetry.

Most of the mathematical fractals are self-similar. Usually, they can be described by iterative algorithms, the resulting fractal (after infinity iterations) has structures on all scales. Nature or physical fractals are self-similar just within a few scales. One of the simplest self-similar objects is the Cantor set, whose iterative construction at successive 'generations' is shown in Fig 3.1. If we enlarge the box of generation 3 by a factor of three, we obtain a set of intervals that is identical to the generation 2 object. In general, at generation k we can enlarge part of the object by a factor of three and obtain the object of generation (k-1). For the Cantor set, the enlarged part overlaps the original object exactly; we call such an exactly self-similar object a deterministic fractal. However, many objects existing in nature are random. Despite this randomness, such natural objects may be self-similar in a statistical sense. One classic example is the coastline of a continent. If we study two maps with different magnifications

representing a typical coastline, they look similar. There is no way to distinguish between them, if we are not already familiar with the particular coastline. In fact, we cannot even determine which map has the higher magnification. Unlike the case of deterministic fractals, the two maps at two different magnifications do not overlap, but nonetheless, their statistical properties are the same. Objects with inherent randomness that are self-similar only in a statistical sense are called random fractals or statistical fractals.

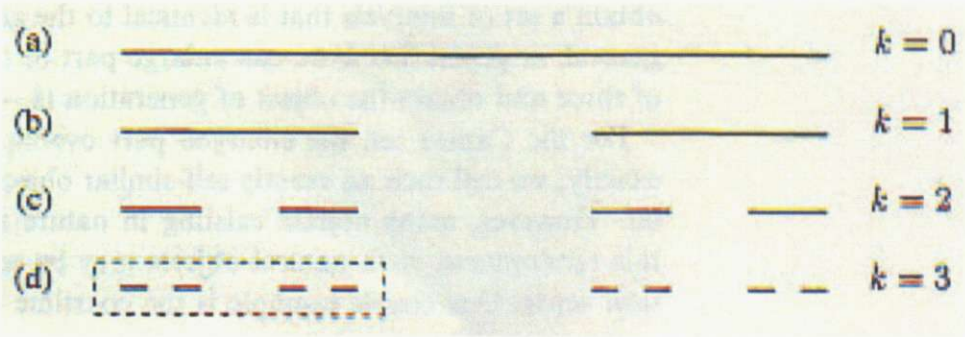

Fig. 3.1 Construction of the Cantor set

3.2 Fractal dimension

How big is a fractal? When are two fractals similar to on another in some sense? What experimental measurements might we make to tell if two different fractals may be metrically equivalent? There are various numbers associated with fractals which can be used to compare them. They are generally referred to as fractal dimensions. They are attempts to quantify a subjective feeling which we have about how densely the fractal occupies the metric space in which it lies. Fractal dimensions provide an objective means for comparing fractals.

In brief, in fractal geometry, the fractal dimension, D, is a statistical quantity that gives an indication of how completely a fractal appears to fill space, as one zooms down to finer and finer scales. There are many specific definitions of fractal dimension and none of them should be treated as the universal one. From the theoretical point of view the most important are the Hausdorff dimension, the packing dimension and, more

generally, the Renyi dimensions. On the other hand the box-counting dimension and correlation dimension are widely used in practice, partly due to their ease of implementation.

Although for some classical fractals all these dimensions do coincide, in general they are not equivalent. For example, what is the dimension of the Koch snowflake? It has topological dimension one, but it is by no means a curve-- the length of the curve between any two points on it is infinite. No small piece of it is line-like, but neither is it like a piece of the plane or any other. In some sense, we could say that it is too big to be thought of as a one-dimensional object, but too thin to be a two-dimensional object, leading to the question of whether its dimension might best be described in some sense by number between one and two. This is just one simple way of motivating the idea of fractal dimension.

3.3 Calculation of the fractal dimension

There are two main approaches to generate a fractal structure. One is growing from a unit object, and the other is to construct the subsequent divisions of an original structure, like the Sierpinski triangle (Fig.3.2). Here we follow the second approach to define the dimension of fractal structures.

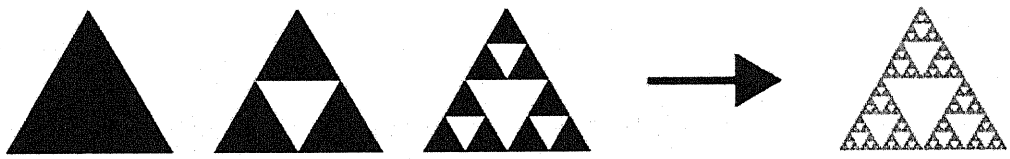

Fig. 3.2 Sierpinski triangle

If we take an object with linear size equal to 1 residing in Euclidean dimension, and reduce its linear size to be L in each spatial direction, it takes N(L) number of self similar objects to cover the original object (Fig. 3.3).

If we take an object residing in Euclidean dimension D and reduce its linear size by

1/r in each spatial direction, its measure (length, area, or volume) would increase to $N=r^D$ times the original. This is pictured in the next figure. We consider $N=r^D$, take the log of both sides, and get log(N) = D log(r). If we solve for D: D = log(N)/log(r) The point: examined this way, D need not be an integer, as it is in Euclidean geometry. It could be a fraction, as it is in fractal geometry. This generalized treatment of dimension is named after the German mathematician, Felix Hausdorff. It has proved useful for describing natural objects and for evaluating trajectories of dynamic systems.

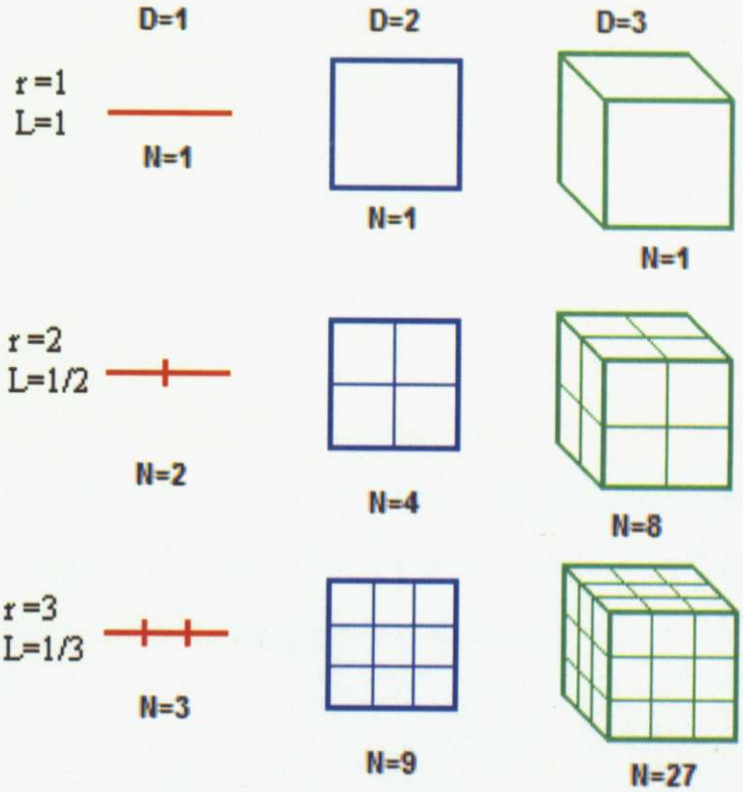

Fig. 3.3 Another way to define dimension

However, the dimension defined by the equation 3.1 is still equal to its topological or Euclidean dimension.

$$D = \frac{\log N(L)}{\log(1/L)} \tag{3.1}$$

By applying the above equation to fractal structure, we can get the dimension of

fractal structure (which is more or less the Hausdorff dimension) as a non-whole number as expected.

$$D = \lim_{\varepsilon \to 0} \frac{\log N(\varepsilon)}{\log(1/\varepsilon)} \tag{3.2}$$

where N(ε) is the number of self-similar structures of linear size ε needed to cover the whole structure.

Closely related to the Hausdorff dimension is the box-counting dimension, sometimes known as the packing dimension, which considers, if the space were divided up into a grid of boxes of size ε, how does the number of boxes scale that would contain part of the attractor?

To calculate this dimension for a fractal D_0, imagine this fractal lying on an evenly-spaced grid, and count how many boxes are required to cover the set. The box-counting dimension is calculated by seeing how this number changes as we make the grid finer. Suppose that N(ε) is the number of boxes of side length ε required to cover the set. Then the box-counting dimension is defined as:

$$D_0 = \lim_{\varepsilon \to 0} \frac{\log N(\varepsilon)}{\log(1/\varepsilon)} \tag{3.3}$$

If the limit does not existthen one must talk about the upper box dimension and the lower box dimension which correspond to the upper limit and lower limit respectively in the expression above. In other words, the box-counting dimension is well defined only if the upper and lower box dimensions are equal. Both are strongly related to the more popular Hausdorff dimension. Only in very specialized applications is it important to distinguish between the three [19].

Chapter 4

Computer simulation of the cluster dynamic growth

As there are lots of models in the field of investigation of fractals, computation is a way to compare the nature with the models. In this chapter, we will simulate the cluster dynamic growth process in the DLA and RLA models. These simulations process are carried out using the MatLab program. The purpose of the simulation is to capture the characteristics of the simulation aggregate' structure and understand deeply the traditional aggregation models. Then the extended models Multi-Types DLA and Multi-Types RLA will be introduced and be used to perform the simulation process. In the simulation process, we will get some relational simulation results and make the discussion.

4.1 Diffusion-Limited Aggregation model

DLA is one common computation model and applied widely in many fields. For DLA model, one approach is to simulate the random walk of the particles and their aggregation. This model has been found to be relevant to a large variety of processes including fluid-fluid displacement in porous media, dielectric breakdown, electrodeposition and possibly growth processes. The DLA model illustrates that simple growth and aggregation models could lead to valuable insights into important physical and chemical processes.

4.1.1 Methodology of the DLA model simulation program

This simulation region is set in a two dimensional squared lattice, L by L with L^2 sites. The simulation procedure will imagine the computer screen as the 'ground' for the fractal cluster to grow and the site is called pixel that makes of the screen. Only one particle can occupy a pixel. The particle will be shown as a point in the squared lattice.

Starting with a single particle, we fix this particle at the center of the squared lattice as the stationary seed. A second moving particle is 'created' in a random position where not particle sites at some distance from the stationary seed. There are eight sites encircle this particle, marked from 1 to 8 (shown in the Fig. 4.1). 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 (shown as in the Fig. 4.2). 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 procedure is shown in the Figure 4.3.

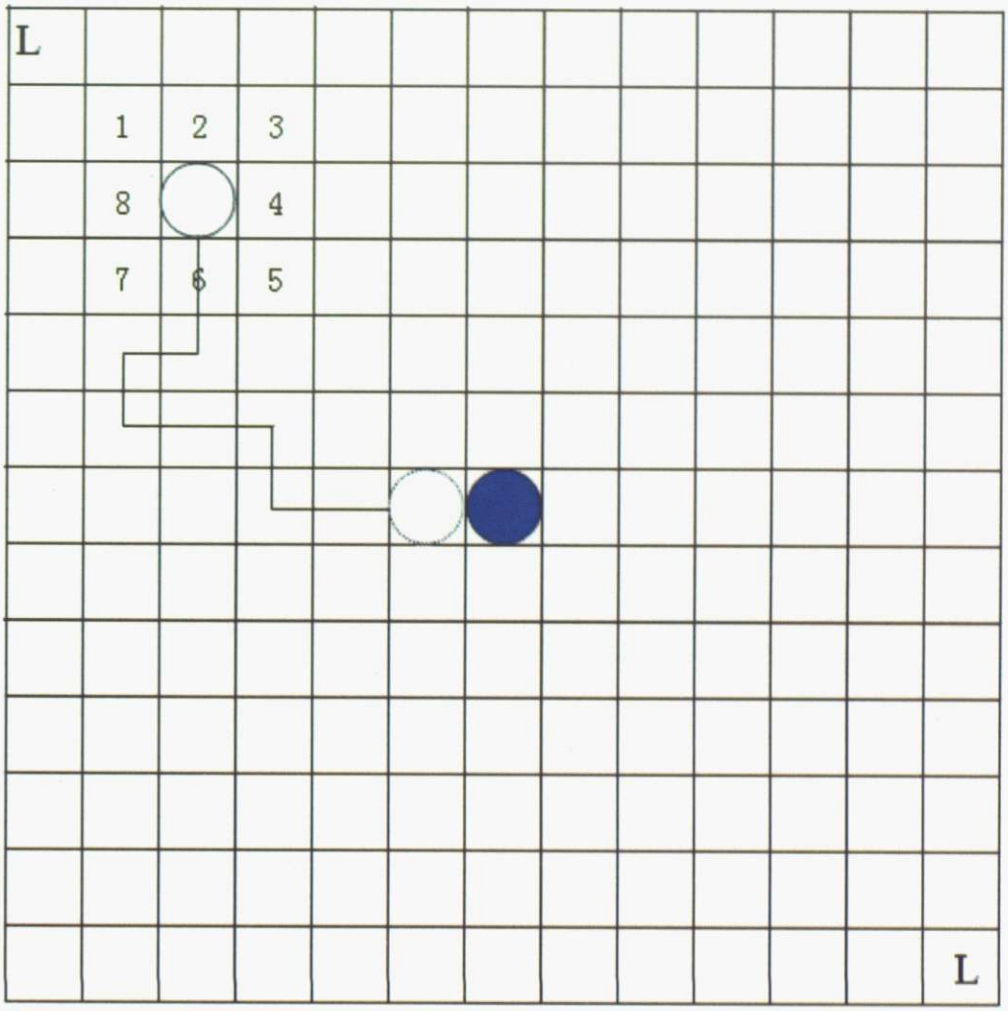

Fig. 4.1 Particle Brownian motion in DLA model

As the increasing the number of the simulation particle, the size of the simulated aggregate will also increase. So the scale of the squared lattice should be adapted to the simulation particle number.

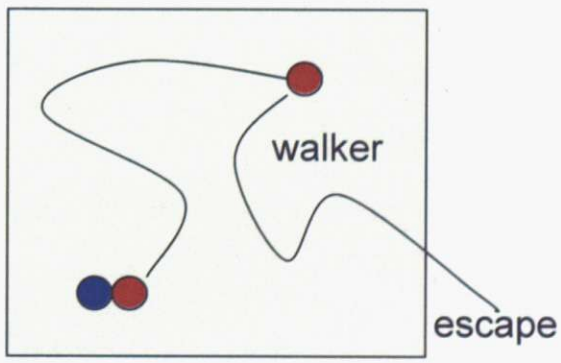

Fig. 4.2 Particle escapes from the simulation region

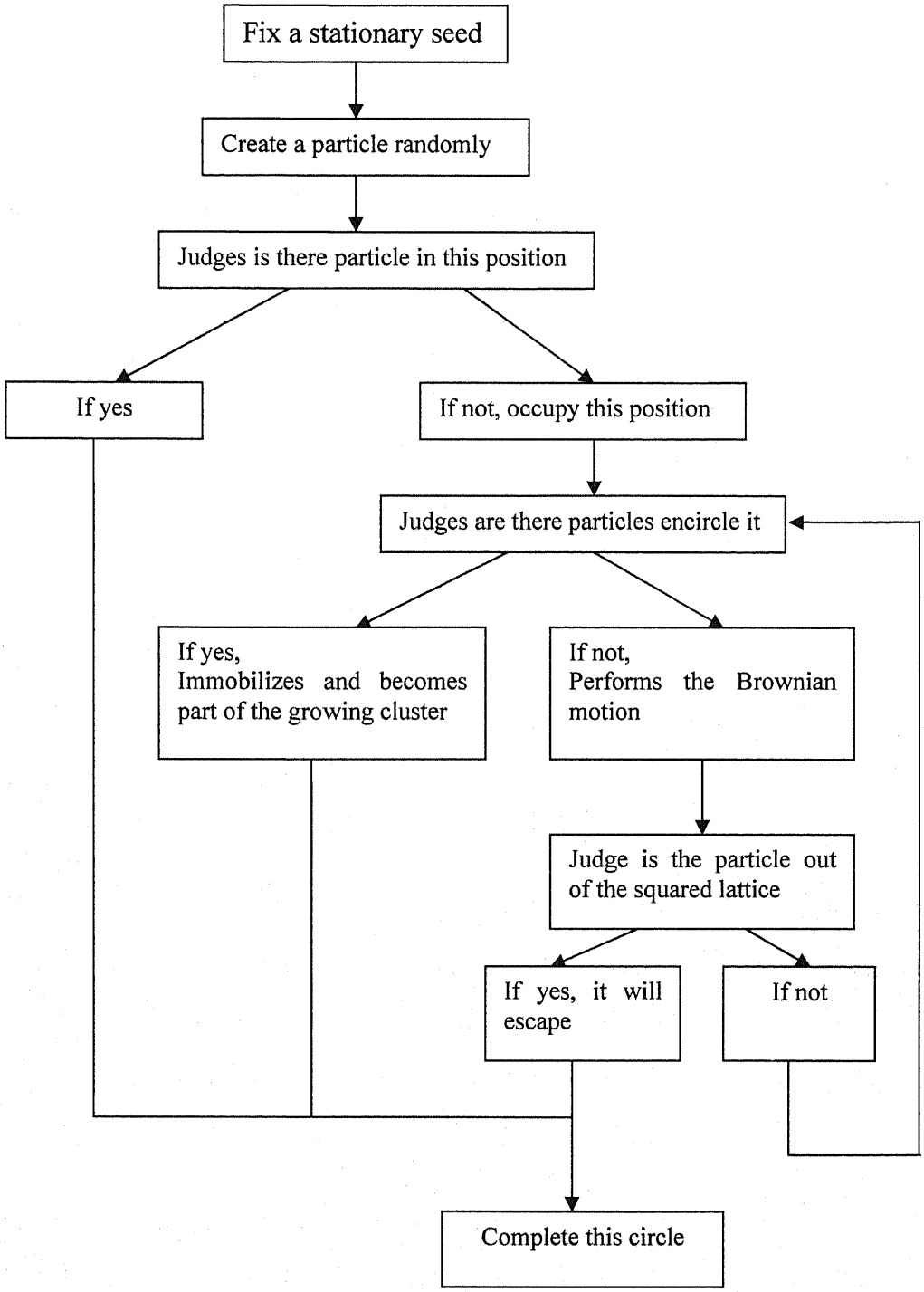

Fig. 4.3 The procedure of the particle aggregation

4.1.2 Computer simulation result

Figure 4.4 shows a simulating result of the DLA model. This simulation is performed

in a in a two dimensional squared lattice of 200 by 200.

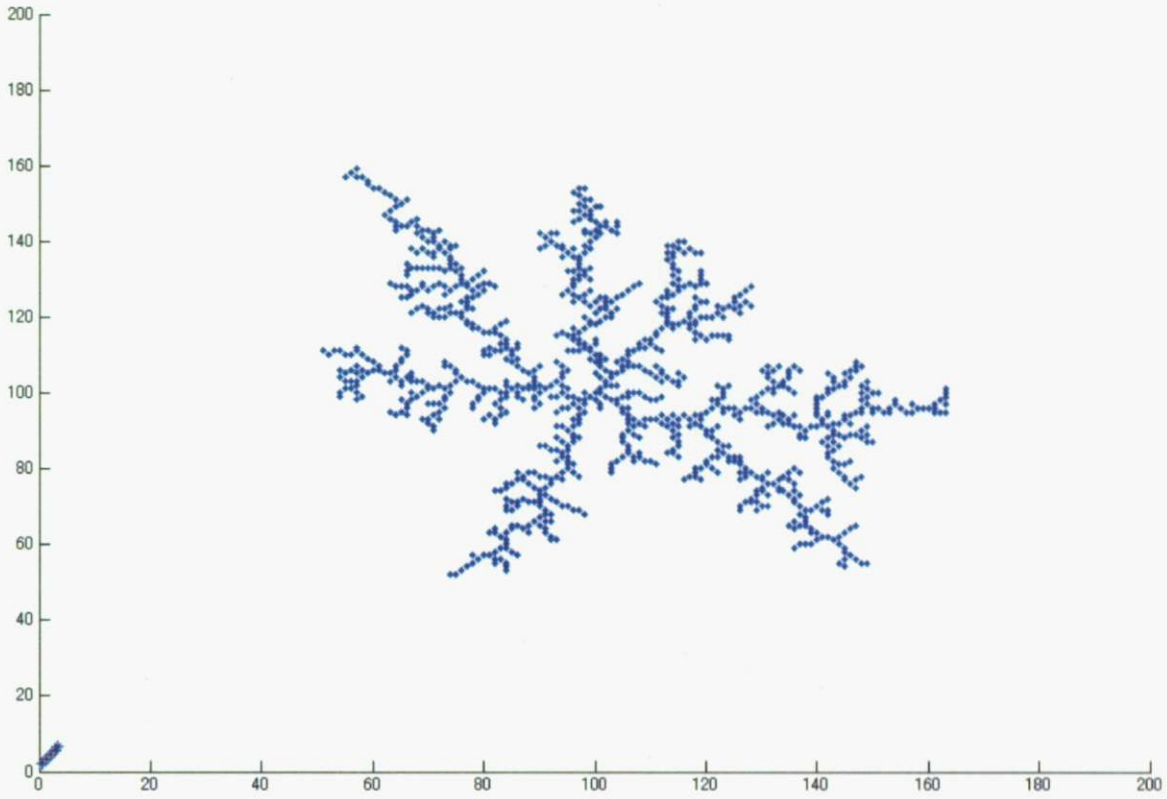

Fig. 4.4 Simulation result of the DLA model

The total number of the simulation particle is 20000, but because of the random walk, most of them have escape form the simulation region. The resulted aggregate only contains 1049 particles, which fractal dimension is 1.5353 calculated by the box-counting method. This aggregate shows the obvious self-similarity, open and intricate branch structure and the obvious shielding effect.

4.1.3 Calculation method of the fractal dimension

Here we apply the box counting method to calculate the two-dimensional fractal dimension, D. In this study, box dimension is determined by counting the number (N) of particles around the center particle, as a function of distance away from the seed particle. This function and relationship are shown as the Figure 4.5 and Equation 4.1 [51].

$$N_{(r)} = r^{D} \tag{4.1}$$

where $N_{(r)}$ is the sum of all primary particles contained within a circle of radius r; s is the distance away form the seed particle; D is the box dimension of the aggregate structure.

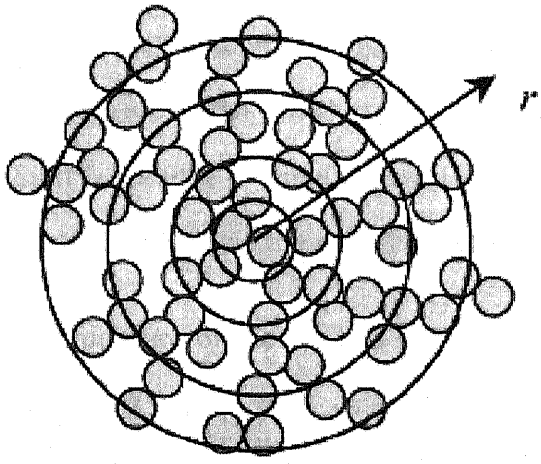

Fig. 4.5 Variation of contained particle number as a function of increasing radius

Take the log of both sides, and D can be found as the slope of the plot of (log N(r)) versus (log r). So the fractal dimension can be obtained by Equation 4.2. The range of the radius 'r' is limited by the size of the aggregate.

$$D = \lim_{r \to 0} \frac{\lg(N_{(r)})}{\lg(r)} \tag{4.2}$$

4.2 Reaction-Limited Aggregation model

4.2.1 Methodology of the RLA model simulation program

Because of the substantial repulsive force remains between particles in the RLA model that induces the particles or clusters must overcome an energy barrier before the aggregating clusters can contact each other and become irreversibly joined. This means that one particle or cluster must collide with other particles or clusters for many times before it can stick and become part of the growing aggregate. This idea provides the basis of the RLA model. So it is possible to simulate reaction-limited aggregation using the diffusion-limited aggregation with a sticking probability (σ).

The practical simulation procedure of the RLA is similar to that of the DLA, but 'creates' a random number (ran) before each collision to control the aggregation mechanism and the stickiness possibility (σ) can be regarded as the energy barrier. Then compare the random number (ran) with the sticking probability (σ), if it meets the condition: ran > σ, the particle will stick to the growing cluster, otherwise, the particle should go on the Brownian motion (shown in the Figure 4.6).

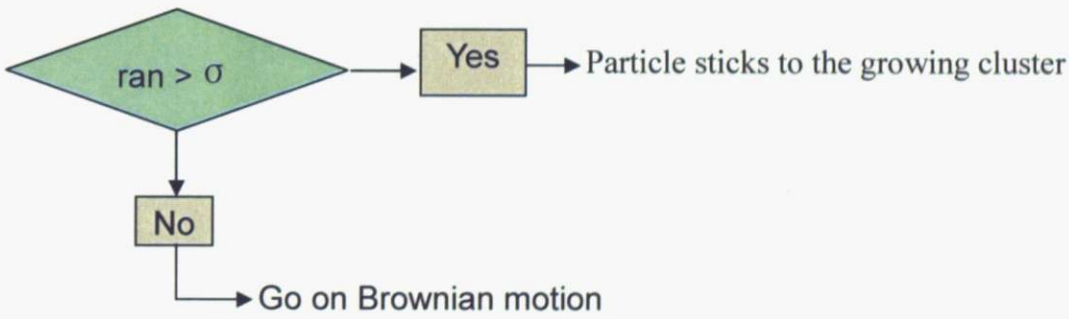

Fig. 4.6 Stickiness control condition

4.2.2 Computer simulation result

Figure 4.6 shows a simulating result of the RLA model. This simulation is also

performed in a in a two dimensional squared lattice of 200 by 200.

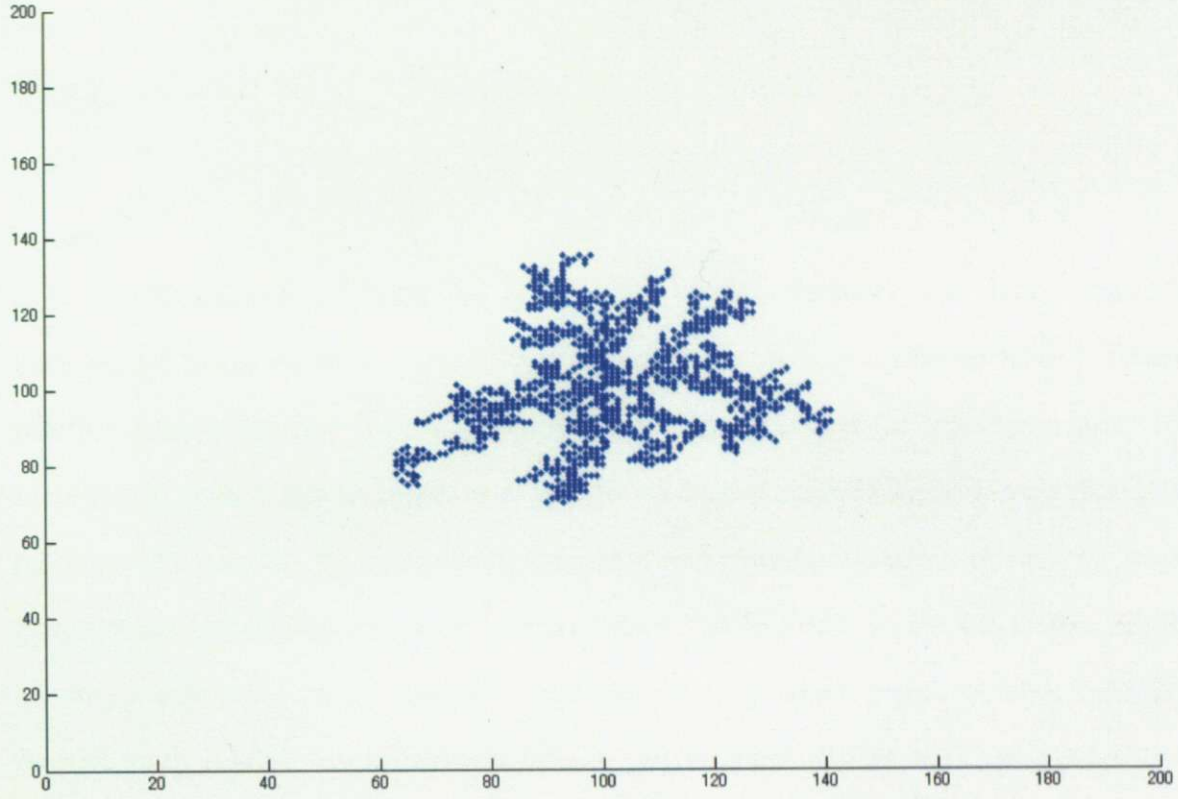

Fig. 4.6 Simulation result of the RLA model

This simulation is performed by 30000 particles with stickiness possibility of 0.10 and result in the aggregate contains 1766 particles with the fractal dimension of 1.6334. The fractal dimension is also calculated using the box-counting method. In contrast to the simulation result of the DLA model, the aggregate formed in the RLA model is more dense (see Fig. 4.4), that means the monomer particles have more chances to move into the inside of the growing aggregate.

Chapter 5

Extended Simulation Model

In natural systems or industrial systems, it is very common that many types of particles are to aggregate and grow. These different types of particles may have different reaction probability and stickiness possibility. So the aggregation mechanism may be more complex than that in single-type system because of various physical and chemical reasons. Researching the particles aggregation and clusters dynamic growth in these practical systems is very necessary and important. For example, in the wastewater, there are many different types of pollutant particles. How to make these pollutant particles deposit more quickly and effectively, how to get the much denser and drier silt are two important targets in the wastewater treatment plant. Computer simulation of particles aggregation in such similar systems conditions can help to understand and improve the treatment techniques. But the present studies and simulations mostly limited in the certain particle type and cannot describe the multi-types particles system. So the traditional DLA and RLA model are not suitable in this system condition. In this chapter, the extended models: multi-types DLA and multi-types RLA models are extended to describe and investigate such multi-types particles aggregation growth behavior and mechanism.

5.1 Multi-types DLA

The Multi-types DLA model can base on the diffusion limited aggregation but adds a 'type' constraint condition to each particle to control the particles sticking behavior when they collide. If it meets the conditions the two approaching particles will stick

together once they collide; if not, there is only collision but not stickiness.

We also set different colors for different types of particles to distinguish them. That was shown in the Table 5.1.

Table 5.1 The particle type' marks and restrictive conditions

SN	Particle Type	Type color	Restrictive Condition
1	A	Blue	Can not stick to A type particles
2	B	Red	Can not stick to B type particles
3	C	Green	Can not stick to C type particles
4	D	Purple	Can not stick to D type particles
5	E	Black	Can not stick to E type particles

In the simulation procedure, the type of the seed particle is random. Both of the position and type of the created walker particles are also random. Here the occurrence probability of each particle types is equal. The probability also can be adapted to the concentration of each particle type in the practical natural or industrial systems.

The restrictive condition of the particle stickiness can be adapted to different practical condition of the natural and industrial systems. This simulating procedure only sets a simple restrictive condition: the same type of particles can not stick together. That means for the particles with different type once they collide they will stick together and form points for new clusters. The process of restrictive condition controlling particle stickiness is shown in the Figure 5.1.

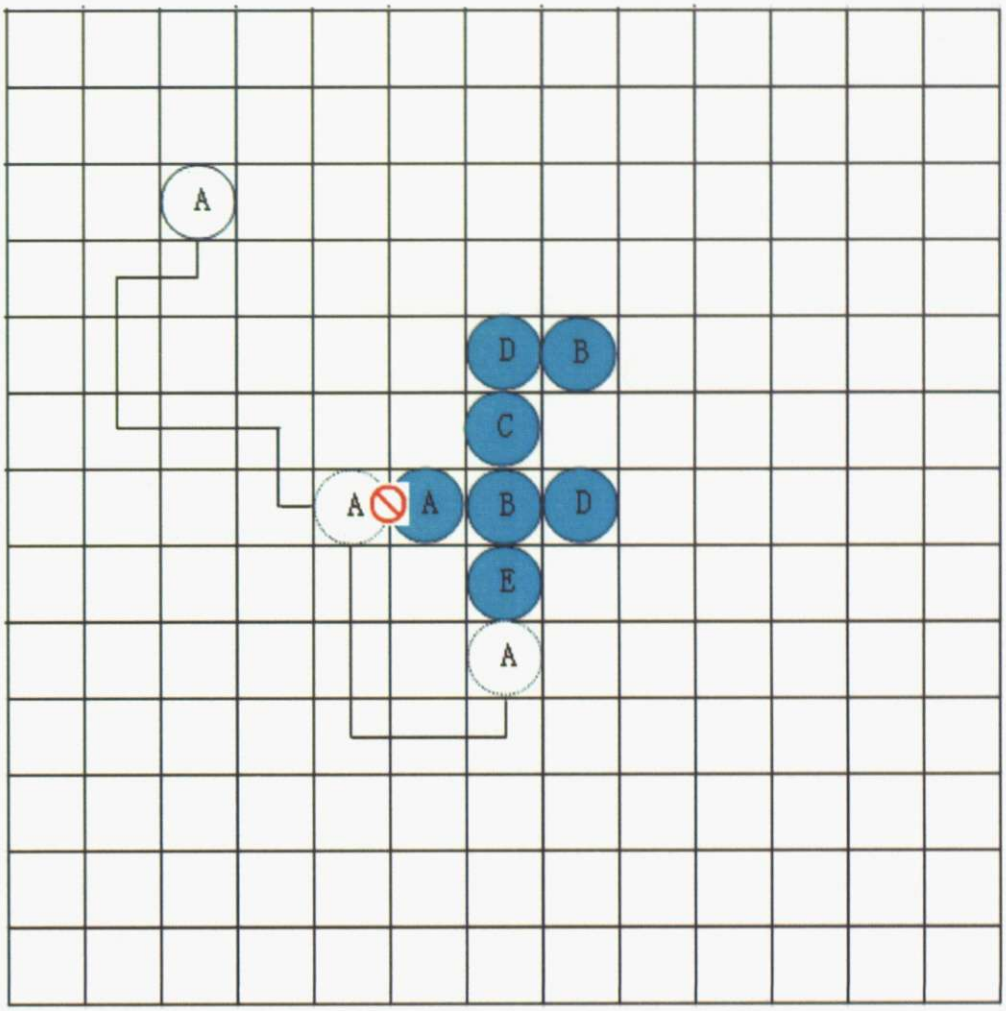

Fig. 5.1 The diagram of restrictive condition controlling the particle stickiness

The simulation procedure of the multi-types DLA model is based on that of traditional DLA model in which particles also perform the random walking (Brownian motion) until they stick to other particles or clusters and form points of the new clusters. But once the collision occurs, it should judge whether the particle meets the restrictive condition. If yes, a bond will occur; if not, it will go on the Brownian motion. For example, in the Figure 5.1, if particle of type 'A' collide with other type 'A' particles, they cannot stick together. So this particle has to go on Brownian motion until it sticks to another particle of other types.

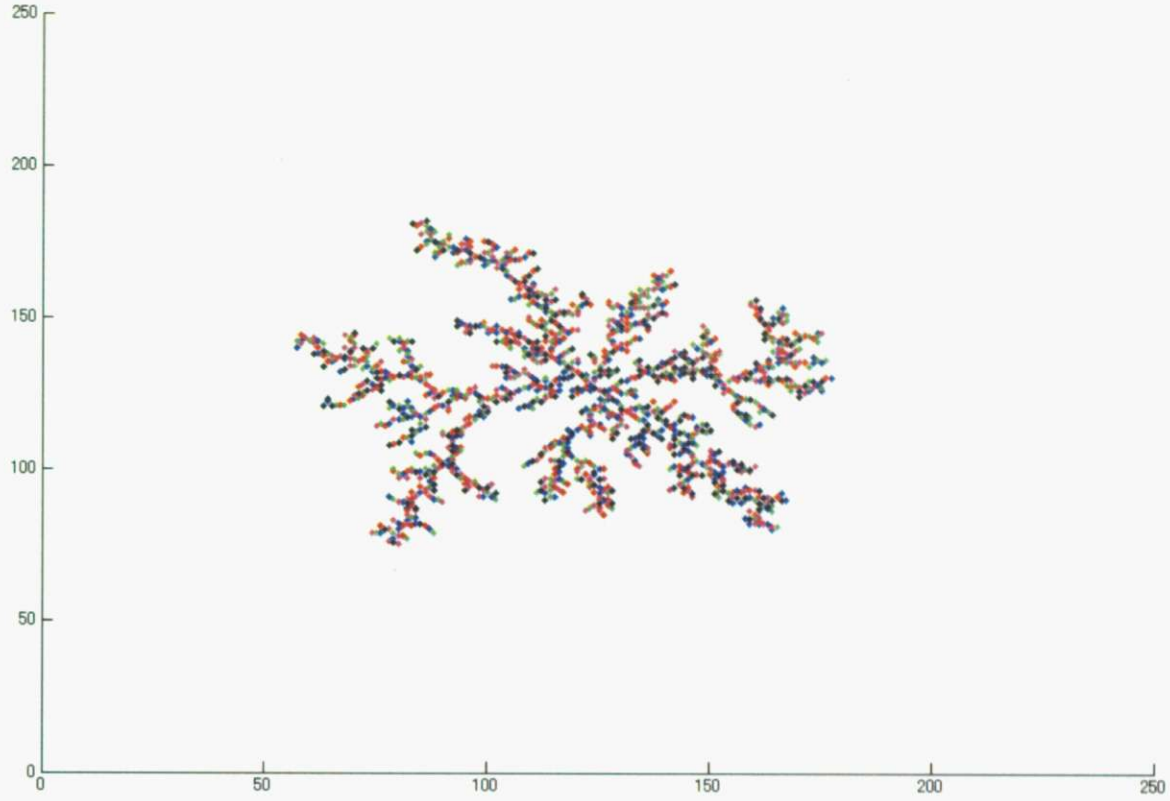

Fig. 5.2 Simulation result of the Multi-types DLA model

Figure 5.2 shows a simulation result of the Multi-types DLA model within a squared lattice of 250 by 250. This simulation is performed by 30000 particles and results in a branch structure aggregate containing 1341 particles. The fractal dimension of this aggregate is 1.5661. This aggregate also has obvious shielding effect.

5.2 Multi-types RLA

As the same as the rule in multi-types DLA model, a 'type' property also added to each particle to control how particle stick together when they collide in this multi-types RLA model. The particle type property, type color, type restrictive condition and other conditions are the same as that in the multi-types DLA model shown in the above table.

But it is different from the above models, for the stationary seed, it is not only one particle but a cluster, which contains five particles of five types. These fiver particles are

arranged together in a line and fixed in the center of the squared lattice as a cluster seed to which following particles stick. This setting can make sure the stickiness probability of each type particle is equal.

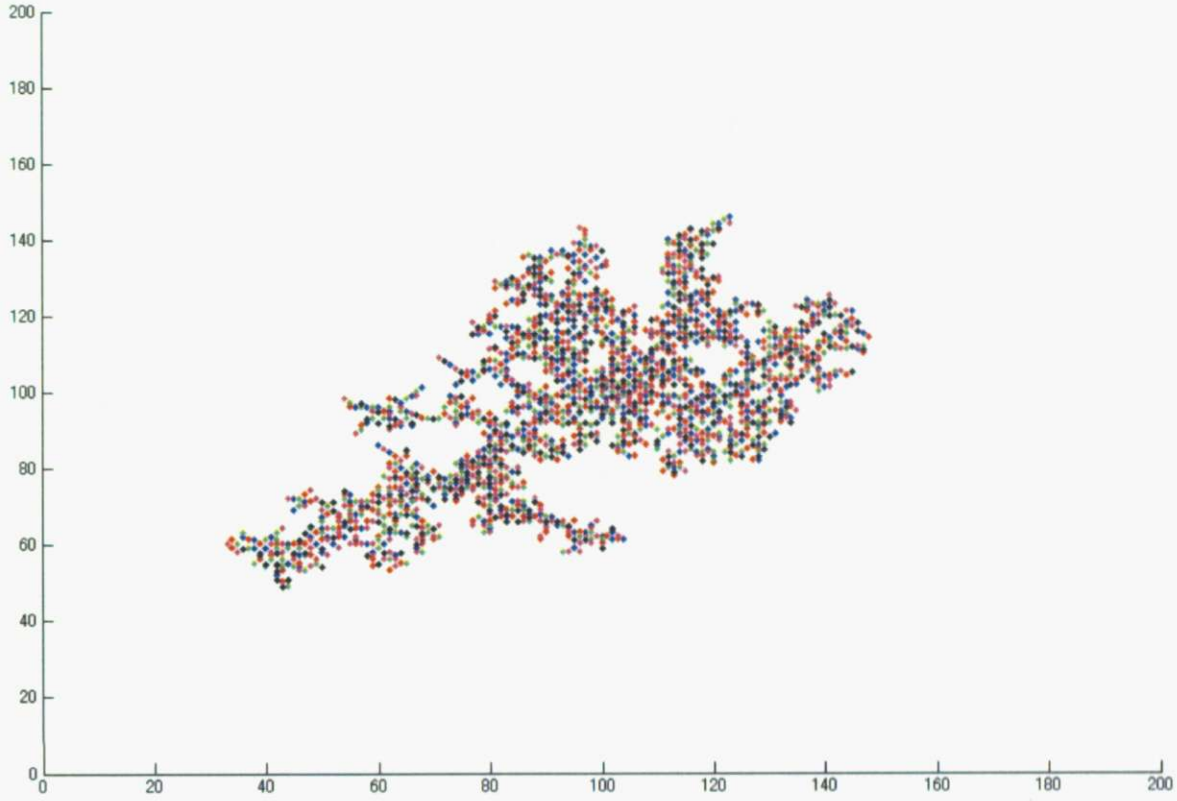

Fig. 5.3 Simulation result of the Multi-types RLA model

Figure 5.3 shows a simulation result of the Multi-types RLA model within a squared lattice of 200 by 200. This simulation is performed by 40000 particles with stickiness possibility of 0.10 and results in a branch structure aggregate containing 1858 particles. The fractal dimension of this aggregate is 1.6342.

Chapter 6

Simulation results and discussion

In this chapter, the simulation results and data of each model will be shown and discussed. The comparisons of the result between different models also will be made and analyzed. A method of selecting the calculated values with higher reliability and veracity in this simulation and calculation process will be also explained.

6.1 Simulation results of DLA model

Because the simulation particles are released randomly and perform the random walking, we need to investigate the influence of the simulation time on the aggregate structure and fractal dimension of the aggregate. Figure 6.1 shows the simulation results of different simulation times: fifteen times and thirty times in the DLA model. The simulation particle number and fractal dimension are shown in the Table 6.1. The diagram indicates that the average fractal dimension value of fifteen times' simulation is similar to that of thirty times. Hence, all the simulation programs will be performed for 15 times to obtain the average value of the fractal dimension.

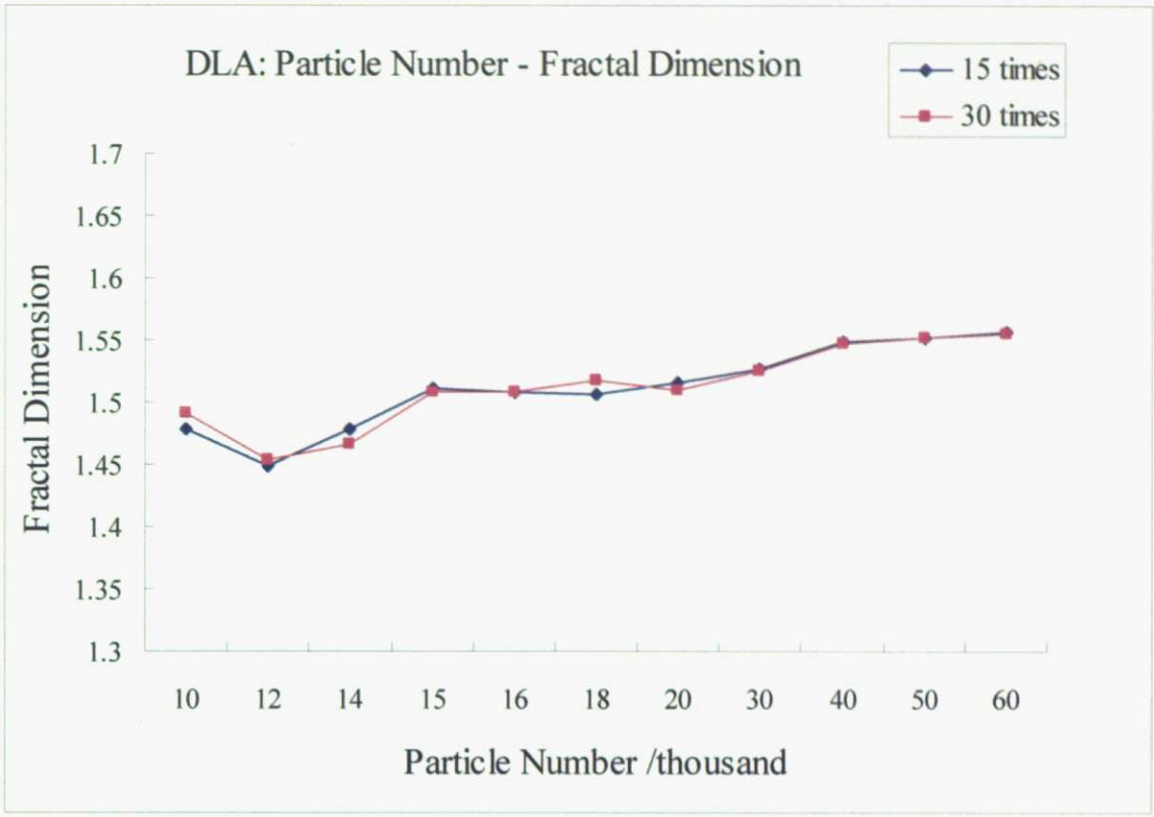

Fig. 6.1 Relationship between simulation times and fractal dimension in DLA mode

Table 6.1 Fractal dimension value of different simulation times in DLA model

Simulation Particle Number	Fractal Dimension	
	Simulating 15 times	Simulating 30 times
10000	1.4774	1.4899
12000	1.4477	1.4524
14000	1.4779	1.4655
15000	1.5113	1.508
16000	1.5079	1.5083
18000	1.5065	1.5169

20000	1.515	1.5093
30000	1.5258	1.5249
40000	1.5481	1.5474
50000	1.5519	1.5522
60000	1.5567	1.5548

The curve in the Figure 6.1 presents the stationary trend increasing the simulation particle number; this implies that the fractal dimension will almost retain a constant when simulation particle number increases along. This also indicates the obvious shielding effect of the branched aggregate in the DLA model.

6.2 Simulation results of RLA model

6.2.1 Relation between stickiness possibility and fractal dimension

In order to investigate the influence of stickiness possibility on the fractal dimension of the aggregate, the program will be performed with different stickiness possibility from 0.1 to 1.0. The total released simulation particles are twenty thousand in the simulation program. Figure 6.2 shows the relationship between the stickiness possibility and fractal dimension in RLA model. Each of the fractal dimension value with different stickiness possibility is shown in the Table 6.2.

From Figure 6.2, fractal dimension of RLA aggregate structure has somewhat change with increasing the stickiness possibility. The bigger stickiness possibility leads to the bigger fractal dimension generally. But this change is so small. This may be because of the less simulation particles and bigger stickiness possibility. This situation will be investigated in the future simulation work.

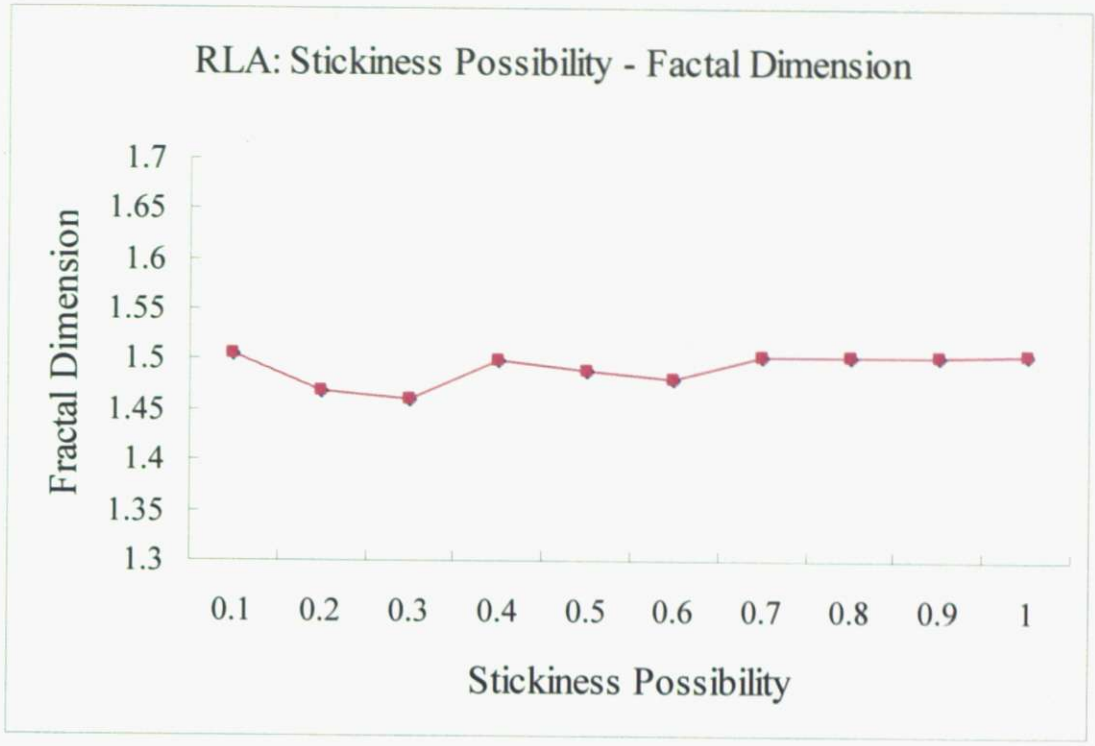

Figure 6.2 Relation between stickiness possibility and fractal dimension in RLA model

Table 6.2 Fractal dimension value of aggregate resulted in different stickiness possibilities

stickiness possibility	Fractal Dimension
0.1	1.5061
0.2	1.4674
0.3	1.4603
0.4	1.4995
0.5	1.4877
0.6	1.4796
0.7	1.504
0.8	1.5036
0.9	1.5039
1	1.5042

When the stickiness possibility is equal to one, RLA model will change to DLA

model. From this aspect, the aggregation structure will become more and more ramified and open with the stickiness possibility increasing.

6.2.2 Relation between simulation particle number and fractal dimension

In order to investigate the relationship between the simulation particle number and the fractal dimension, the simulation program of RLA model will be performed with different released simulation particles. Figure 6.3 shows the simulation result with the stickiness possibility of 0.5.

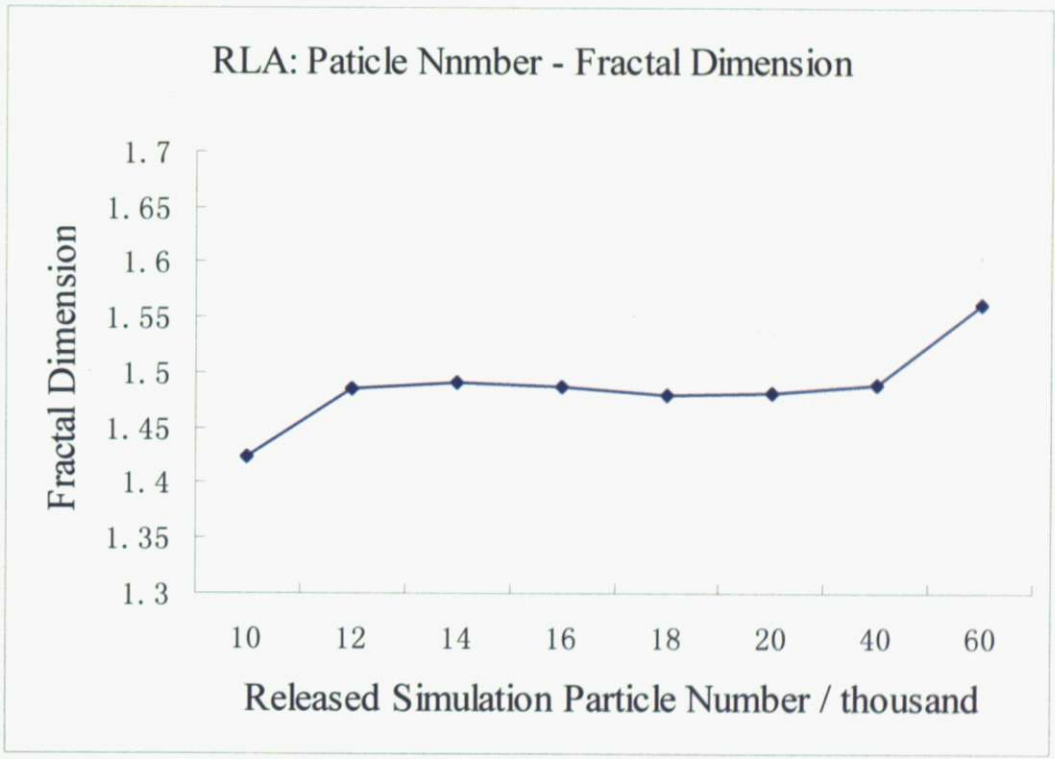

Fig. 6.3 The relation between fractal dimension and released simulation particle number in RLA model

The fractal dimension values of the aggregate structures are shown in the Table 6.3.

Table 6.3 Fractal dimension of aggregate structure resulted from different released particle number

Particle Number /thousand	Fractal Dimension
10	1.4242
12	1.4854
14	1.491
16	1.4866
18	1.48
20	1.4805
40	1.4879
60	1.5616

From the Figure 6.3, the value of fractal dimension has less change when the number of released simulation particle is less than forty thousand. But is has a obvious increase when the number of released particles increases from forty thousand to sixty thousand. This will be a valuable property that can be used in some industrial fields. This will be investigated further in the future work.

6.3 Comparing the result of DLA and RLA

Firstly, let us see the two images of the simulated aggregate structure of DLA model and RLA mode. The simulation results of the DLA model and RLA model, with the same number of released simulation particles are shown in the Figure 6.6.

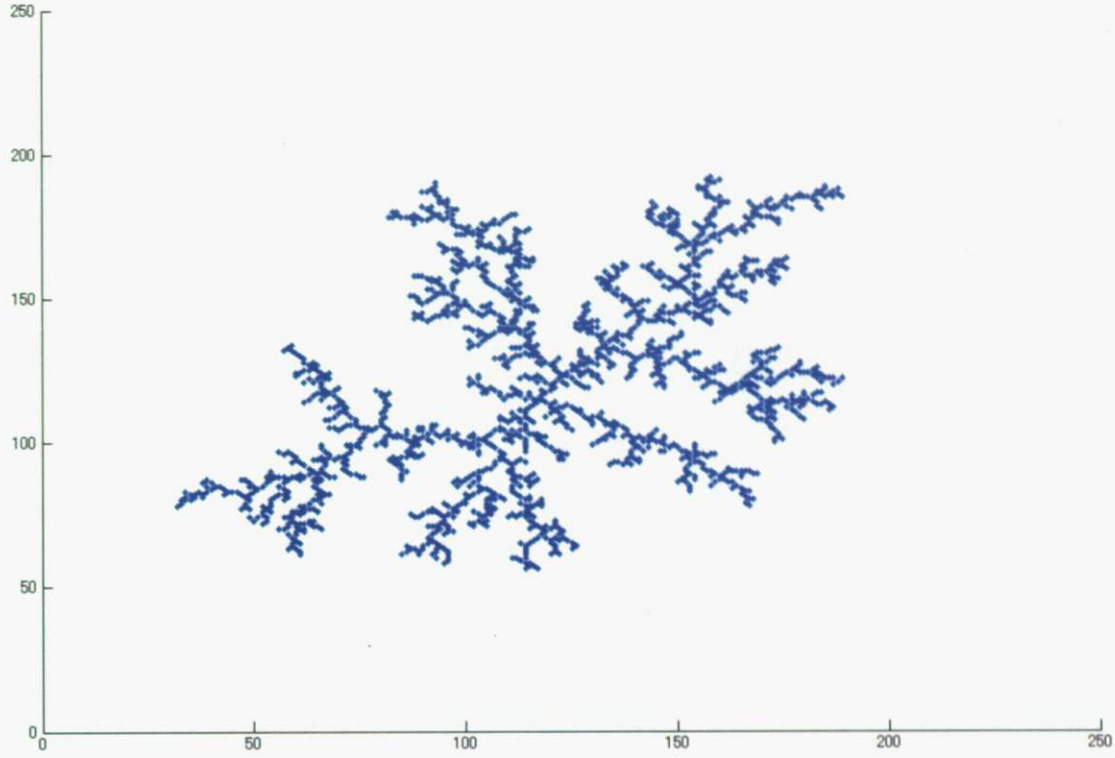

Fig. 6.4 Simulated aggregate structure in the DLA model resulted from 30000 released simulation particles

For the image in the Figure 6.4, the simulation region is set in a two dimensional squared lattice of 250 by 250; the total number of released simulation particles is 30000.

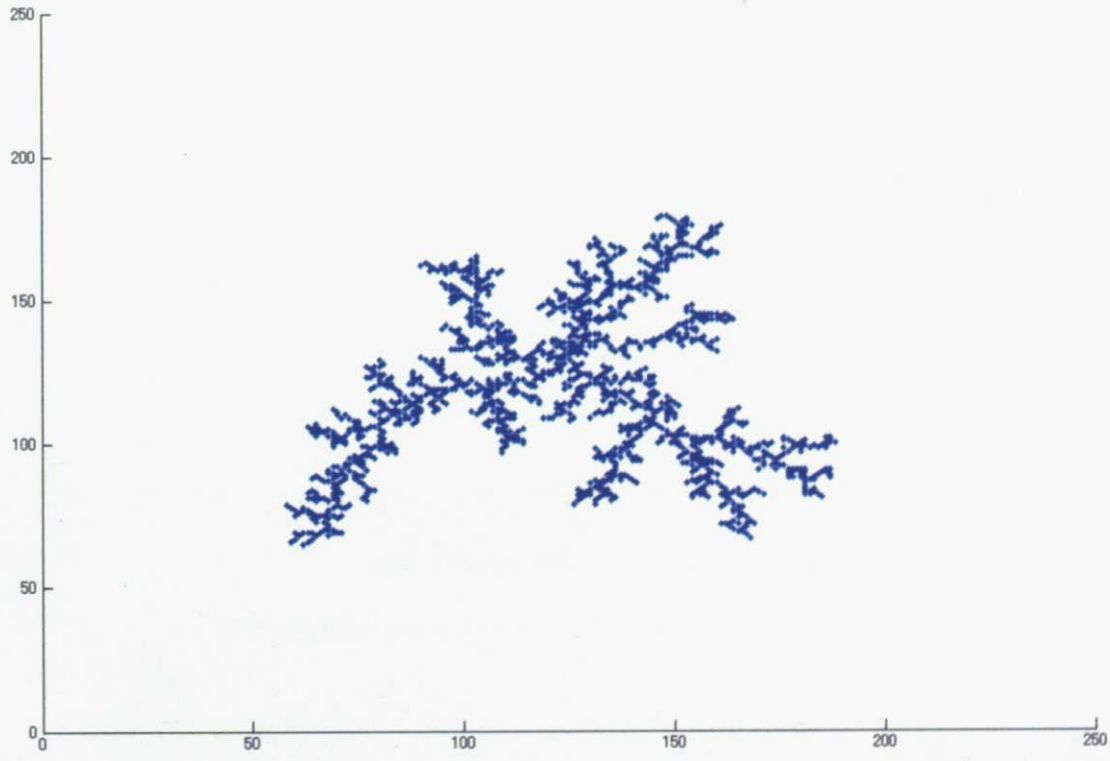

Fig. 6.5 Simulated aggregate structure in the RLA model resulted from 30000 released simulation particles with the stickiness possibility of 0.5

For the above image, the simulation region is set in a two dimensional squared lattice of 250 by 250; the stickiness possibility of simulation particles is 50% and the total number of released simulation particles is 30000.

From the above two figures, it seems that the density of the aggregate structure formed in the RLA model is bigger than that formed in the DLA model. Bur the Figure 6.6 shows that most of the fractal dimensions calculated by the box-counting method of DLA model are little bigger than that of the RLA model. This indicates that the aggregate form in DLA model is more dense.

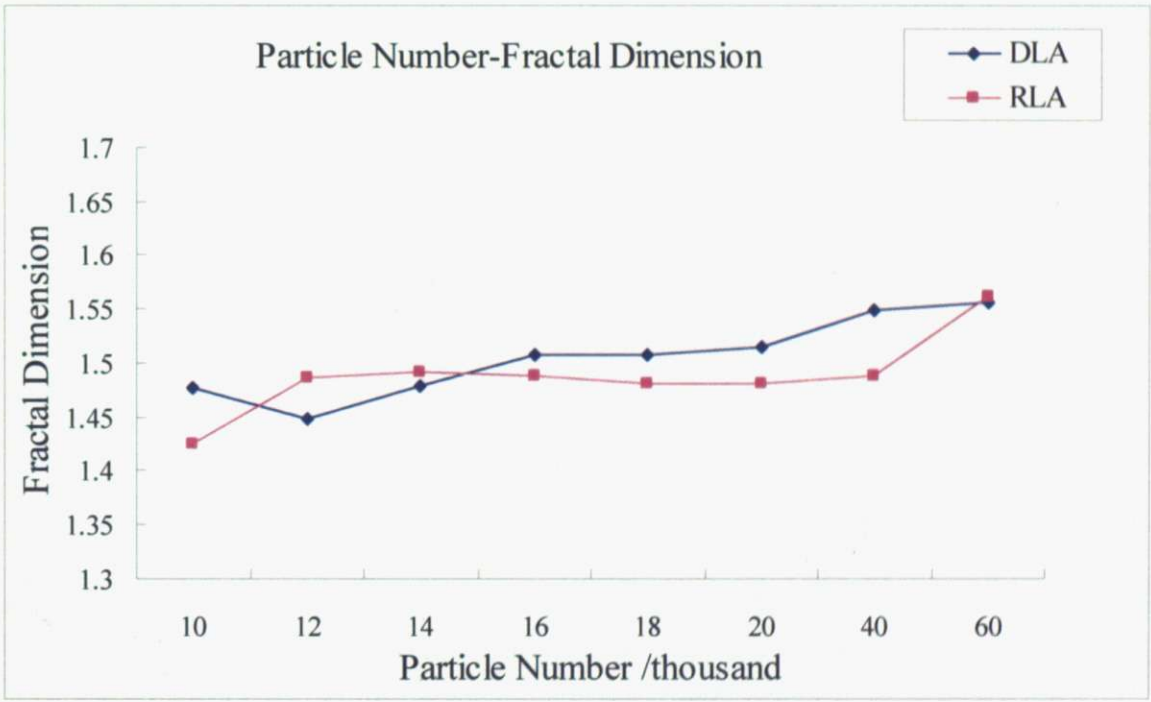

Fig. 6.6 Fractal dimension of DLA and RLA model changes with the total released particle number
(the stickiness possibility in RLA model is 0.5)

The numbers of particles contained in different radiuses' circles, which centre is set in the position of the seed particle, are shown in the Table 6.4. All of these aggregates are simulated by 20000 released particles.

Table 6.4 The number of particles contained in different radiuses' circles

Radius	DLA	RLA									
		Different Stickiness Possibility									
		0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
2	9	18	16	13	12	12	11	10	10	10	10
4	25	49	39	35	29	30	28	26	25	25	23
8	72	147	113	94	85	81	80	77	70	69	64
16	207	399	326	293	257	247	235	218	213	208	188
32	594	631	699	704	705	678	639	624	626	610	604

From the Table 6.4, for every stickiness possibility, the number of particle contained in the same radius of circle in the RLA model is bigger than that in the DLA model. This means that the aggregate structure formed in the RLA model is much denser than the aggregate structure formed in the DLA model. This agrees with that the image shows.

Why does the fractal dimension reflect different result?

1) This seems to present that the total number of released particles is not enough to eliminate the random effect.

2) When calculating the fractal dimension using the box-counting method, in order to adopt the more credible fractal dimension value, some different calculated values will be selected based on the correlation coefficient. The value with the biggest correlation coefficient will be chosen, which may be a smaller one.

This will be investigated in the future research work.

6.4 Simulation results of the Multi-types DLA model

In order to investigate the relationship between the limiting condition and the fractal dimension of the aggregate structure in the extended DLA model: Multi-types DLA model, a simple limiting condition – the particle of the same type can not stick together is set in the simulation program.

Figure 6.7 shows the relationship between the total released particle number and fractal dimension of the Type DLA model.

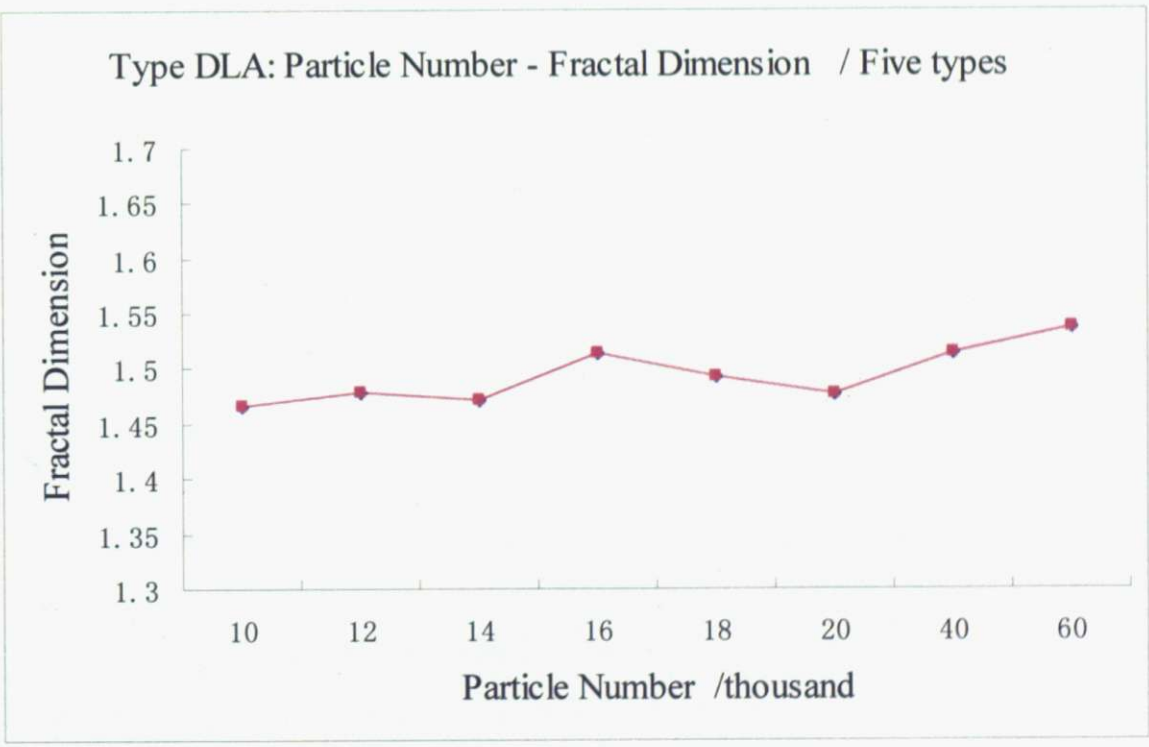

Fig. 6.7 Relationship between the released particle number and fractal dimension of the Type DLA model

From the Figure 6.7, the value of fractal dimension has only somewhat changed. It means that this limiting condition has not remarkable influences on the fractal dimension of the aggregate structure in the Type DLA model. The data of Figure 6.7 are filled in the Table 6.5.

Table 6.5 Fractal dimension values of the aggregates formed by different amounts of released particles in Type DLA

Particle Number	Fractal Dimension
10	1.4652
12	1.4772
14	1.4715
16	1.5139
18	1.492
20	1.4767
40	1.5127
60	1.5369

In order to extend a more useful and effective simulation model, the limiting condition should base on the actual and special condition of the practical field that this extended model can be applied to. Fox example, if want to extend a model to apply in the wastewater treatment, the detail and data about the chemical, physical and biologic condition should be carefully collected and analyzed. Then make the limiting condition in the extended model. This will be investigated in the future work.

6.5 Simulation results of the Multi-types RLA model

The limiting condition and particle type number are the same as that in the Multi-types DLA model. Figure 6.8 shows the relation between the total released particle number and fractal dimension of the Type RLA model.

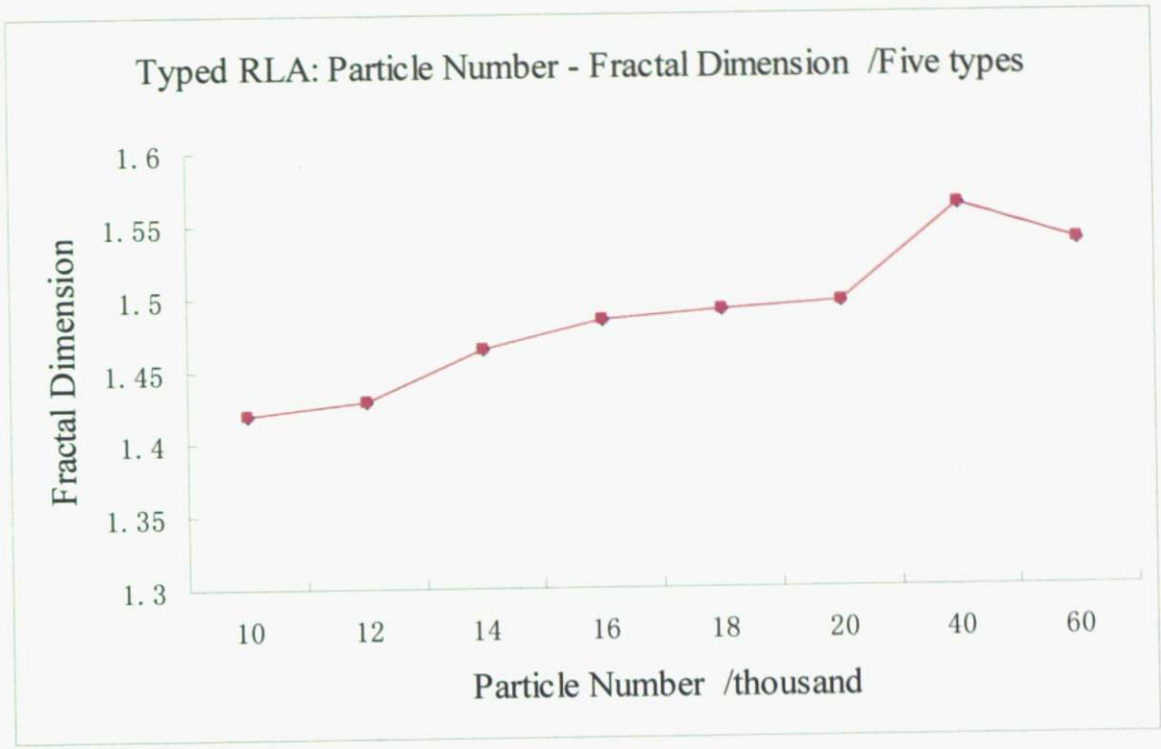

Fig. 6.8 Relationship between the released particle number and fractal dimension of the Type RLA model

From the Figure 6.8, the fractal dimension of the aggregate increase with increasing the number of released simulation particle. The data are shown in the Table 6.6.

Table 6.6 Fractal dimension values of the aggregates formed by different amounts of released particles in Type RLA

Particle Number	Fractal Dimension
10	1.4192
12	1.4287
14	1.4638
16	1.4832
18	1.49
20	1.4956
40	1.5621
60	1.537

Figure 6.9 shows the relationship between the stickiness possibility and fractal dimension in the Type RLA model. The stickiness possibility also differ form 0.1 to 1.0 and the total released simulation particles are twenty thousand in the simulation program. Each of the fractal dimension value with different stickiness possibility is shown in the Table 6.7.

From Figure 6.9, the fractal dimension of different stickiness possibility in Type RLA is shifted bigger around 1.5 and this change is irregular.

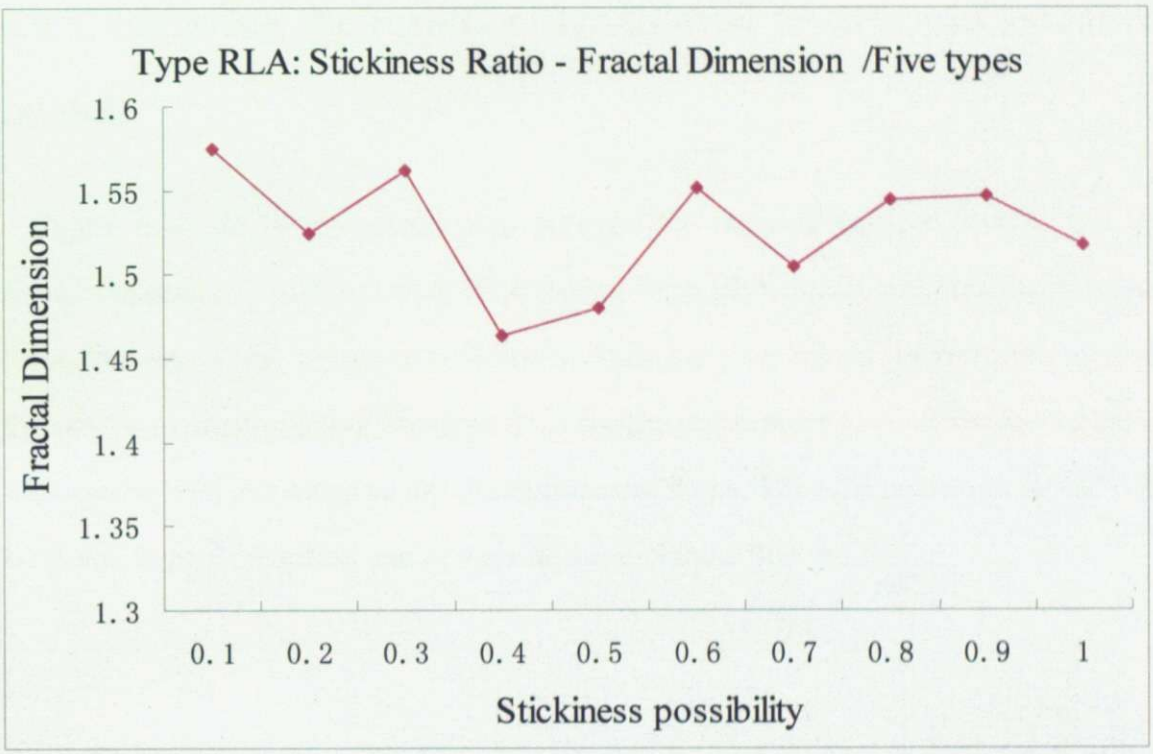

Fig. 6.9 Relationship between the stickiness possibility and fractal dimension in the Type RLA model

Table 6.7 Fractal dimension value of different stickiness possibility in the Type RLA model

Particle Number	Fractal Dimension
0.1	1.5743
0.2	1.5239

0.3	1.5611
0.4	1.4629
0.5	1.479
0.6	1.5506
0.7	1.504
0.8	1.5439
0.9	1.5464
1	1.517

6.6 Comparing the results of traditional models and extended models

Figure 6.10 shows the relationship between the released particle number and the fractal dimensions in DLA model, RLA model, Type DLA model and Type RLA model. From this figure, the curves of different models have somewhat different, but present the similar increasing trend. The type RLA has the much more obvious increasing trend. This can be well explained as the simulation conditions. The type constraint in the Type DLA and Type RLA model can be seen as the stickiness possibility.

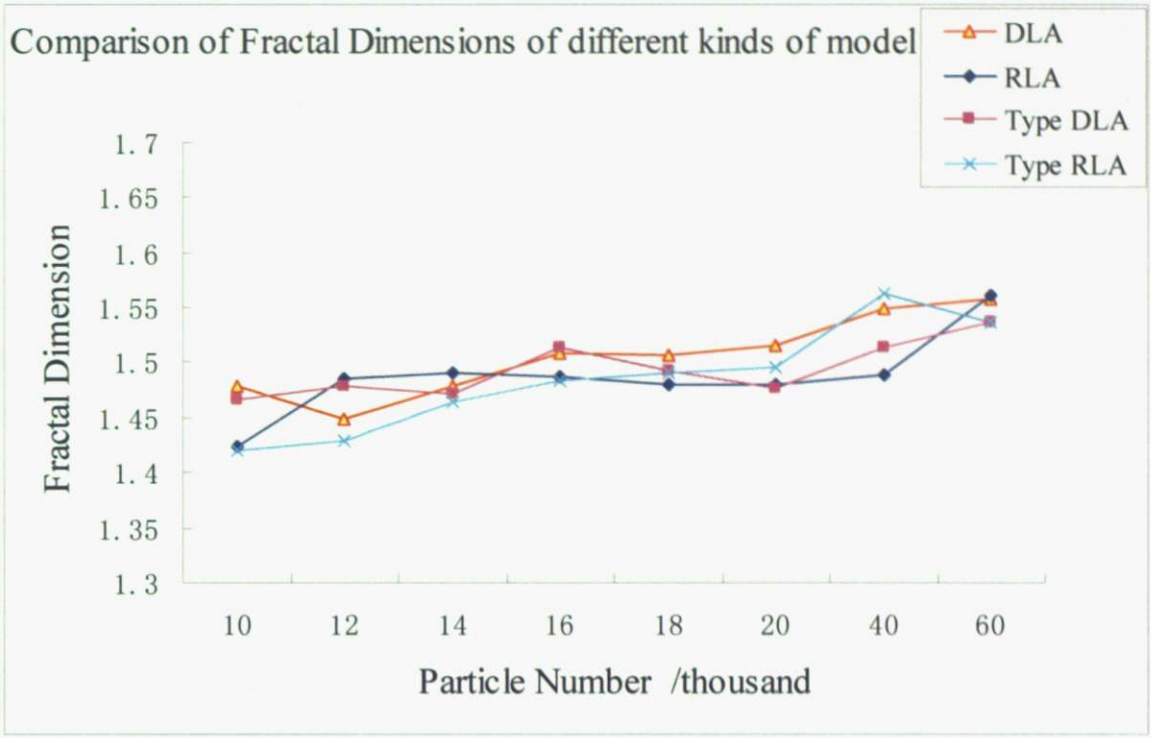

Fig. 6.10 Relationship between the released particle number and the fractal dimensions in DLA model, RLA model, Type DLA model and Type RLA model

6.7 Ensuring the reliability and veracity of the data

How to adopt the data with higher reliability and veracity is the common focus in scientific works.

When calculate the fractal dimension of the aggregate using the box-counting method, we will face on the focus of how to ensure the data's reliability and veracity.

The calculation method of fractal dimension is explained here. For example, in the DLA model, if the number of released simulation is smaller than 30000, we need to calculate five values of the particle number (PN) contained in five circles with the radius of 2, 4, 8, 16 and 32. If there are 60000 released particles, we can calculate seven values of the particle number contained in seven circles. The detailed data are shown in

the Table 6.8.

Table 6.8 Detailed values of one time of simulation with 60000 released particles in the DLA model

Circle Radius	Particle Number (PN)	Fractal Dimension			
		D_1	D_2	D_3	D_4
2	10	1.4925	1.5315	1.5548	1.4962
4	21				
8	67				
16	216				
32	636				
64	1973				
128	3861				

In this case, we need to select a best fractal dimension value D from the four fractal dimension values (**D_1, D_2, D_3 and D_4**) calculated by the anterior four, five, six, seven values of the particle number PN using the least multiply method.

How to select one value from the D_1, D_2, D_3 and D_4 which has the highest reliability and veracity?

Here we can use the value of the correlation coefficient of some values of PN as the selection standard rule. The value of the correlation coefficient (CC) in the simulation is shown in the Table 6.9.

Table 6.9 Correlation Coefficient values

Circle Radius	Particle Number (PN)	Correlation Coefficient			
		CC_1	CC_2	CC_3	CC_4
2	10	0.9979998	0.998572	0.9989844	0.9978659
4	21				
8	67				
16	216				
32	636				
64	1973				
128	3861				

From the Table 6.9, the biggest one is CC_3. It means that the anterior five values of PN have the best linear relation. Based on the value of correlation coefficient, we can select the value of $\mathbf{D_3}$ as the fractal dimension of the aggregate in this time of simulation.

Chapter 7

Conclusion

The present study of the theory and knowledge of colloid particle collision, aggregate dynamic growth, fractal theory and fractal simulation model let the author understand and have the interest in researching the aggregates' growth process and which fractal property and founding the model to simulate such cluster dynamic growth process.

In the previous research, the author simulated the particle aggregating process using the traditional models and the extended models and got the relational result. Analyzing and discussing these results leads to the following conclusions:

1) In the DLA model, there are somewhat change of fractal dimension with increasing the released simulation particle number. When the number of the released simulation particle is more than forty thousand, the fractal dimension will shift smaller around 1.55. This indicates the obvious shielding effect of the aggregate formed in the DLA model.

2) In the RLA model, the bigger stickiness possibility will lead to the bigger fractal dimension generally. But this change is so small that may because of the less released simulation particle in the program and the bigger interval of the stickiness possibility.

3) In the RLA model, the fractal dimension has somewhat change when the number of the released simulation particle differs from twelve thousand to forty thousand. But when the number is bigger than forty thousand the fractal dimension will increase obviously.

4) Comparing the simulation result of the DLA model with the RLA model, both of the image of simulated aggregate structure and the numbers of particle contained

in different radiuses of circle indicate that the density of the aggregate formed in the RLA model is bigger than that in the DLA model using the same number of released simulation particle. But the fractal dimension calculated using the box-counting method shows the contrary result. The possible reason of such difference has been discussed in the above chapter and this situation will be investigated in the future work.

5) In the extended Type DLA model, the limiting condition that control the particle stickiness in this program seems not especial influence on the fractal dimension. To develop this extended model, the limiting condition should base on the special condition of the practical field that this extended model can be applied to.

6) Comparing the relationship between the released particle number and the fractal dimension in DLA model, RLA model and Type DLA model, the relationship curve of the Type RLA has much more obvious increasing trend. The type constraint in the extended model can be seen as the stickiness possibility that leads to the Type RLA has duple limits of 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 dynamic growth 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.

Complementing the former investigations and simulation results, this study provide an enough overview to integrate the available simulation models taking into account of more natural, industrial and scientific fields, such as the chemical, electrical and environmental engineering fields and so on. It is also helpful to extend the suitable models applied in some special fields such as the colloid collision system, wastewater treatment plant and so on.

Chapter 8

Directionality of the Future Research

The research that has been done during the master course is one part of the final research of environment simulation. The research purpose during the master course is to develop basic simulation codes on the aggregate growth which is one of key processed of contamination and decontamination. The future research plan in the earlier period of the doctor course is shown below.

1) Select a set of experimental data from the specific application systems, such as the colloid diffusion and deposition, water pollution and so on. These data should include the aggregate structure characteristics and the physical and chemical properties, such as the solution temperature, particle type, particle concentration, particle size, interparticle forces, chemical reactions properties, and so on.

2) Compare these selected experimental data with the simulation results and evaluate the models developed in his research through qualitative reasoning as pattern formation as well as parametric studies in terms of underlying mechanisms.

3) Articulate the research agenda on how to control aggregate growth by taking advantage of available simulation models and data, paying attentions on the aggregate structure characteristics such as the fractal dimension, aggregate structure shape and so on.

4) Develop an inverse problem solving approach to bridge given experimental data in terms of available models and adaptive reasoning.

5) Propose a set of practical methods to control aggregation growth with respect to typical environmental conditions such as temperature, colloid characteristics, surfaces and so on.

Reference

[1] Rajat K. Chakraborti, Kevin H. Gardner, Joseph F. Atkinson and John E. Van Benschoten, Water Research 37, 873-883 (2003)

[2] Jackson, G. A., and Lochmann S. E., Effect of coagulation on nutrient and light limitation of an algal bloom, Limnology and Oceanography, 37: 77-89 (1992)

[3] S. Harada, R. Tanaka, H. Nogami and M. Sawada, J. Colloid Interface Sci. 301, 123-129 (2006)

[4] Tucker, M., Sigafoos, J. and Bushell, H., Use of noncontingent reinforcement in the treatment of challenging behavior, BehaviorModification, 22, 529–547 (1998)

[5] S. Tang, J. M. Preece, C. M. McFarkane and Z. Zhang, J. Colloid Interface Sci. 221, 114-123 (2000)

[6] Vold J. M., Journal of Colloid Science, 18, 684-695 (1963)

[7] P. Meakin, Phys. Rev. A 27, 1495 (1983)

[8] T.A. Witten and L.M. Sander, Physical Review Letter 47, 1400 (1981)

[9] JiZhong Zhang, Fractal, Tsinghua University Press, 166-187 (1995)

[10] Venkataramana Runkana, P. Somasundaran and P. C. Kapur, American Institute of Chemical Engineers, Vol. 51, No. 4, 1233-1245, April (2005)

[11] R. Jullien and M. Kolb, J. Phys. A17, L639 (1984)

[12] M. Kold and R. Jullien, J. Phys. Lett. 45, L977 (1984)

[13] Edward Kostansek, JCT Research, Vol. 1, No. 1, 41-44, January (2004)

[14] Botet, R. and Jullien, R., J. Phys. A: Math. Gen., 17, 2517 (1984)

[15] Derjaguin, B. and Landau, L., Acta Physicochim., USSR, 14, 633 (1941)

[16] Vervey, E. and Overbeek, J., Theory of the Stability of Lyophobic Colloids, Elsevier, Amsterdam, the Netherlands (1949)

[17] Barnsley, Michael F. and Hawley Rising, Fractals Everywhere, Boston: Academic Press Professional, ISBN 0-12-079061-0 (1993)

[18] Falconer Kenneth, Techniques in Fractal Geometry, John Willey and Sons, ISBN, 0-471-92287-0 (1997)

[19] Albert-Laszlo Barabasi and H. Eugene Stanley, Fractal Concepts in Surface Growth, Cambridge University Press, 29-37 (1995)

[20] Rajat K. Chakrabortia, Kevin H. Gardner, Joseph F. Atkinson, John E. Van Benschoten, Water Research 37, 873-883 (2003)