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Fractals in two-dimensional model of colored diffusion-limited aggregation

V. Tchijov, J. Keller Torres, and S. Rodríguez-Romo
Centro de Investigaciones Teóricas
Universidad Nacional Autónoma de México, Campus Cuautitlán
Apartado postal 95, Cuautitlán Izcalli, 54768 Edo. de México, Mexico

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Abstract. A two-dimensional model for random diffusion-limited aggregation of particles of two different types (colors A and B) on a square lattice is studied by computer simulation. Two parameters are essential to the model—the distance d between two initial seed particles, and the probability p for a randomly moving particle to be A-colored. Intensive numerical experiments are carried out for different values of d and p. The competing growth of two-colored fractal structures exhibit significant instability at $p = 0.5$ and small d which leads to a noticeable number of non-symmetric aggregates. Quantitative characteristics of clusters such as their fractal dimension, coordination number, and averaged ratio of the number of A- and B-colored particles in two-colored aggregates are calculated.

Resumen. En este artículo se estudia un modelo bidimensional de agregación al azar de dos tipos diferentes de partículas (colores A y B) limitado por difusión, en una rejilla cuadrada, usando para ello simulación por computadora. Existen dos parámetros esenciales en el modelo: la distancia d entre dos partículas iniciales llamada semillas y la probabilidad p de que una partícula que se mueve al azar sea de color A. Se realizaron númerosos experimentos computacionales para diferentes valores de d y p. La competencia en el crecimiento de las estructuras fractales bicolores exhibe inestabilidad significativa cuando $p = 0.5$ y d pequeña, lo cual conduce a un número notable de agregados no simétricos. Se calculan algunas cantidades características de los cúmulos, tales como dimensión fractal, número de coordinación y relación promedio del número de partículas de los dos colores.

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1. Introduction

Diffusion-controlled cluster formation, or diffusion-limited aggregation (DLA), is a non-equilibrium irreversible growth process that gives rise to low-density random fractal objects. A wide variety of phenomena in nature and human activities lead to formation of the DLA aggregates: metal-particle aggregation, coagulation of aerosols, crystal growth governed by heat diffusion, solidification of alloys, electrodeposition, electrical breakdown of dielectrics, fluid flow in porous media, moving interface between liquids of different viscosities (viscous fingering), secondary oil recovery, etc. [1–3].

Various models of the growth of such aggregates have been proposed and studied so far. The simplest one is the lattice model of Eden [4] in which particles are added at random, one by one, to the nearest neighbors of already occupied sites. The Eden model leads to a relatively compact cluster while a large number of experimental observations of the DLA growth phenomena indicate structures whose density correlation falls off as a fractional power of distance. The DLA model that reproduces experimentally observed structures was proposed by Witten and Sander in 1981 [5]. In this model, one seed particle forms the initial aggregate. Other particles appear a long distance from the aggregate and perform a Brownian motion (simple random walk) on a lattice until they come in contact with the structure and attach to it, or "die" having wandered far away from the cluster. It was shown [5] that this model exhibits a fractional power-law behavior of a density-density correlation function.

Since 1981, a great deal of investigations was carried out developing and expanding the original DLA model. The subjects of studies were: on-lattice and off-lattice models, scaling properties and large scale effects, fractal dimension and symmetry of DLA structures, cluster-cluster aggregation, etc. [6–22]. Though easy enough to formulate, the DLA phenomenon was found very difficult to study theoretically. One possible approach is based on hitting probabilities of moving particles [23, 24] and involves computer simulations. In fact, the main means of getting quantitative information on the DLA cluster growth still involves computational experiments.

A new model of diffusion-limited aggregation called the Colored DLA model was developed in Ref. 25 which adds a new feature to the original model of Witten and Sander—the competing growth of two fractal objects. In Ref. 25, the structure of the interface between these objects was the main subject of investigation. In the present paper, we report on intensive numerical studies of the two-dimensional Colored DLA model. We pay particular attention to the influence of the two parameters of the model on fractal growth—distance d between two initial seed particles and probability p for a randomly moving particle to be A-colored. We present a qualitative description and quantitative analysis of the two-dimensional fractal structures in the Colored DLA model.

2. Colored DLA model

Following Ref. 25, let us introduce the Colored DLA model in two-dimensional space. Two particles of two different types (colors) A and B are put on a square lattice at distance d from each other, with the origin of the Cartesian coordinate system at the middle point between the particles. A long distance from this initial aggregate, at a random point on a circumference S_0 of radius $R_0 \gg d$ a new particle is added, with the probability p of being A-colored and probability $(1-p)$-B-colored. This particle then performs a Brownian motion (*i.e.*, simple random walk) on a lattice. If it reaches any site of the lattice located at distance $R_d \gg d$ from the origin, it is "killed" and a new particle starts off at a random point on the circumference S_0, with the probability p of being A-colored. The rules of interaction between particles are defined as follows. If the particle reaches the point adjacent to the aggregate of the same color, it becomes a part of the growing cluster. This rule is similar to the one of the original DLA model of Witten and Sander. However, if the particle reaches the point next to any particle of the cluster of a different color, it is "killed." The procedure is repeated until clusters of sufficient sizes are formed.

Two parameters are essential to the model: the distance d between two initial seed particles and the probability p for the particle to be A-colored. Clearly, for the reasons of symmetry it suffices to restrict the study to the case $0 < p \leq 0.5$. The question of our main interest is the influence of these parameters on the fractal growth phenomenon.

In our computational experiments we utilized the procedure of the particles' generation proposed in Ref. 6. We chose R_d and R_0 to be equal to $kR_{\max}$ and $R_{\max} + \Delta R$, respectively, where $k = 3$, $\Delta R = 10$ lattice units, and $R_{\max}$ is the maximum distance of particles in both clusters from the origin. Thus, distances at which particles are added or "killed" change dynamically in the process of clusters' formation. To speed up the calculations we multiplied the elementary step of diffusing particle by factors 2, 4, 8, etc., whenever the particle was at distances $R_{\max} + 10$, $R_{\max} + 20$, $R_{\max} + 40$, etc., from the origin [6].

Our programs were written in Borland C++ and run on 66 MHz Pentium system. We considered the following values of the distance d between the two initial particles and of the probability p for a particle to be A-colored: $d = 2$, 10, 40 and 100 lattice units and $p = 0.1$, 0.2, 0.3, 0.4 and 0.5. For each pair of d and p we generated the ensemble of 25 to 100 two-colored fractal structures containing 3000 particles in the largest cluster of the two. Some calculations were duplicated on a Silicon Graphics workstation to produce aggregates of up to 30 000 particles. The structures obtained were qualitatively the same as those of 3000 particles (see below).

The results of our computer simulations of two-dimensional Colored DLA model are presented in the next section.

3. TWO-DIMENSIONAL FRACTAL STRUCTURES

Firstly, we present a qualitative description of fractal structures obtained in our computational experiments.

For equal probability of generation of the color of a particle (*i.e.*, in the case $p = 0.5$) cluster structures are almost symmetric for distances between initial seed particles $d = 100$. Figure 1 displays a typical structure. All of the 100 experiments performed for $p = 0.5$, $d = 100$ exhibit the aggregates looking very much like the one presented in Fig. 1.

The picture is completely different when $p = 0.5$ and $d = 2$. We have found that among the 100 computational experiments conducted for this pair of parameters, three typical structures occur: aggregates that may be called "symmetric" (containing approximately an equal number of particles (Fig. 2a), structures in which one of the fractals develops as "a branch" (Fig. 2b) and, finally, two-colored aggregates in which one of the clusters suppresses the growth of the second one (Fig. 2c). The growth of one cluster was suppressed by the other in the 7% cases. This remarkable fact is intrinsically embedded in the two-colored DLA model and points out a significant instability of the competing cluster formation in the case $p = 0.5$, $d = 2$.

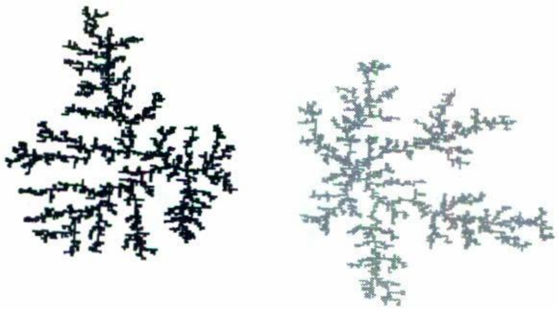


FIGURE 1. A typical structure for $p = 0.5$, $d = 100$.

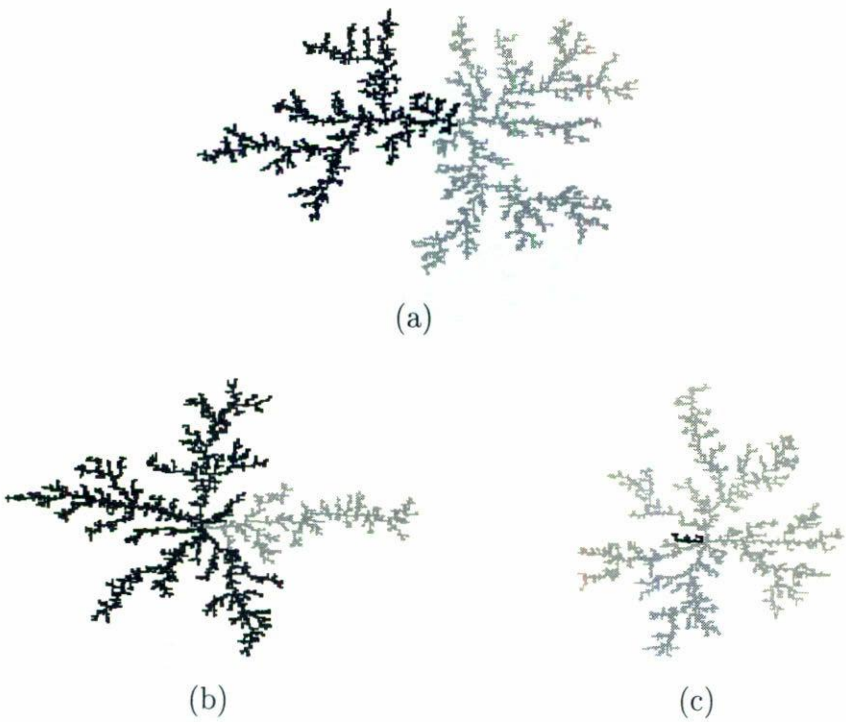
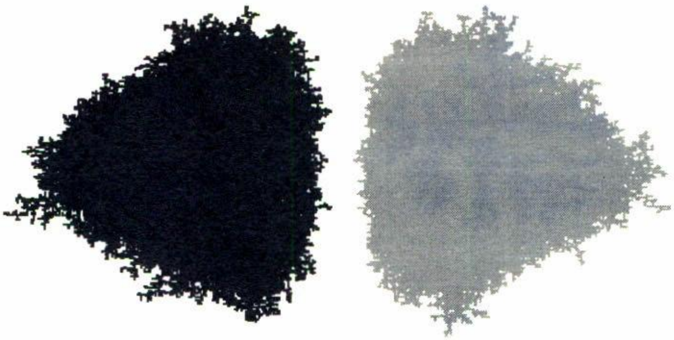


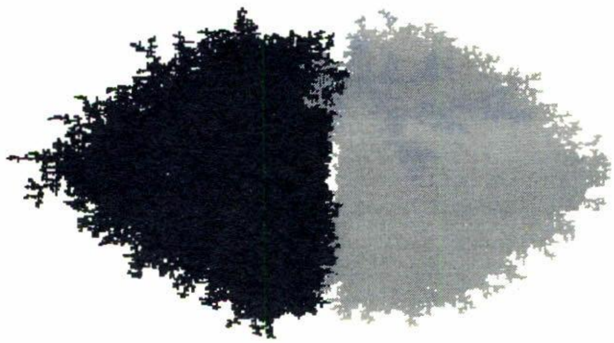
FIGURE 2. Three different representative cluster aggregates for $p = 0.5$, $d = 2$: (a) "symmetric" structure; (b) "branched" structure; (c) one cluster is suppressed by the other.

Figure 3 shows the superposition of one hundred two-colored cluster structures for $p = 0.5$, $d = 100$ (Fig. 3a) and $p = 0.5$, $d = 40$ (Fig. 3b). The superposition shows a triangular profile of a picture rather than a circular one, indicating that clusters' fingers extend faster in the direction along the axis connecting two initial particles. A similar phenomenon has been discovered by Ball and Brady [9] in the superposition of clusters of the original DLA model.

For comparison, twenty five two-colored aggregates have been superimposed for $p = 0.3$, $d = 100$ and $p = 0.3$, $d = 40$ (Fig. 4a and 4b, respectively). Similarly, for the low

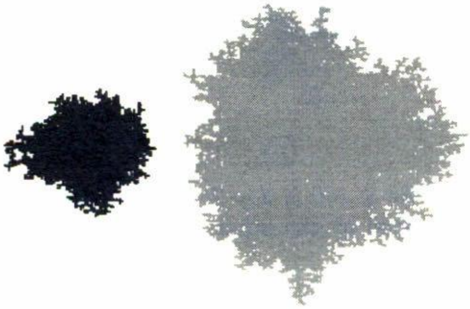


(a)

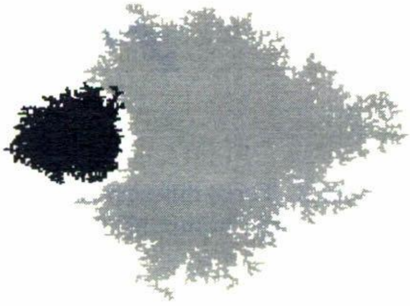


(b)

FIGURE 3. Superposition of 100 two-colored aggregates: (a) $p = 0.5$, $d = 100$; (b) $p = 0.5$, $d = 40$.



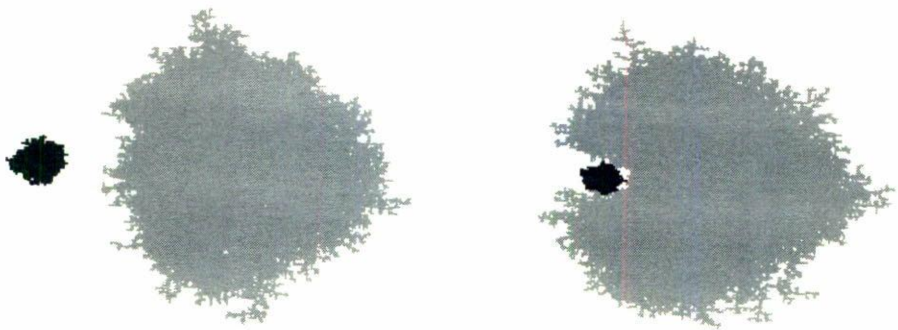
(a)



(b)

FIGURE 4. Superposition of 25 two-colored aggregates: (a) $p = 0.3$, $d = 100$; (b) $p = 0.3$, $d = 40$.

value of the probability for a particle to be A-colored, $p = 0.1$, one hundred aggregates have been superimposed for $d = 100$ (Fig. 5a) and seventy three for $d = 40$ (Fig. 5b). The pictures, of course, are no longer symmetric with respect to both fractals. Figures 4 and 5 show how B-colored clusters "embrace" A-colored ones.



(a) (b)

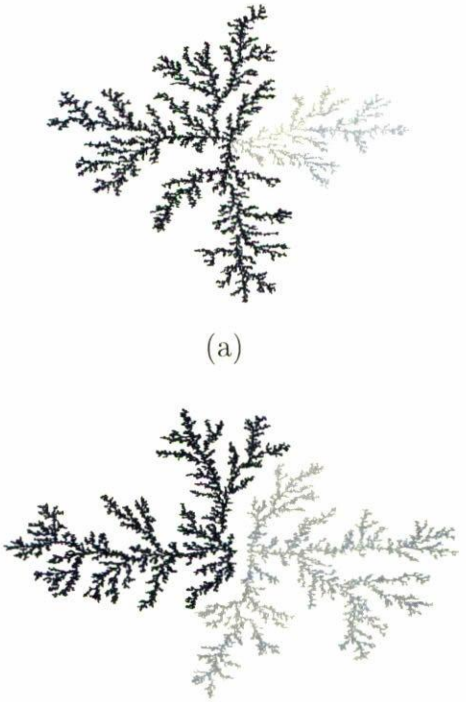
FIGURE 5. (a) Superposition of 100 two-colored aggregates for $p = 0.1$, $d = 100$; (b) superposition of 73 aggregates for $p = 0.3$, $d = 40$.

A qualitative analysis of the superposition of two-colored fractals (Figures 3–5) confirms, to some extent, the electrostatic analogy in the description of the two-dimensional cluster formation presented in Ref. 25.

A "one-branched" fractal structure containing 30 000 particles in the larger cluster and 9132 particles in the smaller one (in the case of $p = 0.5$, $d = 2$) is shown in Fig. 6a. Figure 6b displays "symmetric" aggregates for $p = 0.5$ and $d = 40$. One can see that large structures are similar to those obtained in experiments with 3000 particles in the larger cluster of the two.

Now we pass to a quantitative description of our computational experiments. For the values of $p = 0.1,\ 0.2.\ 0.3,\ 0.4$ and 0.5 and the values of $d = 2,\ 10,\ 40,\ 100$, and for each experiment conducted for a given pair of parameters p and d, we have calculated a ratio of the number N_2 of particles of B-colored cluster to the number N_1 of particles of A-colored cluster. In all our experiments except for those with $p = 0.5$, the number N_2 was larger than N_1 so that $N_2/N_1 > 1$ (recall that p is the probability for a particle to be A-colored). This is not the case for $p = 0.5$. As an example, Fig. 7 shows the ratio N_2/N_1 (on the logarithmic scale) *vs.* the number of experiment for $p = 0.5$ and $d = 100$. The ratio N_2/N_1 (also on the logarithmic scale) *vs.* the number of experiment for $p = 0.5$ and $d = 2$ is displayed in Fig. 8. One can see almost symmetric oscillations of the ratio N_2/N_1 near the value 1.0. Note also a striking difference between the two pictures: in the former case (Fig. 7) there are no significant deviations of N_2/N_1 from 1.0, whereas in the latter case (Fig. 8) the oscillations are very strong, almost chaotic even on the logarithmic scale. The points in Fig. 8 with very large deviations from the value 1.0 correspond to the above mentioned typical case of the suppressed clusters. It follows from Figs. 7 and 8 that in order to get the appropriate mean values corresponding to the numbers of particles in both fractals, it is more convenient to use the logarithm of the ratio of numbers of particles than the ratio itself .

Let $N_{\min} = \min(N_1, N_2)$ and $N_{\max} = \max(N_1, N_2)$. In the case $p \neq 0.5$ the non-negative value $\log(N_{\max}/N_{\min})$ is exactly the same as $\log(N_2/N_1)$. For $p = 0.5$, the value $\log(N_{\max}/N_{\min})$ is a rough measure of the symmetry (or non-symmetry) of a two-colored aggregate since the necessary condition for the structure to be symmetric is



(a)

(b)

FIGURE 6. (a) Colored DLA structure containing 30 000 A-colored particles (black cluster) and 9132 B-colored particles (gray cluster) for $p = 0.5$, $d = 2$; (b) The aggregate with 20 000 A-colored particles (black cluster) and 19 051 B-colored particles (gray cluster) for $p = 0.5$, $d = 40$.

$\log(N_{\max}/N_{\min}) = 0$. At the same time, the mean value of $\log(N_{\max}/N_{\min})$ (defined below) is not equal to zero as it would be for $\log(N_2/N_1)$.

The individual configurations of two-colored fractal structures produced in simulation runs for a given pair of p and d are statistically independent of each other. Therefore, the standard error analysis applies [26]. Let l_i denote the value of $\log(N_{\max}/N_{\min})$ obtained in the trial i ($i = 1, \ldots, n$). The average we take is the simple arithmetic average

$$\langle \log(N_{\max}/N_{\min}) \rangle \equiv \langle l \rangle = \frac{1}{n} \sum_{i=1}^{n} l_i,$$

and its error is estimated as

$$\left[\frac{1}{n(n-1)} \sum_{i=1}^{n} (l_i - \langle l \rangle)^2 \right]^{1/2}.$$

The values $\langle \log(N_{\max}/N_{\min}) \rangle$ averaged over the total number of experiments within each given pair of p and d, together with its estimated error are presented in Table I. The upper number in each entry of Table I gives the value of $\langle \log(N_{\max}/N_{\min}) \rangle$. The lower number is the estimated error. As one can see, for a given value of the probability p the error

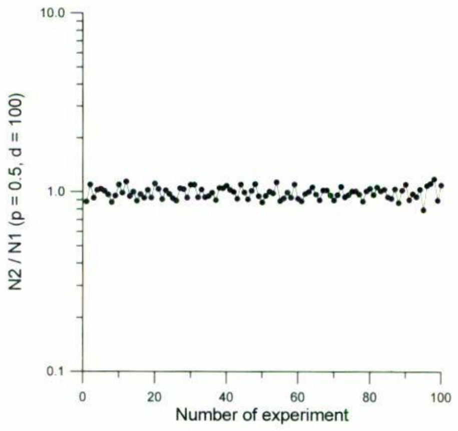


FIGURE 7. Relative number of particles in both clusters *vs.* the number of experiment, for $p = 0.5$, $d = 100$.

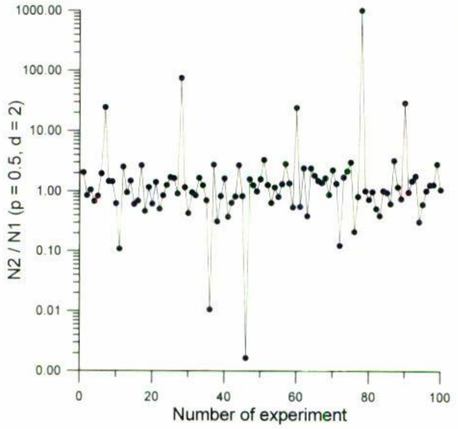


FIGURE 8. Relative number of particles in both clusters *vs.* the number of experiment, for $p = 0.5$, $d = 2$.

grows when the distance d between initial seeds changes from 100 to 10 lattice units. This increase reflects an important fact observed in our computational experiments: significant instability (for small d) of the initial stages of competing cluster formation caused by the mutual screening of two-colored fractals. In the case of $p = 0.5$ this instability leads to three typical cluster structures described above, with substantially different number of particles. The effect attenuates with increasing d. The values of $\langle \log(N_{\max}/N_{\min}) \rangle$ *vs.* probability p for distances between the two initial particles $d = 2$, 10, 40, and 100, according to the data presented in Table I, are plotted in Fig. 9.

In order to evaluate the influence of the competing cluster formation in the Colored DLA model on the fractal properties of clusters, the fractal dimensions D of both two-colored structures of the large aggregate shown in Fig. 6a were estimated in the most interesting case $p = 0.5$, $d = 2$. To this end, the radius of gyration R_g was calculated

TABLE I. Averaged logarithm (base 10) of the ratio of numbers of particles in both structures, $\langle \log(N_{\max}/N_{\min}) \rangle$, (upper value), and its estimated error (lower value).

d \ p	0.1	0.2	0.3	0.4	0.5
2	3.055	2.713	2.179	1.049	3.449×10^{-1}
	3.701×10^{-2}	1.024×10^{-1}	1.319×10^{-1}	1.375×10^{-1}	5.115×10^{-2}
10	2.559	1.884	1.128	6.262×10^{-1}	1.096×10^{-1}
	5.078×10^{-2}	3.194×10^{-2}	5.266×10^{-2}	3.150×10^{-2}	1.089×10^{-2}
40	1.672	1.154	7.419×10^{-1}	3.916×10^{-1}	4.709×10^{-2}
	9.063×10^{-3}	1.149×10^{-2}	1.146×10^{-2}	9.388×10^{-3}	3.909×10^{-3}
100	1.366	9.225×10^{-1}	5.983×10^{-1}	2.921×10^{-1}	2.799×10^{-2}
	7.268×10^{-3}	7.775×10^{-3}	6.122×10^{-3}	6.601×10^{-3}	1.926×10^{-3}

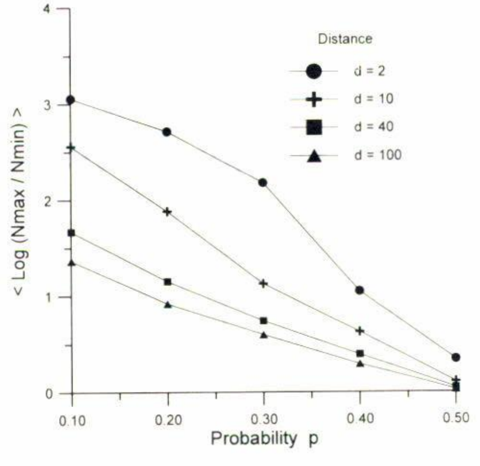


FIGURE 9. The values of $\langle \log(N_{\max}/N_{\min}) \rangle$ *vs.* probability p for distances between the two initial particles $d = 2,\ 10,\ 40$, and 100, according to data presented in Table I.

which has a power-law dependence on the number of particles in a cluster for sufficiently large N: $R_g \sim N^{\beta}$ [27]. The fractal dimension D is given by $D = 1/\beta$. The radius of gyration R_g of an N-particle aggregate is defined as

$$R_g^2 = \frac{1}{N} \sum_{i=1}^{N} \Big[R_i - R_c(N) \Big]^2,$$

where R_i is the radius-vector of the i-th particle and $R_c(N)$ is the radius-vector of the center of mass of the aggregate (we consider each particle to have a mass equal to 1). By

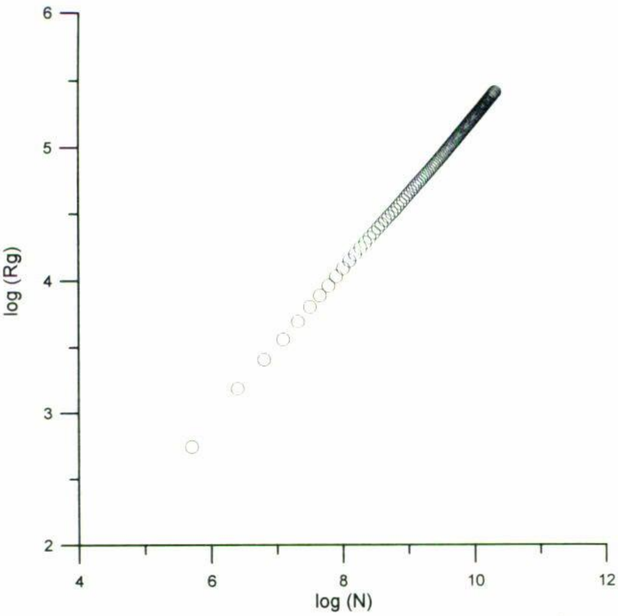


FIGURE 10. Dependence of radius of gyration R_g on cluster size N during the formation of the A-colored cluster of 30 000 particles shown in Fig. 6a.

using the recurrent relationships

$$R_g^2(N) = \frac{N-1}{N} R_g^2(N-1) + \frac{N-1}{N^2}\Big[R_c(N-1) - R_N\Big]^2$$

$$R_c(N) = \frac{N-1}{N} r_c(N-1) + \frac{1}{N} R_N$$

it is possible to plot R_g versus N in the process of the cluster growth. Figures 10 and 11 show how the radius of gyration increases with increasing cluster size during the simulation of the structure presented in Fig. 6a. Figure 10 depicts the logarithm of the radius of gyration of a A-colored cluster containing 30 000 particles *vs.* the logarithm of the number of particles. The figure illustrates that $R_g \sim N^\beta$ for large N with $\beta = 0.575$. Similarly, Fig. 11 shows the logarithm of the radius of gyration of the B-colored "branch" cluster containing 9132 particles *vs.* the logarithm of the number of particles. The corresponding value of β is 0.581. The fractal dimensions of A- and B-colored structures presented in Fig. 6a are 1.739 and 1.721, respectively. The obtained values of β and D are very close to those reported by Meakin [6] for conventional DLA model which means that the competing cluster growth does not affect noticeably the fractal dimension of the two-colored aggregates.

Finally, for each pair of parameters p and d the mean coordination number (*i.e.*, the mean number of neighbors of a particle in a cluster) was calculated by averaging over B-colored fractals containing 3000 particles. The results are presented in Table II. One can see that the averaged coordination number is not sensitive to the variations of p and d and is very close to the value found by Meakin [6].

TABLE II. Averaged coordination number for the clusters of color B (upper value), and its estimated error (lower value).

d \ p	0.1	0.2	0.3	0.4	0.5
2	2.182 1.128×10^{-3}	2.189 2.350×10^{-3}	2.184 2.998×10^{-3}	2.186 2.098×10^{-3}	2.180 1.246×10^{-3}
10	2.186 2.274×10^{-3}	2.181 2.188×10^{-3}	2.189 1.739×10^{-3}	2.184 2.298×10^{-3}	2.189 1.512×10^{-3}
40	2.185 1.479×10^{-3}	2.186 1.836×10^{-3}	2.185 2.050×10^{-3}	2.183 2.460×10^{-3}	2.185 1.196×10^{-3}
100	2.183 1.784×10^{-3}	2.184 2.349×10^{-3}	2.185 2.589×10^{-3}	2.185 2.948×10^{-3}	2.185 1.148×10^{-3}

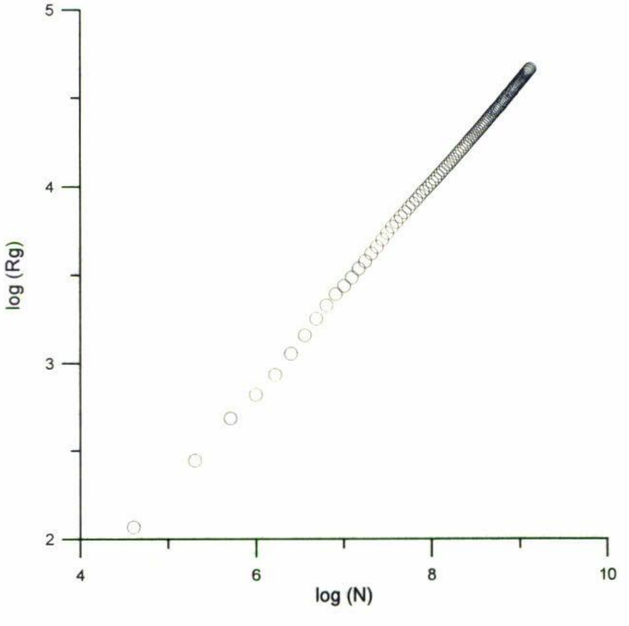


FIGURE 11. Dependence of radius of gyration R_g on cluster size N during the formation of the B-colored cluster of 9132 particles shown in Fig. 6a.

4. CONCLUSIONS

The results presented in this paper pertain to the two-dimensional Colored DLA model [25]. We have performed intensive computer simulations of two-dimensional two-colored fractal structures devoting main attention to the qualitative and quantitative dependence of random fractal aggregates on the two parameters of the model: the distance d between initial seed particles, and the probability p of a diffusing particle to being

A-colored. A significant instability of the initial stages of the competing cluster growth was found for small d and $p = 0.5$ which results in a formation of substantially different aggregates (Fig. 2). Pictures obtained by the superposition of structures produced for various d and p provide an additional insight on the cluster growth phenomenon and confirm, to some extent, the electrostatic analogy developed in [25]. The calculation of the averaged coordination number of a particle indicate that this important quantity is not affected by the competing cluster growth of the Colored DLA model. Our experiments with two-colored aggregates of large size have indicated that the fractal dimension of clusters is also insensitive to the competing cluster formation and is very close to the value of the original DLA model.

The Colored DLA model can be generalized by introducing a sticking probability of a particle to a cluster of the same color, by performing computational experiments in higher dimensions, and by varying a method of particle generation. In the forthcoming paper we intend to report on the mentioned generalization and present a theoretical study of the Colored DLA phenomenon. Note that our DLA model with two species is different from the one recently presented in Ref. 28.

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