# Simulation of Liesegang Pattern Formation Using Lattice Boltzmann Method in three Dimensions

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***Abstract*-The Liesegang pattern formation in three dimensional reaction-diffusion systems is numerically simulated using a lattice Boltzmann method. The reaction and diffusion processes are characterized using the multicomponent lattice Boltzmann equation with three dimensions and fifteen directions. The precipitation and aggregation of the reaction product are modeled based on the supersaturation mechanism. The stratification of the Liesegang pattern in the cubic enclosure can be clearly identified. The interference of the quasiperiodic waves in the Liesegang pattern provides evidence for the interactions between the dynamical processes arise from multisource reactants.**

***Keywords-Liesegang pattern formation, reaction-diffusion system, lattice Boltzmann method, three dimensions***

## I. INTRODUCTION

Reaction-diffusion systems have attracted much attention over the past few years due to the pattern formation frequently encountered in nature [1]. The development of numerical simulation approaches renews the interest of the oscillatory zonations of systems operating far from equilibrium, including chemical waves, Turing structures and Liesegang phenomena, etc [2]. The reaction-diffusion system can be described by the following set of coupled rate equations [3]

$$\frac{\partial \rho_s}{\partial t} - \eta_s \nabla^2 \rho_s = R_s \quad , \tag{1}$$

where t is the time, $\nabla^2$ the Laplacian operator with respect to the spatial coordinate r, s(r,t) the mass density at time t and position r, and s the diffusion coefficient. The subscript s denotes different chemical species. The right-hand side of the equation, Rs, represents the reaction term which depends on the local densities of all chemical species that react with s and the reaction mechanism. The Liesegang phenomena, which were discovered a century ago, presents a particular example within the classification of the pattern formation in reaction-diffusion systems and can be characterized by several empirical regularities [4]. The description in terms of the rate equations is a kind of mean field approach, which is not sufficient to characterize the microscopic dynamics of the system. In order to investigate the process of the Liesegang pattern formation in a first principle manner, Chopard and Droz proposed a cellular automata approach, which takes into consideration the spontaneous aggregation and precipitation in the reaction-diffusion systems [5]. In the past decades, the lattice Boltzmann method (LBM) has developed into a promising numerical scheme for simulating dynamical processes in fluids, which originated from the lattice gas automata and the cellular automata [6]. The LBM is found numerically to be at least as stable, accurate, and computationally efficient as traditional computational fluid dynamics methods [7]. In this paper, the LBM model is employed to simulate the Liesegang pattern formation in three dimensions.

## II. MODEL AND SIMULATION

The model is defined in a three-dimensional cubic enclosure filled with the solution of the chemical species B, which is uniformly distributed with concentration b0. The chemical species A, with concentration a0, diffuses from the source and chemically reacts with B. This reaction will produce a new chemical species C with a reaction constant ı, which can be written as $A + B \to C$ . The dynamic processes in the Liesegang pattern formation adopted were proposed by Dee [8], who considered the supersaturation mechanism as a crucial role in the pattern formation based on the Ostwald's theory. The product C diffuses in the solution and nucleation occurs to form the species D with a reaction constant , which can be written as $C \to D$ , provided that the local concentration of C reaches some threshold value. These processes can be described by the aforementioned rate equations [5,8].

The following multicomponent lattice Boltzmann equation describes the evolution of the distribution function fs(r,i,t) of species s with velocity ei at some dimensionless time, t, and some dimensionless position, r

$$f_s\left(r + e_i, i, t+1\right) - f_s\left(r, i, t\right) = \Omega_s\left(r, i, t\right) \quad . \tag{2}$$

where s(r,i,t) is the collision operator for the species s that can be divided into a reactive term sR and a nonreactive term sN. The reactive term can be expressed as the distribution of Rs over different directions proportional to the weights ws,i, which is dependent on the lattice symmetry [9]

$$\Omega_{sR} = w_{s,i} R_s \quad , \tag{3}$$

where ws,i is determined by the D3Q15 model of three dimensions with fifteen directions. The nonreactive term of the collision adopts the single relaxation time approximation of Bhatnagar, Gross, and Krook (BGK)

$$\Omega_{sN} = -\frac{1}{\tau_s}\left[ f_s\left(r, i, t\right) - f_s^{\mathrm{eq}}\left(r, i, t\right) \right] \quad . \tag{4}$$

where relaxation time s is related to the diffusion coefficient s of each chemical species by s = 3 s + 0.5.

The equilibrium distribution function depends on the local density s(r,t) and local velocity vs(r,t). In a pure reaction diffusion system, the velocity of macroscopic flow approximates to zero, hence, the equilibrium distribution function can be reduced to [3]

$$f_s^{\mathrm{eq}}(r,i,t) = w_{s,i}\rho_s = w_{s,i}\sum_i f_s(r,i,t) \quad . \tag{5}$$

The nucleation of the chemical species D consists of two processes of precipitation and aggregation according to Chopard, who proposed cellular automata rules for the Liesegang pattern formation [5]. The species C spontaneously precipitates to become D once the local density reaches a threshold C. The species C aggregates when it enters into the vicinity of D, provided that the local density of C is aboveD, and the species C always aggregates if it enters into the same site of D. The vicinity of one site is considered as $3\times3\times3$ neighborhood in a three dimensional lattice. The reaction constants C and D are two control parameters of the model and it is reasonable to assume that C >D.

## III. RESULTS AND DISCUSSION

The simulation results of the Liesegang pattern formation by the LBM in three dimensional enclosures are presented in this section. The LBM codes are implemented by the C/C++ programming language. The calculations are preformed on a computer with Pentium dual core CPU 2.8 GHz and 2 GB RAM.

The cubic enclosure is defined on a lattice of $100\times100\times100$, and the species concentrations are initially set as a0 = 1.0, b0 = 0.1 and c0 = d0 = 0. The reaction constant is assumed to be 1 = 1.0 for simplicity, the nucleation threshold $C = 9.8\times10^{-3}$ and the aggregation threshold $D = 7.6\times10^{-3}$. The diffusion coefficients of the chemical species A, B and C are set as a = 0.7 and b = c = 0.07, respectively. A single source of the species A is settled at the center of the cubic enclosure. The species A diffuses from the source into the solution of B and reacts to produce the species C, which also diffuses until it precipitates to form the species D. The profile of the local concentration of the species C and D at different time steps are illustrated in Figure. 1.

The upper of Figure 1 gives the snapshots of the concentration profile of the species C, and the bottom gives those of the species D, correspondingly. The cross section are so made that the source of the species A is located at the center. The bright zones in the pictures denote the high concentration and vice versa. The reaction front moves forwards in the radial direction and the precipitate D species deplete their surroundings of the species C. The local concentration of C drops from the supersaturation and the precipitation stops with the formation of one layer of the Liesegang pattern. However, the diffusion and reaction processes continue and the reaction front moves outside. The local concentration of the species C will reach supersaturation again, which restarts the precipitation and forms a new layer of the species D outside the old one with a larger radius. The thickness of the outer layers and the intervals among them are larger than those of the inner layers, which is in agreement with the empirical regularities, including the Jablczynski spacing law, etc.

The simulation result at t = 2000 time steps is illustrated by a three dimensional plot as shown in Figure. 2. The projection of the pattern onto x-y plane is also included for clarity. The stratification of the Liesegang pattern can be clearly identified.

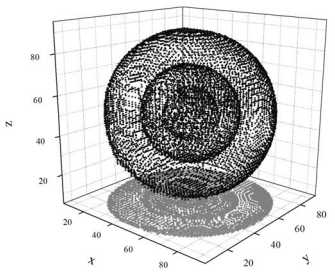


Figure 2. Three dimensional plot of the Liesegang pattern with a single source.

The profiles of the three dimensional Liesegang pattern with a single source are presented in Figure. 3, wherein the sections are made at different z coordinates. The numbers of the Liesegang rings are different with z, which indicates that the Liesegang patterns in three dimensions be considered in different perspectives as compared with those in two dimensions.

The Liesegang pattern formation with multisource reactants in a three dimensional enclosure is investigated by numerical simulation using the LBM. The reactant sources of the chemical species A with the concentration a0 = 1.0 are randomly dispersed within a cubic enclosure filled with the solution of the species B, which is uniformly distributed with the concentration b0 = 0.1. In this simulation, the diffusion coefficients of the species A, B and C and the control parameters 1, C and D take the same values as those in the single source simulation. Figure. 4 presents the simulation results at t = 2000 time steps in a three dimensional plot. The stratification of the Liesegang pattern can be readily identified, nevertheless, more complicated structures are exhibited.

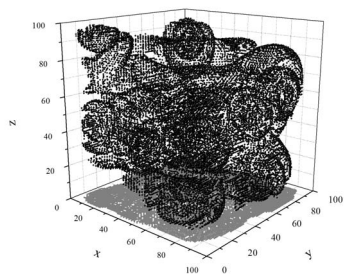


Figure 4. Three dimensional plot of the Liesegang pattern with multisource reactants.

The profiles of the three dimensional Liesegang pattern with multisource reactants are illustrated in Figure. 5, wherein the sections are made at different z coordinates. The interference of the quasiperiodic waves in the Liesegang pattern reveals the interaction between the processes of the pattern formation in the reaction-diffusion systems.

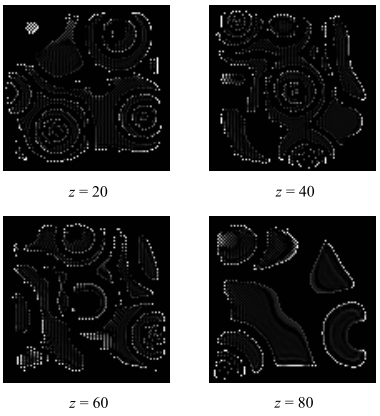


Figure 5. Profiles of the Liesegang pattern with multisource reactants.

## IV. CONCLUSION

The Liesegang pattern formation is simulated using the LBM in cubic enclosures of reaction-diffusion systems. The oscillatory zonations have been observed from the numerical results of three dimensional simulations. The interference of the waves in the Liesegang pattern with multisource reactants reveals the interaction between the processes of the pattern formation in the systems. The LBM provides a feasible approach to simulate the Liesegang pattern formation in three dimensional reaction-diffusion systems.

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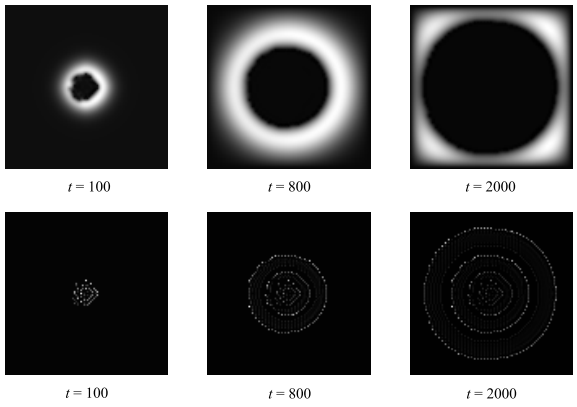


Figure1. Snapshot of concentration of the species *C* and *D* at different time steps.

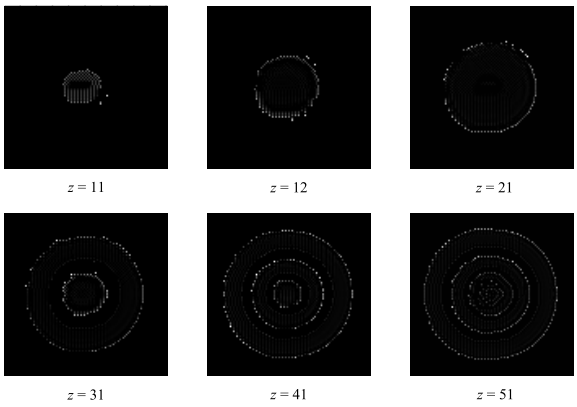


Figure 3. Profiles of the Liesegang pattern.

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