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Three-species reaction–diffusion processes on scale-free networks

Ki-Ho Chang [a], Soon-Hyung Yook [b], Soo Yong Kim [c], Kyungsik Kim [d,*], Deock-Ho Ha [e]

[a] Global Environment System Research Laboratory, National Institute, of Meteorological Research, KMA, Seoul 156-720, Republic of Korea
[b] Department of Physics, Kyung Hee University, Seoul 130-701, Republic of Korea
[c] Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Republic of Korea
[d] Department of Physics, Pukyong National University, Busan 608-737, Republic of Korea
[e] Department of Information and Communication Engineering, Pukyong National University, Busan 608-737, Republic of Korea

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ABSTRACT

We study the novel three-species reaction–diffusion processes of scale-free networks that are significantly different from numerical calculations manipulated on regular and small-world lattices. The inverse particle density for the three-species process scales according to the power-law with a scaling exponent $\alpha = 1.5$ for $\gamma > 3$. It is, however, found from numerical results that the inverse particle density scales in a different way depending on time t when $\gamma < 3$. In the early time regime, $\alpha \simeq 1.5$, but the inverse particle density increases exponentially over time. We also discuss the possible relationship with the dynamical properties of random walks. In particular, we measure the ratio between the number of inactive and active bonds which shows the segregation of the particles.

1. Introduction

During the past three decades, considerable efforts have been directed toward theoretical and numerical investigation of the reaction segregation phenomena in physics, chemistry, biology, and chemical engineering. There have been many important breakthroughs in analytical and numerical methods to address reaction–diffusion processes. The seminal work of Ovchinnikov and Zeldovich [1] was crucial in research of the segregation phenomenon, and the binary reaction has primarily been investigated in relation to the processes of ternary reactions in many scientific phenomena [2–7]. The segregation of reactants has been investigated in a reaction–diffusion process based on the assumption that the scaling form for $A + B \rightarrow C$ has almost been verified by computer simulation and experiment [8,9]. To date, analytical and numerical methods for chemical reaction processes have led to results obtained from the deterministic rate equations and the field theories. However, at present, there exist intriguing methods using intrinsically and novel for both small-world and scale-free networks. Nevertheless, there remain open and innovating problems that need to be studied in relation to the reaction–diffusion process.

While multi-species reactions may occur rarely in several scientific fields, several researchers of reaction–diffusion processes of multi-species have treated this as importantly as more complicated reactions. Even though much effort has been directed toward developing the two-species reaction–diffusion model in Barabási–Albert and other scale-free networks [10,11], a three-species reaction–diffusion system of for scale-free networks has not yet been intensively investigated. In this paper, we focus on the three-species reaction–diffusion process using a static model for scale-free networks. In particular,

* Corresponding author. Tel.: +82 51 629 5562; fax: +82 51 629 5549.
E-mail address: kskim@pknu.ac.kr (K. Kim).

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we numerically estimate the inverse particle density in the three-species reaction–diffusion process. The fraction and ratio from a numerical simulation is also calculated.

2. Theory

The inverse particle density of the surviving particles in the reactions of $A+A \to 0$ and $A+B \to 0$ type scales classically on a d-dimensional regular lattice as

$$\frac{1}{\rho(t)} - \frac{1}{\rho_0} \sim t^{\alpha}, \tag{1}$$

where $\rho(t)$ is the particle density at $t = t$, and ρ_0 is the initial particle density. In a d-dimensional space the scaling exponent α is known to satisfy d/d_c for $d \leq d_c$ and $\alpha = 1$ for $d > d_c$, and the critical dimension $d_c = 2$ for $A + A \to 0$, $d_c = 4$ for $A + B \to 0$, and $d_c = 2$ for $A + B + C \to 0$.

The reaction–diffusion process has been studied numerically: both the global reaction rate and the reaction front increased as $t^{1/2}$ at very early times [12]. From the decay process [13,14] of $A + 2B \to C$, the diffusion equation under the initial reactant segregation is given by

$$\frac{\partial}{\partial t}A(x,t) = D_A\nabla^2 A(x,t) - kA(x,t)B^2(x,t), \tag{2}$$

where $A(x, t)$ and $B(x, t)$ are the particle densities, D_A is the diffusion coefficient of reactants $A(x, t)$, and k is the microscopic reaction constant. From the lowest order of the perturbation theory, the global reaction rates $R(t)$ on both the early time and long time behaviors scale as a power law $t^{1/2}$ and $t^{-1/2}$, respectively. In the case of the $A + B \to 0$ the process on a regular lattice network was introduced for Lévy walks using the following reaction–diffusion equation [15]:

$$\frac{\partial}{\partial t}A(\vec{r},t) = D_A LA(\vec{r},t) - KA(\vec{r},t)B(\vec{r},t), \tag{3}$$

where $A(\vec{r}, t)$ and $B(\vec{r}, t)$ are the particle densities, D_A a generalized diffusion coefficient, K the reaction rate, and L the operator for Lévy-enhanced diffusion. The particle densities in this case can be calculated as

$$A(t) = B(t) \sim t^{d/2\beta} \quad \text{for } \beta > d/2, \tag{4}$$

where three marginal values are $\beta = 1$ for $d = 2$, $\beta = 3/2$ for $d = 3$, and $\beta = 2$ for $d = 4$.

It was found from the two-particle reaction process [15] that the particle density for Lévy walks is distributed as $P(n) \sim n^{-1-\nu}$ for $n > 0$ and $1 < \nu < 2$, and that the segregation disappears in $d = 3$ dimension for $\nu < 3/2$. Also, asymptotic long-time scaling has been found in the ternary reaction–diffusion process with initially separated reactants [14].

In the following a one-dimensional diffusion-reaction system of $A + B + C \to 0$ is introduced such that $A(x, t)$, $B(x, t)$, and $C(x, t)$ are the particle densities for three-species A, B, and C existing at a position x at time t. We assume that the three species are initially distributed separately on the axis x. The rate equation for $A(x, t)$ has the form:

$$\frac{\partial}{\partial t}A(x,t) = D_A\nabla^2 A(x,t) - \kappa A(x,t)B(x,t)C(x,t), \tag{5}$$

where D_A is the diffusion constant for one species A, and κ is the reaction rate. The solution for $A(x, t)$, $B(x, t)$, and $C(x, t)$ is obtained as $A(x,t) = A_0\phi(\frac{x}{at^{1/2}})$, $B(x,t) = B_0\phi(\frac{x}{bt^{1/2}})$, and $C(x,t) = C_0[1 - \phi(\frac{x}{ct^{1/2}})]$, where $\phi(x) = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{x} \mathrm{d}x e^{-x^2}$. From the result of previous works [8,16], given that the global reaction rate $R(t)$ is defined by $R(t) = \int_{-\infty}^{\infty} \mathrm{d}x R(x,t)$ for $R(x,t) = \kappa A(x,t)B(x,t)C(x,t)$, the time dependence of the global reaction rates $R(t)$ was shown to behave as $R(t) \sim t^{1/2}$ $(t^{-1/2})$ in the early (long) time limit.

In scale-free networks, the Laplacian operators in Eq. (5) should be replaced by the network Laplacian operator. For example, the matrix representation $N \times N$ of the network Laplacian L is defined as follows: the diagonal elements are $L_{xx} = k_x$ (k_x = a number of links in node x), and the off-diagonal elements are $L_{xy} = -1$ if node x and y are connected, $L_{xy} = 0$ otherwise. This result on numerous important physical quantities such as that the first passage time and spreading velocity will be different from those expected in regular lattices [17]. Thus, theoretical studies on diffusion-reaction systems in scale-free networks are of particular interest.

The decay process in a reaction–diffusion system with three species on small-world lattices [18] was recently discussed, and its global reaction rate has also been analyzed by numerical simulation before and after the crossover. The bimolecular chemical reaction in scale-free networks [19] was studied for the generation of the depletion zone and the segregation of the reactants. It was found that the reaction–diffusion processes in scale-free networks are different in nature compared with regular lattice models, due to the small diameter of the networks and the existence of hubs. Similarly, the inverse particle density in an uncorrelated scale-free network [20] is shown to cross over to a linear behavior. Gallos and Argyrakis [21] have dealt mainly with the reaction–diffusion process of two species on a scale-free network between correlated and uncorrelated configuration models, and they revealed that the two models are identical when $\gamma = 3.0$.

Among several scale-free models [22–24], we introduce the static model reported by Goh et al. [24] as follows: there are N nodes ($i = 1, 2, \ldots, N$) as a system initiated by Erdös–Rányi model, and the weight $p_i = i^{-\alpha}$ is assigned to each node. After we select two nodes (i, j) with probabilities equal to the normalized weights, we add a link between them unless one already exists. This procedure is repeated until mN degrees are made in the system, where the mean degree is $2m$. It is then found that the degree distribution scales as the power law, $P(k) \sim k^{-\gamma}$, where the scaling exponent γ is given by $\gamma = (1 + \alpha)/\alpha$ for the control parameter α in [0, 1). For our reaction–diffusion process, the model will be henceforth constructed with a characteristic degree distribution $p(k) \sim k^{-\gamma}$ on a static model [24] in scale-free networks, which has the fixed number of nodes N_0 and a scaling exponent γ. The static method is to some extent different from the Barabási–Albert model [25] and the correlated and uncorrelated configuration models [21] in scale-free networks, but we expect to obtain similar results to these methods.

3. Numerical results and conclusion

To numerically calculate the particle density, we analyze the reaction–diffusion process of $A + B + C \to 0$ on the static model. We assume that three species of reactants are distributed randomly. For our diffusion-reaction system, after one species reactant is chosen at random, the direction of its movement is chosen at random with equal weight to one of its linked neighbor nodes. When two species of reactants meet each other on the same node, by the intermediate process existing concurrently, the combined two species of reactants can be formed. If two species of reactants meet the third reactant, these reactants react and immediately leave the network.

To understand the spatial contribution of three-species, we can calculate the number of contact particles as a function of the time step. At time t the fraction $\rho_{A+AB+AC}(t)$ is defined as the number of contacts between three-species for over the total possible number of contacts:

$$\rho_{A+AB+AC}(t) = \rho_A(t) + \rho_{AB}(t) + \rho_{AC}(t), \tag{6}$$

where ρ_{AB} and ρ_{AC} are, respectively, $A + B$ and $A + C$ intermittent reactants. The particles (A, AB and AC) can be regarded as active particles that are similar to species A in the $A + B \to 0$ system. In Fig. 2, we also measure the inverse particle density of the active particles, which contains A species, as

$$\frac{1}{\rho_{A+AB+AC}(t)} - \frac{1}{\rho_0} = \frac{1}{\rho_A(t) + \rho_{AB}(t) + \rho_{AC}(t)} - \frac{1}{\rho_0}. \tag{7}$$

In this case the ratio Q_{ABC} is calculated as

$$Q_{ABC} = \frac{\rho_{ABC}}{\rho_{AB} + \rho_{BC} + \rho_{AC}}, \tag{8}$$

where ρ_{ABC} denotes the number of contacts between three-species compared with the number of three-species ρ_A, ρ_B, and ρ_C denotes the existence of depletion and segregation zones. ρ_{BC} are also $B + C$ intermittent reactants. In this scheme, we make use of Eqs. (7) and (8) to compute the inverse particle density of the active particles and the fraction on scale-free networks. The inverse particle densities and fraction from the results of the obtained measures can be compared numerically with other cases of scale-free networks.

To simulate our process, the respective particle density for A, B, and C corresponds to the value of 10% on a number of nodes $\rho_0 = 1.5 \times 10^4$ of the scale-free network. The diffusion constant in our case takes the same value for each reactant, and the reaction rate is $K = 1/500$. During a simulation performed on 5×10^3 realizations, we numerically estimate the particle density, fraction, and ratio in the reaction–diffusion process of $A + B + C \to 0$ on the static model in scale-free networks.

As can be seen from Fig. 1, the particle density $1/\rho_A(t)$-$1/\rho_0$ has an exponential form, as the scaling exponent γ decreases on scale-free networks.

In Fig. 2, we measure the density of all kinds of particles having particle A. From the data, we find that $\gamma = 3$ is marginal. The measured scaling exponent α is 1.5 for $\gamma \geq 3$. In the case of $\gamma = 2.5$ and $t < 10$, we obtain $\alpha \approx 1.5$ and increases to 2.0 for an intermediate time interval, $10 < t < 50$. As γ is decreased further, the slope of the intermediate interval continuously increases and decays exponentially when $\gamma \to 2.0$. From the definition of our model, the dynamics can be analyzed by a two-stepped two particle reaction. In the first step, intermediate particles such as AB, AC, and so on are created. Then, in the next step, the intermediate particles are annihilated when they encounter the proper counter particles. Therefore, as noted in Ref. [26], the second moment of $P(k)$ plays an important role in predicting the dynamical behavior of our model, which shows good agreement with the present numerical results. However, the measurement presented in Fig. 2 shows that the scaling behavior of three species model is completely different from that of Gallos' calculations [19].

As shown in Fig. 3, we find that Q_{ABC} increases in different ways depending on γ. In the initial transient regime ($t < 10$), Q_{ABC} of both $\gamma = 2.5$ and $\gamma = 3.5$ increase in the same manner. For $t > 10$, Q_{ABC} for $\gamma = 2.5$ satisfies the power-law $Q_{ABC} \sim t^{1.2}$. However, Q_{ABC} for $\gamma = 3.5$ increases much slower than that for $\gamma = 2.5$. The crossover occurs around $t \approx 10$ which coincides with the results obtained in Fig. 2.

In summary, we have studied the reaction–diffusion process $A+B+C \to 0$ of three species on a static model of scale-free networks. The inverse particle densities and fraction of three species are calculated numerically. There exists a crossover

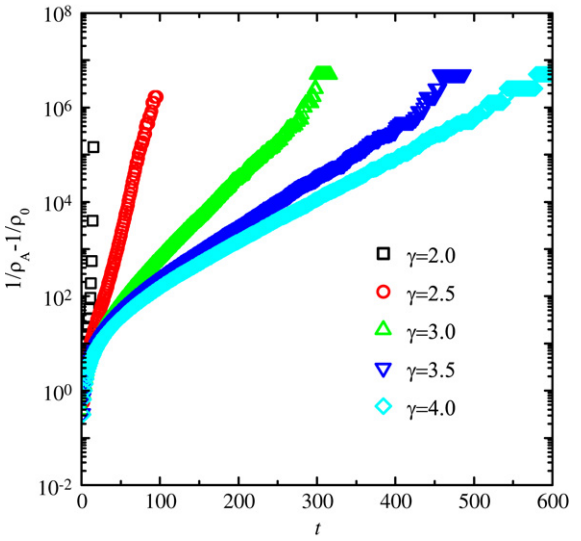

Fig. 1. (Color on line) Particle density $1/\rho_A(t)$-$1/\rho_0$ on scale-free networks of $\gamma = 2.0$ (black), 2.5 (red), 3.0 (green), 3.5 (dense blue), and 4.0 (blue).

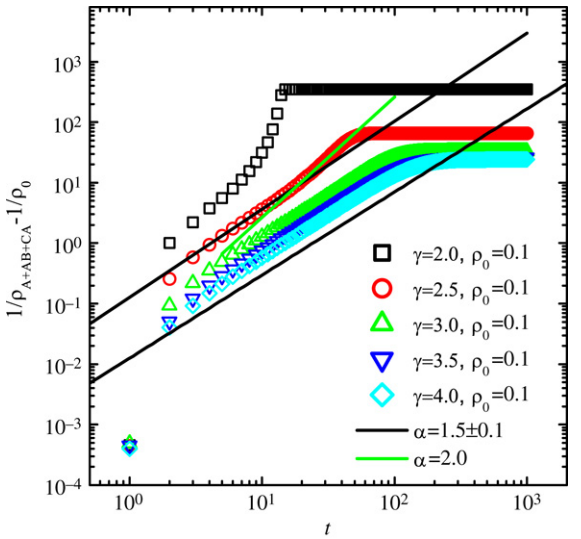

Fig. 2. (Color on line) Fractions $1/\rho_{A+AB+AC}(t) - 1/\rho_0$ obtained from simulated results for $\gamma = 2.0$ (black), 2.5 (red), 3.0 (green), 3.5 (dense blue), and 4.0 (blue) of scale-free networks. The black solid lines represent $\alpha = 1.5$ and the green line denotes $\alpha = 2.0$.

having different scaling exponents between short and long time regimes. An analogous situation arises in the two-species reaction. The most interesting result obtained here is that the scaling exponents of the particle density are slightly different from that of $A + A$ and $A + B$ reaction [15], but the inverse particle densities and fraction show a increasing trend at a long time limit, similar to one or two species diffusion-reaction systems. It is found that the scaling exponents of the particle density presented are smaller than those of a two-species reaction [19–21]. In order for two-species of reactants to meet each other, the second moment become a crucial factor. While this lends itself to a better understanding of the simulated data, it diverges in the region of $\gamma < 3.0$. This means that two-species reactants have extremely high probabilities of meeting in the hubs in scale-free networks.

Furthermore, we have found that the chemical reaction of three species of reactants occurs equivalently in both regular and small-world networks at an early time regime, but the decay process in a small-world network proceeds slightly faster than in the case of a regular network in a long-time regime. It is anticipated that the calculations of reaction–diffusion processes will continue to increase in importance in the future and potential to impact challenging problems in theoretical physics and chemistry. We believe that our model will be useful in other reaction–diffusion studies of multi-species.

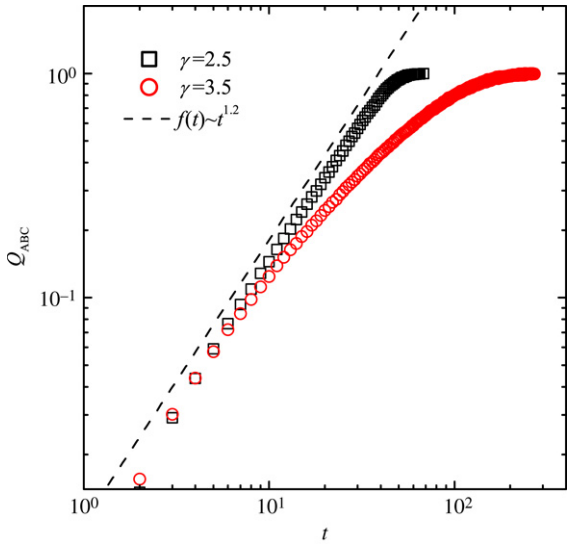

Fig. 3. (Color on line) Ratios Q_{ABC} obtained from simulated results on scale-free networks of $\gamma = 2.5$ (red square) and 3.5 (red circle). The dashed line denotes $Q_{ABC}(t) \sim t^{1.2}$.

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