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Kinetics of catalytically activated duplication in aggregation growth*

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We propose a catalytically activated duplication model to mimic the coagulation and duplication of the DNA polymer system under the catalysis of the primer RNA. In the model, two aggregates of the same species can coagulate themselves and a DNA aggregate of any size can yield a new monomer or double itself with the help of RNA aggregates. By employing the mean-field rate equation approach we analytically investigate the evolution behaviour of the system. For the system with catalysis-driven monomer duplications, the aggregate size distribution of DNA polymers $a_k(t)$ always follows a power law in size in the long-time limit, and it decreases with time or approaches a time-independent steady-state form in the case of the duplication rate independent of the size of the mother aggregates, while it increases with time increasing in the case of the duplication rate proportional to the size of the mother aggregates. For the system with complete catalysis-driven duplications, the aggregate size distribution $a_k(t)$ approaches a generalized or modified scaling form.

Keywords: aggregation, catalytically activated reaction, rate equation, kinetic behavior
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1. Introduction

The aggregation phenomenon is of considerable importance in a variety of fields such as astronomy where planetary systems form via collisions of planetesimals,[1] chemical physics where polymeric chains chemically bond and form polymeric networks or gels,[2,3] and social science.[4−8] Typically, the general mechanism of irreversible aggregation (coagulation) is described by the reaction scheme $A_i + A_j \xrightarrow{K(i,j)} A_{i+j}$, where A_i denotes the mass of cluster i (a cluster containing i units) and $K(i,j)$ is the reaction kernel, which generally depends on the sizes of the two clusters. In the last few decades much work has been done on understanding this kind of nonequilibrium aggregate growth,[9−22] and the results imply that the evolution of the systems is highly sensitive to the details of the underlying dynamics.

Recently, considerable interest has been aroused in a variety of aggregation phenomena involving catalytically activated reactions (CARs),[23−26] where particles react only in the presence of another agent-a catalyst, and remain chemically inactive otherwise. These processes are widespread in nature and used in a variety of technological and industrial applications,[27] even in sociology and economy. Burlatsky and Moreau[28] and Oshanin and Blumen[29] proposed a three-molecule catalytically activated reaction model, in which the elementary reaction step is $A+B+C \rightarrow$ product (where A and B represent two different types of stable species and C is a catalytic substance), and they incisively analysed its kinetics by extending the Smoluchowski approach. Lin *et al*[30] introduced the mutually catalyzed birth of population and assets in exchange-driven aggregation growth to study the interaction between the population and the asset aggregates. In our recent work,[31] we studied the competition between catalyzed birth and catalyzed death in exchange-driven aggregation growth, the results show that this competition between the two mechanisms gives rise to much more abundant kinetic behaviours.

In the present paper, we introduce another catalytically activated aggregation growth model: the catalysis-driven duplication process. In our model,

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there are two kinds of aggregates (A and B species aggregates). Any two aggregates of the same type can bond themselves together according to the above-mentioned binary coagulation reaction with the rate kernels $I(i,j)$ and $J(i,j)$ for A and B species, respectively. Meanwhile, an A species aggregate of any size can produce a new monomer through duplicating a simple structural unit under the catalysis of B species. The catalysis-driven duplication process can be described by the reaction, $A_i + B_j \xrightarrow{K(i,j)} A_i + A_1 + B_j$, with the rate kernel (or equivalently, duplication probability) $K(i,j)$. This is an extreme case of incomplete replication. For the complete duplication case, an A species aggregate of any size can double itself with the help of the B catalyst, which can be described by the reaction, $A_i + B_j \xrightarrow{L(i,j)} 2A_i + B_j$, with the rate kernel $L(i,j)$. By discussing the evolution behaviours, we find that in the catalysis-driven monomer duplication case, the aggregate size distribution of A species $a_k(t)$ always follows a power law in size in the long-time limit, and in the complete catalysis-driven duplication case, $a_k(t)$ takes a generalized scaling form or a modified scaling form.

We think our catalysis-driven duplication model can mimic many real phenomena in nature and society. For example, it is well known that the replication of DNA is essential during each cell cycle and the duplication process cannot take place in the absence of an RNA primer, so we may consider the replication of DNA as a catalytically activated reaction and the catalyst as an RNA primer. Specifically, during the replication of DNA, the DNA helix unwinds at first so that each strand of the double helix could act as a template, then an RNA primer is synthesized (this process can be reasonably considered as aggregation growth), resulting in the transfer of genetic information from the DNA molecule to the messenger RNA, and after the daughter molecules created, the genetic information is transferred from the messenger RNA to the daughter molecules. Thus with the help of the primer RNA, a complete replication of DNA is finished.[32] Moreover, it has been observed that the end-to-end aggregation of DNA fragments can occur to form long linear DNA chains, and during the replication of DNA both complete and incomplete replications of a template can occur with a certain probability.[33] Additionally, it is believed that this catalysis-driven duplication in the aggregation growth process also occurs in many biological, chemical and economical systems, and this model may provide a fairly useful description of such natural phenomena.

The present paper is organized as follows. In Section 2, we introduce a model of coagulation with catalytically activated monomer duplications and describe the outline of the generalized Smoluchowski's rate equation approach to study the kinetic evolution behaviours of the aggregate size distributions. In Section 3, we introduce the model of coagulation with complete catalytically activated duplications, and discuss the kinetic scaling behaviours of the aggregate size distributions. Finally, a brief summary is given in Section 4.

2. Aggregation growth with catalytically activated monomer duplications

In this model, we discuss the simplest incomplete duplication case where only a monomer of A species can be duplicated, driven by the B catalyst. In some practical duplication processes, the size of the mother aggregate plays no role, while in some other cases, it plays an important role. Here, for simplicity, we discuss only two typical cases, i.e., the catalysis-driven duplication probability independent of the size of the mother aggregate and that proportional to the size of the mother aggregate. Moreover, in order to recover the influence of the catalyst on the kinetics of the duplication, we study the evolution of the system in two different subcases, i.e. the systems with and without the coagulation of the catalyst.

2.1. The system with the catalysis-driven duplication probability independent of the size of the mother aggregate

We first discuss the case where the catalysis-driven duplication rate kernel is independent of the size of the mother aggregate, it only depends on the size of the catalyst aggregate, that is, $K(i,j) = Kj^{\upsilon}$, where the parameter υ denotes a geometric index characterizing the catalytic surface of a j-mer, e.g., for compact clusters $\upsilon = 2/3$,[34] and it is found that for many chemical and biological systems, $0 < \upsilon < 1$.

So in the present paper, we only discuss the case of $0 < \upsilon < 1$. Since our system is assumed to be of spatial homogeneity in the mean-field limit, the theoretical approach to the model can be based on the Smoluchowski rate equation, in which it is assumed that the reaction proceeds at a rate proportional to the reactant concentrations. The governing rate equation for this model then reads

$$\frac{\mathrm{d}a_1}{\mathrm{d}t} = -a_1\sum_{j=1}^{\infty} I(1,j)a_j + K\sum_{i=1}^{\infty} a_i \sum_{j=1}^{\infty} j^{\upsilon} b_j, \tag{1}$$

$$\frac{\mathrm{d}a_k}{\mathrm{d}t} = \frac{1}{2}\sum_{i+j=k} I(i,j)a_i a_j - a_k\sum_{j=1}^{\infty} I(k,j)a_j \quad (k>1), \tag{2}$$

$$\frac{\mathrm{d}b_k}{\mathrm{d}t} = \frac{1}{2}\sum_{i+j=k} J(i,j)b_i b_j - b_k\sum_{j=1}^{\infty} J(k,j)b_j. \tag{3}$$

In Eq.(1), the first term on the right-hand side accounts for the loss in $a_1(t)$ due to the self-coagulation processes that the A_1 aggregates bond to any other aggregates, while the second term accounts for the gain in $a_1(t)$ due to the monomer birth driven by the catalytically activated duplication. In Eq.(2) [similarly in Eq.(3)], the first term on the right-hand side accounts for the gain in $a_k(t)$ due to the coagulation processes between $a_i(t)$ and $a_{k-i}(t)$ aggregates ($i = 1, 2, ..., k-1$), while the second term accounts for the loss in $a_k(t)$ due to merging processes that the $a_k(t)$ aggregates bond with any other aggregates.

For simplicity, we assume that the self-coagulation rate kernels of species A and B are both independent of the sizes of the reactants, namely, $I(i,j) = I, J(i,j) = J$, where I and J are two constants. It is sound for some chemical and biological systems, especially for the polymerization of chain-shaped polymers which have only two energetic reactive edges. Then equations (1)–(3) can be reduced to

$$\frac{\mathrm{d}a_1}{\mathrm{d}t} = -Ia_1 M_0^A(t) + KM_0^A(t)M_{\upsilon}^B(t), \tag{4}$$

$$\frac{\mathrm{d}a_k}{\mathrm{d}t} = \frac{I}{2}\sum_{i+j=k} a_i a_j - Ia_k M_0^A(t) \quad (k>1), \tag{5}$$

$$\frac{\mathrm{d}b_k}{\mathrm{d}t} = \frac{J}{2}\sum_{i+j=k} b_i b_j - Jb_k M_0^B(t), \tag{6}$$

where $M_{\upsilon}^B(t) = \sum_{j=1}^{\infty} j^{\upsilon} b_j(t)$ is the υ-th moments of B species, especially, $M_0^B(t) = \sum_{j=1}^{\infty} b_j(t)$ and $M_1^B(t) = \sum_{j=1}^{\infty} jb_j(t)$ denote the total number and the total mass of B species aggregates (similarly for A species aggregates) at time t, respectively.

We first study the evolution behaviour of the B catalyst. The rate equation (6) can be solved with the help of ansatz (the application of this ansatz has been thoroughly discussed in our previous works[30,31]):

$$b_k(t) = B(t)[b(t)]^{k-1}. \tag{7}$$

We consider the simplest but important case of the monodisperse initial condition,

$$b_k(0) = B_0\delta_{k1}. \tag{8}$$

Substituting expression (7) into Eq.(6), we can transform the rate equation (6) into the following differential equations:

$$\frac{\mathrm{d}b}{\mathrm{d}t} = \frac{JB}{2}, \quad \frac{\mathrm{d}B}{\mathrm{d}t} = -\frac{JB^2}{1-b} \tag{9}$$

with the corresponding initial condition

$$b = 0, \quad B = B_0 \quad \text{at} \quad t = 0. \tag{10}$$

From Eq.(9) one can easily obtain

$$b(t) = \frac{JB_0 t}{JB_0 t + 2}, \quad B(t) = \frac{4B_0}{(JB_0 t + 2)^2}. \tag{11}$$

So we derive the accurate solution to the aggregate size distribution of the B catalyst,

$$b_k(t) = 4B_0(JB_0 t + 2)^{-2}\left(1 - \frac{2}{JB_0 t + 2}\right)^{k-1}. \tag{12}$$

In the scaling regime of $k \gg 1$ and $t \gg 1$, it can be asymptotically rewritten as

$$b_k(t) \simeq 4J^{-2}B_0^{-1}t^{-2}\exp(-x), \quad x = 2J^{-1}B_0^{-1}kt^{-1}, \tag{13}$$

which satisfies the conventional scaling law,[9]

$$f_k(t) \simeq t^{-\alpha}\Phi[k/S(t)], \quad S(t) \propto t^{\beta} \tag{14}$$

with the scaling function $\Phi(x) = \exp(-x)$. $S(t) = \frac{1}{2}JB_0 t$ is the characteristic size of the B aggregates, which plays a role analogous to the correlation length in critical phenomena. And $\alpha = 2$ and $\beta = 1$ are the scaling exponents.

We then focus on the kinetics of A aggregates. From Eq.(4), we find that the influence of species-B-catalyzed species A duplication is reflected by the υ-th moments of the B catalyst, which can be easily obtained from expression (12) as

$$M_\upsilon^B(t) = \sum_{j=1}^{\infty} j^\upsilon b_j(t) \simeq \Gamma(1+\upsilon)B_0\left(1+\frac{1}{2}JB_0t\right)^{\upsilon-1}. \quad (15)$$

Summing up Eqs.(4) and (5) yields

$$\frac{\mathrm{d}M_0^A}{\mathrm{d}t} = -\frac{I}{2}(M_0^A)^2 + KM_0^AM_\upsilon^B. \quad (16)$$

From this equation, we determine the asymptotical implicit solution for the total number of A aggregates in the long-time limit,

$$M_0^A(t) \simeq \frac{2K}{I}M_\upsilon^B(t). \quad (17)$$

Substituting expression (17) into Eq.(4), we obtain the asymptotical implicit solution of $a_1(t)$ at large times,

$$a_1(t) \simeq \frac{1}{2}M_0^A(t). \quad (18)$$

Substituting this relationship between a_1 and M_0^A into Eq.(5), one can obtain the asymptotical implicit solution of $a_2(t)$, and the rest can then be deduced by analogy. Here, we only give the asymptotical and brief expression of $a_k(t)$ in the long-time limit,

$$a_k(t) \simeq c_kM_0^A(t). \quad (19)$$

Here, c_k is a set of constants satisfying the recurrence formula

$$c_k = \frac{1}{2}\sum_{i+j=k} c_ic_j, \quad (20)$$

and $c_1 = 1/2$. The recurrence formula (20) can be obtained straightforwardly from Eq.(5) after equating the right-hand side to zero. We compute the value of c_k for $1 \le k \le 1000$ and find that c_k can be expressed as $c_k \simeq 0.3k^{-1.5}$, i.e. it may take the power-law form, $c_k \sim k^{-\alpha}$, $\alpha \simeq 1.5$. This is illustrated in Fig.1. Thus, the aggregate size distribution can be rewritten as

$$a_k(t) \sim k^{-\alpha}M_0^A(t) \simeq \frac{2K}{I}\Gamma(1+\upsilon)B_0k^{-\alpha}\left(1+\frac{1}{2}JB_0t\right)^{\upsilon-1} \sim k^{-\alpha}t^{-(1-\upsilon)}, \quad (21)$$

which indicates that the aggregate size distribution of A species evolves as a power law in size k and decays with time sub-linearly in the long-time limit.

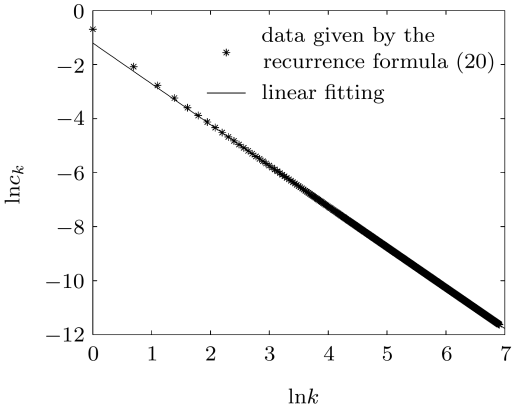


Fig.1. Log-log plot of the constants c_k vs k. The slope of the linear fit line is 1.512 ± 0.003 for $1 \le k \le 1000$.

For the $J = 0$ special case where the B catalyst does not coagulate by itself, the kinetics of the system can be exactly solved.

The υ-th moments of B aggregates is conserved in this case, $M_\upsilon^B(t) = \sum_{j=1}^{\infty} j^\upsilon b_j(t) = b_1(t) = B_0$, then the governing equation (4) reduces to

$$\frac{\mathrm{d}a_1}{\mathrm{d}t} = -Ia_1M_0^A(t) + KB_0M_0^A(t). \quad (22)$$

Summing up Eqs.(22) and (5), we obtain

$$\frac{\mathrm{d}M_0^A}{\mathrm{d}t} = -\frac{I}{2}(M_0^A)^2 + KB_0M_0^A. \quad (23)$$

This Bernoulli equation can be exactly solved to be

$$M_0^A(t) = \frac{2KB_0M_0^A(0)\mathrm{e}^{KB_0t}}{2KB_0 - IM_0^A(0) + IM_0^A(0)\mathrm{e}^{KB_0t}}, \quad (24)$$

where $M_0^A(0)$ is the initial total number of aggregates A at $t = 0$. And it is easy to find $M_0^A(t) \simeq 2KB_0/I$ in the long-time limit. So, the final value of the total number $M_0^A(t)$ is independent of the initial concentration data $M_0^A(0)$.

We then determine the aggregate size distribution $a_k(t)$. Substituting expression (24) into Eq.(22), we can deduce the exact solution of $a_1(t)$,

$$a_1(t) = \frac{KB_0}{I} - \frac{KB_0 - Ia_1(0)}{I}\left[\frac{2KB_0 - IM_0^A(0) + IM_0^A(0)\mathrm{e}^{KB_0t}}{IM_0^A(0)}\right]^{-2}, \tag{25}$$

where $a_1(0)$ is the initial concentration of monomers. In the long-time limit, we have

$$a_1(t) \simeq \frac{KB_0}{I} = \frac{2KB_0}{I}c_1. \tag{26}$$

In a way similar to that in the former case where the B catalyst can coagulate by itself, substituting expressions (24) and (26) into Eq.(5), we can derive the asymptotical expression of $a_k(t)$ in the long-time limit as

$$a_k(t) \simeq \frac{2KB_0}{I}c_k \sim k^{-\alpha}, \tag{27}$$

which decays as power law in size k and is independent of time, so we can conclude that the system will eventually evolve to a steady state.

2.2. The system with the catalysis-driven duplication probability proportional to the size of the mother aggregate

We then discuss the case where the catalysis-driven duplication rate kernel is proportional to the size of the mother aggregate, that is, $K(i,j) = Kij^{\upsilon}$. Equation (4) is then rewritten as

$$\frac{\mathrm{d}a_1}{\mathrm{d}t} = -Ia_1M_0^A + KM_1^AM_{\upsilon}^B, \tag{28}$$

while the governing rate equations for $a_k(t)$ $(k > 1)$ and $b_k(t)$ are the same as Eqs.(5) and (6) respectively.

Multiplying Eq.(5) with k and then summing them up with Eq.(28), we obtain

$$\frac{\mathrm{d}M_1^A}{\mathrm{d}t} = KM_1^AM_{\upsilon}^B. \tag{29}$$

Equation (29) yields the asymptotical solution of the total mass,

$$\begin{aligned} M_1^A(t) &= M_1^A(0)\mathrm{e}^{KM_{\upsilon}^Bt} \\ &\simeq M_1^A(0)\mathrm{e}^{KB_0^{\upsilon}\Gamma(1+\upsilon)(J/2)^{\upsilon-1}t^{\upsilon}}. \end{aligned} \tag{30}$$

We then determine the total number of the system, summing up Eqs.(28) and (5), we obtain

$$\frac{\mathrm{d}M_0^A}{\mathrm{d}t} = -\frac{I}{2}(M_0^A)^2 + KM_1^AM_{\upsilon}^B. \tag{31}$$

From this equation, we determine the asymptotical implicit solution for the total number of A aggregates in the long-time limit,

$$M_0^A(t) \simeq \left[\frac{2K}{I}M_1^A(t)M_{\upsilon}^B(t)\right]^{1/2}. \tag{32}$$

Substituting expression (32) into Eqs.(28) and (5), we derive the asymptotical implicit solution of $a_k(t)$ at large times,

$$\begin{aligned} a_k(t) &\simeq c_kM_0^A(t) \\ &\simeq C_1k^{-\alpha}t^{(\upsilon-1)/2}\mathrm{e}^{C_2t^{\upsilon}} \\ &\sim k^{-\alpha}t^{(\upsilon-1)/2}\mathrm{e}^{C_2t^{\upsilon}}, \end{aligned} \tag{33}$$

where $C_1 = [2^{2-\upsilon}KB_0^{\upsilon}M_1^A(0)\Gamma(1+\upsilon)J^{\upsilon-1}/I]^{1/2}$ and $C_2 = [KB_0^{\upsilon}\Gamma(1+\upsilon)J^{\upsilon-1}/2^{\upsilon}]^{1/2}$. Expression (33) implies that the aggregate size distribution $a_k(t)$ approaches a power law in size k and grows with time as $t^{(\upsilon-1)/2}\mathrm{e}^{C_2t^{\upsilon}}$.

When $J = 0$, the B catalyst cannot coagulate by itself, equation (28) becomes

$$\frac{\mathrm{d}a_1}{\mathrm{d}t} = -Ia_1M_0^A + KB_0M_1^A. \tag{34}$$

Multiplying Eq.(5) with k and then summing them up with Eq.(34), we obtain

$$\frac{\mathrm{d}M_1^A}{\mathrm{d}t} = KB_0M_1^A. \tag{35}$$

It yields the exact solution $M_1^A(t) = M_1^A(0)\,\mathrm{e}^{KB_0t}$.

Then summing up Eqs.(34) and (5) yields

$$\frac{\mathrm{d}M_0^A}{\mathrm{d}t} = -\frac{I}{2}(M_0^A)^2 + KB_0M_1^A. \tag{36}$$

In the long-time limit, from Eq.(36) we obtain the asymptotical implicit solution of the total number,

$$M_0^A(t) \simeq \left[\frac{2KB_0}{I}M_1^A(t)\right]^{1/2}. \tag{37}$$

Substituting expression (37) into Eqs.(34) and (5), we derive the asymptotical implicit solution of $a_k(t)$ at large times,

$$a_k(t) \simeq c_kM_0^A(t) \simeq C_3k^{-\alpha}\mathrm{e}^{\frac{KB_0}{2}t}. \tag{38}$$

where $C_3 = [2KB_0M_1^A(0)/I]^{1/2}$. Expression (38) implies that the aggregate size distribution $a_k(t)$ approaches a power law in size k and increases with time exponentially.

3. Aggregation growth with complete catalytically activated duplications

In this section, we investigate another model in which the complete catalysis-driven duplications of A aggregates can occur. The corresponding rate equations for this model are then written as

$$\frac{\mathrm{d}a_k}{\mathrm{d}t} = \frac{1}{2}\sum_{i+j=k} I(i,j)a_i a_j - a_k\sum_{j=1}^{\infty} I(k,j)a_j + a_k\sum_{j=1}^{\infty} L(i,j)b_j, \tag{39}$$

$$\frac{\mathrm{d}b_k}{\mathrm{d}t} = \frac{1}{2}\sum_{i+j=k} J(i,j)b_i b_j - b_k\sum_{j=1}^{\infty} J(k,j)b_j. \tag{40}$$

In Eq.(39), the newly-introduced third term on the right-hand side accounts for the gain in the concentration of A species due to the complete duplication processes driven by B species. Equation (40) is the same as Eq.(3), and the kinetics of the B catalyst has been discussed in the former model, so we study only the evolution behaviour of A aggregates in this section. We consider here a simple case with the constant coagulation rate kernels $I(i,j) = I$, $J(i,j) = J$, and the catalysis-driven complete duplication rate kernel $L(i,j) = Lj^{\upsilon}$. We find the system can be solved with the help of the ansatz

$$a_k(t) = A(t)[a(t)]^{k-1}. \tag{41}$$

Substituting the ansatz (41) into Eq.(39), it can be transformed into

$$\frac{\mathrm{d}a}{\mathrm{d}t} = \frac{IA}{2}, \tag{42}$$

$$\frac{\mathrm{d}A}{\mathrm{d}t} = -\frac{IA^2}{1-a} + LAM_{\upsilon}^{B}. \tag{43}$$

Under the monodisperse initial condition $a_k(0) = A_0\delta_{k1}$ (A_0 is the initial aggregate concentrations of A species), from the above equations one can obtain

$$A(t) = A_0(1-a)^2E(t) \tag{44}$$

with the shorthand notation $E(t) = \exp[L\int_0^t M_{\upsilon}^{B}(t')\mathrm{d}t'] \simeq \mathrm{e}^{C_4t^{\upsilon}}$, $C_4 = 2^{1-\upsilon}LB_0^{\upsilon}\Gamma(1+\upsilon)\upsilon^{-1}J^{\upsilon-1}$.

Substituting expression (44) into Eq.(42), we can deduce the following equation:

$$\frac{\mathrm{d}(1-a)}{\mathrm{d}t} = -\frac{IA_0}{2}(1-a)^2E(t). \tag{45}$$

This is a Bernoulli equation, and can be straightforwardly solved to be

$$a(t) = 1 - \left[1 + \frac{IA_0}{2}F(t)\right]^{-1}, \tag{46}$$

with the shorthand notation $F(t) = \int_0^t E(t')\mathrm{d}t' \simeq (\upsilon C_4)^{-1}t^{1-\upsilon}\mathrm{e}^{C_4t^{\upsilon}}$.

We then derive the aggregate size distribution of A aggregates,

$$\begin{aligned} a_k(t) &= A(t)a^{k-1}(t) \\ &= A_0E(t)\left[1 + \frac{IA_0}{2}F(t)\right]^{-2} \\ &\quad\times\left\{1 - \left[1 + \frac{IA_0}{2}F(t)\right]^{-1}\right\}^{k-1}. \end{aligned} \tag{47}$$

In the scaling regime of $k \gg 1$ and $t \gg 1$, expression (47) reduces to

$$\begin{aligned} a_k(t) &\simeq 4I^{-2}A_0^{-1}C_4^2\upsilon^2t^{2(\upsilon-1)}\mathrm{e}^{-C_4t^{\upsilon}}\exp(-x), \\ x &= (2\upsilon C_4)^{-1}IA_0kt^{1-\upsilon}\mathrm{e}^{C_4t^{\upsilon}}, \end{aligned} \tag{48}$$

which indicates that the aggregate size distribution approaches the modified scaling form (see, e.g. Ref.[30])

$$a_k(t) \sim t^{-\gamma}S^{-1}(t)\Phi[k/S(t)], \tag{49}$$

where $\gamma = 1 - \upsilon$ is the scaling exponent and $S(t) \sim t^{1-\upsilon}\mathrm{e}^{C_4t^{\upsilon}}$ is the typical aggregate size.

It is also instructive to investigate the total number and the total mass of the system. Using ansatz (41), the total number and total mass of A species can be expressed as

$$M_0^A(t) = \sum_{j=1}^{\infty} a_j(t) = \frac{A}{(1-a)},$$

and

$$M_1^A(t) = \sum_{j=1}^{\infty} ja_j(t) = \frac{A}{(1-a)^2}. \tag{50}$$

Substituting expressions (44) and (46) into expression (50), we derive the asymptotical solution of the total number and the total mass,

$$M_0^A(t) \simeq 2I^{-1}C_4\upsilon t^{-(1-\upsilon)},$$

and

$$M_1^A(t) \simeq A_0\mathrm{e}^{C_4t^{\upsilon}}. \tag{51}$$

Expression (51) indicates that the total number $M_0^A(t)$ decreases sublinearly with time while the total mass $M_1^A(t)$ increases with time exponentially.

In the $J = 0$ case, the B catalyst cannot coagulate by itself, under the monodisperse initial condition $b_k(0) = B_0\delta_{k1}$, equation (39) becomes

$$\frac{\mathrm{d}a_k}{\mathrm{d}t} = \frac{I}{2}\sum_{i+j=k} a_i a_j - Ia_k M_0^A + LB_0 a_k. \quad (52)$$

In this special case, the system can be exactly solved.

Summing up Eq.(52) over all k, we obtain

$$\frac{\mathrm{d}M_0^A}{\mathrm{d}t} = -\frac{I}{2}(M_0^A)^2 + LB_0 M_0^A. \quad (53)$$

From Eq.(53) one readily derives the exact solution of the total number of A aggregates,

$$M_0^A(t) = \frac{2LB_0 A_0 \mathrm{e}^{LB_0 t}}{2LB_0 - IA_0 + IA_0\mathrm{e}^{LB_0 t}}. \quad (54)$$

Obviously, the total number $M_0^A(t) \simeq 2LB_0/I$ in the long-time limit. On the other hand, multiplying Eq.(52) with k and then summing them up, we obtain the differential equation for the total mass of A species,

$$\frac{\mathrm{d}M_1^A}{\mathrm{d}t} = LB_0 M_1^A, \quad (55)$$

which can be straightforwardly integrated to give

$$M_1^A(t) = M_1^A(0)\mathrm{e}^{LB_0 t}. \quad (56)$$

This shows that the total mass of A species grows exponentially with time and diverges finally.

Next, we determine the solution of the aggregate size distribution. With the help of expression (41), we recast Eq.(52) into

$$\frac{\mathrm{d}a}{\mathrm{d}t} = \frac{IA}{2}, \quad (57)$$

$$\frac{\mathrm{d}A}{\mathrm{d}t} = -\frac{IA^2}{1-a} + LB_0 A. \quad (58)$$

Using the above technique, we derive the exact expression of the aggregate size distribution,

$$\begin{aligned} & a_k(t) \\ &= 4A_0 L^2 B_0^2 \mathrm{e}^{LB_0 t}(2LB_0 - IA_0 + IA_0\mathrm{e}^{LB_0 t})^{-2} \\ &\quad \times[1 - 2LB_0(2LB_0 - IA_0 + IA_0\mathrm{e}^{LB_0 t})^{-1}]^{k-1}. \end{aligned} \quad (59)$$

In the scaling region of $k \gg 1$ and $t \gg 1$, expression (59) can be approximately rewritten as

$$\begin{aligned} a_k(t) &\simeq 4L^2 B_0^2 A_0^{-1} I^{-2} \mathrm{e}^{-LB_0 t}\exp(-x), \\ x &= 2LB_0(IA_0)^{-1} k\,\mathrm{e}^{-LB_0 t}. \end{aligned} \quad (60)$$

Expression (60) indicates that the aggregate size distribution of A species approaches the generalized scaling form (see, e.g. Ref.[30])

$$a_k(t) \sim [f(t)]^{-w}\,\Phi[k/S(t)], \quad S(t) \propto [f(t)]^{-z}, \quad (61)$$

where $f(t)$ is an increasing function of time, w and z are two exponents which can describe the dynamic scaling properties of the aggregate size distribution and $S(t)$ is the typical size. For this case, $f(t) = \mathrm{e}^t$, $w = z = LB_0$, and the typical size grows exponentially with time, $S(t) \propto \mathrm{e}^{LB_0 t}$. Moreover, expression (61) also indicates that each $a_k(t)$ asymptotically has the same value for $k \ll IA_0\mathrm{e}^{LB_0 t}/2LB_0$ at large times, while it decays exponentially with size k for $k \gg IA_0\mathrm{e}^{LB_0 t}/2LB_0$.

4. Summary

We have proposed an irreversible aggregation model of two species with catalysis-driven duplications, in which any two aggregates of the same species can coagulate themselves and, meanwhile, the aggregates of A species of any size can duplicate a monomer or itself under the catalysis of B species aggregates. Based on the mean-field theory, we have analytically investigated the evolution of the aggregate size distribution of the two species by means of the rate equation approach. The aggregate size distribution of A species $a_k(t)$ are found to be crucially dependent on the details of the concrete catalysis-driven duplication rate kernels and the coagulation of B catalyst.

In the system with catalysis-driven monomer duplications, the concentration of the A aggregates of any size always follows a power law in size k. And in the case of the duplication rate independent of the size of the mother aggregates, namely, $K(i,j) = Kj^v$, $a_k(t)$ decreases with time sublinearly when the B catalyst coagulates by itself, while the system evolves to a steady state when the B catalyst does not coagulate. In the case of the duplication rate proportional to the size of the mother aggregates, namely, $K(i,j) = Kij^v$, $a_k(t)$ always increases with time. And when the B catalyst does not coagulate by itself, $a_k(t)$ grows with time exponentially, when the B catalyst coagulates, it still grows with time but not exponentially. For the system with complete catalysis-driven duplications, when the B catalyst coagulates by itself, the aggregate size distribution $a_k(t)$ approaches a modified scaling form, and when the B catalyst does not coagulate by itself, $a_k(t)$ satisfies a generalized scaling form.

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