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Solvable aggregation model with monomer annihilation

Jianhong Ke* and Zhenquan Lin
Department of Physics, Wenzhou Normal College, Wenzhou 325027, China

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We propose a simple model in which irreversible aggregations occur between any two clusters of the same species and monomer annihilations occur between any two clusters of different species. We investigate the mean-field rate equation to analyze kinetics of the system under symmetrical initial conditions. In the constant-reaction-rate case, the cluster-mass distribution of either species approaches a conventional scaling form and both species survive finally; while for the system with a fast rate kernel, both species scale according to a modified form and no species can survive at the end.

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The kinetics of irreversible aggregation and annihilation processes is an important subject of extensive research in the recent few decades [1–4]. In a general aggregation model with annihilation, the system consists of at least two distinct species, and an irreversible aggregation occurs between any two clusters of the same species while an irreversible annihilation occurs simultaneously between any two clusters of different species. Recently, considerable works have been devoted to understanding the evolution of the cluster-mass distribution in the irreversible aggregation-annihilation process, and it was found that the evolution behavior of the cluster-mass distribution may obey a scaling law in the long-time limit [5–10].

For the annihilation reaction, most of these works have focused on two types of schemes, partial annihilation and complete annihilation. The former is described by the scheme $A_i+B_j\rightarrow A_{i-j}$ $(i\geqslant j)$ or $A_i+B_j\rightarrow B_{j-i}$ $(i<j)$ [6–8]. Here, A_i denotes an aggregate of A species consisting of size i and B_j represents a cluster of B species consisting of size j, and after the annihilation reaction, the cluster with larger size is conserved with the monomer difference $|i-j|$ of the reactants. The latter is a pairwise annihilation of the aggregates according to the scheme $A_i+B_j\rightarrow$inert, that is, the binary annihilation between any two clusters of different species always yields the inert product, independent of the reactant masses [9,10]. On the other hand, all the results of the investigations on these aggregation processes with partial or complete annihilation imply that at most one species can survive at the end. In particular, all the species will annihilate each other completely under the symmetrical initial conditions. In most situations of the natural science and technology, it may be reasonable to assume the above-mentioned schemes for the annihilation process. However, there also exist many situations in which both reactant clusters can survive together after the annihilation. The classical example is that an animal species can coexist with its natural enemies in the natural world.

In order to study the general mechanisms, we introduce a “monomer annihilation” model as an attempt to account for the coexisting phenomena. In our model, irreversible aggregations occur between any two clusters of the same species,

$$A_i+A_j\rightarrow A_{i+j}\,,\quad B_i+B_j\rightarrow B_{i+j}\,, \tag{1}$$

and a monomer annihilation between different species reads

$$A_i+B_j\rightarrow A_{i-1}+B_{j-1}\,. \tag{2}$$

The two-species case also contains the generic multispecies behavior. Therefore, we can first focus on the two-species case and then generalize it to the multispecies situation. We study our model in the mean-field limit. The mean-field approximation neglects the spatial fluctuation of the reactant densities and, therefore, applies to the case in which the spatial dimension d of the system is greater than or equal to a critical dimension d_c [6,9]. It was found that for pure aggregation processes, $d_c=2$ [11]. Sokolov and Blumen verified that for irreversible aggregation processes with partial annihilation the marginal dimension is 2 [8], and Ben-Naim and Krapivsky also found that for irreversible aggregation system with complete annihilation the critical dimension is $d_c=2$ [9]. Since our model interpolates between the pure aggregation and the general aggregation-annihilation processes, it is natural to expect that for our model the critical dimension is the same, $d_c=2$.

We first investigate the two-species aggregation-annihilation process. The concentrations of A and B clusters consisting of k mers are denoted by a_k and b_k, respectively. Here we consider a simple model with a constant reaction rate kernel. All the annihilation reaction rates are equal to a constant J, and the aggregation rates of A and B clusters equal the constants I_1 and I_2, respectively. The mean-field theory assumes that the reaction proceeds with a rate proportional to the concentrations of the reactants. Then the mean-field rate equations for this two-species system read

$$\frac{da_k}{dt}=I_1\left(\frac{1}{2}\sum_{i+j=k}a_ia_j-a_k\sum_{j=1}^{\infty}a_j\right)-J(a_k-a_{k+1})\sum_{j=1}^{\infty}b_j\,,$$

$$\frac{db_k}{dt}=I_2\left(\frac{1}{2}\sum_{i+j=k}b_ib_j-b_k\sum_{j=1}^{\infty}b_j\right)-J(b_k-b_{k+1})\sum_{j=1}^{\infty}a_j\,. \tag{3}$$

We consider the simplest but important case with the monodisperse initial conditions

$$a_k(0)=A_0\delta_{k1}\,,\quad b_k(0)=B_0\delta_{k1}\,. \tag{4}$$

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*Electronic address: kejianhong@yahoo.com.cn

The governing rate equations (3) can then be solved with the help of ansatz [6]

$$a_k(t)=A(t)[a(t)]^{k-1}, \quad b_k(t)=B(t)[b(t)]^{k-1}. \tag{5}$$

Substituting Eqs. (5) into Eqs. (3), we can transform the rate equations (3) into the differential equations as follows:

$$\frac{da}{dt}=\frac{I_1}{2}A, \quad \frac{dA}{dt}=-\frac{I_1A^2}{1-a}-JAB\frac{1-a}{1-b},$$
$$\frac{db}{dt}=\frac{I_2}{2}B; \quad \frac{dB}{dt}=-\frac{I_2B^2}{1-b}-JAB\frac{1-b}{1-a}. \tag{6}$$

Introducing two variables, $\alpha(t)=[1-a(t)]^{-1}$ and $\beta(t)=[1-b(t)]^{-1}$, we recast Eqs. (6) to

$$\frac{d^2\alpha}{dt^2}=-\frac{2J}{I_2\alpha\beta}\frac{d\alpha}{dt}\frac{d\beta}{dt}, \quad \frac{d^2\beta}{dt^2}=-\frac{2J}{I_1\alpha\beta}\frac{d\alpha}{dt}\frac{d\beta}{dt}, \tag{7}$$

with the initial conditions

$$\alpha=\beta=1, \quad \frac{d\alpha}{dt}=\frac{1}{2}I_1A_0, \quad \frac{d\beta}{dt}=\frac{1}{2}I_2B_0 \quad \text{at } t=0. \tag{8}$$

It is obvious that for our model the mass difference between the two species is conserved,

$$M_A(t)-M_B(t)=\sum_{k=1}^{\infty}k[a_k(t)-b_k(t)]$$
$$=\frac{2}{I_1}\frac{d\alpha}{dt}-\frac{2}{I_2}\frac{d\beta}{dt}\equiv A_0-B_0. \tag{9}$$

From Eq. (9), one can obtain

$$I_2\alpha-I_1\beta=\frac{I_1I_2}{2}(A_0-B_0)t+I_2-I_1. \tag{10}$$

Under the symmetrical initial condition, $A_0=B_0$, we find $I_2\alpha-I_1\beta=I_2-I_1$. Equations (7) then reduce to

$$\frac{d\alpha}{dt}=\frac{I_1}{2}A_0\left(\frac{I_1}{I_2}\right)^{2J/(I_2-I_1)}\left(1-\frac{I_2-I_1}{I_2}\alpha^{-1}\right)^{-2J/(I_2-I_1)}$$
$$\text{for } I_1\neq I_2,$$
$$\frac{d\alpha}{dt}=\frac{I_1}{2}A_0\exp\left(\frac{2J}{I_1\alpha}-\frac{2J}{I_1}\right) \quad \text{for } I_1=I_2. \tag{11}$$

From Eqs. (11), we cannot derive the exact solution of $\alpha(t)$ and then turn to determine its asymptotic solution at large times. The system is assumed to reach its steady state at $t\to\infty$ and the corresponding steady conditions are given as follows:

$$\frac{da}{dt}=\frac{1}{\alpha^2}\frac{d\alpha}{dt}=0, \quad \frac{dA}{dt}=\frac{2}{I_1\alpha^2}\frac{d^2\alpha}{dt^2}-\frac{4}{I_1\alpha^3}\left(\frac{d\alpha}{dt}\right)^2=0. \tag{12}$$

Thus, we can conclude that either $\alpha\to\infty$ or $d\alpha/dt\to 0$ at $t\to\infty$. Further, from Eqs. (11), we know that for this case $\alpha\to\infty$ at $t\to\infty$. Hence, $\alpha\gg 1$ at $t\gg 1$. In the long-time limit, Eqs. (11) can be asymptotically rewritten as

$$\frac{d\alpha}{dt}\simeq C_1, \tag{13}$$

where $C_1=(I_1A_0/2)(I_1/I_2)^{2J/(I_2-I_1)}$ for $I_1\neq I_2$ and $C_1=(I_1A_0/2)\exp(-2J/I_1)$ for $I_1=I_2$. Equation (13) can be directly solved to yield the asymptotic solution of $\alpha(t)$ at large time,

$$\alpha(t)\simeq C_1t. \tag{14}$$

From Eqs. (10) and (14), one can then determine the asymptotic solution of $\beta(t)$ at large times

$$\beta(t)\simeq C_2t, \tag{15}$$

where $C_2=I_2C_1/I_1$. Thus, we obtain the asymptotic solutions of the cluster-mass distributions

$$a_k(t)\simeq\frac{2}{I_1C_1}t^{-2}(1-C_1^{-1}t^{-1})^{k-1},$$
$$b_k(t)\simeq\frac{2}{I_2C_2}t^{-2}(1-C_2^{-1}t^{-1})^{k-1}. \tag{16}$$

Further, Eqs. (16) can be rewritten as

$$a_k(t)\simeq\frac{2}{I_1C_1}t^{-2}\exp(-x), \quad b_k(t)\simeq\frac{2}{I_2C_2}t^{-2}\exp(-y), \tag{17}$$

which are valid in the scaling region $k\gg 1$, $t\gg 1$, $x=(k/C_1)t^{-1}=\text{finite}$, and $y=(k/C_2)t^{-1}=\text{finite}$. These exhibit that the cluster-mass distribution of either species approaches a conventional scaling form [6]

$$c_k(t)\simeq t^{-2}\Phi[k/S(t)], \quad S(t)\propto t, \tag{18}$$

where $c_k(t)$ denotes the concentration of the k-mer aggregates and $S(t)$ is the characteristic mass for such an irreversible aggregation system. In this model, the scaling function is exponential, $\Phi(x)=\exp(-x)$. Moreover, the typical mass $S(t)$ of either species grows as t. It is also instructive to compute the total concentration and the total mass of the aggregates. In the long-time limit, we obtain the total concentrations

$$N_A(t)=\sum_{k=1}^{\infty}a_k(t)\simeq\frac{2}{I_1}t^{-1}, \quad N_B(t)=\sum_{k=1}^{\infty}b_k(t)\simeq\frac{2}{I_2}t^{-1}, \tag{19}$$

and the total mass densities

$$M_A(t)=M_B(t)=\sum_{k=1}^{\infty}ka_k(t)\simeq\frac{2C_1}{I_1}. \tag{20}$$

These indicate that the total concentration of either species decays as t^{-1} and the total mass of either species retains a certain value at $t \gg 1$. The results also imply that for the symmetrical initial case, both species are conserved by the dynamics of this irreversible aggregation-annihilation process, which is quite different from the results for the conventional aggregation-annihilation processes [6,7,9,10].

For the asymmetrical initial case, $A_0 > B_0$, it is difficult for us to derive the explicit solutions of the cluster-mass distributions. However, we can draw several important conclusions on the basis of the results of the above-mentioned symmetrical initial case, which are confirmed by some numerical computations. From Eq. (9), we find that $d\alpha/dt = I_1(A_0-B_0)/2 + (I_1/I_2)d\beta/dt \geq I_1(A_0-B_0)/2$. Meanwhile, since $d\alpha/dt = C_1$ in the $A_0 = B_0$ case at $t \to \infty$ [see Eqs. (13)], we can conclude that for the $A_0 > B_0$ case $d\alpha/dt > C_1$ at large times. Hence, if $C_1 \geq I_1(A_0-B_0)/2$, i.e., $A_0/B_0 \leq [1-\exp(-2J/I_1)]^{-1}$ for $I_1 = I_2$ or $A_0/B_0 \leq [1-(I_1/I_2)^{2J/(I_2-I_1)}]^{-1}$ for $I_1 \neq I_2$, we find that $d\beta/dt \simeq C_3 > 0$ and $d\alpha/dt \simeq I_1(A_0-B_0)/2 + C_3$ in the long-time limit (here C_3 is a finite constant), which are similar to Eq. (13). Thus, we know that the cluster-mass distribution of either species approaches the conventional scaling form (18) and both species can be conserved by the dynamics of the system. This result is confirmed by some numerical computations. On the other hand, when $A_0 \gg B_0$ (especially for the case in which there exists only one monomer of *B* species in the beginning of the process), *B* species will be annihilated completely by *A* species and only *A* clusters survive finally. Thus, we know that for the $A_0 \gg B_0$ case, the mass distribution of *A* clusters also satisfies the conventional scaling form (18), while the conventional scaling description breaks down for *B* clusters.

It is obvious that for the asymmetrical initial case, there exists a critical ratio γ_c of A_0/B_0 which divides the two different evolution regimes. When $A_0/B_0 < \gamma_c$, both species scale according to the conventional scaling form (18) and survive together at the end; however, for the $A_0/B_0 > \gamma_c$ case, only *A* clusters can survive finally. Our results imply that $\gamma_c > [1-\exp(-2J/I_1)]^{-1}$ for the $I_1 = I_2$ case and $\gamma_c > [1-(I_1/I_2)^{2J/(I_2-I_1)}]^{-1}$ for the $I_1 \neq I_2$ case. Unfortunately, we cannot determine the exact value of γ_c. If the details of the reaction events are given, the critical ratio γ_c may be asymptotically determined by numerical computation.

In the *n*-species ($n > 2$) case, we set all the aggregation rates equal to *I* and the annihilation rates *J*. Under the symmetrical monodisperse initial conditions, the governing rate equation reads

$$\frac{dc_k}{dt} = I\left(\frac{1}{2}\sum_{i+j=k} c_i c_j - c_k \sum_{j=1}^{\infty} c_j\right) - (n-1)J(c_k - c_{k+1})\sum_{j=1}^{\infty} c_j, \tag{21}$$

where $c_k(t)$ denotes the concentration of the *k*-mer clusters of any species and $c_k(0) = \delta_{k1}$. By employing the above-mentioned technique, we solve Eq. (21) and obtain the asymptotic scaling solution of $c_k(t)$ as follows:

$$c_k(t) \simeq \frac{2}{IC_4} t^{-2} \exp(-x), \quad x = (k/C_4)t^{-1}, \tag{22}$$

where $C_4 = (I/2)\exp[-2(n-1)J/I]$. This implies that for the symmetrical initial case, the evolution of each species obeys the conventional scaling law (18). Moreover, all species can be conserved by the dynamics of the aggregation process with monomer annihilation, which is independent of the species number *n* as well as the ratio between the reaction rates *J* and *I*. On the other hand, the final surplus mass of each species is equal to a finite constant $\exp[-2(n-1)J/I]$ that depends on the species number *n* and on the ratio of reaction rates.

In order to go deep into the kinetics of the irreversible aggregation with monomer annihilation, we then turn to discuss a two-species model with a fast annihilation rate kernel. In this system, the rate of the annihilation between A_k and B_j clusters is proportional to their masses *k* and *j*, with the proportionality coefficient *J*. Then the rate equations read

$$\begin{aligned}\frac{da_k}{dt} &= I_1\left(\frac{1}{2}\sum_{i+j=k} a_i a_j - a_k \sum_{j=1}^{\infty} a_j\right) - J[ka_k - (k+1)a_{k+1}]\sum_{j=1}^{\infty} jb_j,\\ \frac{db_k}{dt} &= I_2\left(\frac{1}{2}\sum_{i+j=k} b_i b_j - b_k \sum_{j=1}^{\infty} b_j\right) - J[kb_k - (k+1)b_{k+1}]\sum_{j=1}^{\infty} ja_j.\end{aligned} \tag{23}$$

Under the initial conditions (4), with the help of ansatz (5) we recast Eqs. (23) to

$$\begin{aligned}\frac{da}{dt} &= \frac{I_1}{2}A + \frac{Ja^2B}{(1-b)^2} - \frac{JaB}{(1-b)^2},\\ \frac{dA}{dt} &= -\frac{I_1A^2}{1-a} + \frac{2JaAB}{(1-b)^2} - \frac{JAB}{(1-b)^2},\\ \frac{db}{dt} &= \frac{I_2}{2}B + \frac{Jb^2A}{(1-a)^2} - \frac{JbA}{(1-a)^2},\\ \frac{dB}{dt} &= -\frac{I_2B^2}{1-b} + \frac{2JbAB}{(1-a)^2} - \frac{JAB}{(1-a)^2}.\end{aligned} \tag{24}$$

It should be pointed out that for this model the mass difference between the two species is also conserved. For the symmetrical initial case, $A_0 = B_0 = C_0$, we have $M_A(t) \equiv M_B(t)$, i.e., $A/(1-a)^2 \equiv B/(1-b)^2$. Thus, from Eqs. (24) we obtain

$$\frac{d[A/(1-a)^2]}{dt}=\frac{d[B/(1-b)^2]}{dt}=-J\frac{A^2}{(1-a)^4}. \quad (25)$$

Equation (25) can be directly solved to yield

$$\frac{A}{(1-a)^2}=\frac{B}{(1-b)^2}=\frac{C_0}{JC_0t+1}. \quad (26)$$

By making use of Eq. (26) we solve Eqs. (24) and then obtain the asymptotic solutions of $a_k(t)$ and $b_k(t)$ at large times,

$$a_k(t)\simeq C_5\left(\frac{I_1}{I_1+2J}\right)^k t^{-1}\exp(-x), \quad x=C_6kt^{-1},$$

$$b_k(t)\simeq C_7\left(\frac{I_2}{I_2+2J}\right)^k t^{-1}\exp(-y), \quad y=C_8kt^{-1}, \quad (27)$$

where $C_5=4J/(I_1+2J)^2$, $C_6=2/[(I_1+2J)C_0]$, $C_7=4J/(I_2+2J)^2$, and $C_8=2/[(I_2+2J)C_0]$. The results show that the cluster-mass distribution of either species does not approach the conventional definition (18) but satisfies a modified scaling form $c_k(t)\simeq h^k t^{-1}\Phi[k/S(t)]$, $S(t)\propto t$. Here, h is a constant and $0<h<1$. This modified scaling form also indicates that the two different mass scales, a growing scale and a time-independent scale, are associated with either species. The growing scale for either species is the same, $S(t)\sim t$, which is forced by the aggregation-annihilation process. The time-independent scale for A species is $S_A\simeq(I_1+2J)/2J$ while that for B species is $S_B\simeq(I_2+2J)/2J$. It is the time-independent scale that dominates the evolution behavior of the species in the long-time limit. Ben-Naim and Krapivsky also found that this nonuniversal phenomenon exists in the irreversible aggregation-annihilation processes [6,9]. In the long-time limit, the total concentration and the total mass of A species are $N_A(t)\simeq 2t^{-1}/(I_1+2J)$ and $M_A(t)\simeq t^{-1}/J$, and those of B species are $N_B(t)\simeq 2t^{-1}/(I_2+2J)$ and $M_B(t)\simeq t^{-1}/J$. These indicate that both the total concentration and the total mass of either species decay as t^{-1} in the long-time limit. So, both species annihilate each other completely at the end.

Finally, we turn to the asymmetrical initial case, $A_0>B_0$. From Eqs. (24), we obtain

$$\frac{d[A/(1-a)^2]}{dt}=\frac{d[B/(1-b)^2]}{dt}=-J\frac{AB}{(1-a)^2(1-b)^2}. \quad (28)$$

Since $A/(1-a)^2-B/(1-b)^2\equiv A_0-B_0$, it is obvious that $M_A(t)\to A_0-B_0$ and $M_B(t)\to 0$ at $t\to\infty$. Thus, one can easily solve Eqs. (24) to obtain the asymptotic solutions

$$a_k(t)\simeq C_9t^{-2}\exp(-x), \quad x=C_{10}kt^{-1},$$

$$b_k(t)\simeq C_{11}\exp[-J(A_0-B_0)kt], \quad (29)$$

where $C_9=4/[I_1^2(A_0-B_0)]$, $C_{10}=2/[I_1(A_0-B_0)]$, and $C_{11}=(A_0-B_0)B_0/A_0$. The results show that the evolution behavior of A clusters satisfies the conventional scaling law (18) while B clusters do not scale. For this case, the total concentration of A clusters decays as t^{-1} in the long-time limit while that of B clusters decays rapidly as $\exp[-J(A_0-B_0)t]$. Moreover, only A clusters can survive at the end.

In summary, we have proposed a simple irreversible aggregation model with monomer annihilation. Based on the mean-field assumption, we analyzed the kinetics of the irreversible aggregation-annihilation process with a constant-rate kernel. The results indicate that for the symmetrical initial case, the cluster-mass distribution of each species satisfies the conventional scaling form and all species can be conserved by the dynamics of the aggregation-annihilation system. However, for the two-species case in which the initial mass of one species is by far greater than that of another one, only the species with the larger initial concentration scales according to the conventional scaling law and survives at the end. We have also investigated the two-species model with a fast annihilation rate kernel and found that its kinetic behavior is quite different from that of the constant-rate-kernel model. Under the symmetrical initial conditions, the evolution behavior of either species obeys the modified scaling law and both species annihilate each other completely at the end. For the asymmetrical initial case, the evolution of the heavy species with the larger initial concentration approaches the conventional scaling form while the light species does not scale. Hence, only the heavy species can survive finally.

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