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1999 J. Phys. A: Math. Gen. 32 781

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J. Phys. A: Math. Gen. **32** (1999) 781–793. Printed in the UK PII: S0305-4470(99)91005-3

A 'triangle' of interconnected coagulation models

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Received 26 January 1998, in final form 7 August 1998

Abstract. A number of new coagulation models depending on a parameter is derived. The dependence is considered in two different ways. If the parameter takes its maximal value then in the first case we obtain a new discrete kinetic equation. We demonstrate that its continuous version is simply the Oort–Hulst's coagulation model. In the second case, the maximum of the corresponding parameter yields the Smoluchowski coagulation equation. At the minimal values of both parameters we arrive at another new kinetic equation. These three models form a 'triangle' connecting the two known coagulation equations 'situated' in its vertexes (Smoluchowski and Oort–Hulst equations) via an alteration of the parameters. Also, a comparative analysis of these three models is presented. As an advantage of the Oort–Hulst approach we compute the coagulation front and establish a connection between the infringement of the mass conservation law and convergence of the coagulation front to infinity.

0. Preliminaries

We are concerned with disperse systems containing particles of different masses (volumes) that can undergo mutual interactions resulting in a change of their masses. Such systems take place in astronomy (forming of cosmic objects), atmospheric science (evolution of clouds), chemistry (polymer reactors and colloids), etc. If the average mass of particles (i.e. the relation of total mass of all particles divided by the amount of all particles) increases in time then this process is called coagulation. Usually, it is assumed that a coagulation process may be considered as merging two colliding particles. This assumption leads to the well known Smoluchowski coagulation equation [1], which is often written either in the continuous, or discrete forms. However, there is another continuous coagulation model by Oort and van de Hulst [2] written in a convenient form by Safronov [3]. The second model is used in astronomy to analyse cosmic objects (creation of stars, planets, evolution of nebulae, galaxies, clouds of cosmic dust, etc) [2–5], in atmosphere science [6–10] and in technical installations [7, 11].

We derive two one-parameter families of discrete coagulation models. The more values of the parameters, the more intensive a coagulation process we have. We prove that the maximum value of the parameter of the first family yields a discrete balance equation. It turns out that this equation is the discrete version of the Oort–Hulst coagulation equation (section 3), written earlier in the continuous form. The minimum value of the parameter gives us a new discrete kinetic equation with low intensity of coagulation. It plays an auxiliary role in our analysis.

Then we consider another one-parameter family of kinetic equations (section 2). We demonstrate, that the maximum value of the second parameter yields the discrete version of the renowned Smoluchowski coagulation equation. The minimum of the second parameter leads us to the same auxiliary discrete kinetic equation.

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So, we obtain three discrete coagulation models, which can be presented as a triangle. One side of the triangle connects the discrete version of the Oort–Hulst's equation and the auxiliary kinetic equation, provided that the values of the first parameter change. Another side connects the discrete Smoluchowski equation and the same auxiliary kinetic model if values of the second parameter change. So, through the auxiliary kinetic model we establish the interconnection between the basic Smoluchowski and Oort–Hulst coagulation equations.

After that we compare a number of mathematical properties of both basic coagulation equations. We conclude that, usually, these equations yield almost the same results and thus can both be applied to the analysis of disperse systems yielding a wider treatment of coagulation processes. Some of the mathematical properties of these equations differ and, hence, can be treated as useful complements of each other. As an example of such a useful completion we compute the speed of the coagulation front. Such computations become possible only after taking the Oort–Hulst equation into account.

As a more advanced example, we observe that the famous phenomenon of breaking down the mass conservation law at the intensive coagulation rate happens at the same time moment as when the coagulation front goes to infinity. This observation allows us to reveal some new classes of coagulation kernels yielding the breaking down of the mass conservation law.

1. A family of discrete coagulation models

We consider a disperse system possessing the following properties:

(1) the system is sufficiently rarefied to assume that colliding particles do not undergo any influence of other particles;
(2) average collision time (microscopic time) is essentially less than the time of changing the distribution function;
(3) there exist some random forces, which blend the disperse system such that the motion of particles between collision acts (including the process of their approach) is statistically independent;
(4) masses (volumes) of all particles are proportional to some $m_0 > 0$.

Let us consider the following mechanism of growth of particles as a result of the collisions of pairs of particles of masses (volumes) im_0 and jm_0. Hereinafter we assume for definiteness $i \geqslant j$. We call the particles of mass im_0, i-mers. m_0 is the mass of the smallest particles in the system.

Let a collision of an i-mer and a j-mer yield fragmentation of j-mer onto α monomers ($\alpha = \alpha(j)$) and a $j-\alpha$-mer. Each of those α monomers joins instantly to an i-mer (different for each monomer). It is worth pointing out that the consideration of such a joining the resultant monomers to i-mers is a mathematical convenience rather than a physical reality.

Thus, as a result of one collision act we have α new $i+1$-mers and one $j-\alpha$-mer (figure 1). The parameter $\alpha(j)$ is supposed to be non-decreasing with respect to the variable j.

From the balance reasonings we come to the following kinetic model:

$$\frac{\mathrm{d}c_i\ (t)}{\mathrm{d}t} = c_{i-1}(t)\sum_{j=1}^{i-1} K_{i-1,j}\alpha(j)c_j(t) - c_i(t)\sum_{j=1}^{i} K_{i,j}\alpha(j)c_j(t)$$
$$- \sum_{j=i}^{\infty} K_{i,j}c_i(t)c_j(t) + \sum_{m(i)}\sum_{j=m(i)}^{\infty} K_{m(i),j}c_{m(i)}(t)c_j(t) \qquad i \geqslant 1 \tag{1}$$

where $c_i(t)$ is the concentration of i-mers at time moment t, $K_{i,j}$ for $i \neq j$ is equal to the intensity rate of collisions of i-mers and j-mers; this rate is supposed to be prescribed by

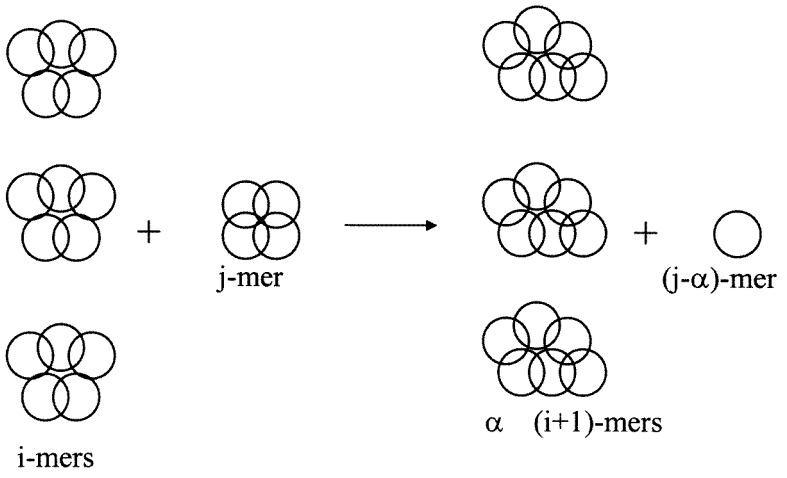

Figure 1. ($\alpha = 3$.)

the process considered. From the physical point of view it is clear that this function must be symmetric for all arguments $i, j \geqslant 1$: $K_{i,j} = K_{j,i}$. The values $K_{i,i}$ are equal to half of the collisions' rate for the particles of mass i. This phenomenon is caused by double reducing of pairs of particles, which can interact.

The first summand in the right-hand side of (1) yields the income of i-mers into the disperse system due to collisions of $i-1$-mers and monomers formed by fragmented j-mers. If $i = 1$ then we set it equal to zero. The second summand describes the decay of i-mers as a result of merging monomers to them. The multiplayer α in the first and the second summands demonstrates that α monomers take part in the collision act. The third and fourth terms describe decay and income of i-mers due to fragmentation of i-mers (third) and fragmentation of m-mers (fourth). In the last double summand a larger j-mer 'bites off' m-mer $\alpha(m)$ monomers, and the i-mer rest of m-mer appears in the system. It is clear that the positive integer value m satisfies the correlation

$$i + \alpha(m) = m. \tag{2}$$

Here each term should be positive and an integer. For example, if we have $\alpha(j) = j - 1$, then at $i = 1$ equation (2) has infinitely many solutions $m \geqslant 2$, and the fourth summand becomes equal to

$$\sum_{m=2}^{\infty} \sum_{j=m}^{\infty} K_{m,j} c_m c_j.$$

If equation (2) has no solutions then the fourth summand should be omitted (e.g., at $\alpha(m) = m$). However, often equation (2) has a unique root m, and the fourth summand in (1) transforms to

$$\sum_{j=m}^{\infty} K_{m,j} c_m c_j.$$

If we supply equation (1) by non-negative initial data $c_i(0)$ then it is possible to observe that solutions of (1) are non-negative, too. To demonstrate that, we use the following integral form of (1):

$$c_i(t) = \exp\left\{ -\int_0^t \left(\sum_{j=1}^{i} K_{i,j} \alpha(j) c_j(s) + \sum_{j=i}^{\infty} K_{i,j} c_j(s) \right) \mathrm{d}s \right\}$$

$$\times\left(c_i(0)+\int_0^t \exp\left\{\int_0^s\left[\sum_{j=1}^{i}K_{i,j}\alpha(j)c_j(s_1)+\sum_{j=i}^{\infty}K_{i,j}c_j(s_1)\right]\mathrm{d}s_1\right\}\right.$$

$$\left.\times\left[c_{i-1}(s)\sum_{j=1}^{i-1}K_{i-1,j}\alpha(j)c_j(s)+\sum_{m(i)}\sum_{j=m(i)}^{\infty}K_{m(i),j}c_{m(i)}(s)c_j(s)\right]\mathrm{d}s\right). \qquad (3)$$

If initial data $c_i(0)$ are strictly positive, then for truncated coagulation kernels $K_{m,j} = 0,\ m, j \geqslant N_0$, we easily obtain positivity of $c_i(t)$ for all $i \geqslant 1,\ t > 0$ by assuming that there is a time t_0 and a number i_0 such that $c_{i_0}(t_0) = 0$ and by arriving from (3) to a contradiction. If initial data are not strictly positive, then we approximate them by positive initial data and obtain the non-negativity of a solution by passing to a limit. The non-negativity of a solution for a non-truncated kernel is more complicated, it can be proved along with the existence theorem by approximating $K_{m,j}$ by a sequence of truncated kernels, generating the corresponding sequence of non-negative solutions of (3), and then passing to a limit which is a solution of (3). The non-negativity of the obtained limit is obvious.

If $\alpha = 1$ then we obtain from (1) the following kinetic equation:

$$\frac{\mathrm{d}c_i}{\mathrm{d}t} = c_{i-1}\sum_{j=1}^{i-1}K_{i-1,j}c_j - c_i\sum_{j=1}^{i}K_{i,j}c_j - \sum_{j=i}^{\infty}K_{i,j}c_ic_j + c_{i+1}\sum_{j=i+1}^{\infty}K_{i+1,j}c_j \qquad i \geqslant 1. \quad (4)$$

At $\alpha(j) = j$ (i.e. if the smaller particle is completely destroyed onto monomers, which 'stuck' instantly to larger particles) then we derive from (1)

$$\frac{\mathrm{d}c_i}{\mathrm{d}t} = c_{i-1}\sum_{j=1}^{i-1}K_{i-1,j}jc_j - c_i\sum_{j=1}^{i}K_{i,j}jc_j - \sum_{j=i}^{\infty}K_{i,j}c_ic_j. \qquad (5)$$

In this case the fourth summand of (1) is absent since smaller particles are completely destroyed without a rest (the fourth summand describes the contribution of such 'rests'). Mathematically, this means that the above-mentioned equation $i + \alpha(m) = m$ has no roots m.

Let us verify if equations (4), (5) possess the mass conservation law

$$M_1 \stackrel{\text{def}}{=} \sum_{i=1}^{\infty} ic_i(t) \stackrel{?}{=} \text{const}. \qquad (6)$$

With this aim we multiply (5) by i and summarize it over $1 \leqslant i \leqslant \infty$. Then we obtain

$$\frac{\mathrm{d}M_1}{\mathrm{d}t} = \sum_{i=1}^{\infty}\sum_{j=1}^{i-1}ijK_{i-1,j}c_{i-1}c_j - \sum_{i=1}^{\infty}\sum_{j=1}^{i}ijK_{i,j}c_ic_j - \sum_{i=1}^{\infty}\sum_{j=i}^{\infty}iK_{i,j}c_ic_j.$$

In the third summand we replace the order of summation and get the summation over $\sum_{j=1}^{\infty}\sum_{i=1}^{j}$. Then in the second and the third terms we 'bite off' the summand at $j = i$ and make the replacement $i = i' + j',\ j = j'$. Then,

$$\frac{\mathrm{d}M_1}{\mathrm{d}t} = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}(i+j)jK_{i+j-1,j}c_{i+j-1}c_j - \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}(i+j)jK_{i+j,j}c_{i+j}c_j$$

$$-\sum_{i=1}^{\infty}i(i+1)K_{i,i}c_i^2 - \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}jK_{i+j,j}c_{i+j}c_j.$$

After a number of replacements like $i = i + 1$ we obtain zero and, thus, come to the mass conservation law. Similar reasonings demonstrate the mass conservation for equation (4).

So, the alteration of the parameter $\alpha(j)$ from 1 to j connects the coagulation models (4) and (5).

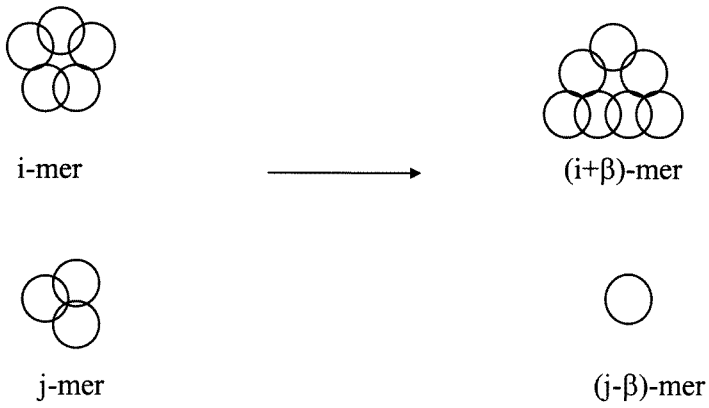

Figure 2. ($\beta = 2$.)

2. Another family of discrete coagulation models

In this section we establish a connection between model (4) and the renowned Smoluchowski coagulation equation. Let us consider another mechanism of an elementary collision act between particles i and j, $i \geqslant j$. Namely, we suppose that the larger particle i 'bites off' j-mer and β-mer ($\beta = \beta(j) \leqslant j$) and, thus, the size of the larger particle becomes equal to $i + \beta$. The size of j-mer becomes equal to $j - \beta$ (figure 2). It is natural to assume that $\beta(j)$ has non-decreasing dependence on the variable j. The balance reasonings yield the following kinetic equation

$$\frac{\mathrm{d}c_i(t)}{\mathrm{d}t} = \sum_{j=1}^{n} K_{i-\beta,j} c_{i-\beta}(t) c_j(t) - c_i(t) \sum_{j=1}^{i} K_{i,j} c_j(t) - c_i(t) \sum_{j=i}^{\infty} K_{i,j} c_j(t) + \sum_{m(i)} \sum_{j=m(i)}^{\infty} K_{m(i),j} c_{m(i)}(t) c_j(t) \qquad \beta = \beta(j) \tag{7}$$

where the first summand is responsible for income of i-mer particles due to 'gluing' $i-\beta$-mers and β-mers that were chipped off j-mers ($\beta \leqslant j$). The upper boundary n of the summation is determined by the following inequalities

$$i - \beta(n) \geqslant n \qquad i - \beta(n+1) < n + 1. \tag{8}$$

This system of inequalities has a unique solution n since we assume a non-decreasing dependence $\beta(j)$ on j.

The negative terms of (7) describe the decay of i-mers due to collisions with j-mers. It can be derived from two negative summands in (1) putting in the first of them $\alpha = 1$, because, unlike (1), an elementary collision act deals now with one i-mer only.

The last summand in (7) is defined as the corresponding summand in (1). It yields an income of i-mer rests after collisions of m-mers and j-mers, $j \geqslant m$. The values m are determined by the equation $i + \alpha(m) = m$, where all terms should be positive.

Substituting $\beta = 1$ in (7) again yields kinetic equation (4). If $\beta(j) = j$ (i.e. i-mer and j-mer just merge, resulting into $i + j$-mer), then inequalities (8) yield $n = [i/2]$ with $[i/2]$ equal to the integer part of $[i/2]$. In view of the symmetry $K_{i,j} = K_{j,i}$ we observe that equation

(7) transforms to the classical Smoluchowski equation [1]

$$\frac{\mathrm{d}c_i}{\mathrm{d}t} = \frac{1}{2}\sum_{j=1}^{i-1} K_{i-j,j}c_{i-j}c_j - c_i\sum_{j=1}^{\infty} K_{i,j}c_j. \tag{9}$$

Unlike the previous equations, where the values $K_{i,i}$ are less than twice real intensities of mutual collisions of i-mers, in (9) the coefficient $\frac{1}{2}$ is directly written before the first summand and is taken into account in the second summand uniting both negative terms of (7) (there the term at $j = i$ is taken into account twice). So, the values $K_{i,i}$ in (9) are equal to real intensities without dividing them by two. If we rewrite the first summand (7) as

$$\sum_{j=1}^{n} K_{i-j,j}c_{i-j}c_j \qquad n = \begin{cases} (i-1)/2 & \text{for odd } i \\ i/2 & \text{for even } i \end{cases} \tag{10}$$

then its similarity to the corresponding summand of (9) is more clear. The solution of system (8) for this case is written in (10).

The celebrated continuous version of (9) is presented below:

$$\frac{\partial c(x,t)}{\partial t} = \frac{1}{2}\int_0^x K(x-y,y)c(x-y,t)c(y,t)\,\mathrm{d}y - c(x,t)\int_0^{\infty} K(x,y)c(y,t)\,\mathrm{d}y. \tag{11}$$

Its derivation from (9) is well known [12].

3. Passage to the Oort–Hulst equation

A remarkable observation is that the passage to limit $m_0 \to 0$ in (5) yields the well known continuous coagulation model

$$\frac{\partial c(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left[c(x,t)\int_0^x yK(x,y)c(y,t)\,\mathrm{d}y\right] - \int_x^{\infty} K(x,y)c(x,t)c(y,t)\,\mathrm{d}y. \tag{12}$$

In fact, to pass to a continuous form of (5), we introduce the disrtibution finction $c(x,t)$ describing distribution of particles in mass x at time t, i.e., $c(x,t)\,\mathrm{d}x$ is equal to the number of particles with masses from $(x, x+\mathrm{d}x)$ at time t. Since the mass of i-mers is equal to im_0, then $c_i(t) = c(im_0,t)m_0$. Since $K_{i,j} = K(im_0, jm_0)$, then

$$K_{i,j}c_i(t)c_j(t) = K(im_0, jm_0)c(im_0,t)c(jm_0,t)m_0^2. \tag{13}$$

Consequently, using the replacement $x = im_0$, we obtain

$$\begin{aligned}\frac{\partial c(x,t)}{\partial t} = -\frac{1}{m_0}\Bigg[&c(x,t)\sum_{j=1}^{x/m_0} K(x, jm_0)c(jm_0,t)jm_0 \\ &-c(x-m_0,t)\sum_{j=1}^{x/m_0-1} K(x-m_0, jm_0)c(jm_0,t)jm_0\Bigg]m_0 \\ &-c(x,t)\sum_{j=i}^{\infty} K(x, jm_0)c(jm_0,t)m_0.\end{aligned}$$

Observing, that these sums are just the integral Darboux sums, we pass to limit $m_0 \to 0$, and obtain (12). Equation (12) was derived by a completely different methods by Oort and van de Hulst [2] and was rewritten in the form (12) by Safronov [3]. So, it turns out that equation (12) is the continuous version of the new discrete equation (5). It is interesting to mention that there were no discrete versions of (12) earlier. Usually, continuous limit equations are derived from their discrete analogues. As an example we can present the basic Smoluchowski coagulation

equation, which was first derived in its discrete form in 1916 [1], and only in 1928 was its continuous version written by Müller [12]. Another, more recent example, can be found in [13], where the authors first derive a discrete monomer–monomer model for heterogeneous catalysis, and then they pass to the limit equation in a continuous form. Other interesting related models can be found in [14, 15].

Some reasonings, slightly related to our derivation of equation (5), can be found in [11, p 131] where the authors noted some connection between (12) and the following process: l particles of mass x during time Δt collide with small particles of mass μ/l, $\mu < x$. This connection is derived on the basis of a series expansion of some functions and a truncation of the series without proper justification (also, cf [6, p 45 and 7, pp 154–5]).

The Oort–Hulst equation (12) can be treated as a model of continuous growth [3, 7]. In fact, if we assume that all particles grow up as a result of joining lesser particles, then the first integral of the right-hand side of (12) is equal to $\mathrm{d}x/\mathrm{d}t$, and the whole first summand is only changing $c(x, t)$ due to joining the particles with masses y, $y < x$. Hence, without the last term equation (12) is a one-dimensional continuity equation with 'density' $c(x, t)$ and 'velocity' $\mathrm{d}x/\mathrm{d}t$. The second term in (12) is the decay of particles of mass x as a result of their 'sedimentation' on larger particles. So, a particle preserves its 'individuality' at collisions with smaller particles, and loses it at collisions with larger particles. In other words, the collisions of particles of mass x with smaller particles change the mass of particles x, the collisions with larger particles change the number of particles x. This procedure gives the average and smoothed rate of growth of all particles of a certain radius.

It is worth mentioning that in works [4, 5] the coagulation model (12) was applied to the analysis of the evolution of different cosmic objects. A similar approach for coagulation growth, involving a small number of uniquely sized large droplets falling through a homogeneous, randomly distributed collection of smaller droplets, was used to compute the coagulation processes in atmosphere clouds by Telford [8], who solved Oort–Hulst equation (12) without the second term in the right-hand side. In later papers [9, 10] it was shown numerically and analytically, respectively, that the method of [8] (and, consequently, equation (12)) yielded results similar to the common kinetic Smoluchowski approach. Also, it is pointed out in [7, 11] that (12) is also useful for the investigation of processes in technical installations (nozzles and engines).

Hence, we can say that there exists a 'coagulation triangle' whose vertexes are constituted by models (4), (5), and (9), and its two sides are formed by the 'intermediate' models (1), (7) at $1 \leqslant \alpha(j) \leqslant j$ and $1 \leqslant \beta(j) \leqslant j$, respectively.

In the next section we discuss some common features and distinctions between the coagulations models (4), (5) and (9).

4. Comparative mathematical analysis of the coagulation models

(1) Mass conservation. There are many works devoted to the physical and mathematical analysis of the Smoluchowski equations (9), (11) (see, e.g., [16]). The mass conservation law for this equation is well known. It holds if the sums over infinite interval

$$\sum_{j=1}^{\infty} j K_{i,j} c_j$$

are bounded. These sums appear at the formal summation of the equation with weight i. In this case for the first moment of solution $M_1(t)$ we have $M_1 = \text{const}$. As we have already seen, the direct summation of (4) and (5) with weight i also yields the mass conservation provided that the corresponding infinite sums are bounded.

(2) Dissipation law. The zero moment $M_0 = \sum c_i$ of solutions means the total number of particles in the unite volume of the disperse system. Due to coagulation this value should decrease in time. Summation of (4) and (5) leads us to the necessary inequality

$$\mathrm{d}M_0(t)/\mathrm{d}t \leqslant 0$$

that additionally justifies these models.

(3) Becker–Döring equations. Let us impose the 'admissibility' condition that for the case of the simplest kinetics when collisions may occur with monomers only, all coagulation models should yield the same equation. In this case

$$K_{i,j} = \begin{cases} k_i & j = 1 \\ k_j & i = 1 \\ 0 & \text{otherwise} \end{cases}$$

and all the models considered (4), (5), and (9) give us the Becker–Döring cluster equations [17, 18]

$$\frac{\mathrm{d}c_i(t)}{\mathrm{d}t} = k_{i-1}c_{i-1}c_1 - k_i c_i c_1 \qquad i \geqslant 2$$
$$\frac{\mathrm{d}c_1(t)}{\mathrm{d}t} = -k_1 c_1^2 - \sum_{j=1}^{\infty} k_j c_1 c_j.$$

So, the 'admissibility condition' is fulfilled.

(4) Singular equilibriums. Following [19–21], the continuous versions (12) and (11) of the basic 'vertex' models should have singular equilibrium solutions of the form

$$L(x, y) \stackrel{\text{def}}{=} K(x, y)c(x)c(y) = (x + y)^{-3}.$$

The direct check confirms that both stationary equations (11) and (12) have such a solution.

(5) Spreading of perturbations. An important difference between the Smoluchowski and Oort–Hulst models is that the Smoluchowski equation spreads perturbation with infinite speed. To demonstrate this fact let $K \equiv 1$ and let equation (9) be provided with initial data $c_0 = (1, 0, 0, 0, \ldots)$. Passing to the generating function $G(z, t) = \sum_{i=1}^{\infty} z^i c_i(t)$, we obtain

$$\frac{\partial G}{\partial t} = \frac{1}{2}G^2(z, t) - G(z, t)G(1, t) \qquad G_0(z) = z$$

whence

$$G(z, t) = \sum_{i=1}^{\infty} z^i \frac{(t/2)^{i-1}}{(1 + t/2)^{i+1}}.$$

Consequently,

$$c_i(t) = \frac{(t/2)^{i-1}}{(1 + t/2)^{i+1}} > 0 \qquad \text{for all} \quad t > 0, \quad i \geqslant 1. \tag{14}$$

Therefore, zero initial data become positive instantly for any large i. Hence, the non-zero initial value at $i = 1$ spreads with infinite speed. This lack is similar to the same property for, e.g., the heat equation and mathematically means the presence of parabolic properties for (9), (11).

Unlike the Smoluchowski equation, the Oort–Hulst equation (12) does not possess this lack. In fact, we differentiate (12) and rewrite it as

$$\frac{\partial c(x,t)}{\partial t} + v(x,t)\frac{\partial c(x,t)}{\partial x} = -c(x,t)\left(\int_0^x y\partial_1 K(x,y)c(y,t)\,\mathrm{d}y\right) - xK(x,x)c(x,t)^2 - c(x,t)\int_x^\infty K(x,y)c(y,t)\,\mathrm{d}y \tag{15}$$

where

$$v(x,t) = \int_0^x yK(x,y)c(y,t)\,\mathrm{d}y$$

and $\partial_1 K(x,y)$ means differentiating K with respect to the first variable. Let $x(s)$ be a solution of the characteristic equation $\mathrm{d}x/\mathrm{d}t = v(x,t)$. Then the substitution

$$c(x,t) = \exp\left\{-\int_0^t \left[K(x(s),x(s))c(x(s),s)x(s) - \int_0^{x(s)} y\partial_1 K(x(s),y)c(y,s)\,\mathrm{d}y - \int_{x(s)}^\infty K(x(s),y)c(y,s)\,\mathrm{d}y\right]\mathrm{d}s\right\}\cdot u(x,t) \tag{16}$$

yields

$$\frac{\partial u(x,t)}{\partial t} + v(x,t)\frac{\partial u(x,t)}{\partial x} = 0. \tag{17}$$

From (16) we see, that functions $c(x,t)$ and $u(x,t)$ are equal or not equal to zero at the same points. The characteristic equation for (15), (17) has the following form:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = v(x,t). \tag{18}$$

From simple equation (17) we conclude that if $c_0(x_1) = 0$, then $c(x_1,t)$ becomes positive not earlier than at time moment t_1 when the first characteristic curve $x(s)$ with non-zero starting value x_0 arrives at the point x_1 (figure 3). So, equation (12) ensures physically meaningful boundedness of the perturbation propagation speed, and, thus, allows us to compute the coagulation front. Mathematically that means that (12) possesses some hyperbolic properties.

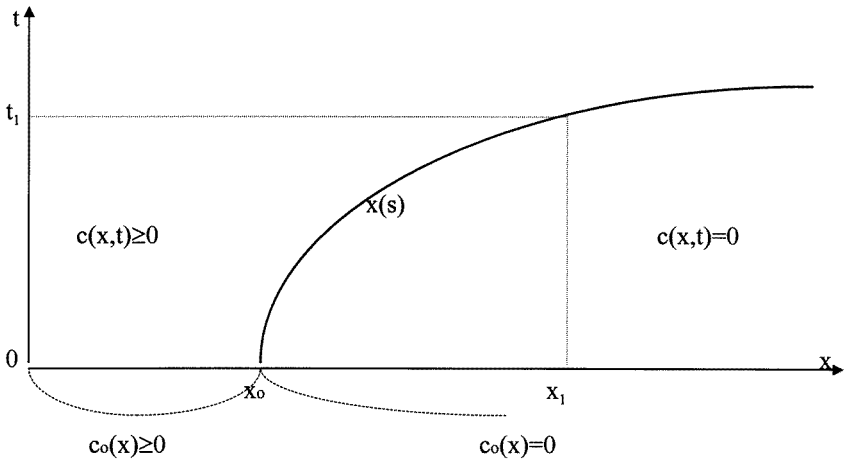

Figure 3.

5. Computing the coagulation front

To demonstrate the reasonings of section 4(5), let us estimate the coagulation front in some cases. Let $c_0(x) = 0$ if $x \geqslant x_0$. Then the characteristic curve, beginning at the point x_0, splits the plane to two parts such that $c(x, t) = 0$ if the point (x, t) is to the right of that characteristic. This characteristic curve we call the boundary characteristic or just the coagulation front. From characteristic equation (18) we see that coagulation front satisfies the following equation:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \int_0^x yK(x, y)c(y, t)\,\mathrm{d}y = \int_0^\infty yK(x, y)c(y, t)\,\mathrm{d}y \tag{19}$$

at the initial value $x(0) = x_0$.

So, if $K(x, y) = C = \text{const}$ then

$$x(t) = x_0 + C \cdot M_1 t \tag{20}$$

where M_1 is the constant first moment of the solution.

If the coagulation kernel is additive, i.e. $K(x, y) = (x + y)$, then from (19):

$$\frac{\mathrm{d}x}{\mathrm{d}t} = M_2(t) + M_1 x.$$

Hence,

$$x(t) = \exp(M_1 t)\left\{x_0 + \int_0^t \exp(-M_1 s)M_2(s)\,\mathrm{d}s\right\}. \tag{21}$$

It is rather complicated to find out the second moment $M_2(t)$ from the Oort–Hulst equation (12). In fact, from (12) we observe

$$\frac{\mathrm{d}M_k(t)}{\mathrm{d}t} = \int_0^\infty \int_0^x yK(x, y)c(x, t)c(y, t)[kx^{k-1} - y^{k-1}]\,\mathrm{d}y\,\mathrm{d}x \qquad k \geqslant 0. \tag{22}$$

So, for the additive kernel we have

$$\begin{aligned}\frac{\mathrm{d}M_2(t)}{\mathrm{d}t} &= 4M_2(t)M_1 - 3\int_0^\infty \int_x^\infty x^2 yc(x, t)c(y, t)\,\mathrm{d}y\,\mathrm{d}x \\ &\quad -2\int_0^\infty \int_x^\infty xy^2 c(x, t)c(y, t)\,\mathrm{d}y\,\mathrm{d}x \\ &\quad -\int_0^\infty \int_x^\infty x^3 c(x, t)c(y, t)\,\mathrm{d}y\,\mathrm{d}x \geqslant 4M_2(t)M_1 \\ &\quad -3\left[\int_0^\infty \int_x^\infty x^2 yc(x, t)c(y, t)\,\mathrm{d}y\,\mathrm{d}x + \int_0^\infty \int_x^\infty xy^2 c(x, t)c(y, t)\,\mathrm{d}y\,\mathrm{d}x\right] \\ &= M_1 M_2(t).\end{aligned} \tag{23}$$

To derive (23) we have utilized the following inequalities:

$$\int_0^\infty \int_0^x x^k y^k c(x)c(y)\,\mathrm{d}y\,\mathrm{d}x = \tfrac{1}{2}\left(\int_0^\infty x^k c(x)\,\mathrm{d}x\right)^2 \tag{24}$$

$$\int_x^\infty y^k c(y)\,\mathrm{d}y \leqslant \frac{1}{x}\int_x^\infty y^{k+1} c(y)\,\mathrm{d}y. \tag{25}$$

Finally, we obtain from (23):

$$M_1 M_2(t) \leqslant \frac{\mathrm{d}M_2(t)}{\mathrm{d}t} \leqslant 2M_1 M_2(t). \tag{26}$$

Then $M_2(0)\exp(M_1 t) \leqslant M_2(t) \leqslant M_2(0)\exp(2M_1 t)$.

The Smoluchowski equation (11) yields

$$\frac{\mathrm{d}M_k(t)}{\mathrm{d}t} = \frac{1}{2}\int_0^\infty \int_0^\infty K(x,y)c(x,t)c(y,t)[(x+y)^k - x^k - y^k]\,\mathrm{d}y\,\mathrm{d}x \qquad k \geqslant 0. \tag{27}$$

From (27) we obtain for the case $K(x, y) = (x + y)$ the result, similar to (26):

$$\frac{\mathrm{d}M_2(t)}{\mathrm{d}t} = 2M_2(t)M_1. \tag{28}$$

So, for convenience we can use equality (28) instead of inequality (26). Substituting (28) into (21), we conclude that for additive coagulation kernels the coagulation front grows faster than for constant kernels (cf (20)):

$$x(t) = \exp(M_1 t)\{x_0 + M_2(0)t\}. \tag{29}$$

Similar reasonings give us front estimates for many coagulation kernels. For example, if for some positive constants a and b

$$K(x,y) = \begin{cases} ax + by & x \geqslant y \\ ay + bx & y \geqslant x \end{cases}$$

then for boundary characteristics,

$$\frac{\mathrm{d}x}{\mathrm{d}t} = axM_1 + bM_2(t).$$

Observing from (11) that

$$\min\{a,b\}M_1M_2 \leqslant \frac{\mathrm{d}M_2}{\mathrm{d}t} \leqslant \max\{a,b\}M_1M_2$$

we obtain for $a > b$ the following estimate for coagulation front:

$$\mathrm{e}^{aM_1t}\left\{x_0 + bM_2(0)\frac{1-\exp[-(a-b)M_1t]}{(a-b)M_1}\right\} \leqslant x(t) \leqslant \mathrm{e}^{aM_1t}\{x_0 + bM_2(0)t\}.$$

The similar correlation holds for the case $b > a$.

Let us consider now the coagulation front for multiplicative coagulation kernels $K(x, y) = xy$. From (19) we see that

$$x(t) = x_0 \exp\left(\int_0^t M_2(s)\,\mathrm{d}s\right).$$

For the Smoluchowski equation (11) we have unboundedness of the second moment $M_2(t)$ at the critical moment $t_{\mathrm{cr}} = [M_2(0)]^{-1}$:

$$M_2(t) = M_2(0)(1 - M_2(0)t)^{-1}.$$

Taking into account inequalities (24), (25), we also obtain for $K(x, y) = xy$ the unboundedness of the second moment:

$$\frac{M_2(0)}{1 - M_2(0)t/2} \leqslant M_2(t) \leqslant \frac{M_2(0)}{1 - M_2(0)t}.$$

For this model $[M_2(0)]^{-1} \leqslant t_{\mathrm{cr}} \leqslant 2[M_2(0)]^{-1}$.

So, we can see that the coagulation front goes to infinity as $t \to t_{\mathrm{cr}}$.

Let us pay attention to another effect of influence of the infinity—breaking up the mass conservation law at the same critical time t_{cr}. It is well known that this effect for Smoluchowski equation (11) is caused by the trend of the second moment of solutions M_2 to go to infinity (see, e.g., [22–28]). So, it turns out that convergence to infinity of the coagulation front means the breaking down of the mass conservation law. This observation allows us to establish the infringement of mass conservation law for a number of other coagulation kernels [29].

6. Conclusions

We derive three basic discrete coagulation models connected via alteration of the parameters, which describe collisions of patricles. Therefore, we can say that these equations form a triangle of interconnected coagulation models.

It turns out, that one of these three models is a discrete version of the well known Oort–Hulst continuous coagulation equation. Another model is the celebrated Smoluchowski equation. The third model corresponds to collisions with minimal intensity because it is derived at the smallest value of parameters α, β connecting (4) and (5), and (4) and (9), respectively.

If the coagulation kernel $K(x, y)$ grows more slowly than $x \cdot y$ then the mass conservation law is valid for all described coagulation types. Also, the particle dissipation law holds. Reducing all discrete equations to the same Becker–Döring system additionally justifies the validity of three basic coagulation models (4), (5) and (9), situated in the vertexes of the coagulation 'triangle' introduced in this paper.

Comparing the continuous Smoluchowski and Oort–Hulst equations yields the same singular equilibrium solution. This fact is an additional reason for the opinion that these equations similarly describe the real coagulation processes.

The Oort–Hulst equation (12) allows us to estimate the speed of the coagulation front. We do that for some cases. Such an estimation is impossible using only the Smoluchowski equation.

We establish a connection between convergence of the coagulation front to infinity and break down the mass conservation law at intensive coagulation rates. It turns out that coagulation front goes to infinity at the same critical time as mass conservation breaks.

Acknowledgments

PBD is obliged to V I Agoshkov, A E Arinstein, and V P Shutyaev for stimulating discussions. He would also like to thank the referees for very useful remarks to the paper. This work is supported by the Russian Foundation for Basic Researches, grant no 97-01-00333.

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