

A “triangle” of interconnected coagulation models¹

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 at the first case we obtain a new discrete kinetic equation. We demonstrate that its continuous version is just the Oort-Hulst’s coagulation model. At the second case the maximum of the corresponding parameter yields the Smoluchowski’s 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 nowadays coagulation equations “situated” in its vertexes (Smoluchowski and Oort-Hulst equations) via 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 infringement of the mass conservation law and convergence of the coagulation front to infinity.

Preliminaries

We are concerned with disperse systems containing particles of different masses (volumes) that can undergo mutual interactions resulting in changing 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 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’s coagulation equation [1], which is often written either in the continuous or in 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 analyze cosmic objects (creation of stars,

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planets, evolution of nebulae, galaxies, clouds of cosmic dust, etc.) [2, 3, 4, 5], in atmosphere science [6, 7, 8, 9, 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 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 only 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's coagulation equation. The minimum of the second parameter leads us to the same auxiliary discrete kinetic equation.

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 values of the first parameter change. Another side connects the discrete Smoluchowski's 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 basic Smoluchowski and Oort-Hulst coagulation equations.

After that we compare a number of mathematical properties of both basic coagulation equations. We conclude that these equations yield usually almost the same results and, thus, they both can be applied to the analysis of disperse systems yielding more wide treatment of coagulation processes. Some of mathematical properties of these equations differ, and, hence, they can be treated as useful complements of each other. As an example of such a useful completion we compute the speed of 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 when the coagulation front goes to infinity. This observation allows to reveal some new classes of coagulation kernels yielding the breaking down 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 an 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 collisions of pairs of particles of masses (volumes) im_0 and jm_0 , hereinafter we assume for definiteness $i \geq j$. We call the particles of mass im_0 as i -mers. m_0 is mass of 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:

$$\begin{aligned} \frac{dc_i(t)}{dt} = & c_{i-1}(t) \sum_{j=1}^{i-1} K_{i-1,j} \alpha(j) c_j(t) - c_i(t) \sum_{j=1}^i K_{i,j} \alpha(j) c_j(t) \\ & - \sum_{j=i}^{\infty} K_{i,j} c_i(t) c_j(t) + \sum_{m(i)} \sum_{j=m(i)}^{\infty} K_{m(i),j} c_{m(i)}(t) c_j(t), \quad i \geq 1, \end{aligned} \quad (1)$$

where $c_i(t)$ is concentration of i -mers at the 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 the process considered. From the physical point of view it is clear that this function must be symmetric for all arguments $i, j \geq 1$: $K_{i,j} = K_{j,i}$. The values $K_{i,i}$ are equal to the 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 decay of i -mers as a result of merging monomers to them. The multiplier 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

$$i + \alpha(m) = m. \quad (2)$$

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

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

If the 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 just 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):

$$\begin{aligned} c_i(t) = & \exp \left\{ - \int_0^t \left(\sum_{j=1}^i K_{i,j} \alpha(j) c_j(s) - \sum_{j=i}^{\infty} K_{i,j} c_j(s) \right) ds \right\} \\ & \times \left(c_i(0) + \int_0^t \exp \left\{ \int_0^s \left[\sum_{j=1}^i K_{i,j} \alpha(j) c_j(s_1) - \sum_{j=i}^{\infty} K_{i,j} c_j(s_1) \right] ds_1 \right\} \right. \\ & \left. \times \left[c_{i-1}(s) \sum_{j=1}^{i-1} K_{i-1,j} \alpha(j) c_j(s) + \sum_{m(i)}^{\infty} \sum_{j=m(i)}^{\infty} K_{m(i),j} c_{m(i)}(s) c_j(s) \right] ds \right). \quad (3) \end{aligned}$$

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

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

$$\frac{dc_i}{dt} = c_{i-1} \sum_{j=1}^{i-1} K_{i-1,j} c_j - c_i \sum_{j=1}^i K_{i,j} c_j - \sum_{j=i}^{\infty} K_{i,j} c_i c_j + c_{i+1} \sum_{j=i+1}^{\infty} K_{i+1,j} c_j, \quad i \geq 1. \quad (4)$$

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)

$$\frac{dc_i}{dt} = c_{i-1} \sum_{j=1}^{i-1} K_{i-1,j} j c_j - c_i \sum_{j=1}^i K_{i,j} j c_j - \sum_{j=i}^{\infty} K_{i,j} c_i c_j. \quad (5)$$

In this case the forth summand of (1) is absent since smaller particles are completely destroyed without a rest (the forth summand describes 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

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

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

$$\frac{dM_1}{dt} = \sum_{i=1}^{\infty} \sum_{j=1}^{i-1} i j K_{i-1,j} c_{i-1} c_j - \sum_{i=1}^{\infty} \sum_{j=1}^i i j K_{i,j} c_i c_j - \sum_{i=1}^{\infty} \sum_{j=i}^{\infty} i K_{i,j} c_i c_j.$$

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,

$$\begin{aligned} \frac{dM_1}{dt} &= \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} (i+j)jK_{i+j-1,j}c_{i+j-1}c_j - \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} (i+j)jK_{i+j,j}c_{i+j}c_j \\ &\quad - \sum_{i=1}^{\infty} i(i+1)K_{i,i}c_i^2 - \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} jK_{i+j,j}c_{i+j}c_j. \end{aligned}$$

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).

2 Another family of discrete coagulation models

In this section we establish a connection between model (4) and the renowned Smoluchowski's coagulation equation. Let us consider another mechanism of an elementary collision act between particles i and j , $i \geq j$. Namely, we suppose that the larger particle i "bites off" j -mer an β -mer ($\beta = \beta(j) \leq j$) 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 naturally to assume that $\beta(j)$ has non-decreasing dependence on the variable j . The balance reasonings yield the following kinetic equation

$$\begin{aligned} \frac{dc_i(t)}{dt} &= \sum_{j=1}^n K_{i-\beta,j}c_{i-\beta}(t)c_j(t) - c_i(t) \sum_{j=1}^i K_{i,j}c_j(t) \\ &\quad - c_i(t) \sum_{j=i}^{\infty} K_{i,j}c_j(t) + \sum_{m(i)}^{\infty} \sum_{j=m(i)}^{\infty} K_{m(i),j}c_{m(i)}(t)c_j(t), \quad \beta = \beta(j), \quad (7) \end{aligned}$$

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 ($\beta \leq j$). The upper boundary n of summation is determined by the following inequalities

$$i - \beta(n) \geq n, \quad i - \beta(n+1) < n+1. \quad (8)$$

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

Substituting $\beta = 1$ in (7) yields again the 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 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's equation [1]

$$\frac{dc_i}{dt} = \frac{1}{2} \sum_{j=1}^{i-1} K_{i-j,j} c_{i-j} c_j - c_i \sum_{j=1}^{\infty} K_{i,j} c_j. \quad (9)$$

Unlike the previous equations, where the values $K_{i,i}$ are twice less than real intensities of mutual collisions of i -mers, in (9) the coefficient $1/2$ 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

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

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

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

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

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

3 Passage to the Oort-Hulst equation

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

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

In fact, to pass to a continuous form of (5), we introduce the distribution function $c(x, t)$ describing distribution of particles in mass x at time t , i.e., $c(x, t)dx$ is equal to the number of particles with masses from $(x, x + dx)$ 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

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

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

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

Observing, that these sums are just the integral Darboux sums, we pass to limit $m_0 \rightarrow 0$, 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 firstly derived in its discrete form in 1916 [1], and only in 1928 its continuous version was written by Müller [12]. Another, more recent example, can be found in [13], where the authors firstly derive a discrete monomer-monomer model for heterogeneous catalysis, and then pass to 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 series expansion of some functions and truncation of the series without proper justification (also, cf. [6], p. 45 and [7], pp. 154–155).

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 more less particles, then the first integral of the right-hand side of (12) is equal to dx/dt , and the whole first summand is just changing $c(x, t)$ due to joining the particles with masses y , $y < x$. Hence, without the last term the equation (12) is a one-dimensional continuity equation with the "density" $c(x, t)$ and the "velocity" dx/dt . 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. By other words, the collisions of particles of mass x with smaller particles change 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.

In worth mentioning that in works [4, 5] coagulation model (12) was applied to analysis of 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 for computing 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)) yields the results, similar to common kinetic Smoluchowski's approach. Also, it is pointed out in [7, 11] that (12) is also useful for 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 two sides are formed by the "intermediate" models (1), (7) at $1 \leq \alpha(j) \leq j$ and $1 \leq \beta(j) \leq j$, 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 is a lot of works devoted to physical and mathematical analysis of the Smoluchowski's 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

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

are bounded. These sums appear at the formal summation of the equation with the 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

$$dM_0(t)/dt \leq 0$$

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]

$$\begin{aligned} \frac{dc_i(t)}{dt} &= k_{i-1}c_{i-1}c_1 - k_i c_i c_1, \quad i \geq 2, \\ \frac{dc_1(t)}{dt} &= -k_1 c_1^2 - \sum_{j=1}^{\infty} k_j c_1 c_j. \end{aligned}$$

So, the “admissibility condition” is fulfilled.

4. Singular equilibriums. Following [19, 20, 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 Smoluchowski’s and Oort-Hulst’s 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 $c_0 = (1, 0, 0, 0, \dots)$. Passing to the generating function $G(z, t) = \sum_{i=1}^{\infty} z^i c_i(t)$, we obtain

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

whence

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

Consequently,

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

Therefore zero initial data become positive instantly for any large i . Hence, the nonzero 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

$$\begin{aligned} \frac{\partial c(x, t)}{\partial t} + v(x, t) \frac{\partial c(x, t)}{\partial x} &= -c(x, t) \left(\int_0^x y \partial_1 K(x, y) c(y, t) dy \right) \\ &\quad - xK(x, x)c(x, t)^2 - c(x, t) \int_x^{\infty} K(x, y)c(y, t) dy, \end{aligned} \quad (15)$$

where

$$v(x, t) = \int_0^x yK(x, y)c(y, t) dy$$

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 $dx/dt = v(x, t)$. Then the substitution

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

yields

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

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

$$\frac{dx}{dt} = v(x, t) \quad (18)$$

From simple equation (17) we conclude that if $c_0(x_1) = 0$, then $c(x_1, t)$ becomes positive not earlier than at the time moment t_1 when the first characteristic curve $x(s)$ with nonzero 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, allow to compute the coagulation front. Mathematically that means that (12) possesses some hyperbolic properties.

5 Computing the coagulation front

To demonstrate the reasonings of subsection 4.5, let us estimate the coagulation front in some cases. Let $c_0(x) = 0$ if $x \geq x_0$. 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 characteristics. This characteristic curve we call the boundary characteristics or just the coagulation front. From characteristic equation (18) we see that coagulation front satisfies the following equation

$$\frac{dx}{dt} = \int_0^x y K(x, y)c(y, t)dy = \int_0^\infty y K(x, y)c(y, t)dy \quad (19)$$

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

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

$$x(t) = x_0 + C \cdot M_1 t, \quad (20)$$

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):

$$\frac{dx}{dt} = M_2(t) + M_1 x.$$

Hence,

$$x(t) = \exp(M_1 t) \left\{ x_0 + \int_0^t \exp(-M_1 s) M_2(s) ds \right\}. \quad (21)$$

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

$$\frac{dM_k(t)}{dt} = \int_0^\infty \int_0^x y K(x, y) c(x, t) c(y, t) [kx^{k-1} - y^{k-1}] dy dx, \quad k \geq 0. \quad (22)$$

So, for the additive kernel we have

$$\begin{aligned} \frac{dM_2(t)}{dt} &= 4M_2(t)M_1 - 3 \int_0^\infty \int_x^\infty x^2 y c(x, t) c(y, t) dy dx \\ &\quad - 2 \int_0^\infty \int_x^\infty x y^2 c(x, t) c(y, t) dy dx - \int_0^\infty \int_x^\infty x^3 c(x, t) c(y, t) dy dx \\ &\geq 4M_2(t)M_1 - 3 \left[\int_0^\infty \int_x^\infty x^2 y c(x, t) c(y, t) dy dx \right. \\ &\quad \left. + \int_0^\infty \int_x^\infty x y^2 c(x, t) c(y, t) dy dx \right] = M_1 M_2(t). \end{aligned} \quad (23)$$

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

$$\int_0^\infty \int_0^x x^k y^k c(x) c(y) dy dx = \frac{1}{2} \left(\int_0^\infty x^k c(x) dx \right)^2 \quad (24)$$

$$\int_x^\infty y^k c(y) dy \leq \frac{1}{x} \int_x^\infty y^{k+1} c(y) dy. \quad (25)$$

Finally, we obtain from (23):

$$M_1 M_2(t) \leq \frac{dM_2(t)}{dt} \leq 2M_1 M_2(t). \quad (26)$$

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

The Smoluchowski's equation (11) yields

$$\frac{dM_k(t)}{dt} = \frac{1}{2} \int_0^\infty \int_0^\infty K(x, y) c(x, t) c(y, t) [(x + y)^k - x^k - y^k] dy dx, \quad k \geq 0. \quad (27)$$

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

$$\frac{dM_2(t)}{dt} = 2M_2(t)M_1. \quad (28)$$

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)]:

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

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

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

then for boundary characteristics,

$$\frac{dx}{dt} = axM_1 + bM_2(t).$$

Observing from (11) that

$$\min\{a, b\}M_1M_2 \leq \frac{dM_2}{dt} \leq \max\{a, b\}M_1M_2,$$

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

$$e^{aM_1 t} \left\{ x_0 + bM_2(0) \frac{1 - \exp[-(a - b)M_1 t]}{(a - b)M_1} \right\} \leq x(t) \leq e^{aM_1 t} \{x_0 + bM_2(0)t\}.$$

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

$$x(t) = x_0 \exp\left(\int_0^t M_2(s) ds\right).$$

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

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

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

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

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

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

Let us pay our 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's equation (11) is caused by trend of the second moment of solutions M_2 to infinity (see, e.g., [22, 23, 24, 25, 26, 27, 28]). So, it turns out, that convergence to infinity of the coagulation front means breaking down the mass conservation law. This observation allows to establish infringement of mass conservation law for a number of other coagulation kernels [29].

Conclusions

We derive three basic discrete coagulation models connected via alteration of the parameters, which describe collisions of particles. 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 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 justifies additionally the validity of three basic coagulation models (4), (5) and (9), situated in the vertexes of the coagulation "triangle" introduced in this paper.

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

The Oort-Hulst equation (12) allows 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 the coagulation front to infinity and breaking 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.

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