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Uniqueness of post-gelation solutions of a class of coagulation equations

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Abstract

We prove well-posedness of global solutions for a class of coagulation equations which exhibit the gelation phase transition. To this end, we solve an associated partial differential equation involving the generating functions before and after the phase transition. Applications include the classical Smoluchowski and Flory equations with multiplicative coagulation rate and the recently introduced symmetric model with limited aggregations. For the latter, we compute the limiting concentrations and we relate them to random graph models.

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1. Introduction

1.1. Coagulation models

In this paper we deal with the problem of uniqueness of post-gelation solutions of several models of coagulation, namely Smoluchowski's and Flory's classical models, and the corresponding models with limited aggregations recently introduced by Bertoin [3].

Smoluchowski's coagulation equations describe the evolution of the concentrations of particles in a system where particles can perform pairwise coalescence, see e.g. [1,18,23]. In the original model of Smoluchowski [29], a pair of particles of mass, respectively, m and m', coalesce at rate $\kappa(m, m')$ and produce a particle of mass m + m'. In the discrete setting, the evolution of the concentration $c_t(m)$ of particles of mass $m \in \mathbb{N}^*$ at time $t \ge 0$ is given by the following system

$$\frac{\mathrm{d}}{\mathrm{d}t}c_t(m) = \frac{1}{2}\sum_{m'=1}^{m-1}\kappa(m,m')c_t(m')c_t(m-m') - \sum_{m'\geqslant 1}\kappa(m,m')c_t(m)c_t(m').$$
(1.1)

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Norris considered in [24] far more general models of *cluster coagulation*, where the rate of coalescence does not depend only on the mass of the particles but also on other parameters. In this general setting, most results on existence and uniqueness are obtained before a critical time, known as the *gelation time*, while the global behavior of the solutions after gelation, and in particular uniqueness, is not known.

An example of a solvable cluster coagulation model is Bertoin's *model with limited aggregations* [3], which we shall simply call the *model with arms*. In this case, particles have a mass but also carry a certain number of potential links, called *arms*. Two particles of mass *m* and *m'* may coagulate only if they have a positive number of arms, say *a* and *a'*. When they coagulate, an arm of each is used to create the bond and both arms are then deactivated, hence creating a particle with a + a' - 2 arms and mass m + m'. The coagulation rate of these two particles is *aa'*. Therefore, if $c_t(a, m)$ is the concentration of particles with $a \in \mathbb{N} = \{0, 1, ...\}$ arms and mass $m \in \mathbb{N}^* = \{1, 2, ...\}$, then the coagulation reads

$$\frac{\mathrm{d}}{\mathrm{d}t}c_t(a,m) = \frac{1}{2}\sum_{a'=1}^{a+1}\sum_{m'=1}^{m-1}a'(a+2-a')c_t(a',m')c_t(a+2-a',m-m') -\sum_{a'\ge 1}\sum_{m'\ge 1}aa'c_t(a,m)c_t(a',m').$$
(1.2)

For monodisperse initial concentrations, i.e. $c_0(a, m) = \mathbb{1}_{\{m=1\}}\mu(a)$, with $\mu = (\mu(a))_{a \in \mathbb{N}}$ a measure on \mathbb{N} with unit mean, it is proved in [3] that this equation has a unique solution on some interval [0, T), where $T = +\infty$ if and only if $K \leq 1$, where

$$K := \sum_{a \ge 1} a(a-1)\mu(a).$$

$$(1.3)$$

In other words, if particles at time 0 have, on average, few arms, Eq. (1.2) has a unique solution defined for all $t \ge 0$. When this is the case, as time passes, all available arms are used to create bonds and only particles with no arms remain in the system. The limit concentrations $c_{\infty}(0, m)$ as $t \to +\infty$ of such particles turn out to be related to the distribution of the total population generated by a sub-critical Galton–Watson branching process (see e.g. [2]) started from two ancestors: see [3,4] and Section 1.4 below.

1.2. The gelation phase transition

A formal computation shows that solutions of (1.1) with multiplicative kernel $\kappa(m, m') = mm'$ should have constant mass

$$M_t := \sum_{m \ge 1} mc_t(m), \quad t \ge 0, \tag{1.4}$$

i.e. $\frac{d}{dt}M_t = 0$. It is however well known that if large particles can coagulate sufficiently fast, then one may observe in finite time a phenomenon called *gelation*, namely the formation of particles of infinite mass, the *gel*. These particles do not count in the computation of the mass so from the gelation time on, M_t starts to decrease.

The reason why (1.2) can be solved, is that it can be transformed into a solvable PDE involving the generating function of $(c_t)_{t \ge 0}$. In Eq. (1.1), this transformation is also possible for several particular choices of the kernel $\kappa(m, m')$, namely when κ is constant, additive or multiplicative: see e.g. [5]. In the multiplicative case $\kappa(m, m') = mm'$, which is our main concern here, the total mass is a parameter of (1.1) and of the associated PDE, which is therefore easy to solve only when $(M_t)_{t\ge 0}$ is known. Existence and uniqueness of solutions of (1.1) are thus easy up to gelation, since in this regime, the total mass M_t is constant.

After gelation, the gel may or may not interact with the other particles. If it does, Eq. (1.1) has to be modified into Flory's equation (3.1). Else, the gel is inert, in which case Smoluchowski's equation continues to hold. Obviously, they are identical before gelation.

Occurrence of gelation depends heavily on the choice of the coagulation rate $\kappa(m, m')$, and in the multiplicative case, gelation always occurs [10,12,17]. After gelation, the mass is not known, so M_t itself becomes an unknown of the equation, and well-posedness of the equation is then much less trivial. The multiplicative kernel is therefore

particularly interesting, since it exhibits a non-trivial behavior but can still be studied in detail by means of explicit computations.

The same phenomenon of gelation has been observed in [3] for (1.2) for monodisperse initial concentrations c_0 . A formal computation shows that the mean number of arms A_t

$$A_t := \sum_{a,m \ge 1} ac_t(a,m), \quad t \ge 0,$$

satisfies the equation $\frac{d}{dt}A_t = -A_t^2$ and should therefore be equal to $\frac{1}{1+t}$ for all $t \ge 0$. In fact, this explicit expression holds only until a critical time, which is shown to be equal to 1/(K-1) if K > 1 and to $+\infty$ if $K \le 1$, where K is defined in (1.3). Again, the associated PDE is easy to solve before gelation since then, A_t is known, while afterwards, the PDE contains the unknown parameter A_t .

1.3. Main result

In this paper we investigate the global behavior of Smoluchowski's equation with arms (1.2) before, at and after the gelation phase transition, proving existence and uniqueness of global solutions for a large class of initial conditions. The technique used, as in [3], is to transform the equation into a PDE. Since the total number of arms $(A_t)_{t\geq 0}$ is not a priori known, this PDE is non-local, unlike the one obtained in the regime before gelation. This is the main difficulty we have to deal with. We use a modification of the classical method of characteristics to show uniqueness of solutions to this PDE, and hence to (1.2). We can consider initial conditions $(c_0(a, m), a \in \mathbb{N}, m \in \mathbb{N}^*)$ with an initial infinite number of arms, that is, such that

$$A_0 := \sum_{a,m \ge 1} ac_0(a,m)$$

is infinite, and show that there is a unique solution "coming down from infinity sufficiently fast", i.e. such that, for positive t,

$$\int_{0}^{t} A_s^2 \, \mathrm{d}s < +\infty.$$

Note however that this is no technical condition, but a mere assumption to ensure that the equation is well defined.

We also consider a modification of this model which corresponds to Flory's equation for the model with arms. In this setting, the infinite mass particles, that is, the gel, interact with the other particles. We also prove existence, uniqueness and study the behavior of the solutions for this model.

In both cases, our technique provides a representation formula allowing to compute various quantities, as the mean number of arms in the system and the limiting concentrations. In Flory's case, we extend to all possible initial concentrations the computations done in [3] in absence of gelation. In the first model, a slight modification appears which calls for a probabilistic interpretation; see Section 1.4 below.

This seems to be the first case of a cluster coagulation model for which global well-posedness in presence of gelation can be proven. Another setting to which these techniques could be applied is the *coagulation model with mating* introduced in [22].

1.4. Limiting concentrations

In [3], explicit solutions to (1.2) are given for monodisperse initial conditions $c_0(a, m) = \mu(a)\mathbb{1}_{\{m=1\}}$ for some measure μ on \mathbb{N} with unit first moment. In particular, when there is no gelation, i.e. $K \leq 1$ where K is as in (1.3), and $\mu \neq \frac{1}{2}\delta_2$, there are limiting concentrations

$$c_{\infty}(a,m) = \frac{1}{m(m-1)} v^{*m}(m-2) \mathbb{1}_{\{a=0\}}, \quad m \ge 2,$$

where $\nu(m) = (m + 1)\mu(m + 1)$ is a probability measure on \mathbb{N} different from δ_1 . This formula clearly resembles the well-known formula of Dwass [7], which provides the law of the total progeny *T* of a Galton–Watson process with reproduction law ν , started from two ancestors:

$$\mathbb{P}(T=m) = \frac{2}{m} \nu^{*m} (m-2), \quad m \ge 2.$$

The similarity between the two formulas is no coincidence and is explained in [4] by means of the configuration model. For basics on Galton–Watson processes, see e.g. [2].

Let us briefly explain the result of [4], referring e.g. to [26] for more results on general random graphs. The configuration model aims at producing a random graph whose vertices have a prescribed degree. To this end, consider a number *n* of vertices, each being given independently a number of arms (that is, half-edges) distributed according to μ . Then, two arms in the system are chosen uniformly and independently, and form an edge between the corresponding vertices. This procedure is repeated until there are no more available arms. Hence, one arrives to a final state which can be described as a collection of random graphs. Then Corollary 2 in [4] and the discussion below show that, when there is no gelation, the proportion of trees of size *m* tends to $c_{\infty}(0, m)$ when the number *n* of vertices tends to infinity. Hence, the final states in the configuration model and in Smoluchowski's equation with arms coincide. This shows that the former is a good discrete model for coagulation.

Interestingly, the absence-of-gelation condition $K \leq 1$ is equivalent to (sub)-criticality of the Galton–Watson branching process with reproduction law ν , i.e. to almost sure extinction of the progeny, while K > 1 and gelation at finite time are equivalent to super-criticality of the GW process.

In this paper, we obtain the limiting concentrations for (1.2) and its modified version when there is gelation. Let us start with the modified model, which is the counterpart of Flory's equation for the model with arms. In this case, and with the same notations as above, we obtain the limit concentrations

$$c_{\infty}(a,m) = \frac{1}{m(m-1)} \nu^{*m}(m-2) \mathbb{1}_{\{a=0\}}, \quad m \ge 2,$$

that is, the same explicit form as the one obtained in absence of gelation. Again, this formula can be interpreted both in terms of a configuration model and of a super-critical Galton–Watson branching process. The relation between Flory's equation with arms and the configuration model is natural, since in both cases all particles interact with each other, no matter what their size is. It is worth noticing that, even though the limit concentrations have the same form with or without gelation, still some mass is eventually lost in presence of gelation, see (6.4) below.

We also obtain the limiting concentrations for Smoluchowski's equation with arms, namely

$$c_{\infty}(a,m) = \frac{1}{m(m-1)} \beta_{\infty}^{m-1} \nu^{*m}(m-2) \mathbb{1}_{\{a=0\}}$$

where β_{∞} is some constant, which is 1 when there is no gelation, and is greater than 1 otherwise, see Section 6.2. However, the probabilistic interpretation of β_{∞} is unclear. One can recover Smoluchowski's equation with arms from discrete models by preventing big particles from coagulating, as is done in [13] for the standard Smoluchowski equation, but the precise meaning of β_{∞} still seems to require some labor.

1.5. Bibliographical comments

Smoluchowski's equation (1.1) has been extensively studied; we refer to the reviews [1,18,23]. Conditions on the kernel κ are known for absence or presence of gelation, though this requires a precise definition of gelation, see e.g. [11], or [14] in a probabilistic setting. For a general class of kernels Smoluchowski's solution has a unique solution before gelation [23,6,12,18], and in the multiplicative case gelation always occurs [10,12,17].

For the monodisperse initial condition $c_0(m) = \mathbb{1}_{\{m=1\}}$, the first proof of existence and uniqueness to (1.1) before gelation is given in [20], and a proof of global existence and uniqueness can be found in [15]. The case of general nonzero initial conditions has been considered by several papers in the Physics literature [8,9,19,25,31], and by at least one mathematical paper [27], which however treats in full details only the regime before gelation, see Remark 2.7 below. The same authors also provide in [28] an exact formula for the post-gelation mass of (1.1), but with no rigorous proof.

Thus, a clear statement about well-posedness of (1.1) for the most general initial conditions still seems to be missing, and our paper tries to fill this gap. We adapt the classical method of characteristics for generating functions, see [5,3], which yields easily uniqueness before gelation for a multiplicative kernel [21]. We can in particular consider initial concentrations with infinite total mass, i.e. such that

$$M_0 := \int_{(0,+\infty)} m c_0(\mathrm{d}m) = +\infty,$$

as long as $\int_{(0,+\infty)} (m \wedge 1) c_0(dm) < +\infty$. This covers for instance initial conditions of the type $c_0(dm) = C_p m^{-p} dm$ with $p \in [1, 2)$.

Our main concern is uniqueness, since existence of solutions has been obtained in a much more general setting by analytic [16,17,24] or probabilistic [13,14] means. However, the case of an infinite initial mass seems to have been considered only in [16] in the discrete case, so we refer to Section 2.4 below for a proof.

1.6. Plan of the article

We start off in Section 2 by considering existence, uniqueness and representation formulas for global solutions of (1.1), introducing and exploiting all main techniques which are needed afterwards to tackle the same issues in the case of (1.2). We prove that for the most general initial conditions $\mu_0(dm)$, a positive measure on $(0, +\infty)$, Smoluchowski's equation with a multiplicative kernel has a unique solution before and after gelation. We also show existence and uniqueness for the modified version of Smoluchowski's model, namely Flory's equation, in Section 3. The techniques used are generalized in Sections 4 and 5, where we prove analogous results for the models with arms. We compute the limiting concentrations in Section 6, which are not trivial, in comparison with the standard Smoluchowski and Flory cases, for which they are always zero.

2. Smoluchowski's equation

In this section we develop our method in the case of Eq. (1.1), proving existence, uniqueness and representation formulas for global solutions. Let us first fix some notations.

- *M*⁺_f is the set of all non-negative finite measures on (0, +∞). *M*⁺_c is the set of all non-negative Radon measures on (0, +∞).
- For $\mu \in \mathcal{M}_c^+$ and $f \in L^1(\mu)$ or $f \ge 0$,

$$\langle \mu, f \rangle = \int_{(0,+\infty)} f(m) \,\mu(\mathrm{d}m)$$

We will write *m* for the function $m \mapsto m$, m^2 for $m \mapsto m^2$, etc.

- For $\phi: (0, +\infty) \to \mathbb{R}$ and $m, m' > 0, \Delta \phi(m, m') = \phi(m + m') \phi(m) \phi(m')$.
- $C_c(0, +\infty)$ is the space of continuous functions on $(0, +\infty)$ with compact support.
- For a function $(t, x) \mapsto \phi_t(x), \phi'_t(x)$ is the partial derivative of ϕ with respect to x.
- $\frac{\partial^+}{\partial t}$ or $\frac{d^+}{dt}$ denotes the right partial derivative with respect to t.

We are interested in Smoluchowski's equation (1.1) with multiplicative coagulation kernel $\kappa(m, m') = mm'$. Note that the second requirement in the following definition is only present for the equation to make sense.

Definition 2.1. Let $\mu_0 \in \mathcal{M}_c^+$. We say that a family $(\mu_t)_{t \ge 0} \subset \mathcal{M}_c^+$ solves Smoluchowski's equation if

- for every t > 0, $\int_0^t \langle \mu_s(\mathrm{d}m), m \rangle^2 \mathrm{d}s < +\infty$,
- for all $\phi \in C_c(0, +\infty)$ and t > 0

$$\langle \mu_t, \phi \rangle = \langle \mu_0, \phi \rangle + \frac{1}{2} \int_0^t \langle \mu_s(\mathrm{d}m) \mu_s(\mathrm{d}m'), mm' \Delta \phi(m, m') \rangle \mathrm{d}s, \qquad (2.1)$$

• if $\langle \mu_0, m^2 \rangle < +\infty$, then $t \mapsto \langle \mu_t, m^2 \rangle$ is bounded in a right neighborhood of 0.

The global behavior of this equation has been studied first for monodisperse initial conditions (i.e. $\mu_0 = \delta_1$), in which case it can be proven that there is a unique solution $(\mu_t)_{t\geq 0}$ on \mathbb{R}^+ , which is also explicit, see [20,15]. This solution clearly exhibits the gelation phase transition. Up to the gelation time $T_{gel} = 1$, the total mass $\langle \mu_t, m \rangle$ is constant and equal to 1, and then it decreases: $\langle \mu_t, m \rangle = 1/t$ for $t \ge 1$. Moreover, the second moment $\langle \mu_t, m^2 \rangle$ is finite before time 1, and then infinite on $[1, +\infty)$. It is also known in the literature that for any nonzero initial conditions, there is a gelation time $0 < T_{gel} < +\infty$, such that there is a unique solution to (2.1) on $[0, T_{gel})$, and $\langle \mu_t, m^2 \rangle \to +\infty$ when $t \to T_{gel}^{-1}$: see e.g. [12].

Theorem 2.2. Let $\mu_0 \in \mathcal{M}_c^+$ be a non-null measure such that

$$\langle \mu_0, m \wedge 1 \rangle = \int_{(0, +\infty)} (m \wedge 1) \, \mu_0(\mathrm{d}m) < +\infty.$$
(2.2)

We can then define

 $M_0 := \langle \mu_0, m \rangle \in (0, +\infty], \qquad K := \langle \mu_0, m^2 \rangle \in (0, +\infty],$

and the function

$$g_0(x) := \langle \mu_0, mx^m \rangle = \int_{(0, +\infty)} mx^m \, \mu_0(\mathrm{d}m), \quad x \in [0, 1]$$
(2.3)

with $g_0(1) = M_0 \in (0, +\infty]$. Let

$$T_{\text{gel}} := 1/K \in [0, +\infty).$$
 (2.4)

Then Smoluchowski's equation (2.1) has a unique solution on \mathbb{R}^+ . It has the following properties.

- (1) The total mass $M_t = \langle \mu_t, m \rangle$ is continuous on $[0, +\infty)$. It is constant on $[0, T_{gel}]$ and strictly decreasing on $[T_{gel}, +\infty)$. It is analytic on $\mathbb{R}^+ \setminus \{T_{gel}\}$.
- (2) If the following limit exists

$$\nu := -\lim_{x \to 1^{-}} \frac{(g'_0(x))^3}{g'_0(x) + xg''_0(x)} \in [-\infty, 0].$$

then the right derivative $\dot{M}_{T_{gel}}$ of M at $t = T_{gel}$ is equal to v.

(3) Let $m_0 = \inf \operatorname{supp} \mu_0 \in [0, +\infty)$. When $t \to +\infty$,

$$\frac{1}{tM_t} \to m_0.$$

(4) The second moment $\langle \mu_t, m^2 \rangle$ is finite for $t \in [0, T_{gel})$ and infinite for $t \in [T_{gel}, +\infty)$.

Remark 2.3.

- This result allows to recover the pre- and post-gelation formulas obtained with no rigorous proof in some earlier papers [9,8,15,19,27,28,25]. The decrease of the mass in 1/t when $m_0 > 0$ was also observed in these papers. Also, some upper bounds in 1/t for the mass were proven in [11,17].
- If m = 0, the mass tends to 0 more slowly than 1/t: small particles need to coagulate before any big particle can appear, and they coagulate really slowly. For instance, a straightforward computation shows that if $\mu_0(dm) = e^{-m} dm$, then $M_t \sim t^{-2/3}$. More generally, the explicit formula in Proposition 2.6 allows to compute M_t for any initial conditions.

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• With this formula, it is easy to check that $\dot{M}_{T_{gel}+}$ can be anything from $-\infty$ to 0. For instance, $\dot{M}_{T_{gel}+} = 0$ for $g_0(x) = (1-x)\log(1-x) + x$, $\dot{M}_0 = -\infty$ for $g_0(x) = \sqrt{1-x}\log(1-x) + x$, and for $0 < \alpha < +\infty$, $\dot{M}_0 = -\alpha$ for $g_0(x) = 1 - \sqrt{1-x^{2\alpha}}$. In particular, M need not be convex on $[T_{gel}, +\infty)$.

2.1. Preliminaries

Let μ_0 be defined as in the previous statement. We shall prove that, starting from μ_0 , there is a unique solution to (2.1) on \mathbb{R}^+ , and give a representation formula for this solution. This allows to study the behavior of the moments. Let us start with some easy lemmas. So take a solution $(\mu_t)_{t\geq 0}$ to (2.1) and set

$$M_t = \langle \mu_t, m \rangle. \tag{2.5}$$

The two following lemmas are easy to prove, using monotone and dominated convergence.

Lemma 2.4. $(M_t)_{t \ge 0}$ is monotone non-increasing and right-continuous. Moreover, $M_t < +\infty$ for all t > 0.

Proof. Take $\phi^K(m) = m$ for $m \in [0, K]$, $\phi^K(m) = 2K - m$ for $m \in [K, 2K]$, and $\phi^K(m) = 0$ for $m \ge 2K$, so that $\phi^K \in C_c$. Plugging ϕ^K in Smoluchowski's equation (2.1), letting $K \to +\infty$ and using Fatou's lemma readily shows that $(M_t)_{t\ge0}$ is monotone non-increasing. Note also that $t \mapsto M_t = \sup_K \langle \mu_t, \phi^K \rangle$ is the supremum of a sequence of continuous functions and so is lower semi-continuous, which implies, for a monotone non-increasing function, right-continuity. Finiteness of M_t is now obvious since $s \mapsto M_s^2$, and hence $s \mapsto M_s$, are integrable by Definition 2.1. \Box

Lemma 2.5. Assume that $t \mapsto \langle \mu_t, m^2 \rangle$ is bounded on some interval $[0, T_0]$. Then $M_t = M_0$ for $t \in [0, T_0]$.

By Lemma 2.4, $\langle \mu_t, m \rangle < +\infty$ for t > 0, so that we can define

$$g_t(x) = \langle \mu_t, mx^m \rangle = \int_{(0, +\infty)} mx^m \, \mu_t(\mathrm{d}m), \quad x \in [0, 1], \ t > 0,$$
(2.6)

which is the generating function of $m \mu_t(dm)$. Then, using a standard approximation procedure, it is easy to see that *g* satisfies

$$\begin{cases} g_t(x) = g_0(x) + \int_0^t x \left(g_s(x) - M_s \right) \frac{\partial^+ g_s}{\partial x}(x) \, \mathrm{d}s, & t \ge 0, \ x \in (0, 1), \\ g_t(1) = M_t, & t \ge 0. \end{cases}$$
(2.7)

It is well known, and will be proven again below, that $M_t = M_0$ for all $t \leq T_{gel}$, since then, the PDE (2.7) can be solved by the method of characteristics: the function $\phi_t(x) : [0, 1] \mapsto [0, 1]$

$$\phi_t(x) = x e^{t(M_0 - g_0(x))}, \quad x \in [0, 1], \ t \leq T_{\text{gel}}$$

is one-to-one and onto, has an inverse $h_t : [0, 1] \mapsto [0, 1]$ and we find

$$g_t(x) = g_0(h_t(x)), \quad x \in [0, 1], \ t \leq T_{gel}$$

However M_t is not necessary constant for $t > T_{gel}$ and the form of ϕ_t has to be modified; we thus define

$$\phi_t(x) = x\alpha_t e^{-tg_0(x)}, \quad x \in [0, 1], \ t > 0$$
(2.8)

where

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$$\alpha_t := \exp\left(\int_0^t M_s \,\mathrm{d}s\right), \quad t \ge 0. \tag{2.9}$$

For $t > T_{gel}$, M_t is possibly less than M_0 and ϕ_t , which depends explicitly on $(M_s)_{s \in [0,t]}$, is possibly neither injective nor surjective. We shall prove that it is indeed possible to find $\ell_t \in (0, 1)$ such that $\phi_t(x) : [0, 1] \mapsto [0, \ell_t]$ is one-to-one and ℓ_t is uniquely determined by g_0 .

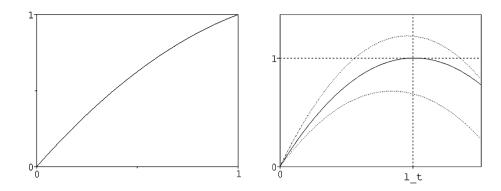


Fig. 1. ϕ_t before and after gelation. The dotted lines represent what ϕ_t may look like. The solid one is the actual ϕ_t .

2.2. Uniqueness of solutions

Using an adaptation of the method of characteristics, we are going to prove the following result. Note that in [27], this properties are claimed to be true but a proof seems to lack. We will use the same techniques in the proof of Theorem 4.2 for the model with arms, but they are easier to understand in the present case.

Proposition 2.6. Let $(\mu_t)_{t \ge 0}$ be a solution of Smoluchowski's equation (2.1).

(1) For all $t \in [0, T_{gel}]$, $M_t = M_0 = g_0(\ell_t)$, where $\ell_t := 1$. For all $t > T_{gel}$, $M_t = g_0(\ell_t)$ where $\ell_t \in (0, 1)$ is uniquely defined by

$$\ell_t g_0'(\ell_t) = \frac{1}{t}.$$
(2.10)

Moreover ℓ_t *and* $\phi_t(\cdot)$ *satisfy*

$$\phi'_t(\ell_t) = 0, \qquad \phi_t(\ell_t) = 1 > \phi_t(x), \quad \forall x \in (0, 1).$$
(2.11)

(2) For all t > 0, the function $\phi_t(\cdot)$ defined in (2.8) has a right inverse

$$h_t: [0,1] \mapsto [0,\ell_t], \quad \phi_t(h_t(x)) = x, \quad x \in [0,1],$$
(2.12)

and

$$g_t(x) = g_0(h_t(x)), \quad t > 0, \ x \in [0, 1].$$
 (2.13)

- (3) The functions $(\ell_t)_{t \ge 0}$ and $(M_t)_{t \ge 0}$ are continuous.
- (4) $(\mu_t)_{t\geq 0}$ is uniquely defined by μ_0 .

Remark 2.7.

- For all $t \leq T_{gel}$, $M_t = M_0$, $\ell_t = 1$ and $\phi_t : [0, 1] \mapsto [0, 1]$ is one-to-one and onto. The first thing one needs to prove is that for all $t > T_{gel}$, $\ell_t < 1$, i.e. there is indeed $x \in [0, 1]$ such that $\phi_t(x) = 1$, see Lemma 2.9; the second one, is that $\ell_t = m_t$, i.e. $\phi_t(\cdot)$ has an absolute maximum at ℓ_t , see Lemma 2.10. In other words, one has to exclude the dotted lines as possible profiles of $\phi_t(\cdot)$ in Fig. 1. These properties are not obvious, since ϕ_t depends on $(M_s)_{s \in [0,t]}$ which is, at this point, unknown. All other properties are derived from these two.
- In [27, Section 6] one finds a discussion of post-gelation solutions, in particular of the results of our Proposition 2.6. However this discussion falls short of a complete proof, since the two above-mentioned properties are not proven. In particular, no precise statement about what initial conditions can be considered is given.

The following lemma is a list of obvious but useful properties satisfied by g and ϕ .

Lemma 2.8. The function g defined in (2.6) satisfies the following properties.

- (a1) $(t, x) \mapsto g_t(x)$ is finite and continuous on $[0, +\infty) \times [0, 1)$;
- (a2) For all $x \in [0, 1)$, $t \mapsto g_t(x)$ is right differentiable on $(0, +\infty)$;
- (a3) For all $t \ge 0$, $x \mapsto g_t(x)$ is analytic on (0, 1) and monotone non-decreasing;
- (a4) For all t > 0, $x \mapsto g_t(x) \in [0, +\infty]$ is continuous on [0, 1].

The function ϕ *defined in* (2.8) *satisfies the following properties.*

- (b1) ϕ_t is continuous on [0, 1] and analytic on (0, 1);
- (b2) $\phi_t(0) = 0, \phi_t(1) = e^{-\int_0^t (M_0 M_s) \, ds} \in [0, 1];$
- (b3) $\phi'_t(x) = \alpha_t e^{-tg_0(x)} (1 txg'_0(x))$ for $x \in (0, 1)$;
- (b4) For $t \leq T_{gel}$, ϕ_t is increasing. For $t > T_{gel}$, $x \mapsto xg'_0(x)$ is increasing, $\phi'_t(0) > 0$ and $\phi'_t(1) < 0$. In particular, for $t > T_{gel}$, there is precisely one point $m_t \in (0, 1)$ such that

$$\phi'_t(m_t) = 0;$$
 (2.14)

(b5) For $t > T_{gel}$, ϕ_t is increasing on $[0, m_t]$ and decreasing on $[m_t, 1]$.

Moreover,

- (c1) The map $(t, x) \mapsto \phi_t(x)$ is continuous on $\mathbb{R}^+ \times [0, 1)$;
- (c2) The map $(t, x) \mapsto \phi'_t(x)$ is continuous on $\mathbb{R}^+ \times (0, 1)$;
- (c3) For every $x \in [0, 1)$, $t \mapsto \phi_t(x)$ is right differentiable and

$$\frac{\partial^+ \phi_t}{\partial t} = \phi_t(x) \left(M_t - g_0(x) \right) \quad x \in [0, 1), \ t \ge 0.$$

$$(2.15)$$

Property (b5) implies that there are at most two points in (0, 1) where ϕ_t equals 1. Take ℓ_t to be the smallest, if any, i.e.

$$\ell_t = \inf\{x \ge 0; \ \phi_t(x) = 1\} \quad (\inf\emptyset := 1).$$
(2.16)

Lemma 2.9.

(1) For every $t \ge 0$ and every $x \in [0, \ell_t]$

$$g_t(\phi_t(x)) = g_0(x).$$
 (2.17)

(2) For all $t \in [0, T_{gel}]$, $\ell_t = 1$, and for $t > T_{gel}$, $0 < \ell_t < 1$. In particular, for all t > 0, $\phi_t(\ell_t) = 1$ and

$$g_0(\ell_t) = g_t(1) = M_t. \tag{2.18}$$

(3) Finally, $t \mapsto \ell_t$ is monotone non-increasing and continuous on \mathbb{R}^+ .

Proof. (1) Let us first prove that there exists $\tau > 0$ such that (2.17) holds for $t \in [0, \tau[$. Fix 0 < a < b < 1. Since $0 < \min_{[a,b]} \phi_0 < \max_{[a,b]} \phi_0 < 1$, then by property (c1) there is $\tau > 0$ such that

$$0 < \min_{[a,b]} \phi_t < \max_{[a,b]} \phi_t < 1, \quad \forall t \in [0,\tau).$$

So, for a fixed $x \in [a, b]$, the function

$$u_t := g_t(\phi_t(x)) - g_0(x)$$

is well defined and using (2.7) and (2.15), we see that

$$u_t = \int_0^t \left(\frac{\partial^+ g_s}{\partial s} (\phi_s(x)) + \frac{\partial g_s}{\partial x} (\phi_s(x)) \frac{\partial^+ \phi_s}{\partial s}(x) \right) ds = \int_0^t \gamma_s u_s \, ds$$

where

$$\gamma_t := \frac{\partial g_t}{\partial x} (\phi_t(x)) \phi_t(x), \quad t > 0.$$

Since $x \in [0, 1)$, $\sup_{t \in [0, \tau)} |\gamma_t| < +\infty$ and therefore $u_t \equiv 0$. Hence (2.17) holds for $x \in [a, b]$ and $t \in [0, \tau[$. Since both terms of (2.17) are analytic functions of x on $(0, \ell_t)$, by analytic continuation, (2.17) actually holds on $(0, \ell_t)$, and hence on $[0, \ell_t]$ by continuity.

(2) Let us now extend this formula to $t \in \mathbb{R}^+$. Let

$$T = \sup\{t > 0: \forall s \in [0, t], \forall x \in [0, \ell_s], g_s(\phi_s(x)) = g_0(x)\} \ge \tau > 0,$$

assume $T < +\infty$, and denote by ℓ the left limit of $(\ell_t)_{t \ge 0}$ at T. First, ℓ cannot be 0, since otherwise we would get when $s \to T^-$

$$1 = \phi_s(\ell_s) = \ell_s \alpha_s e^{-sg_0(\ell_s)} \to 0.$$

For every $t < T^-$, $0 < \ell \leq \ell_t$, so for every $x \in (0, \ell)$, $g_t(\phi_t(x)) = g_0(x)$ and $\phi_t(x) < 1$. Using the continuity property (c1) and passing to the limit when $t \to T^-$ in this equality, we get

$$g_T(\phi_T(x)) = g_0(x), \quad \forall x \in (0, \ell).$$

By the same reasoning as in point (i), we obtain a T' > T such that $g_t(\phi_t(x)) = g_0(x)$ for all $t \in [T, T')$ and x in a non-empty open subset of $(0, \ell)$. By analyticity and continuity, the formula $g_t(\phi_t(x)) = g_0(x)$ holds for every $t \in [T, T')$ and $x \in [0, \ell_t]$. This contradicts the definition of T, and so $T = +\infty$. This concludes the proof of point (1) of the lemma.

(3) For the statement (2) of the lemma, let us show first that $\langle \mu_t, m^2 \rangle$ is bounded on $[0, T_0)$, for every $T_0 \in [0, T_{gel})$. Let T' be the smallest time when this fails (provided of course that $T_{gel} > 0$). By assumption (see Definition 2.1), T' > 0. Differentiating (2.17) with respect to x and having x tend to $\ell_t = 1$ gives, for t < T',

$$g'_t(1) = \langle \mu_t, m^2 \rangle = \frac{1}{1 - tK}$$

This quantity explodes only when $t = T_{gel} = 1/K$, so $T' = T_{gel}$.

(4) The boundedness of $(\langle \mu_t, m^2 \rangle)_{t \in [0, T_{00}]}$ just proven for all $T_0 \in [0, T_{gel})$ and Lemma 2.5 imply that for $t \in [0, T_{gel})$, $M_t = M_0$. By the definition (2.8) of ϕ_t , it follows that $\phi_t(1) = 1$ for $t \in [0, T_{gel})$. But ϕ_t is increasing, so $\ell_t = 1$ for $t \in [0, T_{gel})$. Assume now that for some $t > T_{gel}$, $\ell_t = 1$. Then (2.17) holds on [0, 1], and this is impossible since the right term is an increasing function of x, whereas the left one decreases in a left neighborhood of 1 since $\phi'_t(1) < 0$. The fact that $\phi_t(\ell_t) = 1$ follows then directly from the definition of ℓ_t and the continuity of $\phi_t(\cdot)$. Finally, the inequality $\ell_t > 0$ is obvious since $\phi_t(0) = 0$, and computing (2.17) at $x = \ell_t$ gives (2.18). This concludes the proof of (2).

(5) We know that $\ell_t = 1$ and $M_t = M_0$ for all $t < T_{gel}$. Now, g_0 is strictly increasing and continuous. Since $(M_t)_{t \ge 0}$ is monotone non-increasing and right-continuous by Lemma 2.4, so is $(\ell_t)_{t \ge 0}$ by (2.18). To get left-continuity of $(\ell_t)_{t>T_{gel}}$, consider $t > T_{gel}$, and let ℓ be the left limit of ℓ_s at t. We have $\ell \le \ell_{t+(t-T_{gel})/2} < 1$, so by the continuity property (c1) above,

$$1 = \phi_s(\ell_s) \xrightarrow[s \to t^-]{} \phi_t(\ell).$$

Hence $\phi_t(\ell) = 1$. Assume $\ell > \ell_t$ (that is, ℓ is the second point where ϕ_t reaches 1). Take $x \in (\ell_t, \ell)$. By property (b5), $\phi_t(x) > 1$. But on the other hand, $x < \ell \leq \ell_s$ for s < t, so $\phi_s(x) \leq 1$, and so $\phi_t(x) \leq 1$, and this is a contradiction. So $\ell = \ell_t$ and $(\ell_t)_{t \geq 0}$ is indeed continuous. This concludes the proof of (3) and of the lemma. \Box

Finally, we will see that for $t > T_{gel}$, $\ell_t = m_t$, so that ϕ_t increases from 0 to 1, which is its maximum, and then decreases. To this end, recall that $(\ell_t)_{t \ge 0}$ is monotone non-increasing and that $(\ell_t)_{t \ge 0}$ and $(\phi_t)_{t \ge 0}$ are continuous, so the chain rule for Stieltjes integrals and (2.15) give

$$1 = \phi_t(\ell_t) = \phi_0(\ell_0) + \int_0^t \phi_s'(\ell_s) \, \mathrm{d}\ell_s + \int_0^t \frac{\partial^+ \phi_s}{\partial s}(\ell_s) \, \mathrm{d}s$$
$$= 1 + \int_0^t \phi_s'(\ell_s) \, \mathrm{d}\ell_s + \int_0^t \phi_s(\ell_s) \big(M_s - g_0(\ell_s)\big) \, \mathrm{d}s$$

that is, with (2.18),

$$\phi_t'(\ell_t) \, \mathrm{d}\ell_t = 0. \tag{2.19}$$

Hence, $d\ell_t$ -a.e. $\phi'_t(\ell_t) = 0$, i.e. $\ell_t = m_t$. This is actually true for all $t > T_{gel}$, as we shall now prove. This result also has its counterpart in the model with arms, namely part (3) of the proof of Theorem 4.2.

Lemma 2.10. For every $t > T_{gel}$, $\phi'_t(\ell_t) = 0$, i.e. $\ell_t = m_t$, the point where ϕ_t attains its maximum. In particular,

$$\ell_t g_0'(\ell_t) = \frac{1}{t}, \quad \forall t > T_{\text{gel}}.$$
(2.20)

Proof. First, recall that ϕ_t is increasing on $[0, \ell_t]$, so that $\phi'_t(\ell_t) \ge 0$, that is

$$\ell_t g_0'(\ell_t) \leqslant \frac{1}{t}.$$
(2.21)

Assume now that there is a $t > T_{gel}$ such that $\phi'_t(\ell_t) > 0$, and consider

 $s = \sup \left\{ r \in (T_{\text{gel}}, t): \phi_r'(\ell_r) = 0 \right\}.$

As noted before, $t \mapsto \ell_t$ is strictly decreasing for $t > T_{gel}$ for any $t > T_{gel}$, so $d\ell_t([T_{gel}, T_{gel} + \varepsilon[) > 0$ for all $\varepsilon > 0$. Hence there are points r < t where $\phi'_r(\ell_r) = 0$, and thus the definition of *s* does make sense.

Take now (r_n) a sequence of points such that $T < r_n < t$, $\phi'_r(\ell_r) = 0$ and (r_n) converges to *s*. Since $0 < \ell_s < 1$, by property (c2) above, we get

$$0 = \phi'_{r_n}(\ell_{r_n}) \to \phi'_s(\ell_s)$$

so that $\phi'_s(\ell_s) = 0$. This shows that s < t, and that for $r \in (s, t)$, $\phi'_r(\ell_r) > 0$. Hence, by continuity of $(\ell_r)_{r \ge 0}$ and by (2.19), $(\ell_r)_{r \in [s,t]}$ is constant. This gives

$$\frac{1}{s} = \ell_s g'_0(\ell_s) = \ell_t g'_0(\ell_t) \leqslant \frac{1}{t}$$

which is a contradiction since s < t. In particular, $\phi'_t(\ell_t) = 0$ implies (2.20). \Box

Proof of Proposition 2.6. By Lemma 2.10, necessarily $M_t = M_0$ on $[0, T_{gel}]$ and for $t > T_{gel}, M_t := g_t(1) = g_0(\ell_t)$, where

$$\ell_t g_0'(\ell_t) = \frac{1}{t}.$$
(2.22)

Since $x \mapsto xg'_0(x)$ is strictly increasing from [0, 1] to [0, K], where $K = \langle \mu_0, m^2 \rangle = 1/T_{gel}$, this equation has a unique solution for $t > T_{gel}$. Hence M_t is uniquely defined. Therefore α_t and ϕ_t are uniquely determined by g_0 , so we can define ϕ_t as in (2.8), and Lemma 2.9 shows that $g_t(\phi_t(x)) = g_0(x)$ for $x \in [0, \ell_t]$, and that ϕ_t is a bijection from $[0, \ell_t]$ to [0, 1]. So it has a right inverse h_t , and compounding by h_t in the previous formula gives

$$g_t(x) = g_0(h_t(x))$$
(2.23)

for all $x \in [0, 1]$, $t \ge 0$. Thus g_t can be expressed by a formula involving only g_0 and in particular, $(\mu_t)_{t\ge 0}$ depends only on μ_0 . This shows the uniqueness of a solution to Smoluchowski's equation (2.1). \Box

2.3. Behavior of the moments

In this paragraph, we will study the behavior of the first and second moment of $(\mu_t)_{t\geq 0}$ as time passes, showing how to prove rigorously and recover the results of [9]. For more general coagulation rates, one can obtain upper bounds of the same nature, see [17].

First consider the mass $M_t = \langle \mu_t, m \rangle$. We will always assume that $T_{gel} < +\infty$. Let us start with the following lemma.

Lemma 2.11. Let $v \in \mathcal{M}_c^+$ be a measure which integrates $x \mapsto y^x$ for small enough y > 0. Let m_0 be the infimum of *its support. Then*

$$\lim_{y\to 0^+} \frac{\langle v, xy^x \rangle}{\langle v, y^x \rangle} = m_0.$$

Proof. First, note that $xy^x \ge m_0 y^x$ ν -a.e. so

$$\liminf_{y\to 0} \frac{\langle v, xy^x \rangle}{\langle v, y^x \rangle} \ge m_0.$$

Let us prove now that

$$\limsup_{y\to 0}\frac{\langle v, xy^x\rangle}{\langle v, y^x\rangle}\leqslant m_0.$$

Assume this is not true. Then, up to extraction of a subsequence, we may assume that there exists $\alpha > 0$ such that for arbitrary small $y \in (0, 1)$, $\langle v, xy^x \rangle \ge (m_0 + \alpha) \langle v, y^x \rangle$. Hence $\langle v, (x - m_0 - \alpha)y^x \rangle \ge 0$, so

$$\langle \nu, (x - m_0 - \alpha) y^x \mathbb{1}_{\{x > m_0 + \alpha\}} \rangle \ge \langle \nu, (m_0 + \alpha - x) y^x \mathbb{1}_{\{m_0 \le x \le m_0 + \alpha\}} \rangle.$$

$$(2.24)$$

But

$$\left\langle \nu, (m_0 + \alpha - x) y^x \mathbb{1}_{\{m_0 \leqslant x \leqslant m_0 + \alpha\}} \right\rangle \geq \left\langle \nu, (m_0 + \alpha - x) y^x \mathbb{1}_{\{m_0 \leqslant x \leqslant m_0 + \alpha/2\}} \right\rangle$$
$$\geq \left\langle \nu, (m_0 + \alpha - x) \mathbb{1}_{\{m_0 \leqslant x \leqslant m_0 + \alpha/2\}} \right\rangle y^{m_0 + \alpha/2}$$

and

$$\left\langle v, (x-m_0-\alpha)y^x \mathbb{1}_{\{x>m_0+\alpha\}} \right\rangle \leq \left\langle v, (x-m_0-\alpha)\mathbb{1}_{\{x>m_0+\alpha\}} \right\rangle y^{m_0+\alpha}$$

With (2.24), this shows that

$$\left\langle \nu, (x-m_0-\alpha)\mathbb{1}_{\{x>m_0+\alpha\}}\right\rangle y^{\alpha/2} \ge \left\langle \nu, (m_0+\alpha-x)\mathbb{1}_{\{m_0\leqslant x\leqslant m_0+\alpha/2\}}\right\rangle$$

and having y tend to zero gives

 $0 \ge \langle \nu, (m_0 + \alpha - x) \mathbb{1}_{\{m_0 \le x \le m_0 + \alpha/2\}} \rangle$

which is a contradiction since $\nu([m_0, m_0 + \alpha/2]) > 0$. \Box

Corollary 2.12. The mass of the system is continuous and positive. It is strictly decreasing on $[T_{gel}, +\infty)$. Moreover, denote $m_0 = \inf \text{supp } \mu_0$. Then

$$\lim_{t \to +\infty} \frac{1}{tM_t} = m_0.$$

Proof. Recall that $M_t = g_0(\ell_t)$ so the first properties follow from Lemma 2.9. Denote now $\nu(dm) = m\mu_0(dm)$. For $t > T_{gel}, \ell_t g'_0(\ell_t) = 1/t$, so

$$\frac{1}{tM_t} = \frac{\langle v, x\ell_t^x \rangle}{\langle v, \ell_t^x \rangle}$$

and since $\ell_t \to 0$ when $t \to +\infty$, this tends to m_0 by Lemma 2.11. \Box

We can also study the behavior of the mass for small times. Recall that before gelation, the mass is constant at 1. We have seen that it is continuous at the gelation time. We may then wonder if its derivative is continuous, that is if $\dot{M}_{T_{oel}+}$ is zero or not.

Lemma 2.13. The right derivative of M at T_{gel} is given by

$$\dot{M}_{T_{\text{gel}}+} = -\lim_{x \to 1^{-}} \frac{g_0'(x)^3}{g_0'(x) + xg_0''(x)} \in [-\infty, 0]$$

provided the limit exists.

Proof. For $t > T_{gel}$, $f(\ell_t) = 1/t$ with $f(x) = xg'_0(x)$, and $0 < \ell_t < 1$. But $f'(\ell_t) \neq 0$, so by the inverse mapping theorem, $(\ell_t)_{t\geq 0}$ is differentiable and

$$\dot{\ell}_t = -\frac{1}{t^2 f'(\ell_t)}.$$

Using the fact that $M_t = g_0(\ell_t)$, it is then easy to see that

$$\dot{M}_t = -\ell_t^2 \frac{g_0'(\ell_t)^3}{g_0'(\ell_t) + \ell_t g_0''(\ell_t)}$$

Since $(\ell_t)_{t \ge 0}$ is continuous at T_{gel} and $\ell_{T_{gel}} = 1$, the result follows. \Box

Recall that the gelation time is precisely the first time when the second moment $\langle \mu_t, m^2 \rangle$ of $(\mu_t)_{t \ge 0}$ becomes infinite. It actually remains infinite afterwards.

Corollary 2.14. For all $t \ge T_{gel}$, $\langle \mu_t, m^2 \rangle = +\infty$.

Proof. Note that

$$\left\langle \mu_t, m^2 \right\rangle = g_t'(1),$$

this formula being understood as a monotone limit. By (2.17), for $x < \ell_t$

$$\phi_t'(x)g_t'(\phi_t(x)) = g_0'(x).$$

When $x \to \ell_t^-$, $\phi_t'(x) \to 0$ by Lemma 2.10, and $g_0'(x) \to g_0'(\ell_t) \neq 0$ since $\ell_t > 0$. So

$$g'_t(\phi_t(\ell_t)) = g'_t(1) = +\infty. \quad \Box$$

2.4. Existence of solutions

Existence of solutions of (2.1) is a well-known topic, see e.g. [13]. However, the case $M_0 = +\infty$ is apparently new, so that we give a short proof for the general case based on previous papers, mainly [27].

Let now $\mu_0 \in \mathcal{M}_f^+$ be as in the statement of Theorem 2.2 and let us set g_0 as in (2.3), ℓ_t and M_t as in point (1) of Proposition 2.6, α_t and ϕ_t as in (2.9) and (2.8). Then it is easy to see that ϕ_t admits a right inverse h_t satisfying (2.12), and we can thus define

$$g_t(x) := g_0(h_t(x)), \quad t \ge 0, \ x \in [0, 1].$$

It is an easy but tedious task to check that g_t satisfies (2.7) and all properties (a1)–(a4) above. In particular, if $g_0(1) = +\infty$ then $h_t(1) < 1$ and therefore $g_t(1) < +\infty$ for all t > 0. Following [27], we can now prove the following.

Proposition 2.15. For all t > 0 there exists $\mu_t \in \mathcal{M}_f^+$ such that

$$g_t(x) = \langle \mu_t, mx^m \rangle = \int_{(0, +\infty)} mx^m \, \mu_t(\mathrm{d}m), \quad x \in [0, 1].$$

Proof. Let t > 0 be fixed. We set for all $y \ge 0$

$$\Phi(y) := g_0(e^{-y}), \qquad \Gamma(y) := tg_0(e^{-y}), \qquad G(y) := \Gamma(y) + y - \log \alpha_t = -\log \phi_t(e^{-y}).$$

We recall that $f:[0, +\infty) \mapsto [0, +\infty)$ is completely monotone if f is continuous on $[0, +\infty)$, infinitely many times differentiable on $(0, +\infty)$ and

$$(-1)^k \frac{d^k f}{dy^k}(y) \ge 0, \quad \forall k \ge 0, \ y \in (0, +\infty).$$

It is easy to see that Φ and Γ are completely monotone. Moreover, G has a right inverse

$$G^{-1}:[0,+\infty)\mapsto \left[\log(1/\ell_t),+\infty\right), \quad G^{-1}(y)=-\log h_t\left(e^{-y}\right), \quad y \ge 0,$$

and therefore by the definitions

$$g_0(h_t(e^{-y})) = \Phi(G^{-1}(y)), \quad y \ge 0.$$

By [27, Theorem 3.2], $\Phi \circ G^{-1}$ is completely monotone and therefore, by Bernstein's Theorem, there exists a unique $\nu_t \in \mathcal{M}_f^+$ such that

$$g_t(e^{-y}) = g_0(h_t(e^{-y})) = \Phi(G^{-1}(y)) = \int_{(0,+\infty)} e^{-ym} v_t(\mathrm{d}m), \quad y \ge 0.$$

Since $g_t(1) < +\infty$ for all t > 0, we obtain that $\langle v_t, m \rangle < +\infty$, so that we can set $\mu_t(dm) := m v_t(dm)$, and we have found that there is a unique $\mu_t \in \mathcal{M}_f^+$ such that

$$g_t(x) = g_0(h_t(x)) = \int_{(0,+\infty)} x^m m \,\mu_t(\mathrm{d}m), \quad x \in (0,1]. \qquad \Box$$

In order to show that $(\mu_t)_{t \ge 0}$ is a solution of Smoluchowski's equation in the sense of Definition 2.1, we have to check that $\int_0^{\varepsilon} M_t^2 dt < +\infty$ for all $\varepsilon > 0$. This is the content of the next result.

Lemma 2.16. If $(\mu_t)_{t \ge 0}$ is the family constructed in Proposition 2.15, then for all $\varepsilon > 0$, $\int_0^{\varepsilon} \langle \mu_s, m \rangle^2 ds < +\infty$.

Proof. If $M_0 < +\infty$ then there is nothing to prove, since $(M_t)_{t \ge 0}$ is monotone non-increasing, so let us consider the case $M_0 = +\infty$ and thus $T_{gel} = 0$. Since $M_t = g_0(\ell_t)$ is bounded and continuous for $t \in [\delta, \varepsilon]$ for all $\delta \in (0, \varepsilon)$, we have by (2.10) and (2.3)

$$\begin{split} \int_{\delta}^{\varepsilon} M_t^2 \, \mathrm{d}t &= \int_{\delta}^{\varepsilon} g_0^2(\ell_t) \, \mathrm{d}t = \varepsilon g_0^2(\ell_{\varepsilon}) - \delta g_0^2(\ell_{\delta}) - \int_{\delta}^{\varepsilon} 2t g_0(\ell_t) g_0'(\ell_t) \, \mathrm{d}\ell_t \\ &\leqslant \varepsilon g_0^2(\ell_{\varepsilon}) - \int_{\delta}^{\varepsilon} 2g_0(\ell_t) \, \frac{\mathrm{d}\ell_t}{\ell_t} = \varepsilon g_0(\ell_{\varepsilon}) + 2 \int_{\ell_{\varepsilon}}^{\ell_{\delta}} g_0(y) \, \frac{\mathrm{d}y}{y} \\ &\leqslant \varepsilon g_0(\ell_{\varepsilon}) + \frac{2}{\ell_{\varepsilon}} \Big\langle \mu_0, \frac{m}{1+m} \Big\rangle \leqslant \varepsilon g_0(\ell_{\varepsilon}) + \frac{2}{\ell_{\varepsilon}} \langle \mu_0, m \wedge 1 \rangle. \end{split}$$

Letting $\delta \downarrow 0$, by (2.2) we obtain the desired result. \Box

We now finish the proof of existence of a solution by showing that $(\mu_t)_{t\geq 0}$ indeed solves (2.1). By choosing $x = e^{-y}$, $y \ge 0$, in (2.7), we find an equality between Laplace transforms. Since the Laplace transform is one-to-one, then we obtain (2.1).

Remark 2.17. In the proof of uniqueness, we may only require that $\langle \mu_0, my^m \rangle < +\infty$ for every $y \in [0, 1)$. However, the same kind of computation as in Lemma 2.16 shows that if this the case, but $\langle \mu_0, m \wedge 1 \rangle = +\infty$, then $\int_0^t M_s^2 ds = +\infty$ for all t > 0, in contradiction with Definition 2.1 of a solution.

3. Flory's equation

We will now consider the modified version of Smoluchowski's equation, also known as *Flory's equation*, with a multiplicative kernel.

Definition 3.1. Let $\mu_0 \in \mathcal{M}_c^+$. We say that a family $(\mu_t)_{t \ge 0} \subset \mathcal{M}_c^+$ solves Flory's equation (2.1) if

- for every t > 0, $\int_0^t \langle \mu_s(\mathrm{d}m), m \rangle^2 \, \mathrm{d}s < +\infty$,
- for all $\phi \in C_c(0, +\infty)$ and t > 0

$$\langle \mu_t, \phi \rangle = \langle \mu_0, \phi \rangle + \frac{1}{2} \int_0^t \langle \mu_s(\mathrm{d}m) \, \mu_s(\mathrm{d}m'), mm' \Delta \phi(m, m') \rangle \mathrm{d}s$$
$$- \int_0^t \langle \mu_s, \phi \rangle \langle \mu_0(\mathrm{d}m) - \mu_s(\mathrm{d}m), m \rangle \mathrm{d}s, \tag{3.1}$$

• if $\langle \mu_0, m^2 \rangle < +\infty$, then $t \mapsto \langle \mu_t, m^2 \rangle$ is bounded in a right neighborhood of 0.

In Eq. (3.1), the mass that vanishes in the gel interacts with the other particles. It is a modified Smoluchowski's equation, where a term has been added, representing the interaction of the particles of mass m with the gel, whose mass is

$$\langle \mu_0 - \mu_s, m \rangle$$

i.e. precisely the missing mass of the system. Notice that in this case the equation makes sense only if $\langle \mu_0, m \rangle < +\infty$.

The mass is expected to decrease faster in this case than for (2.1). This is actually true, as we can see in the following result.

Theorem 3.2. Let $\mu_0 \in \mathcal{M}_c^+$ be a non-null measure such that $\langle \mu_0, m \rangle < +\infty$, and set

$$M_0 := \langle \mu_0, m \rangle \in (0, +\infty), \qquad K := \langle \mu_0, m^2 \rangle \in (0, +\infty]$$

Let $T_{gel} := 1/K \in [0, +\infty)$. Then Flory's equation (3.1) has a unique solution $(\mu_t)_{t \ge 0}$ on \mathbb{R}^+ . It has the following properties.

(1) We have $M_t = g_0(l_t)$, where $l_t = 1$ for $t \leq T_{gel}$ and, for $t > T_{gel}$, l_t is uniquely defined by

$$l_t = e^{-t(M_0 - g_0(l_t))}, \quad l_t \in [0, 1).$$

Therefore $t \mapsto M_t$ is continuous on $[0, +\infty)$, constant on $[0, T_{gel}]$, strictly decreasing on $[T_{gel}, +\infty)$ and analytic on $\mathbb{R}^+ \setminus \{T_{gel}\}$.

(2) The function $\phi_t(x) = xe^{t(M_0 - g_0(x))}$ has a right inverse $h_t : [0, 1] \to [0, l_t]$. The generating function g_t of $(\mu_t)_{t \ge 0}$ is given for $t \ge 0$ by

$$g_t(x) = g_0(h_t(x)).$$

(3) Let $m_0 = \inf \operatorname{supp} \mu_0 \ge 0$. Then, when $t \to +\infty$,

$$M_t e^{m_0 t} \rightarrow m_0 \mu_0(\{m_0\})$$

and for every $\epsilon > 0$

 $M_t e^{(m_0+\epsilon)t} \to +\infty.$

(4) The second moment $\langle m^2, c_t \rangle$ is finite on $\mathbb{R}^+ \setminus \{T_{gel}\}$ and infinite at T_{gel} .

Remark 3.3.

- Norris [24, Theorem 2.8] has a proof of global uniqueness of Flory's equation (3.1) for slightly less general initial conditions (μ₀ such that (μ₀, 1 + m) < +∞), but for a much more general model.
- When $m_0 > 0$, it was already observed (Proposition 5.3 in [10]) that the mass decays (at least) exponentially fast (see also [8,25,31]).

Proof of Theorem 3.2. The proof is very similar to (and actually easier than) that of Theorem 2.2.

(1) Arguing as in the proof of Lemma 2.4, we obtain easily that $(M_t)_{t \ge 0}$ is monotone non-increasing and rightcontinuous. As in Lemma 2.5, if $t \mapsto \langle \mu_t, m^2 \rangle$ is bounded on some interval $[0, T_0]$, then $M_t = M_0$ for $t \in [0, T_0]$ and therefore $(\mu_t)_{t \ge 0}$ is a solution of Smoluchowski's equation (2.1) on $[0, T_0]$.

(2) Consider initial concentrations μ_0 as in the statement, a solution $(\mu_t)_{t \ge 0}$ to Flory's equation and $g_t(x)$, $x \in [0, 1]$, generating function of $m \mu_t(dm)$. Then g_t solves the PDE

$$\frac{\partial g_t}{\partial t} = x(g_t - M_0)\frac{\partial g_t}{\partial x}, \quad \forall t > 0, \ x \in [0, 1],$$
(3.2)

the same as the one obtained for Smoluchowski's equation before gelation. It may be solved using the method of characteristics. Indeed, the mapping

$$\phi_t(x) = x e^{t(M_0 - g_0(x))} = x + \int_0^t (M_0 - g_0(x)) \phi_s(x) \,\mathrm{d}s, \tag{3.3}$$

has the following properties

- (d1) $\phi_t(0) = 0, \phi_t(1) = 1.$
- (d2) For all $t \ge 0$, $\phi'_t(x) = e^{t(M_0 g_0(x))}(1 txg'_0(x))$.
- (d3) For $t \leq T_{gel}$, $\phi_t(\cdot)$ is increasing; therefore, $\phi_t(x) \in [0, 1]$ for all $x \in [0, 1]$ and $\phi_t(x) = 1$ if and only if x = 1.
- (d4) For $t > T_{gel}$, $\phi_t(\cdot)$ is increasing on $[0, m_t]$ and decreasing on $[m_t, 1]$, where m_t is the unique $x \in (0, 1)$ such that $\phi'_t(x) = 0$, i.e. such that $txg'_0(x) = 1$.
- (d5) For $t > T_{gel}$, $\phi_t(m_t) > 1$, since $\phi_t(1) = 1$ and $\phi'_t(1) < 0$. Therefore there is a unique $l_t \in (0, m_t)$ such that $\phi_t(l_t) = 1$.
- (d6) For $t > T_{\text{gel}}$, $\phi'_t(l_t) \neq 0$, since $l_t < m_t$ (see Fig. 2).

Setting $l_t := 1$ for $t \leq T_{gel}$, ϕ_t is thus a continuous bijection from $[0, l_t]$ to [0, 1], with continuous inverse function $h_t : [0, 1] \mapsto [0, l_t]$. By using (3.2) and (3.3) and arguing as in parts (i) and (ii) of the proof of Lemma 2.9, we can see that the function $u_t(x) := g_t(\phi_t(x)) - g_0(x)$ satisfies $u_t(x) = u_0(x) = 0$ for all $t \ge 0$ and $x \in [0, l_t]$. Therefore the only solution of the PDE (3.2) is given by

$$g_t(x) = g_0(h_t(x)), \quad t \ge 0, \ x \in [0, 1].$$
 (3.4)

Flory's equation has thus a unique solution on \mathbb{R}^+ , and its generating function is g_t .

(3) We have seen in (d5) above that, for $t > T_{gel}$, there is a unique $l_t \in [0, 1)$ such that $\phi_t(l_t) = 1$. The relation $\phi_t(l_t) = 1$ with $l_t \in [0, 1)$ is equivalent to $l_t = e^{-t(M_0 - g_0(l_t))}$ with $l_t \in [0, 1)$. This relation implies that $t \mapsto l_t$ is analytic for $t > T_{gel}$. A differentiation shows that

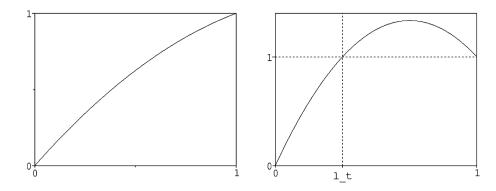


Fig. 2. ϕ_t before and after gelation.

$$\frac{dl_t}{dt} = -\frac{(M_0 - g_0(l_t))l_t}{1 - tg'_0(l_t)l_t} < 0, \quad t > T_{\text{gel}},$$

since $g'_0(l_t)l_t < g'_0(m_t)m_t = 1/t$ and $g_0(l_t) < g_0(1) = M_0$. Let ℓ be the limit of l_t as $t \downarrow T_{gel}$: then we obtain $\ell = e^{-T_{gel}(M_0 - g_0(\ell))}$, i.e. $\phi_{T_{gel}}(\ell) = 1$. By (d3) above, this is equivalent to $\ell = 1$.

(4) Since $M_t = g_t(1) = g_0(h_t(1)) = g_0(l_t)$, the properties of $t \mapsto M_t = g_0(l_t)$ follow from those of $t \mapsto l_t$. Recall now that $\phi_t(l_t) = 1$, that is

$$\log(l_t) = t \left(g_0(l_t) - 1 \right). \tag{3.5}$$

If the limit *l* of l_t as $t \to +\infty$ were nonzero, then passing to the limit in this equality would give $\log(l) = -\infty$. So l = 0 and

$$\log l_t \sim -t. \tag{3.6}$$

• Assume m > 0. Now, obviously $g_0(x) \leq x^m$, so

$$\log(tg_0(l_t)) = \log l_t + \log g_0(l_t) \leq \log t + m \log l_t \to -\infty.$$

Hence $tg_0(l_t) \to 0$ and (3.5) yields $\log l_t + t \to 0$. Hence $l_t^m \sim e^{-mt}$. Finally

$$\lim_{t \to +\infty} M_t e^{mt} = \lim_{t \to +\infty} \frac{g_0(l_t)}{l_t^m} = m\mu_0(\{m\})$$

since by dominated convergence, $g_0(x)x^{-m} \to m\mu_0(\{m\})$ when $x \to 0$. Now, by monotone convergence, if m' > m, then $g_0(x)x^{-m'} \to +\infty$ when x tends to 0, whence

$$\lim_{t \to +\infty} M_t e^{m't} = \lim_{t \to +\infty} \frac{g_0(l_t)}{l_t^{m'}} = +\infty.$$

Assume now m = 0 and let ε > 0. By monotone convergence g₀(x)x^{-ε} → +∞ as x ↓ 0, so using (3.6) we see that g(l_t)e^{-εt} → +∞ as t ↑ +∞, which is the desired result.

(5) Finally, (3.4) gives for x < 1 and $t > T_{gel}$

$$g'_t(x) = g'_0(h_t(x))h'_t(x) = \frac{g'_0(h_t(x))}{\phi'_t(h_t(x))}.$$

When $x \uparrow 1$, $h_t(x) \uparrow l_t < 1$, and $\phi'_t(h_t(x)) \to \phi'_t(l_t) \neq 0$ by (d6) above. So $\langle \mu_t, m^2 \rangle = g'_t(1) < +\infty$. (6) Existence of a solution of (3.1) follows arguing as in Section 2.4. \Box

Corollary 3.4. Let $\mu_0 \in \mathcal{M}_c^+$ such that $\langle \mu_0, m \rangle < +\infty$ and let $(\mu_t^S)_{t \ge 0}$ and $(\mu_t^F)_{t \ge 0}$ be the solutions of (2.1), respectively, (3.1). Then

- $\mu_t^S \equiv \mu_t^F$ for all $t \leq T_{gel} := 1/\langle \mu_0, m^2 \rangle$; $\langle \mu_t^F, m \rangle < \langle \mu_t^S, m \rangle$ for all $t > T_{gel}$.

Proof. For all $t \leq T_{gel}$, $\langle \mu_t^F, m \rangle = \langle \mu_0^F, m \rangle$ and therefore μ_t^F solves (2.1), so that by uniqueness of Smoluchowski's equation we have that $\mu_t^S = \mu_t^F$. For $t > T_{gel}$ we have that $\langle \mu_t^F, m \rangle = g_0(l_t)$ while $\langle \mu_t^S, m \rangle = g_0(\ell_t)$, where l_t and ℓ_t are defined respectively by

$$l_t = e^{-t(M_0 - g_0(l_t))}, \quad l_t \in [0, 1)$$

and

$$\ell_t g_0'(\ell_t) = \frac{1}{t}.$$

In points (d4) and (d5) of the proof of Theorem 3.2, we have shown that $l_t < m_t$ where $tm_t g'_0(m_t) = 1$, so that $m_t = \ell_t < l_t$. Hence $\langle \mu_t^F, m \rangle = g_0(\ell_t) < g_0(l_t) = \langle \mu_t^S, m \rangle$. \Box

As anticipated, the mass decreases faster in Flory's case than for Smoluchowski's equation. In particular, in Flory's case $\langle \mu_t, m^2 \rangle$ becomes finite immediately after gelation, the mass remaining however continuous (we can think that the big particles, which have the biggest influence on this second moment, disappear into the gel). Moreover, if inf supp $\mu_0 > 0$ then the mass decays exponentially fast, which is to be compared with the slow decrease in 1/t in Smoluchowski's equation.

Remark 3.5. The mass in Flory's equation may decrease slower if $\inf \operatorname{supp} \mu_0 = 0$. For instance, if $\mu_0(dm) = e^{-m} dm$, then $M_t \sim t^{-2}$.

4. The model with limited aggregation

We now turn to our main interest, namely Eq. (1.2). We apply the same techniques as above in a slightly more complicated setting. After giving all details in Smoluchowski's case, we will give a shorter proof and focus on the differences with the proof of Theorem 2.2. As above, we can transform the system (1.2) into a non-local PDE problem, which we are able to solve, thus obtaining existence and uniqueness to (1.2). More precisely, we consider the following system.

Definition 4.1. Let $c_0(a, m) \ge 0$, $a \in \mathbb{N}$, $m \in \mathbb{N}^*$. We say that a family $(c_t(a, m))$, $t \ge 0$, $a \in \mathbb{N}$, $m \in \mathbb{N}^*$, is a solution of Smoluchowski's equation (4.1) if

- for every t > 0, ∫₀^t ⟨c_s, a⟩² ds < +∞,
 for all a ∈ N, m ∈ N* and t > 0,

$$c_{t}(a,m) = c_{0}(a,m) + \int_{0}^{t} \frac{1}{2} \sum_{a'=1}^{a+1} \sum_{m'=1}^{m-1} a'(a+2-a')c_{s}(a',m')c_{s}(a+2-a',m-m') ds$$

-
$$\int_{0}^{t} \sum_{a' \ge 1} \sum_{m' \ge 1} aa'c_{s}(a,m)c_{s}(a',m') ds, \qquad (4.1)$$

• if $\langle c_0, a^2 \rangle < +\infty$, then $t \mapsto \langle c_t, a^2 \rangle$ is bounded in a right neighborhood of 0.

Because of the interpretation of a as a variable counting the number of arms a particle possesses, it is more natural to state (4.1) in the discrete setting, as in [3]. In particular, since at each coagulation two arms are removed from the system, a non-integer initial number of arms would lead to an ill-defined dynamics. One could however with no difficulty consider an initial distribution of masses on $(0, +\infty)$.

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It is easy to see that (c_t) is a solution to this equation if and only if the function

$$k_t(x, y) := \sum_{a=1}^{+\infty} \sum_{m=1}^{+\infty} ac_t(a, m) x^{a-1} y^m,$$
(4.2)

defined for $t \ge 0$, $y \in [0, 1]$ and $x \in [0, 1)$, satisfies

$$\begin{cases} k_t(x, y) = k_0(x, y) + \int_0^t \left[\left(k_s(x, y) - xA_s \right) \frac{\partial k_s}{\partial x}(x, y) - A_s k_s(x, y) \right] \mathrm{d}s, \\ A_t := k_t(1, 1) = \langle c_t, a \rangle. \end{cases}$$
(4.3)

We may solve this PDE with the same techniques as above and obtain the following result.

Theorem 4.2. Consider initial concentrations $c_0(a, m) \ge 0$, $a \in \mathbb{N}$, $m \in \mathbb{N}^*$ such that $\langle c_0, 1 \rangle < +\infty$, $A_0 := \langle c_0, a \rangle \in (0, +\infty]$ and with $K := \langle c_0, a(a-1) \rangle \in [0, +\infty]$. Then $K = +\infty$ whenever $A_0 = +\infty$. Let

$$T_{\text{gel}} = \begin{cases} \frac{1}{K - A_0} & \text{if } A_0 < K < +\infty, \\ 0 & \text{if } K = +\infty, \\ +\infty & \text{if } K \leqslant A_0 < +\infty. \end{cases}$$
(4.4)

Then Eq. (4.1) has a unique solution defined on \mathbb{R}^+ . When $T_{gel} < +\infty$, this solution enjoys the following properties.

(1) The number of arms $A_t := \langle c_t, a \rangle$ is continuous, strictly decreasing, and for all t > 0

$$A_t \leqslant \frac{A_0}{1+tA_0} \quad \text{if } A_0 < +\infty, \qquad A_t \leqslant \frac{1}{t} \quad \text{if } A_0 = +\infty.$$

$$(4.5)$$

If we set

$$\alpha_t = \exp\bigg(\int\limits_0^t A_s \,\mathrm{d}s\bigg),$$

then α_t is given by

 $\alpha_t = 1 + A_0 t$ for $t < T_{gel}$

and for $t \ge T_{gel}$

$$\alpha_t = \begin{cases} \Gamma^{-1}(1 + A_0 T_{\text{gel}} + t - T_{\text{gel}}) & \text{if } A_0 < +\infty, \\ \Gamma^{-1}(1 + t) & \text{if } A_0 = +\infty, \end{cases}$$
(4.6)

where

$$\Gamma(x) = 1 + A_0 T_{\text{gel}} + \int_{1+A_0 T_{\text{gel}}}^x \frac{dr}{k_0(H(1/r))}, \quad x \ge 1 + A_0 T_{\text{gel}},$$

and $H : [G(0), G(1)) \mapsto [0, 1)$ is the right inverse of the increasing function

$$G:[0,1) \mapsto \left[G(0), G(1)\right), \quad G(x) := x - \frac{k_0(x,1)}{k'_0(x,1)}, \quad x \in [0,1),$$

$$(4.7)$$

with $G(0) := G(0^+) \leq 0$ *, and*

$$0 < G(1) := G(1^{-}) = \begin{cases} 1 - \frac{A_0}{K} & \text{if } A_0 < +\infty, \\ 1 & \text{if } A_0 = +\infty. \end{cases}$$

(2) Let k_0 be defined as in (4.2), and

$$A_t = \langle c_t, a \rangle, \qquad \alpha_t = \exp\left(\int_0^t A_s \,\mathrm{d}s\right), \qquad \beta_t = \int_0^t \frac{1}{\alpha_s^2} \,\mathrm{d}s. \tag{4.8}$$

Consider

$$\phi_t(x, y) := \alpha_t \left(x - \beta_t k_0(x, y) \right), \quad t \ge 0, \ x, y \in [0, 1].$$

Then

• $\phi_t(\cdot, 1)$ attains its maximum at a point ℓ_t such that $\phi_t(\ell_t, 1) = 1$. For $t \leq T_{gel}$, $\ell_t = 1$, and for $t > T_{gel}$, $0 < \ell_t < 1$ and

$$\frac{\partial \phi_t}{\partial x}(\ell_t, 1) = 0. \tag{4.9}$$

In particular, for $t > T_{gel}$, ℓ_t is given by

$$\ell_t = H\bigg(\frac{1}{\alpha_t}\bigg),\tag{4.10}$$

where *H* is the right inverse of the function *G* defined above.

- For every $y \in [0, 1]$, $\phi_t(\cdot, y)$ has a right inverse $h_t(\cdot, y) : [0, 1] \mapsto [0, 1]$.
- (3) The generating function k_t defined by (4.2) is given by

$$k_t(x, y) = \frac{1}{\alpha_t} k_0 (h_t(x, y), y)$$
(4.11)

for $y \in [0, 1]$, $x \in [0, 1]$. In particular, for t > 0

$$\alpha_t A_t = \alpha_t k_t(1, 1) = k_0(\ell_t, 1), \qquad A_t = \frac{k_0(\ell_t, 1)}{1 + \int_0^t k_0(\ell_s, 1) \, \mathrm{d}s}.$$
(4.12)

(4) The second moment $\langle c_t, a^2 \rangle$ is finite on $[0, T_{gel})$, infinite on $[T_{gel}, +\infty)$.

4.1. Proof

The only major difference with respect to the proof of Theorem 2.2 is the additional variable y in the generating function $k_t(x, y)$. However, the variable y plays the role of a parameter in the PDE (4.3), and this allows to adapt all above techniques.

Proof of Theorem 4.2. The case $K \le A_0 < +\infty$, for which $T_{gel} = +\infty$ has already been treated in [3, Theorem 2], so that we can restrict here to the cases where $T_{gel} < +\infty$. When $T_{gel} > 0$, Theorem 2 in [3] also shows that $\alpha_t = 1 + A_0 t$ on $[0, T_{gel})$ (this however also requires that $\langle a^2, c_t \rangle$ be bounded in a neighborhood of 0: see point (3) of the proof of Lemma 2.9).

(1) First, by setting $u_t(x, y) := \alpha_t k_t(\phi_t(x, y), y) - k_0(x, y)$, we can see, arguing as in points (i)–(ii) of the proof of Lemma 2.9, that for all $y \in (0, 1]$ and t > 0 there exists $\ell_t^0(y) < \ell_t(y) \in (0, 1]$ such that

$$\alpha_t k_t (\phi_t(x, y), y) = k_0(x, y), \quad \forall t \ge 0, \ y \in (0, 1], \ x \in \left[\ell_t^0(y), \ell_t(y)\right]$$
(4.13)

and $\phi_t(\cdot, y) : [\ell_t^0(y), \ell_t(y)] \mapsto [0, 1]$ is a continuous bijection and has a continuous right inverse $h_t(\cdot, y) : [0, 1] \mapsto [\ell_t^0(y), \ell_t(y)]$ (see Fig. 3).

(2) We denote for simplicity

$$k_t(x) := k_t(x, 1), \qquad \phi_t(x) := \phi_t(x, 1), \quad t \ge 0, \ x \in [0, 1].$$

For y = 1, we set $\ell_t(1) = \ell_t$, i.e.

$$1 = \phi_t(\ell_t) = \alpha_t \big(\ell_t - \beta_t k_0(\ell_t) \big), \quad t \ge 0.$$

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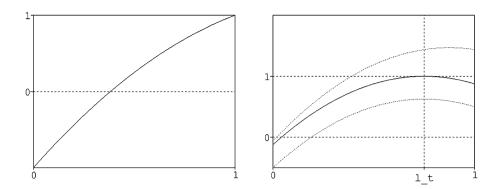


Fig. 3. $\phi_t(\cdot, 1)$ before and after gelation. The dotted lines represent what ϕ_t may look like. The solid one is the actual ϕ_t .

Arguing as in points (iv)–(v) of the proof of Lemma 2.9, we can see that $\ell_t = 1$ for all $t \leq T_{gel}$ and $\ell_t < 1$ for all $t > T_{gel}$. Moreover, $t \mapsto \ell_t$ is continuous and monotone non-increasing. Since ϕ_t is increasing on $[0, \ell_t], \phi'_t(\ell_t) \ge 0$, i.e.

$$\beta_t \leqslant \frac{1}{k'_0(\ell_t)},$$

so that

$$1 = \alpha_t \left(\ell_t - \beta_t k_0(\ell_t) \right) \geqslant \alpha_t G(\ell_t), \tag{4.14}$$

where we set $G(x) := x - \frac{k_0(x)}{k'_0(x)}, x \in [0, 1)$. Notice that

$$G'(x) = 1 - \frac{(k'_0(x))^2 - k_0(x)k''_0(x)}{(k'_0(x))^2} = \frac{k_0(x)k''_0(x)}{(k'_0(x))^2} > 0,$$

since k_0 is strictly convex (there is no gelation whenever $k_0'' \equiv 0$). Moreover $G(0) \leq 0$ and

$$G(1) = 1 - \frac{A_0}{K}$$
 if $A_0 < +\infty$, $G(1) = 1$ if $A_0 = +\infty$

Indeed, $k'_0(1) = K = \langle c_0, a(a-1) \rangle$ and, if $k_0(1) = A_0 = +\infty$, then

$$\lim_{x \uparrow 1} \frac{k_0(x)}{k'_0(x)} = 0$$

since, if $\liminf_{x\uparrow 1} \frac{k_0(x)}{k'_0(x)} > \varepsilon > 0$, then $k_0(1) \leq k_0(1-\delta)e^{\delta/\varepsilon} < +\infty$, for some $\delta > 0$, contradicting $k_0(1) = +\infty$. In any case, *G* has an inverse *H*, and H(1/x) is defined for $x \in [1 + A_0T_{gel}, +\infty)$.

(3) Computing (4.13) at $(x, y) = (\ell_t, 1)$ we obtain

$$k_0(\ell_t) = \alpha_t k_t(1) = \alpha_t A_t = \frac{\mathrm{d}^+ \alpha_t}{\mathrm{d}t}.$$
(4.15)

Let us notice that

$$\phi_t(x) = x + \int_0^t \left(A_s \phi_s(x) - \frac{k_0(x)}{\alpha_s} \right) \mathrm{d}s.$$

Then by (4.15), analogously to (2.19) above,

$$0 = \mathrm{d}\phi_t(\ell_t) = \left(A_t\phi_t(\ell_t) - \frac{k_0(\ell_t)}{\alpha_t}\right)\mathrm{d}t + \phi_t'(\ell_t)\,\mathrm{d}\ell_t = \phi_t'(\ell_t)\,\mathrm{d}\ell_t.$$

In particular, for $d\ell_t$ -a.e. t, $\phi'_t(\ell_t) = 0$, i.e. $\beta_t = 1/k'_0(\ell_t)$, and therefore

$$1 = \alpha_t \left(\ell_t - \beta_t k_0(\ell_t) \right) = \alpha_t G(\ell_t), \quad d\ell_t \text{-a.e. } t.$$

Then, by (4.14), we can write (note that H is well defined on the considered interval)

$$\ell_t \leq H\left(\frac{1}{\alpha_t}\right), \quad \forall t > T_{\text{gel}}, \qquad \ell_t = H\left(\frac{1}{\alpha_t}\right), \quad d\ell_t \text{-a.e. } t$$

Now, by (4.15), setting $\Lambda :]1 + A_0 T_{gel}, +\infty[\mapsto]0, 1[, \Lambda(z) := k_0(H(\frac{1}{z})),$

$$\frac{\mathrm{d}^+\alpha_t}{\mathrm{d}t} \leqslant \Lambda(\alpha_t), \quad \forall t > T_{\text{gel}}, \qquad \frac{\mathrm{d}^+\alpha_t}{\mathrm{d}t} = \Lambda(\alpha_t), \quad \mathrm{d}\ell_t \text{-a.e. } t$$

Since $\alpha_t > 1 + A_0 T_{gel}$ for any $t > T_{gel}$, we obtain that $k_0(\ell_t) \leq \Lambda(\alpha_t) < 1$ for all $t > T_{gel}$. In particular, $d\ell_t$ is not identically equal to 0. Suppose that for some $t > T_{gel}$ we have $\phi'_t(\ell_t) > 0$. We set

$$s := \sup\{r < t: \phi'_r(\ell_r) = 0\} = \max\{r < t: \phi'_r(\ell_r) = 0\}.$$

Then for all $r \in]s, t[$ we must have $\phi'_r(\ell_r) > 0$. Then for all $r \in]s, t[$ we have $\ell_r = \ell_s$. But, by definition of β ,

$$\beta_r > \beta_s = \frac{1}{k'_0(\ell_s)} = \frac{1}{k'_0(\ell_r)}$$

and this is a contradiction. Therefore for all $t > T_{gel}$, we have $\dot{\alpha}_t = \Lambda(\alpha_t)$ for all $t > T_{gel}$ and the only solution of this equation with $\alpha_{T_{gel}} = 1 + A_0 T_{gel}$ is given by (4.6).

(4) In order to prove (4.12), let us note that by the preceding results

$$\frac{d\alpha_t}{dt} = \alpha_t A_t = \alpha_t k_t (1, 1) = k_0(\ell_t, 1),$$

$$A_t = \frac{d}{dt} \log \alpha_t = \frac{d}{dt} \log \left(1 + \int_0^t k_0(\ell_s, 1) \, ds \right) = \frac{k_0(\ell_t, 1)}{1 + \int_0^t k_0(\ell_s, 1) \, ds}.$$

The rest of the proof follows the same line as that of Theorem 2.2. \Box

5. The modified version

Let us finally consider Flory's version of the model with arms. As in the case of Flory's equation (3.1), we can consider only initial concentrations c_0 such that $A_0 = \langle c_0, a \rangle < +\infty$. Then, the equation we are interested in is

$$\frac{\mathrm{d}}{\mathrm{d}t}c_t(a,m) = \frac{1}{2}\sum_{a'=1}^{a+1}\sum_{m'=1}^{m-1}a'(a+2-a')c_t(a',m')c_t(a+2-a',m-m') - \sum_{a'\ge 1}\sum_{m'\ge 1}aa'c_t(a,m)c_t(a',m') - \left(\frac{A_0}{1+tA_0} - \sum_{a',m'\ge 1}a'c_t(a',m')\right)ac_t(a,m).$$
(5.1)

With the same techniques as above, we can prove the following result.

Theorem 5.1. Consider initial concentrations $c_0(a, m) \ge 0$, $a \in \mathbb{N}$, $m \in \mathbb{N}^*$ such that $A_0 := \langle c_0, a \rangle \in (0, +\infty)$ and with $K := \langle c_0, a(a-1) \rangle \in [0, +\infty]$. Let T_{gel} be defined as in (4.4). Then Eq. (5.1) has a unique solution defined on \mathbb{R}^+ . When $T_{gel} < +\infty$, this solution enjoys the following properties.

(1) We have

$$A_t = \frac{1}{1 + tA_0} k_0(l_t)$$
(5.2)

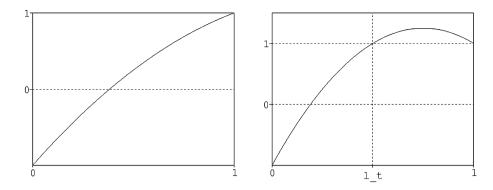


Fig. 4. $\phi_t(\cdot, 1)$ before and after gelation.

where $l_t = 1$ for $t \leq T_{gel}$ and, for $t > T_{gel}$, l_t is uniquely defined by

$$l_t = \frac{t}{1 + tA_0} k_0(l_t), \quad l_t \in [0, 1)$$

Therefore $t \mapsto A_t$ is continuous and strictly decreasing on $[0, +\infty)$ and analytic on $\mathbb{R}^+ \setminus \{T_{gel}\}$.

(2) The function $\phi_t(x, y) = (1 + tA_0)x - tk_0(x, y)$ has, for every $y \in [0, 1]$, a right inverse $h_t(\cdot, y) : [0, 1] \rightarrow [0, l_t]$. The generating function k_t defined in (4.2) is given for $t \ge 0$ by

$$k_t(x, y) = \frac{1}{1 + tA_0} k_0 (h_t(x, y), y).$$
(5.3)

(3) The second moment $\langle a^2, c_t \rangle$ is finite on $\mathbb{R}^+ \setminus \{T_{gel}\}$ and infinite at T_{gel} .

Proof. The proof follows the same line of reasoning as the one of Theorem 3.2. First, for every $y \in [0, 1]$, $\phi_t(\cdot, y)$, as defined in the statement, has the following properties:

- (i) $\phi_t(0, y) \leq 0, \phi_t(1, y) \geq \phi_t(1, 1) = 1;$
- (ii) For $t \leq T_{gel}$, $\phi_t(\cdot, y)$ is increasing, and in particular, there are unique $0 \leq l_t^0(y) < l_t(y) \leq 1$ such that $\phi_t(l_t^0(y), y) = 0$ and $\phi_t(l_t(y), y) = 1$;
- (iii) For $t > T_{gel}$, $\phi_t(\cdot, y)$ is increasing then decreasing for, and in particular, there are unique $0 \le l_t^0(y) < l_t(y) < 1$ such that $\phi_t(l_t^0(y), y) = 0$ and $\phi_t(l_t(y), y) = 1$ (see Fig. 4).

In any case, it is easy to check that for $x \in [l_t^0(y), l_t(y)]$,

$$\exp\left(\int_{0}^{t} A_{s} \,\mathrm{d}s\right) k_{t}\left(\phi_{t}(x, y), y\right) = k_{0}(x, y)$$

where A_t is defined by (5.2). Then, the properties above show that $\phi_t(\cdot, y)$ has a right inverse h_t defined on [0, 1], and compounding by h_t in the previous equation shows that (5.3) holds. The other properties then follow easily. \Box

6. Limiting concentrations

We compute here some explicit formulas for the concentrations and their limit for the two models above. In the standard Smoluchowski and Flory cases, particles keep coagulating, and they all eventually disappear into the gel: $c_t(m) \rightarrow 0$ for every $m \ge 1$. When the aggregations are limited, there may remain some particles in the system, since whenever a particle with no arms is created, it becomes inert, and so it will remain in the medium forever. In the following, we consider monodisperse initial conditions, i.e. $c_0(a, m) = \mu(a) \mathbb{1}_{\{m=1\}}$ for a measure μ on \mathbb{N} . We also denote

$$v(m) = (m+1)\mu(m+1).$$

In [3], it is assumed that ν is a probability measure, what we do not require. The results of [3] can hence be recovered by taking $A_0 = 1$ below. Now, note the two following facts.

• Eqs. (4.5) and (5.2) readily show that

$$c_{\infty}(a,m) := \lim_{t \to +\infty} c_t(a,m) = 0, \quad a \ge 1,$$
(6.1)

that is, only particles with no arms remain in the medium (else, a coagulation "should" occur).

• There is an arbitrary concentration of particles with no arms at time 0, and they are the only particles with no arms and mass 1 which will still be in the medium in the final state. Hence, the limit concentrations $c_{\infty}(0, 1) = c_0(0, 1)$ have no physical meaning. We will thus only consider $c_{\infty}(0, m)$ for $m \ge 2$.

Note now that if at time 0, each particle has zero or more than two arms, then obviously, this property still holds for any positive time. Rigorously, this is easy to check with the representation formula (4.11) or (5.3). Then, because of (6.1),

$$c_{\infty}(m) = 0$$

for each $m \ge 2$. We thus rule out this trivial case by assuming that

 $\nu(0) > 0.$ (6.2)

This is actually a technical assumption which is needed to apply Lagrange's inversion formula in the proof of the following corollaries. We will relate our results to a population model known as the Galton–Watson process. For some basics on this topic, see e.g. the classic book [2]. The formula providing the total progeny of these processes was first obtained by Dwass in [7].

6.1. Modified model

Corollary 6.1. Let $c_t(a, m)$ be the solution to Flory's equation with arms (5.1) and with initial conditions $c_0(a, m) = \mu(a)\mathbb{1}_{\{m=1\}}$ with $\mu(1) > 0$.

• For all $t \ge 0$, $m \ge 2$, $a \ge 0$,

$$c_t(a,m) = \frac{(a+m-2)!}{a!m!} \frac{t^{m-1}}{(1+tA_0)^{a+m-1}} v^{*m}(a+m-2).$$

• In particular, there are limiting concentrations $c_{\infty}(a, m) = c_{\infty}(m)\mathbb{1}_{\{a=0\}}$ with

$$c_{\infty}(m) = \frac{1}{m(m-1)} \nu^{*m}(m-2).$$
(6.3)

Proof. With the notation of Theorem 5.1, we have

$$(1+tA_0)h_t(x, y) - tyk_0(h_t(x, y)) = x, \qquad k_t(x, y) = \frac{1}{1+tA_0}yk_0(h_t(x, y)).$$

Up to some obvious changes (just replace 1 + t by $1 + tA_0$), these are precisely the equations solved in Section 3.2 of [3] under the assumption (6.2). Theorem 2 and Corollary 2 therein hence give the desired result (with only 1 + t replaced by $1 + tA_0$). \Box

If $A_0 = 1$, which we may always assume up to a time-change, we observe as in [3] that $2(m-1)c_{\infty}(0,m)$ is the probability for a Galton–Watson process with reproduction law ν , started from two ancestors, to have total progeny m. This Galton–Watson process is (sub)critical when $K := \sum_{a \ge 1} a(a-1)\mu(a) \le 1$, that is, by Theorem 5.1, when there is no gelation, and supercritical when K > 1. Denote by p_{ν} its extinction probability, i.e. the smallest root of $k_0(x) = x$, so $p_{\nu} = 1$ when $K \le 1$ and $p_{\nu} < 1$ when K > 1. Let us compute the mass at infinity, as in [3], by writing

$$\begin{split} M_{\infty} &:= \sum_{m \ge 1} m c_{\infty}(m) = c_{\infty}(1) + \sum_{m \ge 2} \frac{1}{m-1} \nu^{*m}(m-2) \\ &= c_{\infty}(1) + \sum_{a \ge 0} \nu(a) \sum_{m \ge a+2} \frac{1}{m-1} \nu^{*m-1}(m-2-a) \\ &= c_{\infty}(1) + \sum_{a \ge 0} \nu(a) \sum_{n \ge a+1} \frac{1}{n} \nu^{*n}(n-1-a). \end{split}$$

Now, the Lagrange inversion formula [30] shows that

$$\frac{a+1}{n}\nu^{*n}(n-1-a)$$

is precisely the coefficient of x^n in the analytic expansion of $\phi(x)$ around 0, where ϕ is the unique solution to $\phi(x) = xk(\phi(x))$. Hence

$$\sum_{n \ge a+1} \frac{1}{n} v^{*n} (n-1-a) = p_{\nu},$$

where p_{ν} is defined above. Note also that $c_{\infty}(1) = \mu(0)$, so finally

$$M_{\infty} = c_{\infty}(1) + \sum_{a \ge 0} \nu(a) \frac{1}{a+1} p_{\nu}^{a+1} = \sum_{a \ge 0} \mu(a) p_{\nu}^{a}.$$
(6.4)

The mass at time 0 is $M_0 = \sum \mu(a)$, so when there is no gelation, $p_v = 1$ and no mass is lost in the gel. When there is gelation, $p_v < 1$ and the mass $M_0 - M_\infty > 0$ is lost in the gel. By Dwass' formula [7], M_∞ is also the probability that a Galton–Watson process, with reproduction law μ for the ancestor and ν for the others, has a finite progeny.

6.2. Non-modified model

Corollary 6.2. Let $c_t(a, m)$ be the solution to Smoluchowski's equation with arms (4.1) and with initial conditions $c_0(a, m) = \mu(a) \mathbb{1}_{\{m=1\}}$ with $\mu(1) > 0$.

• For all $t \ge 0$, $m \ge 2$, $a \ge 0$,

$$c_t(a,m) = \frac{(a+m-2)!}{a!m!} \frac{\beta_t^{m-1}}{\alpha_t^a} v^{*m}(a+m-2)$$

where α_t and β_t are defined in Theorem 4.2.

• In particular, there are limiting concentrations $c_{\infty}(a,m) = c_{\infty}(m)\mathbb{1}_{\{a=0\}}$ with

$$c_{\infty}(m) = \frac{1}{m(m-1)} \beta_{\infty}^{m-1} \nu^{*m}(m-2)$$
(6.5)

where β_{∞} is defined by

$$\beta_{\infty} = \frac{1}{k_0'(c)} = \frac{c}{k_0(c)}$$

and c is the unique solution to $k'_0(c) = k_0(c)/c$. Moreover, $\beta_{\infty} = 1$ when there is no gelation, and $\beta_{\infty} > 1$ otherwise.

Proof. As for Corollary 6.1, the proof of the formula for $c_t(a, m)$ is the same as in [3, Section 3.2], just replacing $1 + tA_0$ by α_t and t by $\alpha_t\beta_t$. So we just have to find the limit of β_t . First (4.6) shows that $\alpha_t \to +\infty$, hence, by (4.10), $\ell_t \to \ell_\infty = H(0)$. Now, (4.9) gives $\beta_t = 1/k'_0(\ell_t)$, so β_t tends to

$$\beta_{\infty} = \frac{1}{k_0'(H(0))}$$

where by definition c := H(0) is the unique solution to $k'_0(c) = k_0(c)/c$. Finally, when there is gelation, $\alpha_t < 1 + t$ after gelation because of (4.6), so by (4.8), $\beta_{\infty} > 1$. \Box

By a similar computation as above, we may also compute the mass at infinity in this case and get

$$M_{\infty} = \sum_{a \ge 0} \mu(a) c^a$$

where c is defined in the corollary. Note that c is the slope of the straight line passing by 0 and tangent to the graph of k, so $c > p_{\nu}$. In particular, less mass is lost than in Flory's case.

A final remark is that despite the striking resemblance between formulas (6.5) and (6.3), the meaning of the factor β_{∞} is unclear. A probabilistic interpretation using the configuration model may explain its appearance.

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