

## The post-gelation behaviour of the coagulation equation with product kernel

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It is well known that solutions of the coagulation equation do not conserve mass if the coagulation kernel grows too rapidly. The phenomenon whereby conservation of mass breaks down in finite time is known as gelation and is physically interpreted as being caused by the appearance of an infinite “gel” or “superparticle.” In this paper we discuss the post-gelation behaviour of the coagulation equation with product kernel.

### 1 Formulation

The general coagulation equation may be written as

$$(1.1) \quad \begin{aligned} \frac{\partial c}{\partial t}(\lambda, t) &= \frac{1}{2} \int_0^\lambda K(\lambda - \mu, \mu) c(\lambda - \mu, t) c(\mu, t) d\mu - c(\lambda, t) \int_0^\infty K(\lambda, \mu) c(\mu, t) d\mu, \\ c(\lambda, 0) &= c_0(\lambda). \end{aligned}$$

Equation (1.1) represents the evolution of particles  $c(\lambda, t)$  of size  $\lambda \geq 0$  at time  $t \geq 0$  undergoing a change in size governed by reaction kernel  $K$ . A physical interpretation of the terms in (1.1) can be found in Melzak [?].

We consider the coagulation equation with the separable bilinear kernel

$$K(\lambda, \mu) = \theta(\lambda)\theta(\mu),$$

where  $\theta(\lambda) = \alpha + \beta\lambda$ ,  $\alpha, \beta \geq 0$ . This kernel contains both the constant kernel and product kernel as special cases. For this kernel it is well known that gelation occurs in finite time if and only if  $\beta > 0$ . We examine the behaviour in the post-gelation regime.

The approach we employ is to transform Eq. (1.1) into a first order quasilinear PDE using Laplace transforms. Let

$$(1.2) \quad u(x, t) := \int_0^\infty e^{-\lambda x} \theta(\lambda) c(\lambda, t) d\lambda;$$

$$(1.3) \quad N(t) := \int_0^\infty \theta(\lambda) c(\lambda, t) d\lambda;$$

$$(1.4) \quad h(x) := \int_0^\infty e^{-\lambda x} \theta(\lambda) c_0(\lambda) d\lambda.$$

Multiply Eq. (1.1) by  $e^{-\lambda x}$  and integrate to obtain the following first-order PDE for the transform variable  $u$ :

$$(1.5) \quad \frac{\partial u}{\partial t} + \beta(u - N(t)) \frac{\partial u}{\partial x} = \frac{\alpha}{2} u^2 - \alpha N(t) u, \quad x, t > 0,$$

$$(1.6) \quad u(x, 0) = h(x), \quad x \geq 0,$$

$$(1.7) \quad u(0, t) = N(t), \quad t \geq 0,$$

where (1.7), which comes from (1.2) and (1.3), is in effect a compatibility condition for  $u$  along  $x = 0$ . This initial value problem for  $u$  is unusual in that the function  $N(t)$  in (1.5) and (1.7) is itself unknown and must be determined as part of the solution.

In principle one now proceeds to solve the PDE (using the method of characteristics or otherwise), then take the inverse Laplace transform to get the solution to the original coagulation equation. The problem, however, is that it is almost impossible to get an explicit solution to the PDE, let alone being able to compute its inverse Laplace transform. The only case for which an explicit solution has to date been found is for the pure product kernel ( $\alpha = 0$ ) with monodisperse initial conditions (see Ernst, et al. [?]).

While an explicit solution to the PDE is difficult to obtain, we show in [?] that analysis of the post-shock regime leads to a formula for the total mass  $M(t)$  that depends on the initial particle concentration and a solution of an initial value problem. If we let  $T_0$  denote the gelation time, then the mass is given by

$$(1.8) \quad M(t) = M_0 + \frac{1}{\beta} \int_0^{\xi_0(t)} h'(\zeta) e^{-\frac{\alpha}{\beta}\zeta} d\zeta, \quad \forall t \geq 0,$$

where  $\xi_0(t) \equiv 0$  for  $t \in [0, T_0)$  and, for  $t \in [T_0, \infty)$ , satisfies

$$(1.9) \quad \xi_0' = \frac{\beta^2 h'^2(\xi_0)}{\beta h''(\xi_0) - \frac{\alpha}{2} h'(\xi_0)} e^{-\alpha \xi_0 / \beta}, \quad \xi_0(T_0) = 0.$$

When  $\alpha = 0$  and  $\beta = 1$ , which corresponds to the pure product kernel, Eq. (1.9) reduces to

$$\xi_0' = \frac{h'^2(\xi_0)}{h''(\xi_0)}, \quad \xi_0(T_0) = 0,$$

from which we recover the formulas obtained by Ernst, et al. [?], namely

$$(1.10) \quad h'(\xi_0(t)) = -\frac{1}{t}, \quad M(t) = h(\xi_0(t)).$$

## 2 Examples

We give several examples where the mass can be computed explicitly.

*Example 1.*

For initial particle concentration  $c_0(\lambda) = \lambda^p \delta(\lambda - q)$ , where  $p \geq 0$  and  $q > 0$  are constant, we get

$$h(x) = (\alpha + \beta q) q^p e^{-qx},$$

which leads to a gelation time of  $T_0 = [\beta(\alpha + \beta q) q^{p+1}]^{-1}$ , an initial mass of  $M_0 = q^{p+1}$  and

$$M(t) = \begin{cases} M_0, & t \in [0, T_0), \\ \frac{(\alpha + 2\beta q) M_0}{2(\alpha + \beta q) \frac{t}{T_0} - \alpha}, & t \in [T_0, \infty). \end{cases} \quad \square$$

The remainder of the examples are for the pure product kernel  $K(\lambda, \mu) = \lambda\mu$ . For these cases  $\xi_0$  and the mass  $M$  are given by Eqs. (1.10).

*Example 2.*

For initial particle concentration  $c_0(\lambda) = \lambda^p e^{-q\lambda}$ , where  $p > -1$  and  $q > 0$  are constant, we get

$$h(x) = \frac{\Gamma(p+2)}{(q+x)^{p+2}},$$

which leads to

$$(2.1) \quad M(t) = \begin{cases} M_0, & t \in [0, T_0), \\ M_0 \left(\frac{T_0}{t}\right)^{\frac{p+2}{p+3}}, & t \in [T_0, \infty), \end{cases}$$

where

$$T_0 = \frac{q^{p+3}}{\Gamma(p+3)}, \quad M_0 = \frac{\Gamma(p+2)}{q^{p+2}}. \quad \square$$

For both of the previous examples, the mass  $M$  has a discontinuity in the derivative at the gelation point  $t = T_0$ . It is possible to construct examples for which the derivative of  $M$  is continuous at the gelation point. This is done by choosing an initial particle concentration  $c_0$  that has its first two moments finite, but its third moment infinite. One such example follows (another can be found in [?]).

*Example 3.*

For initial particle concentration

$$c_0(\lambda) = \frac{e^{-\frac{1}{4\lambda}}}{2\sqrt{\pi\lambda^{\frac{7}{2}}}},$$

we get  $h(x) = 2(\sqrt{x} + 1)e^{-\sqrt{x}}$  and  $T_0 = 1$ , and the mass given by

$$(2.2) \quad M(t) = \begin{cases} 2, & t \in [0, 1), \\ \frac{2(1 + \ln t)}{t}, & t \in [1, \infty). \end{cases} \quad \square$$

## REFERENCES

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