

The impact of random fluctuations on the gelation process

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Abstract

We investigate the Smoluchowski equation for the coagulation process of a system of aerosol particles. The objective is the influence of random perturbations in the presence of a source and a sink. To this aim, a Monte Carlo process is constructed and it is shown that fluctuations have a destabilizing effect: Particle systems are forced to gelate i.e. to form "macroparticles" of infinite mass.

Key words: Smoluchowski equation, gelation, random perturbations.

1 Introduction

1.1 Moment solutions of the Smoluchowski equation

An *aerosol system* is an ensemble of particles suspended in a fluid (gas or liquid). The interaction dynamics of aerosol particles is governed by *coagulation* and *fragmentation*. Here, coagulation describes the process in which two particles with masses m_1 and m_2 cluster and build one particle with mass $m_1 + m_2$. Fragmentation means the opposite dynamics: one particle with some mass m may fragment into two particles with masses c and $m - c$. This process is not considered in this paper. *Gelation* is the effect that particles cluster within a finite time to *macroparticles* of infinite mass. The investigation of gelation phenomena plays an important role in a number of applications, e.g. for the modelling of soot formation in engines, or the development of pollution substances in the air.

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The classical instrument to describe the evolution of aerosol systems is the *Smoluchowski equation* [4]. In its discrete, space independent form it governs the evolution of a state vector $\mathbf{f}(t) = (f_i(t))_{i=1}^{\infty}$ which contains the number densities f_i of particles with mass $i \in \mathbb{N}$ at time t . The equation reads

$$\partial_t \mathbf{f} = S[\mathbf{f}, \mathbf{f}], \quad (1.1)$$

with the Smoluchowski coagulation operator defined by

$$S[\mathbf{f}, \mathbf{f}]_i = \frac{1}{2} \cdot \sum_{j=1}^{i-1} K(j, i-j) f_j f_{i-j} - f_i \cdot \sum_{j=1}^{\infty} K(i, j) f_j \quad . \quad (1.2)$$

In general, the kernel $K(.,.)$ is nonnegative and symmetric (cf. [1]). In this paper we restrict for the sake of simplicity to multiplicative kernels of the form

$$K(i, j) = i^\gamma \cdot j^\gamma \quad (1.3)$$

with some $\gamma \in (1/2, 1]$. As is well known from theory, such interaction kernels will lead to gelation. Denote the α -th moment ($\alpha \geq 0$) as $m_\alpha = \sum i^\alpha f_i$. As long as all series in (1.2) are convergent, the zeroth moment m_0 (number of particles) is strictly decreasing. The first moment m_1 (total mass) is a conserved quantity. This is no longer valid after the first time of gelation, since then mass leaves the state space at $i = \infty$. The second moment $m_2 = \sum i^2 \cdot f_i$ diverges not later than at gelation time. In this paper we denote – not in complete agreement with literature – as the *gelation time* (or ”explosion time”) the time of divergence of the second moment. (In practice it turns out that both times either agree or lie close together.)

It is an easy matter to establish the following evolution (in-) equalities for the lowest moments.

$$\partial_t m_0 < 0, \quad (1.4)$$

$$\partial_t m_1 = 0, \quad (1.5)$$

$$\partial_t m_2 = m_{1+\gamma}^2 \leq m_2^2 \quad (1.6)$$

as long as $m_2 < \infty$. A particularly simple case occurs if $\gamma = 1$. Then equation (1.6) turns into

$$\partial_t m_2 = m_2^2 \quad (1.7)$$

indicating a finite gelation time.

1.2 Fluctuations

Fluctuations in the gelation process have (at least) two aspects, a *numerical* and a *physical* one. First, a convenient method for the modelling of coagulation systems are Monte Carlo schemes, like the *Markus-Lushnikov process* and variants (for a review, see [1]), and the process proposed in [2] which is now called the *mass flow process*. Random fluctuations in these processes are inevitable and might perturb the solutions one wants to obtain. Second, fluctuations are also a physical phenomenon, since physical particle systems are finite systems. In this respect, one might try to find out the effect of random perturbations.

The objective of the paper is to investigate the role of fluctuations in the gelation process – in the space homogeneous and the space dependent case (in a 1D interval). In the *space homogeneous* case in the presence of a sink, it will turn out that fluctuations divide the realizations of the Monte Carlo process into diverging and decaying trajectories. If a source is introduced, fluctuations force all trajectories to diverge. In the *space dependent* case, we model coagulation (as usual) as a local phenomenon and introduce diffusion as spatial dynamics with complete absorption at the bounds of the finite interval. If a source (with strength s) in the middle of the interval is introduced, the *deterministic* model exhibits a *fold bifurcation*: For s smaller than a certain threshold s_0 , there exist two stationary solutions of the problem, one of them stable, the other unstable. For $s > s_0$, there exists no stationary solution, and all solutions of the time dependent problem diverge. The *stochastic* model, obtained by an appropriate Monte Carlo system, reveal the stable state as a *metastable* one: Trajectories are first attracted by it but finally (after a long random time) are destabilized and diverge.

The scope of the paper is as follows. First (Section 5) we introduce the mass flow process and derive an appropriately modified process for the second moment equation, represented as an N -particle system. Then (Section 3) we investigate a homogeneous Smoluchowski equation with sink and source and reveal its bifurcation structure. The behavior of the corresponding Monte Carlo scheme is analyzed: without source, the trajectories are separated into diverging ones and ones decaying to 0. In the presence of a source, all trajectories diverge. After this (Section 4) we turn to the space dependent case, including a localized source, diffusion and absorbing boundaries (serving as a sink). Again the bifurcation structure is analyzed. Numerical experiments exhibit one

of the two stationary states as stable, the other one as unstable. In the Monte Carlo simulations, the former stable state turns out to be metastable.

2 Stochastic algorithms

For sake of simplicity we choose the coefficient $\alpha = 1$ in the Smoluchowski equation in all what follows.

2.1 The mass-flow algorithm

A very useful numerical tool for the simulation of the Smoluchowski equation is the so-called *mass-flow* algorithm which has been proposed in [2] and theoretically investigated in [3]. It is a Monte Carlo scheme for the sequence $\mathbf{g} = (g_i)_{i=1}^{\infty} := (i \cdot f_i)_{i=1}^{\infty}$. The evolution equation for \mathbf{g} reads (see [2])

$$\partial_t \mathbf{g} = \tilde{S}[\mathbf{g}, \mathbf{g}], \quad (2.1)$$

with

$$\tilde{S}[\mathbf{g}, \mathbf{g}]_i = \sum_{j=1}^{i-1} j g_j g_{i-j} - i g_i \cdot \sum_{j=1}^{\infty} g_j \quad (2.2)$$

resp. in its Euler discretized formulation

$$\mathbf{g}(t + \Delta t) = \mathbf{g}(t) + \Delta t \cdot \tilde{S}[\mathbf{g}(t), \mathbf{g}(t)] \quad . \quad (2.3)$$

Since $\sum g_i$ is a conserved quantity (up to gelation time), we may assume $\sum g_i = 1$.

In the mass flow scheme, \mathbf{g} is represented (in a sense described below) by an N -particle ensemble $\mathbf{c} = (c_i)_{i=1}^N \in \mathbb{N}^N$, where the label c_i describes the position of the i -th particle in state space $\mathbb{N} = \{1, 2, 3, \dots\}$. Define a sequence Δt_k of time steps, $t_k := \sum_{i=1}^k \Delta t_i$, and identify the number k with t_k (i.e. $\mathbf{c}(k)$ is understood as $\mathbf{c}(t_k)$). The time evolution is very simple. The following pseudo-code describes the transition from one time step to the next.

2.1 Mass flow algorithm: Given the random vector $\mathbf{c}(k) =: (c_i)_{i=1}^N$, the vector $\mathbf{c}(k+1) =: (c'_i)_{i=1}^N$ is determined by the following sequence.

- (1) FOR $i = 1$ TO N DO
- (2) choose random variables $j \in \{1, \dots, N\}$ and $\nu \in [0, 1]$
- (3) IF $\nu \leq \Delta t_k \cdot c_i$, THEN $c'_i := c_i + c_j$ ELSE $c'_i := c_i$

Given a vector $\mathbf{c} \in \mathbb{N}^N$, define the vector $\mathbf{n}[\mathbf{c}] = \mathbf{n} = (n_i)_{i=1}^\infty \in \mathbb{R}^{\mathbb{N}}$ by

$$n_j := \frac{1}{N} \cdot \#\{i \in \{1, \dots, N\} | c_i = j\} \quad . \quad (2.4)$$

As was shown in [2], in the limit $N \rightarrow \infty$, $\mathbf{n}(k)$ converges (componentwise) to the solution $\mathbf{g}(k)$ of the Euler-discretized equation (2.3), if the initial condition ($k = 0$) does.

2.2 An MC algorithm for the second-moment equation

2.2.1 The second moments of the mass flow process

Since $\mathbf{c}(k)$ is an approximation of the solution of the discretized equation (2.3), the sum

$$\bar{c}(k) := \frac{1}{N} \cdot \sum_{i=1}^N c_i(k) = \sum_{j=1}^{\infty} j \cdot n_j(k) \quad (2.5)$$

should be an approximation of the second moment $m_2(k) = \sum j^2 f_j(k) = \sum j g_j(k)$. Thus, in the limit $N \rightarrow \infty$ it should be a solution of the Euler-discretized moment equation

$$a(k+1) = a(k) + \Delta t_k \cdot a(k)^2 \quad . \quad (2.6)$$

Indeed, this can be proven. The transition from $\bar{c}(k)$ to $\bar{c}(k+1)$ consists of a sum $\sum_{i=1}^N \Delta c_i$ of increments; here, $\Delta c_i = c_{\pi(i)}/N$ with probability $\Delta t_k \cdot c_i$, and $\Delta c_i = 0$ else. Elementary calculations show

2.2 Lemma: (a) Expectations:

$$\mathbf{E}(\bar{c}(k+1) | \bar{c}(k)) = \bar{c}(k) + \Delta t_k \cdot (\bar{c}(k))^2 \quad . \quad (2.7)$$

(b) Variances:

$$\mathbf{E}((\bar{c}(k+1))^2 | \bar{c}(k)) = (\bar{c}(k))^2 + 2\Delta t_k \cdot (\bar{c}(k))^3 + (\Delta t_k)^2 \cdot \mathbf{E} \left(\sum_{i=1}^N c_i \cdot \frac{c_{\pi_i}}{N} \right)^2 \quad (2.8)$$

If we define $a^{(k)} := \mathbf{E}\bar{c}(k)$, then simple arguments lead to

2.3 Proposition: The evolution of $a^{(k)}$ is given by

$$a^{(k+1)} = a^{(k)} + \Delta t_k \cdot ((a^{(k)})^2 + \mathbf{Var}(a^{(k)})) \geq a^{(k)} + \Delta t_k \cdot (a^{(k)})^2 \quad . \quad (2.9)$$

Thus $a^{(k)}$ is a supersolution converging to the discretized equation for $N \rightarrow \infty$, since $\mathbf{Var}(a^{(k)}) \rightarrow_{N \rightarrow \infty} 0$.

2.2.2 Reduced model processes

For the sake of numerical efficiency it is extremely useful to simplify the process by replacing the increments and the transition probabilities by mean values. As a result, the increment is a sum of i.i.d. random variables:

$$\bar{c}(k+1) = \bar{c}(k) + \sum_{i=1}^N \Delta c_i \quad (2.10)$$

where

$$\Delta c_i = \begin{cases} \bar{c}(k)/N & \text{with probability } \Delta t_k \cdot \bar{c}(k) \\ 0 & \text{else} \end{cases} \quad (2.11)$$

We refer to this as to a *reduced process*, since it operates on a σ -algebra smaller than that of the original process. In analogy to Lemma 2.2 we find

2.4 Lemma: (a) Expectations:

$$\mathbf{E}(\bar{c}(k+1)|\bar{c}(k)) = \bar{c}(k) + \Delta t_k \cdot (\bar{c}(k))^2 \quad . \quad (2.12)$$

(b) Variances:

$$\begin{aligned} \mathbf{E}((\bar{c}(k+1))^2|\bar{c}(k)) &= (\bar{c}(k))^2 + 2\Delta t_k \cdot \left(1 + \frac{1}{2N}\right) (\bar{c}(k))^3 \\ &\quad + (\Delta t_k)^2 \cdot \left(1 - \frac{1}{N}\right) (\bar{c}(k))^4 \end{aligned} \quad (2.13)$$

This shows that this process exhibits the same asymptotic behavior as that of section 2.2.1 for large N and small Δt .

Since $\Delta t_k \cdot \bar{c}(k)$ has to be bounded by 1, Δt_k has to be adapted to the state $\bar{c}(k)$. To overcome this, we arrive at the final process used in the following by changing (2.11) into

$$\Delta c_i = \begin{cases} \bar{c}(k) & \text{with probability } \Delta t_k \cdot \bar{c}(k)/N \\ 0 & \text{else} \end{cases} \quad (2.14)$$

Of course, this modification increases the variance of the process; however, for bounded N it should reproduce the qualitative behavior of the original reduced process.

3 Coagulation with sink and source

3.1 The model equation

As a preparation for the full problem in Section 4, we consider a space-homogeneous Smoluchowski equation with time-independent sink and source. The system under study reads

$$\partial_t f_i = S[\mathbf{f}, \mathbf{f}]_i - \lambda f_i + s_i \quad , \quad (3.1)$$

where $S[\mathbf{f}, \mathbf{f}]$ is defined by (1.2), λ and s_i are nonnegative, and

$$s := \sum_{i=1}^{\infty} i^2 s_i < \infty \quad . \quad (3.2)$$

The equation for the second moment $m_2 = \sum i^2 f_i$ reads

$$\partial_t m_2 = m_2^2 - \lambda m_2 + s \quad . \quad (3.3)$$

Whether m_2 diverges in finite time, depends on the initial condition $m_2(0)$ and on λ and s . With methods from standard ODE theory we find the exact solution.

3.1 Theorem: (a) Suppose $s < \lambda^2/4$. If $m_2(0) = \lambda/2 + \mu$ with $\mu = \sqrt{\lambda^2/4 - s}$, then $m_2(\cdot)$ is constant. Otherwise define $z_0 := (m_2(0) - \lambda/2 - \mu)^{-1}$. Then

$$m_2(t) = \frac{\lambda}{2} + \mu + \frac{\mu}{-1 + (\mu z_0 + 1) \cdot \exp(-\mu t)} \quad . \quad (3.4)$$

The solution converges to the steady state $\lambda/2 - \mu$ if $z_0 < 0$ and diverges in finite time if $z_0 > 0$.

(b) If $s > \lambda^2/4$, then

$$m_2(t) = \lambda/2 + \sigma \cdot \tan((\sigma(t + c)) \tag{3.5}$$

with $\sigma = \sqrt{s - \lambda^2/4}$ and $c = [\arctan((m_2(0) - \lambda/2)/\sigma)]/\sigma$. The solution explodes at some time $t_\infty \leq \pi/(2\sigma)$.

The stationary solutions of equation (3.3) exhibit a *fold bifurcation* in the sense described below. This is interesting since precisely the same structure will be found in the space dependent model problem of Section 4.

3.2 Corollary: For $s > \lambda^2/4$ there exists no steady solution to (3.3). For $s = \lambda^2/4$, the only steady solution is $m_2 = \lambda/2$. For $s < \lambda^2/4$, there are the two steady solutions $\lambda/2 \pm \sqrt{\lambda^2/4 - s}$, the lower of which is stable, the other unstable.

3.2 A Monte Carlo model process

Our main concern at this place is the behaviour of Monte Carlo solutions in the presence of sinks and sources. In order to understand their behaviour it is sufficient to establish a simplified model process.

Let A_n (time step t_n), $n \in \mathbb{N}$, be a stochastic process with state space \mathbb{N} . Given a weight $1/ng$ (with $ng \in \mathbb{N}$ sufficiently large), $a_n := A_n/ng$ should represent a stochastic solution of (3.3). We interpret A_n as an ensemble of A_n particles, each of which increases with an amount of A_n with probability $\Delta t/ng$ and decreases by 1 with probability $\lambda\Delta t$. The corresponding computer program section reads as follows.

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g := 0
FOR k:=1 TO A_n DO
  p := random      {random number in (0, 1)}
  IF p < Δt/ng THEN g := g + A_n
  ELSE IF p > 1 - λΔt THEN g := g - 1
A_{n+1} := A_n + g
a_{n+1} := A_{n+1}/ng

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Following the usual arguments, it is easy to prove that $\mathbf{E}(A_n)$ is a solution of the discretized version of (3.3) with source $s = 0$. This is an easy consequence of

3.3 Proposition: For $n = 1, 2, 3, \dots$,

$$\mathbf{E}(a_{n+1}|a_n = a) = a + \Delta t \cdot (a^2 - a) \quad . \quad (3.6)$$

For $n \rightarrow \infty$, realizations A_n might converge to 0, diverge to ∞ or move in a bounded domain. The following theorem proves that 0 and ∞ attract almost all of the trajectories.

3.4 Theorem: Almost surely, $\lim_{n \rightarrow \infty} A_n = \infty$ or $\lim_{n \rightarrow \infty} A_n = 0$. For all initial values $A_0 = a_0 > 0$, the realizations may go to 0 and to ∞ with positive probability, i.e.

$$P(\lim_{n \rightarrow \infty} A_n = \infty | A_0) > 0 \quad \text{and} \quad P(\lim_{n \rightarrow \infty} A_n = 0 | A_0) > 0 \quad (3.7)$$

whenever $A_0 > 0$.

Proof: *Step (1):* Choose any constants \underline{C} and \overline{C} satisfying $0 < \underline{C} < ng < \overline{C} < \infty$. Choose $n_0 \in \mathbb{N}$ arbitrary. Then

$$P(\underline{C} \leq A_n \leq \overline{C} \quad \text{for all } n \geq n_0) = 0 \quad . \quad (3.8)$$

Proof: It is easy to show that there exists a number N of time steps and a probability $p > 0$ such that for any $A_{n_0} \in (\underline{C}, \overline{C})$

$$P(A_{n_0+N} \notin [\underline{C}, \overline{C}] | A_{n_0}) \leq p \quad . \quad (3.9)$$

The event $\underline{C} \leq A_{n_0} \leq \overline{C}$ for all $n \geq n_0$ implies the event $\underline{C} \leq A_{n_0+kN} \leq \overline{C}$ for all $k \in \mathbb{N}$ and thus has probability 0.

Step (2): We have the following recurrence properties of A_N with respect to the lines \overline{C} and \underline{C} .

(i) If \bar{C} is large enough, then there exists $\bar{p} < 1$ such that

$$P(A_n \text{ crosses line } \bar{C} \text{ at least once} \mid A_0 \geq \bar{C}) \leq \bar{p}. \quad (3.10)$$

(ii) For any fixed $\underline{C} > 0$ there exists $\underline{p} > 0$ such that

$$P(A_n \text{ hits the zero line} \mid A_0 \leq \underline{C}) \geq \underline{p}. \quad (3.11)$$

Proof of (i): The increments $A_{n+1} - A_n$ take values in $[-A_n, A_n^2]$. Necessary for the condition $A_{n+1} - A_n < A_n$ is that no more than one of the A_n particles has an increment of A_n (see program section). Thus we easily find that

$$\begin{cases} P(A_{n+1} - A_n < A_n) < p[A_n] = \left(1 - \frac{\Delta t}{ng}\right)^{A_n-1} \left[\left(1 - \frac{\Delta t}{ng}\right) + A_n \frac{\Delta t}{nf}\right] \\ P(A_{n+1} - A_n \geq A_n) > 1 - p[A_n] \end{cases} \quad (3.12)$$

Notice that $p[A_n]$ is monotonely decaying to 0 for $A_n \nearrow \infty$. We choose $A_0 \geq \bar{C}$ arbitrary and calculate the probability

$$P^{(k)} = \prod_{j=0}^{k-1} (1 - p[A_j]) \quad (3.13)$$

for the event

$$2^k A_0 \leq 2^{k-1} A_1 \leq \dots \leq 2A_{k-1} \leq A_k. \quad (3.14)$$

For ξ sufficiently large we have the estimate

$$p[\xi] \leq a^\xi \quad \text{for some } a \in (0, 1) \quad . \quad (3.15)$$

Now a classical formula (see [5, Sec. 0.7.5]),

$$P^{(k)} \searrow P^\infty \geq \prod_{j=0}^{\infty} (1 - a^{2^j}) = \frac{a}{1+a} \quad . \quad (3.16)$$

Thus with positive probability, A_n will not return to \bar{C} .

Step (3): Choose \bar{C} as in *step (2)(i)*, and $\underline{C} := \bar{C}$. A_n can pass this line only a finite number of times, since the recurrence probabilities from below and above are bounded away from 1. If A_n remains in $[0, \bar{C}]$ after finitely many steps, it is absorbed from 0 at

finite time. In the other case, $A_n \nearrow \infty$ for $n \rightarrow \infty$ (which follows again by comparison with the classical random walk). \circ

We conclude, whatever value for A_0 we choose, fluctuations separate trajectories in those converging to 0 and those diverging. It is, however, obvious that for the discretized scheme A_n cannot diverge *in finite time*, since each time step Δt allows only a finite increment. A consequence of the theorem is that it is e.g. not possible to find the longtime behaviour for the solution of problem (3.3) with small initial value (this solution should converge) by taking ensemble averages of the stochastic process. Averages will diverge as soon as there is a single diverging trajectory in the ensemble. Fig. 1 shows a couple of numerical trajectories.

Finally, let us include a source > 0 into the model process. This is readily achieved by adding randomly new particles. In this case, the limiting state $A_n \searrow 0$ is prohibited. A slight modification of the proof of Theorem 3.4 yields

3.5 Corollary: In the case of a source $s > 0$, almost all trajectories satisfy $A_n \nearrow \infty$.

4 A spatial coagulation model with source

4.1 An initial boundary value problem

4.1.1 The problem

We now combine the coagulation process with a diffusion in the spatial domain $[-1, 1]$. A source of aerosols of strength $s \geq 0$ is introduced at $x = 0$; the boundary of $[-1, 1]$ is totally absorbing and serves as a sink. The initial boundary value problem (IBVP) under consideration for the second moment function $a : [0, T] \times [-1, 1] \rightarrow \mathbb{R}_+$ reads

$$\partial_t a = \partial_{xx} a + a^2 + s \cdot \delta_{x=0} \quad , \quad (4.1)$$

$$0 = a(-1) = a(1) \quad , \quad (4.2)$$

with initial conditions to be specified.

4.1.2 Stationary solutions

For the following it is useful to study the stationary boundary value problem (BVP)

$$\partial_{xx}a = -a^2 - s \cdot \delta_0 \quad , \quad a(-1) = a(1) = 0 \quad . \quad (4.3)$$

A solution of (BVP) has to satisfy the ODE

$$\partial_{xx}a = -a^2 \quad \text{in } [-1, 0) \quad \text{and in } (0, 1] \quad (4.4)$$

and the interface jump condition for $\partial_x a$,

$$\partial_x a(0-) - \partial_x a(0+) = s \quad . \quad (4.5)$$

One finds easily that solutions have to satisfy the symmetry condition

$$a(-x) = a(x) \quad , \quad (4.6)$$

and thus

$$\partial_x a(0-) = -\partial_x a(0+) = s/2 \quad . \quad (4.7)$$

Therefore we may restrict to the solution in the left interval $[-1, 0]$. We shift the interval by transforming $x \rightarrow x + 1$ and consider as a modified problem on \mathbb{R}_+ the initial value problem (IVP)

$$\partial_{xx}b = -b^2 \quad , \quad b(0) = 0 \quad , \quad \partial_x b(0) = \alpha \quad . \quad (4.8)$$

If necessary, we denote $b(x) =: b[\alpha](x)$ to indicate the dependence of b on the initial value $\partial_x b(0) = \alpha$. We have to find $\alpha > 0$ such that $\partial_x b[\alpha](1) = s/2$.

Solutions of (4.7) are convex functions satisfying (for $\partial_x b(0) > 0$) the asymptotic behavior $\lim_{x \rightarrow \infty} b(x) = -\infty$. Multiplying with $\partial_x b$ and setting $\partial_x b = \alpha$, we find after integration the equation

$$\partial_x b = \begin{cases} +\sqrt{\alpha^2 - \frac{2}{3}b^3} & \text{as long as } b(x) \leq (1.5 \cdot \alpha^2)^{1/3} \\ -\sqrt{\alpha^2 - \frac{2}{3}b^3} & \text{else} \end{cases} \quad (4.9)$$

From the convexity of b follows easily by application of standard ODE techniques

4.1 Lemma: (a) For $\alpha > 0$ there exists a unique $x_0(\alpha) \in (0, \infty)$ with

$$\partial_x b(x) \begin{cases} \geq 0 & \text{for } x \leq x_0(\alpha) \\ < 0 & \text{else} \end{cases} \quad (4.10)$$

(b) $x_0(\alpha)$ is continuous and strictly monotonically decreasing, and

$$\lim_{\alpha \searrow 0} x_0(\alpha) = \infty \quad , \quad \lim_{\alpha \nearrow \infty} x_0(\alpha) = 0 \quad . \quad (4.11)$$

Define $\alpha_0 > 0$ as that value, for which $x_0(\alpha_0) = 1$. Then it is obvious that the BVP (4.4) has two solutions: one with $\partial_x a(-1) = 0$ and one with $\partial_x a(-1) = \alpha_0$. Values $\alpha > \alpha_0$ imply $\partial_x b(1) = \partial_x a(0) < 0$ which corresponds to a negative source s . Since we assume $s \geq 0$, the only range for α is $[0, \alpha_0]$. We now define the function

$$\Psi : [0, \alpha_0] \rightarrow \mathbb{R}_+ \quad , \quad \Psi(\alpha) = \partial_x b[\alpha](1) \quad . \quad (4.12)$$

Ψ is continuous, satisfies $\Psi(0) = \Psi(\alpha_0) = 0$, and is strictly positive for $\alpha \in (0, \alpha_0)$. Thus Ψ assumes its maximum ψ_{max} at (at least) one point α_{max} . For all values $\tilde{\psi} < \psi_{max}$, there exist *at least* two points α_1, α_2 with $\Psi(\alpha_1) = \Psi(\alpha_2) = \tilde{\psi}$. A more detailed analysis shows that there are *exactly* two points. This proves that the space of stationary solutions exhibits the structure of a fold bifurcation.

4.2 Theorem: There exists an $s_0 > 0$ such that the BVP (4.3) has

$$\begin{cases} \text{no solution} & \text{for } s > s_0 = 2a'(0-) \\ \text{exactly one solution} & \text{for } s = s_0 \\ \text{two solutions} & \text{for } s < s_0 \end{cases} \quad (4.13)$$

This situation is illustrated in Fig. 2 which shows the dependance of $a'(-1)$ on $a'(0) = s/2$.

4.2 Numerical simulations

4.2.1 Discretization of the IBVP

As a basis for the numerical simulation we choose the following *discretization*. We determine some sufficiently large $N \in \mathbb{N}$ and define a step size $\Delta x = 1/N$, and for

$k = -N, \dots, N$, $x_k = k \cdot \Delta x$. In the numerical experiments described below we chose $N = 40$ (4.2.2) resp. $N = 20$ (4.2.3). The dynamics is modelled by operator splitting. Alternatingly, the

$$\begin{aligned} \text{diffusion step:} \quad & \partial_t a = \partial_{xx} a \text{ and the} \\ \text{coagulation step:} \quad & \partial_t a = a^2 + s \cdot \delta_0 \end{aligned}$$

are performed for a time step of length Δt . This is a quite rough discretization, but it exhibits all features which we want to illuminate in this paper.

In a first step, we calculate the bifurcation structure observed in Theorem (4.2). Fig. 2 shows the value of $a'(0-)$ (abscissa) (which we denote for short $a'(0)$) depending on the choice of $\alpha = a'(-1)$. As the maximal value for $a'(0)$ we find $a'(0)_{\max} \approx 0.87$. Corresponding to formula (4.13), for sources stronger than $s_0 = 2a'(0)_{\max} \approx 1.74$, there exists no stationary solution to (the discretized version of) (4.1). For $0 \leq s < s_0$, there are two solutions *stat1* and *stat2*.

4.2.2 Stability of stationary solutions

We test numerically the stability of the two solutions *stat1* and *stat2* for $s = 1.5864$. The corresponding initial conditions for the BVP are $a'(-1) = 1.3004$ and $a'(-1) = 2.5$. Both solutions $\text{stat1} \leq \text{stat2}$ are shown in Fig. 3. For the test we investigate the asymptotic behavior (large t) for solutions of the IBVP with initial data $a(0, x)$ close to one of the stationary solutions, and for $a(0, x) = 0$.

Fig. 4 shows the evolution corresponding to $a(0) = 0$, displaying the time steps $25 \cdot 2^k$, $k = 0, \dots, 7$. The two dotted lines correspond to the stationary solutions. For fixed $x \in (-1, 1)$, $a(t, x)$ is strictly increasing with t , and there is a clear numerical indication that $a(t) \rightarrow \text{stat1}$. In the next experiment we choose initial data $a(0) < \text{stat2}$, with $0.99 \cdot \text{stat2} < a < \text{stat2}$, obtained by subtracting a random function (in x) from *stat2*. Fig. 5 illustrates that $a(t)$ stays for a long time close to *stat2* (approximately 2000 time steps) and is eventually attracted by *stat1* (after 8000 time steps, $a(t) \approx \text{stat1}$). The same experiment with $a(0) > \text{stat2}$ leads to a diverging solution as displayed in Fig. 6. Here, $a(t)$ remains for a long time near *stat2* (solid lines illustrate the time steps 1000 and 2000), then increases with moderate speed (the dashed lines represent the time steps 2500 and 2600) and finally explodes in a short time (dotted lines, showing time steps 2620, 2640 and 2660; time step 2670 leads to an overflow exception).

These examples are clear indications that $stat1$ is a stable and $stat2$ an unstable stationary solution to (4.1), (4.2).

Finally, we want to test the influence of (small) random fluctuations in the *initial conditions*. We find that choosing initial conditions as slight random perturbations of $stat2$ leads to splitting up of the random solutions into diverging ones and ones converging to $stat1$. Fig. 7 shows $a(t, 0) - stat1(0)$ (in logarithmic scale) for a couple of realizations. We recognize a picture resembling that of Fig. 1 for the homogeneous case.

4.2.3 Metastability of $stat1$

As a last example we want to test the effect of random fluctuations of the *coagulation process* and of the *diffusion*. As source we take $s = 1.72$ (which is close to the maximal value $s_0 = 1.74$; thus the two stationary solutions are quite close together). Furthermore, $ng = 50$. We again start with initial condition $a(0) = 0$ and expect the numerical solution to approximate $stat1$. Indeed, $a(t)$ approximates $stat1$ after 1000 time steps (see Fig. 8) and seems to be kept by $stat1$. However, after approximately 3000 time steps it starts to increase and finally explodes after time step 4130 (Fig. 9).

Our interpretation is that due to fluctuations a major portion of the random system crosses the line of $stat2$ and becomes destabilized. Thus the system exhibits a typical feature which in other contexts has been observed and which is denoted as *metastability*. The time scale for destabilization will rapidly increase with increasing ng (and thus reduced fluctuations). The effect, however, will be still observable.

References

- [1] D. J. Aldous. Deterministic and stochastic models for coalescence (aggregation, coagulation): a review of the mean-field theory for probabilists. *Bernoulli*, 5:3–48, 1999.
- [2] H. Babovsky. On a Monte Carlo scheme for Smoluchowski's coagulation equation. *Monte Carlo Methods and Applications*, 5:1–18, 1999.
- [3] A. Eibeck and W. Wagner. Stochastic particle approximations for Smoluchowski's coagulation equation. *Ann. Appl. Probab.* 11:1137–1165, 2001.

- [4] M. Smoluchowski. Versuch einer mathematischen Theorie der Koagulationskinetik kolloider Lösungen. *Z. Phys. Chem.*, 92:129–168, 1917.
- [5] E. Zeidler (Ed). *Teubner Taschenbuch der Mathematik*. Teubner, 1996.

Figures

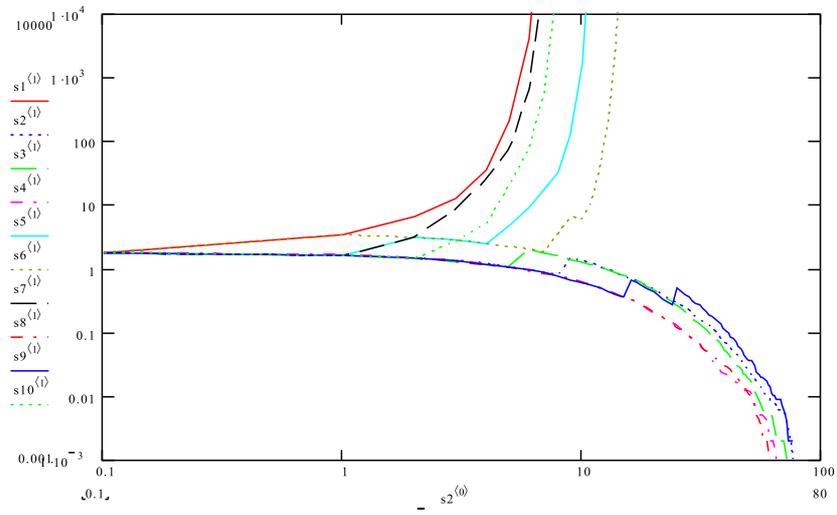


Fig. 1: MC realizations for homogeneous model with sink

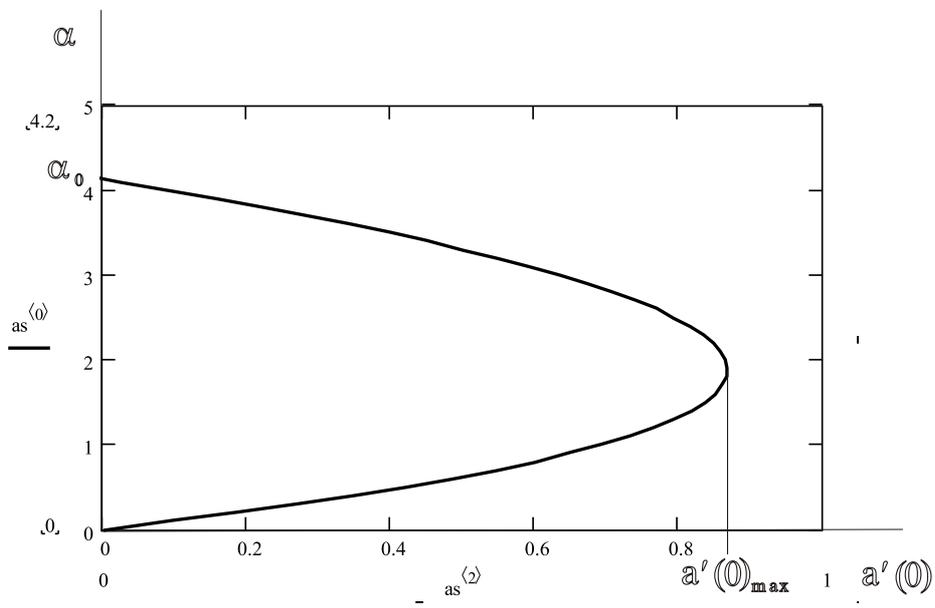


Fig. 2: Bifurcation structure of stationary BVP

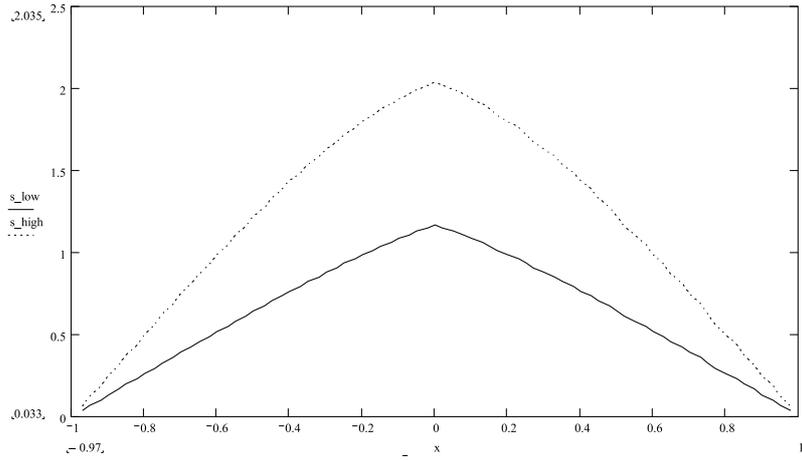


Fig. 3: Stationary solutions of BVP for fixed source $s < s_0$

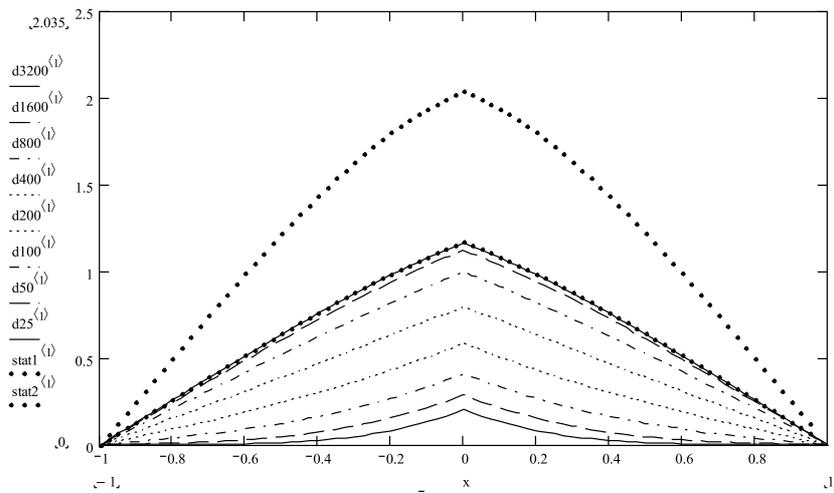


Fig. 4: Solutions of evolution problem (IBVP), $a(0) = 0$

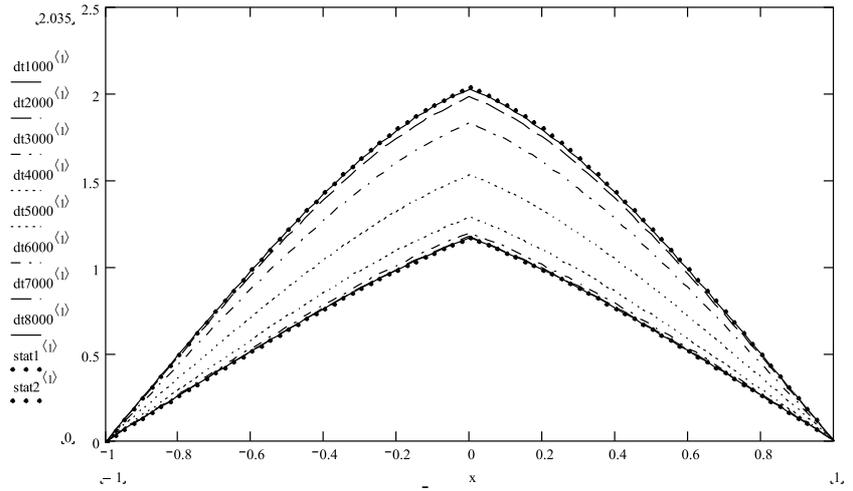


Fig. 5: Solutions of evolution problem (IBVP), $a(0)$ slightly below $stat2$

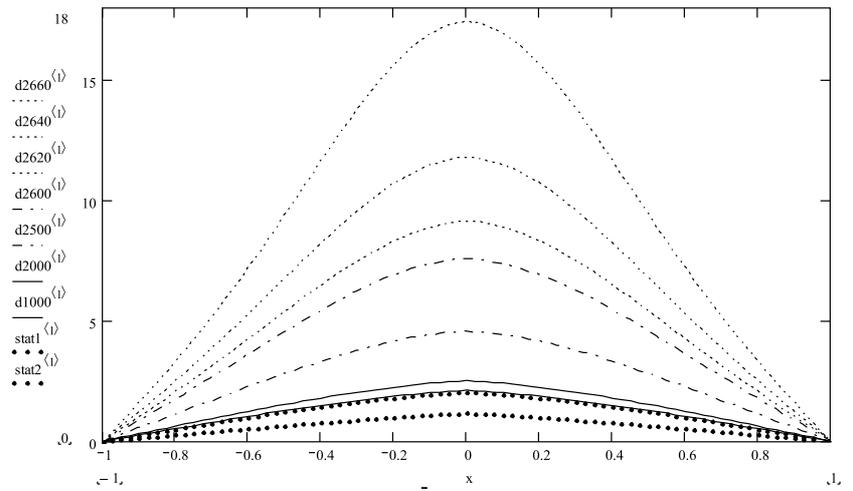


Fig. 6: Solutions of evolution problem (IBVP), $a(0)$ slightly above $stat2$

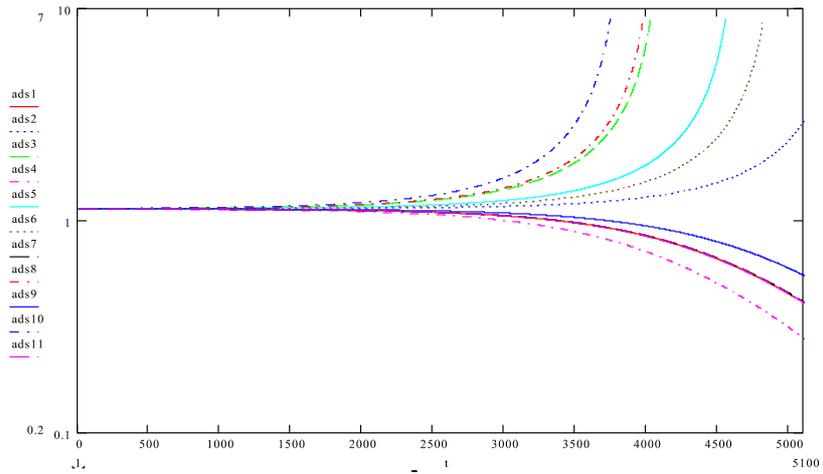


Fig. 7: Solutions $a(t, 0)$ of evolution problem (IBVP), $a(0, x)$ random perturbation around *stat2*

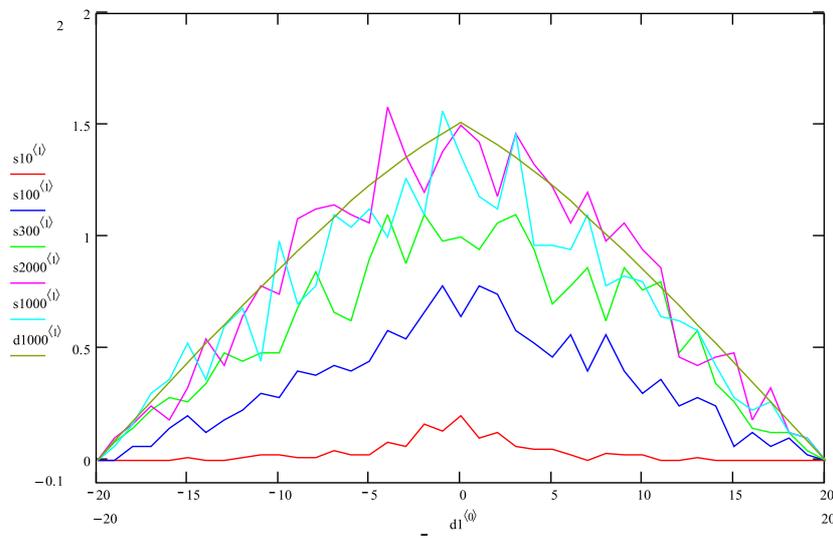


Fig. 8: MC solution of IBVP, $a(0) = 0$: attraction to *stat1*

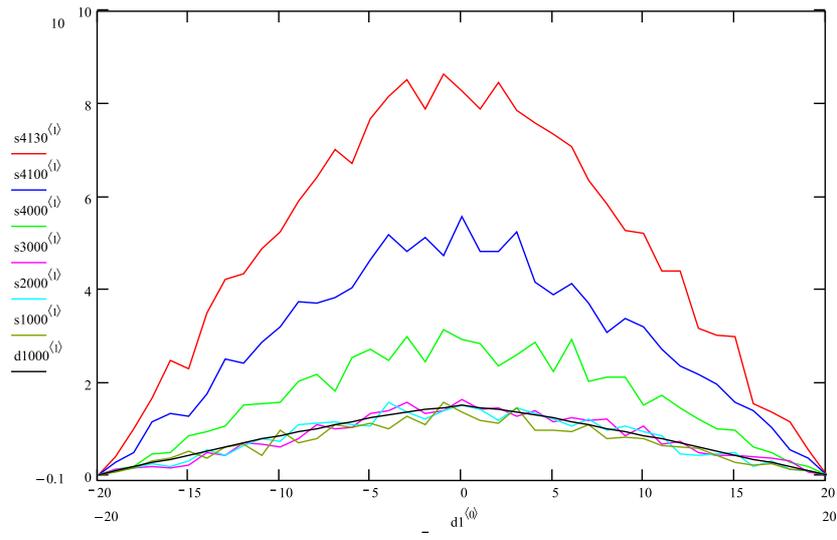


Fig. 9: Continuation of Fig. 8: destabilization