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PAPERS

A Becker–Döring model with injection and irreversible fragmentation

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Abstract

We introduce and analyse a variant of the Becker–Döring equations that models the growth of clusters through the gain or loss of monomers. Motivated by enzymatic reactions in biology, this model incorporates irreversible fragmentation and monomers injection. We establish the well-posedness of the equations under suitable conditions on the kinetic rates. Then, as in the Becker–Döring equations, we distinguish two cases for the long-time behaviour of our solution; however, the distinction is made from the constant rate injection of monomers. While under strong fragmentation rate the system may exhibit infinite steady states, we prove that for low injection rate and moderate fragmentation, the solution converges locally exponentially fast to the steady state. Finally, we present an efficient scheme that preserves the asymptotic and allows fast computation by sub-sampling the clusters.

1. Introduction

In their article [9], Becker and Döring provided one of the earliest descriptions of particle growth in the theory of nucleation from supersaturated vapour, which subsequently gave the name to the model. This model describes the growth and decay of clusters, consisting of identical monomers, only by the addition and removal of monomers. The modern formulation of the equations seems to go back to Burton [14] to study condensations phenomena at different pressures and was popularised among mathematicians by Penrose and Lebowitz [43]. Since then, the model has been applied in a variety of fields, including but not limited to physics, chemistry and biology. Initial mathematical results were proved by Ball, Carr and Penrose [5, 7], then the mathematical aspect of these equations has been studied in detail. Well-posedness and many aspects of the long-time behaviour of solutions are understood [16, 15, 32] and many other works, as well as the emergence of phase transition [42]. However, there are still open questions, see, e.g. [31] and [46].

We also point out the fact that the Becker–Döring equations are a specific case of general discrete coagulation-fragmentation equations. Therefore, classical results, mainly on the well-posedness, can be applied. First, mathematical results were proved by Ball and Carr [6], Carr [17], Carr and da Costa [18], and da Costa [19] on the well-posedness and the asymptotic behaviour of solutions. Another proof of existence was found by Laurençot [35] extending existence result of Carr and da Costa [18].

In this work, we study a variant of Becker–Döring equations. We have in mind specific applications to biology with polymerisation of biomolecules such as fibrin clots formation. It is thus natural to consider *open systems* in which monomers arise from a reaction cascades (e.g. fibrinogen conversion to fibrin protein), and a fragmentation process undergoes an irreversible process such as fibrin digestion by plasmin [39]. In our version of Becker–Döring equations, we consider a model where injection of

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monomers is constant, which may represent synthesis of fibrin monomer, and the detached monomer from fragmentation is not able to go through the coagulation process again. The reactions taking place are given by

$$\begin{cases} (1) + (i) \xrightarrow{a_i} (i+1), \ i \geq 1, \\ (i) \xrightarrow{b_i} (i-1), \ i \geq 3, \\ (2) \xrightarrow{b_2} \emptyset, \\ \emptyset \xrightarrow{\lambda} (1), \end{cases}$$

where (i) represents the concentration of clusters of size i. The non-negative numbers a_i and b_i denote, respectively, the coagulation and fragmentation coefficients. It is important to note that the $(2) \xrightarrow{b_2} \emptyset$ reaction is the result of a specific choice that was made, namely that a 2-polymer should disappear and not form a single monomer. The degradation of the 2-polymer is presumed to occur in a manner that both monomers are degraded. We believe that with slight adaptations, our results hold with considering the reaction $(2) \xrightarrow{b_2} (1)$.

The infinite system of ordinary differential equations associates to the reaction scheme is

$$\begin{cases} \dfrac{d}{dt}C_1(t) = \lambda - \displaystyle\sum_{j=1}^{+\infty} a_j C_1(t) C_j(t) - a_1 C_1(t)^2, \\ \dfrac{d}{dt}C_i(t) = J_{i-1}(t) - J_i(t), \qquad\qquad i \geq 2, \end{cases} \tag{1.1}$$

where, for all $i \geq 1$,

$$J_i(t) = a_i C_1(t) C_i(t) - b_{i+1} C_{i+1}(t). \tag{1.2}$$

The unknowns are the functions $C = (C_i(t))_{i \geq 1}$ that depend on time $t \geq 0$ and where, for each $i \in \mathbb{N}^*$, $C_i(t)$ denotes the concentration of i-particles clusters per unit of volume at time t. The quantity J_i does not represent the rate of change of a reversible reaction as in the Becker–Döring equations, but for convenience, we keep this notation.

Some work already exists on models close to Becker–Döring and close to ours. The first modification was to add monomers injection; it appears in submonolayer epitaxial growth [2, 4], in nucleation theory for thin film growth [44]. The first mathematical work was done by Blackman and Marshall [10], they discussed scaling behaviour and growth exponent for a constant rate source; then by Wattis [45] where he studied self-similar behaviour of solutions for a time-dependent monomer input and size-independent rate coefficients. He has already shown that with a slight modification, the long-time behaviour of solutions may become complex and depend strongly on the production rate. We also mention the works of da Costa et al. [21, 22] and [23], which, with constant rate coefficients, complement some of the formal results in [10] and [45]. Recently, Niethammer et al. [41] introduced a depletion term representing clusters removal. As our model, the chemical reaction network is open, it then becomes unclear whether long-time convergence towards steady-state holds. In their case, they provide evidence for the persistence of oscillations in time. We also mention the work of Bolton and Wattis [13], in which they considered a model with injection, competition and inhibition.

There exist other modifications of the Becker–Döring equations but differs to ours, for example, the work of Doumic et al. [24] introduces a bi-monomeric model explaining oscillations. We also mention the work of Wattis [47] in which the fragmentation rates depend on the total number of clusters present in the system and the works of Laurençot and Wrzosek [36] and [37] in which they added space diffusion.

Some literature exists on continuous models with mass loss, more specifically on coagulation and fragmentation equations with discrete and continuous mass loss. The first mathematical work was done by Edwards [27], and a more recent work was done by Blair et al. [11]. A part of the book of Banasiak, Lamb and Laurençot [8] treats those equations using semigroups techniques. Different authors [1] and [3] considered a hybrid model of fragmentation still with discrete and continuous mass loss.

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In this work, we start by proving well-posedness of (1.1). The proof of existence follows that of Laurençot [34], which, as for the proof of Ball et al. [6] and [7], relies on a truncated system and compactness arguments to obtain the limit. Uniqueness is more classical and follows the initial work of Ball and Carr [6]. As in the Becker–Döring equations, two distinct cases appear; however, here it does not depend on the initial mass, since our system does not preserve it, but instead on the production rate λ. There is a threshold λ_s, which dictates significant change in the dynamic. In the sub-critical case $\lambda \leq \lambda_s$, it may occur that

- either there exists a unique steady state for $b_i \leq ia_i$,
- or there exists an infinite number of steady states for $b_i > i^\nu a_i$ with $\nu > 1$.

We prove that if λ is sufficiently small and $a_i < b_i \leq i$, then the steady state is locally exponentially asymptotically stable. This corresponds to b_i strong enough but not too much (moderate); these conditions will be made precise in the Section 2.2.3. In the super-critical case $\lambda > \lambda_s$, contrary to the Becker–Döring equations, we do not find a Lyapunov functional; thus, we were not able to prove a result in the super-critical case. The question remains open, but we expect some self-similar behaviour of the solution [45]. We end this work with a numerical scheme. We develop, on the conservative truncation, a well-balanced and coarse-grained scheme, which consists of sub-sampling the clusters at some given size, preserving the asymptotics. The scheme is based on the flux approximation scheme of Ducan and Soheili [26] and the well-balanced scheme of Goudon and Monasse [29]. This scheme can be used on the classical Becker–Döring equations.

2. Main results

In this section, we introduce some notations, hypotheses and state the main results. Details and proofs are presented in their respected section. Before starting our existence and uniqueness result, we provide the definition of a solution to (1.1).

Definition 2.1. *Let $T \in (0, +\infty]$. A solution $C = (C_i)_{i\geq 1}$ of (1.1) on $[0, T)$ is a sequence of non-negative functions satisfying the following conditions for all $i \geq 1$, $t \in [0, T)$,*

(i) $C_i \in \mathcal{C}^0([0, t))$, $\displaystyle\sum_{j=1}^{+\infty} a_j C_j \in \mathrm{L}^1(0, t)$,

(ii) *and there holds*

$$\begin{cases} C_1(t) = C_1(0) + \lambda t - \displaystyle\int_0^t C_1(s) \sum_{j=1}^{+\infty} a_j C_j(s) - a_1 C_1(s)^2 ds, & i = 1 \\ C_i(t) = C_i(0) + \displaystyle\int_0^t [J_{i-1}(s) - J_i(s)]\, ds, & i \geq 2. \end{cases}$$

We start by stating the weak form of (1.1), which is very useful to compute moments or to find some uniform bounds.

Proposition 2.2. *Let C be a solution of (1.1). For all compactly supported sequences $(\varphi_i)_{i\geq 1}$, we have*

$$\frac{d}{dt} \sum_{i=1}^{+\infty} \varphi_i C_i = \lambda \varphi_1 - \varphi_2 b_2 C_2 + \sum_{i=1}^{+\infty} [\varphi_{i+1} - \varphi_i - \varphi_1]\, a_i C_1 C_i + \sum_{i=3}^{+\infty} [\varphi_{i-1} - \varphi_i]\, b_i C_i. \tag{2.1}$$

We can write it under another form as follows:

$$\frac{d}{dt} \sum_{i=1}^{+\infty} \varphi_i C_i = \varphi_1 \left(\lambda - b_2 C_2 - \sum_{i=2}^{+\infty} b_i C_i \right) + \sum_{i=1}^{+\infty} [\varphi_{i+1} - \varphi_i - \varphi_1]\, (a_i C_1 C_1 - b_{i+1} C_{i+1}). \tag{2.2}$$

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We define the following Banach spaces in which solutions will lie. Let $\alpha \geq 0$, we define the following subspaces of $\ell^1(\mathbb{R})$,

$$X_\alpha := \left\{ x = (x_k)_{k\geq 1} \in \mathbb{R}^{\mathbb{N}} : \|x\|_{X_\alpha} := \sum_{k=1}^{+\infty} k^\alpha |x_k| < +\infty \right\},$$

and we denote X_α^+ its positive cone. Some of these spaces have physical meaning, for example, the norm in $X_0 = \ell^1$ is proportional to the total number of clusters, or the norm of X_1 is proportional to the mass of all the clusters in our system. Some properties of these spaces can be found in the review of da Costa [20, Section 2.1].

2.1. Well-posedness

We state the main results on existence and uniqueness of solutions under some assumptions on the kinetic coefficients, mainly on the coagulation ones, and on the initial data. Let $\alpha \in [0, 1]$.

(H1) There exists $a \geq 0$ such that $0 \leq a_i \leq ai^\alpha$ and $b_i \geq 0$ for all $i \geq 1$.

In the classical proof of existence from Ball, Carr and Penrose [7] or for the general coagulation-fragmentation equations from [6] or [34], the natural space for the existence is X_1 since the equations are mass preserving. Here, equations (1.1) do not preserve mass; therefore, we can consider a larger space for the existence, in which mass does not necessarily have meaning or may blow up. We have the following existence results in X_α for $\alpha \in [0, 1]$.

Theorem 2.3 (Existence and moment spreading). *Let $C^{init} \in X_\alpha^+$. Under the hypothesis (H1), there exists at least one solution $C \in \mathcal{C}^0([0, +\infty), X_\alpha^+)$ to (1.1) with initial data $C(0) = C^{init}$. Moreover, if there exists $\mu \geq \alpha$ such that*

$$\sum_{i=1}^{+\infty} i^\mu C_i^{init} < +\infty,$$

then any solution satisfies for all $T > 0$

$$\sup_{t\in[0,T]} \sum_{i=1}^{+\infty} i^\mu C_i(t) < +\infty.$$

We actually prove a more general result including more than just power law moments but a wider class, see Section 3. This theorem is inspired by [34, Theorem 2.5], and it generalises [18, Theorem 3.3], which proves moment spreading in coagulation-fragmentation equations.

Theorem 2.4 (Partial uniqueness). *Let $C^{init} \in X_\alpha^+$ and $T \in (0, +\infty]$. Under the hypothesis (H1), there exists at most one solution C to (1.1) on $[0, T)$ with initial condition $C(0) = C^{init}$ such that*

$$C \in \mathrm{L}^\infty([0, t], X_\alpha^+) \text{ and } \sum_{i=1}^{+\infty} i^{2\alpha} C_i \in \mathrm{L}^1(0, t) \text{ for all } t \in (0, T). \tag{2.3}$$

Theorem 2.5 (Well-posedness). *Let $C^{init} \in X_{2\alpha}^+$ and $T \in (0, +\infty]$. Under the hypothesis (H1), there exists a unique solution C to (1.1) on $[0, T)$ with initial condition $C(0) = C^{init}$. Moreover, this solution satisfies*

$$C \in \mathcal{C}^0([0, t], X_\alpha^+) \text{ and } \sum_{i=1}^{+\infty} i^{2\alpha} C_i \in \mathrm{L}^1(0, t) \text{ for all } t \in (0, T).$$

Theorem 2.5 is an immediate consequence of Theorems 2.4 and 2.3. The partial uniqueness result Theorem 2.4 is inspired by [6, Theorem 4.2] and [34, Proposition 5.1] and state uniqueness under moments control. Laurençot and Mischler [35, Theorem 2.1] gave another proof of uniqueness, on the

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Becker–Döring equations, without the assumption on moments control, but with an assumption on coefficients $(b_i)_{i\geq 1}$. Their proof is based on estimates of distribution tails and mass conservation. The proof of Theorem 2.4 is given in Section 4.

In the remainder, we will always assume that the kinetics coefficients satisfy the condition (H1) for some suitable $\alpha \in [0, 1]$.

2.2. Long-time behaviour

2.2.1. Uniform-in-time bound

The first uniform-in-time bound is an upper bound on $C_1(t)$. We obtain directly from the equation on C_1 that for all $t \in [0, +\infty)$, we have

$$C_1(t) \leq \kappa(\lambda, C^{init}) := \max\left\{C_1^{init}, \sqrt{\frac{\lambda}{2a_1}}\right\}. \tag{2.4}$$

We prove an upper uniform-in-time bound on exponential moments under strong fragmentation, and this will allow us to prove the local exponential stability of a steady state. The following proposition is inspired by a similar result in [32, Lemma 3.3].

Proposition 2.6 (Exponential moments uniform-in-time bound). *Assume that the kinetics coefficients satisfy the following conditions:*

$$\forall i \geq 1,\ a_i \geq \underline{a} > 0. \tag{2.5}$$

Let $\lambda \geq 0$ *and* C^{init} *small enough such that*

$$\kappa(\lambda, C^{init}) < \inf_{i\geq 1} \frac{b_i}{a_i}, \tag{2.6}$$

and there exists $\nu > 0$ *such that*

$$\sum_{i=1}^{+\infty} e^{\nu i} C_i^{init} < +\infty. \tag{2.7}$$

Then, there exists a constant $\Xi_1 > 0$ *such that for all* $t \geq 0$,

$$\sum_{i=1}^{+\infty} e^{\nu i} C_i(t) \leq \Xi_1, \tag{2.8}$$

where Ξ_1 *depends only on* λ, $(a_i)_{i\geq 1}$, $(b_i)_{i\geq 1}$, ν *and initial data.*

We also prove, under some hypotheses on the kinetic coefficients, an upper bound on the mass and a lower bound on C_1. Details and proofs are presented in Section 5.1.

2.2.2. Steady states

We define the detailed balance coefficients Q_i by

$$Q_1 := 1,\ \ Q_i := \prod_{j=2}^{i} \frac{a_{j-1}}{b_j},\ \text{pour } i \geq 2. \tag{2.9}$$

These coefficients play a significant role in the long-term behaviour of the solutions. It is from these coefficients that two significant quantities are defined. The first quantity is the *critical monomer density*, denoted z_s, which is defined as the radius of convergence of the power series $\sum a_i Q_i z^i$. This quantity is also called *monomer saturation density*, hence the subscript. The second quantity is the *critical*

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production threshold, denoted λ_s, which is defined as follows:

$$\lambda_s := \sup_{z \le z_s} \sum_{j=1}^{+\infty} a_j Q_j z^{j+1} + a_1 z^2. \tag{2.10}$$

We emphasise that both z_s and λ_s are completely determined by the coefficients a_i and b_i.

Remark 2.7. *As the function $z \mapsto a_j Q_j z^{j+1}$ is increasing, the critical production threshold can be rewritten, when the series converges, as follows:*

$$\lambda_s = \sum_{j=1}^{+\infty} a_j Q_j z_s^{j+1} + a_1 z_s^2.$$

In the following, we add two hypotheses that can be readily verified in the case of constant coefficients, certain power laws or Niethammer's coefficients [40, (1.5) and (1.6)]. These conditions are as follows.

(H2) There exists $\underline{a} > 0$ and $\underline{b} > 0$ such that $\inf_{i \ge 1} a_i = \underline{a}$ and $\inf_{i \ge 1} b_i = \underline{b}$,

(H3) There exists $l > 0$ such that $\lim_{i \to +\infty} \dfrac{Q_{i+1}}{Q_i} = \dfrac{1}{l z_s}$,

(H4) $\lim_{i \to +\infty} \dfrac{a_{i+1}}{a_i} = \lim_{i \to +\infty} \dfrac{b_{i+1}}{b_i} = l$.

Remark 2.8. *Hypotheses (H3) and (H4) imply that* $\lim_{i \to +\infty} \frac{b_i}{a_i} = z_s$.

Whether or not a steady state exists depends on the critical production rate λ_s and the production rate λ and, more particularly, on their comparison. By steady state, we understand a constant solution C, in particular, $\sum_{i=1}^{+\infty} a_i C_i < \infty$.

Theorem 2.9 (Steady states). *Under the assumptions (H2)–(H4), we have the two following possibilities:*

1. *(Sub-critical) If $\lambda \le \lambda_s$, then there exists a unique $z \le z_s$ verifying*

$$\lambda = \sum_{j=1}^{+\infty} a_j Q_j z^{j+1} + a_1 z^2 \tag{2.11}$$

   such that $(Q_i z^i)_{i \ge 1}$ is a steady state. Moreover, if $b_i \le i a_i$ for $i \gg 1$, then $(Q_i z^i)_{i \ge 1}$ is the unique steady-state or if $b_i > i^\nu a_i$ for $i \gg 1$ and $\nu > 1$, then there is an infinity of steady state.
2. *(Super-critical) Else $\lambda > \lambda_s$, and then there exists no steady state.*

2.2.3. Local exponential stability

The objective is to determine the long-term behaviour of the solution. We do not find a Lyapunov functional; consequently, we used the linearised system of equations. We analyse the spectral properties of the linearised operator, which can be represented as a perturbation of the one studied in the work of Cañizo and Lods [15].

In what follows, we assume the additional hypothesis:

(H5) $\exists\, \beta \in [0,1], \exists\, b > 0,\ \forall i \ge 1,\ b_i \le b i^\beta$.

Remark 2.10. *We point out that Remark 2.8 with $z_s \neq 0$ and (H2) implies that* $\inf_{i \ge 1} \frac{b_i}{a_i}$ *is a positive constant.*

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Theorem 2.11 (Local exponential convergence). *Assume (H1)–(H5). Let $\lambda < \lambda_s$ and C^{init} such that*

$$\kappa(\lambda, C^{init}) < \inf_{i\geq 1} \frac{b_i}{a_i} \tag{2.12}$$

and that (2.7) holds for some $\nu > 0$. Let $C = (C_i)_{i\geq 1}$ a solution of (1.1) with initial condition C^{init}. Take z satisfying (2.11). Then, there exists some $\eta \in (0, \nu)$, some $K, \varepsilon > 0$ and some $\mu_* > 0$ such that if

$$\frac{8b}{\sqrt{z}}\sqrt{\sum_{i=1}^{+\infty} i^{2\beta} Q_i z^i} \sup_{k\geq 1}\left(\sum_{j=k+1}^{+\infty} Q_j z^j\right)\left(\sum_{j=1}^{k} \frac{1}{a_j Q_j z^j}\right) < 1 \tag{2.13}$$

and

$$\sum_{i=1}^{+\infty} \exp(\eta i)|C_i^{init} - Q_i z^i| \leq \varepsilon, \tag{2.14}$$

then

$$\sum_{i=1}^{+\infty} \exp(\eta i)|C_i(t) - Q_i z^i| \leq K \exp(-\mu_* t),\ \forall t \geq 0. \tag{2.15}$$

Remark 2.12. *Condition (2.13) is a sufficient condition. One might ask whether this condition is ever met. To address this, we give the following examples.*

Example 2.13 (Constant coefficients). *Constant kinetics coefficients $a_i = a$ and $b_i = b$ satisfy hypotheses (H1)–(H5) for some a, b well choose. The condition (2.12) becomes either $C_1^{init} < \frac{b}{a}$ or $\lambda < 2\frac{b^2}{a}$. The condition (2.13) becomes*

$$\frac{(z_s - z)^{5/2}}{8 z z_s^{5/2}} > 1.$$

Since the left-hand side goes to $+\infty$ when z goes to 0, this condition holds for λ small enough. Indeed, recalling the definition of z (2.11), we see that the smaller λ is, the smaller z is too.

Example 2.14 (Linear coefficients). *Linear coefficients $a_i = ai$ and $b_i = bi$ satisfy hypotheses (H1)–(H5) for some a, b well choose. The condition (2.13) becomes for z small enough*

$$\frac{32z}{\sqrt{z_s}(z_s - z)} < 1.$$

As before, since the left-hand side goes to 0 when z goes to 0, this condition holds for λ small enough.

Details for Examples 2.13 and 2.14 are, respectively, presented in Appendices A.1 and A.2.

2.3. Numerical simulations

To simulate our equations numerically, we need to truncate our system, since we obviously cannot keep an infinite number of ordinary differential equations. We, therefore, have different ways of truncating our system. Generally speaking, for coagulation-fragmentation equations, there are two 'natural' truncations: conservative truncation and non-conservative truncation. Conservative truncation means that

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clusters of the maximum size cannot grow in size through the coagulation process, and those clusters are not the result of fragmentation; we have the following system of equations:

$$\begin{cases} \dfrac{d}{dt}C_1(t) = \lambda - \displaystyle\sum_{j=1}^{n-1} a_j C_1(t) C_j(t) - a_1 C_1(t)^2, & i = 1, \\ \dfrac{d}{dt}C_i(t) = J_{i-1}(t) - J_i(t), & 1 < i < n, \\ \dfrac{d}{dt}C_n(t) = J_{n-1}(t), & i = n. \end{cases} \tag{2.16}$$

This truncation corresponds to $J_i = 0$ for $i \geq n$. Another truncation exists, taking $J_n = a_n C_1 C_n$, referred to as non-conservative truncation, which means that at the size of truncation, we are allowing this maximum size to coagulate and as before no aggregates of this size are the result of depolymerisation.

To numerically simulate these previous systems, we can just use standard Ordinary Differential Equation (ODE) schemes (e.g. Runge-Kutta 4); however, choosing a large truncation n may involve very long computation time. Therefore, the goal is to develop a coarse-grain scheme, consisting of sub-sampling the clusters at some given size, preserving the asymptotics of the system.

The main idea is to see our truncation (2.16) as some discretisation of a particular Partial Differential Equation (PDE) for some size step Δx, in which the size of the aggregates x is a continuous variable. Let $n \geq 2$ be an integer, the aforementioned PDE is the following:

$$\frac{\partial C(t,x)}{\partial t} = -\frac{\partial J(t,x)}{\partial x}, \text{ in } [0,T] \times (1,n), \tag{2.17}$$

with

$$J(t,x) = -a(x)Q(x)C(t,1)^{x+1/2}\frac{\partial}{\partial x}\left(\frac{C(t,x)}{Q(x)C(t,1)^x}\right), \tag{2.18}$$

where the functions $a(x), b(x)$, and $Q(x)$ are the step functions of the discrete quantities a_i, b_i, and Q_i. Formally, (2.18) is obtained through the following discretisation with $\Delta x = 1$

$$\begin{aligned} J_i(t) &= \frac{1}{\Delta x}\left(a_{i-1}C_1C_{i-1} - a_{i-1}\frac{Q_{i-1}}{Q_i}C_1\right) \\ &= -a_{i-1}Q_{i-1}C_1^i\frac{1}{\Delta x}\left(\frac{C_i}{Q_iC_1^i} - \frac{C_{i-1}}{Q_{i-1}C_1^{i-1}}\right) \approx J\left(t, i-\frac{1}{2}\right). \end{aligned} \tag{2.19}$$

To which we add boundary conditions, the right one depends on the truncation that we are considering, and the left one comes from C_1. This idea is, in particular, presented by Duncan and Soheili [26]. Thus, taking another discretisation of the PDE, for example, with a non-uniform mesh, and simulating the PDE on this mesh should approach the desired solution. To that end, we are going to use the idea presented by Goudon and Monasse [29]. We mention the work of Bolton and Wattis [12], in which they develop a coarse-grain scheme on the Becker–Döring equations. Details are presented in Section 6.

2.4. Open questions

We highlight some questions that remain open. The uniqueness of a solution without the moment control, as in [35, Theorem 2.1], is open since no quantity is preserved. The long-time behaviour of the solution, except for our local stability result, remains open even in the sub-critical case, and especially when there exists an infinity of steady states. The behaviour of the solution in the super-critical case is even more unclear since no steady state exists.

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3. Existence

To prove Theorem 2.3, we follow the idea of Laurençot from [34]. To start, we introduce three sets of functions that are going to be useful later

$$\mathcal{K}_1 := \left\{U \in C^1([0,+\infty)) \cap \mathrm{W}^{2,\infty}_{loc}(0,+\infty) : U \geq 0,\ U \text{ convex},\ U(0)=0,\ U'(0)\geq 0,\ \text{et } U' \text{ concave}\right\},$$

$$\mathcal{K}_{1,\infty} := \left\{U \in \mathcal{K}_1 :\ \lim_{r\to+\infty} U'(r) = \lim_{r\to+\infty} \frac{U(r)}{r} = +\infty\right\},$$

$$\mathcal{K}_2 := \left\{U \in \mathcal{C}^2([0,+\infty),\mathbb{R}_+) : U(0)=U'(0)=0,\ U' \text{ convex satisfying the } \Delta_2-\text{condition}\right\},$$

with the Δ_2-condition being

$$U'(2r) \leq k_U U'(r),\ \forall r \geq 0,\ \text{and some } k_U > 0. \tag{3.1}$$

Remark 3.1. *The function $x \mapsto x^m$ belongs to $\mathcal{K}_1$ for $m \in [1,2]$, belongs to $\mathcal{K}_{1,\infty}$ for $m \in (1,2]$ and belongs to $\mathcal{K}_2$ for $m \geq 2$.*

As mentioned in the beginning, we prove a more general result than Theorem 2.3, which considers propagation of general moments. It reads as follows:

Theorem 3.2 (Existence and moment spreading). *Let $C^{init} \in X^+_\alpha$. Under the hypothesis (H1), and assume that there exists $U \in \mathcal{K}_1 \cup \mathcal{K}_2$ such that*

$$\sum_{i=1}^{+\infty} U(i^\alpha) C_i^{init} < +\infty. \tag{3.2}$$

Then, there exists at least one solution $C \in \mathcal{C}^0([0,+\infty), X^+_\alpha)$ to (1.1) with initial data $C(0) = C^{init}$, and for each $T \in (0,+\infty)$,

$$\sup_{t\in[0,T]} \sum_{i=1}^{+\infty} U(i^\alpha) C_i(t) < +\infty. \tag{3.3}$$

Theorem 2.3 follows by taking $U(x) = x^m$ for $m \geq 1$.

3.1. Preliminary results

As in many works on similar coagulation-fragmentation equations (e.g. [6, 7, 17] or [18]), the existence of a solution to (1.1) satisfying $C(0) = C^{init}$ comes by taking the limit of solutions to a finite number system of differential equations obtained by truncating our system of equations (1.1). More precisely, let $n \geq 3$, and recall the system of n ordinary differential equations (2.16), to which we still add the initial condition

$$C_i^n(0) = C_i^{init} \geq 0,\ 1 \leq i \leq n. \tag{3.4}$$

As in the infinite system, we can write the weak form of this system of equations. It reads as follows:

$$\frac{d}{dt}\sum_{i=1}^{n} \varphi_i C_i = \lambda\varphi_1 - \varphi_2 b_2 C_2 + \sum_{i=1}^{n-1} \left[\varphi_{i+1} - \varphi_i - \varphi_1\right] a_i C_1 C_i + \sum_{i=3}^{n} \left[\varphi_{i-1} - \varphi_i\right] b_i C_i. \tag{3.5}$$

To start, we prove the well-posedness of the truncated system of equations (2.16).

Proposition 3.3. *Let $n \geq 3$ and $C^{init} \in X^+_\alpha$. There exists a unique solution $C^n \in \mathcal{C}^1([0,+\infty),\mathbb{R}^n)$ to (2.16) satisfying $C_i^n(0) = C_i^{init}$ for $i = 1,\dots,n$. This solution satisfies $C_i^n(t) \geq 0$ for all $t \geq 0$ and $i = 1,\dots,n$ and*

$$C_i^n(t) \leq \sum_{i=1}^{n} i^\alpha C_i^n(t) \leq \lambda T + \|C^{init}\|_{X^+_\alpha} \tag{3.6}$$

for all $T \in (0,+\infty)$ and $i = 1,\dots,n$.

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Proof. The proof is a straightforward application of the Cauchy–Lipschitz theorem. The non-negativity follows from [25, Theorem 7.1 (Positivity)]. The fact that

$$\frac{d}{dt}\sum_{i=1}^{n} C_i^n(t) \le \lambda$$

entails non-explosion in finite time. Moreover, using (3.5) with $\varphi_i = i^\alpha$ and since $\alpha \in [0,1]$, we obtain

$$\frac{d}{dt}\sum_{i=1}^{n} i^\alpha C_i^n = \lambda - 2^\alpha b_2 C_2^n + \sum_{i=1}^{n-1}\left[(i+1)^\alpha - i^\alpha - 1\right] a_i C_i^n C_1^n + \sum_{i=3}^{n}\left[(i-1)^\alpha - i^\alpha\right] b_i C_i^n \le \lambda,$$

which entails (3.6). □

Our objective is now to show that we can extract from the sequence $(C^n)_{n\ge 1}$, even if we take $C_i^n = 0$ for $i > n$, a sub-sequence, which converges, and the limit is a solution, i.e. satisfies the Definition 2.1. In order to do that, we need to establish the following two lemmas.

Lemme 3.4. *Let $T \in (0,+\infty)$ and $U \in \mathcal{K}_1 \cup \mathcal{K}_2$. There exists a constant γ_T depending only on a, U, C^{init}, and T such that for all $n \ge 3$ and $t \in [0,T]$, we have*

$$\sum_{i=1}^{n} U(i^\alpha) C_i^n(t) \le \gamma_T \sum_{i=1}^{n} U(i^\alpha) C_i^{init} + \lambda U(1) T \gamma_T \tag{3.7}$$

Proof. Let $n \ge 3$ and $M_U^n(t) := \sum_{i=1}^{n} U(i^\alpha) C_i^n(t)$. We have for $t \ge 0$

$$\begin{aligned}\frac{d}{dt}M_U^n(t) \le{}& \lambda U(1) - U(2^\alpha) b_2 C_2^n(t) + \sum_{i=3}^{n}\left[U((i-1)^\alpha) - U(i^\alpha)\right] b_i C_i^n(t)\\ &+ \sum_{i=1}^{n-1}\left[U((i+1)^\alpha) - U(i^\alpha) - U(1)\right] a_i C_i^n(t) C_1^n(t)\end{aligned}$$

Noticing, for all $i \ge 1$ and $\alpha \in [0,1]$, $(i+1)^\alpha \le i^\alpha + 1$, and as $U \in \mathcal{K}_1 \cup \mathcal{K}_2$, U is increasing, thus $U((i+1)^\alpha) \le U(i^\alpha + 1)$ for all $i \ge 1$. Moreover, from [34, Lemma 3.2], there exists a constant m_U depending only on U such that for all $i \ge 1$

$$(i^\alpha + 1)(U(i^\alpha + 1) - U(i^\alpha) - U(1)) \le m_U(i^\alpha U(1) + U(i^\alpha)). \tag{3.8}$$

Therefore, by (H1) and (3.8), we obtain

$$\begin{aligned}\frac{d}{dt}M_U^n(t) \le{}& \lambda U(1) - U(2^\alpha) b_2 C_2^n(t) + \sum_{i=3}^{n}\left[U((i-1)^\alpha) - U(i^\alpha)\right] b_i C_i^n(t)\\ &+ a m_U \sum_{i=1}^{n-1}(i^\alpha U(1) + U(i^\alpha)) C_i^n(t) C_1^n(t),\end{aligned}$$

with a, respectively, m_U, the constant from (H1), respectively (3.8). As U is increasing, $U((i-1)^\alpha) - U(i^\alpha) \le 0$ for all $i \ge 1$, thus

$$\begin{aligned}\frac{d}{dt}M_U^n(t) &\le \lambda U(1) + 2a m_U M_\alpha^n(t) M_U^n(t)\\ &\le \lambda U(1) + 2a m_U\left(\lambda T + \|C^{init}\|_{X_\alpha}\right) M_U^n(t)\end{aligned}$$

Therefore, using Grönwall's lemma, we conclude

$$M_U^n(t) \le \left(M_U^n(0) + \lambda U(1) T\right) e^{2a m_U\left(\lambda T + \|C^{init}\|_{X_\alpha}\right) T}$$

which ends the proof. □

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Lemme 3.5. *Let $T \in (0, +\infty)$. For each $i \geq 1$, there exists a constant $\Gamma_i(T)$ depending only on $a, i, \|C^{init}\|_{X_\alpha}$ et T such that, for all $n \geq i$,*

$$\left\| \frac{d}{dt} C_i^n \right\|_{\mathrm{L}^1(0,T)} \leq \Gamma_i(T). \tag{3.9}$$

Proof. From Proposition 3.3, there exists a constant K_T such that $\left|C_i^n(t)\right| \leq K_T$ for all $i \geq 1$. Hence, for $i \geq 2$, $\left|\frac{d}{dt} C_i^n(t)\right|$ is uniformly bounded in $\mathrm{L}^1(0, T)$ according to n, thanks to equations (2.16). It remains to bound $\left|\frac{d}{dt} C_1^n(t)\right|$, which follows from the bound

$$\int_0^T \sum_{i=1}^{n-1} a_i C_1^n C_i^n \leq K_T a \int_0^T \sum_{i=1}^{n} i^\alpha C_i^n \leq TaK_T^2. \qquad \square$$

3.2. Proof of existence theorem

We are now in a position to prove Theorem 3.2. However, let us not forget a refined version of the de La Vallée–Poussin theorem for integrable functions from [38, Proposition I.1.1], which we are going to need. That is the key point of Laurençot's proof in [34, Theorems 2.3 and 2.5] that enables him to provide a different kind of proof without the need for cleverly decomposing the sums as in [6, Theorems 2.4 and 2.5].

Theorem 3.6 (de La Vallée-Poussin). *Let $(\Omega, \mathcal{B}, \mu)$ a measured space, and let $w \in \mathrm{L}^1(\Omega, \mathcal{B}, \mu)$. Then, there exists a function $V \in \mathcal{K}_{1,\infty}$ such that*

$$V(|w|) \in \mathrm{L}^1(\Omega, \mathcal{B}, \mu).$$

Proof of Theorem 3.2. First, we want to apply Theorem 3.6 with $\Omega = \mathbb{N}^*$. To that end, we define the measure μ by

$$\mu(I) = \sum_{i \in I} C_i^{init}, \quad I \subset \mathbb{N} \setminus \{0\}.$$

The condition $C^{init} \in X_\alpha^+$ ensures that the function $x \mapsto x^\alpha$ belongs to $\mathrm{L}^1(\Omega, \mathcal{B}, \mu)$. Therefore, using Theorem 3.6, there exists a function $U_0 \in \mathcal{K}_{1,\infty}$ such that $x \mapsto U_0(x^\alpha)$ belongs to $\mathrm{L}^1(\Omega, \mathcal{B}, \mu)$, i.e.

$$\mathcal{U}_0 := \sum_{i=1}^{+\infty} U_0(i^\alpha) C_i^{init} < \infty. \tag{3.10}$$

Moreover, for $n \geq i$,

$$C_i^n(t) \leq M_\alpha^n(t) \leq \lambda T + \|C^{init}\|_{X_\alpha}, \text{ on } [0, T], \tag{3.11}$$

and by Lemma 3.5, the sequence $(C_i^n)_{n \geq i}$ is bounded in $\mathrm{L}^\infty(0, T) \cap \mathrm{W}^{1,1}(0, T)$ for each $i \geq 1$ and $T \in (0, \infty)$. Therefore, using Helly's theorem [33, Théorème 5 (p. 372)], there exists a subsequence of $(C_i^n)_{n \geq i}$, still denoted $(C_i^n)_{n \geq i}$, and a sequence C of bounded variation functions such that

$$\lim_{n \to \infty} C_i^n(t) = C_i(t), \quad \forall i \geq 1, \ \forall t \geq 0. \tag{3.12}$$

Thus, using (3.11) and (3.12), we have $C \in X_\alpha^+$, with

$$\|C(t)\|_{X_\alpha^+} \leq \lambda T + \|C^{init}\|_{X_\alpha}. \tag{3.13}$$

It now remains to show that the potential candidate C is indeed a solution of (1.1), satisfying $C(0) = C^{init}$. To that end, we need to show two estimates. First, as $U_0 \in \mathcal{K}_{1,\infty}$, using Lemma 3.4 and

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(3.10), we have for all $T \geq 0$, and $n \geq 3$,

$$\sum_{i=1}^{n} U_0(i^\alpha) C_i^n(t) \leq \xi(T), \quad t \in [0, T], \tag{3.14}$$

where the constant $\xi(T)$ depend only on a, C^{init}, U_0, and T.

Let $T \in (0, +\infty)$ and $m \geq 2$, considering $C_i^n = 0$ if $i \geq n$, the previous estimate becomes, for $n \geq m + 1$,

$$\sum_{i=1}^{m} U_0(i^\alpha) C_i^n(t) \leq \xi(T), \quad t \in [0, T].$$

Thanks to (3.12), we can pass to the limit when $n \to +\infty$ in the previous estimates; thus, it stays true substituting C_i^n by C_i. We then pass to the limit on $m \to +\infty$, and we obtain

$$\sum_{i=1}^{+\infty} U_0(i^\alpha) C_i(t) \leq \xi(T), \quad t \in [0, T]. \tag{3.15}$$

Second, using (H1) and (3.13), we obtain for all $i \geq 1$

$$\sum_{j=1}^{+\infty} a_j C_j \in \mathrm{L}^1(0, T). \tag{3.16}$$

Now, we state that, for all $i \geq 1$, we have

$$\lim_{n \to +\infty} \left\| C_1^n \sum_{j=1}^{n-1} a_j C_j^n - C_1 \sum_{j=1}^{+\infty} a_j C_j \right\|_{\mathrm{L}^1(0,T)} = 0, \tag{3.17}$$

$$\lim_{n \to +\infty} \left\| a_i C_i^n C_1^n - a_i C_i C_1 \right\|_{\mathrm{L}^1(0,T)} = 0, \tag{3.18}$$

$$\lim_{n \to +\infty} \left\| b_i C_i^n - b_i C_i \right\|_{\mathrm{L}^1(0,T)} = 0. \tag{3.19}$$

The last two assertions (3.18) and (3.19) come from (3.12), (3.13), (3.6) and from Lebesgue-dominated convergence theorem. It remains to prove the first assertion (3.17). Let $i \geq 1$ fixed, and $m \geq 2$. As before, using (3.12), (3.13) and (3.6) and Lebesgue-dominated convergence theorem, we obtain for $m \leq n - 1$,

$$\lim_{n \to +\infty} \left\| \sum_{j=1}^{m} a_j \left(C_1^n C_j^n - C_1 C_j \right) \right\|_{\mathrm{L}^1(0,T)} = 0. \tag{3.20}$$

Moreover, for $n - 1 \geq m + 1$, and using (H1), (3.13) and (3.15), we obtain

$$\begin{aligned}
\left\| \sum_{j=m+1}^{+\infty} a_j C_1 C_j \right\|_{\mathrm{L}^1(0,T)} &\leq a\left(\lambda T + \|C^{init}\|_{X_\alpha}\right) \left\| \sum_{j=m+1}^{+\infty} j^\alpha C_j \right\|_{\mathrm{L}^1(0,T)} \\
&\leq a\left(\lambda T + \|C^{init}\|_{X_\alpha}\right) \sup_{j \geq m+1} \frac{j^\alpha}{U_0(j^\alpha)} \left\| \sum_{j=m+1}^{+\infty} U_0(j^\alpha) C_j \right\|_{\mathrm{L}^1(0,T)} \\
&\leq a\left(\lambda T + \|C^{init}\|_{X_\alpha}\right) T \xi(T) \sup_{j \geq m+1} \frac{j^\alpha}{U_0(j^\alpha)}.
\end{aligned} \tag{3.21}$$

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Likewise, using (H1), (3.6) and (3.14), we obtain

$$\begin{aligned}\left\|\sum_{j=m+1}^{n-i} a_j C_1^n C_j^n\right\|_{\mathrm{L}^1(0,T)} &\le a\big(\lambda T + \|C^{init}\|_{X_\alpha}\big)\left\|\sum_{j=m+1}^{+\infty} j^\alpha C_j^n\right\|_{\mathrm{L}^1(0,T)}\\ &\le a\big(\lambda T + \|C^{init}\|_{X_\alpha}\big)\sup_{j\ge m+1}\frac{j^\alpha}{U_0(j^\alpha)}\left\|\sum_{j=m+1}^{+\infty} U_0(j^\alpha)C_j^n\right\|_{\mathrm{L}^1(0,T)}\\ &\le a\big(\lambda T + \|C^{init}\|_{X_\alpha}\big)T\xi(T)\sup_{j\ge m+1}\frac{j^\alpha}{U_0(j^\alpha)}. \end{aligned} \tag{3.22}$$

Therefore, combining (3.20)–(3.22), we obtain that for all $m \ge 2$,

$$\limsup_{n\to+\infty}\left\|\sum_{j=1}^{n-1} a_j C_1^n C_j^n - \sum_{j=1}^{+\infty} a_j C_1 C_j\right\|_{\mathrm{L}^1(0,T)} \le 2a\big(\lambda T + \|C^{init}\|_{X_\alpha}\big)T\xi(T)\sup_{j\ge m+1}\frac{j^\alpha}{U_0(j^\alpha)}.$$

As U_0 belongs to $\mathcal{K}_{1,\infty}$, we have that the right-hand side of the above inequality tends to 0 when $m \to +\infty$, thus we obtain (3.17).

Now, thanks to (3.12) and (3.17)–(3.19), passing to the limit in n we obtain (*ii*) of the Definition 2.1. By (3.16), we recover the continuity of C_i for all $i \ge 1$. Therefore, we have shown that $C = (C_i)_{i\ge1} \in X_\alpha^+$ is a solution of (1.1) on $[0,T]$ satisfying $C(0) = C^{init}$. Note that the continuity of $C(\cdot)$ comes from the uniform convergence thanks to Dini's theorem of the sequence of continuous functions $\left(\sum_{i=1}^{n} i^\alpha C_i(\cdot)\right)_{n\ge1}$ on $[0,T]$.

To conclude, we only need to show that the solution constructed in the previous proof enjoys the additional property (3.3). As $U \in \mathcal{K}_1 \cup \mathcal{K}_2$, (3.3) follows from Lemma 3.4 and the convergence (3.12). □

4. Uniqueness

We first need some estimates on a solution that satisfies (2.3). These are as follows:

Lemme 4.1. *A solution C of (1.1) on $[0,T)$ which satisfy the condition (2.3) also satisfies, for all $t \in (0,T)$,*

$$\lim_{n\to+\infty}\int_0^t n^\alpha a_n C_n(s)C_1(s)ds = 0, \tag{4.1}$$

$$\lim_{n\to+\infty}\int_0^t \sum_{i=n}^{+\infty} a_i C_i(s)C_1(s)ds = 0. \tag{4.2}$$

Proof. Let $n \ge 2$ and $t \in (0,T)$, recalling (H1), we have

$$\int_0^t n^\alpha a_n C_1 C_n ds \le \int_0^t \sum_{i=n}^{+\infty} i^\alpha a_i C_i C_1 ds \le a\int_0^t \sum_{i=n}^{+\infty} i^{2\alpha} C_i C_1 ds.$$

and

$$\int_0^t \sum_{i=n}^{+\infty} a_i C_i C_1 ds \le a\int_0^t \sum_{i=n}^{+\infty} i^{2\alpha} C_i C_1 ds.$$

Therefore, both assertions (4.1) and (4.2) come from Lebesgue-dominated convergence theorem using (2.4) and (2.3). □

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Proof of Theorem 2.4. Let $C=(C_i)_{i\geq 1}$ and $D=(D_i)_{i\geq 1}$ denote two solutions of (1.1) on $[0,T)$ with $C(0)=D(0)=C^{init}$, which satisfy (2.3). For $i\geq 1$, defines

$$z_i := C_i - D_i, \text{ and } g_i := i^\alpha \operatorname{sign}(z_i),$$

where sign denotes the sign function, i.e. $\operatorname{sign}(x)=\frac{x}{|x|}$ for $x\in\mathbb{R}^*$ and $\operatorname{sign}(0)=0$. Now, we fix $n\geq 2$, and $t\in(0,T)$. The goal is to show that $\|z(t)\|_{X_\alpha}=0$, which will entail the desired uniqueness result.

Note that if $f\in AC(\mathbb{R})$, then $|f|\in AC(\mathbb{R})$, and therefore

$$\frac{d}{dt}|f(t)| = \operatorname{sign}(f(t))\frac{df}{dt}(t) \text{ a.e. in } \mathbb{R}.$$

Since C and D are absolute continuous functions, z is also an absolute continuous function, and therefore, using the integral form of (1.1), we obtain

$$\begin{aligned}
\sum_{i=1}^{n} i^\alpha |z_i(t)| = \sum_{i=1}^{n} g_i z_i(t) = &- \int_0^t \sum_{j=1}^{+\infty} g_1 a_j [C_1(s)C_j(s) - D_1(s)D_j(s)] + g_1 a_1 \left[C_1(s)^2 - D_1(s)^2\right] ds \\
&+ \sum_{i=2}^{n} \int_0^t g_i a_{i-1} \left[C_{i-1}(s)C_1(s) - D_{i-1}(s)D_1(s)\right] ds \\
&- \sum_{i=2}^{n} \int_0^t g_i a_i \left[C_i(s)C_1(s) - D_i(s)D_1(s)\right] ds \\
&+ \sum_{i=2}^{n} \left(- \int_0^t g_i b_i \left[C_i(s) - D_i(s)\right] ds + \int_0^t g_i b_{i+1} \left[C_{i+1}(s) - D_{i+1}(s)\right] ds \right) \\
= &\int_0^t \sum_{i=1}^{n-1} (g_{i+1} - g_i - g_1) a_i [C_i(s)C_1(s) - D_i(s)D_1(s)] ds \\
&- \int_0^t g_n a_n [C_1(s)C_n(s) - D_1(s)D_n(s)] ds \\
&- \sum_{i=n}^{+\infty} \int_0^t g_1 a_i \left[C_i(s)C_1(s) - D_i(s)D_1(s)\right] ds \\
&+ \sum_{i=2}^{n} \left(- \int_0^t g_i b_i \left[C_i(s) - D_i(s)\right] ds + \int_0^t g_i b_{i+1} \left[C_{i+1}(s) - D_{i+1}(s)\right] ds \right).
\end{aligned}$$

However, $C_i(s)C_1(s) - D_i(s)D_1(s) = C_i(s)z_1(s) + D_1(s)z_i(s)$, therefore

$$\begin{aligned}
\sum_{i=1}^{n} i^\alpha |z_i(t)| \leq &\int_0^t \sum_{i=1}^{n-1} (g_{i+1} - g_i - g_1) a_i [C_i(s)z_1(s) + z_i(s)D_1(s)] ds \\
&- \int_0^t g_n a_n [C_1(s)C_n(s) - D_1(s)D_n(s)] ds \\
&- \sum_{i=n}^{+\infty} \int_0^t g_1 a_i \left[C_i(s)C_1(s) - D_i(s)D_1(s)\right] ds \\
&+ \sum_{i=2}^{n} \left(- \int_0^t g_i b_i \left[C_i(s) - D_i(s)\right] ds + \int_0^t g_i b_{i+1} \left[C_{i+1}(s) - D_{i+1}(s)\right] ds \right).
\end{aligned}$$

As $\operatorname{sign}(x)\leq 1$ for all $x\in\mathbb{R}$, we have for all $i,j\geq 1$,

$$\begin{aligned}
(g_{i+j} - g_i - g_j) z_j &= ((i+j)^\alpha \operatorname{sign}(z_{i+j}) - i^\alpha \operatorname{sign}(z_i) - j^\alpha \operatorname{sign}(z_j)) z_j \\
&= ((i+j)^\alpha \operatorname{sign}(z_{i+j}z_j) - i^\alpha \operatorname{sign}(z_i z_j) - j^\alpha) |z_j| \\
&\leq ((i+j)^\alpha + i^\alpha - j^\alpha) |z_j| \\
&\leq 2i^\alpha |z_j|. \qquad (4.3)
\end{aligned}$$

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Moreover, using (H1), we obtain

$$\sum_{i=2}^{n}\left(-\int_0^t g_i b_i z_i(s)ds+\int_0^t g_i b_{i+1}z_{i+1}(s)ds\right)=\int_0^t\sum_{i=2}^{n-1}g_{i-1}b_i z_i(s)-\sum_{i=2}^{n}g_i b_i z_i(s)ds$$
$$=-\int_0^t\sum_{i=2}^{n-1}(g_i-g_{i-1})b_i z_i(s)ds-\int_0^t\underbrace{n^\alpha b_n|z_n(s)|}_{\geq 0}ds.$$

However, $(g_i-g_{i-1})z_i=(i^\alpha-(i-1)^\alpha\text{sign}(z_{i-1}z_i))|z_i|\geq 0$, this entails that

$$\sum_{i=2}^{n}\left(-\int_0^t g_i b_i z_i(s)ds+\int_0^t g_i b_{i+1}z_{i+1}(s)ds\right)\leq 0. \tag{4.4}$$

Therefore, using (4.3) and (4.4), we have

$$\sum_{i=1}^{n}i^\alpha|z_i(t)|\leq\int_0^t\sum_{i=1}^{n-1}a_i i^\alpha|z_1(s)|C_i(s)+\sum_{i=1}^{n-1}a_i|z_i(s)|D_1(s)ds$$
$$-\int_0^t g_n a_n[C_1(s)C_n(s)-D_1(s)D_n(s)]ds$$
$$-\int_0^t\sum_{i=n}^{+\infty}g_1 a_i\left[C_i(s)C_1(s)-D_i(s)D_1(s)\right]ds. \tag{4.5}$$

We now treat one by one the three terms on the right-hand side of the above inequality.
First term: Using (H1), we have

$$\int_0^t\sum_{i=1}^{n-1}a_i i^\alpha|z_1(s)|C_i(s)ds+\int_0^t\sum_{i=1}^{n-1}a_i|z_i(s)|D_1(s)ds$$
$$\leq\int_0^t\sum_{i=1}^{n}i^\alpha a_i C_i(s)\sum_{i=1}^{n}|z_i(s)|+\sum_{i=1}^{n}a_i|z_i(s)|\sum_{i=1}^{n}i^\alpha D_i(s)ds$$
$$\leq\int_0^t\left(\sum_{i=1}^{n}i^\alpha a_i C_i(s)+a\sum_{i=1}^{n}i^\alpha D_i(s)\right)\sum_{i=1}^{n}i^\alpha|z_i(s)|ds.$$

Using (2.3) and Lebesgue-dominated convergence theorem, we obtain

$$\lim_{n\to+\infty}\int_0^t\sum_{i=1}^{n-1}a_i i^\alpha|z_1(s)|C_i(s)+\sum_{i=1}^{n-1}a_i|z_i(s)|D_1(s)ds$$
$$\leq\int_0^t\left(\sum_{i=1}^{+\infty}i^\alpha a_i C_i(s)+a\big(\lambda T+\|C^{init}\|_{X_\alpha}\big)\right)\sum_{i=1}^{+\infty}i^\alpha|z_i(s)|ds. \tag{4.6}$$

Second term: As $-g_n[C_1C_n-D_1D_n]\leq n^\alpha[C_1C_n+D_1D_n]$, we have

$$-\int_0^t g_n a_n[C_1(s)C_n(s)-D_1(s)D_n(s)]ds\leq\int_0^t n^\alpha a_n C_1(s)C_n(s)ds+\int_0^t n^\alpha a_n D_1(s)D_n(s)ds.$$

Using (H1) and (4.1) from Lemma 4.1, we obtain

$$\lim_{n\to+\infty}-\int_0^t g_n a_n[C_1(s)C_n(s)-D_1(s)D_n(s)]ds=0. \tag{4.7}$$

Third term: We have

$$-\int_0^t\sum_{i=n}^{+\infty}g_1 a_i\left[C_i(s)C_1(s)-D_i(s)D_1(s)\right]ds\leq\int_0^t\sum_{i=n}^{+\infty}a_i C_1(s)C_i(s)ds+\int_0^t\sum_{i=n}^{+\infty}a_i D_1(s)D_i(s)ds.$$

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Therefore, using (4.2) from Lemma 4.1, we obtain

$$\lim_{n\to+\infty} -\int_0^t \sum_{i=n}^{+\infty} g_1 a_i \left[C_i(s)C_1(s) - D_i(s)D_1(s)\right] ds = 0. \tag{4.8}$$

Passing to the limit $n \to +\infty$ in (4.5), the previous estimations (4.6)–(4.8) entail that

$$\sum_{i=1}^{+\infty} i^\alpha |z_i(t)| \le \int_0^t \left(\sum_{i=1}^{+\infty} i^\alpha a_i C_i(s) + a\big(\lambda T + \|C^{init}\|_{X_\alpha}\big)\right) \sum_{i=1}^{+\infty} i^\alpha |z_i(s)| ds.$$

Then, applying Grönwall's lemma, we obtain that for all $t \in [0, T)$,

$$\sum_{i=1}^{+\infty} i^\alpha |z_i(t)| \le 0,$$

which entails $C = D$ and ends the proof. □

5. Long-time behaviour

5.1. Uniform-in-time bound

We start by proving Proposition 2.6.

Proof of Proposition 2.6. Let $M > 1$, for convenience, we rewrite condition (2.6) as

$$\frac{b_i}{a_i} \ge M\kappa \text{ for all } i \ge 1. \tag{5.1}$$

Let $t \ge 0$ and $\mu \in (1, M)$. We have the following formal computations:

$$\begin{aligned}
\frac{d}{dt}\sum_{i=1}^{+\infty} \mu^i C_i(t) &= \mu\left(\lambda - \sum_{j=1}^{+\infty} a_j C_j(t) C_1(t) - a_1 C_1(t)^2\right) + \sum_{i=2}^{+\infty} \mu^i (J_{i-1}(t) - J_i(t)) \\
&= \mu\left(\lambda - \sum_{j=1}^{+\infty} a_j C_j(t) C_1(t) - a_1 C_1(t)^2\right) + (\mu-1)\sum_{i=1}^{+\infty} \mu^i J_i + \mu(a_1 C_1(t)^2 - b_2 C_2(t)) \\
&\le \mu\lambda - \mu a_1 C_1(t)^2 + (\mu-1)\sum_{i=1}^{+\infty} \mu^i (a_i C_i(t) C_1(t) - b_{i+1} C_{i+1}(t)) + \mu(a_1 C_1(t)^2 - b_2 C_2(t)) \\
&= \mu\lambda + (\mu-1)\sum_{i=1}^{+\infty} \mu^{i-1} a_i \left(\mu C_1(t) - \frac{b_i}{a_i}\right) C_i(t) + (\mu-1) b_1 C_1(t) - \mu b_2 C_2(t) \\
&= \mu\lambda + \frac{(\mu-1)}{\mu}\sum_{i=1}^{+\infty} \mu^i a_i \left(\mu C_1(t) - \frac{b_i}{a_i}\right) C_i(t) + (\mu-1) b_1 C_1(t) - \mu b_2 C_2(t) \\
&\le \mu\lambda + (\mu-1) b_1 C_1(t) + \frac{(\mu-1)}{\mu}\sum_{i=1}^{+\infty} \mu^i a_i \left(\mu C_1(t) - \frac{b_i}{a_i}\right) C_i(t).
\end{aligned}$$

Then, using (2.4) and (5.1) and denoting $\varepsilon = (M-\mu)\kappa > 0$, we have

$$\begin{aligned}
\frac{d}{dt}\sum_{i=1}^{+\infty} \mu^i C_i(t) &\le \mu\lambda + (\mu-1) b_1 \kappa - \varepsilon \frac{\mu-1}{\mu}\sum_{i=1}^{+\infty} a_i \mu^i C_i(t) \\
&\le \mu\lambda + (\mu-1) b_1 \kappa - \varepsilon \frac{\mu-1}{\mu} \underline{a} \sum_{i=1}^{+\infty} \mu^i C_i(t).
\end{aligned}$$

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Therefore, using Grönwall's lemma, we obtain for all $t \geq 0$ and $\mu \in (1, M)$,

$$\sum_{i=1}^{+\infty} \mu^i C_i(t) \leq \sum_{i=1}^{+\infty} \mu^i C_i^{init} + \frac{\lambda\mu + (\mu-1)b_1\kappa}{\varepsilon \frac{\mu-1}{\mu} \underline{a}} := \Xi_1,$$

where Ξ_1 depends only on λ, $(a_i)_{i\geq 1}$, $(b_i)_{i\geq 1}$, μ and the initial condition. Taking $\nu = \ln(\mu)$, we have the desired estimation (2.8).

The rigorous proof can be left to the reader, as it consists in reproducing these estimates on the truncated system (2.16), (3.4) and then letting $n \to +\infty$ using $C_i^n \to C_i$ and $\sum_{i=1}^n \mu^i C_i^n \to \sum_{i=1}^{+\infty} \mu^i C_i$. □

As mention in the beginning, we have an upper bound on the mass and lower bound on $C_1(t)$.

Proposition 5.1 (Mass uniform-in-time bound). *Let $b > 0$. Assume that $C^{init} \in X_1^+$ and that the kinetics coefficients satisfy the following conditions:*

$$\forall i \geq 1,\ b_i \geq bi. \tag{5.2}$$

Then, for all $t \geq 0$,

$$\sum_{i=1}^{+\infty} iC_i(t) \leq \max\left\{\sum_{i=1}^{+\infty} iC_i^{init}, \frac{\lambda + b_1\kappa}{b}\right\}. \tag{5.3}$$

Proof of Proposition 5.1. Recalling (2.1) and using the assumption (5.2) and the uniform-in-time bound of C_1 (2.4), we have for all $t \geq 0$,

$$\begin{aligned}\frac{d}{dt}\sum_{i=1}^{+\infty} iC_i(t) &= \lambda - b_2C_2 - \sum_{i=2}^{+\infty} b_iC_i \\ &\leq \lambda - 2bC_2 + b_1C_1 - b\sum_{i=1}^{+\infty} iC_i \\ &\leq \lambda + b_1\kappa - b\sum_{i=1}^{+\infty} iC_i.\end{aligned}$$

Therefore, for all $t \geq 0$,

$$\sum_{i=1}^{+\infty} iC_i(t) \leq \max\left\{\sum_{i=1}^{+\infty} iC_i^{init}, \frac{\lambda + b_1\kappa}{b}\right\}.$$ □

Proposition 5.2 (C_1 uniform-in-time positivity). *Let $a, b > 0$. Assume that the kinetics coefficients satisfy the following conditions:*

$$\forall i \geq 1,\ a_i \leq ai \ \text{ and } \ b_i \geq bi. \tag{5.4}$$

Then, there exists a constant $\eta > 0$ and $t_1 \geq 0$ such that for all $t \geq t_1$, we have

$$C_1(t) \geq \eta. \tag{5.5}$$

Proof of Proposition 5.2. First, using (5.4) and the uniform-in-time bound of the mass (5.3), we have for all $t \geq 0$,

$$\sum_{i=1}^{+\infty} a_iC_i(t) \leq a\sum_{i=1}^{+\infty} iC_i(t) \leq a\max\left\{\sum_{i=1}^{+\infty} iC_i^{init}, \frac{\lambda + b_1\kappa}{b}\right\}.$$

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Then, for all $t \geq 0$, we have

$$\begin{aligned}\frac{d}{dt}C_1(t) &= \lambda - \sum_{j=1}^{+\infty} a_j C_j(t) C_1(t) - a_1 C_1(t)^2 \\ &\geq \lambda - a \max\left\{\sum_{i=1}^{+\infty} i C_i^{init}, \frac{\lambda + b_1\kappa}{b}\right\} C_1(t) - a_1 C_1(t)^2.\end{aligned}$$

Therefore, as long as $C_1 \leq \min\left\{1, a\max\left\{\sum_{i=1}^{+\infty} iC_i^{init}, \frac{\lambda+b_1\kappa}{b}\right\} + a\right\}$, we have

$$\begin{aligned}\frac{d}{dt}C_1(t) &\geq \lambda - \left[a \max\left\{\sum_{i=1}^{+\infty} i C_i^{init}, \frac{\lambda + b_1\kappa}{b}\right\} + a_1\right] C_1(t) \\ &\geq \lambda - \left[a \max\left\{\sum_{i=1}^{+\infty} i C_i^{init}, \frac{\lambda + b_1\kappa}{b}\right\} + a\right] C_1(t) \geq 0.\end{aligned}$$

Hence, there exists $t_1 \geq 0$ such that for all $t \geq t_1$,

$$C_1(t) \geq \frac{1}{2}\min\left\{1, a\max\left\{\sum_{i=1}^{+\infty} iC_i^{init}, \frac{\lambda + b_1\kappa}{b}\right\} + a\right\} =: \eta. \qquad \square$$

5.2. Steady states

In this subsection, we prove Theorem 2.9. Let $C = (C_i)_{i\geq 1}$ a constant solution. From (1.1), we obtain

$$J_{i-1} = J_i, \ \forall i \geq 2.$$

Therefore, there exists $J \in \mathbb{R}$ such that

$$J_i = J, \ \forall i \geq 1. \tag{5.6}$$

We then have three possibilities: either $J = 0$, or $J > 0$ or $J < 0$. We immediately obtain that there is no steady state with a positive flux $J > 0$. Indeed, from (H1) and the positivity of solutions, we have

$$a_i C_1 C_i = J + b_{i+1} C_{i+1} \geq J.$$

Therefore,

$$\sum_{i=1}^{+\infty} a_i C_1 C_i \geq \sum_{i=1}^{+\infty} J = +\infty,$$

which means that there is no steady state when $J > 0$ due to the equation on C_1.

The case $J = 0$ gives the steady-state $(Q_i z^i)_{i\geq 1}$. Assuming that a steady state exists, we denote it C^{eq}, the equation (5.6) entails the following relation:

$$a_i C_1^{eq} C_i^{eq} = b_{i+1} C_{i+1}^{eq}, \ \forall i \geq 1.$$

Thus,

$$C_i^{eq} = \left(\prod_{j=2}^{i} \frac{a_{j-1}}{b_j}\right)\left(C_1^{eq}\right)^i = Q_i\left(C_1^{eq}\right)^i, \ \forall i \geq 1.$$

The steady state is therefore entirely determined by C_1^{eq}; to determine this value, we use the first equation of the system (1.1), which has not yet been used. We, therefore, have that C_1^{eq} is a solution of the following equation in z

$$\lambda = \sum_{j=1}^{+\infty} a_j Q_j z^{j+1} + a_1 z^2. \tag{5.7}$$

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By comparing with the critical production threshold λ_s defined in (2.10), the equation (5.7) admits a unique solution when $\lambda \leq \lambda_s$, which verifies $z \leq z_s$.

The last case is the negative flux $J < 0$. Using equation (5.6), we have

$$J(z) := a_i z g_i(z) - b_{i+1} g_{i+1}(z), \quad \forall i \geq 1, \tag{5.8}$$

where z and functions $g_i(z)$ designate a constant solution. In other words, we search for a steady state

$$C_i = g_i(z),$$

for all $i \geq 1$, with $g_1(z) = z$.

We now want to determine J and the g_i functions. To do this, we start from (5.8), divide the two members of this equality by $a_i Q_i z^{i+1}$, and using (2.9), we obtain

$$\frac{J(z)}{a_i Q_i z^{i+1}} = \frac{a_i z g_i(z)}{a_i Q_i z^{i+1}} - \frac{b_{i+1} g_{i+1}(z)}{a_i Q_i z^{i+1}} = \frac{g_i(z)}{Q_i z^i} - \frac{g_{i+1}(z)}{Q_{i+1} z^{i+1}} \tag{5.9}$$

Summing from $i = 1$ to $k - 1$, we obtain

$$J(z) \sum_{i=1}^{k-1} \frac{1}{a_i Q_i z^{i+1}} = 1 - \frac{g_k(z)}{Q_k z^k}. \tag{5.10}$$

Rewriting (5.10), we obtain the expression of $g_k(z)$ for all $k \geq 2$:

$$g_k(z) = Q_k z^k \left[1 - J(z) \sum_{i=1}^{k-1} \frac{1}{a_i Q_i z^{i+1}} \right], \tag{5.11}$$

and we also find $g_1(z) = z$.

In order for the sequence $(g_k(z))_{k \geq 1}$ to be a steady state, it needs to be summable against $(a_k)_{k \geq 1}$. We have

$$\sum_{k=2}^{+\infty} a_k g_k(z) = \sum_{k=2}^{+\infty} a_k Q_k z^k - J(z) \sum_{k=2}^{+\infty} a_k Q_k z_k \left(\sum_{i=1}^{k-1} \frac{1}{a_i Q_i z^{i+1}} \right).$$

From the definition of z_s as the radius of convergence of a power series, we observe that if $z > z_s$, then the series $\sum a_k Q_k z^k$ is divergent; therefore, there is no steady state in the super-critical case. We now suppose that $z \leq z_s$. We have for all $k \geq 1$,

$$\begin{aligned} a_k g_k(z) = a_k Q_k z^k \left[1 - J(z) \sum_{i=1}^{k-1} \frac{1}{a_i Q_i z^{i+1}} \right] &> |J(z)| a_k Q_k z_k \sum_{i=1}^{k-1} \frac{1}{a_i Q_i z^{i+1}} \\ &= |J(z)| \frac{a_k}{b_k} + \sum_{i=1}^{k-2} \frac{a_k Q_k}{a_i Q_i} z^{k-(i+1)} \end{aligned} \tag{5.12}$$

Therefore, using (H3) and (H4), if $z_s < +\infty$, then $a_k g_k(z)$ does not converge towards 0, and therefore, the series diverge. This implies that there is no steady state in the super-critical case, and no other steady state in the sub-critical case when z_s is finite.

It remains to prove the uniqueness of the steady state or the existence of an infinite number of steady-state depending on the comparison of the kinetics rates.

First case: $b_i \leq i a_i$ for $i \gg 1$. Recalling the expression (5.11), we show that in this case they are not summable against $(a_k)_{k \geq 1}$. Let $h(x) = \sum_{k=1}^{+\infty} a_k Q_k x^k$ for $x \in [0, z_s)$; noticing that all derivatives of h are

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increasing in x and using (2.9), we have

$$\begin{aligned}\sum_{k=2}^{+\infty} a_k g_k(z) &\geq |J| \sum_{k=2}^{+\infty} a_k Q_k z^k \sum_{i=1}^{k-1} \frac{1}{a_i Q_i z^{i+1}} = |J| \sum_{i=2}^{+\infty} \frac{1}{a_i Q_i z^{i+1}} \sum_{k=i+1}^{+\infty} a_k Q_k z^k \\ &= |J| \sum_{i=2}^{+\infty} \frac{1}{a_i Q_i z^{i+1}} \int_0^z h^{(i+1)}(t) \frac{(z-t)^i}{i!} dt \geq \frac{|J|}{z} \sum_{i=2}^{+\infty} \frac{1}{a_i Q_i z^i} \frac{h^{(i+1)}(0)}{i!} \int_0^z (z-t)^i dt \\ &= \frac{|J|}{z} \sum_{i=2}^{+\infty} \frac{(i+1)a_{i+1}}{b_{i+1}} \int_0^z \left(1 - \frac{t}{z}\right)^i dt = |J| \sum_{i=2}^{+\infty} \frac{a_{i+1}}{b_{i+1}} \\ &\geq |J| \sum_{i=2}^{+\infty} \frac{1}{i} = +\infty.\end{aligned}$$

Which proves that in this case, there is no other steady state.

Second case: $b_i > i^\nu a_i$ for $i \gg 1$ with $\nu > 1$. Using the relation (5.6), we obtain for $J < 0$

$$C_{i+1} = \frac{a_i z C_i + |J|}{b_{i+1}} \ \forall i \geq 1 \text{ and } C_1 = z.$$

Solving the recurring sequence, we obtain for $i \geq 2$

$$C_i = |J| \sum_{k=0}^{i-2} \frac{Q_i}{a_{i-1-k} Q_{i-1-k}} z^k + Q_i z^i.$$

First, we prove that this sequence is summable against $(a_i)_{i\geq 1}$. Since $\sum a_i Q_i z^i$ is finite for $z < z_s$, it remains to prove that the first term is summable against $(a_i)_{i\geq 1}$. We have

$$\sum_{i=1}^{+\infty} a_i \sum_{k=0}^{i-2} \left(\frac{Q_i}{a_{i-1-k} Q_{i-1-k}}\right) z^k = \sum_{k=0}^{+\infty} \sum_{i=k+2}^{+\infty} \frac{a_i Q_i}{a_{i-1-k} Q_{i-1-k}} z^k = \sum_{k=0}^{+\infty} \underbrace{\left[\sum_{j=2}^{+\infty} \frac{a_{j+k} Q_{j+k}}{a_{j-1} Q_{j-1}}\right]}_{:=\gamma_k} z^k$$

For all $k \geq 0$, we prove that $\gamma_k < +\infty$. Let $k \geq 0$, there exists $j_0 \gg 1$ such that for $j \geq j_0$ we have $Q_{j+k} \leq Q_j$. Thus, using (H4), the sequence of ratio is bounded by $K \geq 0$ and the hypothesis of the second case, we have

$$\sum_{j\geq j_0} \frac{a_{j+k} Q_{j+k}}{a_{j-1} Q_{j-1}} \leq \sum_{j\geq j_0} \frac{a_{j+k} Q_j}{a_{j-1} Q_{j-1}} = \sum_{j\geq j_0} \frac{a_{j+k}}{b_j} \leq \sum_{j\geq j_0} \frac{a_{j+k}}{j^\nu a_j} \leq K^{k+1} \sum_{j\geq j_0} \frac{1}{j^\nu} < +\infty.$$

This is where the hypothesis of the second case, mainly $\nu > 1$, is crucial. Otherwise, $\gamma_k = +\infty$ and the computation does not allow us to conclude. Computing the ratio of γ_k, we have

$$\frac{\gamma_{k+1}}{\gamma_k} = \frac{\sum_{j=2}^{+\infty} \frac{a_{j+k+1} Q_{j+k+1}}{a_{j-1} Q_{j-1}}}{\sum_{j=2}^{+\infty} \frac{a_{j+k} Q_{j+k}}{a_{j-1} Q_{j-1}}} = \frac{\sum_{j=2}^{+\infty} \frac{a_{j+k} Q_{j+k}}{a_{j-1} Q_{j-1}} \frac{a_{j+k+1}}{b_{j+k+1}}}{\sum_{j=2}^{+\infty} \frac{a_{j+k} Q_{j+k}}{a_{j-1} Q_{j-1}}}.$$

However, for $k \gg 1$ using the hypothesis of the second case, we have

$$\frac{a_{j+k+1}}{b_{j+k+1}} < \frac{a_{j+k+1}}{(j+k+1)^\nu a_{j+k+1}} < \frac{1}{(k+1)^\nu}.$$

Therefore,

$$\frac{\gamma_{k+1}}{\gamma_k} \leq \frac{1}{(k+1)^\nu} \xrightarrow{k\to+\infty} 0.$$

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Using D'Alembert's ratio test, the sum $\sum a_i C_i$ converges for all $z \geq 0$. To obtain a steady state, it remains to satisfy the first equation and if there is any condition on λ, z or J. The equation

$$a_1 z^2 + z|J| \sum_{k=0}^{+\infty} \gamma_k z^k + \sum_{k=1}^{\infty} a_k Q_k z^{k+1} = \lambda$$

admits, for all $J < 0$, a unique z such that the above equation is satisfied, since the left-hand side of the equation is a strictly increasing function of z from 0 to $+\infty$. We, therefore, obtain an infinity of steady states parameterised by J.

Remark 5.3. *Note that every sequence, even increasing sequence, cannot be compared in the previous two cases. However, both cases already show the critical point at which the existence of a unique or of multiple steady states changes drastically. In the case of power law coefficients, the two cases are exhaustive.*

5.3. Local exponential stability: Sub-critical case

Let $\Theta_i = Q_i z^i$ for all $i \geq 1$. We introduce the ansatz $C_i = \Theta_i(1 + h_i)$ where h_i denotes the fluctuation around Θ_i. We introduce the Hilbert space $\mathcal{H} := \ell^2(\Theta_i)$ and a subspace $\mathcal{H}_\mathcal{D} = \ell^2(\Theta_i(1 + \sigma_i^2))$ namely

$$\mathcal{H} = \left\{ h = (h_i)_{i\geq 1} : \|h\|_\mathcal{H} := \left(\sum_{i=1}^{+\infty} \Theta_i h_i^2 \right)^{1/2} < \infty \right\},$$

and

$$\mathcal{H}_\mathcal{D} = \left\{ h = (h_i)_{i\geq 1} : \|h\|_{\mathcal{H}_\mathcal{D}} := \left(\sum_{i=1}^{+\infty} \Theta_i (1 + \sigma_i^2) h_i^2 \right)^{1/2} < \infty \right\},$$

where the sequence $(\sigma_i)_{i\geq 1}$ is defined later in (5.19). The inner scalar product of $\mathcal{H}$ is denoted by $\langle \cdot, \cdot \rangle_\mathcal{H}$. We define two linear operators S and P on $\mathcal{H}$ by the following weak form

$$\sum_{i=1}^{+\infty} S_i(h)\Theta_i \varphi_i = \sum_{i=1}^{+\infty} [\varphi_{i+1} - \varphi_i - \varphi_1] a_i \Theta_1 \Theta_i (h_i + h_1 - h_{i+1}), \tag{5.13}$$

and

$$\sum_{i=1}^{+\infty} P_i(h)\Theta_i \varphi_i = -\varphi_1 \left(a_1 \Theta_1^2 h_2 + \sum_{i=1}^{+\infty} a_i \Theta_1 \Theta_i h_{i+1} \right), \tag{5.14}$$

for any compactly supported sequences $(h_i)_{i\geq 1}$ and $(\varphi_i)_{i\geq 1}$. We denote by L the sum of the previous operators, namely

$$L = S + P. \tag{5.15}$$

We also define a bilinear operator Γ by the following weak form

$$\sum_{i=1}^{+\infty} \Gamma_i(f, g)\Theta_i \varphi_i = \frac{1}{2} \sum_{i=1}^{+\infty} a_i \Theta_1 \Theta_i (f_1 g_i + f_i g_1)(\varphi_{i+1} - \varphi_i - \varphi_1),$$

for any compactly supported sequences $(f_i)_{i\geq 1}$, $(g_i)_{i\geq 1}$, and $(\varphi_i)_{i\geq 1}$. We note that $\Gamma(0, 0) = 0$.

The fluctuation h satisfies

$$\frac{d}{dt} h_i(t) = L_i(h(t)) + \Gamma_i(h(t), h(t)). \tag{5.16}$$

The aforementioned decomposition of the linear operator L is due to the fact that the operator S is the linear operator studied by Cañizo and Lods [15] for the Becker–Döring equations. Consequently, it is

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established that S is a symmetric operator in $\mathcal{H}$ and dissipative. Cañizo and Lods proved that the operator S admits a spectral gap in $\mathcal{H}$, and they have also proved a lower bound on this spectral gap. In order to prove that the steady state is then locally exponentially stable, it is necessary to establish estimates on the quadratic term Γ. However, finding estimates on the quadratic term Γ in a weighted ℓ^2 space is quite complicated. The approach proposed by Cañizo and Lods [15] is to extend the operator S in some weighted ℓ^1 space, with the aim of showing that the operator S still has a spectral gap in this space. Then, we control the quadratic term in this weighted ℓ^1 space, which is more treatable.

Our goal is to prove the same spectral gap holds whenever we control the perturbation operator P.

Remark 5.4. *We may also write the operator S in the strong form, for all compactly supported sequence* $h = (h_i)_{i\geq 1}$,

$$S_1(h) = -\frac{1}{\Theta_1}\left(W_1(h) + \sum_{k=1}^{+\infty} W_k(h)\right), \quad S_i(h) = \frac{1}{\Theta_i}\left(W_{i-1}(h) - W_i(h)\right),\ i \geq 2, \tag{5.17}$$

where

$$W_k(h) = a_k\Theta_1\Theta_k(h_k + h_1 - h_{k+1}). \tag{5.18}$$

As well as the operator L, for all compactly supported sequence $h = (h_i)_{i\geq 1}$,

$$L_i(h) = -\sigma_i h_i + \sum_{j=1}^{+\infty} \xi_{i,j} h_j, \quad \text{for } i \geq 1,$$

where σ_i *are defined by*

$$\sigma_1 = 3a_1 z + \sum_{i=1}^{+\infty} a_i\Theta_i, \quad \sigma_i = a_i z + b_i \ \text{ for } i \geq 2, \tag{5.19}$$

and $\xi_{i,j} = 0$ *for* $j \notin \{1, i-1, i+1\}$. *The other* $\xi_{i,j}$ *are not equal to zero but are not relevant in the following.*

The operator L is in general not continuous on $\mathcal{H}$; however, we give a dense subspace $\mathcal{H}_{\mathcal{D}}$ of $\mathcal{H}$ in which it is bounded:

Lemme 5.5. *Assume hypotheses (H1)–(H5). Then, there exists a constant* $K > 0$, *depending only on z and the coefficients* $(a_i)_{i\geq 1}$ *and* $(b_i)_{i\geq 1}$, *such that for any compactly supported sequence* $h = (h_i)_{i\geq 1}$, *we have*

$$\|L(h)\|_{\mathcal{H}} \leq K\|h\|_{\mathcal{H}_{\mathcal{D}}}.$$

Proof. Using triangular inequality, it is sufficient to prove this bound separately for S then P. We already know from Cañizo and Lods [15, Lemma 2.4] that this is true for the operator S. We prove it for the operator P. We show equivalently that

$$|\langle P(h), \phi\rangle_{\mathcal{H}}| \leq K\|h\|_{\mathcal{H}_{\mathcal{D}}}\|\phi\|_{\mathcal{H}}, \ \text{for all } \phi \in \mathcal{H}.$$

We have from the weak form of P (5.14), and using Cauchy–Schwarz's inequality,

$$\begin{aligned}|\langle P(h), \phi\rangle_{\mathcal{H}}| &\leq \sqrt{\Theta_1}\|\phi\|_{\mathcal{H}}\left(a_1\Theta_1|h_2| + \sum_{i=1}^{+\infty} a_i\Theta_i|h_{i+1}|\right)\\ &\leq K\|\phi\|_{\mathcal{H}}\left(\sum_{i=1}^{+\infty}\Theta_i\right)^{\frac{1}{2}}\left(\sum_{i=1}^{+\infty} a_i^2\Theta_i|h_{i+1}|^2\right)^{\frac{1}{2}}.\end{aligned}$$

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However, using (H3) and the definition of $(\sigma_i)_{i\geq 1}$ (5.19), we have

$$\left(\sum_{i=1}^{+\infty} a_i^2\Theta_i|h_{i+1}|^2\right)^{\frac{1}{2}} = \sum_{i=1}^{+\infty}\frac{\Theta_{i+1}}{\Theta_i}b_{i+1}^2\Theta_{i+1}|h_{i+1}|^2$$
$$\leq K\sum_{i=2}^{+\infty}\sigma_i^2\Theta_i|h_i|^2 \leq K\|h\|_{\mathcal{H}_\mathcal{D}}.$$

Combining the previous inequalities, we obtain the desired estimation on P and therefore on L. □

Proposition 5.6. *Assume (H1)–(H5). If (2.13) is satisfied, then the operator L admits a spectral gap $\mu_1 > 0$.*

Proof. As mentioned earlier, the operator S has been studied by Cañizo and Lods [15]. They proved that the eigenvalues are non-positive and that S admits a spectral gap $\mu_0 > 0$ when $z \in (0, z_s)$. Moreover, they found [15, Theorem 2.15] a lower bound on the spectral gap; namely,

$$\frac{1}{4D} \leq \mu_0,$$

where

$$D := \sup_{k\geq 1}\left(\sum_{j=k+1}^{+\infty} Q_j z^j\right)\left(\sum_{j=1}^{k}\frac{1}{a_j Q_j z^j}\right) \in (0, +\infty). \tag{5.20}$$

The fact that D is finite comes from our hypotheses on the coefficients (H1)–(H5). Moreover, for all $h \in \mathcal{H}$, using the definition of P and (H5), we have

$$\|P(h)\|_{\mathcal{H}}^2 \leq \frac{4b^2}{z}\left(\sum_{k=1}^{+\infty} k^\beta\Theta_k h_k\right)^2.$$

Then, using Cauchy–Schwarz's inequality, we obtain

$$\|P(h)\|_{\mathcal{H}}^2 \leq \frac{4b^2}{z}\left(\sum_{k=1}^{+\infty} k^{2\beta}Q_k z^k\right)\|h\|_{\mathcal{H}}^2,$$

this means that

$$|||P||| \leq \frac{2b}{\sqrt{z}}\sqrt{\sum_{k=1}^{+\infty} k^{2\beta}Q_k z^k} < +\infty. \tag{5.21}$$

We now compare the bound on the norm of P and the one on the spectral gap μ_0. A sufficient condition for the norm $|||P|||$ to be smaller than the spectral gap μ_0 is

$$\frac{1}{4D} > \frac{2b}{\sqrt{z}}\sqrt{\sum_{k=1}^{+\infty} k^{2\beta}Q_k z^k},$$

which is exactly

$$\frac{8b}{\sqrt{z}}\sqrt{\sum_{i=1}^{+\infty} i^{2\beta}Q_i z^i}\sup_{k\geq 1}\left(\sum_{j=k+1}^{+\infty} Q_j z^j\right)\left(\sum_{j=1}^{k}\frac{1}{a_j Q_j z^j}\right) < 1. \tag{2.13}$$

Using [28, Theorem III.1.3] on bounded perturbation operator, we have that under the condition (2.13) the linearised operator L admits a spectral gap $\mu_1 > 0$. □

To prove that the steady-state $(Q_i z^i)_{i\geq 1}$ of the full system (1.1) is locally exponentially stable, we now need to find some estimates on the quadratic term $\Gamma(h, h)$. As previously announced, we extend the operator L in a weighted ℓ^1 space.

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Let $\eta \in (0, \frac{1}{2}\log(\frac{z_s}{z}))$. We introduce two subspaces of ℓ^1, $\mathcal{Z} = \ell^1(e^{\eta i}\Theta_i)$ and $\mathcal{Z}_{\mathcal{D}} = \ell^1((1+\sigma_i)e^{\eta i}\Theta_i)$ namely

$$\mathcal{Z} = \left\{ h = (h_i)_{i\geq 1} : \|h\|_{\mathcal{Z}} := \sum_{i=1}^{+\infty} e^{\eta i}\Theta_i |h_i| < +\infty \right\},$$

and

$$\mathcal{Z}_{\mathcal{D}} = \left\{ h = (h_i)_{i\geq 1} : \|h\|_{\mathcal{Z}_{\mathcal{D}}} := \sum_{i=1}^{+\infty} (1+\sigma_i)e^{\eta i}\Theta_i |h_i| < +\infty \right\}.$$

The choice of η ensures that the space $\mathcal{Z}$ is larger than the previous Hilbert space $\mathcal{H} = \ell^2(\Theta)$, since

$$\|h\|_{\mathcal{Z}} = \sum_{k=1}^{+\infty} \exp(\eta i)\Theta_i |h_i| \leq \left(\sum_{i=1}^{+\infty} h_i^2 \Theta_i\right)^{\frac{1}{2}} \left(\sum_{i=1}^{+\infty} \exp(2\eta i)\Theta_i\right)^{\frac{1}{2}} = \left(\sum_{i=1}^{+\infty} \exp(2\eta i)\Theta_i\right)^{\frac{1}{2}} \|h\|_{\mathcal{H}},$$

and the last factor in the previous inequality is finite for $\eta < \frac{1}{2}\log(\frac{z_s}{z})$. Indeed, we have

$$\sum_{i=1}^{+\infty} Q_i z^i \exp(2\eta i) = \sum_{i=1}^{+\infty} Q_i r^i \text{ where } r = \exp(2\eta + \log(z)),$$

and recalling that the radius of convergence of the power series $\sum iQ_i z^i$ is z_s, then the above sum is finite whenever $r < z_s$, this is exactly when $\eta < \frac{1}{2}\log(z_s/z)$.

As before, the operator L is in general not continuous on $\mathcal{Z}$; however, we give a dense subspace $\mathcal{Z}_{\mathcal{D}}$ of $\mathcal{Z}$ in which it is bounded:

Lemme 5.7. *Assume hypotheses (H1)–(H5). Then, there exists a constant $K > 0$, depending only on $(a_i)_{i\geq 1}$, $(b_i)_{i\geq 1}$, z and η, such that for all compactly supported sequence $h = (h_i)_{i\geq 1}$, we have*

$$\|L(h)\|_{\mathcal{Z}} \leq K\|h\|_{\mathcal{Z}_{\mathcal{D}}}.$$

Proof. Using triangular inequality, it is sufficient to prove this bound separately for S then P. We already know from Cañizo and Lods [15, Lemma 3.3] that this is true for the operator S. We prove it for the operator P. Recalling the definition of P and using (H5), we have

$$\begin{aligned}\|P(h)\|_{\mathcal{Z}} &\leq \exp(\eta) z \left(\frac{1}{z}\left(b_2\Theta_2|h_2| + \sum_{k=2}^{+\infty} b_k\Theta_k|h_k|\right)\right) \\ &\leq 2b\exp(\eta)\sum_{k=1}^{+\infty} k^{\eta}\Theta_k|h_k|.\end{aligned}$$

Then, using that $k^{\beta} \leq K(\eta,\beta)\exp(\eta k)$ for all $k \geq 1$ and the positivity of σ_k (5.19) for all $k \geq 1$, we have

$$\begin{aligned}\|P(h)\|_{\mathcal{Z}} &\leq K(\eta,\beta)\sum_{k=1}^{+\infty} \exp(\eta k)\Theta_k|h_k| \\ &\leq K(\eta,\beta)\sum_{k=1}^{+\infty} (1+\sigma_k)\exp(\eta k)\Theta_k|h_k| = C\|h\|_{\mathcal{Z}_{\mathcal{D}}}.\end{aligned}$$

Combining this estimation with the one on S, we obtain the desired estimation. □

Following Cañizo and Lods [15], we extend the operator L to an unbounded operator on $\mathcal{Z}$ that has a positive spectral gap using techniques based upon a suitable decomposition of the linearised operator into a dissipative part and a "regularising" part. To extend the operator, we use [15, Theorem 3.1],

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which is a slight improvement over some of the consequences of the work of Gualdani, Mischler and Mouhot [30].

Theorem 5.8 (Extension of the spectral gap). *Assume hypotheses (H1)–(H5). Let* $\eta \in (0, \frac{1}{2}\log(\frac{z_s}{z}))$. *If (2.13) is satisfied, then the extension of* L *on* $\mathcal{Z}_\mathcal{D}$ *that we note* Λ *generates a strongly continuous semigroup* $(\exp(t\Lambda))_{t\geq 0}$ *on* $\mathcal{Z}_\mathcal{D}$ *and there exists* $\mu_* \in (0, \mu_1]$, *a constant* $K > 0$ *such that*

$$\|\exp(t\Lambda)x\|_\mathcal{Z} \leq K\exp(-\mu_* t)\|x\|_\mathcal{Z}, \ \forall t \geq 0 \text{ and } x \in \mathcal{Z}. \tag{5.22}$$

Proof. The proof follows the one of [15, Theorem 3.5]; to that end, we apply [15, Theorem 3.1]. The main modification is to add the operator P in the regularising part of the decomposition of Λ. We mean that an operator $\mathcal{A}$ is regularising if for all $h \in \mathcal{Z}$, $\mathcal{A}h \in \mathcal{H}$. We just have to show that this is true for our operator P. Let $h \in \mathcal{Z}$, we have

$$\begin{aligned}\|P(h)\|_\mathcal{H}^2 &\leq \frac{4b^2}{z}\left(\sum_{k=1}^{+\infty} b_k Q_k z^k h_k\right)^2 \\ &\leq \frac{4b^2}{z}K(\beta,\eta)\|h\|_\mathcal{Z}^2.\end{aligned}$$

Then, the proof is straightforward following the proof of [15, Theorem 3.5]. We obtain that our operator has a spectral gap $\mu_* \in (0, \mu_1)$. □

5.3.1. Proof of Theorem 2.11

As stated before, we can obtain an estimation on the quadratic term in a weighted ℓ^1 space. Indeed, Cañizo and Lods [15, Proposition 3.2] proved an estimation on the quadratic term Γ, it reads as follows:

Proposition 5.9. *Let* $\eta \in (0, \frac{1}{2}\log(\frac{z_s}{z}))$. *There is a constant* $K > 0$, *depending only on* $(a_i)_{i\geq 1}$, $(b_i)_{i\geq 1}$, *and* z, *such that*

$$\|\Gamma(h,h)\|_\mathcal{Z} \leq K\|h\|_\mathcal{Z}\|h\|_{\mathcal{Z}_\mathcal{D}}, \ \forall h \in \mathcal{Z}_\mathcal{D}. \tag{5.23}$$

Let $\eta \in (0, \min\{\nu, \frac{1}{2}\log\frac{z_s}{z}\})$, where ν comes from (2.7). The fluctuation h satisfies (5.16) in $\mathcal{Z}$, namely

$$\frac{d}{dt}h = \Lambda h + \Gamma(h,h).$$

Therefore, if $(V_t)_{t\geq 0}$ denotes the semigroup generates by Λ, we have

$$h(t) = V_t h(0) + \int_0^t V_{t-s}\Gamma(h(s),h(s))ds.$$

Using Proposition 5.9 and Theorem 5.8, we have for some constant $C > 0$,

$$\begin{aligned}\|h(t)\|_\mathcal{Z} &\leq \|V_t h(0)\|_\mathcal{Z} + \int_0^t \|V_{t-s}\Gamma(h(s),h(s))\|_\mathcal{Z} ds \\ &\leq K\|h(0)\|_\mathcal{Z}\exp(-\mu_* t) + K\exp(-\mu_* t)\int_0^t \exp(\mu_* s)\|\Gamma(h(s),h(s))\|_\mathcal{Z} ds \\ &\leq K\|h(0)\|_\mathcal{Z}\exp(-\mu_* t) + K\exp(-\mu_* t)\int_0^t \exp(\mu_* s)\|h(s)\|_\mathcal{Z}\|h(s)\|_{\mathcal{Z}_\mathcal{D}} ds,\end{aligned}$$

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For any $\upsilon \in (0, \nu - \eta)$, using Cauchy–Schwarz's inequality, we have

$$\begin{aligned}\|h(t)\|_{\mathcal{Z}_{\mathcal{D}}} &= \sum_{i=1}^{+\infty} |h_i(t)| i\Theta_i \exp(\eta i) \\ &\leq \left(\sum_{i=1}^{+\infty} |h_i(t)| i\Theta_i \exp(\eta i - \upsilon i)\right)^{\frac{1}{2}} \left(\sum_{i=1}^{+\infty} |h_i(t)| i\Theta_i \exp(\eta i + \upsilon i)\right)^{\frac{1}{2}}.\end{aligned}$$

However, $i \exp(-\upsilon i) \leq K$, and $i \exp(\eta i + \upsilon i) \leq K \exp(\nu i)$, for all $i \geq 1$. Therefore, we deduce from (2.8) that

$$\|h(t)\|_{\mathcal{Z}_{\mathcal{D}}} \leq K \|h(t)\|_{\mathcal{Z}}^{\frac{1}{2}} \left(\sum_{i=1}^{+\infty} |h_i(t)| \Theta_i \exp(\nu i)\right)^{\frac{1}{2}} \leq K \Xi_1^{\frac{1}{2}} \|h(t)\|_{\mathcal{Z}}^{\frac{1}{2}}, \ \forall t \geq 0.$$

All-in-one, we have

$$\|h(t)\|_{\mathcal{Z}} \leq K \|h(0)\|_{\mathcal{X}} \exp(-\mu_* t) + K \exp(-\mu_* t) \int_0^t \exp(\mu_* s) \|h(s)\|_{\mathcal{Z}}^{\frac{3}{2}} ds.$$

Let $u(t) = \|h(t)\|_{\mathcal{Z}} \exp(\mu_* t)$, we have

$$\begin{aligned}u(t) &\leq K \|h(0)\|_{\mathcal{Z}} + K \int_0^t u(s) \|h(s)\|_{\mathcal{Z}}^{\frac{1}{2}} ds \\ &\leq K\varepsilon + K \int_0^t \exp\left(-\frac{\mu_*}{2} s\right) u(s)^{\frac{3}{2}} ds.\end{aligned}$$

Using Grönwall's lemma, we have for some $K > 0$ and ε small enough,

$$u(t) \leq K.$$

This means that

$$\|h(t)\|_{\mathcal{Z}} \leq K \exp(-\mu_* t), \ \forall t \geq 0,$$

which is exactly what we want. Indeed, recalling the ansatz $C_i = \Theta_i(1 + h_i)$, we have

$$\|h(t)\|_{\mathcal{Z}} = \sum_{i=1}^{+\infty} e^{\eta i} Q_i z^i |h_i(t)| = \sum_{i=1}^{+\infty} e^{\eta i} |C_i(t) - Q_i z^i|,$$

and therefore, the previous inequality is exactly (2.15).

6. Numerical simulations

6.1. Numerical scheme

In this section, we describe a numerical scheme used for the conservative truncation (2.16). At the end, we will make a few comments about the non-conservative truncation.

Let $n \geq 2$ be an integer. Recalling the PDE (2.17) and (2.18), it remains to add the boundary conditions. As we are considering the conservative truncation, we have on the right side of our domain the following boundary condition:

$$J(t, n) = 0. \tag{6.1}$$

Now, on the left side of our domain, which is the production of monomers, we have the following ODE:

$$\frac{d}{dt} C(t, 1) = \lambda - \int_1^n a(x) C(t, 1) C(t, x) dx - a(1) C(t, 1)^2. \tag{6.2}$$

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6.1.1. Verification of the choice of PDE

We verify that with the right discretisation and the right mesh, we retrieve our system of equations (2.16). To do this, we use a uniform mesh with a size step $\Delta x = 1$, giving

$$C_i(t) \approx C(t,i),\ i = 1,\dots,n.$$

We discretise (2.17) using centre differences

$$\left.\frac{\partial J(t,x)}{\partial x}\right|_{x=x_i} \approx \frac{J(t,x_{i+1/2}) - J(t,x_{i-1/2})}{\Delta x},$$
$$\left.\frac{\partial}{\partial x}\left(\frac{C(t,x)}{Q(x)C(t,1)^x}\right)\right|_{x=x_{i+1/2}} \approx \frac{1}{\Delta x}\left(\frac{C_{i+1}(t)}{Q_{i+1}C_1^{i+1}(t)} - \frac{C_i(t)}{Q_i C_1^i(t)}\right).$$

Therefore, since $\Delta x = 1$ and from (2.19), we obtain

$$\left.\frac{\partial C(t,x)}{\partial t}\right|_{x=i} = -\left.\frac{\partial J(t,x)}{\partial x}\right|_{x=i} \approx \frac{J_{i-1}(t) - J_i(t)}{\Delta x} = \frac{d}{dt}C_i(t).$$

We just need to check the case $i = 1$, which comes from the left boundary condition (6.2). Using the rectangle rule to approximate the integral, we have

$$\frac{d}{dt}C(t,1) = \lambda - \int_1^n a(x)C(t,1)C(t,x)dx - a(1)C(t,1)^2 \approx \lambda - \sum_{j=1}^{n-1} a_j C_1(t)C_j(t) - a_1 C_1(t)^2 = \frac{d}{dt}C_1(t).$$

We have indeed found back our ODE (2.16) with a given scheme and a given mesh.

6.1.2. Reaction-diffusion (RD) scheme

We now follow the idea in [29] on a non-uniform mesh. Let $K > 0$ and $\mathbb{L}$ the set of all the nodes in our non-uniform mesh:

$$\mathbb{L} = \{n_1,\dots,n_K : n_j < n_{j+1},\ n_1 = 1,\ n_K = n\}.$$

We then define the following size step:

$$\Delta x_{j+1/2} = n_{j+1} - n_j \text{ and } \Delta x_j = n_{j+1/2} - n_{j-1/2} \text{ where } n_{j+1/2} = \frac{n_{j+1} + n_j}{2} \text{ with } n_j, n_{j+1} \in \mathbb{L}.$$

Using finite volume scheme, we discretise (2.17) and (2.18) as follows:

$$C_{n_j}^{k+1} - C_{n_j}^k = \frac{\Delta t}{\Delta x_j}\left(J_{n_{j-1/2}}^{k+1} - J_{n_{j+1/2}}^{k+1}\right), \tag{6.3}$$

with

$$J_{n_{j-1/2}}^{k+1} = -a_{n_{j-1/2}} Q_{n_{j-1/2}} \left(C_1^k\right)^{n_{j-1/2}+1/2} \frac{1}{\Delta x_{j-1/2}}\left(\frac{C_{n_j}^{k+1}}{Q_{n_j}\left(C_1^k\right)^{n_j}} - \frac{C_{n_{j-1}}^{k+1}}{Q_{n_{j-1}}\left(C_1^k\right)^{n_{j-1}}}\right). \tag{6.4}$$

At this point, it remains to choose what is $a_{n_{j-1/2}}$ and $Q_{n_{j-1/2}}$. To remain consistent with the discrete equations (i.e. when we take the step size equal to 1), we impose $a_{n_{j-1/2}} = a_{n_{j-1}}$ et $Q_{n_{j-1/2}} = Q_{n_{j-1}}$. We have tried to impose something else, and the numerical results were not satisfying. Let $M_{n_j}^k = Q_{n_j}\left(C_1^k\right)^{n_j}$, we have

$$Q_{n_{j-1}}\left(C_1^k\right)^{n_{j-1}} = M_{n_{j-1}} = \sqrt{M_{n_{j-1}}M_{n_j}}\sqrt{\frac{M_{n_{j-1}}}{M_{n_j}}} = \sqrt{M_{n_{j-1}}M_{n_j}}\sqrt{\prod_{k=n_{j-1}+1}^{n_j}\frac{b_k}{a_{k-1}}}\left(\sqrt{C_1^k}\right)^{-(n_j-n_{j-1})}.$$

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Using the above equality, we can rewrite (6.3), we obtain for all $2 \le j \le K-1$,

$$C_{n_j}^{k+1} - C_{n_j}^k = \frac{\Delta t}{\Delta x_j}\sqrt{M_j^k}\left(\frac{a_{n_j}\sqrt{C_1^k}}{\Delta x_{j+1/2}}\sqrt{\prod_{k=n_j+1}^{n_{j+1}}\frac{b_k}{a_{k-1}}}\frac{C_{n_{j+1}}^{k+1}}{\sqrt{M_{n_j}^k}} + \frac{a_{n_{j-1}}\sqrt{C_1^k}}{\Delta x_{j-1/2}}\sqrt{\prod_{k=n_{j-1}+1}^{n_j}\frac{b_k}{a_{k-1}}}\frac{C_{n_{j-1}}^k}{\sqrt{M_{n_{j-1}}^k}}\right.$$
$$\left. - \left(\frac{a_{n_j}}{\Delta x_{j+1/2}}\left(\sqrt{C_1^k}\right)^{n_{j+1}-n_j+1} + \frac{a_{n_{j-1}}}{\Delta x_{j-1/2}}\left[\prod_{k=n_{j-1}+1}^{n_j}\frac{b_k}{a_{k-1}}\right]\left(\sqrt{C_1^k}\right)^{1-(n_j-n_{j-1})}\right)\frac{C_{n_j}^{k+1}}{\sqrt{M_{n_j}^k}}\right).$$

Let $h_{n_j}^* := \dfrac{C_{n_j}^{k+1}}{\sqrt{M_{n_j}^k}}$ and $h_{n_j} = \dfrac{C_{n_j}^k}{\sqrt{M_{n_j}^k}}$, we then have for all $2 \le j \le K-1$,

$$h_{n_j}^* = h_{n_j}^k + \frac{\Delta t}{\Delta x_j}\left(\frac{a_{n_j}}{\Delta x_{j+1/2}}\sqrt{\prod_{k=n_j+1}^{n_{j+1}}\frac{b_k}{a_{k-1}}}\sqrt{C_1^k}h_{n_{j+1}}^* + \frac{a_{n_{j-1}}}{\Delta x_{j-1/2}}\sqrt{\prod_{k=n_{j-1}+1}^{n_j}\frac{b_k}{a_{k-1}}}\sqrt{C_1^k}h_{n_{j-1}}^*\right.$$
$$\left. - \left(\frac{a_{n_j}}{\Delta x_{j+1/2}}\left(\sqrt{C_1^k}\right)^{n_{j+1}-n_j+1} + \frac{a_{n_{j-1}}}{\Delta x_{j-1/2}}\left[\prod_{k=n_{j-1}+1}^{n_j}\frac{b_k}{a_{k-1}}\right]\left(\sqrt{C_1^k}\right)^{1-(n_j-n_{j-1})}\right)h_{n_j}^*\right).$$

As mentioned in the beginning of this section, we present this scheme on the conservative truncation (2.16); thus, we impose the zero flux condition on the right boundary, meaning $J_{n_{K+1/2}} = 0$. This condition may be rewritten as follows:

$$\frac{C_{n_{K+1}}^{k+1}}{M_{n_{K+1}}^k} = \frac{C_{n_K}^{k+1}}{M_{n_K}^k}, \quad \forall k > 0. \tag{6.5}$$

Therefore, the scheme becomes

$$C_1^{k+1} = C_1^k + \Delta t\left(\lambda - C_1^{k+1}\left(\sum_{j=1}^{K-1} a_{n_j}\Delta x_{j+1/2}C_{n_j}^k + a_1 C_1^k\right)\right)$$
$$h_1^* = \frac{1}{\sqrt{C_1^k}}\frac{C_1^k + \lambda\Delta t}{1 + \Delta t\left(\sum_{j=1}^{K-1} a_{n_j}\Delta x_{j+1/2}C_{n_j}^k + a_1 C_1^k\right)}$$
$$h_{n_j}^* = h_{n_j}^k + \frac{\Delta t}{\Delta x_j}\left(\frac{a_{n_j}}{\Delta x_{j+1/2}}\sqrt{\prod_{k=n_j+1}^{n_{j+1}}\frac{b_k}{a_{k-1}}}\sqrt{C_1^k}h_{n_{j+1}}^* + \frac{a_{n_{j-1}}}{\Delta x_{j-1/2}}\sqrt{\prod_{k=n_{j-1}+1}^{n_j}\frac{b_k}{a_{k-1}}}\sqrt{C_1^k}h_{n_{j-1}}^*\right.$$
$$\left. - \left(\frac{a_{n_j}}{\Delta x_{j+1/2}}\left(\sqrt{C_1^k}\right)^{n_{j+1}-n_j+1} + \frac{a_{n_{j-1}}}{\Delta x_{j-1/2}}\left[\prod_{k=n_{j-1}+1}^{n_j}\frac{b_k}{a_{k-1}}\right]\left(\sqrt{C_1^k}\right)^{1-(n_j-n_{j-1})}\right)h_{n_j}^*\right)$$
$$h_{n_K}^* = h_{n_K} + \frac{\Delta t}{\Delta x_K}\left(\frac{a_{n_{K-1}}}{\Delta x_{K-1/2}}\sqrt{\prod_{k=n_{K-1}+1}^{n_K}\frac{b_k}{a_{k-1}}}\sqrt{C_1^k}h_{n_{K-1}}\right.$$
$$\left. - \frac{a_{n_{K-1}}}{\Delta x_{K-1/2}}\left[\prod_{k=n_{K-1}+1}^{n_K}\frac{b_k}{a_{k-1}}\right]\left(\sqrt{C_1^k}\right)^{1-(n_K-n_{K-1})}h_{n_K}\right). \tag{6.6}$$

Numerically to implement (6.6), we solve the following linear system:

$$\left(I_{K-1} - \Delta t\mathrm{W}^k\right)H^* = H + \beta^k, \tag{6.7}$$

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where

$$H^* = \begin{pmatrix} h_2^* \\ \vdots \\ \vdots \\ \vdots \\ h_{n_K}^* \end{pmatrix}, \quad H = \begin{pmatrix} h_2 \\ \vdots \\ \vdots \\ \vdots \\ h_{n_K} \end{pmatrix}, \quad \beta^k = \frac{\Delta t}{\Delta x_2 \Delta x_{2-1/2}} a_{n_1} \sqrt{C_1^k} \sqrt{\prod_{k=n_1+1}^{n_2} \frac{b_k}{a_{k-1}}} \begin{pmatrix} h_1^* \\ 0 \\ \vdots \\ \vdots \\ 0 \end{pmatrix},$$

and the tri-diagonal matrix

$$\mathsf{W}^k = \begin{pmatrix} -\omega_{n_2}^k & \alpha_{n_{2+1/2}} & 0 & \cdots & 0 & 0 \\ \gamma_{n_{3-1/2}} & -\omega_{n_3}^k & \alpha_{n_{3+1/2}} & & \vdots & \vdots \\ 0 & \gamma_{n_{4-1/2}} & -\omega_{n_4}^k & & 0 & \\ \vdots & & & & \alpha_{n_{K-3/2}} & 0 \\ 0 & \cdots & 0 & \gamma_{n_{K-3/2}} & -\omega_{n_{K-1}}^k & \alpha_{n_{K-1/2}} \\ 0 & \cdots & \cdots & 0 & \gamma_{n_{K-1/2}} & -\nu_{n_K}^k \end{pmatrix},$$

with for $2 \leq j \leq K-1$,

$$\omega_{n_j}^k = \frac{1}{\Delta x_j} \left(\frac{a_{n_j}}{\Delta x_{j+1/2}} \left(\sqrt{C_1^k} \right)^{n_{j+1}-n_j+1} + \frac{a_{n_{j-1}}}{\Delta x_{j-1/2}} \left[\prod_{k=n_{j-1}+1}^{n_j} \frac{b_k}{a_{k-1}} \right] \left(\sqrt{C_1^k} \right)^{1-(n_j-n_{j-1})} \right),$$

$$\alpha_{n_{j+1/2}} = \frac{1}{\Delta x_j} \frac{a_{n_j}}{\Delta x_{j+1/2}} \sqrt{\prod_{k=n_j+1}^{n_{j+1}} \frac{b_k}{a_{k-1}}} \sqrt{C_1^k}, \quad \gamma_{n_{j-1/2}} = \frac{1}{\Delta x_j} \frac{a_{n_{j-1}}}{\Delta x_{j-1/2}} \sqrt{\prod_{k=n_{j-1}+1}^{n_j} \frac{b_k}{a_{k-1}}} \sqrt{C_1^k},$$

and

$$\nu_{n_K}^k = \frac{1}{\Delta x_K} \frac{a_{n_{K-1}}}{\Delta x_{K-1/2}} \left[\prod_{k=n_{K-1}+1}^{n_K} \frac{b_k}{a_{k-1}} \right] \left(\sqrt{C_1^k} \right)^{1-(n_K-n_{K-1})}.$$

Remark 6.1. *As opposed to uniform mesh, the matrix* W^k *is no longer symmetric, which can translate in a loss of computation time. Therefore, to symmetrise this matrix while keeping the tri-diagonal form, we can multiply the matrix by*

$$\Theta = \operatorname{diag} \left(\frac{\Delta x_j}{\Delta x_1} \right)_{2 \leq j \leq K}.$$

The scheme on h^* (6.6) is unconditionally stable in time and size. Indeed, the only restriction could be on the time step because of Euler's explicit–implicit scheme for C_1, but this scheme is also unconditionally stable. We have

$$C_1^{k+1} \left(1 + \Delta t \left(a_1 C_1^k + \sum_{j=1}^{K-1} a_{n_j} \Delta x_{j+1/2} C_{n_j}^k \right) \right) = C_1^k + \Delta t \lambda$$

thus

$$C_1^{k+1} \leq C_1^k + \Delta t \lambda,$$

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which leads to, for $0 \leq t^k \leq T$,

$$C_1^k \leq C_1^0 + \lambda t^k \leq C_1^0 + \lambda T.$$

Remark 6.2. *We could just do an Euler explicit scheme for (6.2), but then we would have two conditions on the time step Δt: stability and to preserve positivity. This would lead to having an adaptive time step Δt^k.*

We now have a well-balanced scheme that is unconditionally stable in time and size. However, there is a difference with the uniform mesh with $\Delta x = 1$ or with the ODEs, which is the parameter z of the steady-state. Indeed, equation (6.6) for $j \geq 2$ implies that the steady state is of the form $Q_{n_j}\eta^{n_j}$, and the parameter η is determined with the equation on C_1. The difference comes from the following two equations:

$$\lambda - \sum_{i=1}^{N-1} a_i Q_i z^{i+1} - a_1 z^2 = 0 \text{ and } \lambda - \sum_{j=1}^{K-1} a_{n_j} \Delta x_{n_{j+1/2}} Q_{n_j} \tilde{z}^{n_j+1} - a_{n_1}\tilde{z}^2 = 0, \tag{6.8}$$

which do not have the same solutions. In fact, the difference of the two solutions is of order $Q_{n_l}\tilde{z}^{n_l}$ where l is defined as follows:

$$l = \min\left\{j \in \{1, \ldots, K-1\} \,:\, \Delta x_{j+1/2} > 1\right\}.$$

A difference is expected since we reduce the linear system; therefore, we lost information that translates into a slight difference in the steady state. We note that we can compute the steady state on a uniform mesh with $\Delta x = 1$ and, therefore, choose the right mesh to control the error. Morally, if we choose a mesh with $\Delta x = 1$ for small size and whatever we want for bigger size, then we approach the right steady state.

Remark 6.3 (Non-conservative truncation). *Changing the right boundary condition (6.5) to one taking account things that can leave the system, we obtain the same scheme except for the bottom right term in the iteration matrix. However, the scheme is no longer well-balanced since we still use the same form of steady state. One modification could be to use the steady state of the non-conservative truncation and doing again the same scheme.*

6.2. Numerical results

Before showing numerical results, we have to mention the fact that the conservative truncation (2.16) has the same steady state as the infinite system, meaning $(Q_i z^i)_{i\geq 1}$; however, the z differs due to the truncation. In fact, the conservative truncation (2.16) has a unique steady state, which is this one, no matter λ. There is no sub-critical or super-critical cases in any truncation; indeed, if z_s is finite, then for a fixed n and λ there always exists $z(n) > z_s$ such that $(Q_i z(n)^i)_{1\leq i\leq n}$ is the only steady state of (2.16).

Following the above discussion on z for different meshes, we denote $z_{RK4} = z_{RDU}$ the parameter z obtained with the full sum, meaning with $\Delta x = 1$, and we denote z_{RDNU} the parameter z obtained with a non-uniform mesh. Consequently, we denote $C^{eq}_{RK4} = C^{eq}_{RDU}$ and C^{eq}_{RDNU} the corresponding steady state.

In every numerical simulation used to obtain graphs below, we start with a system containing nothing:

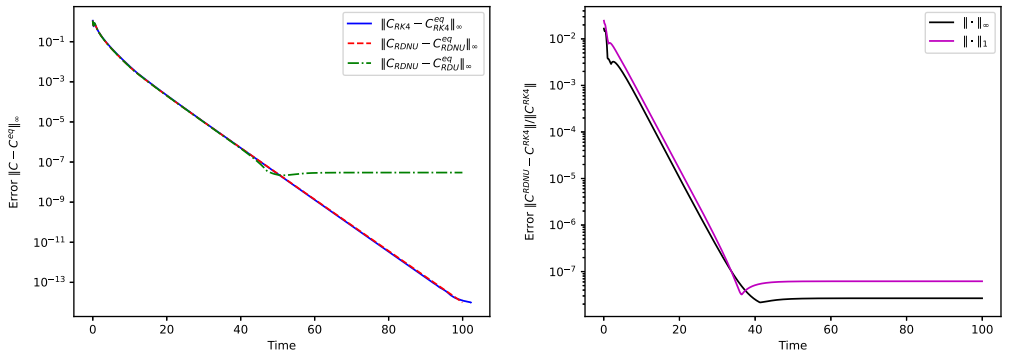
$$C_i(0) = 0, \text{ for } i = 1, \ldots, n.$$

For the size discretisation, we use a non-uniform mesh with $\Delta x = 1$ close to the boundaries and then nodes are spaced evenly on a log scale until the step size reaches the maximum size that we impose.

We start with the convergence towards the steady state of our numerical solution. Figure 1 shows results for a system of size $n = 30000$ with kinetics coefficients and production rate as follows:

$$a_i = i^{1/2},\ b_i = i^{2/3} \text{ and } \lambda = 10. \tag{6.9}$$

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(a) Absolute error (b) Relative error

Figure 1. *Comparison of the convergence towards the steady state. System size $K = 649$ with maximum step size $\Delta x_{max} = 50$. The relative error is only taken from the nodes on the non-uniform mesh, no interpolation is used.*

These parameters give $z_s = +\infty$, and therefore, $\lambda_s = +\infty$ and $\mathtt{z} \approx \mathtt{1.119}$. Using our coarse-grain mesh, we have $|\mathtt{z}_{RDU} - \mathtt{z}_{RDNU}| \leq \mathtt{1.8e{-}8}$.

Figure 1a shows that the numerical solution of our scheme converges towards the steady-state $(Q_i z^i_{RDNU})_{1 \leq i \leq n}$ at the given precision, and the green curve shows what we expected, which is that the two equilibria differ at the expected order of magnitude. Focusing on the red and blue curves, our scheme preserves the exponential decay towards the steady state. Figure 1b shows that the relative error between the numerical solution obtained from our scheme and the one obtained with RK4 scheme (Runge–Kutta method) converges towards the relative error between the different equilibria, which is expected from Figure 1b and (6.8). However, unlike the scheme of Duncan and Soheili [26, Figure 3], the relative error does not behave similarly. Indeed, their relative error is close to 0 for small time but remains around 10^{-2} when the solution reaches the steady state, whereas our relative error is bigger for small time but decreases towards the expected error (the sub-sampling error from (6.8)) as the solution reaches the steady state.

We now compare computation time, since for the super-critical case, we may need to compute very large size for a very long time. We, therefore, want a scheme that is able to reduce the computation time. In our scheme, we take Δx_{max} such that it represents at most 0.05% of the truncation size n. Figure 2 shows that, for large enough truncation size n, it is efficient to use our scheme.

Figure 2a shows results with kinetics coefficients and production rate from (6.9), and Figure 2b shows results with kinetics coefficients and production rate as follows:

$$a_i = i^{1/2},\ b_i = 0.1 + 0.75 i^{1/2} \text{ and } \lambda = 1. \tag{6.10}$$

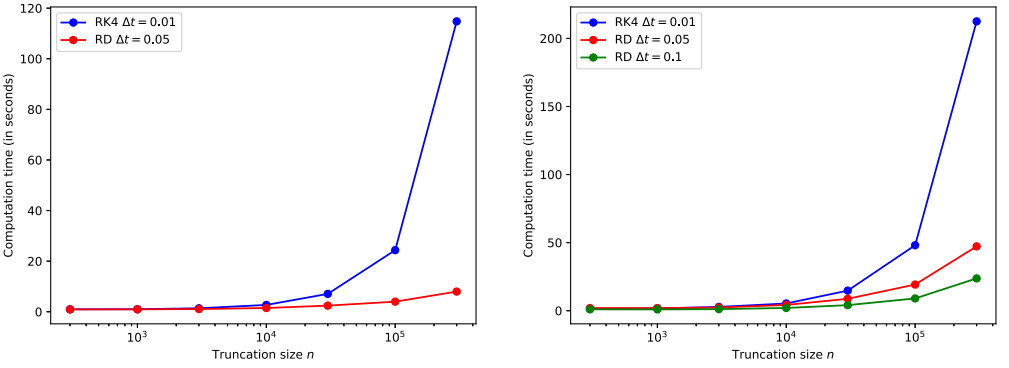
These parameters give $z_s = 0.75$, $\lambda_s \approx \mathtt{5.34375}$ and $\mathtt{z} \approx \mathtt{0.516}$.

We mention that with other coefficients (e.g. (6.11)), the convergence is much slower towards the steady-state and therefore the gain can be much better. Taking the maximum size $n = 30000$ and allowing only Δx_{max} to be roughly 0.05% of n, we reduce the computational time by 65%. Taking Δx_{max} to be roughly 0.5% of n, the reduction becomes 80%. The gain of computational time also comes from the time size, which is 10 times bigger for our scheme.

$$a_i = i^{1/2},\ b_i = 0.05 + 0.1 i^{2/3} \text{ and } \lambda = 10. \tag{6.11}$$

We now compare the dynamics of our numerical solution. We know that the convergence towards the steady state is the same and that for large truncation it is more efficient time wise. However, is the behaviour, quantitatively and qualitatively speaking, of our solution the same or not? Figure 3 shows that it globally conserves the dynamical behaviour of the solution with the same order of magnitude.

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(a) Parameters (6.9) (b) Parameters (6.10)

Figure 2. *Comparison of computation time.*

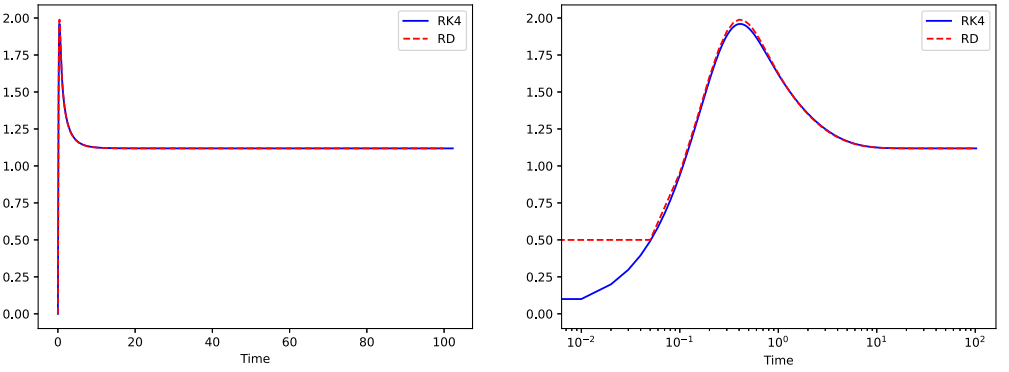


Figure 3. *Comparison of the dynamical behaviour of $C_1(t)$.*

We only show the first coordinate since the dynamical behaviour is led by the latter. We note that in those simulations, neither Δt nor Δx_j is the same as in the RK4 scheme, which already creates an error.

Figure 3 shows results with kinetics coefficients and production rate from (6.9).

One more reason we want to develop a different scheme and not settle for classical ODE schemes is for the super-critical case. Indeed, as stated before, either truncation have a unique steady state, but they are not necessarily the one (or ones) of the infinite system, and moreover, they do not necessarily converge as n goes to infinity to the one (or ones) of the infinite system. In practice, we observe that the numerical solution of the RK4 scheme (Runge–Kutta method) always converges towards the steady state of the truncation even in the theoretical super-critical case.

We might expect a different behaviour of our scheme, leading to hints of what is happening in the super-critical case. There is no steady state, but as in the Becker–Döring equations, it still could converge towards $(Q_i z_s^i)_{i\geq 1}$ in some sense, even if it is not a steady state, unlike in the Becker–Döring equations. We then believe that our scheme may be able to catch a very slow convergence towards this sequence that a classical numerical scheme on the truncation system would definitely not catch.

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Appendix A. Estimations of the sufficient condition

A.1. Constant coefficients

We detail the computation to obtain Example 2.13. Recalling that $a_i = a$ and $b_i = b$ for all $i \geq 1$, we have for $z < z_s$, $\frac{b}{a} = z_s$ and

$$Q_i = \prod_{j=2}^{i} \frac{a_{j-1}}{b_j} = \prod_{j=2}^{i} \frac{a}{b} = \left(\frac{a}{b}\right)^{i-1} = \frac{1}{z_s^{i-1}}.$$

Thus,

$$\sum_{k=1}^{+\infty} Q_k z^k = z_s \sum_{k=1}^{+\infty} \left(\frac{z}{z_s}\right)^k = \frac{z z_s}{z_s - z},$$

and

$$\sum_{j=1}^{k} \frac{1}{a_j Q_j z^j} = \frac{1}{a} \sum_{j=1}^{k} \frac{z_s^{j-1}}{z^j} = \frac{1}{a z_s} \frac{\frac{z}{z_s} - \left(\frac{z_s}{z}\right)^{k+1}}{1 - \frac{z}{z_s}} = \frac{1}{a} \frac{1 - \left(\frac{z_s}{z}\right)^k}{z - z_s},$$

and

$$\sum_{j=k+1}^{+\infty} Q_j z^j = z_s \sum_{j=k+1}^{+\infty} \left(\frac{z}{z_s}\right)^j = \frac{z}{1 - \frac{z}{z_s}} - \frac{z - z_s \left(\frac{z}{z_s}\right)^{k+1}}{1 - \frac{z}{z_s}} = \frac{z_s^2}{z_s - z} \left(\frac{z}{z_s}\right)^{k+1}.$$

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We then obtain

$$\left(\sum_{j=k+1}^{+\infty} Q_j z^j\right)\left(\sum_{j=1}^{k} \frac{1}{a_j Q_j z^j}\right) = -\frac{1}{a}\frac{z_s^2}{(z_s-z)^2}\left(\frac{z}{z_s}\right)^{k+1} + \frac{1}{a}\frac{zz_s}{(z_s-z)^2}.$$

Therefore, the condition (2.13) becomes

$$\frac{8b}{\sqrt{z}}\sqrt{\frac{zz_s}{z_s-z}}\frac{1}{a}\frac{zz_s}{(z_s-z)^2} < 1,$$

which is, after simplification,

$$\frac{8zz_s^{5/2}}{(z_s-z)^{5/2}} < 1.$$

A.2. Linear coefficients

We detail the computation to obtain the Example 2.14. Recalling that $a_i = ai$ and $b_i = bi$ for all $i \geq 1$, we have for $z < z_s$, $\frac{b}{a} = z_s$ and

$$Q_i = \prod_{j=2}^{i} \frac{a_{j-1}}{b_j} = \prod_{j=2}^{i} \frac{a(j-1)}{bj} = \left(\frac{a}{b}\right)^{i-1} \prod_{j=2}^{i} \frac{j-1}{j} = \left(\frac{a}{b}\right)^{i-1} \frac{1}{i} = \frac{1}{iz_s^{i-1}}.$$

Thus,

$$\begin{aligned}\sum_{i=1}^{+\infty} i^2 Q_i z^i &= z\sum_{i=1}^{+\infty} i\left(\frac{z}{z_s}\right)^{i-1} = z\sum_{i=1}^{+\infty}\left[\left(\frac{z}{z_s}\right)^i\right]' \\ &= z\left[\sum_{i=1}^{+\infty}\left(\frac{z}{z_s}\right)^i\right]' = z\left(\frac{\frac{z}{z_s}}{1-\frac{z}{z_s}}\right)' \\ &= \frac{zz_s}{(z_s-z)^2},\end{aligned}$$

and

$$\sum_{j=1}^{k} \frac{1}{a_j Q_j z^j} = \frac{1}{a}\sum_{j=1}^{k} \frac{z_s^{j-1}}{z^j} = \frac{1}{az_s}\frac{\frac{z}{z_s} - \left(\frac{z_s}{z}\right)^{k+1}}{1-\frac{z}{z_s}} = \frac{1}{a}\frac{1-\left(\frac{z_s}{z}\right)^k}{z-z_s},$$

and

$$\begin{aligned}\sum_{j=k+1}^{+\infty} Q_j z^j &= \frac{b}{a}\sum_{j=k+1}^{+\infty} \frac{1}{j}\left(\frac{z}{z_s}\right)^j = z_s\sum_{j=k+1}^{+\infty}\int_0^z \left(\frac{x}{z_s}\right)^{j-1} dx \\ &= z_s\int_0^z \frac{\left(\frac{x}{z_s}\right)^k}{1-\frac{x}{z_s}}dx.\end{aligned}$$

Therefore, the condition (2.13) becomes

$$\frac{8z_s^{3/2}}{z_s-z}\sup_{k\geq 1}\left(\int_0^z \frac{\left(\frac{x}{z_s}\right)^k}{1-\frac{x}{z_s}}dx\right)\left(\frac{1-\left(\frac{z_s}{z}\right)^k}{z-z_s}\right) < 1.$$

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However, for $z < \dfrac{z_s}{2}$ (z small enough), we have $\dfrac{1}{z_s - z} < \dfrac{2}{z_s}$. Thus, for $k \geq 1$,

$$\begin{aligned}\left(\int_0^z \frac{\left(\frac{x}{z_s}\right)^k}{1-\frac{x}{z_s}}dx\right)\left(\frac{1-\left(\frac{z_s}{z}\right)^k}{z-z_s}\right) &< \frac{4}{z_s^2}\int_0^z \left(\frac{x}{z_s}\right)^k\left[\left(\frac{z_s}{z}\right)^k - 1\right] \\ &< \frac{4}{z_s^2}\frac{z_s}{k+1}\left(\frac{z}{z_s}\right)^{k+1}\left[\left(\frac{z_s}{z}\right)^k - 1\right] \\ &< \frac{4}{z_s}\frac{1}{k+1}\frac{z}{z_s} \\ &< \frac{4z}{z_s^2}.\end{aligned}$$

Therefore, the condition (2.13) is true when

$$\frac{32z}{\sqrt{z_s}(z_s - z)} < 1.$$

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