Cross-diffusion limit for a reaction-diffusion system with fast reversible reaction

Dieter Bothe, Michel Pierre, Guillaume Rolland

Abstract

We consider a reaction-diffusion system which models a fast reversible reaction of type $C_1 + C_2 \rightleftharpoons C_3$ between mobile reactants inside an isolated vessel. Assuming mass action kinetics, we study the limit when the reaction speed tends to infinity in case of unequal diffusion coefficients and prove convergence of a subsequence of solutions to a weak solution of an appropriate limiting pde-system, where the limiting problem turns out to be of cross-diffusion type. The proof combines the L^2-approach to reaction-diffusion systems having at most quadratic reaction terms with a thorough exploitation of the entropy functional for mass action systems. The limiting cross-diffusion system has unique local strong solutions for sufficiently regular initial data, while uniqueness of weak solutions is in general open but is shown to be valid under restrictions on the diffusivities.

Keywords: QSSA, Pseudo-steady-state approximation, instantaneous limit, weak global solution

1 Introduction

The main goal of this paper is to identify the limit as $k \to +\infty$ for the following reaction-diffusion system

$$(R^K) \begin{cases} \left.\begin{aligned} \partial_t c_1 - d_1 \Delta c_1 &= -k(c_1 c_2 - \kappa c_3) \\ \partial_t c_2 - d_2 \Delta c_2 &= -k(c_1 c_2 - \kappa c_3) \\ \partial_t c_3 - d_3 \Delta c_3 &= +k(c_1 c_2 - \kappa c_3) \end{aligned}\right\} \text{ on } (0,+\infty) \times \Omega, \\ \partial_\nu c_1 = \partial_\nu c_2 = \partial_\nu c_3 = 0 \text{ on } (0,+\infty) \times \partial\Omega, \\ c_1(0,\cdot) = c_1^0,\ c_2(0,\cdot) = c_2^0,\ c_3^0(0,\cdot) = c_3^0. \end{cases} \tag{1}$$

where Ω is a bounded regular subset of $\mathbb{R}^N$ (we assume throughout the paper that $\partial\Omega$ is of class C^2), ∂_ν denotes the exterior normal derivative to $\partial\Omega$, $\kappa > 0, d_i > 0$ and the initial data c_i^0 are nonnegative. We denote $K = (k, \kappa)$.

This system is a classical model for the chemical reaction

$$C_1 + C_2 \underset{k^b}{\overset{k^f}{\rightleftharpoons}} C_3\,, \tag{2}$$

when the reaction takes place in an isolated domain represented by Ω where diffusive transport of the species C_i occurs. We assume that the reaction follows the law of mass action with positive rate constants k^f and k^b for the forward and backward reaction, respectively, and that linear Fickian diffusion applies. We also impose no-flux conditions at the boundary. This leads to the system (R^K), where $c_i(t, x)$ represents the molar concentration of the species C_i at time t and position $x \in \Omega$.

To understand the reason and the meaning of letting $k \to +\infty$ in this system, let us look at the time scales for both mechanisms diffusion and reaction. For this purpose, we need to consider the reaction-diffusion system (1) in its dimensionless form. The latter is of the same type as (1), but with differently defined model parameters: the c_i then denote dimensionless concentrations, obtained by normalizing the molar concentrations with a characteristic reference value c_0. The independent variables time and space are also normalized by appropriate characteristic values τ and l, respectively. Then, in the non-dimensional form of (1), the model parameters are

$$d_i = \frac{D_i}{D_0}, \qquad k = \frac{k^f c_0\, l^2}{D_0}, \qquad \kappa = \frac{k^b}{k^f c_0},$$

where we have already chosen the diffusion time scale $\tau_{\text{diff}} = l^2/D_0$ as the characteristic time τ with D_0 denoting a characteristic diffusivity. Note that both k and κ are time scale ratios, namely

$$k = \frac{\tau_{\text{diff}}}{\tau^f_{\text{reac}}}, \qquad \kappa = \frac{\tau^f_{\text{reac}}}{\tau^b_{\text{reac}}}.$$

The quantity k^f/k^b is called the equilibrium constant of the reversible reaction. Let us note in passing that for fixed equilibrium constant, one can always assume $\kappa = 1$ by choosing $c_0 = k^f/k^b$.

Now, diffusion in liquids or especially in solids is a relatively slow process. For example, even in an actively mixed aqueous system the smallest achievable concentration length scales are typically about $l \simeq 10^{-6}m$, often considerably larger. Therefore, with typical diffusivities in water of about $D_0 \simeq 10^{-9}m^2s^{-1}$, a conservative estimate for τ_{diff} is given by $\tau_{\text{diff}} \geq 10^{-3}s$. In systems without agitation it will be several magnitudes larger. On the other hand, chemical transformations can be extremely fast, depending on the reaction mechanism. For instance in case of the neutralization $H^+ + OH^- \rightleftharpoons H_2O$, the forward reaction can have a time scale as small as $\tau^f_{\text{reac}} \simeq 10^{-11}s$. Other examples for fast reversible reactions include dissociations, other ionic as well as radical reactions; cf. [11] for more details on chemical reaction mechanisms and rates. Therefore, in many actual experiments one or several reactions are much faster than the diffusive transport processes.

For concrete reversible reactions the equilibrium constants can often be obtained from the literature or by means of measurements, while the individual rate constants are usually unknown, especially for fast reactions. On the other side, it is reasonable to expect that during the evolution, according to (R^K), the chemical composition $c(t, \cdot)$ will be close to the manifold on which the fast reversible reaction is in equilibrium, driven by the diffusive transport processes. This is the motivation to study rigorously what happens at the limit as $k \to +\infty$ in the system (R^K). More precisely, we are interested in the slightly more general limit $K = (k, \kappa) \to (+\infty, \kappa^\infty)$, where $\kappa^\infty > 0$.

To understand better what may happen at the limit, let us first recall *what happens for the associated O.D.E.*, that is the same system as above, but without diffusion. Let $c=(c_1,c_2,c_3)$ be the solution and let us set $c_i(t)=\kappa\tilde{c}_i(k\kappa\, t)$. We are led to the system

$$(\tilde{C})\quad \begin{cases} \frac{d}{dt}\begin{pmatrix}\tilde{c}_1\\ \tilde{c}_2\\ \tilde{c}_3\end{pmatrix} & = & \begin{pmatrix}-\tilde{c}_1\tilde{c}_2+\tilde{c}_3\\ -\tilde{c}_1\tilde{c}_2+\tilde{c}_3\\ \tilde{c}_1\tilde{c}_2-\tilde{c}_3\end{pmatrix} \\ \tilde{c}(0) & = & \kappa(c_1^0,c_2^0,c_3^0) \qquad \in \mathbb{R}_+^3. \end{cases}$$

It is easy to check that this system has a global nonnegative and uniformly bounded solution on $[0,\infty)$ (note that $\tilde{c}_1(t)+\tilde{c}_2(t)+2\tilde{c}_3(t)=\kappa(c_1^0+c_2^0+2c_3^0))$. If we assume for simplicity that κ is fixed (say $\kappa=1$), then the limit as $k\to+\infty$ of the original system is exactly described through the asymptotic behavior of $\tilde{c}(t)$ as $t\to+\infty$. It is well known (and easy to check) that the entropy function

$$V(\tilde{c}):=\sum_{i=1}^{3}\tilde{c}_i\log(\frac{\tilde{c}_i}{\tilde{c}_i^*})+(\tilde{c}_i-\tilde{c}_i^*)$$

is a Lyapunov function for $(\tilde{C})$, where $\tilde{c}_1^*,\ \tilde{c}_2^*,\ \tilde{c}_3^*$ are positive numbers such that $\tilde{c}_1^*\tilde{c}_2^*=\tilde{c}_3^*$. From this, the compactness of the trajectories and La Salle's invariance principle, we deduce that $\tilde{c}_i(t), i=1,2,3$ converge as $t\to+\infty$ to the unique nonnegative solution $(c_1^\infty,c_2^\infty,c_3^\infty)$ of

$$\begin{cases} c_1^\infty c_2^\infty & = & c_3^\infty \\ c_1^\infty+c_3^\infty & = & c_1^0+c_3^0 \\ c_2^\infty+c_3^\infty & = & c_2^0+c_3^0 \end{cases}$$

Going back to the solution $c=(c_1,c_2,c_3)$ of the first system, this implies that

$$\forall\,\alpha>0,\ \forall\, i=1,2,3,\quad \|c_i-c_i^\infty\|_{L^\infty([\alpha,+\infty))}\underset{k\to+\infty}{\longrightarrow}0.$$

In other words, the limit system is "constant", which means that a constant equilibrium is reached very quickly when k is large. Note that there is a boundary layer at t=0 if $c_1^0c_2^0\neq\kappa c_3^0$.

For the treatment of more general O.D.E.-systems with several fast reversible reactions and additional slow processes, see [7].

The mathematical analysis is quite more involved for the limit of the full reaction-diffusion system. As we will see, global existence of classical solutions still holds for each (k,κ). In the case $d_1=d_2=d_3=d$ of equal diffusion coefficients, some of the features of the O.D.E. system remain also valid. In particular, if we set $U=c_1+c_2+2c_3$, then $\partial_t U-d\Delta U=0$, and by maximum principle

$$\|c_1(t)+c_2(t)+2c_3(t)\|_{L^\infty(\Omega)}\le\|c_1^0+c_2^0+2c_3^0\|_{L^\infty(\Omega)}. \tag{3}$$

Together with positivity, this implies a uniform bound on the solution, uniformly in time. This property was exploited in [6], together with the Lyapunov property of the entropy function –which remains also valid here– to prove convergence in some adequate sense of the solution of (R^K) as $k \to +\infty$ to the solution of the limit system

$$\begin{cases} \partial_t(c_1+c_3) - d\Delta(c_1+c_3) = 0 \quad \text{in} \quad (0,\infty)\times\Omega, \\ \partial_t(c_2+c_3) - d\Delta(c_2+c_3) = 0 \quad \text{in} \quad (0,\infty)\times\Omega, \\ \partial_\nu(c_1+c_3) = \partial_\nu(c_2+c_3) = 0 \quad \text{on} \quad (0,\infty)\times\partial\Omega, \\ c_1(0)+c_3(0) = c_1^0+c_3^0,\ c_2(0)+c_3(0) = c_2^0+c_3^0 \quad \text{in} \quad \Omega, \\ c_1c_2 = \kappa^\infty c_3 \quad \text{in} \quad \Omega. \end{cases} \tag{4}$$

Note that the first four lines of this system completely determine the two sums c_1+c_3 and c_2+c_3. Coupling with the fifth equation and the positivity of the c_i's, this implies uniqueness of classical solutions for the above system.

Now the situation when the diffusion coefficients are different from each other is quite more difficult to analyze and this is the main purpose of the present paper. In particular, the uniform estimate (3) is no longer valid, although a global classical solution, bounded for all $T>0$, does exist for (R^K); for the readers convenience, this is recalled in Section 2. Moreover, the limit system is quite more difficult to understand.

The following is one of the main results of this paper, where we employ the common notation $Q_T = (0,T)\times\Omega$, $\Sigma_T = (0,T)\times\partial\Omega$.

Theorem 1 *Let $K^n := (k_n,\kappa_n) \overset{n\to+\infty}{\longrightarrow} (+\infty,\kappa^\infty)$ with $\kappa^\infty > 0$ and let $c^n = (c_1^n, c_2^n, c_3^n)$ be the solution of (R^{K_n}) on $[0,\infty)$ with initial data $c^0 = (c_1^0,c_2^0,c_3^0) \in L^\infty(\Omega,\mathbb{R}_+^3)$. Then, up to a subsequence, $(c^n)_{n\in\mathbb{N}}$ converges for all $T>0$ in $L^2(Q_T)^3$ to a limit $c=(c_1,c_2,c_3)$, solution of the following for all $T>0$:*

$$\begin{cases} \forall i=1,2,3,\ c_i\in L^2(Q_T),\ \nabla c_i \in L^{\frac{4}{3}}(Q_T)^N, \quad c_i\geq 0, \quad c_1c_2 = \kappa^\infty c_3, \\ \forall \psi \in C^\infty(\overline{Q_T}) \text{ such that } \psi(T)=0, \\ \quad \begin{cases} -\int_\Omega \psi(0)(c_1^0+c_3^0) + \int_{Q_T} -\psi_t(c_1+c_3) + \nabla\psi.\nabla(d_1c_1+d_3c_3) = 0, \\ -\int_\Omega \psi(0)(c_2^0+c_3^0) + \int_{Q_T} -\psi_t(c_2+c_3) + \nabla\psi.\nabla(d_2c_2+d_3c_3) = 0. \end{cases} \end{cases} \tag{5}$$

System (5) is a weak formulation of

$$\begin{cases} \partial_t(c_1+c_3) - \Delta(d_1c_1+d_3c_3) = 0 & \text{in } Q_T, \\ \partial_t(c_2+c_3) - \Delta(d_2c_2+d_3c_3) = 0 & \text{in } Q_T, \\ \partial_\nu(c_1+c_3) = \partial_\nu(c_2+c_3) = 0 & \text{on } \Sigma_T, \\ (c_1+c_3)(0,\cdot) = c_1^0+c_3^0;\ (c_2+c_3)(0,\cdot) = c_2^0+c_3^0 & \text{in } \Omega, \\ c_1c_2 = \kappa^\infty c_3 & \text{in } Q_T. \end{cases} \tag{6}$$

It couples a cross-diffusion system with an algebraic equation. This system is quite harder to understand than (4) which was built of two classical heat equations for the sums c_1+c_3, c_2+c_3. As we will see in Section 3, this limit system can be rewritten in a different way as a 2×2 nonlinear reaction-cross-diffusion system. Using known results (in particular in [1, 2, 3]), we may then prove that it has a classical regular solution, at least on some time-interval $[0,T^*)$, $T^* \leq +\infty$ and for regular enough initial data, and this solution is unique among classical solutions . However, two questions remain open in general:
- Does the solution of (5) coincide with this classical solution on $[0,T^*)$? This is a uniqueness question for the (weak) solutions of (5).
- The solution obtained in (5) is global in time, while the classical regular solution is proved to exist only on some interval $[0,T^*)$, where T^* may be finite.

Can it happen that the solution of (5) is regular for some time, but becomes singular after some finite time?

We give in Section 3 some interesting partial answer to the first question: we prove that, if d_1, d_2 are both close enough to d_3 (with an explicit range), then uniqueness holds for the global (weak) solution of (5). This implies that the whole sequence of approximate solutions c^n converges and not only a subsequence. Moreover, the unique global weak solution of (5) necessarily coincides with the regular one on the interval where this regular solution exists. But even in this restricted range of values for d_1, d_2, d_3, we do not know if the global weak solution is regular for all time.

We also provide another type of uniqueness result: if $|d_1 - d_2|$ belongs to some small interval depending on the $L^\infty((0,T)\times\Omega)$-norm of the regular solution, then the (weak) solution of (5) coincides with this regular one on $[0,T]$. Thus, the whole sequence c^n converges on $[0,T]$. But, this does not say anything about uniqueness of the weak global solution of (5) for large time.

We focus here on the specific reaction (2). However, our approach is rather general and applies for instance to reactions of the type

$$\sum_{i=1}^{p-1} \alpha_i C_i \rightleftharpoons C_p \ . \tag{7}$$

This is discussed in Section 4 together with some further remarks on possible extensions of the tools introduced here to various chemical systems.

Let us finally mention some related work. The case of a single fast reversible reaction of type $A \rightleftharpoons B$ has been treated in [8]. For the resulting RD-system, a priori L^∞-estimates independent of k are available from flow invariance properties which considerably simplify the analysis of convergence of solutions. Using again invariant sets independent of k, a first result on convergence of solutions of (R^K) has been obtained in [6]; note that this approach to (R^K) is restricted to the case of equal diffusivities. In [5] and [9], a coupled system of two reversible reactions of type $A + B \rightleftharpoons C \rightleftharpoons D + E$ is studied. There, in contrast to the present study, the species C is considered highly reactive, modeling the case of a so-called intermediate. For the somewhat less related topic of RD-systems with fast irreversible reactions we refer to [14], [10] and the references therein.

2 Proof of the main theorem

First, let us recall the arguments that prove the global existence of a unique strong solution for the problem (R^K). The local existence of strong solutions is a consequence of a classical result (see e.g. [13, 20, 2]):

Lemma 1 *Let us consider the following $m \times m$-system: for all $i = 1, ..., m$,*

$$\partial_t u_i - d_i \Delta u_i = f_i(u_1, ..., u_m) \text{ in } \mathbb{R}_+ \times \Omega,\ \partial_\nu u_i = 0 \text{ on } \partial\Omega,\ u_i(0) = u_{i0}, \tag{8}$$

where $d_i \in (0, +\infty)$, $f = (f_1, ..., f_m) : \mathbb{R}^m \to \mathbb{R}^m$ is C^1 and $u_{i0} \in L^\infty(\Omega)$. Then, there exists $T > 0$ and a unique classical solution of (8) on $[0, T)$. If T^* denotes *the greatest of these T's, then*

$$\left[\sup_{t\in[0,T^*),1\le i\le m}\|u_i(t)\|_{L^\infty(\Omega)}<+\infty\right]\Rightarrow[T^*=+\infty]. \tag{9}$$

If the nonlinearity $(f_i)_{1\le i\le m}$ *is moroever* **quasi-positive**, *which means*

$$\forall i=1,...,m,\ \forall u_1,...,u_m\ge 0,\ f_i(u_1,...,u_{i-1},0,u_{i+1},...,u_m)\ge 0,$$

then

$$[\forall i=1,...,m,\ u_{i0}\ge 0]\Rightarrow[\forall i=1,...,m,\ \forall t\in[0,T^*),\ u_i(t)\ge 0]\,.$$

In the case of the system (R^K), the nonlinearity is quasi-positive and the initial data are in $L^\infty(\Omega,\mathbb{R}^3_+)$, so the previous lemma yields the local existence and uniqueness of classical, nonnegative solutions. To show that these solutions are global, according to (9), we need an *a priori* estimate for c in $L^\infty((0,T^*)\times\Omega)$. This is not as standard as the local existence result. We may use the following result proved in [18] (see also [16, 17, 12, 19] for earlier proofs).

Lemma 2 *Using the same notations and hypotheses as in Lemma 1, suppose moreover that* f *has at most polynomial growth and that there exists* $\mathbf{b}\in\mathbb{R}^m$ *and a lower triangular invertible matrix* P *with nonnegative entries such that*

$$\forall r\in[0,+\infty)^m,\ Pf(r)\le[1+\sum_{i=1}^m r_i]\,\mathbf{b}\,.$$

Then, for $u_0\in L^\infty(\Omega,\mathbb{R}^m_+)$, *the system* (8) *has a global strong solution.*

In the case of system (R^K), the existence of such a matrix P is obvious thanks to the linear dependence in c_3. Indeed, we may choose for instance

$$P=\begin{bmatrix}1&0&0\\0&1&0\\0&1&1\end{bmatrix},\quad \mathbf{b}=\begin{pmatrix}k\kappa\\k\kappa\\0\end{pmatrix}.$$

Therefore, (R^K) has a unique global strong solution for every K.

Notation. *Throughout the rest of this paper, the solution of* (R^K) *will be denoted by* $c^K=(c_1^K,c_2^K,c_3^K)$.

We are now interested in the fast-reaction limit.

The scheme of the proof of Theorem 1 is the following :

1) The sum of the first and the third equations of (R^K) yields a zero right-hand side: using the L^2-compactness result of Lemma 5, we will deduce that $c_1^K+c_3^K$ is relatively compact in $L^2(Q_T)$ for all $T<\infty$ (see Lemma 4). To check the full assumptions of Lemma 5, we will first use the estimates provided by the entropy inequality of Lemma 3 and use Aubin-Simon type compactness result [21].

2) Similarly $c_2^K+c_3^K$ is relatively compact in $L^2(Q_T)$ as $K\to(+\infty,\kappa^\infty)$.

3) If we knew that, along some subsequence, the c_i^K were converging a.e. on $(0,\infty)\times\Omega$ for each $i=1,2,3$, then, by dominated convergence based on

$$0\le c_1^K\le c_1^K+c_3^K,\;\; 0\le c_2^K\le c_2^K+c_3^K,$$

we would deduce that each c_i^K actually converges in $L^2(Q_T)$ for all $T>0$ (along the considered subsequence). This convergence a.e. would for instance hold if we knew that $k(c_1^Kc_2^K-\kappa c_3^K)$ was bounded in $L^1(Q_T)$ (this would indeed imply the relative compactness of the c_i in $L^1(Q_T)$, see e.g. [4]). This L^1-bound is proved to be valid in [6] when $d_1=d_2=d_3$. But, we are not able to prove it in general.
4) However, we are able to exploit the entropy inequality (see Lemma 3) to prove that c_i does converges a.e. up to a subsequence. Whence the expected convergence of c_i in $L^2(Q_T)$ for all $T<\infty$.
5) To pass to the limit in the weak version (5) of the system, we still need some control on ∇c_i. Again, this is provided by the entropy inequality that we state next.

Lemma 3 *Let $K=(k,\kappa)$ and let $c^K=(c_1^K,c_2^K,c_3^K)$ be the solution of (R^K). Let J be a compact subset of $(0,+\infty)$. Then, there exists $C>0$ independent of $K\in(0,\infty)\times J$ such that, for all $T>0$,*

$$k\int_{Q_T}(c_1^Kc_2^K-\kappa c_3^K)\left[\log(c_1^Kc_2^K)-\log(\kappa c_3^K)\right]+\sum_{i=1}^3 d_i\int_{Q_T}\frac{|\nabla c_i^K|^2}{c_i^K}\le C\,. \quad (10)$$

Proof: We define the nonnegative functions

$$W_i^K=c_i^K\log\left(\frac{c_i^K}{c_i^{K^*}}\right)-(c_i^K-c_i^{K^*}),\;\; W^K=\sum_{i=1}^3 W_i^k,\;\; Z^K=\sum_{i=1}^3 d_iW_i^K,$$

where $c_1^{K^*},c_2^{K^*}$ and $c_3^{K^*}$ are positive numbers such that $c_1^{K^*}c_2^{K^*}=\kappa c_3^{K^*}$. A straightforward computation yields

$$\begin{aligned}
&\partial_tW^K-\Delta Z^K\\
&=-\left(\sum_{i=1}^3 d_i\frac{|\nabla c_i^K|^2}{c_i^K}\right)-k(c_1^Kc_2^K-\kappa c_3^K)\left(\log(\frac{c_1^K}{c_1^{K^*}})+\log(\frac{c_2^K}{c_2^{K^*}})-\log(\frac{c_3^K}{c_3^{K^*}})\right),\\
&=-\left(\sum_{i=1}^3 d_i\frac{|\nabla c_i^K|^2}{c_i^K}\right)-k(c_1^Kc_2^K-\kappa c_3^K)(\log(c_1^Kc_2^K)-\log(\kappa c_3^K)),
\end{aligned}$$

where we used the relation $c_1^{K^*}c_2^{K^*}=\kappa c_3^{K^*}$ to get the last equality. Using the nonnegativity of W^K and the fact that $\int_\Omega \Delta Z^K=\int_{\partial\Omega}\partial_\nu Z^K=0$, we get after integration on Q_T:

$$\begin{aligned}
k\int_{Q_T}(c_1^Kc_2^K-\kappa c_3^K)(\log(c_1^Kc_2^K)-\log(\kappa c_3^K))+\sum_{i=1}^3 d_i\int_{Q_T}\frac{|\nabla c_i^K|^2}{c_i^K}\\
=\int_\Omega W^K(0,\cdot)-\int_\Omega W^K(T,\cdot)\le\int_\Omega W^K(0,\cdot).
\end{aligned}$$

It is easy to see that the right-hand side of the inequality is bounded independently of $K \in (0, \infty) \times J$:

$$\int_\Omega W^K(0,\cdot) = \sum_{i=1}^{3} \int_\Omega W_i^K(0,.) = \sum_{i=1}^{3} \int_\Omega c_i^0 \log(\frac{c_i^0}{c_i^{K^*}}) - (c_i^0 - c_i^{K^*}).$$

By assumption, $c_i^0 \in L^\infty(\Omega)^+$. The right member is bounded if the $c_i^{K^*}$ remain in a compact set of $(0, +\infty)$, and this is the case if we choose for instance $c_1^{K^*} = c_2^{K^*} = 1$ and $c_3^{K^*} = 1/\kappa$, $\kappa \in J$. Therefore, there exists a constant C independent of K, T such that (10) holds.

Remark 1 Note that it is sufficient to assume that $c_i^0 |\log c_i^0| \in L^1(\Omega)$ to obtain the above bound C and consequently to get the estimate (10).

Lemma 4 *The families $(c_1^K + c_3^K)_{K\in(0,+\infty)^2}$, $(c_2^K + c_3^K)_{K\in(0,+\infty)^2}$ are relatively compact in $L^2(Q_T)$ for all $T > 0$.*

Proof: By definition of c^K, $(c_1^K + c_3^K)$ and $(c_2^K + c_3^K)$ are classical solutions of

$$\begin{cases} \left.\begin{array}{l} \partial_t(c_1^K + c_3^K) - \Delta(d_1 c_1^K + d_3 c_3^K) = 0 \\ \partial_t(c_2^K + c_3^K) - \Delta(d_2 c_2^K + d_3 c_3^K) = 0 \end{array}\right\} \text{ on } (0,T)\times\Omega, \\ \partial_\nu(c_1^K + c_3^K) = \partial_\nu(c_2^K + c_3^K) = 0 \text{ on } (0,T)\times\partial\Omega, \\ (c_1^K + c_3^K)(0,\cdot) = c_1^0 + c_3^0,\ (c_2^K + c_3^K)(0,\cdot) = c_2^0 + c_3^0. \end{cases} \tag{11}$$

For $j \in \{1, 2\}$, we define

$$\tilde W_j^K = c_j^K + c_3^K,\ \tilde Z_j^K = d_j c_j^K + d_3 c_3^K,\ d_j^{\min} = \min(d_j, d_3),\ d_j^{\max} = \max(d_j, d_3).$$

Using the nonnegativity of c^K, we see that

$$d_j^{\min}\tilde W_j^K \le \tilde Z_j^K \le d_j^{\max}\tilde W_j^K \quad \text{with } 0 < d_j^{\min} \le d_j^{\max} < +\infty\,,$$

and $(\tilde W_j^K, \tilde Z_j^K)$ is a solution of

$$\begin{cases} \partial_t \tilde W_j^K - \Delta \tilde Z_j^K = 0 & \text{on } (0,T)\times\Omega, \\ \partial_\nu \tilde W_j^K = \partial_\nu \tilde Z_j^K = 0 & \text{on } (0,T)\times\partial\Omega, \\ \tilde W_j^K(0,\cdot) = \tilde W_j^0 := c_j^0 + c_3^0 & \text{on } \Omega\,. \end{cases}$$

After integration in time, we see that $(\tilde W_j^K, \tilde Z_j^K)$ is solution of (12) in the next Lemma 5 with $(W, Z) = (\tilde W_j^K, \tilde Z_j^K)$ and with $W(0) = c_1^0 + c_j^0$. According to this lemma, to prove the relative $L^2(Q_T)$-compactness of $\tilde W_j^K$, it is sufficient to prove that, up to a subsequence, it converges a.e. as $K \to (\infty, \kappa)$.

For this, we will prove that $\zeta_j^K := (1+\tilde W_j^K)^{1/2} = (1+c_j^k+c_3^K)^{1/2}$ is relatively compact in $L^2(Q_T)$. Indeed

$$2\,|\nabla \zeta_j^K| = \left|\frac{\nabla c_j^K + \nabla c_3^K}{\zeta_j^K}\right| \le \frac{|\nabla c_j^K|}{(c_j^K)^{1/2}} + \frac{|\nabla c_3^K|}{(c_3^K)^{1/2}}.$$

By (10) in Lemma 3, $\nabla\zeta_j^K$ is bounded in $L^2(Q_T)^N$. Now

$$2\,\partial_t\zeta_j^K = \frac{\partial_t(c_j^K + c_3^K)}{\zeta_j^K} = \frac{\Delta(d_j c_j^K + d_3 c_3^K)}{\zeta_j^K} = \nabla\cdot f_j^K + g_j^K,$$

$$f_j^K := \frac{\nabla(d_j c_j^K + d_3 c_3^K)}{\zeta_j^K},\ \ g_j^K := \frac{\nabla(d_j c_j^K + d_3 c_3^K)\nabla(c_j^K + c_3^K)}{2(\zeta_j^K)^3}.$$

Again, by (10) in Lemma 3, we have that f_j^K is bounded in $L^2(Q_T)^N$ and g_j^K is bounded in $L^1(Q_T)$. Therefore, $\partial_t\zeta_j^K$ is bounded in

$$L^2(0,T:H^{-1}(\Omega)) + L^1(Q_T) \subset L^1(0,T:Y),\ Y := H^{-1}(\Omega) + L^1(\Omega).$$

Since ζ_j^K is also bounded in $L^2(0,T;H^1(\Omega))$ where $H^1(\Omega)$ is compactly embedded into $L^2(\Omega)\subset Y$, by the Aubin-Simon compactness results (see [21], Corollary 4), ζ_j^K is compact in $L^2(Q_T)$. This ends the proof of Lemma 4, based on the following lemma, inspired from the results in [18] and whose proof is given in the Appendix.

Lemma 5 *Let $0 < d^{\min} \le d^{\max} < +\infty$ and let $\mathcal{G}$ be a bounded subset of $L^2(\Omega)^+$. We denote by $\mathcal{F}$ the family of functions $(W,Z)\in H^1(Q_T)^2$ such that $W(0)\in\mathcal{G}$ and*

$$\begin{cases} W(t) - \Delta\int_0^t Z(s)\,ds = W(0) \text{ on } Q_T,\ \partial_\nu\int_0^t Z(s)\,ds = 0 \text{ on } \Sigma_T,\\ W,Z\ge 0,\\ d^{\min}\le Z/W\le d^{\max}. \end{cases} \quad (12)$$

Then, the family $\mathcal{F}$ is bounded in $L^2(Q_T)^2$ by a constant depending only on $d^{\min}, d^{\max}, \mathcal{G}, T$. Next, let $(W^p,Z^p)_{p\ge0}$ be a sequence in $\mathcal{F}$ converging to (W,Z) weakly in $L^2(Q_T)^2$. Assume that $A^p := Z^p/W^p$ converges to $A := Z/W$ for the weak-$L^\infty(Q_T)$ convergence, namely*

$$\forall\psi\in L^1(Q_T),\ \lim_{p\to\infty}\int_{Q_T}\psi\,A^p = \int_{Q_T}\psi\,A. \quad (13)$$

Then, W^p converges strongly to W in $L^2(Q_T)$. Property (13) holds in particular if W^p converges a.e. or if A^p converges a.e. on Q_T.

Remark 2 More generally, we could choose initial data $c_i^0\in L^2(\Omega)$. Approximating them in $L^2(\Omega)$ by bounded data c_i^n, we could still apply Lemma 5 with $\mathcal{G} = \{(c_j^n + c_3^n)_{n\ge0}\}$ and obtain the same $L^2(Q_T)$ compactness.

Using Lemma 3 and 4, we are now able to show a convergence result for the approximate solutions.

Lemma 6 *Let $\kappa^\infty > 0$ and $K_n := (k_n,\kappa_n) \overset{n\to+\infty}{\longrightarrow} (+\infty,\kappa^\infty)$. We denote by c^n the solution of (R^{K_n}). Then, up to a subsequence, c^n converges to a limit $c = (c_1,c_2,c_3)$ in $L^2(Q_T)^3$ for all $T>0$ and $c_1c_2 = \kappa^\infty c_3$ holds a.e. in Q_T.*

Proof: The entropy inequality (10) yields, with the notations of Lemma 3,

$$\|(c_1^n c_2^n - \kappa_n c_3^n)(\log(c_1^n c_2^n) - \log(\kappa_n c_3^n))\|_{L^1(Q_T)} \leq \frac{C}{k_n} \underset{n\to+\infty}{\longrightarrow} 0,$$

and Lemma 4 guarantees that $(c_1^n + c_3^n)_{n\in\mathbb{N}}$ and $(c_2^n + c_3^n)_{n\in\mathbb{N}}$ are relatively compact in $L^2(Q_T)$. Using a diagonal process, we may assume that this holds for all $T > 0$. Therefore, up to a subsequence,

$$\begin{cases} c_1^n + c_3^n & \underset{n\to+\infty}{\longrightarrow} \alpha \quad \text{in } L^2(Q_T) \text{ and a.e.} \\ c_2^n + c_3^n & \underset{n\to+\infty}{\longrightarrow} \beta \quad \text{in } L^2(Q_T) \text{ and a.e.} \\ (c_1^n c_2^n - \kappa_n c_3^n)(\log(c_1^n c_2^n) - \log(\kappa_n c_3^n)) & \underset{n\to+\infty}{\longrightarrow} 0 \quad \text{in } L^1(Q_T) \text{ and a.e.} \end{cases} \tag{14}$$

for all $T > 0$ with $\alpha, \beta \in L^2((0,\infty) \times \Omega; \mathbb{R}_+)$. ¿From now on, we work with this subsequence. Let $(t,x) \in Q_T$ such that the three pointwise convergence above hold. The sequence $(c^n(t,x))_{n\in\mathbb{N}}$ is bounded in $\mathbb{R}_+^3$, so it has a limit point $l = (l_1, l_2, l_3) \in \mathbb{R}_+^3$. Using (14), we easily see that l is a solution of the system

$$l_1 + l_3 = \alpha, \;\; l_2 + l_3 = \beta, \;\; l_1 l_2 = \kappa^\infty l_3, \tag{15}$$

where we omitted the dependence in (t,x) for $\alpha(t,x)$ and $\beta(t,x)$. Actually, this system has a unique solution in $\mathbb{R}_+^3$, given by

$$(l_1, l_2, l_3) = (\varphi(\alpha,\beta), \varphi(\beta,\alpha), \varphi(\alpha,\beta)\varphi(\beta,\alpha)/\kappa^\infty), \tag{16}$$

where

$$\varphi(\alpha,\beta) := \frac{1}{2}\sqrt{(\kappa^\infty)^2 + (\alpha-\beta)^2 + 2\kappa^\infty(\alpha+\beta)} - (\kappa^\infty + \beta - \alpha).$$

The bounded sequence $(c^n(t,x))_{n\in\mathbb{N}}$ has a unique possible limit point, so it converges to this limit point. This holds for almost all $(t,x) \in Q_T$, so up to a subsequence, c^n converges pointwise to a limit c with $c_1 c_2 = \kappa^\infty c_3$. Finally, we have

$$\begin{cases} c_1^n(t,x) \underset{n\to+\infty}{\longrightarrow} c_1(t,x) \quad \text{for almost every } (t,x) \in Q_T \\ 0 \leq c_1^n \leq c_1^n + c_3^n \underset{n\to+\infty}{\longrightarrow} \alpha \in L^2(Q_T)\,. \end{cases}$$

By dominated convergence, the sequence $(c_1^n)_{n\in\mathbb{N}}$ converges to c_1 in $L^2(Q_T)$. We do the same for c_2^n and c_3^n, which proves the $L^2(Q_T)$ convergence of the subsequence c^n.

Proof of Theorem 1: Lemma 6 guarantees that, up to a subsequence, c^n goes to a limit $c = (c_1, c_2, c_3)$ in $L^2(Q_T)^3$ for all $T > 0$ with $c_1 c_2 = \kappa^\infty c_3$. Using the estimate on the gradients in Lemma 3, for $i = 1,2,3$, we get a bound on $\int_{Q_T} \frac{|\nabla c_i^n|^2}{c_i^n}$ independent of n. This bound can be exploited together with the $L^2(Q_T)$-bound on c^n to get an estimate on ∇c^n. Letting $l, m > 0$, we have

$$\begin{aligned} \int_{Q_T} |\nabla c_i^n|^l &= \int_{Q_T} \frac{|\nabla c_i^n|^l}{(c_i^n)^m}(c_i^n)^m \\ &\leq \left(\int_{Q_T} \frac{|\nabla c_i^n|^{lp}}{(c_i^n)^{mp}}\right)^{1/p} \left(\int_{Q_T} (c_i^n)^{mp'}\right)^{1/p'} \quad \text{(Hölder's inequality)}, \end{aligned}$$

where $p,\ p' \in [1,+\infty]$, $\frac{1}{p}+\frac{1}{p'}=1$. We know that the right-hand side is bounded independently of n for

$$lp=2,\ mp=1,\ mp'=2,$$

so taking $(l,m,p)=(\frac{4}{3},\frac{2}{3},\frac{3}{2})$, we get that $\|\nabla c^n\|_{L^{\frac{4}{3}}(Q_T)}$ is bounded independently of n. Since $L^{\frac{4}{3}}(Q_T)$ is a reflexive space, up to a subsequence, $\forall i=1,2,3$,

$$\forall\, T\in(0,\infty),\ \nabla c_i^n \rightharpoonup \nabla c_i \quad \text{for the weak topology } \sigma(L^{\frac{4}{3}}(Q_T)^N, L^4(Q_T)^N).$$

To use this result, let us write a weaker formulation for the system (11) which involves only the first-order derivatives of c: for all $n\in\mathbb{N}$, c^n is a solution of

$$(R^n)\begin{cases} \forall i=1,2,3,\ c_i^n\in L^2(Q_T),\ \nabla c_i^n\in L^{\frac{4}{3}}(Q_T)^N,\\ \forall \psi\in C^\infty(\overline{Q_T}) \text{ such that } \psi(T)=0,\\ \quad\begin{cases} -\int_\Omega \psi(0)(c_1^0+c_3^0)+\int_{Q_T} -\psi_t(c_1^n+c_3^n)+\nabla\psi\cdot\nabla(d_1c_1^n+d_3c_3^n)=0\\ -\int_\Omega \psi(0)(c_2^0+c_3^0)+\int_{Q_T} -\psi_t(c_2^n+c_3^n)+\nabla\psi\cdot\nabla(d_2c_2^n+d_3c_3^n)=0. \end{cases}\end{cases}$$

Using $c_i^n \underset{n\to+\infty}{\overset{L^2}{\longrightarrow}} c$ and $\nabla c_i^n \underset{n\to+\infty}{\overset{\left(L^{\frac{4}{3}}\right)^N}{\rightharpoonup}} \nabla c$, we can pass to the limit in this formulation and obtain that c is solution of (5).

Remark 3 Actually, we can prove somewhat more regularity of the limit solution. Namely, if we set

$$\mathcal{C}_i(t,x)=\int_0^t c_i(s,x)ds,\ Z_1=d_1\mathcal{C}_1+d_3\mathcal{C}_3,\ Z_2=d_2\mathcal{C}_2+d_3\mathcal{C}_3,$$

then, for all $T<\infty$, $\mathcal{C}_i\in L^\infty(Q_T)$ and

$$Z_1,Z_2\in L^2\left((0,T);H^2(\Omega)\right)\cap L^4\left((0,T);W^{1,4}(\Omega)\right)\cap L^\infty\left((0,T);H^1(\Omega)\right). \quad (17)$$

Indeed, if we set $\mathcal{C}_i^n(t,x)=\int_0^t c_i^n(s,x)ds$, we have after integrating (11) in time

$$c_1^n(t)+c_3^n(t)-\Delta(d_1\mathcal{C}_1^n+d_3\mathcal{C}_3^n)=c_1^0+c_3^0. \quad (18)$$

Using $c_1^n+c_3^n\ge\mu(d_1c_1^n+d_3c_3^n)$ with $\mu=\min\{d_1^{-1},d_3^{-1}\}$, we see that $Z^n=d_1\mathcal{C}_1^n+d_3\mathcal{C}_3^n$ satisfies the inequality

$$\mu\partial_t Z^n-\Delta Z^n\le c_1^0+c_3^0.$$

Therefore, $\|Z^n(t)\|_{L^\infty(\Omega)}\le t\mu^{-1}\|c_1^0+c_3^0\|_{L^\infty(\Omega)}$. The same is valid for $d_2\mathcal{C}_2^n+d_3\mathcal{C}_3^n$. By positivity, all three $\mathcal{C}_i^n$ are bounded in $L^\infty(Q_T)$. This estimate is preserved at the limit for the $\mathcal{C}_i$.

Going back to (18), we see that $\|\Delta Z^n\|_{L^2(Q_T)}$ is bounded independently of n. Therefore $\Delta Z_1\in L^2(Q_T)$ and similarly $\Delta Z_2\in L^2(Q_T)$. Together with the boundary conditions and the regularity of Ω, we deduce that $Z_1,Z_2\in L^2\left((0,T);H^2(\Omega)\right)$. We may then use the Gagliardo-Nirenberg inequality, namely $\|\nabla Z\|^4_{L^4(\Omega)}\le C\|Z\|^2_{L^\infty(\Omega)}\|Z\|^2_{H^2(\Omega)}$, to obtain that $Z_1,Z_2\in L^4\left((0,T);W^{1,4}(\Omega)\right)$.

Finally, let us multiply (18) by $d_1c_1^n+d_3c_3^n$ and integrate on Q_t. We obtain

$$\int_{Q_t}(c_1^n+c_3^n)(d_1c_1^n+d_3c_3^n)+\frac{1}{2}\int_\Omega|\nabla Z_1^n(t)|^2=\int_{Q_T}(d_1c_1^n+d_3c_3^n)(c_1^0+c_3^0),$$

and the right-hand side is bounded independently of n. It provides the last estimate for (17).

3 Study of the limit problem

This section is devoted to an independent study of the non-standard limit problem (5). *Throughout the end of this paper, we assume for simplicity that* $d_3 = 1$ *and* $\kappa_\infty = 1$. This can be done without loss of generality: indeed, by setting $c_i(t,x) = \kappa^\infty \tilde{c}_i(d_3 t, x)$, we have for instance

$$\partial_t(\tilde{c}_1 + \tilde{c}_3) = \Delta(\frac{d_1}{d_3}\tilde{c}_1 + \tilde{c}_3),\ \tilde{c}_1\tilde{c}_2 = \tilde{c}_3.$$

Then, any result with $d_3 = 1, \kappa^\infty = 1$ carries over to the general case by replacing d_i by d_i/d_3 and changing $\tilde{c}$ into c.

3.1 Existence of strong local solutions

Let us consider the limit system in its explicit version (6). We may rewrite it as a 2×2 cross-diffusion system as follows. Let us introduce new unknown functions as

$$x(c_1, c_2) := c_1 + c_1 c_2;\quad y(c_1, c_2) := c_2 + c_1 c_2\ . \tag{19}$$

As seen in (15), (16), we have $(c_1, c_2) = \phi(x, y) = (\varphi(x, y), \varphi(y, x))$, where ϕ defines a C^∞-diffeomorphism from $(0,\infty)^2$ onto itself, which extends to a C^∞-homeomorphism from $[0,\infty)^2$ onto itself. The function $\psi : (0,+\infty)^2 \to (0,+\infty)^2$ with

$$\begin{pmatrix} \psi_1(x,y) \\ \psi_2(x,y) \end{pmatrix} := \begin{pmatrix} d_1 c_1 + c_1 c_2 \\ d_2 c_2 + c_1 c_2 \end{pmatrix}(x, y)$$

is also C^∞. The limit problem (6) can be rewritten as

$$\left\{ \begin{aligned} \partial_t x - \Delta\psi_1(x,y) &= 0 && \text{in } Q_T, \\ \partial_t y - \Delta\psi_2(x,y) &= 0 && \text{in } Q_T, \\ \partial_\nu\left(\psi_1(x,y)\right) = \partial_\nu\left(\psi_2(x,y)\right) &= 0 && \text{on } \Sigma_T, \\ x(0,\cdot) = x^0,\ y(0,\cdot) &= y^0 && \text{in } \Omega. \end{aligned} \right. \tag{20}$$

For the boundary condition, we used that

$$\nabla\left(\psi_i(x,y)\right) = \nabla\left(d_i c_i + c_1 c_2\right) = d_i \nabla c_i + c_1 \nabla c_2 + c_2 \nabla c_1.$$

The new system is a nonlinear cross-diffusion system. We may apply Amann's local existence theory [2, 3]. For this purpose we need to study the spectrum of the Jacobian matrix $D\psi$ of ψ. Let us denote

$$g : \mathbb{R}^2 \to \mathbb{R}^2,\ (c_1, c_2) \mapsto (d_1 c_1 + c_1 c_2, d_2 c_2 + c_1 c_2).$$

With the above notations, we have

$$\forall (x,y) \in (0,+\infty)^2,\quad \psi(x,y) = g \circ \phi(x,y).$$

Differentiating this expression, we get

$$\begin{aligned} D\psi(x,y) &= Dg(\phi(x,y))D\phi(x,y) = Dg(c_1,c_2)D\phi(\phi^{-1}(c_1,c_2)) \\ &= Dg(c_1,c_2)[D\phi^{-1}(c_1,c_2)]^{-1}, \end{aligned}$$

hence

$$(1+c_1+c_2)D\psi\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} d_1+c_2 & c_1 \\ c_2 & d_2+c_1 \end{pmatrix}\begin{pmatrix} 1+c_1 & -c_1 \\ -c_2 & 1+c_2 \end{pmatrix}.$$

We have

$$\begin{aligned} &0 < (1+c_1+c_2)\mathrm{trace}(D\psi) = d_1+d_2+(d_1+1)c_1+(d_2+1)c_2, \\ &0 < \det(D\psi) = d_1d_2+d_1c_1+d_2c_2\,. \end{aligned}$$

Thus, the spectrum of $D\psi(x,y)$ is in $\{z \in \mathbb{C} : \mathrm{Re}\ z > 0\}$ for all $(x,y) \in [0,+\infty)^2$. Therefore, the operator $(x,y) \mapsto \Delta(\psi(x,y))$ with homogeneous Neumann boundary conditions is *normally elliptic* in the sense of [2, 3] and we have

Proposition 1 *Let $s > 0$ and $p \in (\max\{N, N/s\}, +\infty)$. For $c^0 \in W^{s,p}(\Omega, \mathbb{R}^2_+)$, there exists a unique classical and nonnegative solution $c \in C([0,T^*) \times \overline{\Omega}) \cap C^\infty((0,T^*) \times \Omega)$ for the problem (20) on a maximal time interval $[0,T^*)$.*

Remark 4 Note that the above result applies with $s = 1$ and all $p > N$. Global existence would follow from a uniform bound in $W^{1,p}(\Omega)$ on $[0,T^*)$. This question is open here. However, the existence result of Theorem 1 does provide a *global* weak solution to the system (20). We do not know in general if it coincides with the regular one obtained in Proposition 1, even on the interval $[0,T^*)$. The following paragraph gives, however, a partial answer to this question.

3.2 A uniqueness result

Let $D = \{(d_1,d_2) \in \mathbb{R}^2_+ : (d_1-1)^2(d_2-1)^2 < 16d_1d_2\}$.

Theorem 2 *There exists a unique solution to (5) for $(d_1,d_2) \in D$.*

Remark 5 This uniqueness result is interesting since it applies to very weak solutions. An interesting consequence is that, in Theorem 1, the whole sequence c^n converges as $n \to +\infty$ to the unique solution of the limit system on the whole interval $[0,\infty)$. It also proves that, for regular enough initial data, the solution obtained in Theorem 1 coincides with the regular solution of Proposition 1 on $[0,T^*)$. But we do not know if it stays regular for all time (or whether $T^* = +\infty$).

Proof of Theorem 2: Let $c = (c_1,c_2,c_3)$ and $\hat{c} = (\hat{c}_1,\hat{c}_2,\hat{c}_3)$ be two solutions of (5) on $[0,T)$. We define $U = c_1 - \hat{c}_1$, $V = c_2 - \hat{c}_2$, $W = c_3 - \hat{c}_3$. Using the relations $c_1c_2 = c_3$ and $\hat{c}_1\hat{c}_2 = \hat{c}_3$, we have $W = \hat{c}_2U + c_1V$, so that (U,V) is a solution of

$$\left\{ \begin{array}{l} \forall \psi_1,\psi_2 \in C^\infty(\overline{Q_T}) \ \textit{with} \ \ \psi_1(T) = 0 = \psi_2(T), \\ \qquad \int_{Q_T} -\partial_t\psi_1[(1+\hat{c}_2)U + c_1V] + \nabla\psi_1 \cdot \nabla[(d_1+\hat{c}_2)U + c_1V] = 0, \\ \qquad \int_{Q_T} -\partial_t\psi_2[\hat{c}_2U + (1+c_1)V] + \nabla\psi_2 \cdot \nabla[\hat{c}_2U + (d_2+c_1)V] = 0\,. \end{array} \right. \tag{21}$$

We may rewrite this in a vectorial way with the scalar product $<\cdot,\cdot>$ in $\mathbb{R}^2$, namely

$$\int_{Q_T} - < \partial_t\Psi, AX > + < \nabla\Psi, \nabla BX >= 0,$$

where we set

$$X = \left(\begin{array}{c} U \\ V \end{array} \right), \Psi = \left(\begin{array}{c} \psi_1 \\ \psi_2 \end{array} \right), A = \left(\begin{array}{cc} 1+\hat{c}_2 & c_1 \\ \hat{c}_2 & 1+c_1 \end{array} \right), B = \left(\begin{array}{cc} d_1+\hat{c}_2 & c_1 \\ \hat{c}_2 & d_2+c_1 \end{array} \right).$$

Choosing $\Psi = \int_t^T \Phi = \int_t^T (\Phi_1, \Phi_2)$ where $\Phi_1, \Phi_2 \in C^\infty(\overline{Q_T})$, this leads, after an integration by parts in time, to

$$\forall \Phi \in C^\infty(\overline{Q_T})^2, \int_{Q_T} < \Phi, AX > + < \nabla\Phi, \nabla \int_0^t BX >= 0. \tag{22}$$

Note that

$$AX, BX \in L^2(Q_T)^2, \;\; \nabla(BX) \in L^{4/3}(Q_T)^{2N},$$

since $U, V, W \in L^2(Q_T), \nabla U, \nabla V, \nabla W \in L^{4/3}(Q_T)^N$. Property (22) implies that, a.e. on $[0,T]$, $\int_0^t BX$ is solution in a variational sense of

$$\Delta \left(\int_0^t BX \right) = AX \text{ in } \Omega, \;\; \partial_\nu \left(\int_0^t BX \right) = 0 \text{ on } \partial\Omega. \tag{23}$$

Since Ω is assumed to be bounded and with a C^2-boundary, this solution is in $H^2(\Omega)$ for a.e. $t \in (0,T)$ (see Remark 6 below) and even in $L^2\left((0,T); H^2(\Omega)\right)^2$ since $AX \in L^2(Q_T)^2$. Moreover, the boundary condition is valid in a strong sense. Then, (22) leads to

$$\forall \Phi \in L^2(Q_T)^2, \int_{Q_T} < \Phi, AX > - < \Phi, \Delta \int_0^t BX >= 0, \tag{24}$$

where we used the density of $C^\infty(\overline{Q_T})^2$ in $L^2(Q_T)^2$.

Let M be a symmetric positive definite matrix. Then, choosing $\Phi = MBX$ in (24) leads to

$$\int_{Q_T} < MBX, AX >= \int_{Q_T} < MBX, \Delta \int_0^t BX >= \int_{Q_T} < M^{\frac{1}{2}}BX, \Delta \int_0^t M^{\frac{1}{2}}BX > .$$

The last integral above is nonnegative. Indeed, if we set $F(t) = \int_0^t M^{\frac{1}{2}}BX$, we have, *at first only formally*,

$$\int_{Q_T} < \partial_t F, \Delta F >= -\int_{Q_T} < \nabla\partial_t F, \nabla F >= -\frac{1}{2}\int_\Omega \left| \nabla \int_0^T F \right|^2 \leq 0. \tag{25}$$

Actually, this computation is not justified since the conditions in (5) do not imply that $\nabla\partial_t F \in L^2(Q_T)^{2N}$. However, we will prove below (see (28)) that, nevertheless

$$\int_{Q_T} < \partial_t F, \Delta F > \leq 0, \tag{26}$$

so that we do have

$$\int_{Q_T} < MBX, AX > \leq \; 0. \tag{27}$$

Let us continue by proving that we can choose $M = \left[\begin{array}{cc} m_1 & 1 \\ 1 & m_2 \end{array} \right]$ in such a way that the scalar product $< MBY, AY >$ is positive for all $Y \in \mathbb{R}^2 \backslash \{0\}$.

Then, (27) will imply $X = 0$, whence uniqueness. This happens if and only if MBA^{-1} has a symmetric part which is positive definite and which we denote by $\mathrm{Sym}(MBA^{-1})$. We may write

$$(1 + c_1 + \hat{c}_2)MBA^{-1} = P_0 + c_1P_1 + \hat{c}_2P_2$$

where

$$P_0 := \begin{pmatrix} d_1m_1 & d_2 \\ d_1 & d_2m_2 \end{pmatrix}, \; P_1 := \begin{pmatrix} d_1m_1 & m_1 - d_1m_1 + 1 \\ d_1 & -d_1 + m_2 + 1 \end{pmatrix},$$

$$P_2 := \begin{pmatrix} m_1 - d_2 + 1 & d_2 \\ -m_2d_2 + m_2 + 1 & m_2d_2 \end{pmatrix}.$$

Considering the symmetric parts, we have

$$(1 + c_1 + \hat{c}_2)\mathrm{Sym}(MBA^{-1}) = \mathrm{Sym}(P_0) + c_1\mathrm{Sym}(P_1) + \hat{c}_2\mathrm{Sym}(P_2),$$

so that $\mathrm{Sym}(MBA^{-1})$ is positive definite for any $c_1 \geq 0,\ \hat{c}_2 \geq 0$ if and only if $\mathrm{Sym}(P_0)$ is positive definite and $\mathrm{Sym}(P_1), \mathrm{Sym}(P_2)$ are positive. Using the traces and the determinants, this is equivalent to the conditions

$$\left\{ \begin{array}{rcl} m_1m_2 & > & \max\{1, \frac{(d_1+d_2)^2}{4d_1d_2}\} \\ 0 & \leq & d_1(m_1 - 1) + m_2 + 1 \\ 0 & \leq & d_2(m_2 - 1) + m_1 + 1 \\ m_1 & \geq & \frac{(d_2-1)^2}{4d_2}m_2 + \frac{(d_2-1)^2}{2d_2} + \frac{(d_2+1)^2}{4d_2}\frac{1}{m_2} \\ m_2 & \geq & \frac{(d_1-1)^2}{4d_1}m_1 + \frac{(d_1-1)^2}{2d_1} + \frac{(d_1+1)^2}{4d_1}\frac{1}{m_1}\ . \end{array} \right.$$

The first three inequalities are satisfied for m_1, m_2 large enough. The two last inequalities may also be satisfied for m_1, m_2 large enough if

$$\Delta_1\,\Delta_2 < 1, \text{ where } \Delta_1 := \frac{(d_1 - 1)^2}{4d_1},\ \Delta_2 := \frac{(d_2 - 1)^2}{4d_2}.$$

Indeed, we may then choose

$$m_1 = \lambda m_2 \textit{ with } \Delta_2 < \lambda < \Delta_1^{-1},$$

and the two last inequalities are satisfied for m_1, m_2 large enough. The condition $\Delta_1\Delta_2 < 1$ exactly means that $(d_1, d_2) \in D$.

To end the proof of Theorem 2 we need to justify (26). We denote by L the Laplace operator in $L^2(\Omega)$ with Neumann boundary conditions, namely

$$D(L) = \{u \in H^2(\Omega);\ \partial_\nu u = 0 \text{ on } \partial\Omega\},\ \ \forall u \in D(L), Lu = -\Delta u.$$

For $\epsilon > 0$, we denote $J_\epsilon = (I + \epsilon L)^{-1}$ its resolvent and we recall that, for all $v \in L^2(\Omega)$, $J_\epsilon v \to v$ in $L^2(\Omega)$ as $\epsilon \to 0$. Consequently, if $w \in L^2(Q_T)$, then $J_\epsilon w$ converges in $L^2(Q_T)$ to w.

We set $F_\epsilon(t) = J_\epsilon F(t)$ where $F(t) = \int_0^t M^{\frac{1}{2}}BX$. Recall that $F(t) \in D(L)$ (see (23-24)) and $\partial_t F \in L^2(Q_T)$. We have the commutations

$$\partial_t F_\epsilon(t) = J_\epsilon(\partial_t F(t)),\ LF_\epsilon(t) = J_\epsilon LF(t).$$

Consequently, $\partial_t F_\epsilon, LF_\epsilon$ converge in $L^2(Q_T)^2$ to $\partial_t F, LF$. Since F_ϵ is regular enough to make the computation (25), we have

$$\int_{Q_T} < \partial_t F_\epsilon, LF_\epsilon > \geq 0, \tag{28}$$

and this inequality remains valid in the limit as $\epsilon \to 0$, whence (26).

Remark 6 It is not so easy to find references for the uniqueness (up to a constant) of the solution to the variational problem

$$u \in W^{1,p}(\Omega), \forall \psi \in C^\infty(\overline{\Omega}), \int_\Omega \nabla\psi \cdot \nabla u = 0, \tag{29}$$

when $p \in [1,2)$ "only". Since Ω is regular, the above relation is valid by density for all $\psi \in W^{1,p'}(\Omega), p' = p/(p-1)$. If $p = 2$, we may choose $\psi = u$ in (29) which easily yields uniqueness. But, if $p \in [1,2)$, we need a different approach, for instance the following.

Let $\theta : \Omega \to \mathbb{R}$ be a C^∞-function with compact support and $\int_\Omega \theta = 0$. We introduce the solution (unique up to a constant) of

$$v \in H^2(\Omega) \cap W^{1,\infty}(\Omega), -\Delta v = \theta \text{ in } \Omega, \;\; \partial_\nu v = 0 \text{ on } \partial\Omega.$$

(where the regularity $H^2 \cap W^{1,\infty}$ is due to the regularity of Ω). Then, we may choose $\psi = v$ in (29). Next, we need to justify the integration by parts

$$\int_\Omega \nabla v \cdot \nabla u = \int_\Omega (-\Delta v)\; u.$$

For this, we approximate u in $W^{1,p}(\Omega)$ by a sequence of regular functions u_n. The integration by parts is valid for u_n. Then, we pass to the limit. Finally, the relation $0 = \int_\Omega \theta\, u$, for all θ as above, implies that u is a constant function.

3.3 Extra remarks on uniqueness

We just saw that the weak solution of the limit-problem (5) is unique if d_1, d_2 are close enough to d_3. The above sufficient condition may be written as

$$(\frac{d_1}{d_3} - 1)^2 (\frac{d_2}{d_3} - 1)^2 < 16 \frac{d_1 d_2}{d_3^2}$$

in general. This does not include the full case $d_1 = d_2 = d$. Uniqueness can nevertheless be proved directly in this case as follows: going back to the system (21) for the difference of two solutions, and taking the difference of the two equations, we obtain that $U - V$ satisfies the heat equation in a weak sense:

$$\partial_t(U - V) - d\Delta(U - V) = 0, \; or \; (U - V)(t) - d\Delta \int_0^t (U - V)(s) ds = 0.$$

Multiplying by $(U - V)(t)$ and integrating on Q_T yields $\int_{Q_T} (U - V)^2 \leq 0$ (taking into account that we start with a weak solution, this may be justified by regularization as in the proof of Theorem 2). Hence $U = V$. Now, using $W = \hat{c}_2 U + c_1 V = (\hat{c}_2 + c_1)U$, the first equation gives

$$\partial_t[(1 + c_1 + \hat{c}_2)U] - \Delta[((d + c_1 + \hat{c}_2)U] = 0.$$

Integration on $(0,t)$, multiplication by $(d+c_1+\hat{c}_2)U$ and integration on Q_T leads to

$$\int_{Q_T}(1+c_1+\hat{c}_2)(d+c_1+\hat{c}_2)U^2 \leq 0.$$

Whence $U=0$ and then $V=0=W$, i.e. the solution is unique.

More generally, we may expect some uniqueness if d_1 and d_2 are close enough to each other. We may indeed prove the following.

Proposition 2 *Assume the initial data is regular. If d_1 is close enough to d_2, the limit-solution of (5) coincides with the regular solution of Proposition 1.*

Proof: We only indicate the main computations (justifications are the same as in the proof of Theorem 2). By difference of the two equations of (21), we have

$$\partial_t(U-V) - d_2\Delta(U-V) = (d_1-d_2)\Delta U. \tag{30}$$

¿From this, we first deduce

$$\|U-V\|_{L^2(Q_T)} \leq \frac{|d_1-d_2|}{d_2}\|U\|_{L^2(Q_T)}. \tag{31}$$

This may be proved by duality, by introducing the solution of

$$\begin{cases} -[\partial_t\phi + d_2\Delta\phi] = U-V \text{ on } Q_T, \\ \phi(T)=0,\ \partial_\nu\phi = 0 \text{ on } \Sigma_T. \end{cases} \tag{32}$$

Multiplying the equation (30) by ϕ and integrating by parts gives

$$\int_{Q_T}(U-V)^2 = (d_1-d_2)\int_{Q_T}U\Delta\phi \leq |d_1-d_2|\|U\|_{L^2(Q_T)}\|\Delta\phi\|_{L^2(Q_T)}. \tag{33}$$

Multiplying the equation in ϕ by $-\Delta\phi$ leads to

$$\begin{aligned} -\int_{Q_T}\tfrac{1}{2}\partial_t|\nabla\phi|^2 + d_2\int_{Q_T}(\Delta\phi)^2 &= \int_{Q_T}(V-U)\Delta\phi \\ &\leq \tfrac{d_2}{2}\int_{Q_T}(\Delta\phi)^2 + \tfrac{1}{2d_2}\int_{Q_T}(U-V)^2. \end{aligned}$$

Integrating in time the first integral and using its positivity, we deduce

$$\int_{Q_T}(\Delta\phi)^2 \leq \frac{1}{d_2^2}\int_{Q_T}(U-V)^2.$$

Whence (31) using also (33). Next, using the first equation in (21) and "multiplying" it by d_1U+W leads to:

$$\int_{Q_T}(U+W)(d_1U+W) \leq 0.$$

Setting $\zeta = V-U$ and using $W = \hat{c}_2U + c_1(U+\zeta)$, this may be rewritten as

$$\int_{Q_T}[(1+c_1+\hat{c}_2)U + c_1\zeta][(d_1+c_1+\hat{c}_2)U + c_1\zeta] \leq 0.$$

This implies

$$\int_{Q_T}(1+c_1+\hat{c}_2)(d_1+c_1+\hat{c}_2)U^2 + (c_1\zeta)^2 \leq \int_{Q_T}c_1|\zeta U|[d_1+1+2(c_1+\hat{c}_2))],$$

$$\leq \alpha \int_{Q_T} (c_1\zeta)^2 + \frac{1}{4\alpha}\int_{Q_T} [d_1 + 1 + 2(c_1 + \hat{c}_2))]^2 U^2,$$

where we choose $\alpha = \max\left\{2, \frac{(d_1+1)^2}{2d_1}\right\}$ so that, for all $\theta \geq 0$,

$$\frac{1}{4\alpha}[d_1 + 1 + 2\theta]^2 \leq \frac{1}{2}(1+\theta)(d_1+\theta).$$

Finally, we may write

$$\int_{Q_T} (1 + c_1 + \hat{c}_2)(d_1 + c_1 + \hat{c}_2)U^2 \leq 2\alpha \int_{Q_T} (c_1\zeta)^2. \tag{34}$$

Now, we assume that $c = (c_1, c_2)$ is the regular solution so that, for $T < T^*$, $\|c_1\|_{L^\infty(Q_T)} < +\infty$ and we use (31):

$$\int_{Q_T} (1 + c_1 + \hat{c}_2)[d_1 + c_1 + \hat{c}_2]U^2 \leq 2\alpha \|c_1\|^2_{L^\infty(Q_T)} \frac{(d_1 - d_2)^2}{d_2^2} \int_{Q_T} U^2.$$

If

$$d_1 > 2\alpha \|c_1\|^2_{L^\infty(Q_T)} \frac{(d_1 - d_2)^2}{d_2^2},$$

we deduce that $U \equiv 0$. It follows that $V = U = 0 = W$.

Remark 7 This uniqueness result is not as "good" as the one obtained in Theorem 2: first, there uniqueness is obtained for the global weak solution; moreover, it holds for a fixed region of values for d_1, d_2, d_3. Here, the distance required between d_1, d_2 depends on the L^∞-norm of the regular solution. It might tend to zero if the solution becomes singular in finite time. And it may then happen that a bifurcation appears with multiple weak solutions. This is an open question.

3.4 A third way to write the limit system

It turns out that there is still one more "formal" way to write the limit problem. We are not able to derive more information with it than we already did, but it seems nevertheless worth being mentioned.

Let us make the following computation for the limit of $c^K = (c_1^K, c_2^K, c_3^K)$. Let f be the distribution such that

$$k(c_1^K c_2^K - \kappa c_3^K) \quad \overset{K \to (+\infty, \kappa^\infty)}{\longrightarrow} \quad f\,.$$

If c is a solution of the limit problem satisfying $c_1 c_2 = \kappa c_3$, we can differentiate in time this relation:

$$c_2 \partial_t c_1 + c_1 \partial_t c_2 = \kappa \partial_t c_3$$
$$c_2(d_1 \Delta c_1 - f) + c_1(d_2 \Delta c_2 - f) = \kappa(d_3 \Delta c_3 + f).$$

Therefore, there is a unique possible choice for f, namely:

$$f = \frac{d_1 c_2 \Delta c_1 + d_2 c_1 \Delta c_2 - \kappa d_3 \Delta c_3}{c_1 + c_2 + \kappa}\,.$$

Replacing $k(c_1c_2-\kappa c_3)$ by f in (R^K) suggests the new form of the limit system:

$$(R^\infty)\begin{cases} \partial_t c &= (I-P(c))\,D\Delta c \quad \text{for } \ t>0\ ,x\in\Omega\\ \partial_\nu c &= 0 \quad \text{for } \ t>0\ ,x\in\partial\Omega\\ c(0) &= c^0 \quad \text{for } x\in\Omega;\ c^0\in L^\infty(\Omega,\mathbb{R}^3_+)\end{cases}$$

where $D=\operatorname{diag}(d_1,d_2,d_3)$ and

$$P(c)=\frac{1}{c_1+c_2+\kappa}\begin{bmatrix} c_2 & c_1 & -\kappa\\ c_2 & c_1 & -\kappa\\ -c_2 & -c_1 & \kappa\end{bmatrix}.$$

Thus, we are led to a new nonlinear reaction-cross-diffusion system. Unfortunately, it is not possible to use it for the weak solutions expected at the limit since we do not know how to make sense of products like $c_i\Delta c_j$ when the c_i are not regular.

However, a simple analysis indicates that the matrix involved in (R^∞) has its spectrum in the closed right half-plane of the complex plane. Thus, the operator is "normally elliptic", up to adding a positive factor of the identity. Applying again H. Amann's results ([2, 3]), we obtain existence of local classical solutions for all given regular initial data. A difference with the previous 2×2 system (20) is that it is more general in the sense we do not require the initial conditions to satisfy $c_1^0c_2^0=\kappa c_3^0$. It is built into the system that the solutions must satisfy $[c_1c_2-\kappa c_3](t)=[c_1^0c_2^0-\kappa c_3^0]$, but this expression is not necessarily equal to zero. On the other hand, the system (R^∞) does not preserve positivity while its restriction to the manifold $c_1c_2=\kappa c_3$ does.

4 Extensions

As explained in the introduction, the goal of this paper is mainly to understand what happens in a reaction-diffusion system when a reversible reaction is considerably faster than diffusion. We chose to focus on the specific system (1) in order to concentrate on the main difficulties without being disturbed by other technical aspects. However, the techniques we have developed are rather general and can be applied to quite more general situations. Below, we discuss some explicit examples.

4.1 Extension to the chemical reaction $\sum_{i=1}^{p-1}\alpha_iC_i \rightleftharpoons C_p$

We indicate what should be added in the proof of Theorem 1 to extend it to the more general reaction of type

$$\sum_{i=1}^{p-1}\alpha_iC_i \underset{k\kappa}{\overset{k}{\rightleftharpoons}} C_p,\quad \alpha_i\in\mathbb{N}. \tag{35}$$

In the following, the concentration of C_i is denoted by c_i and the reaction term is supposed to be of the form $r(c)=k(\Pi_{i=1}^{p-1}c_i^{\alpha_i}-\kappa c_p)$, according to the mass action law, where $c=(c_1,...,c_p)$. The associated reaction-diffusion system can be written as

$$(R_0^K)\begin{cases} \partial_t c - D\Delta c &= r(c)\nu \quad \text{on } (0,+\infty)\times\Omega,\\ \partial_\nu c &= 0 \quad \text{on } (0,+\infty)\times\partial\Omega,\\ c(0,\cdot) &= c^0 \quad \text{on } \Omega \end{cases} \tag{36}$$

with $D = \mathrm{diag}(d_1, ..., d_p)$, $d_i > 0$, $\nu = (-\alpha_1, ..., -\alpha_{p-1}, 1)$. The reaction term is quasi-positive and, for $c^0 \in L^\infty(\Omega, \mathbb{R}_+^p)$, we have the local existence of nonnegative classical solutions. The global existence still holds since the growth of the reaction term with respect to c_p is linear (Theorem 3.5 in [18] applies as well).

Again, we want to let $(k,\kappa) \mapsto (+\infty, \kappa^\infty)$. Note that

$$\forall i = 1, ..., p-1,\ \partial_t(c_i + \alpha_i c_p) - \Delta(d_i c_i + \alpha_i d_p c_p) = 0. \tag{37}$$

There is a similar entropy inequality as (10) which provides estimates independent on $K = (k,\kappa)$ on the gradients in $L^{4/3}(Q_T)$ and shows that

$$\|(\Pi c_i^{\alpha_i} - \kappa c_p)(\log(\Pi c_i^{\alpha_i}) - \log(\kappa c_p))\|_{L^1(Q_T)} \to 0 \text{ when } (k,\kappa) \to (+\infty, \kappa^\infty).$$

The scheme of the proof is the same as what we did in the proof of Lemma 3: we only need to redefine $W_i = \alpha_i(c_i \log(c_i/c_i^*) - (c_i - c_i^*))$, $W = \sum_{i=1}^p W_i$, $Z = \sum_{i=1}^p d_i W_i$, with $c_1^{*\alpha_1} ... c_{p-1}^{*\alpha_{p-1}} = \kappa c_p^* \neq 0$.

Thanks to (37), and to the estimates coming from the entropy inequality, it is also possible to use Lemma 5 to get the compactness in $L^2(Q_T)$ of $c_i^K + \alpha_i c_p^K$, $1 \leq i \leq p-1$.

Let $K_n := (k_n, \kappa_n) \to (+\infty, \kappa^\infty)$ and let c^n be the classical solution of $(R_0^{K_n})$ on Q_T. Up to a subsequence, $(c_i^n + \alpha_i c_p^n)_{1\leq i\leq p-1}$ converges to a limit $(a_i)_{1\leq i \leq p-1} \in L^2(Q_T)^{p-1}$ for all $T > 0$ and almost everywhere, and $(\Pi_{i=1}^{p-1} c_i^{n\alpha_i} - \kappa_n c_p^n)_{n\in\mathbb{N}}$ converges to 0 almost everywhere. Let $(t,x) \in Q_T$ such that this pointwise convergence holds. The sequence $(c^n(t,x))_{n\in\mathbb{N}}$ is bounded and a limit point $l = (l_1, ..., l_p)$ for this sequence is a solution in $\mathbb{R}_+^p$ of the system

$$(s)\begin{cases} l_1 + \alpha_1 l_p &= a_1(t,x)\\ \quad\vdots & \\ l_{p-1} + \alpha_{p-1} l_p &= a_{p-1}(t,x)\\ l_1^{\alpha_1} \cdots l_{p-1}^{\alpha_{p-1}} &= \kappa^\infty l_p\ . \end{cases} \qquad (a_1, ..., a_{p-1})(t,x) \in [0,\infty)^{p-1} \tag{38}$$

Lemma 7 *The system (s) has a unique solution $l \in [0,\infty)^p$.*

Proof: Let l, l' be two solutions. Suppose first that $\forall i, a_i(t,x) > 0$. This implies: $\forall i, l_i > 0, l_i' > 0$. Then, taking the logarithm in the last equality of (s), we see that $< \log l - \log l', \nu >= 0$, where $< \cdot, \cdot >$ is the usual scalar product in $\mathbb{R}^p$. The linear relations in (s) can be rewritten as $< L_i, l - l' >= 0$ for some $p-1$ independent vectors $L_i \in \mathbb{R}_+^p$. It is easy to check that $\forall i, < L_i, \nu >= 0$. Therefore, $l - l'$ is parallel to ν. Finally, we have

$$< \log l - \log l', l - l' >= 0 = \sum_{i=1}^p (\log l_i - \log l_i')(l_i - l_i') = 0.$$

Since the function log is increasing on $(0,+\infty)$, we deduce $l = l'$.

Suppose now that $I = \{i \in \{1,...,p-1\} : a_i = 0\}$ is not empty. If l is a solution of (s), we have $l_i = 0$ for $i \in I \cup \{p\}$ and for $j \notin I \cup \{p\}$, $l_j = a_j$, so l is unique.

¿From here on, everything works like in the previous proof: for almost every $(t,x) \in Q_T$, a subsequence of $c^n(t,x)$ is bounded and has a unique limit point, so it converges to this limit point. This shows the pointwise convergence of a subsequence of c^n. Since each c_i^n is dominated by an $L^2(Q_T)$-convergent subsequence, the convergence of the subsequence of c_i^n holds also in $L^2(Q_T)$. Finally, the limit is a solution of the problem

$$\left\{\begin{array}{l} \forall i = 1,...,p,\ c_i \in L^2(Q_T), \nabla c_i \in L^{\frac{4}{3}}(Q_T)^N,\ c_i \geq 0,\ c_1^{\alpha_1} c_2^{\alpha_2} ... c_{p-1}^{\alpha_{p-1}} = \kappa^\infty c_p, \\ \forall i = 1,...,p-1,\ \forall \psi \in C^\infty(\overline{Q_T}) \text{ such that } \psi(T) = 0, \\ \quad -\int_\Omega \psi(0)(c_i^0 + \alpha_i c_p^0) + \int_{Q_T} -\psi_t(c_i + \alpha_i c_p) + \nabla\psi.\nabla(d_i c_i + \alpha_i d_p c_p) = 0. \end{array}\right.$$

4.2 Further possible extensions

One may wonder what happens for a general chemical reaction

$$\sum_{i=1}^{p} \alpha_i C_i \underset{k\kappa}{\overset{k}{\rightleftharpoons}} \sum_{i=1}^{p} \beta_i C_i \ .$$

The corresponding system is similar to (36) except that

$$r(c) = k\left(\Pi_{i=1}^p c_i^{\alpha_i} - \kappa \Pi_{i=1}^p c_i^{\beta_i}\right).$$

We still have $p-1$ independent positive linear relations between the equations which will provide compactness of $p-1$ linearly independent combinations of the solution. Thanks to the reversibility, the entropy inequality will still hold and helps to pass to the limit a.e. and in $L^2(Q_T)$ for all components.

However, a main difference is that the existence of global solutions for (k,κ) fixed is still an open problem in general (see e.g. [18] for more comments). One can nevertheless say that, if we are in a situation where global existence holds for all (k,κ), then passing to the limit as $(k,\kappa) \to (+\infty, \kappa^\infty)$ will be essentially the same as for the previous examples. Some specific features may provide global existence of classical solutions (see e.g. [15]). Recall also that global weak solutions exist for the (k,κ)-system when $\sum_i \beta_i \leq 2$ (or $\sum_i \alpha_i \leq 2$) (see [18]). Our approach can very likely be extended to cases when one starts with weak solutions for the (k,κ) system.

We may also consider the case where the reaction

$$C_1 + C_2 \underset{k\kappa}{\overset{k}{\rightleftharpoons}} C_3 \tag{39}$$

is coupled with some other *slow processes* which would lead to a system

$$\left\{\begin{array}{rcl} \partial_t c - D\Delta c &=& kr(c)\nu + g(c) \\ c(0) &=& c^0 \in L^\infty(\Omega, [0,\infty)^p), \end{array}\right.$$

where, $D = \text{diag}(d_1,...,d_p), d_i > 0,\ r(c) = c_1 c_2 - \kappa c_3,\ \nu = (-1,-1,1,0,...,0)$, and $g : \mathbb{R}^p \to \mathbb{R}^p$ is Lipschitz continuous and quasi-positive. Let us indicate how this situation can be also treated by using the same tools.

Thanks to the linear growth of g and to Lemma 2, the above system has global classical solutions for $K = (k, \kappa)$ fixed. Moreover, the $L^1(\Omega)^p$-norm of $c(t)$ is bounded on any interval. Setting

$$W = \sum_i c_i + c_3,\ Z = \sum_i d_i c_i + d_3 c_3, G = \sum_i g_i + g_3,$$

we have $\partial_t W - \Delta Z = G$.

Using that $G \leq k_1 W + k_2, k_1, k_2 \in (0, \infty)$, we obtain an $L^2(Q_T)$-bound on W as in Lemma 5. At this step, we need an alternative for the entropy inequality (10). The same computation as in the proof of Lemma 3 leads to an inequality where the right-hand side "C" of (10) is to be replaced by $\int_{Q_T} \sum_i g_i(c) \log c_i$ which is also bounded for each T (due to the $L^2(Q_T)$-bound on c_i and the Lipschitz continuity of g; see also [7]).

¿From a slight extension of Lemma 5 to $\partial_t W - \Delta Z = G$, we deduce the $L^2(Q_T)$-compactness of W as $K \to (+\infty, \kappa^\infty)$ as before. From the $L^2(Q_T)$-bound on the c_i and the linear growth of g, we deduce the compactness of each $c_i, i \geq 4$ in $L^2(Q_T)$.

Now, we are left with checking what happens for c_1, c_2, c_3. We still have $L^2(Q_T)$-compactness of $c_1 + c_3, c_2 + c_3$. The rest of the proof is the same and we are led to the limit system

$$\begin{cases} \partial_t(c_1 + c_3) - \Delta(d_1 c_1 + d_3 c_3) = g_1 + g_3 & \text{in } Q_T, \\ \partial_t(c_2 + c_3) - \Delta(d_2 c_2 + d_3 c_3) = g_2 + g_3 & \text{in } Q_T, \\ c_1 c_2 = \kappa^\infty c_3 & \text{in } Q_T, \\ \forall i \geq 4,\ \partial_t c_i - d_i \Delta c_i = g_i(c) & \text{in } Q_T \end{cases}$$

together with initial and boundary conditions.

Note that the above applies in particular to the famous Michaelis-Menten reaction for enzymatic catalysis:

$$C_1 + C_2 \underset{k\kappa}{\overset{k}{\rightleftharpoons}} C_3 \xrightarrow{k_2} C_1 + C_4. \tag{40}$$

In this situation, $g_1 = k_2 c_3, g_2 = k_2 c_3, g_3 = -k_2 c_3$. We identify as above the limit system as $(k, \kappa) \to (+\infty, \kappa^\infty)$. Note that it does not directly lead to the famous Michaelis-Menten homographic limit model which would require one more asymptotics, taking into account small initial concentrations of the enzyme C_1.

5 Appendix

Proof of Lemma 5:

Multiplying the equation in W, Z of Lemma 5 by Z and integrating on Q_T leads to

$$\int_{Q_T} \left[W\, Z + \nabla Z \cdot \nabla \int_0^t Z(s) ds \right] = \int_\Omega W(0) \int_0^T Z(s) ds,$$

or

$$\int_{Q_T} W\,Z + \frac{1}{2}\int_\Omega \left|\nabla \int_0^t Z(s)ds\right|^2 = \int_\Omega W(0)\int_0^T Z(s)ds. \tag{41}$$

We deduce

$$d^{\min}\int_{Q_T} W^2 \leq d^{\max}\sqrt{T}\left[\int_\Omega W(0)^2\right]^{1/2}\left[\int_{Q_T} W^2\right]^{1/2}.$$

The announced $L^2(Q_T)$-bound on W, and therefore on Z, follows.

Now, let (W^p, Z^p) be a sequence in $\mathcal{F}$ such that $W^p(0) \in \mathcal{G}$ and (W^p, Z^p) converges weakly in $L^2(Q_T)^2$ to (W, Z). Let us pass to the limit as $p \to +\infty$ in

$$W^p(t) - \Delta\int_0^t Z^p(s)\,ds = W^p(0),\ \partial_\nu \int_0^t Z^p(s)\,ds = 0 \text{ on } \Sigma_T.$$

Note that $\Delta\int_0^t Z^p(s)\,ds$ is bounded in $L^2(Q_T)$ so that $\int_0^t Z^p(s)\,ds$ is bounded in $L^2\left(0,T;H^2(\Omega)\right)$. Thus, we may pass to the limit (weakly in L^2) to get

$$W(t) - \Delta\int_0^t Z(s)\,ds = W_0,\ \partial_\nu \int_0^t Z(s)\,ds = 0 \text{ on } \Sigma_T,$$

where W_0 is the weak limit in $L^2(\Omega)$ of $W^p(0)$. Now, we multiply the identity

$$W^p(t) - W(t) - \Delta\int_0^t [Z^p - Z](s)\,ds = W^p(0) - W_0,$$

by $Z^p - Z$. As in the computation leading to (41), we will use that

$$\int_{Q_T} -(Z^p - Z)\Delta\int_0^t [Z^p - Z](s)\,ds \geq 0. \tag{42}$$

This may be justified by introducing $Z_h(t) = h^{-1}\int_t^{t+h}[Z^p - Z](s)ds$. Then $Z_h, \Delta\int_0^t Z_h$ converge in $L^2(Q_T)$ respectively to $Z^p - Z, \Delta\int_0^t(Z^p - Z)$. Moreover, $Z_h \in L^2\left(0,T;H^1(\Omega)\right)$ so that the following computation is allowed

$$\int_{Q_T} -Z_h\Delta\int_0^t Z_h(s)ds = \int_{Q_T}\nabla Z_h\nabla\int_0^t Z_h(s)ds = \frac{1}{2}\int_\Omega\left|\nabla\int_0^T Z_h(s)ds\right|^2 \geq 0.$$

And we may pass to the limit as $h \to 0$ to recover (42). It implies

$$\int_{Q_T}(W^p - W)(Z^p - Z) \leq \int_\Omega (W^p(0) - W_0)\int_0^T [Z^p - Z](s)\,ds. \tag{43}$$

Next, let $H^p(t) := \int_0^t Z^p(s)\,ds$. We have

$$\int_\Omega |\nabla H^p(t)|^2 = \int_{Q_t} 2\,\partial_t(\nabla H^p)\,\nabla H^p = -\int_{Q_t} 2\,\partial_t H^p\,\Delta H^p,$$

so that

$$\sup_{t\in[0,T]}\int_\Omega |\nabla H^p(t)|^2 \leq 2\left[\int_{Q_T}(\partial_t H^p)^2\right]^{1/2}\left[\int_{Q_T}(\Delta H^p)^2\right]^{1/2} \leq C < +\infty,$$

since ΔH^p and $\partial_t H^p = Z^p$ are bounded in $L^2(Q_T)$. It follows that H^p is bounded in $L^\infty\left(0,T;H^1(\Omega)\right)\cap H^1\left(0,T;L^2(\Omega)\right)$: by compact embedding of H^1 into L^2 and by Ascoli's Theorem, H^p is compact in $C\left([0,T];L^2(\Omega)\right)$. We deduce that it converges strongly in $C([0,T];L^2(\Omega))$ and the limit is necessarily $\int_0^t Z(s)ds$. Thus the right hand side of (43) tends to zero.

Now, using $Z^p - Z = A^pW^p - A^pW + A^pW - Z$ in the left-hand side of (43), we may write

$$\limsup_{p\to\infty}\int_{Q_T} A^p(W^p-W)^2 + Z^pW - W^pZ - A^pW^2 + WZ \le 0. \tag{44}$$

By assumption (13) and weak-L^2 convergence of (W^p, Z^p) towards (W, Z), $\int_{Q_T} Z^pW - W^pZ - A^pW^2 + WZ$ converges to zero as $p\to\infty$. Using $A^p \ge d^{\min} > 0$, we deduce that $W^p - W$ converges to zero strongly in $L^2(Q_T)$.

Let us now show that, if (W^p, Z^p) converges weakly in $L^2(Q_T)$ to (W, Z) and if moreover W^p converges a.e., then (13) holds. Let W^∞ be the a.e. limit of W^p. Thanks to the $L^2(Q_T)$-bound on W^p, by a Vitali-type argument, it is classical that W^p converges in $L^1(Q_T)$ to W^∞ (and even in $L^q(Q_T)$ for all $q\in[1,2)$). In particular, $W^\infty = W$. Then, note that this implies that any weak$^* - L^\infty(Q_T)$ limit-point A^∞ of A^p is equal to Z/W. Indeed, if $\psi\in C_0^\infty(\Omega)$, $\psi\, W^p$ converges strongly in $L^1(Q_T)$ to ψW, so that, up to convenient subsequences

$$\forall\psi\in C_0^\infty(Q_T),\ \int_{Q_T}\psi\, W^pA^p = \int_{Q_T}\psi\, Z^p \to \int_{Q_T}\psi\, W\, A^\infty = \int_{Q_T}\psi Z.$$

The last equality, valid for all $\psi\in C_0^\infty(Q_T)$, implies that $A^\infty = Z/W$, and it follows that the full sequence A^p converges to $A = Z/W$ in the sense of (13).

Finally, if A^p converges a.e., and if A^∞ denotes its a.e. limit, by dominated convergence (recall that A^p is uniformly bounded), A^p converges in any $L^q(Q_T), q<\infty$ towards A^∞ (and also in weak*-$L^\infty(Q_T)$). To see that $A^\infty = A = Z/W$, we pass to the limit in the identity $Z^p = A^pW^p$ where

$$(Z^p, W^p)\to(Z,W)\ \textit{in weak} - L^2(Q_T)^2,\ \ A^p\to A^\infty\ \textit{strongly in}\ L^2(Q_T),$$

so that $Z = A^\infty\, W$.

References

[1] Amann, H. (1985). *Global existence for semilinear parabolic problems*, J. Reine Angew. Math. **360**: 47–83.

[2] Amann, H. (1993). *Nonhomogeneous linear and quasilinear elliptic and parabolic boundary value problems*, in Function Spaces, Differential Operators and Nonlinear Analysis, H.J. Schmeisser, H. Triebel (ed.), Teubner, Stuttgart, Leipzig: 9–126.

[3] Amann, H. (1990). *Dynamic theory of quasilinear parabolic equations. II. Reaction-diffusion systems*, Diff. Int. Equ. **3**: 13–75.

[4] Baras, P., Pierre, M. (1984). *Problèmes paraboliques semi-linéaires avec données mesures*, Applicable Analysis **18**: 111–149.

[5] Bisi, M., Confort, F., Desvillettes, L. (2007). *Quasi-steady-state approximation for reaction-diffusion equations*, Bull. Inst. Math., Acad. Sin. (N.S.) **2**: 823–850.

[6] Bothe, D. (1999). *Nonlinear Evolutions in Banach Spaces – Existence and Qualitative Theory with Applications to Reaction-Diffusion Systems*, Habilitation thesis, Univ. of Paderborn.

[7] Bothe, D. (2003). *Instantaneous limits of reversible chemical reactions in presence of macroscopic convection*, J. Differ. Equations **193**: 27-48.

[8] Bothe, D., Hilhorst, D. (2003). *A reaction-diffusion system with fast reversible reaction*, J. Math. Anal. Appl. **286**: 125-135.

[9] Bothe D., Pierre, M. (2010). *Quasi-steady-state approximation for a reaction-diffusion system with fast intermediate*, J. Math. Anal. Appl. **368**: 120–132.

[10] Bothe, D., Pierre, M. (2012). *Quasi-steady-state approximation for a reaction-diffusion system with fast intermediate*, Discr. and Cont. Dyn. Syst. - Ser. S **5**: 49–59.

[11] Espenson, J.H. (1995). *Chemical Kinetics and Reaction Mechanisms*, (2^{nd} ed.), McGraw-Hill.

[12] Fitzgibbon, W.B., Hollis, S.L., Morgan, J.J. (1997). *Stability and Lyapunov Functions for Reaction-Diffusion Systems*, SIAM J. Math. Anal. **28**: 595–610.

[13] Henry, D. (1981). *Geometric Theory of semilinear Parabolic Equations*, Lecture Notes in Math. **840**, Springer-Verlag.

[14] Hilhorst, D., Mimura M., Ninomiya, H. (2009). *Fast reaction limit of competition-diffusion systems*, in "Handbook of Differential Equations" (C. M. Dafermos and M. Pokorny, eds.), Elsevier, Evolution Equations **5**.

[15] Laamri, E.-H. (2011). *Global Existence of Classical Solutions for a Class of Reaction-Diffusion Systems*, Acta Applicanda Mathematicae **115**: 153–165.

[16] Martin, R.H, Pierre, M. (1991). *Nonlinear reaction-diffusion systems*, in Nonlinear Equations in the Applied Sciences, W.F. Ames and C. Rogers ed., Math. Sci. Eng. **185**, Acad. Press, New York.

[17] Morgan, J. (1989). *Global existence for semilinear parabolic systems*, SIAM J. Math. Anal. **20**: 1128–1144.

[18] Pierre, M. (2010). *Global Existence in Reaction-Diffusion Systems with Control of Mass: a Survey*, Milan J. Math. **78**: 417–455.

[19] Prüss, J. (2003). *Maximal Regularity for Evolution Equations in L^p-Spaces*, Conf. Sem. Mat. Univ. Bari **285**: 1–39.

[20] Rothe, F. (1984). *Global Solutions of Reaction-Diffusion Systems*, Lecture Notes in Mathematics **1072**, Springer, Berlin.

[21] Simon, J. (1987). *Compact Sets in the Space $L^p(0,T;B)$*, Annali di Matematica pura ed applicata (IV) **146**: 65–96.

Dieter Bothe
Center of Smart Interfaces, TU Darmstadt
Petersenstrasse 32, 64287 Darmstadt, Germany
bothe@csi.tu-darmstadt.de

Michel Pierre
ENS Cachan Bretagne, IRMAR, UEB
Campus de Ker Lann, 35170-Bruz, FRANCE
michel.pierre@bretagne.ens-cachan.fr

Guillaume Rolland
ENS Cachan Bretagne, IRMAR, UEB
Campus de Ker Lann, 35170-Bruz, FRANCE
guillaume.rolland@bretagne.ens-cachan.fr