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About entropy methods for reaction-diffusion equations (**)

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^(**) Received 30^{th} April 2007 and in revised form 26^{th} August 2007. AMS classification 35K57, 35Q80, 35B40, 35B45.

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1 - Introduction

This paper summarizes a series of lectures given by the author at the University of Milano in the winter of 2007. It is devoted to a self-contained and elementary approach to the mathematical properties of reversible reaction-diffusion equations, almost entirely based on the entropy estimate.

The only mathematical prerequisites for this paper are some familiarity with PDEs methods (like, for example, Sobolev inequalities), together with a few basic facts about the solutions to linear parabolic equations.

Our goal is to show how the entropy estimate (which, together with the conservation of atoms, is the only physically relevant estimate) can be used in a systematic way in order to get bounds leading to existence of strong or weak solutions, as well as bounds for the rate of convergence to the equilibrium.

We have decided to present the estimates for three typical systems corresponding to basic chemical reactions involving a few species, rather than introducing general systems with an arbitrary number of species and reactions. We hope that this simplified presentation, which retains many of the difficulties of the general case, will help the readers.

1.1 - Reversible reactions

Our aim is to study reversible reaction processes for a set of chemical species $A_i, i = 1, 2, ..., q$, of the type

(1)
$$a_1 \mathcal{A}_1 + \ldots + a_q \mathcal{A}_q \rightleftharpoons \beta_1 \mathcal{A}_1 + \ldots + \beta_q \mathcal{A}_q, \quad a_i, \beta_i \in \mathbb{N}.$$

We define by $a_i := a_i(t)$ the concentration at time t of species A_i . Then, thanks to the mass action law, the functions $a_i, i = 1, 2, ..., q$, satisfy (Cf. for example [7]) the following system of ordinary differential equations (ODEs):

(2)
$$a_i'(t) = (\beta_i - a_i) \left(l \prod_{j=1}^q a_j^{a_j}(t) - k \prod_{j=1}^q a_j^{\beta_j}(t) \right).$$

Here a_i, β_i are the stoichiometric coefficients, and k > 0, l > 0 are strictly positive reaction rates corresponding to a reversible reaction.

1.2 - Convection; diffusion

We now assume that the chemical reaction happens in a reactor (that is, from the point of view of mathematics, a bounded box $\Omega \subset \mathbb{R}^N$ $(N \ge 1)$, assumed to be smooth (C^2) , bounded and connected), where the molecules of the various species are moving.

We shall concentrate on the case when the molecules of the various species diffuse (each species has its own velocity of diffusion) within a non-reactive background supposed to be at rest. It means that the unknown is $a_i := a_i(t,x) \ge 0$, $i = 1, \ldots, q$ (where $x \in \Omega$). It satisfies (Cf. for example [3]) the following system of partial differential equations (PDE):

$$(3) \hspace{1cm} \partial_t a_i - d_i \, \varDelta_x a_i = (\beta_i - a_i) \Biggl(l \, \prod_{j=1}^q a_j^{a_j} - k \, \prod_{j=1}^q a_j^{\beta_j} \Biggr),$$

where d_i is the diffusion velocity (in the non-reacting background) of species A_i .

Note that many important problems involve some form of convection. The simplest modeling involving such a phenomenon concerns the case when the (non-reactive) fluid is not at rest, but has a velocity $u := u(t, x) \in \mathbb{R}^N$. In this case, equation (3) becomes

$$(4) \hspace{1cm} \partial_t a_i + \nabla_x \cdot (u \, a_i) - d_i \, \varDelta_x a_i = (\beta_i - a_i) \Bigg(l \, \prod_{j=1}^q a_j^{a_j} - k \, \prod_{j=1}^q a_j^{\beta_j} \Bigg).$$

However, the most interesting situation concerns the case of a mixture of reactive gases satisfying reactive Euler equations or reactive Navier-Stokes equations. We refer to [7] for a precise description of such a situation.

We shall assume that the molecules are confined in the reactor, so that the flux of concentration of each species at the boundary $\partial\Omega$ is 0. This gives for equation (3) the homogeneous Neumann boundary condition:

$$(5) n(x) \cdot \nabla_x a_i = 0,$$

where n(x) is (and always will be in the sequel) the outer normal unit vector at point x of $\partial \Omega$.

1.3 - Three typical chemical reactions

We shall from now on concentrate on the three typical chemical reactions

$$(6) A + A \rightleftharpoons B,$$

$$(7) A + B \rightleftharpoons C,$$

and

$$(8) A+B \rightleftharpoons C+D.$$

Without loss of generality, it is convenient to assume that (denoting by $|\Omega|$ the measure of Ω)

$$(9) l = k = 1, |\Omega| = 1.$$

This can be obtained (for example in the case of eq. (8)) thanks to the rescaling $t \to \frac{1}{k} t, x \to |\Omega|^{\frac{1}{N}} x, (a,b,c,d) \to \frac{k}{l} (a,b,c,d).$

Then, we first describe the system associated to $A+A\rightleftharpoons B.$ It can be written as:

(10)
$$\begin{cases} \partial_t a - d_a \Delta_x a = -2 (a^2 - b), \\ \partial_t b - d_b \Delta_x b = a^2 - b, \end{cases}$$

together with the homogeneous Neumann conditions

(11)
$$n(x) \cdot \nabla_x a = 0, \quad n(x) \cdot \nabla_x b = 0 \quad x \in \partial \Omega,$$

and the nonnegative initial data

(12)
$$a(0,x) = a_{in}(x) \ge 0, \quad b(0,x) = b_{in}(x) \ge 0.$$

Then, we turn to the system associated to $A + B \rightleftharpoons C$. It writes

(13)
$$\begin{cases} \partial_t a - d_a \Delta_x a = -ab + c, \\ \partial_t b - d_b \Delta_x b = -ab + c, \\ \partial_t c - d_c \Delta_x c = ab - c, \end{cases}$$

with a, b, c satisfying homogeneous Neumann conditions

(14)
$$n(x) \cdot \nabla_x a = 0$$
, $n(x) \cdot \nabla_x b = 0$, $n(x) \cdot \nabla_x c = 0$ $x \in \partial \Omega$,

and the nonnegative initial data

(15)
$$a(0,x) = a_{in}(x) \ge 0, \qquad b(0,x) = b_{in}(x) \ge 0, \qquad c(0,x) = c_{in}(x) \ge 0.$$

Finally, we write down the system associated to $A + B \rightleftharpoons C + D$:

(16)
$$\begin{cases} \partial_t a - d_a \Delta_x a = -ab + cd, \\ \partial_t b - d_b \Delta_x b = -ab + cd, \\ \partial_t c - d_c \Delta_x c = ab - cd, \\ \partial_t d - d_d \Delta_x d = ab - cd, \end{cases}$$

with a, b, c, d satisfying homogeneous Neumann conditions

(17)
$$\begin{cases} n(x) \cdot \nabla_x a = 0, & n(x) \cdot \nabla_x b = 0, & x \in \partial \Omega, \\ n(x) \cdot \nabla_x c = 0, & n(x) \cdot \nabla_x d = 0 & x \in \partial \Omega, \end{cases}$$

and the nonnegative initial data

(18)
$$\begin{cases} a(0,x) = a_{in}(x) \ge 0, & b(0,x) = b_{in}(x) \ge 0, \\ c(0,x) = c_{in}(x) \ge 0, & d(0,x) = d_{in}(x) \ge 0. \end{cases}$$

1.4 - Plan of the paper

The rest of the paper is devoted to the mathematical study of the systems (10) - (12), (13) - (15), and (16) - (18).

In section 2 are presented the basic a priori estimates for our equations: it is proven there that strong solutions (with strictly positive initial data) are strictly positive, satisfy a set of conservation laws (that is, the conservation of the number of atoms of each kind), and (this will be systematically used in the sequel) an entropy estimate. By exploiting these estimates, a priori L^p bounds are proven (with p > 1 depending on the dimension).

Section 3 is devoted to the treatment of the Cauchy problem for our equations. For systems (10) – (12) and (13) – (15), it is possible to obtain an L^{∞} a priori estimate, either thanks to a maximum principle, or to the use of the properties of the heat kernel. This enables to prove the existence (and uniqueness) of a strong solution for those systems. The situation is completely different for system (16) – (18). No L^{∞} a priori estimate is known in this case, except in dimension 1 (and, thanks to a very recent work, Cf. [8], in dimension 2). It is however possible to prove the existence of weak solutions to this system in L^2 (for any dimension), thanks to a method based on duality arguments.

Finally, we present in Section 4 an estimate of exponential decay toward equilibrium for the solution of system (10) - (12). This estimate is a direct consequence of the entropy inequality, together with a Cziszar-Kullback type inequality.

2 - A priori estimates; formal computations

We now prove the standard a priori estimates for systems (10) – (12), (13) – (15), and (16) – (18). For this, we assume that we have strong (for example $C^2([0, T[\times \overline{\Omega})])$ for some T > 0) solutions of one of these systems.

2.1 - Strict positivity

We begin with the question of strict positivity. The following proposition gives a classical general sufficient condition on the coefficients of a parabolic equation for propagation of strict positivity:

Proposition 2.1. Let Ω be a smooth (C^2) bounded open set of \mathbb{R}^N , T > 0, and d > 0. We also consider coefficients $a \in C^2([0,T] \times \overline{\Omega})$ and $b \in C^2([0,T] \times \overline{\Omega}, \mathbb{R}_+)$. We suppose that u := u(t,x) is a solution in $C^2([0,T] \times \overline{\Omega})$ to equation

(19)
$$\partial_t u(t,x) - d \Delta_x u(t,x) = a(t,x) u(t,x) + b(t,x),$$

together with Neumann boundary condition and initial datum

$$\nabla_x u(t, x) \cdot n(x) = 0, \qquad u(0, x) = u_{in}(x) > 0,$$

where $u_{in} \in C^2(\overline{\Omega})$.

Then, for all $t \in [0, T]$ and $x \in \Omega$, u(t, x) > 0.

Proof of Proposition 2.1. We define $t_0 > 0$ as the infimum of times t > 0 such that there exists $x_0 \in \overline{\Omega}$ satisfying $u(t_0, x_0) = 0$. For $t \in [0, t_0[$, we can consider

 $f(t,x) = \ln u(t,x)$. Then, f satisfies the inequality

$$\partial_t f(t,x) - d \Delta_x f(t,x) = a(t,x) + \frac{b(t,x)}{u(t,x)} + d \frac{|\nabla_x u(t,x)|^2}{u(t,x)^2} \ge - ||a||_{\infty},$$

$$\nabla_x f(t, x) \cdot n(x) = 0, \qquad f(0, x) = \ln u_{in}(x) \ge -\|\ln u_{in}\|_{\infty}.$$

We consider (for any $\varepsilon > 0$) the auxiliary quantity $f^{\varepsilon}(t,x) = f(t,x) + \|a\|_{\infty} t + \|\ln u_{in}\|_{\infty} + \varepsilon(t+1)$. This quantity satisfies the inequality,

$$\partial_t f^{\varepsilon} - d \Delta_x f^{\varepsilon} \geq \varepsilon$$
,

together with Neumann boundary condition and initial datum

$$\nabla_x f^{\varepsilon} \cdot n(x) = 0, \qquad f^{\varepsilon}(0, x) \ge \varepsilon.$$

We define $t_1 \leq t_0$ as the infimum of times t > 0 such that there exists $x_0 \in \overline{\Omega}$ satisfying $f^{\varepsilon}(t_1, x_0) = 0$. Note that (according to the definition of t_1), the function $x \mapsto f^{\varepsilon}(t_1, x)$ reaches its infimum at point x_0 , and that $t_1 > 0$.

If $x_0 \in \Omega$, then $\Delta_x f^{\varepsilon}(t_1, x_0) \ge 0$, so that $\partial_t f^{\varepsilon}(t_1, x_0) > 0$. Since $t_1 > 0$, this is impossible.

If $x_0 \in \partial \Omega$, then, we know that $\nabla_x u(t_1, x_0) \cdot \tau(x_0) = 0$ (where $\tau(x_0)$ is any vector tangeant to $\partial \Omega$ at point x_0), so that thanks to the Neumann boundary condition, $\nabla_x f^{\varepsilon}(t_1, x_0) = 0$. Therefore, $\Delta_x f^{\varepsilon}(t_1, x_0) \geq 0$, and we conclude as in the case when $x_0 \in \Omega$.

Finally, $t_1 = t_0$, so that $f^{\varepsilon}(t,x) > 0$ when $t \in [0,t_0[$, and (letting ε go to 0), $f(t,x) \ge -\|a\|_{\infty} t - \|\ln u_{in}\|_{\infty}$ (still when $t \in [0,t_0[$). This finally ensures that $t_0 = T$, so that Proposition 2.1 is proven.

This proposition can be used directly for proving the strict positivity of the concentrations in systems (10) - (12), (13) - (15) and (16) - (18).

Proposition 2.2. Let T > 0, Ω be a bounded regular C^2 domain of \mathbb{R}^N , $d_a, d_b > 0$ (together with $d_c, d_d > 0$, depending on the system considered) be diffusivity constants, $a_{in} := a_{in}(x) > 0$, $b_{in} := b_{in}(x) > 0$ (together with $c_{in} := c_{in}(x) > 0$, $d_{in} := d_{in}(x) > 0$ depending on the system considered) be initial data in $C^2(\overline{\Omega})$. Let also a := a(t, x), b := b(t, x) (together with c := c(t, x), d := d(t, x), depending on the system considered) be solutions in $C^2([0, T[\times \overline{\Omega})$ of one of the systems (10) – (12), (13) – (15), or (16) – (18).

Then, for all $t \in [0, T[$ and $x \in \Omega$, one has a(t, x) > 0, b(t, x) > 0 (and c(t, x) > 0, d(t, x) > 0 depending on the system considered).

Proof of Proposition 2.2. We consider only the system (10) - (12), since the other ones can be treated in the same way.

It is enough to consider the time t_0 defined as the infimum of the times t where there exists $x_0 \in \overline{\Omega}$ such that $a(t,x_0)=0$ or $b(t,x_0)=0$. On the interval $[0,t_0]$, it is possible to put the two equations of system (10) under the form (19). Then, one can use Proposition 2.1 in order to show that $a(t_0,\cdot)>0$ and $b(t_0,\cdot)>0$, which leads to a contradiction.

2.2 - Conservation of the number of atoms

We begin by noticing that the flow of equations (10) - (12), (13) - (15), or (16) - (18), conserves a quantity equivalent to the total L^1 -norm:

Proposition 2.3. Let T > 0, Ω be a bounded regular (C^2) open set of \mathbb{R}^N , $d_a, d_b > 0$ (together with $d_c, d_d > 0$, depending on the system considered) be diffusivity constants, $a_{in} := a_{in}(x) > 0$, $b_{in} := b_{in}(x) > 0$ (together with $c_{in} := c_{in}(x) > 0$, $d_{in} := d_{in}(x) > 0$ depending on the system considered) be initial data in $C^2(\overline{\Omega})$. Let also a := a(t, x), b := b(t, x) (together with c := c(t, x), d := d(t, x), depending on the system considered) be solutions in $C^2([0, T] \times \overline{\Omega})$ of one of the systems (10) – (12), (13) – (15), or (16) – (18).

Then, for all $t \in [0, T]$ and $x \in \Omega$, one has the following properties of conservation:

1. For system (10) - (12):

(20)
$$M := \int_{\Omega} (a(t,x) + 2b(t,x)) dx = \int_{\Omega} (a_{in}(x) + 2b_{in}(x)) dx.$$

2. For system (13) - (15):

(21)
$$\begin{cases} M_1 := \int_{\Omega} (a(t,x) + c(t,x)) dx = \int_{\Omega} (a_{in}(x) + c_{in}(x)) dx, \\ M_2 := \int_{\Omega} (b(t,x) + c(t,x)) dx = \int_{\Omega} (b_{in}(x) + c_{in}(x)) dx. \end{cases}$$

3. Finally, for system (16) - (18):

(22)
$$\begin{cases} M_{1} := \int_{\Omega} (a(t,x) + c(t,x)) dx = \int_{\Omega} (a_{in}(x) + c_{in}(x)) dx, \\ M_{2} := \int_{\Omega} (b(t,x) + c(t,x)) dx = \int_{\Omega} (b_{in}(x) + c_{in}(x)) dx, \\ M_{3} := \int_{\Omega} (b(t,x) + d(t,x)) dx = \int_{\Omega} (b_{in}(x) + d_{in}(x)) dx. \end{cases}$$

Proof of Proposition 2.3. Those conservations are simply obtained by taking linear combinations of the equations, and by integrating on the domain Ω , taking into account the Neumann boundary condition.

This ends the proof of Proposition 2.3.

Taking into account the properties of strict positivity and the previous properties of conservation, we see that there is a natural $L^{\infty}([0,T];L^{1}(\Omega))$ estimate for all the concentrations appearing in systems (10) - (12), (13) - (15), and (16) - (18).

2.3 - Entropy estimate

Our main tool in the sequel will be the entropy/entropy dissipation conservation property. In order to state it precisely, we introduce the following definitions of entropy E_i and entropy dissipation D_i (i = 1, ..., 3 corresponds to each system), defined as functions of the concentrations, seen as functions of x. For a general definition of the entropy of a mixture of reactive species, we refer to [7].

We start with system (10) - (12):

(23)
$$E_{1}(a,b) := \int_{\Omega} \left(a \left(\ln a - 1 \right) + b \left(\ln b - 1 \right) \right) dx,$$

$$D_{1}(a,b) = d_{a} \int_{\Omega} \frac{\left| \nabla_{x} a \right|^{2}}{a} dx + d_{b} \int_{\Omega} \frac{\left| \nabla_{x} b \right|^{2}}{b} dx$$

$$+ \int_{\Omega} (a^{2} - b) \left(\ln (a^{2}) - \ln b \right) dx.$$

Then, we turn to system (13) - (15):

(25)
$$E_{2}(a,b,c) := \int_{\Omega} \left(a \left(\ln (a) - 1 \right) + b \left(\ln (b) - 1 \right) + c \left(\ln (c) - 1 \right) \right) dx,$$

$$D_{2}(a,b,c) = d_{a} \int_{\Omega} \frac{|\nabla_{x}a|^{2}}{a} dx + d_{b} \int_{\Omega} \frac{|\nabla_{x}b|^{2}}{b} dx + d_{c} \int_{\Omega} \frac{|\nabla_{x}c|^{2}}{c} dx$$

$$+ \int_{\Omega} (ab - c) \left(\ln (ab) - \ln c \right) dx.$$

Finally, we introduce the quantities corresponding to system (16) - (18):

$$E_{3}(a,b,c,d) := \int_{\Omega} (a (\ln(a) - 1) + b (\ln(b) - 1) + c (\ln(c) - 1) + d (\ln(d) - 1)) dx,$$

$$(27) \qquad + c (\ln(c) - 1) + d (\ln(d) - 1)) dx,$$

$$D_{3}(a,b,c,d) := d_{a} \int_{\Omega} \frac{|\nabla_{x}a|^{2}}{a} dx + d_{b} \int_{\Omega} \frac{|\nabla_{x}b|^{2}}{b} dx + d_{c} \int_{\Omega} \frac{|\nabla_{x}c|^{2}}{c} dx$$

(28) $+ d_d \int_{\Omega} \frac{|\nabla_x d|^2}{d} \, dx + \int_{\Omega} (a \, b - c \, d) \, (\ln (a \, b) - \ln (c \, d)) \, dx \, .$

We are able to prove the following a priori estimates:

Proposition 2.4. Let T > 0, Ω be a bounded regular (C^2) open set of \mathbb{R}^N , $d_a, d_b > 0$ (together with $d_c, d_d > 0$, depending on the system considered) be diffusivity constants, $a_{in} := a_{in}(x) > 0$, $b_{in} := b_{in}(x) > 0$ (together with $c_{in} := c_{in}(x) > 0$, $d_{in} := d_{in}(x) > 0$ depending on the system considered) be initial data in $C^2(\overline{\Omega})$. Let also a := a(t, x), b := b(t, x) (together with c := c(t, x), d := d(t, x), depending on the system considered) be solutions in $C^2([0, T] \times \overline{\Omega})$ of one of the systems (10) – (12), (13) – (15), or (16) – (18).

Then, for all $t \in [0,T]$ and $x \in \Omega$, one has the following identity: (for the $i \in \{1,\ldots,3\}$ corresponding to the system under consideration)

$$\partial_t E_i = -D_i.$$

Moreover, this identity entails the following a priori estimate (for all $T \in]0, +\infty]$):

(30)
$$\sup_{t \in [0,T]} E_i(t) + \int_0^T D_i(s) \, ds \le E_i(0).$$

Proof of Proposition 2.4. Note first that we already know that our solutions are strictly positive, so that we can compute quantities like the logarithms of concentrations. Then, we detail the computation only in the case of system (10) - (12):

$$\partial_t E_1 = \int_{\Omega} (\ln a \, \partial_t a + \ln b \, \partial_t b) \, dx$$

$$=-\int\limits_{\Omega}\!\left(d_a\,rac{\left|
abla_xa
ight|^2}{a}+d_b\,rac{\left|
abla_xb
ight|^2}{b}
ight)dx$$

$$+ \int_{\partial\Omega} (\ln a \, \nabla_x a \cdot n(x) + \ln b \, \nabla_x b \cdot n(x)) \, d\sigma(x)$$
$$+ \int_{\Omega} (-2 \, \ln a \, (a^2 - b) + \ln b \, (a^2 - b)) \, dx.$$

We conclude by using the Neumann boundary condition.

The a priori estimate is obtained by integrating between times 0 and t (0 < t < T) identity (29). This concludes the proof of Proposition 2.4.

2.4 - Consequences of the entropy estimate

The a priori estimate obtained above can be exploited in order to obtain L^p type bounds for our solutions. More precisely, it is possible to obtain the following proposition (Cf. [5]):

Proposition 2.5. Let T > 0, Ω be a bounded regular (C^2) and connected open set of \mathbb{R}^N , $d_a, d_b > 0$ (together with $d_c, d_d > 0$, depending on the system considered) be diffusivity constants, $a_{in} := a_{in}(x) > 0$, $b_{in} := b_{in}(x) > 0$ (together with $c_{in} := c_{in}(x) > 0$, $d_{in} := d_{in}(x) > 0$ depending on the system considered) be initial data in $C^2(\overline{\Omega})$. Let also a := a(t, x), b := b(t, x) (together with c := c(t, x), d := d(t, x), depending on the system considered) be solutions in $C^2([0, T] \times \overline{\Omega})$ of one of the systems (10) - (12), (13) - (15), or (16) - (18).

Then, for all $t \in [0, T]$ and $x \in \Omega$, and for a denoting any concentration appearing in one of the three systems, there exists C > 0 depending only on the initial data and the diffusivity constants such that:

(31)
$$\|a\|_{L^{\inf(1+2/N,2)}([0,T]\times\Omega)} \le C (1+T)^{\sup(2,N/(N+2))}.$$

Proof of Proposition 2.5. Thanks to the a priori estimate (30), we see that for any concentration a appearing in any of the three systems considered (that is, a = a, b, c or d), there exists a constant C depending only on the initial data (in fact, the initial entropy of the mixture) such that

(32)
$$\iint\limits_{0}^{T} |\nabla_{x}\sqrt{a}|^{2} dxdt \leq C.$$

We use the Sobolev-Wirtinger estimate (valid for $u \in H^1(\Omega)$, where Ω is a

bounded, regular, and connected open set of \mathbb{R}^N of volume 1, Cf. [1]):

(33)
$$\left(\int\limits_{\Omega} |u(x) - \bar{u}|^{p^*} dx\right)^{2/p^*} \le K \int\limits_{\Omega} |\nabla_x u|^2 dx,$$

where
$$\bar{u} = \int_{\Omega} u(y) \, dy$$
, $p^* = \frac{2N}{N-2}$, and $K := K(\Omega)$.

When N=2, this estimate is true for all $p^* \in [1, +\infty[$, and when N=1, it is replaced by the stronger inequality

(34)
$$\left(\sup_{x\in\Omega}|u(x)-\bar{u}|\right)^2 \leq K\int\limits_{\Omega}|\nabla_x u|^2\,dx.$$

Thanks to the Poincaré-Wirtinger inequality, estimate (32) becomes

$$\int\limits_0^T igg(\int\limits_\Omega igg| \sqrt{a(t,x)} - \int\limits_\Omega \sqrt{a(t,y)} \, dy igg|^{p^*} \, dx igg)^{2/p^*} \, dt \leq C.$$

Then,

$$\begin{split} &\int\limits_{0}^{T} \bigg(\int\limits_{\Omega} \left| \sqrt{a(t,x)} \, \right|^{p^*} dx \bigg)^{2/p^*} \, dt \\ &\leq 2^{2(p^*-1)/p^*} \int\limits_{0}^{T} \bigg(\int\limits_{\Omega} \left| \sqrt{a(t,x)} - \int\limits_{\Omega} \sqrt{a(t,y)} \, dy \, \right|^{p^*} \, dx \bigg)^{2/p^*} \, dt \\ &+ 2^{2(p^*-1)/p^*} \int\limits_{0}^{T} \bigg(\int\limits_{\Omega} \sqrt{a(t,x)} \, dx \bigg)^{2} \, dt \\ &\leq 2^{2(p^*-1)/p^*} \left(C + \int\limits_{0}^{T} \int\limits_{\Omega} a(t,x) \, dx dt \right). \end{split}$$

Using the conservation of number of atoms (20), (21), or (22), and the definition of p^* , we see that that for some constant C depending only on the initial data,

(35)
$$\int_{0}^{T} \left(\int_{C} |a(t,x)|^{N/(N-2)} dx \right)^{(N-2)/N} dt \le C (1+T).$$

When N = 2, this estimate is replaced by

$$\int_{0}^{T} \left(\int_{C} \left| a(t,x) \right|^{p} dx \right)^{1/p} dt \le C (1+T),$$

for all $p \in [1, +\infty[$.

Finally, when N = 1, it becomes

$$\int\limits_{0}^{T} \left(\sup_{x \in \Omega} a(t, x) \right) dt \le C (1 + T).$$

We shall now interpolate estimate (35) with the estimate coming out of the conservation of number of atoms:

$$\sup_{t \in [0,T]} \int_{\Omega} a(t,x) \, dx \le C.$$

We compute

$$\int_{0}^{T} \int_{\Omega} (a(t,x))^{1+2/N} dx dt \le \int_{0}^{T} \int_{\Omega} a(t,x) (a(t,x))^{2/N} dx dt$$

$$\le \int_{0}^{T} \left(\int_{\Omega} (a(t,x))^{N/(N-2)} dx \right)^{(N-2)/N} \left(\int_{\Omega} a(t,x) dx \right)^{2/N} dt$$

$$\le \left[\int_{0}^{T} \left(\int_{\Omega} (a(t,x))^{N/(N-2)} dx \right)^{(N-2)/N} dt \right] \times \sup_{t \in [0,T]} \left(\int_{\Omega} a(t,x) dx \right)^{2/N}$$

$$\le C (1+T) C^{2/N}.$$

Finally, we see that for some constant C depending only on the initial data (and when $N \ge 3$),

$$||a||_{L^{1+2/N}([0,T]\times\Omega)} \le C (1+T)^{N/(N+2)}.$$

This estimate is replaced by

(36)
$$||a||_{L^p([0,T]\times\Omega)} \le C (1+T)^{1/p}$$

for all $p \in [1, 2[$ when N = 2, and by

(37)
$$||a||_{L^2([0,T]\times\Omega)} \le C(1+T)^{1/2}$$

when N=1.

In order to treat the case N=2, we use a refinement of Sobolev-Wirtinger's inequality.

2.5 - Trudinger's inequality

In order to obtain estimate (36) in the case when N=2, we first recall Trudinger's inequality (Cf. [1]), which is a limit case of Poincaré inequality, saying that (when Ω is a bounded and regular (C^2) open set of \mathbb{R}^2), there are two absolute strictly positive constants s_0 and C_0 such that, for all $u \in H^1(\Omega)$,

(38)
$$\int_{\Omega} \exp\left(s_0 \frac{|u(x)|^2}{\|u\|_{H^1(\Omega)}^2}\right) \le C_0.$$

As a consequence, we can also find two strictly positive absolute constants s and C such that (for all functions $u \in H^1(\Omega)$),

(39)
$$\int_{\Omega} \frac{|u(x)|^2}{\|u\|_{H^1(\Omega)}^2} \exp\left(s \frac{|u(x)|^2}{\|u\|_{H^1(\Omega)}^2}\right) \le C.$$

Using this inequality for $u = \sqrt{a}(t, \cdot)$, and integrating in time between 0 and T, we get the estimate

$$\int\limits_0^T\int\limits_\Omega a(t,x)\,\exp\!\left(\frac{s\,a(t,x)}{\|\sqrt{a}(t,\cdot)\|_{H^1(\Omega)}^2}\right)dxdt\leq C\int\limits_0^T\|\sqrt{a}(t,\cdot)\|_{H^1(\Omega)}^2\,dt$$

$$(40) \leq C(1+T).$$

We note that thanks to Young's inequality (valid for $x, y, \gamma > 0$)

$$xy \le e^{\gamma x} + \frac{y}{\gamma} \left(\log \left(\frac{y}{\gamma} \right) - 1 \right),$$

applied to $\gamma = \frac{\log a}{a} + \frac{s}{q}$ and x = y = a, we have for all a > e and s, q > 0,

$$a^2 \leq a \, e^{\frac{sa}{q}} + \frac{a}{\frac{\log a}{a} + \frac{s}{q}} \left(\log \left(\frac{a}{\frac{\log a}{a} + \frac{s}{q}} \right) - 1 \right) \leq a \, e^{\frac{sa}{q}} + \frac{aq}{s} \log{(a^2)}.$$

Using this last inequality with s being the constant in inequality (39), $q = \|\sqrt{a}(t,\cdot)\|_{H^1(\Omega)}^2$ and $a = \max(e, a(t,x))$, and using also estimates (40) and (the first

part of) (30), we end up with

$$\begin{split} \|a\|_{L^2([0,T]\times\Omega)}^2 &\leq \|\min\{a,e\}\|_{L^2([0,T]\times\Omega)}^2 + \|\max\{a,e\}\|_{L^2([0,T]\times\Omega)}^2 \\ &\leq e^2\,T + \int\limits_0^T \int\limits_\Omega a(t,x)\,\exp\!\left(\frac{s\,a(t,x)}{\|\sqrt{a}(t,\cdot)\|_{H^1(\Omega)}^2}\right) dxdt \\ &\quad + \frac{2}{s}\int\limits_0^T \!\left(\int\limits_\Omega a(t,x)\,\log\left(a(t,x)\right) dx\right) \|\sqrt{a}(t,\cdot)\|_{H^1(\Omega)}^2 dt \\ &\leq e^2\,T + C\,(1+T) + \frac{2}{s}\,C\,(1+T), \end{split}$$

which is exactly estimate (37), but in dimension 2.

3 - Existence, uniqueness and smoothness

In this section, we study the traditional problems associated to the systems we are interested in (that is, systems (10) - (12), (13) - (15), and (16) - (18)), that is, existence, uniqueness and smoothness of the solutions. More precisely, we shall show that for the two first systems, existence ans uniqueness of a smooth solution holds, while we only can prove existence of a weak solution to the third system (except in small dimensions).

3.1 - Linear parabolic equations

We begin by recalling a few classical facts about linear parabolic equations.

3.1.1 - Existence, uniqueness and smoothness for linear parabolic equations

We first state the following theorem (Cf. for example [11]) for the heat equation with Neumann boundary condition:

Theorem 3.1. We consider a smooth (C^2) bounded and connected open subset Ω of \mathbb{R}^N . Let $u_{in} \in C^2(\overline{\Omega})$ be an initial datum (compatible with the Neumann boundary condition) and $\phi \in L^p([0,T] \times \Omega)$ (for some T > 0 and $p \in]1, +\infty[$) be a right-hand side.

Then, there exists a unique weak solution $u \in L^p([0,T] \times \Omega)$ to the linear

parabolic initial-boundary value problem:

(41)
$$\begin{cases} \partial_t u - d \, \Delta_x u = \phi, \\ \nabla_x u \cdot n = 0 \quad on \quad \partial \Omega, \\ u(0, x) = u_{in}(x). \end{cases}$$

Moreover, $u \in W^{1,p}(]0,T[\times \Omega)$.

Finally, if we know that for some $a \in]0,1[$, $\phi \in C^{0,a}([0,T] \times \overline{\Omega})$, then $u \in C^{1,a}([0,T] \times \overline{\Omega})$, and if $\phi \in C^{1,a}([0,T] \times \overline{\Omega})$, then $u \in C^{2}([0,T] \times \overline{\Omega})$. Note that in this last case, the solution is in fact strong.

3.1.2 - The case of the 1D heat equation

In the one-dimensional case, it is easy to give a complete explicit formula for problem (41), using Fourier series.

Proposition 3.1. Let $u_{in} \in C^2([0,1])$ be an initial datum (compatible with the Neumann boundary condition) and $\phi \in C^2([0,T] \times [0,1])$ be a second member. Then, the unique solution u := u(t,x) to eq. (41) is given by the formula

$$\begin{split} u(t,x) &= \frac{1}{2\sqrt{\pi}} \int\limits_{-1}^{1} \tilde{u_{in}}(y) \sum_{k=-\infty}^{\infty} \frac{1}{\sqrt{d\,t}} \, e^{-\frac{(2k+x-y)^2}{4\,d\,t}} dy \\ &+ \frac{1}{2\sqrt{\pi}} \int\limits_{0}^{t} \int\limits_{-1}^{1} \tilde{\phi}(s,y) \sum_{k=-\infty}^{\infty} \frac{1}{\sqrt{d\,(t-s)}} \, e^{-\frac{(2k+x-y)^2}{4\,d\,(t-s)}} dy \, ds \, , \end{split}$$

where

(42)
$$\tilde{u_{in}}(x) = \begin{cases} u_{in}(x) & x \in [0, 1], \\ u_{in}(-x) & x \in [-1, 0], \end{cases}$$

and

(43)
$$\tilde{\phi}(t,x) = \begin{cases} \phi(t,x) & x \in [0,1], \\ \phi(t,-x) & x \in [-1,0]. \end{cases}$$

Proof of Proposition 3.1. The proof uses Fourier series, which simplify when (41) is mirrored evenly around x = 0, i.e. when the functions are extended like

(44)
$$\tilde{u}(t,x) = \begin{cases} u(t,x) & x \in [0,1], \\ u(t,-x) & x \in [-1,0], \end{cases}$$

and when $\tilde{\phi}$ and $\tilde{u_{in}}$ are defined analogously by (42), (43). Then, the eigenvalue-problem $\tilde{\psi}_{xx} = \lambda \tilde{\psi}$ on [-1,1] with homogeneous Neumann boundary and periodicity conditions is satisfied by the eigenvalue-eigenfunction pairs

$$(\lambda_k, \tilde{\psi}_k(x)) = (-(k\pi)^2, \cos(k\pi x))$$
 for $k = 0, 1, 2, \dots$

and yields the Fourier representation

$$\tilde{u}(t,x) = \int_{-1}^{1} u_{in}(y) \, dy + 2 \sum_{k=1}^{\infty} e^{\lambda_k dt} \left(\int_{-1}^{1} u_{in}(y) \, \tilde{\psi}_k(y) \, dy \right) \tilde{\psi}_k(x)$$

$$+ \int_{0}^{t} \int_{-1}^{1} \tilde{\phi}(s,y) \, dy ds$$

$$(45)$$

$$+2\sum_{k=1}^{\infty}\int\limits_{0}^{t}e^{\lambda_{k}d\cdot(t-s)}\Biggl(\int\limits_{-1}^{1}\tilde{\phi}(s,y)\,\tilde{\psi}_{k}(y)dy\Biggr)ds\,\tilde{\psi}_{k}(x)\,.$$

Thanks to Poisson's summation formula (Cf. for example [18] in this context), we can write down the final form of the explicit solution to the 1-D heat equation with Neumann boundary condition:

$$\begin{split} \tilde{u}(t,x) &= \frac{1}{2\sqrt{\pi}} \int_{-1}^{1} u_{in}(y) \sum_{k=-\infty}^{\infty} \frac{1}{\sqrt{d\,t}} \, e^{-\frac{(2k+x-y)^{2}}{4\,d\,t}} dy \\ &+ \frac{1}{2\sqrt{\pi}} \int_{0}^{t} \int_{-1}^{1} \tilde{\phi}(s,y) \sum_{k=-\infty}^{\infty} \frac{1}{\sqrt{d\,(t-s)}} \, e^{-\frac{(2k+x-y)^{2}}{4\,d\,(t-s)}} dy \, ds \, . \end{split}$$

This ends the proof of Proposition 3.1.

3.2 - Nonlinear reaction-diffusion equations with bounded r.h.s.

We now turn to the problem of building solutions to nonlinear reaction-diffusion systems. Thanks to a simple fixed point argument in L^2 , it is classical to prove the following theorem, which holds when the nonlinearity lies in the space $W^{1,\infty}$ of bounded and Lipschitz-continuous functions (we refer for example to [13] for many results on reaction-diffusion systems including variants of the result below):

Proposition 3.2. Let Ω be a bounded and regular (C^2) open set of \mathbb{R}^N , and let D be a diagonal matrix with entries $d_i > 0$, i = 1, ..., k. We consider an initial

datum $U_{in} \in C^2(\overline{\Omega}, \mathbb{R}^k)$ compatible with the Neumann boundary condition, and $f \in C^2(\mathbb{R}^k; \mathbb{R}^k)$. We suppose moreover that $f \in W^{1,\infty}(\mathbb{R}^k; \mathbb{R}^k)$ (space of bounded and globally Lipschitz-continous functions), which means that there exists K > 0, such that for all $x, y \in \mathbb{R}^k$,

$$|f(x)| \le K,$$
 $|f(x) - f(y)| \le K|x - y|.$

Then, there exists a unique strong solution $U \in C^2(\mathbb{R}_+ \times \overline{\Omega}; \mathbb{R}^k)$ to equation

(47)
$$\begin{cases} \partial_t U - D \Delta_x U = f(U), \\ n \cdot \nabla_x U = 0 \quad \text{for} \quad x \in \partial \Omega, \\ U(0, x) = U_{in}(x). \end{cases}$$

Proof of Proposition 3.2. We introduce $U_0(t,x)=U_{in}(x)$. According to Theorem 3.1 for linear parabolic equations, we know that for any integer $n\geq 0$, there exists a (unique) function $U_{n+1}\in C^2(\mathbb{R}_+\times\overline{\Omega};\mathbb{R}^k)$ such that

(48)
$$\begin{cases} \partial_t U_{n+1} - D \Delta_x U_{n+1} = f(U_n), \\ n(x) \cdot \nabla_x U_{n+1}(t, x) = 0 \quad \text{for} \quad x \in \partial \Omega, \\ U_{n+1}(0, x) = U_{in}(x). \end{cases}$$

We denote

$$r_n(t) = ||U_n - U_{n-1}||_{L^2(\Omega)}^2(t).$$

We multiply the difference of (48) for n + 1 and (48) for n by $U_{n+1} - U_n$, and perform an integration by parts. Denoting by U_n^j the components of U_n , we get

$$\partial_t \int_{\Omega} \frac{1}{2} |U_{n+1} - U_n|^2 dx + \sum_{j=1}^k d_j \int_{\Omega} |\nabla_x (U_{n+1}^j - U_n^j)|^2 dx$$

$$= \int_{\Omega} (U_{n+1} - U_n) (f(U_n) - f(U_{n-1})) dx,$$

so that

$$\int_{\Omega} |U_{n+1} - U_n|^2 dx(t) \le \int_{0}^{t} \left\{ \int_{\Omega} |U_{n+1} - U_n|^2 dx(s) + K \int_{\Omega} |U_n - U_{n-1}|^2 dx(s) \right\} ds,$$

which we can rewrite as

$$r_{n+1}(t) \leq \int\limits_0^t ig(r_{n+1}(s) + K\,r_n(s)ig)\,ds.$$

Then, we observe that

$$r_1(t) \le R_T := 2 \|U_{in}\|_{L^2(\Omega)}^2 + 2 (\|U_{in}\|_{L^2(\Omega)} + KT)^2$$

for all $t \in [0, T]$. Using the auxiliary quantity

$$w_n(t) = e^{-t} \int\limits_0^t r_n(s) \, ds,$$

it is possible to prove that $w_{n+1}(t) \leq K \int_0^t w_n(s) \, ds$, so that $w_n(t) \leq R_t \frac{(Kt)^{n-1}}{(n-1)!}$. This in turn implies that for all $t \in [0,T]$,

$$r_n(t) \le (2R_T K (1+T) e^T) \frac{(K t)^{n-2}}{(n-2)!}$$

Since this sequence is the general term of a series which converges uniformy on [0, T], and recalling that $L^{\infty}([0, T]; L^{2}(\Omega))$ is complete, we see that U_{n} converges to some function U in this space.

Passing to the limit in eq. (48), we obtain that U is a weak solution of eq. (47) on [0, T].

We now use the "smoothness" part of Theorem 3.1. Since U is a (weak) solution (on [0,T]) of the heat equation with a r.h.s. in L^{∞} , it lies in $W^{1,p}(]0,T[\times\Omega)$ for all p>1, and therefore in $C^{0,a}([0,T]\times\overline{\Omega})$ for all $a\in]0,1[$. Thanks to the hypothesis on f, this is also true of f(U). As a consequence, still using Theorem 3.1, $U\in C^{1,a}([0,T]\times\overline{\Omega})$ for all $a\in]0,1[$, and (still thanks to the hypothesis on f), so does f(U). We use a last time Theorem 3.1, and get that $U\in C^2([0,T]\times\overline{\Omega})$, so that U is a strong solution to the system (47) on [0,T].

Uniqueness of strong solutions to system (47) on [0, T] is easily obtained by noticing that if U, V are two such strong solutions, then taking the difference of the equations for U and V, multiplying by U - V, and integrating by parts, we obtain:

$$\partial_t \|U - V\|_{L^2(\Omega)}(t) \le K \|U - V\|_{L^2(\Omega)}(t).$$

Finally, it is possible to build a unique strong solution U to system (47) on \mathbb{R}_+ by sticking together all the solutions to system (47) on [0, T], with T > 0. This concludes the proof of Proposition 3.2.

3.3 - Nonlinear reaction-diffusion equations with unbounded r.h.s: use of L^{∞} bounds

Proposition 3.2 can be used in order to prove existence (together with uniqueness and smoothness) of solutions to reaction-diffusion systems with general r.h.s, once some L^{∞} bound has been proven for the unknowns. Such bounds are not available in general, but they can be obtained for particular systems (among which (10) - (12) and (13) - (15) in any dimension, and (16) - (18) in small dimension). They can be based either on "geometrical properties" of the r.h.s. (here we shall follow the method described in [9] for systems of two equations), or on the fact that (the nonnegative part of) the r.h.s. is a function of the unknowns that does not increase too much (we refer to [13] for examples of such a situation).

In general, L^{∞} bounds are obtained all the more easily than the system has few equations, and the dimensionality of the space is low.

3.3.1 - Maximum principle

We begin with a maximum (and minimum) principle property of our simplest system (namely system (10) - (12)). It writes like this:

Proposition 3.3 [Minimum and maximum principle]. We assume that Ω is a bounded, smooth (C^2) , and connected open subset of \mathbb{R}^N , and that d_a , d_b are strictly positive diffusivity constants. Let a := a(t,x) and b := b(t,x) be a solution in $C^2([0,T] \times \overline{\Omega})$ to system (10) - (12). We suppose that the initial conditions satisfy:

(50)
$$\forall x \in \bar{\Omega}, \quad 0 < A_0 < a_{in}(x) < A_1, \quad 0 < B_0 < b_{in}(x) < B_1,$$

for some constants $A_0, A_1, B_0, B_1 > 0$.

Then, a and b satisfy the bounds

(51)
$$\forall t \in [0, T], x \in \Omega, \quad \inf(A_0, \sqrt{B_0}) \le a(t, x) \le \sup(A_1, \sqrt{B_1}),$$

(52)
$$\forall t \in [0, T], x \in \Omega, \quad \inf(A_0^2, B_0) \le b(t, x) \le \sup(A_1^2, B_1).$$

Proof of Proposition 3.3. The proof shall be carried out following the ideas of [9]. Let us consider the functions

(53)
$$a^{\varepsilon}(t,x) = a(t,x) e^{\varepsilon t}, \qquad b^{\varepsilon}(t,x) = b(t,x) e^{\varepsilon t}.$$

From equations (10), it follows that the evolution of a^{ε} , b^{ε} is governed by the

system

(54)
$$\begin{cases} \partial_t a^{\varepsilon} - d_a \, \, \varDelta_x a^{\varepsilon} = -2 \left((a^{\varepsilon})^2 \, e^{-\varepsilon t} - b^{\varepsilon} \right) + \varepsilon \, a^{\varepsilon}, \\ \partial_t b^{\varepsilon} - d_b \, \, \varDelta_x b^{\varepsilon} = \left((a^{\varepsilon})^2 \, e^{-\varepsilon t} - b^{\varepsilon} \right) + \varepsilon \, b^{\varepsilon}. \end{cases}$$

We define the set B^{ε} as

$$B^{\varepsilon} = \left\{ \tau > 0 : a^{\varepsilon}(t, x) > \inf(A_0, \sqrt{B_0}), \qquad b^{\varepsilon}(t, x) > \inf(A_0^2, B_0) e^{-\varepsilon t}, \right.$$

$$(55) \qquad \qquad \forall (t, x) \in [0, \tau[\times \bar{\Omega} \right\}.$$

Then, we consider $\tilde{t} = \sup B^{\varepsilon}$. Note first that $\tilde{t} > 0$. Then, there must exist $\tilde{x} \in \overline{\Omega}$ such that at least one of the following equalities holds:

$$a^{\varepsilon}(\tilde{t}, \tilde{x}) = \inf(A_0, \sqrt{B_0})$$
 or $b^{\varepsilon}(\tilde{t}, \tilde{x}) = \inf(A_0^2, B_0) e^{-\varepsilon t}$.

Case 1: $a^{\varepsilon}(\tilde{t}, \tilde{x}) = \inf(A_0, \sqrt{B_0})$. By definition of \tilde{t} and \tilde{x} , the function $x \mapsto a^{\varepsilon}(\tilde{t}, x)$ takes it miminum at point \tilde{x} , so that $\Delta_x a^{\varepsilon}(\tilde{t}, \tilde{x}) \geq 0$. Evaluating the chemical contributions in the first line of (54) at (\tilde{t}, \tilde{x}) , we get

$$\begin{split} &-2\left(a^{\varepsilon}\right)^{2}(\tilde{t},\tilde{x})\,e^{-\varepsilon t}+2\,b^{\varepsilon}(\tilde{t},\tilde{x})+2\,\varepsilon\,a^{\varepsilon}(\tilde{t},\tilde{x})\\ &=&-2\,\inf\left(A_{0},\sqrt{B_{0}}\right)^{2}e^{-\varepsilon t}+2\,b^{\varepsilon}(\tilde{t},\tilde{x})+2\,\varepsilon\,\inf\left(A_{0},\sqrt{B_{0}}\right)\\ &\geq&-2\,\inf\left(A_{0},\sqrt{B_{0}}\right)^{2}e^{-\varepsilon t}+2\,\inf\left(A_{0}^{2},B_{0}\right)e^{-\varepsilon t}+2\,\varepsilon\,\inf\left(A_{0},\sqrt{B_{0}}\right)\\ &>&0 \end{split}$$

Consequently, eq. (54) for a^{ε} implies that $\partial_t a^{\varepsilon}(\tilde{t}, \tilde{x}) > 0$, hence $a^{\varepsilon}(t, \tilde{x}) < a^{\varepsilon}(\tilde{t}, \tilde{x})$ for some $t < \tilde{t}$, contradicting the definition of \tilde{t} .

Case 2: $b^{\varepsilon}(\tilde{t}, \tilde{x}) = \inf(A_0^2, B_0) e^{-\varepsilon t}$. In this case, we have $b^{\varepsilon}(\tilde{t}, \tilde{x}) \leq b^{\varepsilon}(\tilde{t}, x)$ $\forall x \in \Omega$, so that $b^{\varepsilon}(\tilde{t}, x)$ takes its minimum at point $x = \tilde{x}$. Therefore we get, as above, $A_x b^{\varepsilon}(\tilde{t}, \tilde{x}) \geq 0$. As concerns the r.h.s. of the second line of (54), we obtain

$$\begin{split} &(a^{\varepsilon})^2(\tilde{t},\tilde{x})\,e^{-\varepsilon t}-b^{\varepsilon}(\tilde{t},\tilde{x})+\varepsilon\,b^{\varepsilon}(\tilde{t},\tilde{x})\\ &=\quad (a^{\varepsilon})^2(\tilde{t},\tilde{x})\,e^{-\varepsilon t}-\inf\left(A_0^2,B_0\right)e^{-\varepsilon t}+\varepsilon\,\inf\left(A_0^2,B_0\right)e^{-\varepsilon t}\,,\\ &\geq\quad (\inf A_0,\sqrt{B_0})^2\,\,e^{-\varepsilon t}-\inf\left(A_0^2,B_0\right)e^{-\varepsilon t}+\varepsilon\,\inf\left(A_0^2,B_0\right)\,e^{-\varepsilon t}\\ &>\quad 0. \end{split}$$

It follows that $\partial_t b^{\varepsilon}(\tilde{t}, \tilde{x}) > 0$, which leads to a contradiction as in case 1. Consequently, the set B^{ε} is unbounded, and

$$\forall t \geq 0, x \in \Omega, \qquad a^{\varepsilon}(t,x) > \inf\left(A_0, \sqrt{B_0}\right), \qquad b^{\varepsilon}(t,x) > \inf\left(A_0^2, B_0\right) e^{-\varepsilon t}.$$

This means that $a(t,x) > \inf(A_0, \sqrt{B_0}) e^{-\varepsilon t}$ and $b(t,x) > \inf(A_0^2, B_0) e^{-2\varepsilon t}$. Thus, passing to the limit $\varepsilon \to 0$, we have $a(t,x) \ge \inf(A_0, \sqrt{B_0})$ and $b(t,x) \ge \inf(A_0^2, B_0)$.

This ends the proof of the minimum principle for system (10) - (12). The maximum principle can be proven in exactly the same way. We have therefore finished the proof of Proposition 3.3

We are now in position to state a theorem of existence (and uniqueness, smoothness) for system (10) - (12):

Theorem 3.2. Let Ω be a bounded, connected and regular (C^2) open set of \mathbb{R}^N $(N \geq 1)$, and d_a , d_b be strictly positive diffusivity constants. We consider initial data $a_{in}, b_{in} \in C^2(\overline{\Omega})$ (compatible with the Neumann boundary condition) which satisfy the bound:

(56)
$$\forall x \in \overline{\Omega}, \quad 0 < A_0 < a_{in}(x) < A_1, \quad 0 < B_0 < b_{in}(x) < B_1.$$

Then, there exists a unique (strong) solution a, b in $C^2(\mathbb{R}_+ \times \bar{\Omega})$ to system (10) – (12) such that:

$$\forall t \in \mathbb{R}_+, x \in \overline{\Omega}, \quad \inf(A_0, \sqrt{B_0}) \le a(t, x) \le \sup(A_1, \sqrt{B_1}),$$

(57)
$$\inf (A_0^2, B_0) \le b(t, x) \le \sup (A_1^2, B_1).$$

Proof of Theorem 3.2. We consider a function $\chi := \chi(a,b)$ in $C^2(\mathbb{R}^2,\mathbb{R})$ such that $\chi(a,b)=1$ when $|a|,|b|\leq 2\sup(A_1,A_1^2,\sqrt{B_1},B_1)$, and $\chi(a,b)=0$ when |a| or $|b|\geq 4\sup(A_1,A_1^2,\sqrt{B_1},B_1)$.

Then, the function

$$f(a,b) = (-2(a^2 - b)\chi(a,b), (a^2 - b)\chi(a,b))$$

lies in $C^2(\mathbb{R}^2,\mathbb{R}^2)\cap W^{1,\infty}(\mathbb{R}^2,\mathbb{R}^2)$. According to Proposition 3.2, there exists a solution $U=(a,b)\in C^2(\mathbb{R}_+\times\overline{\Omega})$ to the system

(58)
$$\begin{cases} \partial_t U - D \Delta_x U = f(U), \\ n \cdot \nabla_x U = 0 \quad \text{for} \quad x \in \partial \Omega, \\ U(0, x) = (a_{in}(x), b_{in}(x)), \end{cases}$$

where D is a (2×2) diagonal matrix with entries d_a, d_b .

On any interval of time [0,T] for which (for all $x \in \Omega$) $|a(t,x)|, |b(t,x)| \le 2 \sup(A_1,A_1^2,\sqrt{B_1},B_1), (a,b)$ is also a (strong) solution of system (10) – (12), and

according to Proposition 3.3, it satisfies

$$|a(t,x)|, |b(t,x)| \le \sup (A_1, A_1^2, \sqrt{B_1}, B_1).$$

Therefore, the sup of all T such that (for all $x \in \Omega$) $|a(t,x)|, |b(t,x)| \le 2 \sup(A_1, A_1^2, \sqrt{B_1}, B_1)$ is infinite, and therefore (a, b) is a (strong, C^2) solution of system (10) - (12) on \mathbb{R}_+ , which satisfies (thanks to Proposition 3.2) estimate (57).

If we now have two solutions of system (10) - (12) on \mathbb{R}_+ which satisfy estimate (57), they are also solutions of system (58), and thanks to the "uniqueness" part of Proposition 3.2, they are equal. This concludes the proof of Theorem 3.2.

3.3.2 - Using the properties of the heat kernel

We introduce here the idea of using the smoothing properties of the heat kernel in order to obtain L^{∞} bounds for system (13) – (15). Those bounds are only local in time (that is, in $L^{\infty}([0,T]\times\Omega)$ for a given T>0), but we take care of controlling what happens when $T\to +\infty$.

We give complete proofs for system (13) - (15) in dimension 1, and briefly indicate how these proofs can be extended to the case of system (13) - (15) in any dimension, or to the case of system (16) - (18) in dimension 1.

Those proofs are inspired by the book of Rothe [13].

We begin with a standard estimate of the smoothing effect of the heat equation in dimension 1.

Lemma 3.1 (Explicit L^r bounds $(r \ge 1)$ for the 1D heat equation). Let u denote the (unique weak) solution of the 1D heat equation $(t > 0, x \in [0, 1],$ with constant diffusivity d) with homogeneous Neumann boundary condition, i.e.

(59)
$$\partial_t u - d \partial_{xx} u = \phi, \quad \partial_x u(t,0) = \partial_x u(t,1) = 0,$$

and assume for the initial data $u(0,x) = u_{in}(x)$ and for the source term $\phi := \phi(t,x)$ that

(60)
$$u_{in} \in L^{\infty}([0,1]), \qquad \phi \in L^{p}_{loc}([0,+\infty[;L^{p}([0,1])),$$

for some $p \geq 1$.

Then, for any exponent r > 1 such that $\frac{1}{r} + \frac{2}{3} > \frac{1}{p}$ and for all T > 0, the norm $\|u\|_{L^r([0,T]\times[0,1])}$ grows at most polynomially in T like

(61)
$$||u||_{L^{r}([0,T]\times[0,1])} \le T^{1/r} ||a_{in}||_{L^{\infty}[0,1]} + C(1+T^{\frac{3}{2}}) ||\phi||_{L^{p}([0,T]\times[0,1])}.$$

In the case when $p > \frac{3}{2}$, one can take $r = \infty$ in estimate (61).

Proof of Lemma 3.1. We recall that according to Proposition 3.1, the solution of the heat equation (59) is given by formula (42):

(62)
$$u(t,x) = \frac{1}{2\sqrt{\pi}} \int_{-1}^{1} u_{in}(y) \sum_{k=-\infty}^{\infty} \frac{1}{\sqrt{dt}} e^{-\frac{(2k+x-y)^2}{4dt}} dy + \frac{1}{2\sqrt{\pi}} \int_{0}^{t} \int_{-1}^{1} \tilde{\phi}(s,y) \sum_{k=-\infty}^{\infty} \frac{1}{\sqrt{d(t-s)}} e^{-\frac{(2k+x-y)^2}{4d(t-s)}} dy ds.$$

This yields the estimate

(63)
$$||u||_{L^{r}([0,T]\times[-1,1])} \leq \frac{1}{2\sqrt{\pi}} ||\tilde{u_{in}} *_{x} S||_{L^{r}([0,T]\times[-1,1])} + \frac{1}{2\sqrt{\pi}} ||\tilde{\phi} *_{t,x} S||_{L^{r}([0,T]\times[-1,1])},$$

where $S(t,x) := \sum_{k=-\infty}^{\infty} \frac{1}{\sqrt{dt}} e^{-\frac{(2k+x)^2}{4dt}}$ satisfies (for $q \in [1,3[)$

(64)
$$||S(t,\cdot)||_{L^1([-1,1])} = 2\sqrt{\pi}, \qquad ||S||_{L^q([0,T]\times[-1,1])} \le C\left(1+T^{\frac{1}{q}+\frac{1}{2}}\right).$$

The second formula of (64) can be obtained by using (when $n \neq 0$) $(2n + x)^2 \ge |2n + x| \ge 2n - 1$ in order to estimate

$$\begin{split} \|S\|_{L^q([0,T]\times[-1,1])} &\leq \left\| (d\,t)^{-\frac{1}{2}} \left(e^{-\frac{x^2}{4\,dt}} + 2\sum_{n=1}^{\infty} e^{-\frac{2n-1}{4\,dt}} \right) \right\|_{L^q([0,T]\times[-1,1])} \\ &\leq \left\| (d\,t)^{-\frac{1}{2}} e^{-\frac{x^2}{4\,dt}} \right\|_{L^q([0,T]\times[-1,1])} \\ &+ 2\left\| (d\,t)^{-\frac{1}{2}} \left(e^{1/4\,dt} - e^{-1/4\,dt} \right)^{-1} \right\|_{L^q([0,T]\times[-1,1])} \\ &\leq \left(\int\limits_0^T (d\,t)^{-q/2} \, 2\sqrt{\pi} \, \sqrt{\frac{d\,t}{q}} \, \operatorname{erf} \, \left(\frac{\sqrt{q}}{2\sqrt{d\,t}} \right) dt \right)^{1/q} + 4 \left(\int\limits_0^T |2(d\,t)^{1/2}|^q \, dt \right)^{1/q}. \end{split}$$

Returning to (63), we can estimate each term in the right-hand side in order to obtain Lemma 3.1, the last term being the most difficult. In order to treat it, we apply Young's inequality $\|\tilde{\phi}*S\|_{L^r} \leq \|\tilde{\phi}\|_{L^p} \|S\|_{L^q}$ for $\frac{1}{r}+1=\frac{1}{p}+\frac{1}{q}$ (remember that $\frac{1}{r}+\frac{2}{3}>\frac{1}{p}$, which is compatible with $q\in[1,3[)$, and estimate (64) for $\|S\|_{L^q}$. The same is true when $r=\infty$ and $p>\frac{3}{2}$. This concludes the proof of Lemma 3.1.

Remark. The lemma above extends to dimension N>1, with a certain number of changes in the assumption and the conclusion. The main one is that $\frac{1}{r}+\frac{2}{3}>\frac{1}{p}$ is replaced by $\frac{1}{r}+\frac{2}{N+2}>\frac{1}{p}$, so that the solution of the heat equation lies in a L^r space which is not as good as in dimension 1.

We use this lemma in order to prove an a priori L^{∞} estimate for the concentrations solving system (13) – (15) in dimension 1.

Proposition 3.4. Let a_{in} , b_{in} and c_{in} be strictly positive initial data lying in $C^2([0,1])$, and d_a , d_b , d_c be strictly positive diffusivity constants. We consider a, b, c a (strong) solution in $C^2([0,T] \times [0,1])$ of system (13) – (15).

Then, there exists a constant C_T (which grows at most polynomially with T, and depend only on the initial data) such that

(65)
$$||a,b,c||_{L^{\infty}([0,T]\times[0,1])} \leq C_T.$$

Proof of Proposition 3.4. According to Proposition 2.5, we already know that $\|a,b,c\|_{L^2([0,T]\times[0,1])}\leq C_T$, where C_T is (and will systematically be in the sequel of this proof) a constant which grows at most polynomially with T. Then, $\|a-b\,c\|_{L^1([0,T]\times[0,1])}\leq C_T$. We see thanks to Lemma 3.1 that $\|a,b,c\|_{L^r([0,T]\times[0,1])}\leq C_T$ for all r<3. As a consequence, $\|a-b\,c\|_{L^{3/2}([0,T]\times[0,1])}\leq C_T$. A second use of Lemma 3.1 yields $\|a,b,c\|_{L^r([0,T]\times[0,1])}\leq C_T$ for all $r<+\infty$, and a third use of Lemma 3.1 yields $\|a,b,c\|_{L^\infty([0,T]\times[0,1])}\leq C_T$.

This ends the proof of Proposition 3.4.

Remark. We note that the same proof holds for system (16) – (18) in dimension 1.

A variant of this proof (in which the nonnegativity of the concentrations is used: the nonpositive part of the r.h.s of the equations is not estimated) shows that the L^{∞} estimate also remains valid for system (13) – (15) in any dimension.

This a priori estimate enables to prove the existence (and uniqueness, smoothness) of a (strong) solution to system (13) - (15) in dimension 1:

Theorem 3.3. Let a_{in} , b_{in} and c_{in} be strictly positive initial data lying in $C^2([0,1])$, and d_a , d_b , d_c be strictly positive diffusivity constants.

Then, there exists a unique solution $a, b, c \in C^2(\mathbb{R}_+ \times [0,1])$ to system (13) – (15) such that $||a,b,c||_{L^{\infty}([0,T]\times [0,1])} \leq C_T$ (where C_T grows at most polynomially with T).

Proof of Theorem 3.3. We consider a function $\chi_K := \chi_K(a,b,c)$ in $C^2(\mathbb{R}^3,\mathbb{R})$ such that $\chi_K(a,b,c) = 1$ when $|a|,|b|,|c| \leq K$, and $\chi_K(a,b,c) = 0$ when |a| or |b| or $|c| \geq 2K$.

Then, the function

$$f(a, b, c) = ((bc - a)\chi_K(a, b, c), (a - bc)\chi_K(a, b, c), (a - bc)\chi_K(a, b, c))$$

lies in $C^2(\mathbb{R}^3, \mathbb{R}^3) \cap W^{1,\infty}(\mathbb{R}^3, \mathbb{R}^3)$. According to Proposition 3.2, there exists a (strong) solution $U = (a, b, c) \in C^2(\mathbb{R}_+ \times [0, 1])$ to the system

(66)
$$\begin{cases} \partial_t U - D \Delta_x U = f(U), \\ n \cdot \nabla_x U = 0 \quad \text{for} \quad x \in \partial \Omega, \\ U(0, x) = (a_{in}(x), b_{in}(x), c_{in}(x)), \end{cases}$$

where D is the diagonal matrix with entries d_a, d_b, d_c .

On any interval of time [0, T] for which (for all $x \in \Omega$) $|a(t, x)|, |b(t, x)|, |c(t, x)| \le K$, the functions (a, b, c) are also a (strong) solution of system (13) – (15). According to Proposition 3.4, we can thus build a (strong) solution to system (13) – (15) on any interval [0, T] such that $C_T \le K$.

Letting $K \to +\infty$ and using the "uniqueness" part of Proposition 3.2 (on bounded time intervals), we obtain a (strong) solution of system (13) – (15) on \mathbb{R}_+ by sticking together solutions on [0,T] (remember that $C_T < +\infty$ for all T > 0 since C_T grows at most polynomially with T).

Finally, if we now have two solutions of system (13) - (15) on \mathbb{R}_+ which satisfy estimate (65), they are also solutions to system (66) for a certain K on a time interval [0,T] depending on K but arbitrarily large (that is, T is going to $+\infty$ when $K \to +\infty$). Thanks to the "uniqueness" part of Proposition 3.2, they are equal on this time interval. This concludes the proof of Theorem 3.3.

3.4 - Unbounded source: the duality method

3.4.1 - Duality for parabolic equations with non smooth coefficients

We begin with the following proposition, which shows that the solutions of a parabolic differential inequality with bounded coefficients satisfy a natural L^2 bound. We refer to [12] for this type of arguments of duality:

Proposition 3.5. Let T > 0 and Ω be a bounded, connected and regular (C^2) open set of \mathbb{R}^N . We suppose that $A : [0,T] \times \overline{\Omega} \to \mathbb{R}$ is a smooth (belonging to $C^2([0,T] \times \overline{\Omega})$) function such that $A_0 \leq A(t,x) \leq A_1$, for some strictly positive constants A_0 , A_1 .

We assume that $z:[0,T]\times\overline{\Omega}\to\mathbb{R}$ is a strong (belonging to $C^2([0,T]\times\overline{\Omega})$) nonnegative solution to the parabolic inequation:

(67)
$$\begin{cases} \partial_t z - A_x(A z) \le 0, \\ \nabla_x(A z) \cdot n = 0 \quad on \quad \partial \Omega, \\ z(0, \cdot) = z_{in}. \end{cases}$$

Then, there exists a constant C (depending on T, A_0, A_1) such that

$$||z||_{L^2([0,T]\times\Omega)} \le C ||z_{in}||_{L^2(\Omega)}.$$

Proof of Proposition 3.5. For any smooth (C^2) nonnegative function H := H(t, x), let us consider the nonnegative (smooth) solution of the dual problem:

(68)
$$\begin{cases}
-\partial_t w - A \Delta_x w = H, \\
\nabla_x w \cdot n = 0, \text{ on } \partial \Omega, \\
w(T, \cdot) = 0.
\end{cases}$$

Integrating by parts, we see that

$$egin{aligned} &\int\limits_{0}^{T}\int\limits_{\Omega}z\left(\partial_{t}w+AarDelta_{x}w
ight)dxdt = -\int\limits_{0}^{T}\int\limits_{\Omega}w\left(\partial_{t}z-arDelta_{x}(A\,z)
ight)dxdt \ &-\int\limits_{\Omega}z_{in}(x)\,w(0,x)\,dx+\int\limits_{0}^{T}\int\limits_{\partial\Omega}z\,A\,
abla_{x}w\cdot n\,d\sigma(x)\,dt \ &-\int\limits_{0}^{T}\int\limits_{\partial\Omega}w\,
abla_{x}(A\,z)\cdot nd\sigma(x)\,dt. \end{aligned}$$

Using the Neumann boundary conditions, we end up with

(69)
$$-\int_{0}^{T} \int_{\Omega} z(t,x) H(t,x) dx dt \ge -\int_{\Omega} z_{in}(x) w(0,x) dx.$$

Let us estimate $w(0,\cdot)$ in $L^2(\Omega)$. Multiplying eq. (68) by $-\Delta_x w$ and integrating by parts in the variable x gives (for any time $t \in [0,T]$)

$$-\frac{1}{2}\frac{d}{dt}\int_{\Omega} |\nabla_x w(t,x)|^2 dx + \int_{\Omega} A(t,x) \left(\varDelta_x w(t,x)\right)^2 dx$$
$$= -\int_{\Omega} H(t,x) \varDelta_x w(t,x) dx$$
$$\leq \int_{\Omega} \left(\frac{A_0}{2} (\varDelta_x w(t,x))^2 + \frac{1}{2A_0} H^2(t,x)\right) dx.$$

It follows, after integration in time, that

$$\int_{0}^{T} \int_{C} (\Delta_x w(t,x))^2 dx dt \le \frac{1}{A_0^2} \int_{0}^{T} \int_{C} H^2(t,x) dx dt.$$

Integrating eq. (68) between times 0 and T, we obtain

$$w(0,x)+\int\limits_0^T A(s,x)\, extstyle \varDelta_x w(s,x)\, ds=\int\limits_0^T H(s,x)\, ds,$$

so that

$$\int_{\Omega} w(0,x)^2 dx dt \le \left(2T + 2T\frac{A_1^2}{A_0^2}\right) \int_{0}^{T} \int_{\Omega} H^2(t,x) dx dt.$$

Therefore, thanks to estimate (69), we see that

$$\int_{0}^{T} \int_{\Omega} z(t,x) H(t,x) dx dt \leq \int_{\Omega} z_{in}(x) w(0,x) dx
\leq \|z_{in}\|_{L^{2}(\Omega)} \|w(0)\|_{L^{2}(\Omega)}
\leq \left(2 T + 2 T \frac{A_{1}^{2}}{A_{0}^{2}}\right)^{1/2} \|z_{in}\|_{L^{2}(\Omega)} \|H\|_{L^{2}([0,T] \times \Omega)}.$$

By density, this estimate is true for any nonnegative function H in L^2 , and, using $H=H^+-H^-$, we see that for any function H in L^2 , one has $\left(\text{for }C=\left(2\,T+2\,T\,\frac{A_1^2}{A_0^2}\right)^{1/2}\right)$

$$\left| \int_{0}^{T} \int_{\Omega} z(t,x) H(t,x) dx dt \right| \leq C \|z_{in}\|_{L^{2}(\Omega)} \|H\|_{L^{2}([0,T] \times \Omega)}.$$

By duality (L^2 is the dual of itself), this gives a bound for z in $L^2(0,T] \times \Omega$) in terms of $\|z_{in}\|_{L^2(\Omega)}$, and the proof of Proposition 3.5 is ended.

3.4.2 - The $L^2 Log L$ estimate

We shall now follow [5] and use the duality argument of Proposition 3.5 in order to build a weak (L^2) solution to problem (16) - (18):

Theorem 3.4. Let Ω be a bounded, regular (C^2) and connected open set of \mathbb{R}^N , let d_a , d_b , d_c and d_d be strictly positive diffusivity constants, and let a_{in} , b_{in} , c_{in} , d_{in} be strictly positive initial data in $C^2(\overline{\Omega})$.

Then, there exists a weak solution $a,b,c,d \in L^2_{loc}(\mathbb{R}_+;L^2(\Omega))$ to system (16) –(18).

Proof of Theorem 3.4. We introduce the approximated system:

$$\begin{cases}
\partial_{t}a_{n} - d_{a}\Delta_{x}a_{n} = -\frac{a_{n}b_{n} - c_{n}d_{n}}{1 + \frac{1}{n}\left(a_{n}^{2} + b_{n}^{2} + c_{n}^{2} + d_{n}^{2}\right)}, \\
\partial_{t}b_{n} - d_{b}\Delta_{x}b_{n} = -\frac{a_{n}b_{n} - c_{n}d_{n}}{1 + \frac{1}{n}\left(a_{n}^{2} + b_{n}^{2} + c_{n}^{2} + d_{n}^{2}\right)}, \\
\partial_{t}c_{n} - d_{c}\Delta_{x}c_{n} = \frac{a_{n}b_{n} - c_{n}d_{n}}{1 + \frac{1}{n}\left(a_{n}^{2} + b_{n}^{2} + c_{n}^{2} + d_{n}^{2}\right)}, \\
\partial_{t}d_{n} - d_{d}\Delta_{x}d_{n} = \frac{a_{n}b_{n} - c_{n}d_{n}}{1 + \frac{1}{n}\left(a_{n}^{2} + b_{n}^{2} + c_{n}^{2} + d_{n}^{2}\right)},
\end{cases}$$

together with the homogeneous Neumann conditions

(71)
$$\begin{cases} n(x) \cdot \nabla_x a_n = 0, & n(x) \cdot \nabla_x b_n = 0, \\ n(x) \cdot \nabla_x c_n = 0, & n(x) \cdot \nabla_x d_n = 0, & x \in \partial \Omega, \end{cases}$$

and the strictly positive initial data

(72)
$$\begin{cases} a_n(0,x) = a_{in}(x), & b_n(0,x) = b_{in}(x), \\ c_n(0,x) = c_{in}(x), & d_n(0,x) = d_{in}(x). \end{cases}$$

We know thanks to Proposition 3.2 that there exists a unique strong solution to this system, since the right-hand side is C^2 , bounded and globally Lipschitz continuous $(W^{1,\infty})$.

We introduce the quantity $z_n = \phi(a_n) + \phi(b_n) + \phi(c_n) + \phi(d_n)$, where $\phi(x) = x \ln x - x + 1$. Note that ϕ is a nonnegative function whose second derivative is $x \mapsto \frac{1}{x}$. The computation gives

$$\begin{split} \partial_{t}z_{n} - d_{a} \, \varDelta_{x}\phi(a_{n}) - d_{b} \, \varDelta_{x}\phi(b_{n}) - d_{c} \, \varDelta_{x}\phi(c_{n}) - d_{d} \, \varDelta_{x}\phi(d_{n}) \\ = -\ln a_{n} \, \frac{a_{n} \, b_{n} - c_{n} \, d_{n}}{1 + \frac{1}{n} \, (a_{n}^{2} + b_{n}^{2} + c_{n}^{2} + d_{n}^{2})} - \ln b_{n} \, \frac{a_{n} \, b_{n} - c_{n} \, d_{n}}{1 + \frac{1}{n} \, (a_{n}^{2} + b_{n}^{2} + c_{n}^{2} + d_{n}^{2})} \\ + \ln c_{n} \, \frac{a_{n} \, b_{n} - c_{n} \, d_{n}}{1 + \frac{1}{n} \, (a_{n}^{2} + b_{n}^{2} + c_{n}^{2} + d_{n}^{2})} + \ln d_{n} \, \frac{a_{n} \, b_{n} - c_{n} \, d_{n}}{1 + \frac{1}{n} \, (a_{n}^{2} + b_{n}^{2} + c_{n}^{2} + d_{n}^{2})} \\ - d_{a} \, \frac{|\nabla_{x} a_{n}|^{2}}{a_{n}} - d_{b} \, \frac{|\nabla_{x} b_{n}|^{2}}{b_{n}} - d_{c} \, \frac{|\nabla_{x} c_{n}|^{2}}{c_{n}} - d_{d} \, \frac{|\nabla_{x} d_{n}|^{2}}{d_{n}}. \end{split}$$

Therefore,

$$\partial_t z_n - d_a \Delta_x \phi(a_n) - d_b \Delta_x \phi(b_n) - d_c \Delta_x \phi(c_n) - d_d \Delta_x \phi(d_n)$$

$$(73) + d_a \frac{|\nabla_x a_n|^2}{a_n} + d_b \frac{|\nabla_x b_n|^2}{b_n} + d_c \frac{|\nabla_x c_n|^2}{c_n} + d_d \frac{|\nabla_x d_n|^2}{d_n} \le 0,$$

and finally

$$\partial_t z_n - \Delta_x (A_n z_n) < 0,$$

where

$$A_n = rac{d_a \, \phi(a_n) + d_b \, \phi(b_n) + d_c \, \phi(c_n) + d_d \, \phi(d_n)}{z_n}.$$

Note that

$$\forall t > 0, x \in \Omega$$
, $\inf (d_a, d_b, d_c, d_d) \leq A_x(t, x) \leq \sup (d_a, d_b, d_c, d_d)$,

and

$$\nabla_x (A_n z_n) \cdot n(x) = 0$$
 for $x \in \partial \Omega$.

According to Proposition 3.5, we obtain the estimate

$$||z_n||_{L^2([0,T]\times\Omega)} \le C \left(||\phi(a_{in})||_{L^2(\Omega)} + ||\phi(b_{in})||_{L^2(\Omega)} + ||\phi(c_{in})||_{L^2(\Omega)} + ||\phi(d_{in})||_{L^2(\Omega)} \right),$$

where C does not depend on n (but depends on T and the diffusivity constants).

This ensures that the sequences a_n , b_n , c_n and d_n are bounded in the space $L^2(\ln L)^2([0,T]\times\Omega)$. In particular, the quantities a_n b_n and c_n d_n are equiintegrable.

We conclude the proof of Theorem 3.4 in next paragraph, by showing the strong convergence (i.-e. the convergence a.e.) of the sequences a_n , b_n , c_n and d_n .

3.4.3 - Existence of weak L^2 solutions

In the previous paragraph, we proved that there exists for each $n \ge 1$ a smooth solution (a_n, b_n, c_n, d_n) to system (70) - (72).

Moreover, we have shown that the sequences a_n , b_n , c_n and d_n are bounded in $L^2(\ln L)^2([0,T]\times\Omega)$, so that the quantities a_n b_n and c_n d_n are equiintegrable.

We start again from estimate (73). Integrating between times 0 and T and for $x \in \Omega$ this estimate, we see that

$$\int_{\Omega} z_n(T,x) dx + d_a \int_{0}^{T} \int_{\Omega} \frac{\left|\nabla_x a_n\right|^2}{a_n}(t) dx dt + d_b \int_{0}^{T} \int_{\Omega} \frac{\left|\nabla_x b_n\right|^2}{b_n}(t) dx dt + d_c \int_{0}^{T} \int_{\Omega} \frac{\left|\nabla_x c_n\right|^2}{c_n} dx dt + d_d \int_{0}^{T} \int_{\Omega} \frac{\left|\nabla_x d_n\right|^2}{d_n} dx dt \leq \int_{\Omega} z(0,x) dx.$$

As a consequence, we obtain that $\nabla_x(\sqrt{1+a_n})$ is bounded in $L^2([0,T]\times\Omega)$, and therefore in $L^1([0,T]\times\Omega)$.

Then, we compute

$$(\partial_t - d_a \, \varDelta_x) \sqrt{1 + a_n} = rac{d_a}{4} \, rac{\left|
abla_x a_n
ight|^2}{\left(1 + a_n
ight)^{3/2}} + rac{1}{2} \, rac{c_n \, d_n - a_n \, b_n}{\sqrt{1 + a_n} \left(1 + rac{1}{n} \left(a_n^2 + b_n^2 + c_n^2 + d_n^2
ight)
ight)},$$

so that $(\partial_t - d_a \Delta_x) \sqrt{1 + a_n}$ is bounded in $L^1([0, T] \times \Omega)$.

We consider now $g_n = \sqrt{1 + a_n}$, and we prove that this quantity is strongly compact (in $L^1_{loc}(]0, T[\times \Omega)$), using the fact that $\nabla_x g_n$ is bounded in $L^1([0, T] \times \Omega)$ and that $(\partial_t - d_a \Delta_x) g_n$ is also bounded in $L^1([0, T] \times \Omega)$. This is a variant of Aubin's lemma (Cf. [17]).

We denote by ω_v the set $\{x \in \Omega : d(x, \partial \Omega) > v\}$. Let $x \in \omega_v$ (with v positive and such that ω_v is not an empty set), and $k \in \mathbb{R}^N$, with $|k| \leq v$. Since $\nabla_x g_n$ is bounded in $L^1([0, T] \times \Omega)$, we know that

(74)
$$\int_{0}^{T} \int_{C} |g_n(t, x + k) - g_n(t, x)| \, dx dt \le C_T |k| ,$$

where C_T is some constant depending on T.

Then, introducing any smooth function $\phi := \phi(x)$, with compact support in Ω , we have

$$\partial_t \int_{\Omega} g_n \, \phi \, dx = d_a \int_{\Omega} g_n \, \Delta_x \phi \, dx + \int_{\Omega} \beta_n \, \phi \, dx \; ,$$

where β_n is bounded in $L^1([0,T] \times \Omega)$. Therefore

(75)
$$\int_{0}^{T} \left| \partial_{t} \int_{\Omega} g_{n} \phi \, dx \right| dt \leq d_{a} \|g_{n}\|_{L^{1}} \|A_{x} \phi\|_{L^{\infty}} + \|\beta_{n}\|_{L^{1}} \|\phi\|_{L^{\infty}}$$

$$\leq C_{T} \|\phi\|_{W^{2,\infty}}.$$

We introduce v > 0 and a mollifying sequence $\phi_{\delta}(x) = \delta^{-N} \phi(x/\delta)$ of smooth functions with compact support $B(0, \delta)$, so that $B(0, \delta) + \omega_v \subset \Omega$ when $\delta < v$. Then, for any $t \in [\mu, T - \mu] \subset [0, T]$ $(0 < \mu < T/2)$, and for any $h \in \mathbb{R}$, $|h| \le \mu$, we get

$$\begin{split} &\int\limits_{\mu}^{T-\mu}\int\limits_{\omega_{o}} |g_{n}(t+h,x)-g_{n}(t,x)| \, dxdt \\ &\leq \int\limits_{\mu}^{T-\mu}\int\limits_{\omega_{o}} \left|\left(g_{n}*_{x}\phi_{\delta}\right)(t+h,x)-(g_{n}*_{x}\phi_{\delta})(t,x)\right| \, dxdt \\ &+2\int\limits_{0}^{T}\int\limits_{\omega_{o}} \left|\left(g_{n}*_{x}\phi_{\delta}\right)(t,x)-g_{n}(t,x)\right| \, dxdt \\ &\leq \int\limits_{\mu}^{T-\mu}\int\limits_{\omega_{o}} \left|\left(g_{n}*_{x}\phi_{\delta}\right)(t+h,x)-(g_{n}*_{x}\phi_{\delta})(t,x)\right| \, dxdt \\ &+2\,C_{T}\,\delta. \end{split}$$

Using (75), we see that

$$\int\limits_{\mu}^{T-\mu}\int\limits_{\omega_{v}}\left|g_{n}(t+h,x)-g_{n}(t,x)\right|dxdt\\ \leq \int\limits_{t=\mu}^{T-\mu}\int\limits_{x\in\omega_{v}}\left|h\right|\left|\int\limits_{u=0}^{1}\left[\int\limits_{y\in\Omega}g_{n}(\cdot,y)\,\phi_{\delta}(x-y)\,dy\right]'(t+uh)du\right|dxdt\\ +2\,C_{T}\,\delta$$

$$egin{aligned} & \leq \|h\| \int\limits_{x \in \omega_v} \int\limits_{u=0}^1 \int\limits_{t=0}^T \left| \partial_t \int\limits_{y \in \Omega} g_n(t,y) \, \phi_\delta(x-y) \, dy \, \right| dt du dx \ & + 2 \, C_T \, \delta \ & \leq C_T \, \|h\| \int\limits_{x \in \omega} \|\phi_\delta(x-\cdot)\|_{W^{2,\infty}} \, dx + \, 2 \, C_T \, \delta \; . \end{aligned}$$

Finally, optimizing in δ , we get

$$\int_{\mu}^{T-\mu} \int_{\omega_{v}} |g_{n}(t+h,x) - g_{n}(t,x)| dxdt \le C_{T} |h| \delta^{-N-2} + 2C_{T} \delta$$

$$\le C_{T} |h|^{1/(N+3)}.$$

Recalling estimate (74), we obtain

$$\int\limits_{\mu}^{T-\mu}\int\limits_{\omega_{n}}\left|g_{n}(t+h,x+k)-g_{n}(t,x)
ight|dxdt\leq C_{T}\left(\left|h
ight|^{1/\left(N+3
ight)}+\left|k
ight|
ight).$$

This ensures that g_n is a strongly compact sequence in $L^1(]\mu, T - \mu[\times \omega_v)$ for all (sufficiently small) $\mu > 0$, v > 0, or, more simply, that g_n is a strongly compact sequence in $L^1_{loc}(]0, T[\times \Omega)$.

Then, up to extraction of a subsequence, g_n converges a.e., and so does a_n . The same proof applied to the other concentrations shows that b_n , c_n and d_n also converge (up to extraction) a.e.

It is now possible to pass to the limit in the weak formulation of system (70) - (72).

We recall that this formulation (written here only for the first equation) is the following: for any smooth (C^2) test function $\varphi := \varphi(t,x)$ with compact support in $[0,+\infty[\times\overline{\Omega}]]$ and such that $n(x)\cdot\nabla_x\varphi(t,x)=0$ for $x\in\partial\Omega$,

(76)
$$\int_{0}^{+\infty} \int_{\Omega} a_n \, \partial_t \varphi \, dx dt + \int_{\Omega} a_{in}(x) \, \varphi(0, x) \, dx$$

$$+ \int_{0}^{+\infty} \int_{\Omega} d_a \, a_n \, \Delta_x \varphi \, dx dt = \int_{0}^{+\infty} \int_{\Omega} \frac{c_n \, d - a_n \, b_n}{1 + \frac{1}{n} \, (a_n^2 + b_n^2 + c_n^2 + d_n^2)} \, \varphi \, dx dt \, .$$

At this point, let us recall that since a_n converges a.e. (up to a subsequence), and is bounded in $L^2(\ln L)^2([0,T]\times\Omega)$, it converges strongly in $L^2([0,T]\times\Omega)$ to a function a lying in this space (and so do the other concentrations), so that the quantity a_n b_n and c_n d_n , which are equiintegrable, converge respectively to a b and c d in L^1 .

We can pass finally to the limit in the left-hand side of (76), obtaining

(77)
$$\int_{0}^{+\infty} \int_{\Omega} a \ \partial_t \varphi \, dx dt + \int_{\Omega} a_{in} \ \varphi(0,\cdot) \, dx + \int_{0}^{+\infty} \int_{\Omega} d_a \, a \ \Delta_x \varphi \, dx dt.$$

As concerns the right-hand side of (76), we see that

$$\int_{0}^{+\infty} \int_{\Omega} \frac{c_n d - a_n b_n}{1 + \frac{1}{n} (a_n^2 + b_n^2 + c_n^2 + d_n^2)} \varphi \, dx dt$$

converges to

$$\int_{0}^{+\infty} \int_{\Omega} (c d - a b) \varphi \ dxdt \ .$$

We end up in this way with the weak form of the (first equation) of system (16) - (18).

4 - Large time behaviour

4.1 - Entropy dissipation estimate: general theory

We first describe the traditional strategy (sometimes called entropy/entropy dissipation method in the context of kinetic equations) used to get explicit estimates of convergence toward equilibrium for equations where dissipative effects are predominant.

4.1.1 - Lyapounov functionals; De La Salle principle

The principles of the approach described below and many applications can be found in [6].

We consider an abstract equation

$$\partial_t f = A f,$$

where A is an operator which can be linear or nonlinear, and can involve derivatives or integrals.

We suppose that there exists a (bounded below) Lyapounov functional H := H(f) (usually called entropy (or opposite of the entropy)) and a functional D := D(f)

(usually called entropy dissipation) such that (what is called in kinetic theory the first and second part of Boltzmann's H-theorem) holds:

(79)
$$\partial_t H(f) = -D(f) \le 0,$$

(80)
$$D(f) = 0 \iff Af = 0 \iff f = f_{eq},$$

where f_{eq} is a given function.

Then, one can often prove that the decreasing function $t \mapsto H(f(t))$ converges toward its minimum, that $t \mapsto D(f(t))$ converges toward 0, and that as a consequence

$$\lim_{t \to +\infty} f(t) = f_{eq}$$

in a convenient topology (a precise theorem could for example be written down, in the case when *H* is coercive).

Unfortunately, the situation described above is often slightly more intricate, because one has to take into account quantities which are conserved in the evolution of eq. (78). In particular, in eq. (80), f_{eq} is in general not a given function, but a set of functions depending on a number of parameters equal to the number of conserved quantities.

4.1.2 - Use of the Gronwall lemma

In order to obtain an explicit rate of convergence toward equilibrium, one looks for functional inequalities of the form

(82)
$$D(f) > \Phi(H(f) - H(f_{eq})),$$

where $\Phi: \mathbb{R}_+ \to \mathbb{R}_+$ is a function such that $\Phi(x) = 0 \iff x = 0$. One tries to find a function Φ which increases as much as possible near 0.

Note that we look for such an inequality for functions f which are not necessarily solutions of eq. (78) (they do not even depend upon t!). This is a way of transforming a problem on PDEs in a problem of functional inequalities.

In the case when there are conserved quantities in the evolution of eq. (78), it is enough to prove estimate (82) when the corresponding quantities are fixed.

Assuming that estimate (82) holds, we apply it to the function f := f(t) solution of eq. (78) and get thanks to estimate (79) the differential inequality

(83)
$$\partial_t (H(f)(t) - H(f_{eq})) \le -\Phi(H(f)(t) - H(f_{eq})).$$

Then, Gronwall's lemma ensures that

$$(84) H(f)(t) - H(f_{eq}) \le R(t),$$

where R is the reciprocal of a primitive of $-1/\Phi$.

When one can take, for some constant $C_0 > 0$, $\Phi(x) = C_0 x$, one gets $R(t) \leq Cst \, e^{-C_0 t}$. Sometimes, it is however only possible to take $\Phi(x) = Cst_\varepsilon \, x^{1+\varepsilon}$ for some (or all) $\varepsilon > 0$, and consequently $R(t) = Cst_\varepsilon \, t^{-1/\varepsilon}$.

4.1.3 - Cziszar-Kullback inequality

It is often more interesting to estimate $||f(t) - f_{eq}||$ for some norm || ||, than to estimate the more abstract quantity $H(f(t)) - H(f_{eq})$. Therefore, we are interested in inequalities of the form

(85)
$$H(f) - H(f_{eq}) \ge \psi(\|f(t) - f_{eq}\|),$$

where we look for a function $\psi \geq 0$ which increases as much as possible near 0.

Note that since H reaches its minimum at $f = f_{eq}$, we expect at best that ψ behaves quadratically at point 0.

Next proposition, sometimes called Cziszar-Kullback or Pinsker inequality (Cf. [2] and [10]), enables to prove such an estimate in the case when $H(f) = \int\limits_{\Omega} (f \ln f - f)$, where $\Omega \subset \mathbb{R}^N$.

Proposition 4.1. Let Ω be a measurable subset of \mathbb{R}^N and $f,g:\Omega\to R_+$. Then

$$\int_{\Omega} \left(f(x) \ln \left(\frac{f(x)}{g(x)} \right) - f(x) + g(x) \right) dx \ge \left(\frac{3}{2 \int_{\Omega} f(x) dx + 4 \int_{\Omega} g(x) dx} \right) \\
\times \left(\int_{\Omega} |f(x) - g(x)| dx \right)^{2}.$$

Proof of Proposition 4.1. We recall the following elementary inequality, due to Pinsker: for all $u \in \mathbb{R}$,

$$3|u-1|^2 \le (2u+4)(u \log u - u + 1).$$

Then,

$$\begin{split} \int\limits_{\Omega} |f(x) - g(x)| \, dx &= \int\limits_{\Omega} \left| \frac{f(x)}{g(x)} - 1 \right| g(x) \, dx \\ &\leq \int\limits_{\Omega} \sqrt{2 \, \frac{f(x)}{g(x)} + 4} \, \sqrt{\frac{f(x)}{g(x)} \ln \left(\frac{f(x)}{g(x)} \right) - \frac{f(x)}{g(x)} + 1} \, \frac{g(x)}{\sqrt{3}} \, dx \\ &\leq \frac{1}{\sqrt{3}} \, \sqrt{\int\limits_{\Omega} (2 \, f(x) + 4 \, g(x)) \, dx} \, \sqrt{\int\limits_{\Omega} \left(f(x) \ln \left(\frac{f(x)}{g(x)} \right) - f(x) + g(x) \right) \, dx}. \end{split}$$

This concludes the proof of Proposition 4.1.

In the sequel, since we shall use Lyapounov functionals which are sums of quantities like $\int_{\Omega} (a \ln a - a)$, for various concentrations a, we shall have to use Cziszar-Kullback inequality in order to obtain estimates like (85).

4.2 - The case of two reaction-diffusion equations

4.2.1 - Large time behavior: the result

We now present a result which gives an explicit estimate about the speed of convergence of a solution to system (10) - (12) towards equilibrium. This result is extracted from [4].

Theorem 4.1. Let Ω be a bounded, regular (C^2) and connected open set of \mathbb{R}^N ($N \geq 1$) of measure 1, and d_a, d_b be two strictly positive diffusivity constants. Let the initial data a_{in} , b_{in} be two strictly positive functions of $C^2(\overline{\Omega})$ with mass $\int (a_{in} + 2b_{in}) dx = M > 0$.

Then, the unique strictly positive smooth (C^2) solution $t \in \mathbb{R}_+ \mapsto (a(t), b(t))$ to equations (10) – (12) obeys the following estimate of exponential decay toward equilibrium:

$$||a(t,\cdot)-a_{\infty}||_{L^{1}(\Omega)}^{2}+||b(t,\cdot)-b_{\infty}||_{L^{1}(\Omega)}^{2}\leq C_{1}e^{-C_{2}t},$$

where $C_1, C_2 > 0$.

Here, a_{∞} and b_{∞} are the unique nonnegative numbers which satisfy the equation

(86)
$$a_{\infty}^2 = b_{\infty}, \qquad a_{\infty} + 2b_{\infty} = M.$$

4.2.2 - The proof: the entropy dissipation estimate

Proof of Theorem 4.1. We recall that since the initial data are strictly positive and smooth, system (10) – (12) has indeed a unique smooth C^2 solution, which moreover satisfies (for some constants A_0 , A_1 , B_0 and $B_1 > 0$)

(87)
$$\forall t \ge 0, x \in \Omega, \qquad A_0 \le a(t, x) \le A_1, \qquad B_0 \le b(t, x) \le B_1.$$

This is a direct application of Theorem 3.2.

We then prove the following proposition, which corresponds to estimate (82) in the abstract formulation of subsection 4.1:

Proposition 4.2. Let Ω be a bounded, smooth (C^2), and connected subset of \mathbb{R}^N of measure 1. We consider $d_a, d_b > 0$ two strictly positive diffusion constants.

Let $a, b: \Omega \to \mathbb{R}$ be two functions such that (for some constants A_0, A_1, B_0 and $B_1 > 0$

(88)
$$\forall x \in \Omega, \qquad A_0 \le a(x) \le A_1, \qquad B_0 \le b(x) \le B_1,$$

and

(89)
$$\int_{\Omega} (a(x) + 2b(x)) dx = M > 0.$$

Then, there exists a constant C > 0 (depending on Ω , M, d_a , d_b , A_0 , A_1 , B_1 and B_2) such that

$$D_1(a,b) \geq C(E_1(a,b) - E_1(a_{\infty},b_{\infty})),$$

where a_{∞} , b_{∞} are defined by (86), and functionals E_1 , D_1 are defined by formulas (23) and (24).

Proof of Proposition 4.2. We systematically denote the average over Ω of a

quantity z by $\overline{z} = \int\limits_{\Omega} z(x)\,dx$ (remember that Ω is of measure 1). We start with the identity $\frac{|\nabla_x a|^2}{a} \geq \frac{|\nabla_x a|^2}{\|a\|_{L^\infty}}$, and apply Poincaré's inequality (with Poincaré's constant P), so that

$$\int_{\Omega} \frac{\left|\nabla_{x} a\right|^{2}}{a} dx \ge P \int_{\Omega} \frac{\left|a - \bar{a}\right|^{2}}{\|a\|_{L^{\infty}}} dx.$$

We do the same for b, but we also use the identity

$$\int\limits_{\Omega}rac{\left|
abla_{x}b
ight|^{2}}{b}\,dx=4\int\limits_{\Omega}\left|
abla_{x}\sqrt{b}
ight|^{2}dx\geq P\int\limits_{\Omega}\left|\sqrt{b}-\overline{\sqrt{b}}
ight|^{2}dx.$$

Using then the inequality

$$(x-y)(\ln(x) - \ln(y)) \ge 4(\sqrt{x} - \sqrt{y})^2$$

and the L^{∞} bound on a and b, we get (for a strictly positive constant which we denote by C, as any other strictly positive constant in the sequel)

$$(90) \qquad D_{1}(a,b) \geq C \left(\left\| a - \sqrt{b} \right\|_{L^{2}}^{2} + \left\| a - \overline{a} \right\|_{L^{2}}^{2} + \left\| b - \overline{b} \right\|_{L^{2}}^{2} + \left\| \sqrt{b} - \overline{\sqrt{b}} \right\|_{L^{2}}^{2} \right).$$

We shall prove that the r.h.s. of (90) is bounded below by (some constant times) the relative entropy $E(a,b) - E(a_{\infty},b_{\infty})$.

Firstly, we use the conservation law (89) to rewrite the relative entropy as

$$egin{aligned} E_1(a,b) - E_1(a_\infty,b_\infty) &= \int\limits_{arOmega} igg(a \ln igg(rac{a}{a_\infty}igg) - (a-a_\infty) \ &+ b \ln igg(rac{b}{b_\infty}igg) - (b-b_\infty)igg) dx. \end{aligned}$$

We use the elementary inequality

$$\forall a > 0,$$
 $a \ln a - a + 1 \le (a - 1)^2,$

in order to obtain

(91)
$$E_1(a,b) - E_1(a_{\infty},b_{\infty}) \le \frac{1}{a_{\infty}} \|a - a_{\infty}\|_{L^2}^2 + \frac{1}{b_{\infty}} \|b - b_{\infty}\|_{L^2}^2.$$

We see therefore that we only have to show that for some constant C > 0,

$$egin{aligned} \left\| a - \sqrt{b}
ight\|_{L^2}^2 + \left\| a - \overline{a}
ight\|_{L^2}^2 + \left\| b - \overline{b}
ight\|_{L^2}^2 + \left\| \sqrt{b} - \overline{\sqrt{b}}
ight\|_{L^2}^2 \ & \geq C \left(\left\| a - a_{\infty}
ight\|_{L^2}^2 + \left\| b - b_{\infty}
ight\|_{L^2}^2
ight). \end{aligned}$$

We notice that

$$egin{align} \|a-a_\infty\|_{L^2}^2 &\leq 2\left(\|a-\overline{a}\|_{L^2}^2 + |\overline{a}-a_\infty|^2
ight), \ \|b-b_\infty\|_{L^2}^2 &\leq 2\left(\|b-\overline{b}\|_{L^2}^2 + |\overline{b}-b_\infty|^2
ight), \ \|a-\sqrt{b}\|_{L^2} &\geq \left|\overline{a}-\overline{\sqrt{b}}
ight|, \end{aligned}$$

so that we only have to show that for some constant C > 0,

$$\left\| \overline{a} - \overline{\sqrt{b}} \right\|^2 + \left\| \sqrt{b} - \overline{\sqrt{b}} \right\|_2^2 \ge C \left(\left| \overline{a} - a_{\infty} \right|^2 + \left| \overline{b} - b_{\infty} \right|^2 \right).$$

Then, we observe that

$$egin{split} \left| \overline{\sqrt{b}} - \sqrt{\overline{b}} \, \right|^2 &= 2 \sqrt{\overline{b}} \left(\sqrt{\overline{b}} - \overline{\sqrt{b}}
ight) rac{\sqrt{\overline{b}} - \overline{\sqrt{b}}}{2 \sqrt{\overline{b}}} \ &\leq \left\| \sqrt{b} - \overline{\sqrt{b}} \,
ight\|_{L^2}^2 rac{\sqrt{\overline{b}} + \overline{\sqrt{b}}}{2 \sqrt{\overline{b}}} \ &\leq \left\| \sqrt{b} - \overline{\sqrt{b}} \,
ight\|_{L^2}^2. \end{split}$$

Thus, we only have to show that for some constant C > 0,

$$\left|\overline{a}-\sqrt{\overline{b}}\,\right|^2 \geq C\left(\left|\overline{a}-a_\infty
ight|^2+\left|\overline{b}-b_\infty
ight|^2
ight).$$

Note that this is a statement on numbers and not on functions.

We recall that

$$\overline{a} + 2\overline{b} = a_{\infty} + 2b_{\infty}$$

and that $a_{\infty}^2=b_{\infty}$, so that we only have to show that for some constant C>0,

$$|(\overline{a})^2 + \frac{1}{2}\overline{a} - a_{\infty}^2 - \frac{1}{2}a_{\infty}|^2 \ge C|\overline{a} - a_{\infty}|^2.$$

This is easily obtained by noticing that if $f(x) = x^2 + \frac{1}{2}x$, then $|(f^{-1})'(x)| \le 2$. This ends the proof of Proposition 4.2.

4.2.3 - The Cziszar-Kullback type inequality

We now turn to another proposition, which shows that the relative entropy $E_1(a,b)-E_1(a_\infty,b_\infty)$ defined by (23) and (86) controls (from above) the squares of the L^1 -distances to the equilibrium:

Proposition 4.3. Let Ω be an open subset of \mathbb{R}^N of measure 1. For all (measurable) nonnegative functions $a, b : \Omega \to \mathbb{R}$ such that $\int_{\Omega} (a(x) + 2b(x)) dx = M > 0$,

(92)
$$E_1(a,b) - E_1(a_{\infty}, b_{\infty}) \ge C \left(\|a - a_{\infty}\|_{L^1}^2 + \|b - b_{\infty}\|_{L^1}^2 \right),$$

where definitions (23) and (86) have been used.

Proof of Proposition 4.3. We still use the notations $\overline{a} = \int\limits_{\Omega} a\,dx$ and $\overline{b} = \int\limits_{\Omega} b\,dx$, and define $q(x) := x\,\ln x - x$. Then,

$$E_1(a,b) - E_1(a_{\infty}, b_{\infty}) = \int_{\Omega} a \ln\left(\frac{a}{\overline{a}}\right) dx + \int_{\Omega} b \ln\left(\frac{b}{\overline{b}}\right) dx + \left(q(\overline{a}) - q(a_{\infty})\right) + \left(q(\overline{b}) - q(b_{\infty})\right).$$

We first note that thanks to Cziszar-Kullback inequality (Cf. Proposition 4.1),

$$\int_{\Omega} a \ln\left(\frac{a}{\overline{a}}\right) dx \ge \frac{1}{2\overline{a}} \|a - \overline{a}\|_{L^{1}}^{2}, \qquad \int_{\Omega} b \ln\left(\frac{b}{\overline{b}}\right) dx \ge \frac{1}{2\overline{b}} \|b - \overline{b}\|_{L^{1}}^{2},$$

and moreover $\overline{a} \leq M$ and $\overline{b} \leq M/2$ by (89). Then, we consider $Q(\overline{a}) := q(\overline{a}) + q\left(\frac{M-\overline{a}}{2}\right)$ for $\overline{a} \in]0, M[$ and $R(\overline{b}) := q(\overline{b}) + q(M-2\overline{b})$ for $\overline{b} \in]0, M/2[$. Since

(93)
$$Q''(\overline{a}) = \frac{1}{\overline{a}} + \frac{1}{2} \frac{1}{M - \overline{a}} \ge \frac{3 + 2\sqrt{2}}{2M},$$

and

$$(94) R''(\overline{b}) = \frac{1}{\overline{b}} + \frac{4}{M - \overline{b}} \ge \frac{6 + 4\sqrt{2}}{M},$$

we combine 2/3 of (93) and 1/3 of (94) to Taylor-expand

$$(q(\overline{a})-q(a_{\infty}))+(q(\overline{b})-q(b_{\infty}))\geq \frac{3+2\sqrt{2}}{6M}\left|\overline{a}-a_{\infty}\right|^{2}+\frac{3+2\sqrt{2}}{3M}\left|\overline{b}-b_{\infty}\right|^{2}.$$

Finally, we observe that

$$\left\|a-a_{\infty}\right\|_{L^{1}}^{2} \leq \frac{6+2\sqrt{2}}{3+2\sqrt{2}}\left(\left\|a-\overline{a}\right\|_{L^{1}}^{2}+\frac{3+2\sqrt{2}}{3}\left|\overline{a}-a_{\infty}\right|^{2}\right),$$

and

$$\|b-b_{\infty}\|_{L^{1}}^{2} \leq rac{6+2\sqrt{2}}{3+2\sqrt{2}}\left(\|b-\overline{b}\|_{L^{1}}^{2}+rac{3+2\sqrt{2}}{3}\left|\overline{b}-b_{\infty}
ight|^{2}
ight),$$

by Young's inequality. This concludes the proof of Proposition 4.3.

We come back to the proof of Theorem 4.1.

We consider the unique smooth solution $t \mapsto (a(t), b(t))$ to system (10) – (12) obtained at the beginning of the proof. We apply Proposition 4.2 to a = a(t) and b = b(t). This is possible since condition (88) is satisfied thanks to estimate (87), and condition (89) is satisfied thanks to the conservation property (20). As a consequence, we see that

$$D_1(a(t), b(t)) > C(E_1(a(t), b(t)) - E_1(a_{\infty}, b_{\infty})).$$

Thanks to the entropy estimate (29), we obtain

$$\frac{d}{dt}(E_1(a(t), b(t)) - E_1(a_{\infty}, b_{\infty})) \le -C(E_1(a(t), b(t)) - E_1(a_{\infty}, b_{\infty})),$$

and thanks to Gronwall's lemma:

$$E_1(a(t), b(t)) - E_1(a_{\infty}, b_{\infty}) \le (E_1(a_{in}, b_{in}) - E_1(a_{\infty}, b_{\infty})) e^{-Ct}.$$

Using now Proposition 4.3 with a = a(t) and b = b(t) (and noticing again that the conservation property (20) enables to fulfill the assumptions of this proposition), we conclude the proof of Theorem 4.1.

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Abstract

In this work, we present an approach for a certain type of reaction diffusion equations (those coming out of problems of reversible chemistry) based on the relationship between entropy and entropy dissipation. We first discuss the existence, uniqueness and smoothness of solutions for the equations under study. Then, we get an explicit bound of exponential decay describing the large time behavior of those solutions.

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