# EXPLICIT EXPONENTIAL CONVERGENCE TO EQUILIBRIUM FOR MASS ACTION REACTION-DIFFUSION SYSTEMS

KLEMENS FELLNER, BAO QUOC TANG

Abstract. The explicit convergence to equilibrium for reaction-diffusion systems arising from chemical reaction networks is studied. The reaction networks are assumed to satisfy the detailed balance condition and have no boundary equilibria. We use the so-called entropy method in which an entropy-entropy dissipation estimate is derived utilizing the structure of conservation laws. As a consequence, the convergence to equilibrium for solutions follows with computable convergence rates. The applications of the approach are demonstrated in two cases: a single reversible reaction involving arbitrary number of chemical substances and a chain of two reversible reactions arising from enzyme reactions.

## 1. Introduction

In this paper, we study the convergence to equilibrium for a class of reaction-diffusion systems arising from chemical reaction networks by using the so-called entropy method.

The considered reaction-diffusion systems describe networks of chemical reaction with mass action law kinetics under the assumption of a detailed balance condition. In particular, we consider $I$ chemical substances $\mathcal{A}_1, \ldots, \mathcal{A}_I$ reacting in $R$ reversible reactions of the form

$$\alpha_1^r \mathcal{A}_1 + \ldots + \alpha_I^r \mathcal{A}_I \underset{k_{r,f}}{\overset{k_{r,b}}{\rightleftharpoons}} \beta_1^r \mathcal{A}_1 + \ldots + \beta_I^r \mathcal{A}_I$$

for $r = 1, 2, \ldots, R$ with the nonnegative stoichiometric coefficients $\boldsymbol{\alpha}^r = (\alpha_1^r, \ldots, \alpha_I^r) \in (\{0\} \cup [1, \infty))^I$ and $\boldsymbol{\beta}^r = (\beta_1^r, \ldots, \beta_I^r) \in (\{0\} \cup [1, \infty))^I$ and the positive forward and backward reaction rate constants $k_{r,f} > 0$ and $k_{r,b} > 0$. The corresponding reaction-diffusion system for the concentration vector $\mathbf{c} = (c_1, \ldots, c_I) : \Omega \times \mathbb{R}_+ \to [0, +\infty)^I$ reads as

$$\begin{cases} \dfrac{\partial}{\partial t}\mathbf{c} = \operatorname{div}(\mathbb{D}\nabla \mathbf{c}) - \mathbf{R}(\mathbf{c}), & \text{in } \Omega, \\ \nabla \mathbf{c} \cdot \nu = 0, & \text{on } \partial\Omega, \\ \mathbf{c}(x, 0) = \mathbf{c}_0(x), & \text{for } x \in \Omega, \end{cases} \tag{1.1}$$

where $\Omega \subset \mathbb{R}^n$ is a bounded domain with smooth boundary $\partial\Omega$ and normalized volume, i.e. $|\Omega| = 1$, $\mathbb{D} = \operatorname{diag}(d_1(x), \ldots, d_I(x))$ is the positive definite diffusion matrix and the reaction vector $\mathbf{R}(\mathbf{c})$ represents the chemical reactions according to the mass action kinetics, i.e.

$$\mathbf{R}(\mathbf{c}) = \sum_{r=1}^{R} \left(k_{r,f}\mathbf{c}^{\boldsymbol{\alpha}^r} - k_{r,b}\mathbf{c}^{\boldsymbol{\beta}^r}\right)(\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r) \quad \text{with} \quad \mathbf{c}^{\boldsymbol{\alpha}^r} = \prod_{i=1}^{I} c_i^{\alpha_i^r}.$$

By denoting $m = \operatorname{codim}(\operatorname{span}\{\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r : r = 1, 2, \ldots, R\})$, there exists a matrix $\mathbb{Q} \in \mathbb{R}^{m \times I}$ such that $\mathbb{Q}\,\mathbf{R}(\mathbf{c}) = 0$ for all states $\mathbf{c}$. Thus, we have the following conservation laws for (1.1)

$$\int_\Omega \mathbb{Q}\,\mathbf{c}(t)dx = \int_\Omega \mathbb{Q}\,\mathbf{c}_0\,dx \quad \text{or equivalently} \quad \mathbb{Q}\,\overline{\mathbf{c}}(t) = \mathbf{M} := \mathbb{Q}\,\overline{\mathbf{c}_0}$$

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for all $t > 0$ where $\overline{\mathbf{c}} = (\overline{c_1}, \ldots, \overline{c_I})$, with $\overline{c_i} = \int_\Omega c_i(x)dx$, is the spatial average concentration vector and $\mathbf{M} \in \mathbb{R}_+^m$ denote the vector of positive initial masses.

The large time behaviour of solutions to reaction-diffusion systems if a highly active research area, which poses many open problems, in particular for nonlinear problems. Classical analytical methods include e.g. linearisation techniques, spectral analysis, invariant regions and Lyapunov stability arguments.

More recently, the so-called entropy method is proved to be very useful in showing explicit convergence to equilibrium for reaction diffusion systems. The basic idea of the entropy method consists of studying the large-time asymptotics of a dissipative PDE model by looking for a nonnegative convex entropy functional $\mathcal{E}(f)$ and its nonnegative entropy dissipation functional

$$\mathcal{D}(f) = -\frac{d}{dt}\mathcal{E}(f(t))$$

along the flow of the PDE model, which is well-behaved in the following sense: firstly, all states with $\mathcal{D}(f) = 0$, which also satisfy all the involved conservation laws, identify a unique entropy-minimising equilibrium $f_\infty$, i.e.

$$\mathcal{D}(f) = 0 \quad \text{and} \quad \text{conservation laws} \quad \Longleftrightarrow \ f = f_\infty,$$

and secondly, there exists an *entropy entropy-dissipation (EED for short) estimate* of the form

$$\mathcal{D}(f) \geq \Phi(\mathcal{E}(f) - \mathcal{E}(f_\infty)), \qquad \Phi(x) \geq 0, \qquad \Phi(x) = 0 \iff x = 0,$$

for some nonnegative function $\Phi$. We remark, that such an inequality can only hold when all the conserved quantities are taken into account. Moreover, if $\Phi'(0) \neq 0$, one usually gets exponential convergence toward $f_\infty$ in relative entropy $\mathcal{E}(f) - \mathcal{E}(f_\infty)$ with a rate, which can be explicitly estimated.

The entropy method is a fully nonlinear alternative to arguments based on linearisation around the equilibrium and has the advantage of being quite robust with respect to variations and generalisations of the model system. This is due to the fact that the entropy method relies mainly on functional inequalities which have no direct link to the original PDE model. Generalised models typically feature related entropy and entropy-dissipation functionals and previously established EED estimates may very usefully be re-applied.

The entropy method has previously been used for scalar equations: nonlinear diffusion equations (such as fast diffusions [CV03, PD02], Landau equation [DV00]), integral equations (such as the spatially homogeneous Boltzmann equation [TV99, TV00, Vil03]), kinetic equations (see e.g. [DV01, DV05, FNS04]), or coagulation-fragmentation equations (see e.g. [CDF08, CDF08a]). For certain systems of drift-diffusion-reaction equations in semiconductor physics, an entropy entropy-dissipation estimate has been shown indirectly via a compactness-based contradiction argument in [GGH96, GH97, Gro92].

A first proof of EED estimates for systems with explicit rates and constants was established in [DF06, DF07, DF08] in the case of particular reversible reaction-diffusion equations with quadratic nonlinearities.

In this paper, we shall generalise the entropy method to detailed balance reaction-diffusion systems with arbitrary mass action law nonlinearities and, as a consequence, show explicit exponential convergence to equilibrium for (1.1). The analysis in this work uses the *detailed balance condition*, which also allows to assume (without loss of generality due to a suitable scaling argument) that

$$k_{r,f} = k_{r,b} = k_r > 0 \quad \text{for all } r = 1, 2, \ldots, R.$$

The key quantity of our study is the logarithmic entropy (free energy) functional

$$\mathcal{E}(\mathbf{c}) = \sum_{i=1}^{I} \int_\Omega (c_i \log c_i - c_i + 1)\, dx,$$

which decays monotone in time according to the following entropy dissipation functional

$$\mathcal{D}(\mathbf{c}) = -\frac{d}{dt}\mathcal{E}(\mathbf{c}) = \sum_{i=1}^{I} \int_\Omega d_i(x) \frac{|\nabla c_i|^2}{c_i} dx + \sum_{r=1}^{R} k_r \int_\Omega (\mathbf{c}^{\boldsymbol{\alpha}^r} - \mathbf{c}^{\boldsymbol{\beta}^r})(\log \mathbf{c}^{\boldsymbol{\alpha}^r} - \log \mathbf{c}^{\boldsymbol{\beta}^r}) dx \geq 0.$$

For a fixed positive initial mass vector $\mathbf{M} \in \mathbb{R}^m_+$, denote by $\mathbf{c}_\infty$ the detailed balanced equilibrium of (1.1) with mass $\mathbf{M}$, that is the unique vector of positive constants $\mathbf{c}_\infty > 0$, which balances all the reaction rates, i.e.

$$\mathbf{c}_\infty^{\boldsymbol{\alpha}^r} = \mathbf{c}_\infty^{\boldsymbol{\beta}^r}, \qquad \text{for all} \quad r = 1, 2, \ldots, R$$

and satisfies the mass conservation laws

$$\mathbb{Q}\, \mathbf{c}_\infty = \mathbf{M}.$$

The key step of the entropy method in order to prove exponential convergence to equilibrium of (1.1) is the following EED estimate

$$\boxed{\mathcal{D}(\mathbf{c}) \geq \lambda_{\mathbf{M}}(\mathcal{E}(\mathbf{c}) - \mathcal{E}(\mathbf{c}_\infty))} \tag{1.2}$$

for all $\mathbf{c} \in L^1(\Omega; [0, +\infty)^I)$ obeying the mass conservation $\mathbb{Q}\, \overline{\mathbf{c}} = \mathbf{M}$.

Once such a functional inequality is proved, applying it to solutions of the reaction-diffusion system and a classic Gronwall inequality yields exponential convergence in relative entropy with rates, which can be explicitly calculated. By applying moreover a Csiszár-Kullback-Pinsker type inequality one obtains $L^1$-convergence to equilibrium of solutions to (1.1) with the rate $e^{-\lambda_{\mathbf{M}} t/2}$ as $t \to +\infty$.

In [MHM14], by using a convexification argument, the authors proved that such a $\lambda_{\mathbf{M}} > 0$ always exists for system (1.1) under the detailed balance condition and gave an explicit bound of $\lambda_{\mathbf{M}}$ in the case of the quadratic reaction $2X \leftrightharpoons Y$. However, because of the convexification argument, obtaining estimates on $\lambda_{\mathbf{M}}$ seems difficult in the case of more than two substances, e.g. for systems like

$$\alpha \mathcal{A}_1 + \beta \mathcal{A}_2 \leftrightharpoons \gamma \mathcal{A}_3 \qquad \text{or} \qquad \mathcal{A}_1 + \mathcal{A}_2 \leftrightharpoons \mathcal{A}_3 + \mathcal{A}_4.$$

Inspired by ideas from [FLT14, DF08, DF14, FL], this work aims to propose a constructive way to prove the EED estimate (1.2). The main novelty of our method is that, by extensively using the structure of the mass conservation laws, the proof relies on elementary inequalities and has the advantage of providing explicit estimates for the convergence rate $\lambda_{\mathbf{M}}$.

In the following we shall sketch the main ideas of our method to prove (1.2) by dividing the proof into four steps, which are designed as a chain of estimates, which at the end of the day allows to take into account the conservation laws, which are crucial to the validity of (1.2):

**Step 1:** We use an additivity property in order to split the right hand side of (1.2) into two parts

$$\mathcal{E}(\mathbf{c}) - \mathcal{E}(\mathbf{c}_\infty) = \Big(\mathcal{E}(\mathbf{c}) - \mathcal{E}(\overline{\mathbf{c}})\Big) + \Big(\mathcal{E}(\overline{\mathbf{c}}) - \mathcal{E}(\mathbf{c}_\infty)\Big),$$

where the first part $\mathcal{E}(\mathbf{c}) - \mathcal{E}(\overline{\mathbf{c}})$ can be controlled by $\mathcal{D}(\mathbf{c})$ by using the Logarithmic Sobolev Inequality and the second part $\mathcal{E}(\overline{\mathbf{c}}) - \mathcal{E}(\mathbf{c}_\infty)$ contains only spatially averaged terms.

**Step 2:** We estimate $\mathcal{D}(\mathbf{c})$ and $\mathcal{E}(\overline{\mathbf{c}}) - \mathcal{E}(\mathbf{c}_\infty)$ in terms of quadratic forms, since the associated quadratic structures are significantly easier to deal with. By using capital letters as short hand notation for the square roots of various quantities, i.e. $C_i = \sqrt{c_i}$ and $C_{i,\infty} = \sqrt{c_{i,\infty}}$, we have

$$\frac{1}{2}\mathcal{D}(\mathbf{c}) \geq \sum_{i=1}^{I} 2\, d_{i,min}\, \|\nabla C_i\|^2_{L^2(\Omega)} + 2\sum_{r=1}^{R} k_r \left\| \mathbf{C}^{\boldsymbol{\alpha}^r} - \mathbf{C}^{\boldsymbol{\beta}^r} \right\|^2_{L^2(\Omega)},$$

and

$$\mathcal{E}(\overline{\mathbf{c}}) - \mathcal{E}(\mathbf{c}_\infty) \leq K_2 \sum_{i=1}^{I} \left( \sqrt{\overline{C_i^2}} - C_{i,\infty} \right)^2.$$

**Step 3:** In order to be able to use the constrains provided by the conservation laws, we bound the reaction term of $\mathcal{D}(\mathbf{c})$ below by a reaction term of the corresponding spatial averages:

$$\begin{aligned}\frac{1}{2}\mathcal{D}(\mathbf{c}) &\geq \sum_{i=1}^{I} 2 d_{i,min} \|\nabla C_i\|^2_{L^2(\Omega)} + 2\sum_{r=1}^{R} k_r \left\| \mathbf{C}^{\boldsymbol{\alpha}^r} - \mathbf{C}^{\boldsymbol{\beta}^r} \right\|^2_{L^2(\Omega)} \\ &\geq K_3 \left( \sum_{i=1}^{I} \|\nabla C_i\|^2_{L^2(\Omega)} + \sum_{r=1}^{R} \left( \overline{\mathbf{C}}^{\boldsymbol{\alpha}^r} - \overline{\mathbf{C}}^{\boldsymbol{\beta}^r} \right)^2 \right)\end{aligned}$$

where $\overline{\mathbf{C}} = (\overline{C_1}, \ldots, \overline{C_I})$ with $\overline{C_i} = \int_\Omega C_i(x)dx$.

**Step 4:** As a final step, we are left to find a constant $K_1 > 0$ such that

$$K_3 \left( \sum_{i=1}^{I} \|\nabla C_i\|^2_{L^2(\Omega)} + \sum_{r=1}^{R} \left( \overline{\mathbf{C}}^{\boldsymbol{\alpha}^r} - \overline{\mathbf{C}}^{\boldsymbol{\beta}^r} \right)^2 \right) \geq K_1 K_2 \sum_{i=1}^{I} \left( \sqrt{\overline{C_i^2}} - C_{i,\infty} \right)^2. \quad (1.3)$$

To prove this claim, we will employ a change of variable, which allows to quantify the conservation laws in terms of deviations around the equilibrium values, i.e.

$$\overline{C_i^2} = C_{i,\infty}^2 (1+\mu_i)^2, \qquad \mu_i \in [-1, +\infty). \quad (1.4)$$

While the non-negativity of the concentration vector $\mathbf{c}$ provides a natural lower bound $\mu_i \geq 1$, the conservation laws $\mathbb{Q}\,\overline{\mathbf{C}^2} = \mathbb{Q}\,\mathbf{C}_\infty^2$ impose also certain upper bounds on the new variable $\mu_i$.

Then, the proof of (1.3) distinguishes two cases: i) when all $\overline{C_i^2}$ are strictly bounded away from zero and ii) when at least one $\overline{C_{i_0}^2}$ is "small". In the first case, using the ansatz (1.4), (1.3) yields a finite dimensional inequality in terms of the new variables $\mu_1, \ldots, \mu_I$ under the constraints of the conservation laws. In the latter case, we are able to quantitatively estimate that if some $\overline{C_{i_0}^2}$ is much smaller than e.g. its equilibrium value, then such a state is far away from equilibrium in the sense that the left hand side of (1.3) is always bounded below by a positive constant, which is derived by again using the conservation laws. Thus, one obtains (1.3) by choosing a suitable $K_1$ after observing the fact that the right hand side of (1.3) is naturally bounded above by a constant.

We remark that the Steps **1.**, **2.** and **3.** can be proved without using the conservation laws. Hence, we are able to prove these three steps in full generality. Step **4.**, however depends on the structure of conservation laws defined by the matrix $\mathbb{Q}$ of left zero-eigenvectors. Hence the matrix $\mathbb{Q}$ is in general case is not explicit given. This prevents an entirely explicit proof of this step in the general case. However, for a specific model, in which $\mathbb{Q}$ is explicitly known, Step **4.** can be made entirely explicit, as we shall illustrate in terms of two example systems below.

Before stating our main results, let us remark that the question of global existence of (classical, strong or weak) solutions to (1.1) is far open in general. This is due to the lack of sufficiently strong a-priori estimates (maximum/comparison principles do no longer hold except for special systems) in order to control nonlinear terms.

Recently, Fischer [Fis15] proved the global existence of so-called "renormalised solution" for (1.1). All the estimates presented in our paper hold for renormalised solution. Indeed, its shown in [Fis15] that $c_i \log c_i \in L^\infty_{loc}([0,+\infty); L^1(\Omega))$ for all $i = 1, 2, \ldots, I$, which makes the entropy functional $\mathcal{E}(\mathbf{c})$ well defined.

In this paper, we will detail the proposed strategy for two important specific models: the general single reversible reaction with arbitrary number of substances

$$\alpha_1\mathcal{A}_1 + \ldots + \alpha_I\mathcal{A}_I \leftrightharpoons \beta_1\mathcal{B}_1 + \ldots + \beta_J\mathcal{B}_J \tag{1.5}$$

and a chain of two reversible reactions, which generalises the Michaels-Menton model for catalytic enzyme kinetics (see e.g. [Mur02])

$$\mathcal{A}_1 + \mathcal{A}_2 \leftrightharpoons \mathcal{A}_3 \leftrightharpoons \mathcal{A}_4 + \mathcal{A}_5. \tag{1.6}$$

Note that with respect to the general system (1.1), it is more convenient and usual to change of notation for the single reversible reaction (1.5) by splitting the concentration vector $\boldsymbol{c}$ into a left- and a right-concentration vector, i.e.

$$\boldsymbol{c} = (c_1, \ldots, c_I) \to (\boldsymbol{a}, \boldsymbol{b}) = (a_1, \ldots, a_I, b_1, \ldots, a_J).$$

which allows a clearer presentation of the proof.

At first, the reaction-diffusion system modelling (1.5) reads as

$$\begin{cases} \partial_t a_i - \operatorname{div}(d_{a,i}(x)\nabla a_i) = -\alpha_i(\boldsymbol{a}^{\boldsymbol{\alpha}} - \boldsymbol{b}^{\boldsymbol{\beta}}), & i = 1, 2, \ldots, I, \quad x \in \Omega, \\ \partial_t b_j - \operatorname{div}(d_{b,j}(x)\nabla b_j) = -\beta_j(\boldsymbol{a}^{\boldsymbol{\alpha}} - \boldsymbol{b}^{\boldsymbol{\beta}}), & j = 1, 2, \ldots, J, \quad x \in \Omega, \\ \nabla a_i \cdot \nu = \nabla b_j \cdot \nu = 0, & i = 1, \ldots, I, \ j = 1, \ldots, J, \ x \in \partial\Omega \end{cases} \tag{1.7}$$

where $\boldsymbol{a} = (a_1, \ldots, a_I)$ and $\boldsymbol{b} = (b_1, \ldots, b_J)$ denote the two vectors for left- and right-hand side concentrations and $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_I) \in ([1,\infty))^I$ and $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_J) \in ([1,\infty))^I$ the positive vectors of the stoichiometric coefficients assosiated to the single reaction (1.5). Moreover, $\boldsymbol{a}^{\boldsymbol{\alpha}} = \prod_{i=1}^I a_i^{\alpha_i}$ and $\boldsymbol{b}^{\boldsymbol{\beta}} = \prod_{i=1}^J b_i^{\beta_i}$.

This system (1.7) possesses the following $IJ$ mass conservation laws

$$\frac{\overline{a_i}}{\alpha_i} + \frac{\overline{b_j}}{\beta_j} = M_{i,j}, \qquad i = 1, \ldots, I, \ j = 1, \ldots, J, \tag{1.8}$$

from which exactly $m = I + J - 1$ conservation laws are linear independent. That means the matrix $\mathbb{Q}$ in this case has the dimension $\mathbb{Q} \in \mathbb{R}^{(I+J-1)\times(I+J)}$. See Lemma 3.1 for an explicit form of $\mathbb{Q}$. After choosing and fixing $I + J - 1$ linear independent components from the $IJ$ conserved initial masses $(M_{i,j}) \in \mathbb{R}_+^{IJ}$, we denote by $\mathbf{M} = (M_{i,j}) \in \mathbb{R}^{I+J-1}$ the vector of initial masses corresponding to the selected $I + J - 1$ coordinates of $(M_{i,j}) \in \mathbb{R}_+^{IJ}$. The detailed balanced equilibrium $(\boldsymbol{a}_\infty, \boldsymbol{b}_\infty) \in \mathbb{R}_+^{I+J}$ of (1.7) is defined by

$$\begin{cases} \frac{a_{i,\infty}}{\alpha_i} + \frac{b_{j,\infty}}{\beta_j} = M_{i,j} \quad \forall i = 1, 2, \ldots, I, \ \forall j = 1, 2, \ldots, J, \\ \boldsymbol{a}_\infty^{\boldsymbol{\alpha}} = \boldsymbol{b}_\infty^{\boldsymbol{\beta}}. \end{cases}$$

**Theorem 1.1** (Explicit convergence to equilibrium)**.** *Let $\mathbf{M} \in \mathbb{R}_+^{I+J-1}$ be a fixed positive initial mass vector corresponding to $I + J - 1$ linear independent conservation laws (1.8). Denote by $(\boldsymbol{a}_\infty, \boldsymbol{b}_\infty)$ the detailed balanced equilibrium of (1.7).*

*Then, for any nonnegative $(\boldsymbol{a}, \boldsymbol{b}) \in L^1\left(\Omega; [0,\infty)^{I+J}\right)$ satisfying the mass conservation laws (1.8), we have*

$$\mathcal{D}(\boldsymbol{a}, \boldsymbol{b}) \geq \lambda_{\mathbf{M}}(\mathcal{E}(\boldsymbol{a}, \boldsymbol{b}) - \mathcal{E}(\boldsymbol{a}_\infty, \boldsymbol{b}_\infty))$$

*where the constant $\lambda_{\mathbf{M}} > 0$ can be explicitly estimated in terms of the initial mass $\mathbf{M}$, the domain $\Omega$, the positive stoichiometric coefficients $\boldsymbol{\alpha}, \boldsymbol{\beta}$ and the diffusion coefficients $d_{a,i}, 1 \le i \le I$ and $d_{b,j}, 1 \le j \le J$.*

*Consequently, the solution to (1.7) obeys the following exponential convergence to equilibrium*

$$\sum_{i=1}^{I} \|a_i(t) - a_{i,\infty}\|^2_{L^1(\Omega)} + \sum_{j=1}^{J} \|b_j(t) - b_{j,\infty}\|^2_{L^1(\Omega)} \le C_{CKP}^{-1}(\mathcal{E}(\boldsymbol{a}(0), \boldsymbol{b}(0)) - \mathcal{E}(\boldsymbol{a}_\infty, \boldsymbol{b}_\infty))e^{-\lambda_{\mathbf{M}} t}$$

*where $C_{CKP}$ is the constant in a Csiszár-Kullback-Pinsker inequality in Lemma 2.4.*

Secondly, the reaction-diffusion system modelling (1.6) reads as

$$\begin{cases} \partial_t c_1 - \operatorname{div}(d_1(x)\nabla c_1) = -c_1c_2 + c_3, & x \in \Omega, \\ \partial_t c_2 - \operatorname{div}(d_2(x)\nabla c_2) = -c_1c_2 + c_3, & x \in \Omega, \\ \partial_t c_3 - \operatorname{div}(d_3(x)\nabla c_3) = c_1c_2 + c_4c_5 - 2c_3, & x \in \Omega, \\ \partial_t c_4 - \operatorname{div}(d_4(x)\nabla c_4) = -c_4c_5 + c_3, & x \in \Omega, \\ \partial_t c_5 - \operatorname{div}(d_5(x)\nabla c_5) = -c_4c_5 + c_3, & x \in \Omega, \\ \nabla c_i \cdot \nu = 0, \qquad i = 1, 2, \ldots, 5, & x \in \partial\Omega. \end{cases} \tag{1.9}$$

The mass conservation laws of (1.9) are

$$\overline{c_i} + \overline{c_3} + \overline{c_j} = M_{i,j}, \qquad \forall i \in \{1, 2\} \quad \text{and} \quad \forall j \in \{4, 5\} \tag{1.10}$$

and among these there are precisely $m = 3$ linear independent conservation laws, thus $\mathbb{Q} \in \mathbb{R}^{3\times 5}$. In the following, we denote by $\boldsymbol{c} = (c_1, \ldots, c_5)$ the concentration vector and by $(M_{i,j}) = (M_{1,4}, M_{1,5}, M_{2,4}, M_{2,5}) \in \mathbb{R}^4$ the initial mass vector. Note that the initial mass vector $\mathbf{M}$ is fixed once its three linear independent coordinates are fixed, then by a fixed initial mass vector $(M_{i,j}) \in \mathbb{R}^4_+$ we mean that the three linear coordinates are given and the remaining coordinates are subsequently calculated. The detailed balanced equilibrium $\boldsymbol{c}_\infty \in \mathbb{R}^5$ to (1.9) is defined by

$$\begin{cases} c_{i,\infty} + c_{3,\infty} + c_{j,\infty} = M_{i,j}, \qquad \forall i \in \{1,2\} \quad \text{and} \quad \forall j \in \{4,5\}, \\ c_{1,\infty}c_{2,\infty} = c_{3,\infty}, \\ c_{4,\infty}c_{5,\infty} = c_{3,\infty}. \end{cases}$$

**Theorem 1.2** (Explicit convergence to equilibrium)**.** *Let $\mathbf{M} \in \mathbb{R}^3_+$ be a fixed positive initial mass vector corresponding to 3 linear independent conservation laws of (1.9). Denote by $\boldsymbol{c}_\infty$ the detailed balanced equilibrium of (1.9).*

*Then, for any nonnegative measurable function $\boldsymbol{c} = (c_1, \ldots, c_5) \in L^1\left(\Omega; [0, +\infty)^5\right)$ satisfying the mass conservation laws (1.10), we have*

$$\mathcal{D}(\boldsymbol{c}) \ge \lambda_{\mathbf{M}}(\mathcal{E}(\boldsymbol{c}) - \mathcal{E}(\boldsymbol{c}_\infty))$$

*where $\lambda_{\mathbf{M}} > 0$ is a positive constant. which can be explicitly estimated in terms of the initial mass $\mathbf{M}$, the domain $\Omega$ and the diffusion coefficients $d_i, i = 1, 2, \ldots, 5$.*

*As a consequence, the solution $\boldsymbol{c} = (c_1, \ldots, c_5)$ to (1.9) converges exponentially to the equilibrium defined by its initial mass,*

$$\sum_{i=1}^{5} \|c_i(t) - c_{i,\infty}\|^2_{L^1(\Omega)} \le C_{CKP}(\mathcal{E}(\boldsymbol{c}(0)) - \mathcal{E}(\boldsymbol{c}_\infty))e^{-\lambda_{\mathbf{M}} t} \quad \forall t > 0,$$

*where $C_{CKP}$ is the constant in the Csiszár-Kullback-Pinsker inequality.*

The rest of this paper is organized as follows: In Section 2, we give the details of the mathematical settings and the method containing the mentioned four steps. Also in this section, the Steps **1.**, **2.** and **3.** will be proved rigorously and explicitly in the general case. The proofs of Theorems 1.1 and 1.2 are presented in Sections 3 and 4 respectively. Finally, we discuss the further possible applications of our method and some open problems in Section 5.

## 2. Mathematical settings and a general approach

In this section, we first recall the mathematical settings of the reaction network and then we give the details of the proposed method.

2.1. **Mathematical settings.** For convenience to the reader, we will adopt the notations from [MHM14]. Consider $I$ species $\mathcal{A}_1, \ldots, \mathcal{A}_I$ reacting via $R$ reactions according to the mass-action law of the form:

$$\alpha_1^r \mathcal{A}_1 + \ldots + \alpha_I^r \mathcal{A}_I \leftrightharpoons \beta_1^r \mathcal{A}_1 + \ldots + \beta_I^r \mathcal{A}_I \tag{2.1}$$

for $r = 1, 2, \ldots, R$, where $R \in \mathbb{N}$, $\boldsymbol{\alpha}^r = (\alpha_1^r, \ldots, \alpha_I^r) \in (\{0\} \cup [1, +\infty))^I$ and $\boldsymbol{\beta}^r = (\beta_1^r, \ldots, \beta_I^r) \in (\{0\} \cup [1, +\infty))^I$ are the vectors of nonnegative stoichiometric coefficients, and $k_{r,b}, k_{r,f}$ are the the backward and forward reaction rate coefficients.

Denote by $\mathbf{c}(t,x) \in \mathbb{R}^I$ the vector of concentrations, then the reaction-diffusion process is modeled by the semilinear parabolic PDE system

$$\frac{\partial}{\partial t}\mathbf{c} = \mathrm{div}(\mathbb{D}\nabla \mathbf{c}) - \mathbf{R}(\mathbf{c}) \quad \text{in } \Omega \qquad \text{and} \qquad \nabla \mathbf{c} \cdot \nu = 0 \quad \text{in } \partial\Omega, \tag{2.2}$$

subject to nonnegative initial data $\mathbf{c}(x,0) = \mathbf{c}_0(x), x \in \Omega$, where $\Omega \subset \mathbb{R}^N$ is a bounded domain with smooth boundary $\partial\Omega$ which has the outward normal unit vector $\nu$. Note that without loss of generality, we can rescale the spatial variable such that the volume of $\Omega$ is normalised, i.e.

$$|\Omega| = 1.$$

The diffusion matrix is diagonal $\mathbb{D}(x) = \mathrm{diag}(d_i(x))_{i=1,\ldots,I}$ and positive definite. We assume moreover that the diffusion coefficients satisfy

$$d_{i,min} \le d_i(x) \le d_{i,max} \qquad \forall x \in \Omega, \quad \forall i = 1, 2, \ldots, I. \tag{2.3}$$

The reaction vector $\mathbf{R}$, given by the reactions (2.1), is of the mass-action type

$$\mathbf{R}(\mathbf{c}) = \sum_{r=1}^{R} \left(k_{r,f}\mathbf{c}^{\boldsymbol{\alpha}^r} - k_{r,b}\mathbf{c}^{\boldsymbol{\beta}^r}\right)(\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r) \quad \text{with} \quad \mathbf{c}^{\boldsymbol{\alpha}^r} = \prod_{i=1}^{I} c_i^{\alpha_i^r}. \tag{2.4}$$

To determine the mass conservation laws for (2.2), we arrange the stoichiometric coefficients $\boldsymbol{\alpha}^r = (\alpha_1^r, \ldots, \alpha_I^r) \in (\{0\} \cup [1, +\infty))^I$ and $\boldsymbol{\beta}^r = (\beta_1^r, \ldots, \beta_I^r) \in (\{0\} \cup [1, +\infty))^I$ as columns, which gives the stoichiometric matrix

$$W = ((\beta^r - \alpha^r)_{r=1,\ldots,R})^\top \in \mathbb{R}^{R\times I} \tag{2.5}$$

which is also called Wegscheider matrix. Note that according to the mass action law, now we can write $\mathbf{R}(\mathbf{c})$ in the form

$$\mathbf{R}(\mathbf{c}) = -W^\top \mathbf{K}(\mathbf{c}), \qquad \text{where} \quad \mathbf{K}(\mathbf{c}) = [K_r(\mathbf{c}) = k_{r,f}\mathbf{c}^{\boldsymbol{\alpha}^r} - k_{r,b}\mathbf{c}^{\boldsymbol{\beta}^r}]_{r=1,\ldots,R}. \tag{2.6}$$

The range $\mathrm{rg}(W^\top)$ is called the *stoichiometric subspace* and due to (2.6) we have $\mathbf{R}(\mathbf{c}) \in \mathrm{rg}(W^\top)$. We now can determine the mass conservation laws as follows: for $m = \dim\ker(W)$, the codim of $W$, we choose a matrix $\mathbb{Q} \in \mathbb{R}^{m\times I}$ such that $\mathrm{rank}\mathbb{Q} = m$ and $\mathbb{Q}W^\top = 0$, i.e., the rows of $\mathbb{Q}$ form a basis of $\ker(W)$. Since $\mathbf{R}(\mathbf{c}) \in \mathrm{rg}(W^\top)$, we have

$$\mathbb{Q}\,\mathbf{R}\mathbf{c} = 0 \qquad \text{for all } \mathbf{c} \in \mathbb{R}^I. \tag{2.7}$$

By denoting
$$\overline{\mathbf{c}} = (\overline{c_1}, \ldots, \overline{c_I}) \quad \text{ with } \overline{c_i} = \int_\Omega c_i(x)dx \tag{2.8}$$
and using the no-flux boundary condition for $\mathbf{c}$ on $\partial\Omega$, we end up with the conservation laws
$$\frac{d}{dt}\int_\Omega \mathbb{Q}\,\mathbf{c}(t)\,dx = \mathbb{Q}\mathbb{D}\int_{\partial\Omega} \nabla\mathbf{c}\cdot\nu\,\mathrm{d}S - \int_\Omega \mathbb{Q}\mathbf{R}(\mathbf{c})\,dx = 0 \tag{2.9}$$
or equivalently
$$\mathbb{Q}\,\overline{\mathbf{c}}(t) = \mathbb{Q}\,\overline{\mathbf{c}}(0) =: \mathbf{M} \in \mathbb{R}^m \tag{2.10}$$
for all $t > 0$, where we $\mathbf{M}$ denote the initial mass vector.

For physical consideration, we are only allowed to consider nonnegative concentrations as solutions. Thanks to [Pie10], we only have to check that the nonlinear reaction vector $\mathbf{R}(\mathbf{c})$ satisfy a quasi-positivity condition, that is, if $\mathbf{R}(\mathbf{c}) = (R_1(\mathbf{c}), \ldots, R_I(\mathbf{c}))^\top$ then
$$R_i(c_1, \ldots, c_{i-1}, 0, c_{i+1}, \ldots, c_I) \geq 0 \quad \forall i = 1, 2, \ldots I \quad \text{with} \quad c_1, \ldots, c_{i-1}, c_{i+1}, \ldots, c_I \geq 0,$$
which is naturally satisfied by mass action law reactions of the form
$$R_i(\mathbf{c}) = \sum_{r=1}^{R} k_r\left(\mathbf{c}^{\boldsymbol{\alpha}^r} - \mathbf{c}^{\boldsymbol{\beta}^r}\right)(\alpha_i^r - \beta_i^r)$$
for $i = 1, 2, \ldots, I$. Thus, we have

**Lemma 2.1** (Nonnegativity)**.** [Pie10] *If the initial concentration vector $\mathbf{c}_0$ is nonnegative, then the solution vector $\mathbf{c}(t)$ remains nonnegative for all $t > 0$.*

**Definition 2.1** (Equilibrium)**.** *Fix an positive initial mass vector $\mathbf{M} \in \mathbb{R}^m_+$. A state $\mathbf{c}^* \in [0, +\infty)^I$ is called a homogeneous equilibrium (or equilibrium) for (2.2) if*
$$\mathbf{R}(\mathbf{c}^*) = 0 \quad \text{and} \quad \mathbb{Q}\,\mathbf{c}^* = \mathbf{M}.$$

To study the large time behaviour of (2.2), we impose the following crucial assumptions:

(**A1**) System (2.2) satisfies a *detailed balance condition*, that is, there exists an equilibrium $\mathbf{c}_\infty \in (0, +\infty)^I$ such that
$$\forall r = 1, 2, \ldots, R: \qquad k_{r,f}\mathbf{c}_\infty^{\boldsymbol{\alpha}^r} = k_{r,b}\mathbf{c}_\infty^{\boldsymbol{\beta}^r}.$$
This equilibrium $\mathbf{c}_\infty$ is called a *detailed balanced equilibrium.*

(**A2**) There is *no boundary equilibrium*, that is (2.2) does not possess an equilibrium belonging to $\partial[0, +\infty)^I$. Therefore any equilibrium $\mathbf{c}_\infty = (c_{1,\infty}, \ldots, c_{I,\infty})^\top$ to (2.2) satisfies $c_{i,\infty} > 0$ for all $i = 1, 2, \ldots, I$.

**Remark 2.1.**

- *The assumption* (**A1**) *allows to rescale the system such that we can assume $k_{r,f} = k_{r,b} = k_r$ for all $r = 1, 2, \ldots, R$. Thus, the reaction rate constant of each reaction is equal to the reaction rate constant of the reverse reaction. This helps us to see that the free energy functional, or the logarithmic entropy functional (see* (2.11)*) in other words, is a Lyapunov functional, that is it is decreasing along the trajectory of the system* (2.2) *as time is increasing.*
- *The assumption* (**A2**) *is a natural structural assumption in order to prove an entropy-entropy dissipation estimate like state above. In fact, for general systems featuring boundary equilibria, the behaviour near a boundary equilibrium is unclear and can prevent global exponential decay to an asymptotically stable equilibrium as can be seen in example systems. See Remark 2.2 for an example of a system having a boundary equilibrium.*

**Lemma 2.2** (Uniqueness of detailed balanced equilibrium)**.** [GGH96, Lemma 3.4] *If the system* (2.2) *satisfies* (**A1**)*, then* (2.2) *has a unique detailed balanced equilibrium.*

We define the entropy functional

$$\mathcal{E}(\mathbf{c}) = \sum_{i=1}^{I}\int_{\Omega}(c_i\log c_i - c_i + 1)dx, \tag{2.11}$$

which decays monotone in time according to the following entropy dissipation functional

$$\mathcal{D}(\mathbf{c}) = -\frac{d}{dt}\mathcal{E}(\mathbf{c}) = \sum_{i=1}^{I}\int_{\Omega}d_i(x)\frac{|\nabla c_i|^2}{c_i}dx + \sum_{r=1}^{R}k_r\int_{\Omega}(\mathbf{c}^{\boldsymbol{\alpha}^r} - \mathbf{c}^{\boldsymbol{\beta}^r})(\log\mathbf{c}^{\boldsymbol{\alpha}^r} - \log\mathbf{c}^{\boldsymbol{\beta}^r})dx \geq 0. \tag{2.12}$$

**Lemma 2.3** ($L^1$-bounds)**.** *Assume that the initial data $\mathbf{c}_0$ are nonnegative and satisfies $\mathcal{E}(\overline{\mathbf{c}_0}) < +\infty$. Then,*

$$\|c_i(t)\|_{L^1(\Omega)} \leq K := 2(\mathcal{E}(\overline{\mathbf{c}_0}) + I) \qquad \forall t > 0, \quad \forall i = 1, 2, \ldots, I.$$

*Proof.* Integrating (2.12) over $(0,t)$ leads to

$$\sum_{i=1}^{I}\int_{\Omega}(c_i(x,t)\log c_i(x,t) - c_i(x,t) + 1)\,dx \leq \mathcal{E}(\overline{\mathbf{c}_0}) \qquad \forall t > 0.$$

By using the elementary inequalities $x\log x - x + 1 \geq (\sqrt{x}-1)^2 \geq \frac{1}{2}x - 1$ for all $x \geq 0$, we get

$$\frac{1}{2}\sum_{i=1}^{I}\int_{\Omega}c_i(x,t)\,dx \leq \mathcal{E}(\overline{\mathbf{c}_0}) + I.$$

This, combined with the nonnegativity of solutions, completes the proof of the Lemma. $\square$

The following Csiszár-Kullback-Pinsker type inequality shows that the convergence of equilibrium in $L^1(\Omega)$ follows from the convergence of the relative entropy $\mathcal{E}(\mathbf{c}) - \mathcal{E}(\mathbf{c}_\infty)$ to zero. For a generalized Csiszár-Kullback-Pinsker inequality, we refer to the paper [AMTU01]. Here, we give an elementary proof using only the natural bound inheriting from Lemma 2.3.

**Lemma 2.4** (Csiszár-Kullback-Pinsker type inequality)**.** *For all $\mathbf{c} \in L^1(\Omega; [0,+\infty)^I)$ such that $\mathbb{Q}\,\overline{\mathbf{c}} = \mathbb{Q}\,\mathbf{c}_\infty$ and $\overline{c}_i \leq K$ for all $i = 1, 2, \ldots, I$ with some $K > 0$, we have*

$$\mathcal{E}(\mathbf{c}) - \mathcal{E}(\mathbf{c}_\infty) \geq C_{CKP}\sum_{i=1}^{I}\|c_i - c_{i,\infty}\|_{L^1(\Omega)}^2$$

*where the constant $C_{CKP}$ depends only on the domain $\Omega$ and the constant $K$.*

*Proof.* By using the additivity of the relative entropy (see [MHM14, Lemma 2.3]), we have

$$\mathcal{E}(\mathbf{c}) - \mathcal{E}(\mathbf{c}_\infty) = \sum_{i=1}^{I}\int_{\Omega}c_i\log\frac{c_i}{\overline{c}_i}dx + \sum_{i=1}^{I}\left(\overline{c}_i\log\frac{\overline{c}_i}{c_{i,\infty}} - \overline{c}_i + c_{i,\infty}\right). \tag{2.13}$$

Using the classical Csiszár-Kullback-Pinsker inequality, we have

$$\int_{\Omega}c_i\log\frac{c_i}{\overline{c}_i}dx \geq C_0\|c_i - \overline{c}_i\|_{L^1(\Omega)}^2 \tag{2.14}$$

for all $i = 1, 2, \ldots, I$, where the constant $C_0$ depends only on the domain $\Omega$. On the other hand, by applying the elementary inequality $x\log(x/y) - x + y \geq (\sqrt{x} - \sqrt{y})^2$ we obtain

$$\begin{aligned}
\mathcal{E}(\overline{\mathbf{c}}) - \mathcal{E}(\mathbf{c}_\infty) &= \sum_{i=1}^{I}\left(\overline{c}_i \log\frac{\overline{c}_i}{c_{i,\infty}} - \overline{c}_i + c_{i,\infty}\right)\\
&\geq \sum_{i=1}^{I}\left(\sqrt{\overline{c}_i} - \sqrt{c_{i,\infty}}\right)^2 = \sum_{i=1}^{I}\frac{(\overline{c}_i - c_{i,\infty})^2}{\left(\sqrt{\overline{c}_i} + \sqrt{c_{i,\infty}}\right)^2}\\
&\geq \frac{1}{4K}\sum_{i=1}^{I}(\overline{c}_i - c_{i,\infty})^2.
\end{aligned} \tag{2.15}$$

By combining (2.13)–(2.15), we obtain

$$\begin{aligned}
\mathcal{E}(\mathbf{c}) - \mathcal{E}(\mathbf{c}_\infty) &\geq C_0\sum_{i=1}^{I}\|c_i - \overline{c}_i\|^2_{L^1(\Omega)} + \frac{1}{4K}\sum_{i=1}^{I}(\overline{c}_i - c_{i,\infty})^2\\
&\geq \min\{C_0; 1/4K\}\sum_{i=1}^{I}\left(\|c_i - \overline{c}_i\|^2_{L^1(\Omega)} + \|\overline{c}_i - c_{i,\infty}\|^2_{L^1(\Omega)}\right)\\
&\geq \frac{1}{2}\min\{C_0; 1/4K\}\sum_{i=1}^{I}\|c_i - c_{i,\infty}\|^2_{L^1(\Omega)},
\end{aligned}$$

which is the desired inequality with $C_{CKP} = \frac{1}{2}\min\left\{C_0; \frac{1}{4K}\right\}$. □

The following entropy-entropy dissipation estimate is established in [MHM14].

**Theorem 2.5.** [MHM14] *Assume that* (2.2) *satisfies the assumption* (**A1**) *and* (**A2**)*. For a given fixed positive initial mass vector* $\mathbf{M} \in \mathbb{R}^m_+$*, there exists a positive constant* $\lambda_{\mathbf{M}} > 0$ *such that*

$$\mathcal{D}(\mathbf{c}) \geq \lambda_{\mathbf{M}}(\mathcal{E}(\mathbf{c}) - \mathcal{E}(\mathbf{c}_\infty))$$

*for all* $\mathbf{c} \in L^1(\Omega; [0, +\infty)^I)$ *satisfying* $\mathbb{Q}\,\overline{\mathbf{c}} = \mathbf{M}$*, where* $\mathbf{c}_\infty$ *is the detailed balanced equilibrium of* (2.2) *corresponding to* $\mathbf{M}$.

We emphasise that, though this Theorem gives the existence of $\lambda_{\mathbf{M}} > 0$, it seems difficult to extract an explicit estimate of $\lambda_{\mathbf{M}}$ except in some special cases, e.g. a quadratic system arising from the reaction $2X \leftrightharpoons Y$. The main reason is that the method used in [MHM14] to prove this result is crucially based on a convexification argument, which appears very hard (if not impossible) to make explicit for general systems.

In this paper, we propose a constructive way to prove the EED estimate based on the structure of the conservation laws. The method applies elementary estimates and has the advantage of a better computability of the rates and constants of convergence to equilibrium. Before detailing our approach, let us remark about the assumption (**A2**) on the absence of boundary equilibria.

**Remark 2.2** (Boundary equilibrium)**.** *The validity of Theorem 2.5 may fail if the system* (2.2) *has a boundary equilibrium. For example, for the single reversible reaction* $2\mathcal{A} \leftrightharpoons \mathcal{A} + \mathcal{B}$ *with normalised reaction rate constants* $k_f = k_b = 1$*, we consider the following system*

$$\begin{cases}
a_t - \operatorname{div}(\delta_a(x)\nabla a) = -a^2 + ab, & x \in \Omega, \quad t > 0,\\
b_t - \operatorname{div}(\delta_b(x)\nabla b) = a^2 - ab, & x \in \Omega, \quad t > 0,\\
\partial_\nu a = \partial_\nu b = 0, & x \in \partial\Omega, \quad t > 0,\\
a(x, 0) = a_0(x),\ b(x, 0) = b_0(x), & x \in \Omega.
\end{cases} \tag{2.16}$$

*This system has one mass conservation law*

$$\int_\Omega (a(x,t)+b(x,t))dx = \int_\Omega (a_0(x)+b_0(x))dx =: \mathbf{M} > 0 \qquad \forall t>0.$$

*It is easy to see that the system possesses a positive detailed balance equilibrium* $(a_\infty^1, b_\infty^1) = \left(\frac{\mathbf{M}}{2}, \frac{\mathbf{M}}{2}\right)$ *and a boundary equilibrium* $(a_\infty^2, b_\infty^2) = (0,\mathbf{M})$*. Moreover, we have the entropy functional*

$$\mathcal{E}(a,b) = \int_\Omega (a\log a - a + 1)dx + \int_\Omega (b\log b - b + 1)dx$$

*and the entropy dissipation functional*

$$\mathcal{D}(a,b) = \int_\Omega \delta_a(x)\frac{|\nabla a|^2}{a}dx + \int_\Omega \delta_b(x)\frac{|\nabla b|^2}{b}dx + \int_\Omega a(a-b)(\log a - \log b)dx.$$

*By defining* $Z = \{(a,b)\in\mathbb{R}_+^2 : a+b = \mathbf{M}\}$*, we can compute*

$$\lim_{Z\ni(a,b)\to(a_\infty^2,b_\infty^2)} D(a,b) = 0$$

*and*

$$\lim_{Z\ni(a,b)\to(a_\infty^2,b_\infty^2)} (\mathcal{E}(a,b) - \mathcal{E}(a_\infty^1,b_\infty^1)) = \mathbf{M}\log 2 > 0.$$

*Then,* ***there does not exist a global constant*** $\lambda_{\mathbf{M}} > 0$ *such that*

$$\mathcal{D}(a,b) \geq \lambda_{\mathbf{M}}(\mathcal{E}(a,b) - \mathcal{E}(a_\infty^1,b_\infty^1))$$

*for all functions* $a,b:\Omega\to\mathbb{R}_+$ *satisfying* $\int_\Omega (a(x)+b(x))dx = \mathbf{M}$.

*So, in general, if (2.2) has a boundary equilibrium then we cannot expect global exponential convergence to equilibrium but only local convergence, that is, if a trajectory starts from a neighbourhood of the positive equilibrium, then it converges exponentially to equilibrium as time goes to infinity. Interestingly, it is conjectured in the case of ODE reaction systems that even if the system possesses boundary equilibria, a trajectory starting from a positive initial state will always converge to the unique positive equilibrium as time goes to infinity. The reader is referred to [CDSS09] for a discussion of more general systems.*

2.2. **A constructive method to prove the EED estimate.** Though the Theorem 2.5 provides the existence of $\lambda_{\mathbf{M}} > 0$ satisfying the entropy-entropy dissipation estimate, it does not seem to give an explicit estimates for $\lambda_{\mathbf{M}}$ when the reaction network has more than two substances, for example,

$$\alpha\mathcal{A} + \beta\mathcal{B} \leftrightharpoons \gamma\mathcal{C} \quad \text{ or } \quad \mathcal{A}_1 + \mathcal{A}_2 \leftrightharpoons \mathcal{A}_3 + \mathcal{A}_4.$$

Inspired by the works [DF08, DF14, FLT14, FL], we propose a general approach to prove an entropy-entropy dissipation estimate using only the mass conservation laws and which allows explicit estimates of the rates and constants of convergence to equilibrium for a given general reaction-diffusion system of the form (1.1).

By recalling the crucial EED estimate

$$\mathcal{D}(\mathbf{c}) \geq \lambda_{\mathbf{M}}(\mathcal{E}(\mathbf{c}) - \mathcal{E}(\mathbf{c}_\infty)), \tag{2.17}$$

we observe that the right hand side is zero if and only if $\mathbf{c}\equiv\mathbf{c}_\infty$, while the left hand side is zero for all constant states $\mathbf{c}^*\in(0,+\infty)^I$ satisfying $(\mathbf{c}^*)^{\boldsymbol{\alpha}^r} = (\mathbf{c}^*)^{\boldsymbol{\beta}^r}$ $\forall r = 1,2,\ldots,R$ and such a $\mathbf{c}^*$ identifies with $\mathbf{c}_\infty$ if and only if $\mathbb{Q}\,\mathbf{c}^* = \mathbf{M}$. Hence, it the EED estimate (2.17) has crucially to take into account all the conservations laws.

The following notations and elementary inequalities are useful in our proof:

*$L^2(\Omega)$-norm*:

For the rest of this paper, we will denote by $\|\cdot\|$ the usual norm of $L^2(\Omega)$,

$$\|f\|^2 = \int_\Omega |f(x)|^2\,dx.$$

*Spatial averages and square-root abbreviation*:

For a function $f:\Omega\to\mathbb{R}$, the spatial average is denoted by (recall the domain normalisation $|\Omega|=1$)

$$\overline{f} = \int_\Omega f(x)\,dx.$$

Moreover, for a quantity denoted by small letters, we introduce the short hand notation of the same uppercase letter as it's square root, e.g.

$$C_i = \sqrt{c_i}, \quad \text{and} \quad C_{i,\infty} = \sqrt{c_{i,\infty}}.$$

*Additivity of Entropy*: see e.g. [DF08, DF14],[MHM14, Lemma 2.3]

$$\begin{aligned}\mathcal{E}(\mathbf{c}) - \mathcal{E}(\mathbf{c}_\infty) &= (\mathcal{E}(\mathbf{c}) - \mathcal{E}(\overline{\mathbf{c}})) + (\mathcal{E}(\overline{\mathbf{c}}) - \mathcal{E}(\mathbf{c}_\infty))\\ &= \sum_{i=1}^I \int_\Omega c_i \log\frac{c_i}{\overline{c}_i}dx + \sum_{i=1}^I \left(\overline{c}_i \log\frac{\overline{c}_i}{c_{i,\infty}} - \overline{c}_i + c_{i,\infty}\right).\end{aligned} \tag{2.18}$$

*An elementary inequality*:

$$(a-b)(\log a - \log b) \geq 4\left(\sqrt{a}-\sqrt{b}\right)^2.$$

*An elementary function*:

Consider $\Phi:[0,+\infty)\to[0,+\infty)$ defined as (and continuously extended at $z=0,1$)

$$\Phi(z) = \frac{z\log z - z + 1}{(\sqrt{z}-1)^2}.$$

Then, $\Phi$ is increasing and $\lim_{z\to 0}\Phi(z) = 1$ and $\lim_{z\to 1}\Phi(z) = 2$.

**Remark 2.3** (Explicit constants)**.** *We remark that though the approach proposed here allows to explicitly estimate the rate of convergence, the issue of optimal convergence rate goes beyond the method. Therefore, in several places, we will introduce some explicit constants $K_i$ in the sense that $K_i$ can be estimated explicitly, but sometimes we don't give unnecessary long expression of $K_i$ to improve the readability.*

The method of proving the EED estimate (2.17) contains four steps designed as a chain of estimates, which allows to enter the conservation laws in a final step. Among the four steps, **Step 1.**, **Step 2.** and **Step 3.** can be proved for general systems since their proofs do not rely on the structure of the conservation laws. In **Step 4.**, which crucially uses the mass conservation laws defined in (2.10) an explicit constructive proof can be done for a given system (see the examples in Section 3 and Section 4) but for a general system it is unclear how to prove **Step 4.** since the choice of the matrix $\mathbb{Q}$ is not unique n the general case.

Nevertheless, we will see in Section 3 and Section 4 that once the conservation laws are explicitly known, we can finish the proof of **Step 4.** and thus complete the proof of (2.17).

**Step 1 (Use of the Logarithmic Sobelev Inequality):**

The idea of this step is to divide the relative entropy $\mathcal{E}(\mathbf{c}) - \mathcal{E}(\mathbf{c}_\infty)$ into two parts, where the first part is controlled by the diffusion using the Logarithmic Sobolev Inequality and the second part contains only spatial average of concentrations, which have the advantage of obeying the conservation laws as well as having the natural bounds in Lemma 2.3.

We use the additivity of entropy (2.18)

$$\begin{aligned}\mathcal{E}(\mathbf{c}) - \mathcal{E}(\mathbf{c}_\infty) &= (\mathcal{E}(\mathbf{c}) - \mathcal{E}(\overline{\mathbf{c}})) + (\mathcal{E}(\overline{\mathbf{c}}) - \mathcal{E}(\mathbf{c}_\infty)) \\ &= \sum_{i=1}^{I}\int_\Omega c_i \log\frac{c_i}{\overline{c_i}}dx + \sum_{i=1}^{I}\left(\overline{c_i}\log\frac{\overline{c_i}}{c_{i,\infty}} - \overline{c_i} + c_{i,\infty}\right)\end{aligned} \tag{2.19}$$

To control the first integrals, we use the Logarithmic Sobolev Inequality

$$\int_\Omega d_i(x)\frac{|\nabla c_i|^2}{c_i}dx \geq C_{LSI}(d_i)\int_\Omega c_i\log\frac{c_i}{\overline{c_i}}dx$$

and estimate

$$\frac{1}{2}\mathcal{D}(\mathbf{c}) \geq \frac{1}{2}\min\{C_{LSI}(d_1), \ldots, C_{LSI}(d_I)\}(\mathcal{E}(\mathbf{c}) - \mathcal{E}(\overline{\mathbf{c}})).$$

Thus, it remains to prove that

$$\frac{1}{2}\mathcal{D}(\mathbf{c}) \geq K_1(\mathcal{E}(\overline{\mathbf{c}}) - \mathcal{E}(\mathbf{c}_\infty)) \tag{2.20}$$

for an explicit constant $K_1$.

**Step 2 (Transformation into quadratic terms):**

To prove (2.20), we first estimate $\mathcal{D}(\mathbf{c})$ below and $\mathcal{E}(\overline{\mathbf{c}}) - \mathcal{E}(\mathbf{c}_\infty)$ above in terms of $L^2$-distance of the square roots $C_i$ of the concentrations $c_i$. The associated quadratic forms are significantly easier to handle than the logarithmic terms. For $\mathcal{D}(\mathbf{c})$ we estimate

$$\begin{aligned}\mathcal{D}(\mathbf{c}) &= \sum_{i=1}^{I}\int_\Omega d_i\frac{|\nabla c_i|^2}{c_i}dx + \sum_{r=1}^{R}k_r\int_\Omega(\mathbf{c}^{\boldsymbol{\alpha}^r} - \mathbf{c}^{\boldsymbol{\beta}^r})(\log\mathbf{c}^{\boldsymbol{\alpha}^r} - \log\mathbf{c}^{\boldsymbol{\beta}^r})dx \\ &\geq \sum_{i=1}^{I}4d_{i,min}\|\nabla C_i\|^2 + 4\sum_{r=1}^{R}k_r\left\|\mathbf{C}^{\boldsymbol{\alpha}^r} - \mathbf{C}^{\boldsymbol{\beta}^r}\right\|^2\end{aligned} \tag{2.21}$$

by recalling $C_i = \sqrt{c_i}$, $d_i(x) \geq d_{i,min}$, $\mathbf{C} = (C_1, C_2, \ldots, C_I)^\top$ and the elementary inequality $(a-b)(\log a - \log b) \geq 4(\sqrt{a} - \sqrt{b})^2$.

For the second terms on the right hand side of (2.19), we use the function

$$\Phi(z) = \frac{z\log z - z + 1}{(\sqrt{z}-1)^2}$$

which is non-decreasing to estimate

$$\begin{aligned}\mathcal{E}(\overline{\mathbf{c}}) - \mathcal{E}(\mathbf{c}_\infty) &= \sum_{i=1}^{I}\left(\overline{c_i}\log\frac{\overline{c_i}}{c_{i,\infty}} - \overline{c_i} + c_{i,\infty}\right) = \sum_{i=1}^{I}\Phi\left(\frac{\overline{c_i}}{c_{i,\infty}}\right)\left(\sqrt{\overline{c_i}} - \sqrt{c_{i,\infty}}\right)^2 \\ &\leq K_2\sum_{i=1}^{I}\left(\sqrt{\overline{C_i^2}} - C_{i,\infty}\right)^2\end{aligned} \tag{2.22}$$

with

$$K_2 = \max_{i=1,\ldots,I}\left\{\Phi\left(\frac{K}{c_{i,\infty}}\right)\right\}, \tag{2.23}$$

where we used Lemma 2.3 that all $\overline{c_i} \leq K := 2(\mathcal{E}(\overline{\mathbf{c}_0}) + I) > 0$ for all $i = 1, \ldots, I$. From (2.21) and (2.22), we now want to find an explicit constant $K_1 > 0$ such that

$$2\sum_{i=1}^{I}d_{i,min}\|\nabla C_i\|^2 + 2\sum_{r=1}^{R}k_r\left\|\mathbf{C}^{\boldsymbol{\alpha}^r} - \mathbf{C}^{\boldsymbol{\beta}^r}\right\|^2 \geq K_1K_2\sum_{i=1}^{I}\left(\sqrt{\overline{C_i^2}} - C_{i,\infty}\right)^2. \tag{2.24}$$

**Step 3 (Reaction dissipation term and reaction dissipation term of averages):**
The left hand side of (2.24) represents the coupling between diffusion and reaction of the system. In order to be able to use the constrains provided by the conservation laws, we shall bound it below by a reaction term of spatially averaged concentrations. More precisely, by denoting $\overline{\mathbf{C}} = (\overline{C_1}, \ldots, \overline{C_I})^\top$, we have

**Lemma 2.6** (Reaction terms of averages)**.** *There exists an explicit constant $K_3 > 0$ such that*

$$2\sum_{i=1}^{I} d_{i,min}\|\nabla C_i\|^2 + 2\sum_{r=1}^{R} k_r\|\mathbf{C}^{\boldsymbol{\alpha}^r} - \mathbf{C}^{\boldsymbol{\beta}^r}\|^2 \geq K_3\Big(\sum_{i=1}^{I}\|\nabla C_i\|^2 + \sum_{r=1}^{R}\left(\overline{\mathbf{C}}^{\boldsymbol{\alpha}^r} - \overline{\mathbf{C}}^{\boldsymbol{\beta}^r}\right)^2\Big). \tag{2.25}$$

We postpone a proof of this Lemma to the end of this section in order to continue presenting the main ideas of our strategy. It's worth noticing that comparing to [DF08], in which the nonlinearity has a quadratic form and allowed to exploit certain $L^2$-orthogonality structures, Lemma 2.6 is more complicated due to the arbitrary order of the nonlinearity. In the proof of Lemma 2.6 at the end of this section, we introduce new ideas, which are motivated by [FL] and consist of a domain decomposition to overcome the difficulties caused by the nonlinearity. This idea is also applicable to volume-surface reaction-diffusion systems, see [FLT14]. Now, combining (2.24) and (2.25), our goal now is to find an explicit $K_1 > 0$ satisfying

$$\sum_{i=1}^{I}\|\nabla C_i\|^2 + \sum_{r=1}^{R}\left(\overline{\mathbf{C}}^{\boldsymbol{\alpha}^r} - \overline{\mathbf{C}}^{\boldsymbol{\beta}^r}\right)^2 \geq \frac{K_1K_2}{K_3}\sum_{i=1}^{I}\left(\sqrt{\overline{C_i^2}} - C_{i,\infty}\right)^2 \tag{2.26}$$

with $K_2$ is defined in (2.23) and $K_3$ is in (2.25).

**Step 4 (Express averages in terms of the equilibrium):**
Before continuing, we remark that while the previous three steps can be proved in the general case without details of the structure of the conservation laws, this step is rather a *proof of concept* how to proceed to complete the proof of the EED estimate for a specific model, whose conservation laws are explicit given (see Lemmas 3.1 and 4.1 for example of two specific models).

To prove (2.26), we use the ansatz

$$\overline{C_i^2} = C_{i,\infty}^2(1+\mu_i)^2 \quad \text{for all} \quad i = 1, \ldots, I \tag{2.27}$$

or equivalently

$$\overline{\mathbf{C}^2} = \mathbf{C}_\infty^2(\mathbf{1}+\boldsymbol{\mu})^2$$

with $\mathbf{1} = (1, 1, \ldots, 1)^\top \in \mathbb{R}^I$ and $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_I)^\top$. By recalling that $\mathbf{C}^2 = \mathbf{c}$ and $\mathbf{C}_\infty^2 = \mathbf{c}_\infty$, and $\mathbb{Q}\,\overline{\mathbf{c}} = \mathbb{Q}\,\mathbf{c}_\infty = \mathbf{M}$, we have the following algebraic constrains between $\mu_1, \ldots, \mu_I$,

$$\mathbb{Q}\,\mathbf{C}_\infty^2(\mathbf{1}+\boldsymbol{\mu})^2 = \mathbb{Q}\,\mathbf{C}_\infty^2$$

or equivalently

$$\mathbb{Q}\,\mathbf{C}_\infty^2(\boldsymbol{\mu}^2 + 2\boldsymbol{\mu}) = 0. \tag{2.28}$$

By denoting $\delta_i(x) = C_i(x) - \overline{C}_i$ for $x \in \Omega, i = 1, \ldots, I$ and by using (2.27), it follows from $\|\delta_i\|^2 = \overline{C_i^2} - \overline{C_i}^2$ that

$$\overline{C_i} = \sqrt{\overline{C_i^2}} - \frac{\|\delta_i\|^2}{\sqrt{\overline{C_i^2}} + \overline{C_i}} = C_{i,\infty}(1+\mu_i) - \|\delta_i\|^2 R(C_i) \tag{2.29}$$

where we denote $R(C_i) = \left(\sqrt{\overline{C_i^2}} + \overline{C_i}\right)^{-1}$, for all $i = 1, \ldots, I$. We observe that $R(C_i)$ becomes unbounded when $\overline{C_i^2}$ approaches zero. This possibility prevents the use of the ansatz (2.29) in cases where $\overline{C_i^2}$ is small. Therefore, we have to distinguish two cases where $\overline{C_i^2}$ is either "big", say $\overline{C_i^2} \geq \varepsilon^2$, or "small", says $\overline{C_i^2} \leq \varepsilon^2$. We remark that a good value for the constant $\varepsilon > 0$ can be explicitly computed in specific models (See (3.37) in Section 3 or (4.18) in Section 4).

(i) $\overline{C_i^2} \geq \varepsilon^2$ for all $i = 1, \ldots, I$.
In this case, we have

$$R(C_i) = \frac{1}{\sqrt{\overline{C_i^2}} + \overline{C_i}} \leq \frac{1}{\varepsilon} \qquad \forall i = 1, 2, \ldots, I.$$

Thus, we can estimate the left hand side of (2.26) as follows, for all $\theta \in (0, 1)$,

$$\begin{aligned}
&\sum_{i=1}^{I} \|\nabla C_i\|^2 + \sum_{r=1}^{R} \left(\overline{\mathbf{C}}^{\boldsymbol{\alpha}^r} - \overline{\mathbf{C}}^{\boldsymbol{\beta}^r}\right)^2 \\
&\qquad \geq C_P \sum_{i=1}^{I} \|\delta_i\|^2 + \theta \sum_{r=1}^{R} \left[\prod_{i=1}^{I} \left(C_{i,\infty}(1+\mu_i) - \|\delta_i\|^2 R(C_i)\right)^{\alpha_i^r}\right. \\
&\qquad\qquad \left. - \prod_{i=1}^{I} \left(C_{i,\infty}(1+\mu_i) - \|\delta_i\|^2 R(C_i)\right)^{\beta_i^r}\right]^2 \\
&\qquad \geq C_P \sum_{i=1}^{I} \|\delta_i\|^2 + \theta \sum_{r=1}^{R} \left[\mathbf{C}_\infty^{\boldsymbol{\alpha}^r} (\mathbf{1} + \boldsymbol{\mu})^{\boldsymbol{\alpha}^r} - \mathbf{C}_\infty^{\boldsymbol{\beta}^r} (\mathbf{1} + \boldsymbol{\mu})^{\boldsymbol{\beta}^r}\right]^2 \\
&\qquad\quad - \theta\, C(\varepsilon, K) \sum_{i=1}^{I} \|\delta_i\|^2 \\
&\qquad \geq \theta \sum_{r=1}^{R} \left[\mathbf{C}_\infty^{\boldsymbol{\alpha}^r} (\mathbf{1} + \boldsymbol{\mu})^{\boldsymbol{\alpha}^r} - \mathbf{C}_\infty^{\boldsymbol{\beta}^r} (\mathbf{1} + \boldsymbol{\mu})^{\boldsymbol{\beta}^r}\right]^2
\end{aligned} \tag{2.30}$$

if we choose $\theta \in (0, 1)$ such that $\theta C(\varepsilon, K) \leq C_P$ where $C(\varepsilon, K)$ is a constant explicitly depends on $\varepsilon$ and $K$. On the other hand, with the ansatz (2.27), the right hand side of (2.26) becomes

$$\frac{K_1 K_2}{K_3} \sum_{i=1}^{I} \left(\sqrt{\overline{C_i^2}} - C_{i,\infty}\right)^2 = \frac{K_1 K_2}{K_3} \sum_{i=1}^{I} C_{i,\infty}^2 \mu_i^2. \tag{2.31}$$

By using (2.30) and (2.31), we obtain the desired inequality (2.26) provided the following finite dimensional inequality holds

$$\theta \sum_{r=1}^{R} \left[\mathbf{C}_\infty^{\boldsymbol{\alpha}^r} (\mathbf{1} + \boldsymbol{\mu})^{\boldsymbol{\alpha}^r} - \mathbf{C}_\infty^{\boldsymbol{\beta}^r} (\mathbf{1} + \boldsymbol{\mu})^{\boldsymbol{\beta}^r}\right]^2 \geq \frac{K_1 K_2}{K_3} \sum_{i=1}^{I} C_{i,\infty}^2 \mu_i^2 \tag{2.32}$$

under the constrains posed by the conservation laws $\mathbb{Q}\,\mathbf{C}_\infty^2(\boldsymbol{\mu}^2 + 2\boldsymbol{\mu}) = 0$.
To prove (2.32), we seem to need explicit forms of the mass conservation laws represented by $\mathbb{Q}$, which should be known in a specific model but is unclear in the general case. We will give a proof of (2.32) in Lemma 3.3 for a single reversible reaction and in Lemma 4.3 for a chain of reversible reactions in which the conservation laws are explicitly known.

(ii) $\overline{C_{i_0}^2} \leq \varepsilon^2$ for some $i_0 \in \{1, \ldots, I\}$.

In this case, we first bound the right hand side of (2.26) above by using the boundedness of averaged concentrations $\overline{c_i} \le K$ for all $i = 1, \ldots, I$ in Lemma 2.3,

$$\frac{K_1K_2}{K_3}\sum_{i=1}^{I}\left(\sqrt{\overline{C_i^2}} - C_{i,\infty}\right)^2 \le \frac{2K_1K_2}{K_3}\sum_{i=1}^{I}\left(\overline{C_i^2} + C_{i,\infty}^2\right) \le \frac{4KK_1K_2}{K_3}. \tag{2.33}$$

To bound the left hand side of (2.26), we consider two subcases due to different roles of the diffusion.

- (When the diffusion is dominant.) If $\|\delta_{i^*}\|^2 \ge C(\varepsilon, i_0)$ for some $i^* \in \{1, \ldots, I\}$, where $C(\varepsilon, i_0)$ is an explicit constant in terms of $\varepsilon$ and $i_0$ (see (2.36)). Then, the left hand side of (2.26) is bounded below by

$$\sum_{i=1}^{I}\|\nabla C_i\|^2 + \sum_{r=1}^{R}\left(\overline{\mathbf{C}}^{\boldsymbol{\alpha}^r} - \overline{\mathbf{C}}^{\boldsymbol{\beta}^r}\right)^2 \ge C_P\|\delta_{i^*}\|^2 \ge C_PC(\varepsilon, i_0). \tag{2.34}$$

Then, (2.26) follows from (2.33) and (2.34) by choosing $K_1 > 0$ such that

$$K_1 \le \frac{K_3C_PC(\varepsilon, i_0)}{4KK_2}.$$

- (When the diffusion is inefficient)
If $\|\delta_i\|^2 \le C(\varepsilon, i_0)$ for all $i = 1, \ldots, I$. Therefore, we can estimate

$$\overline{C_i}^2 = \overline{C_i^2} - \|\delta_i\|^2 \ge \overline{C_i^2} - C(\varepsilon, i_0) \qquad \forall i = 1, 2, \ldots, I. \tag{2.35}$$

Recall that we have also $\overline{C_{i_0}^2} \le \varepsilon^2$. At this point, by using the mass conservation laws $\mathbb{Q}\,\overline{\mathbf{C}^2} = \mathbf{M} > 0$, we should be able to show that, there exists $1 \le j^* \le I$ such that

$$\overline{C_{j^*}^2} \ge C^*(\varepsilon, i_0, \mathbf{M})$$

for an explicit constant $C^*(\varepsilon, i_0, \mathbf{M})$. Now, by choosing

$$C(\varepsilon, i_0) \le \frac{C^*(\varepsilon, i_0)}{2}, \tag{2.36}$$

we obtain from (2.35) that

$$\overline{C_{j^*}}^2 \ge \frac{C^*(\varepsilon, i_0)}{2}.$$

Combining this and the fact that the system (2.2) does not have boundary equilibria, this leads to the following bound

$$\begin{aligned}\sum_{i=1}^{I}\|\nabla C_i\|^2 + \sum_{i=1}^{I}\left(\overline{\mathbf{C}}^{\boldsymbol{\alpha}^r} - \overline{\mathbf{C}}^{\boldsymbol{\beta}^r}\right)^2 &\ge \sum_{i=1}^{I}\left(\overline{\mathbf{C}}^{\boldsymbol{\alpha}^r} - \overline{\mathbf{C}}^{\boldsymbol{\beta}^r}\right)^2\\ &\ge K^*(\varepsilon, i_0)\end{aligned}$$

where $K^*(\varepsilon, i_0)$ is an explicit constant. This inequality, together with (2.33), implies (2.26) if we choose

$$K_1 \le \frac{K_3K^*(\varepsilon, i_0)}{4KK_2}.$$

For the rest of this section, we give a proof of Lemma 2.6 in Step **3**.

*Proof of Lemma 2.6.* We first prove that

$$\sum_{i=1}^I d_{i,min}\|\nabla C_i\|^2 + 2\sum_{r=1}^R k_r \left\|\mathbf{C}^{\boldsymbol{\alpha}^r} - \mathbf{C}^{\boldsymbol{\beta}^r}\right\|^2 \geq \kappa \sum_{r=1}^R \left(\overline{\mathbf{C}}^{\boldsymbol{\alpha}^r} - \overline{\mathbf{C}}^{\boldsymbol{\beta}^r}\right)^2 \tag{2.37}$$

for an explicit constant $\kappa > 0$. Then, (2.25) follows by choosing

$$K_3 = \min\left\{\min_{i=1,\ldots,I}\{d_{i,min}\};\, \kappa\right\}.$$

The proof of (2.37) introduces pointwise deviations of the concentrations around their spatial averages, which are as follows: for all $i = 1, 2, \ldots, I$, we define

$$\delta_i(x) = C_i(x) - \overline{C}_i, \qquad \text{for } x \in \Omega. \tag{2.38}$$

Thanks to the non-negativity of $C_i$ and Lemma 2.3, we have that $\delta_i \in [-\sqrt{K}; +\infty)$. Fixing a constant $L > \sqrt{K} > 0$, we can decompose $\Omega$ as

$$\Omega = S \cup S^\perp, \tag{2.39}$$

where

$$S = \{x \in \Omega : |\delta_i(x)| \leq L, \quad \forall i = 1, 2, \ldots, I\}. \tag{2.40}$$

We will prove (2.37) on both $S$ and $S^\perp$. On $S$ we have, for all $\gamma \in (0, 2)$,

$$\begin{aligned}\gamma\sum_{r=1}^R k_r \left\|\mathbf{C}^{\boldsymbol{\alpha}^r} - \mathbf{C}^{\boldsymbol{\beta}^r}\right\|^2_{L^2(S)} &= \gamma\sum_{r=1}^R k_r \left\|\prod_{i=1}^I \left(\overline{C}_i + \delta_i\right)^{\alpha_i^r} - \prod_{i=1}^I \left(\overline{C}_i + \delta_i\right)^{\beta_i^r}\right\|^2_{L^2(S)} \\ &\geq \gamma \min_{r=1,\ldots,R}\{k_r\}\sum_{r=1}^R \left\|\overline{\mathbf{C}}^{\boldsymbol{\alpha}^r} - \overline{\mathbf{C}}^{\boldsymbol{\beta}^r}\right\|^2_{L^2(S)} - \gamma\, C(L)\sum_{i=1}^I \|\delta_i\|^2_{L^2(S)},\end{aligned} \tag{2.41}$$

where $C(L)$ is a constant which *does not* depend on $S$. On the other hand, by using the Poincaré inequality,

$$\|\nabla f\|^2 \geq C_P\|f - \overline{f}\|^2 \geq C_P\|f - \overline{f}\|^2_{L^2(S)}, \tag{2.42}$$

we have

$$\sum_{i=1}^I d_{i,min}\|\nabla C_i\|^2 \geq C_P \min_{i=1,\ldots,I}\{d_{i,min}\}\sum_{i=1}^I \|\delta_i\|^2 \geq C_P \min_{i=1,\ldots,I}\{d_{i,min}\}\sum_{i=1}^I \|\delta_i\|^2_{L^2(S)}. \tag{2.43}$$

From (2.41) and (2.43), if we choose $\gamma \in (0, 2)$ such that $4\gamma C(L) \leq C_P \min_{i=1,\ldots,I}\{d_{i,min}\}$, then we have

$$\sum_{i=1}^I d_{i,min}\|\nabla C_i\|^2 + 2\sum_{r=1}^R k_r \left\|\mathbf{C}^{\boldsymbol{\alpha}^r} - \mathbf{C}^{\boldsymbol{\beta}^r}\right\|^2_{L^2(S)} \geq \gamma \min_{r=1,\ldots,R}\{k_r\}\sum_{r=1}^R \left\|\overline{\mathbf{C}}^{\boldsymbol{\alpha}^r} - \overline{\mathbf{C}}^{\boldsymbol{\beta}^r}\right\|^2_{L^2(S)}. \tag{2.44}$$

To estimate (2.37) in $S^\perp$, we note that

$$S^\perp = \{x \in \Omega : \quad \delta_i(x) > L \;\text{ for some }\; i = 1, 2\ldots, I\}. \tag{2.45}$$

Hence,

$$\begin{aligned}|S^\perp| &= \sum_{i=1}^I |\{x \in \Omega : \delta_i(x) > L\}| = \sum_{i=1}^I \left|\{x \in \Omega : \delta_i^2(x) > L^2\}\right| \\ &\leq \frac{1}{L^2}\sum_{i=1}^I \|\delta_i\|^2 \leq \frac{1}{L^2 C_P \min_{i=1,\ldots,I}\{d_{i,min}\}}\sum_{i=1}^I d_{i,min}\|\nabla C_i\|^2.\end{aligned} \tag{2.46}$$

By making use of the following a priori bounds $\overline{C_i} \leq \sqrt{\overline{C_i^2}} \leq \sqrt{K}$ from Lemma 2.3, we can estimate the right hand side of (2.37) in $S^\perp$ as follows

$$\begin{aligned}\sum_{r=1}^{R}\left\|\overline{\mathbf{C}}^{\boldsymbol{\alpha}^r} - \overline{\mathbf{C}}^{\boldsymbol{\beta}^r}\right\|^2_{L^2(S^\perp)} &\leq C(\sqrt{K})\,|S^\perp|\\ &\leq \frac{C(\sqrt{K})}{L^2 C_P \min\limits_{i=1,\ldots,I}\{d_{i,min}\}}\sum_{i=1}^{I} d_{i,min}\|\nabla C_i\|^2 \qquad (\text{use } (2.46)) \\ &\leq \frac{1}{4}\sum_{i=1}^{I} d_{i,min}\|\nabla C_i\|^2,\end{aligned} \tag{2.47}$$

if we choose $L$ to be big enough, e.g. $L^2 \geq \frac{4C(\sqrt{K})}{C_P \min\limits_{i=1,\ldots,I}\{d_{i,min}\}}$. By combining (2.44) and (2.47) we obtain (2.37) with $\kappa = \frac{1}{2}\min\{1, \gamma \min\limits_{r=1,\ldots,R}\{k_r\}\}$. □

## 3. A single reversible reaction - Proof of Theorem 1.1

In this section, we will follow the strategy in Subsection 2.2 to show the explicit convergence to equilibrium for a single reversible reaction of the form

$$\alpha_1\mathcal{A}_1 + \alpha_2\mathcal{A}_2 + \ldots + \alpha_I\mathcal{A}_I \leftrightharpoons \beta_1\mathcal{B}_1 + \beta_2\mathcal{B}_2 + \ldots + \beta_J\mathcal{B}_J$$

for any $I, J \geq 1$. The stoichiometric coefficients $\alpha_i, \beta_j \geq 1$ for $i = 1, \ldots, I$ and $j = 1, \ldots, J$. For the sake of convenience, the forward and backward reaction rate constants are assumed to be one $k_f = k_b = 1$.

As mentioned before, this problem was left as an open problem in [MHM14] whenever $I + J \geq 3$. The reaction is assumed to take place in reaction vessel, i.e. in a bounded domain $\Omega \subset \mathbb{R}^n, n \geq 1$ with sufficiently smooth boundary $\partial\Omega$ (e.g. $\partial\Omega \in C^{2+\epsilon}$ for some $\epsilon > 0$). The mass action reaction-diffusion system reads as

$$\begin{cases}\partial_t a_i - \operatorname{div}(d_{a,i}(x)\nabla a_i) = -\alpha_i\left(\boldsymbol{a}^{\boldsymbol{\alpha}} - \boldsymbol{b}^{\boldsymbol{\beta}}\right), & t > 0,\ x \in \Omega,\ i = 1,\ldots,I,\\ \partial_t b_j - \operatorname{div}(d_{b,j}(x)\nabla b_j) = \beta_j\left(\boldsymbol{a}^{\boldsymbol{\alpha}} - \boldsymbol{b}^{\boldsymbol{\beta}}\right), & t > 0,\ x \in \Omega,\ j = 1,\ldots,J,\\ \partial_\nu a_i = \partial_\nu b_j = 0, \qquad t > 0,\ x \in \partial\Omega, & i = 1,\ldots,I,\ j = 1,\ldots,J,\\ a_i(x,0) = a_{i,0}(x),\ b_j(x,0) = b_{j,0}(x), & x \in \Omega,\ i = 1,\ldots,I,\ j = 1,\ldots,J,\end{cases} \tag{3.1}$$

where $d_{a,i}(x), d_{b,j}(x)$ are diffusion coefficients satisfying

$$d_{min} \leq d_{a,i}(x),\, d_{b,j}(x) \leq d_{max} \qquad \forall x \in \Omega,\ i = 1,\ldots,I,\ j = 1,\ldots,J, \tag{3.2}$$

$\boldsymbol{a} = (a_1, a_2, \ldots, a_I)$, $\boldsymbol{b} = (b_1, b_2, \ldots, b_J)$ are vector concentrations, $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_I) \in [1, +\infty)^I$ and $\boldsymbol{\beta} = (\beta_1, \beta_2, \ldots, \beta_J) \in [1, +\infty)^J$ are vectors of stoichiometric coefficients and we recall the notation

$$\boldsymbol{a}^{\boldsymbol{\alpha}} = \prod_{i=1}^{I} a_i^{\alpha_i} \quad \text{and} \quad \boldsymbol{b}^{\boldsymbol{\beta}} = \prod_{j=1}^{J} b_j^{\beta_j}.$$

The aim of this section is to follow the strategy proposed in Section 2 to show the explicit convergence to equilibrium for the system (3.1). To do that, we first derive the mass conservation laws for (3.1), which are essential in our strategy. Then, (3.1) is shown to satisfy the assumptions (**A1**) and (**A2**), that is (3.1) satisfies the detailed balance condition and has no boundary equilibrium. Theorem 1.1 shows the main result of this section.

**Lemma 3.1** (Mass conservation laws)**.** *The system* (3.1) *obeys* $I + J - 1$ *linear independent mass conservation laws.*

*Then, with respect to the general formulation, we have the matrix* $\mathbb{Q}$ *is defined as*

$$\mathbb{Q} = [v_1, \ldots, v_J, w_2, \ldots, w_I]^\top \in \mathbb{R}^{(I+J-1)\times(I+J)}$$

*where* $v_j$ *and* $w_i$ *are defined in* (3.6) *and* (3.7) *below.*

*Proof.* Recall the equations for $a_i$,

$$\partial_t a_i - \operatorname{div}(d_{a,i}(x)\nabla a_i) = -\alpha_i \left(\boldsymbol{a}^{\boldsymbol{\alpha}} - \boldsymbol{b}^{\boldsymbol{\beta}}\right) \tag{3.3}$$

and for $b_j$,

$$\partial_t b_j - \operatorname{div}(d_{b,j}(x)\nabla b_j) = \beta_j \left(\boldsymbol{a}^{\boldsymbol{\alpha}} - \boldsymbol{b}^{\boldsymbol{\beta}}\right). \tag{3.4}$$

Then, by dividing (3.3) by $\alpha_i$ and (3.4) by $\beta_j$, summation and integration over $\Omega$ yields, thanks to the homogeneous Neumann boundary condition,

$$\frac{d}{dt}\int_\Omega \left(\frac{a_i(x,t)}{\alpha_i} + \frac{b_j(x,t)}{\beta_j}\right) dx = 0 \qquad \forall t > 0.$$

Hence, after introducing the nonnegative partial masses $M_{i,j} := \int_\Omega \left(\frac{a_{i,0}(x)}{\alpha_i} + \frac{b_{j,0}(x)}{\beta_j}\right) dx$, we observe that system (3.1) obeys the following $IJ$ mass conservation laws

$$\frac{\overline{a_i}(t)}{\alpha_i} + \frac{\overline{b_j}(t)}{\beta_j} = M_{i,j} \qquad \forall t > 0, \forall i = 1, \ldots, I, \forall j = 1, \ldots, J, \tag{3.5}$$

where we recall the notation for spatial average, e.g. $\overline{a_i} = \int_\Omega a_i(x)dx$. Fix $I + J - 1$ laws

$$\frac{\overline{a_1}}{\alpha_1} + \frac{\overline{b_j}}{\beta_j} = M_{1,j}, \qquad j = 1, 2, \ldots, I,$$

and

$$\frac{\overline{a_i}}{\alpha_i} + \frac{\overline{b_1}}{\beta_1} = M_{i,1}, \qquad i = 2, 3, \ldots, J.$$

We first show that other laws can be implied from these $I + J - 1$ laws due to

$$\frac{\overline{a_i}}{\alpha_i} + \frac{\overline{b_j}}{\beta_j} = \left(M_{i,1} - \frac{\overline{b_1}}{\beta_1}\right) + \left(M_{1,j} - \frac{\overline{a_1}}{\alpha_1}\right) = M_{i,1} + M_{1,j} - M_{1,1},$$

and then prove that these $I + J - 1$ laws are linear independent. Indeed, it is equivalent to prove that the set of vector $(v_1, \ldots, v_J, w_2, \ldots, w_I)$ is linear independent in $\mathbb{R}^{I+J-1}$ where

$$v_j = \Bigg(\underbrace{\frac{1}{\alpha_1}, 0, \ldots, 0, \frac{1}{\beta_j}}_{I+j}, 0, \ldots, 0\Bigg), \qquad 1 \le j \le J, \tag{3.6}$$

and

$$w_i = \Bigg(\underbrace{\underbrace{0, \ldots, 0, \frac{1}{\alpha_i}}_{i}, 0, \ldots, 0, \frac{1}{\beta_1}}_{I+1}, 0, \ldots, 0\Bigg), \qquad 2 \le i \le I. \tag{3.7}$$

This fact follows from direct computations so we omit it here. $\square$

**Remark 3.1.** *It follows from the Lemma 3.1 that the initial mass vector* $\mathbf{M}$ *is fixed once its* $I + J - 1$ *coordinates* $M_{1,j}$ *with* $1 \le j \le J$ *and* $M_{i,1}$ *with* $2 \le i \le I$ *are fixed. Therefore, from now on, by a fixed initial mass vector* $\mathbf{M}$ *we mean that those coordinates are fixed.*

**Remark 3.2.** *Similar to Lemma 3.1, we can also divide the equation for $a_i$ by $\alpha_i$ and the equation for $a_k$ by $\alpha_k$ for $1 \leq i \neq k \leq I$ and obtain*

$$\frac{d}{dt}\int_{\Omega}\left(\frac{a_i(t,x)}{\alpha_i} - \frac{a_k(t,x)}{\alpha_k}\right)dx = 0 \qquad \forall t \geq 0, \quad 1 \leq i \neq k \leq I, \tag{3.8}$$

*which leads to the following mass conservation laws*

$$\int_{\Omega}\left(\frac{a_i(t,x)}{\alpha_i} - \frac{a_k(t,x)}{\alpha_k}\right)dx = N_{i,k}, \qquad \forall t \geq 0, \quad 1 \leq i \neq k \leq I, \tag{3.9}$$

*with*

$$N_{i,k} := \int_{\Omega}\left(\frac{a_{i,0}(x)}{\alpha_i} - \frac{a_{k,0}(x)}{\alpha_k}\right)dx.$$

*It's also useful to observe that*

$$N_{i,k} = M_{i,j} - M_{k,j}, \qquad \forall 1 \leq j \leq J. \tag{3.10}$$

**Lemma 3.2** (Unique constant positive equilibrium)**.**
*For any fixed positive initial mass vector $\mathbf{M}$, the system (3.1) possesses a unique equilibrium $(\boldsymbol{a}_\infty, \boldsymbol{b}_\infty) \in (0,+\infty)^{I+J}$ solving*

$$\begin{cases} \dfrac{a_{i,\infty}}{\alpha_i} + \dfrac{b_{j,\infty}}{\beta_j} = M_{i,j}, \qquad i = 1,\ldots,I,\ j = 1,\ldots,J,\\ \boldsymbol{a}_\infty^{\boldsymbol{\alpha}} = \boldsymbol{b}_\infty^{\boldsymbol{\beta}}. \end{cases} \tag{3.11}$$

*Consequently, system (3.1) satisfies the assumption (**A1**) and (**A2**).*

*Proof.* From (3.11) and (3.10) we have

$$\frac{a_{i,\infty}}{\alpha_i} - \frac{a_{1,\infty}}{\alpha_1} = M_{i,k} - M_{1,k} = N_{i,1} \tag{3.12}$$

and thus

$$\prod_{i=1}^{I} a_{i,\infty}^{\alpha_i} = a_{1,\infty}^{\alpha_1}\prod_{i=2}^{I}\left(\alpha_i N_{i,1} + \frac{\alpha_i}{\alpha_1}a_{1,\infty}\right)^{\alpha_i}, \tag{3.13}$$

which is a strictly monotone increasing function in $a_{1,\infty}$. From (3.11), we deduce similarly that $b_{j,\infty} = \beta_j M_{1,j} - \frac{\beta_j}{\alpha_1}a_{1,\infty} \geq 0$ and thus

$$\prod_{j=1}^{J} b_{j,\infty}^{\beta_j} = \prod_{j=1}^{J}\left(\beta_j M_{1,j} - \frac{\beta_j}{\alpha_1}a_{1,\infty}\right)^{\beta_j}, \tag{3.14}$$

which is a strictly monotone decreasing function in $a_{1,\infty}$. Thus, when setting equal (3.13) and (3.14), there exists a unique positive solution $a_{1,\infty}$ and consequently a unique positive equilibrium $(\boldsymbol{a}_\infty, \boldsymbol{b}_\infty)$.

It's obvious that the assumption (**A1**) holds. To prove that (**A2**) holds we assume that $a_{i_0,\infty} = 0$ for some $1 \leq i_0 \leq I$. Then, on the one hand $\boldsymbol{a}_\infty^{\boldsymbol{\alpha}} = 0$. On the other hand, from (3.11), $b_{j,\infty} = M_{i_0,j} > 0$ for $j = 1,2,\ldots,J$, thus

$$\boldsymbol{b}_\infty^{\boldsymbol{\beta}} = \prod_{j=1}^{J} M_{i_0,j}^{\beta_j} > 0.$$

This contradicts to $\boldsymbol{a}_\infty^{\boldsymbol{\alpha}} = \boldsymbol{b}_\infty^{\boldsymbol{\beta}}$. Thus $a_{i,\infty} > 0$ for all $i = 1,2,\ldots,I$. Similarly, $b_{j,\infty} > 0$ for all $j = 1,2,\ldots,J$. Therefore, the system (3.1) has no boundary equilibrium. $\square$

The entropy functional for system (3.1) writes as

$$\mathcal{E}(\boldsymbol{a},\boldsymbol{b}) = \sum_{i=1}^{I}\int_{\Omega}(a_i\log a_i - a_i + 1)dx + \sum_{j=1}^{J}\int_{\Omega}(b_j\log b_j - b_j + 1)dx$$

and the entropy dissipation writes as

$$\mathcal{D}(\boldsymbol{a},\boldsymbol{b}) = \sum_{i=1}^{I}\int_{\Omega}d_{a,i}(x)\frac{|\nabla a_i|^2}{a_i}dx + \sum_{j=1}^{J}\int_{\Omega}d_{b,j}(x)\frac{|\nabla b_j|^2}{b_j}dx + \int_{\Omega}(\boldsymbol{a}^{\boldsymbol{\alpha}} - \boldsymbol{b}^{\boldsymbol{\beta}})\log\frac{\boldsymbol{a}^{\boldsymbol{\alpha}}}{\boldsymbol{b}^{\boldsymbol{\beta}}}dx.$$

*Proof of Theorem 1.1.* We follow the strategy in Section 2 to prove this Theorem. Notice that now the mass conservation laws are explicitly known (Lemma 3.1), we can we can proceed the points that were postponed in **Step 4.** of the strategy. For convenience of the reader, we recall the main steps.

- **Step 1 (Use of the Logarithmic Sobelev Inequality).** Thanks to the additivity of the entropy, we have

$$\begin{aligned}\mathcal{E}(\boldsymbol{a},\boldsymbol{b}) - \mathcal{E}(\boldsymbol{a}_\infty,\boldsymbol{b}_\infty) &= (\mathcal{E}(\boldsymbol{a},\boldsymbol{b}) - \mathcal{E}(\overline{\boldsymbol{a}},\overline{\boldsymbol{b}})) + (\mathcal{E}(\overline{\boldsymbol{a}},\overline{\boldsymbol{b}}) - \mathcal{E}(\boldsymbol{a}_\infty,\boldsymbol{b}_\infty))\\ &= \sum_{i=1}^{I}\int_{\Omega}a_i\log\frac{a_i}{\overline{a_i}}dx + \sum_{j=1}^{J}\int_{\Omega}b_j\log\frac{b_j}{\overline{b_j}}dx\\ &\quad + \sum_{i=1}^{I}\left(\overline{a_i}\log\frac{\overline{a_i}}{a_{i,\infty}} - \overline{a_i} + a_{i,\infty}\right) + \sum_{j=1}^{J}\left(\overline{b_j}\log\frac{\overline{b_j}}{b_{j,\infty}} - \overline{b_j} + b_{j,\infty}\right).\end{aligned}$$

By using the Logarithmic Sobolev Inequality, we get

$$\frac{1}{2}\mathcal{D}(\boldsymbol{a},\boldsymbol{b}) \geq \frac{1}{2}\min_{i,j}\{C_{LSI}(d_{a,i}), C_{LSI}(d_{b,j})\}(\mathcal{E}(\boldsymbol{a},\boldsymbol{b}) - \mathcal{E}(\overline{\boldsymbol{a}},\overline{\boldsymbol{b}})). \tag{3.15}$$

Now, it is left to find $K_1 > 0$ such that

$$\frac{1}{2}\mathcal{D}(\boldsymbol{a},\boldsymbol{b}) \geq K_1(\mathcal{E}(\overline{\boldsymbol{a}},\overline{\boldsymbol{b}}) - \mathcal{E}(\boldsymbol{a}_\infty,\boldsymbol{b}_\infty)). \tag{3.16}$$

- **Step 2 (Transform terms into quadratic terms).** By using $\nabla\sqrt{f} = \nabla f/2\sqrt{f}$ and $(a-b)(\log a - \log b) \geq 4(\sqrt{a}-\sqrt{b})^2$, we can estimate

$$\frac{1}{2}\mathcal{D}(\boldsymbol{a},\boldsymbol{b}) \geq 2d_{min}\left(\sum_{i=1}^{I}\|\nabla A_i\|^2 + \sum_{j=1}^{J}\|\nabla B_j\|^2\right) + 2\|\boldsymbol{A}^{\boldsymbol{\alpha}} - \boldsymbol{B}^{\boldsymbol{\beta}}\|^2,$$

where we recall $A_i = \sqrt{a_i}, B_j = \sqrt{b_j}$, $\boldsymbol{A} = (A_1,\ldots,A_I)$ and $\boldsymbol{B} = (B_1,\ldots,B_J)$. On the other hand, by using the increasing function

$$\Phi(z) = \frac{z\log z - z + 1}{(\sqrt{z}-1)^2},$$

we can estimate

$$\begin{aligned}\mathcal{E}(\overline{\boldsymbol{a}},\overline{\boldsymbol{b}}) - \mathcal{E}(\boldsymbol{a}_\infty,\boldsymbol{b}_\infty) &= \sum_{i=1}^{I}\Phi\left(\frac{\overline{a_i}}{a_{i,\infty}}\right)\left(\sqrt{\overline{a_i}} - \sqrt{a_{i,\infty}}\right)^2 + \sum_{j=1}^{J}\Phi\left(\frac{\overline{b_j}}{b_{j,\infty}}\right)\left(\sqrt{\overline{b_j}} - \sqrt{b_{j,\infty}}\right)^2\\ &\leq K_2\left(\sum_{i=1}^{I}\left(\sqrt{\overline{A_i^2}} - A_{i,\infty}\right)^2 + \sum_{j=1}^{J}\left(\sqrt{\overline{B_j^2}} - B_{j,\infty}\right)^2\right)\end{aligned}$$

where we have used $\overline{a_i}, \overline{b_j} \leq K$ thanks to Lemma 2.3 and the constant $K_3$ is defined by

$$K_2 = \max_{i,j}\left\{\Phi\left(\frac{K}{a_{i,\infty}}\right), \Phi\left(\frac{K}{b_{j,\infty}}\right)\right\}.$$

Thus, to prove (3.16) is equivalent to prove for a suitable $K_1$,

$$2d_{min}\left(\sum_{i=1}^{I}\|\nabla A_i\|^2 + \sum_{j=1}^{J}\|\nabla B_j\|^2\right) + 2\|\boldsymbol{A}^{\boldsymbol{\alpha}} - \boldsymbol{B}^{\boldsymbol{\beta}}\|^2$$
$$\geq K_1K_2\left(\sum_{i=1}^{I}\left(\sqrt{\overline{A_i^2}} - A_{i,\infty}\right)^2 + \sum_{j=1}^{J}\left(\sqrt{\overline{B_j^2}} - B_{j,\infty}\right)^2\right) \quad (3.17)$$

- **Step 3 (Reaction dissipation term and reaction dissipation term of averages).** It follows from Lemma 2.6 that

$$2d_{min}\left(\sum_{i=1}^{I}\|\nabla A_i\|^2 + \sum_{j=1}^{J}\|\nabla B_j\|^2\right) + 2\|\boldsymbol{A}^{\boldsymbol{\alpha}} - \boldsymbol{B}^{\boldsymbol{\beta}}\|^2$$
$$\geq K_3\left(\sum_{i=1}^{I}\|\nabla A_i\|^2 + \sum_{j=1}^{J}\|\nabla B_j\|^2 + \left(\overline{\boldsymbol{A}}^{\boldsymbol{\alpha}} - \overline{\boldsymbol{B}}^{\boldsymbol{\beta}}\right)^2\right). \quad (3.18)$$

for an explicit $K_3 > 0$. Then (3.17) follows from (3.18) provided

$$\sum_{i=1}^{I}\|\nabla A_i\|^2 + \sum_{j=1}^{J}\|\nabla B_j\|^2 + \left(\overline{\boldsymbol{A}}^{\boldsymbol{\alpha}} - \overline{\boldsymbol{B}}^{\boldsymbol{\beta}}\right)^2$$
$$\geq \frac{K_1K_2}{K_3}\left(\sum_{i=1}^{I}\left(\sqrt{\overline{A_i^2}} - A_{i,\infty}\right)^2 + \sum_{j=1}^{J}\left(\sqrt{\overline{B_j^2}} - B_{j,\infty}\right)^2\right) \quad (3.19)$$

for a suitable $K_1 > 0$.

- **Step 4 (Express averages in terms of the equilibrium).** We introduce the ansatzs

$$\overline{A_i^2} = A_{i,\infty}^2(1+\mu_i)^2 \quad \text{and} \quad \overline{B_j^2} = B_{j,\infty}^2(1+\xi_j)^2 \quad (3.20)$$

with $\mu_i, \xi_j \in [-1, +\infty)$ for $i = 1, \ldots, I$ and $j = 1, \ldots, J$. With these ansatz, (3.19) becomes

$$\sum_{i=1}^{I}\|\nabla A_i\|^2 + \sum_{j=1}^{J}\|\nabla B_j\|^2 + \left(\overline{\boldsymbol{A}}^{\boldsymbol{\alpha}} - \overline{\boldsymbol{B}}^{\boldsymbol{\beta}}\right)^2 \geq \frac{K_1K_2}{K_3}\left(\sum_{i=1}^{I}A_{i,\infty}^2\mu_i^2 + \sum_{j=1}^{J}B_{j,\infty}^2\xi_j^2\right). \quad (3.21)$$

By using the deviations

$$\delta_i(x) = A_i(x) - \overline{A_i} \quad \forall x \in \Omega, \qquad \text{and} \qquad \eta_j(x) = B_j(x) - \overline{B_j} \quad \forall x \in \Omega,$$

we have

$$\|\delta_i\|^2 = \overline{A_i^2} - \overline{A_i}^2 = \left(\sqrt{\overline{A_i^2}} - \overline{A_i}\right)\left(\sqrt{\overline{A_i^2}} + \overline{A_i}\right) \quad (3.22)$$

thus

$$\overline{A_i} = \sqrt{\overline{A_i^2}} - \frac{\|\delta_i\|^2}{\sqrt{\overline{A_i^2}} + \overline{A_i}} = A_{i,\infty}(1+\mu_i) - Q(A_i)\|\delta_i\|^2 \quad (3.23)$$

with

$$Q(A_i) = \frac{1}{\sqrt{\overline{A_i^2}} + \overline{A_i}}. \quad (3.24)$$

Similarly, we have

$$\overline{B_j} = B_{j,\infty}(1+\xi_j) - Q(B_j)\|\eta_j\|^2. \tag{3.25}$$

From (3.24) we see that $Q(A_i)$ (respectively $Q(B_j)$) becomes unbounded when $\overline{A_i^2}$ (respectively $\overline{B_j^2}$) approaches 0. It makes the ansatz (3.23) and (3.25) not useful in the case $\overline{A_i^2}$ and $\overline{B_j^2}$ are small. Therefore, in the following, we consider two cases: $\overline{A_i^2}$ and $\overline{B_j^2}$ are either "big" or "small".

(i) $\overline{A_i^2} \geq \varepsilon^2$ and $\overline{B_j^2} \geq \varepsilon^2$ for all $i = 1,\ldots,I,\ j = 1,\ldots,J$.
*We remark that $\varepsilon$ can be computed explicitly (see (3.37)).*
In this case we have $Q(A_i)$ and $Q(B_j)$ a bounded as

$$Q(A_i) = \frac{1}{\sqrt{\overline{A_i^2}} + \overline{A_i}} \leq \frac{1}{\sqrt{\overline{A_i^2}}} \leq \frac{1}{\varepsilon}, \quad \text{and similarly} \quad Q(B_j) \leq \frac{1}{\varepsilon},$$

for all $i = 1,2,\ldots,I$ and $j = 1,2,\ldots,J$. We note also that

$$\|\delta_i\|^2 = \overline{A_i^2} - \overline{A_i}^2 \leq \overline{A_i^2} = \overline{a_i} \leq K \quad \text{and} \quad \|\eta_j\|^2 = \overline{B_j^2} - \overline{B_j}^2 \leq K.$$

Hence, by using (3.23) and (3.25), we obtain

$$\begin{aligned}
\left(\overline{\boldsymbol{A}}^{\boldsymbol{\alpha}} - \overline{\boldsymbol{B}}^{\boldsymbol{\beta}}\right)^2 &= \left(\prod_{i=1}^I \overline{A_i}^{\alpha_i} - \prod_{j=1}^J \overline{B_j}^{\beta_j}\right)^2 \\
&= \Bigg(\prod_{i=1}^I \left(A_{i,\infty}(1+\mu_i) + Q(A_i)\|\delta_i\|^2\right)^{\alpha_i} \\
&\qquad - \prod_{j=1}^J \left(B_{j,\infty}(1+\xi_j) + Q(B_j)\|\eta_j\|^2\right)^{\beta_j}\Bigg)^2 \\
&\geq \left(\prod_{i=1}^I A_{i,\infty}^{\alpha_i}(1+\mu_i)^{\alpha_i} - \prod_{j=1}^J B_{j,\infty}^{\beta_j}(1+\xi_j)^{\beta_j}\right)^2 \\
&\quad - C(\varepsilon,K)\left(\sum_{i=1}^I \|\delta_i\|^2 + \sum_{j=1}^J \|\eta_j\|^2\right) \\
&= \left(\boldsymbol{A}_\infty^{\boldsymbol{\alpha}}\left(\boldsymbol{1}+\boldsymbol{\mu}\right)^{\boldsymbol{\alpha}} - \boldsymbol{B}_\infty^{\boldsymbol{\beta}}\left(\boldsymbol{1}+\boldsymbol{\xi}\right)^{\boldsymbol{\beta}}\right)^2 - C(\varepsilon,K)\left(\sum_{i=1}^I \|\delta_i\|^2 + \sum_{j=1}^J \|\eta_j\|^2\right).
\end{aligned} \tag{3.26}$$

Therefore, by choosing $\theta \leq C_P C(\varepsilon,K)^{-1}$ with $C_P$ is the Poincaré inequality, we can estimate

$$\begin{aligned}
&\sum_{i=1}^I \|\nabla A_i\|^2 + \sum_{j=1}^J \|\nabla B_j\|^2 + \left(\overline{\boldsymbol{A}}^{\boldsymbol{\alpha}} - \overline{\boldsymbol{B}}^{\boldsymbol{\beta}}\right)^2 \\
&\qquad \geq \sum_{i=1}^I \|\nabla A_i\|^2 + \sum_{j=1}^M \|\nabla B_j\|^2 - \theta C(\varepsilon,K)\left(\sum_{i=1}^I \|\delta_i\|^2 + \sum_{j=1}^J \|\eta_j\|^2\right) \\
&\qquad\qquad + \theta\left(\boldsymbol{A}_\infty^{\boldsymbol{\alpha}}\left(\boldsymbol{1}+\boldsymbol{\mu}\right)^{\boldsymbol{\alpha}} - \boldsymbol{B}_\infty^{\boldsymbol{\beta}}\left(\boldsymbol{1}+\boldsymbol{\xi}\right)^{\boldsymbol{\beta}}\right)^2 \\
&\qquad \geq \theta\left(\boldsymbol{A}_\infty^{\boldsymbol{\alpha}}\left(\boldsymbol{1}+\boldsymbol{\mu}\right)^{\boldsymbol{\alpha}} - \boldsymbol{B}_\infty^{\boldsymbol{\beta}}\left(\boldsymbol{1}+\boldsymbol{\xi}\right)^{\boldsymbol{\beta}}\right)^2.
\end{aligned} \tag{3.27}$$

Therefore, (3.21) follows from (3.27) provided the following

$$\left(\boldsymbol{A}_{\infty}^{\boldsymbol{\alpha}}\left(\mathbf{1}+\boldsymbol{\mu}\right)^{\boldsymbol{\alpha}}-\boldsymbol{B}_{\infty}^{\boldsymbol{\beta}}\left(\mathbf{1}+\boldsymbol{\xi}\right)^{\boldsymbol{\beta}}\right)^2 \geq \frac{K_1K_2}{\theta K_3}\left(\sum_{i=1}^{I}A_{i,\infty}^2\mu_i^2+\sum_{j=1}^{J}B_{j,\infty}^2\xi_j^2\right). \tag{3.28}$$

for a suitable $K_1 > 0$. This inequality is a consequence of Lemma 3.3 with

$$K_1 \leq \frac{\zeta\theta K_3}{K_2} \tag{3.29}$$

where $\zeta$ is defined as (3.54).

(ii) $\overline{A_i^2} \leq \varepsilon^2$ or $\overline{B_j^2} \leq \varepsilon^2$ for some $i = 1,\ldots,I$, $j = 1,\ldots,J$.
Without loss of generality, we can assume that $\overline{A_{i_0}^2} \leq \varepsilon^2$ for some $1 \leq i_0 \leq I$. In this case, we observe that the right hand side of (3.19) is bounded above. Indeed,

$$\frac{K_1K_3}{K_2}\left(\sum_{i=1}^{I}\left(\sqrt{\overline{A_i^2}}-A_{i,\infty}\right)^2+\sum_{j=1}^{J}\left(\sqrt{\overline{B_j^2}}-B_{j,\infty}\right)^2\right) \leq 4(I+J)K\frac{K_1K_2}{K_3} \tag{3.30}$$

thanks to the natural bounds of $\overline{a_i} \leq K$ and $\overline{b_j} \leq K$ in Lemma 2.3. This gives us a hint to prove (3.19) by showing that the left hand side of (3.19) is bounded below by a positive constant. Therefore, we will consider two subcases due to the contribution of the diffusion represented by the values of $\|\delta_i\|^2$ and $\|\eta_j\|^2$.

- (When the diffusion is dominant.)
  If $\|\delta_{i^*}\|^2 \geq \frac{\varepsilon^2}{\alpha_{i_0}}$ for some $1 \leq i^* \leq I$ or $\|\eta_{j^*}\|^2 \geq \frac{\varepsilon^2}{\alpha_{i_0}}$ for some $1 \leq j^* \leq J$. In this case, thanks to the Poincare inequality $\|\nabla f\|^2 \geq C_P\|f-\overline{f}\|^2$, the left hand side of (3.19) obviously bounded below

$$\sum_{i=1}^{I}\|\nabla A_i\|^2+\sum_{j=1}^{J}\|\nabla B_j\|^2+\left(\overline{\boldsymbol{A}}^{\boldsymbol{\alpha}}-\overline{\boldsymbol{B}}^{\boldsymbol{\beta}}\right)^2 \geq C_P\left(\|\delta_{i^*}\|^2+\|\eta_{j^*}\|^2\right) \geq \frac{C_P\varepsilon^2}{\alpha_{i_0}}. \tag{3.31}$$

  By combining (3.31) and (3.30), we obtain (3.19) whenever

$$K_1 \leq \frac{C_P\varepsilon^2K_3}{4\alpha_{i_0}(I+J)KK_2}. \tag{3.32}$$

- (When the diffusion is inefficient.)
  If $\|\delta_i\|^2 \leq \frac{\varepsilon^2}{\alpha_{i_0}}$ for all $i = 1,\ldots,I$ and $\|\eta_j\|^2 \leq \frac{\varepsilon^2}{\alpha_{i_0}}$ for all $j = 1,\ldots,J$. By using the mass conservation (3.5),

$$\frac{\overline{A_{i_0}^2}}{\alpha_{i_0}}+\frac{\overline{B_j^2}}{\beta_j} = M_{i_0,j}, \tag{3.33}$$

  we have

$$\overline{B_j^2} = \beta_j\left(M_{i_0,j}-\frac{\overline{A_{i_0}^2}}{\alpha_{i_0}}\right) \geq \beta_j\left(M_{i_0,j}-\frac{\varepsilon^2}{\alpha_{i_0}}\right), \tag{3.34}$$

  for all $j = 1,\ldots,J$. Hence, for all $j = 1,\ldots,J$,

$$\overline{B_j}^2 = \overline{B_j^2}-\|\eta_j\|^2 \geq \beta_jM_{i_0,j}-\frac{\beta_j+1}{\alpha_{i_0}}\varepsilon^2. \tag{3.35}$$

Now, we can estimate the left hand side of (3.19) as follows:

$$
\begin{aligned}
\sum_{i=1}^{I}\|\nabla A_i\|^2 &+ \sum_{j=1}^{J}\|\nabla B_j\|^2 + \left(\overline{\boldsymbol{A}^{\boldsymbol{\alpha}}} - \overline{\boldsymbol{B}^{\boldsymbol{\beta}}}\right)^2\\
&\geq \left(\prod_{i=1}^{I}\overline{A_i}^{\alpha_i} - \prod_{j=1}^{J}\overline{B_j}^{\beta_j}\right)^2\\
&\geq \prod_{j=1}^{J}\overline{B_j}^{2\beta_j} - \frac{1}{2}\prod_{i=1}^{I}\overline{A_i}^{2\alpha_i}\\
&\geq \prod_{j=1}^{J}\left[\beta_j M_{i_0,j} - \frac{\beta_j+1}{\alpha_{i_0}}\varepsilon^2\right]^{\beta_j} - \frac{1}{2}\varepsilon^2\prod_{i=1,i\neq i_0}^{I}\overline{A_i^2}^{\alpha_i}\\
&\geq \prod_{j=1}^{J}\left[\beta_j M_{i_0,j} - \frac{\beta_j+1}{\alpha_{i_0}}\varepsilon^2\right]^{\beta_j} - \frac{1}{2}\varepsilon^2\prod_{i=1,i\neq i_0}^{I}M_{i,1}^{\alpha_i}\\
&\geq \frac{1}{2}\prod_{j=1}^{J}\left[\frac{\beta_j M_{i_0,j}}{2}\right]^{\beta_j}
\end{aligned}
\tag{3.36}
$$

if $\varepsilon$ fulfills

$$
\varepsilon^2 \leq \min\left\{\min_{1\leq j\leq J}\left\{\frac{\alpha_{i_0}\beta_j M_{i_0,j}}{2(\beta_j+1)}\right\};\left(\prod_{i=1,i\neq i_0}^{I}M_{i,1}^{\alpha_i}\right)^{-1}\prod_{j=1}^{J}(\beta_j M_{i_0,j})^{\beta_j}\right\}. \tag{3.37}
$$

Therefore, (3.19) follows from (3.30) and (3.36) provided

$$
K_1 \leq \frac{K_3}{8KK_2(I+J)}\prod_{j=1}^{J}\left[\frac{\beta_j M_{i_0,j}}{2}\right]^{\beta_j}. \tag{3.38}
$$

Now, by combining (3.29), (3.32) and (3.38), we can conclude **Step 4.** that we have proved (3.19) with either

$$
K_1 = \frac{\zeta\theta K_3}{K_2}
$$

if $\overline{A_i^2} \geq \varepsilon^2$ and $\overline{B_j^2} \geq \varepsilon^2 \quad \forall i = 1,\ldots,I,\ \forall j = 1,\ldots,J$, or

$$
K_1 = \min\left\{\frac{C_P\varepsilon^2 K_3}{4\alpha_{i_0}(I+J)KK_2}; \frac{K_3}{8KK_2(I+J)}\prod_{j=1}^{J}\left[\frac{\beta_j M_{i_0,j}}{2}\right]^{\beta_j}\right\}
$$

if $\overline{A_{i_0}^2} \leq \varepsilon^2$ for some $1 \leq i_0 \leq J$ or

$$
K_1 = \min\left\{\frac{C_P\varepsilon^2 K_3}{4\beta_{j_0}(I+J)KK_2}; \frac{K_3}{8KK_2(I+J)}\prod_{i=1}^{I}\left[\frac{\alpha_i M_{i,j_0}}{2}\right]^{\alpha_i}\right\}
$$

if $\overline{B_{j_0}^2} \leq \varepsilon^2$ for some $1 \leq j_0 \leq J$.

From (3.15) and (3.16) we obtain the desired entropy-entropy dissipation estimate

$$
\mathcal{D}(\boldsymbol{a},\boldsymbol{b}) \geq \lambda_{\mathbf{M}}(\mathcal{E}(\boldsymbol{a},\boldsymbol{b}) - \mathcal{E}(\boldsymbol{a}_\infty,\boldsymbol{b}_\infty))
$$

with

$$
\lambda_{\mathbf{M}} = \frac{1}{2}\min\left\{\min_{i,j}\{C_{LSI}(d_{a,i}), C_{LSI}(d_{b,j})\};\ 2K_1\right\}.
$$

The exponential convergence to equilibrium for solution to (3.1)

$$\sum_{i=1}^{I}\|a_i(t)-a_{i,\infty}\|^2_{L^1(\Omega)}+\sum_{j=1}^{J}\|b_j(t)-b_{j,\infty}\|^2_{L^1(\Omega)}$$
$$\leq C_{CKP}^{-1}(\mathcal{E}(\boldsymbol{a}(0),\boldsymbol{b}(0))-\mathcal{E}(\boldsymbol{a}_\infty,\boldsymbol{b}_\infty))e^{-\lambda_{\mathrm{M}}t}$$

follows from the entropy-entropy dissipation estimate, the classic Gronwall's lemma and the Ciszár-Kullback-Pinsker inequality

$$\mathcal{E}(\boldsymbol{a},\boldsymbol{b})-\mathcal{E}(\boldsymbol{a}_\infty,\boldsymbol{b}_\infty)\geq C_{CKP}\left(\sum_{i=1}^{I}\|a_i(t)-a_{i,\infty}\|^2_{L^1(\Omega)}+\sum_{j=1}^{J}\|b_j(t)-b_{j,\infty}\|^2_{L^1(\Omega)}\right).$$

□

**Lemma 3.3.** *With $\mu_i$ and $\eta_j$ are defined in (3.20), we can find an explicit constant $\zeta>0$ such that*

$$\left(\boldsymbol{A}_\infty^{\boldsymbol{\alpha}}\left(\boldsymbol{1}+\boldsymbol{\mu}\right)^{\boldsymbol{\alpha}}-\boldsymbol{B}_\infty^{\boldsymbol{\beta}}\left(\boldsymbol{1}+\boldsymbol{\xi}\right)^{\boldsymbol{\beta}}\right)^2\geq\zeta\left(\sum_{i=1}^{I}A_{i,\infty}^2\mu_i^2+\sum_{j=1}^{J}B_{j,\infty}^2\xi_j^2\right). \tag{3.39}$$

*Proof.* The proof of (3.39) relies on relations between $\mu_i$ and $\xi_j$ arising from mass conservation laws (3.5) and (3.9). We first observe that $\mu_i$ and $\xi_j$ are bounded above for all $i=1,\ldots,I$ and $j=1,\ldots,j$. Indeed, from the mass conservation

$$\frac{\overline{a_i}}{\alpha_i}+\frac{\overline{b_j}}{\beta_j}=M_{i,j}\quad\text{ or equivalently }\quad\frac{\overline{A_i^2}}{\alpha_i}+\frac{\overline{B_j^2}}{\beta_j}=M_{i,j}$$

we have

$$\frac{A_{i,\infty}^2(1+\mu_i)^2}{\alpha_i}+\frac{B_{j,\infty}^2(1+\xi_j)^2}{\beta_j}=M_{i,j}.$$

Hence

$$A_{i,\infty}^2(1+\mu_i)^2\leq\alpha_iM_{i,j},$$

which implies that

$$\mu_i\leq-1+\frac{\sqrt{\alpha_iM_{i,j}}}{A_{i,\infty}}=:\mu_{i,max}.$$

Similarly, $\xi_j$ is bounded above as

$$\xi_j\leq-1+\frac{\sqrt{\beta_jM_{i,j}}}{B_{j,\infty}}=:\xi_{j,max}.$$

From (3.9), for all $1\leq i,k\leq I$, we have

$$\frac{\overline{a_i}}{\alpha_i}-\frac{\overline{a_k}}{\alpha_k}=N_{i,k}=\frac{a_{i,\infty}}{\alpha_i}-\frac{a_{k,\infty}}{\alpha_k}$$

thus

$$\alpha_k\left(\overline{A_i^2}-A_{i,\infty}^2\right)=\alpha_i\left(\overline{A_k^2}-A_{k,\infty}^2\right).$$

Hence, by recalling $\overline{A_i^2}=A_{i,\infty}^2(1+\mu_i)^2$ from (3.20) we get

$$\alpha_kA_{i,\infty}^2(\mu_i^2+2\mu_i)=\alpha_iA_{k,\infty}^2(\mu_k^2+2\mu_k).$$

Then, we can write $\mu_i$ in terms of $\mu_k$ as follows

$$\mu_i=\left(\frac{\alpha_iA_{k,\infty}^2}{\alpha_kA_{i,\infty}^2}\frac{\mu_k+2}{\mu_i+2}\right)\mu_k=:R_k(\mu_i)\mu_k.$$

Thanks to $\mu_i \in [-1, \mu_{i,max}]$ and $\mu_k \in [-1, \mu_{k,max}]$, there exist $C_{min} > 0$ and $C_{max} > 0$ such that

$$0 < C_{min} \le R_k(\mu_i)\frac{\alpha_i A_{k,\infty}^2}{\alpha_k A_{i,\infty}^2}\frac{\mu_k + 2}{\mu_i + 2} \le C_{max} < +\infty.$$

Similarly, from the conservation laws

$$\frac{\overline{b_j}}{\beta_j} - \frac{\overline{b_k}}{\beta_k} = \frac{b_{j,\infty}}{\beta_j} - \frac{b_{k,\infty}}{\beta_k} \quad \text{and} \quad \frac{\overline{a_i}}{\alpha_i} + \frac{\overline{b_j}}{\beta_j} = \frac{a_{i,\infty}}{\alpha_i} + \frac{b_{j,\infty}}{\beta_j}$$

we can write

$$\xi_j = \left(\frac{B_{k,\infty}^2}{B_{j,\infty}^2}\frac{\xi_k + 2}{\xi_j + 2}\right)\xi_j =: P_k(\xi_j)\xi_k \quad \text{and} \quad \mu_i = \left(\frac{B_{j,\infty}^2}{A_{i,\infty}^2}\frac{\xi_j + 2}{\mu_i + 2}\right)\xi_j =: -Q_j(\mu_i)\xi_j$$

with

$$C_{min} \le P_k(\xi_j), Q_j(\mu_i) \le C_{max}.$$

Now we can estimate the right hand side of (3.39) as follows

$$\begin{aligned}\sum_{i=1}^{I} A_{i,\infty}^2\mu_i^2 + \sum_{j=1}^{J} B_{j,\infty}^2\xi_j^2 &= \mu_1^2\sum_{i=1}^{I} A_{i,\infty}^2 R_1(\mu_i)^2 + \xi_1^2\sum_{j=1}^{J} B_{j,\infty}^2 P_1(\xi_j)^2\\ &\le C_{max}^2\xi_1^2\left(Q_1(\mu_1)^2\sum_{i=1}^{I} A_{i,\infty}^2 + \sum_{j=1}^{J} B_{j,\infty}^2\right)\\ &\le \zeta_1\xi_1^2\end{aligned} \tag{3.40}$$

with

$$\zeta_1 = C_{max}^2\left(C_{max}^2\sum_{i=1}^{I} A_{i,\infty}^2 + \sum_{j=1}^{J} B_{j,\infty}^2\right). \tag{3.41}$$

To deal with the left hand side of (3.39), first we use $\boldsymbol{A}_\infty^{\boldsymbol{\alpha}} = \boldsymbol{B}_\infty^{\boldsymbol{\beta}}$ to have

$$\left(\boldsymbol{A}_\infty^{\boldsymbol{\alpha}}(\mathbf{1} + \boldsymbol{\mu})^{\boldsymbol{\alpha}} - \boldsymbol{B}_\infty^{\boldsymbol{\beta}}(\mathbf{1} + \boldsymbol{\xi})^{\boldsymbol{\beta}}\right)^2 = \boldsymbol{A}_\infty^{2\boldsymbol{\alpha}}\left((\mathbf{1} + \boldsymbol{\mu})^{\boldsymbol{\alpha}} - (\mathbf{1} + \boldsymbol{\xi})^{\boldsymbol{\beta}}\right)^2 \tag{3.42}$$

and then prove that

$$\left((\mathbf{1} + \boldsymbol{\mu})^{\boldsymbol{\alpha}} - (\mathbf{1} + \boldsymbol{\xi})^{\boldsymbol{\beta}}\right)^2 \ge \zeta_2\xi_1^2 \tag{3.43}$$

or equivalently

$$\left(\prod_{i=1}^{I}(1 + \mu_i)^{\alpha_i} - \prod_{j=1}^{J}(1 + \xi_j)^{\beta_j}\right)^2 \ge \zeta_2\xi_1^2. \tag{3.44}$$

To prove (3.44), we first try to eliminate the nonlinearities raised by $\alpha_i$ and $\beta_j$ on the left hand side and then use the relations between $\mu_i$ and $\xi_j$ to reduce the left hand side into only one variable $\xi_1$. By recalling

$$\mu_i = R_k(\mu_i)\mu_k \quad \text{and} \quad \xi_j = P_k(\xi_j)\xi_k \quad \text{and} \quad \mu_i = -Q_j(\mu_i)\xi_j$$

in which the functions $R_k(\mu_i)$, $P_k(\xi_j)$ and $Q_j(\mu_i)$ are always positive, we see that $\mu_i$ and $\mu_k$ (resp. $\xi_j$ and $\xi_k$) always have the same sign while $\mu_i$ and $\xi_j$ always have the opposite sign. Therefore, we consider two cases depending on the sign of $\mu_1$, that is $-1 \le \mu_1 \le 0$ and $\mu_1 \ge 0$.

- If $-1 \le \mu_1 \le 0$, then we have $-1 \le \mu_i \le 0$ for all $i = 2, \ldots, I$ and $\xi_j \ge 0$ for all $j = 1, \ldots, J$. Then,

$$0 \le (1 + \mu_i)^{\alpha_i} \le (1 + \mu_i) \quad \text{and} \quad (1 + \xi_j)^{\beta_j} \ge (1 + \xi_j) \ge 0 \tag{3.45}$$

thanks to $\alpha_i, \beta_j \geq 1$ for all $i = 1, \ldots, I$ and all $j = 1, \ldots, J$. It follows from (3.45) that

$$\begin{aligned}\left|\prod_{i=1}^{I}(1+\mu_i)^{\alpha_i} - \prod_{j=1}^{J}(1+\xi_j)^{\beta_j}\right| &\geq \prod_{j=1}^{J}(1+\xi_j)^{\beta_j} - \prod_{i=1}^{I}(1+\mu_i)^{\alpha_i} \\ &\geq \prod_{j=1}^{J}(1+\xi_j) - \prod_{i=1}^{I}(1+\mu_i).\end{aligned} \tag{3.46}$$

Since $1 + \xi_j \geq 1$ for all $j = 1, \ldots, J$,

$$\prod_{j=1}^{J}(1+\xi_j) \geq (1+\xi_1). \tag{3.47}$$

On the other hand, since $-1 \leq \mu_i \leq 0$ for all $i = 1, \ldots, I$, we have

$$\begin{aligned}-\prod_{i=1}^{I}(1+\mu_i) &= -\prod_{i=2}^{I}(1+\mu_i) - \mu_1\prod_{i=2}^{I}(1+\mu_i) \\ &\geq -\prod_{i=2}^{I}(1+\mu_i) \\ &\geq -\prod_{i=3}^{I}(1+\mu_i) - \mu_2\prod_{i=3}^{I}(1+\mu_i) \\ &\geq \ldots \\ &\geq -(1+\mu_1).\end{aligned} \tag{3.48}$$

By combining (3.46), (3.47) and (3.48) we obtain

$$\left|\prod_{i=1}^{I}(1+\mu_i)^{\alpha_i} - \prod_{j=1}^{J}(1+\xi_j)^{\beta_j}\right| \geq \xi_1 - \mu_1 \geq 0. \tag{3.49}$$

- If $\mu_1 \geq 0$, then we have $\mu_i \geq 0$ for all $i = 2, \ldots, I$ and $-1 \leq \xi_j \leq 0$ for all $j = 1, \ldots, J$. Applying similar arguments to the former case, we get

$$\begin{aligned}\left|\prod_{i=1}^{I}(1+\mu_i)^{\alpha_i} - \prod_{j=1}^{J}(1+\xi_j)^{\beta_j}\right| &\geq \prod_{i=1}^{I}(1+\mu_i)^{\alpha_i} - \prod_{j=1}^{J}(1+\xi_j)^{\beta_j} \\ &\geq (1+\mu_1) - (1+\xi_1) \\ &= \mu_1 - \xi_1 \geq 0.\end{aligned} \tag{3.50}$$

From the results (3.49) and (3.50) of the two cases, we have

$$\left|\prod_{i=1}^{I}(1+\mu_i)^{\alpha_i} - \prod_{j=1}^{J}(1+\xi_j)^{\beta_j}\right| \geq |\mu_1 - \xi_1|, \tag{3.51}$$

thus,

$$\left(\prod_{i=1}^{I}(1+\mu_i)^{\alpha_i} - \prod_{j=1}^{J}(1+\xi_j)^{\beta_j}\right)^2 \geq |\mu_1 - \xi_1|^2 = (1+Q_1(\mu_1))^2\,\xi_1^2 \geq \zeta_2\xi_1^2 \tag{3.52}$$

with

$$\zeta_2 = (1 + C_{min})^2\,. \tag{3.53}$$

From (3.40), (3.42) and (3.43), we can finish the proof of this Lemma with

$$\zeta = \frac{\boldsymbol{A}_\infty^{2\boldsymbol{\alpha}}\zeta_2}{\zeta_1} = \frac{\boldsymbol{A}_\infty^{2\boldsymbol{\alpha}}(1+C_{min})^2}{C_{max}^2\left(C_{max}^2\sum_{i=1}^I A_{i,\infty}^2 + \sum_{j=1}^J B_{j,\infty}^2\right)} \tag{3.54}$$

thanks to (3.41) and (3.53). □

## 4. Enzymes reversible reactions - Proof of Theorem 1.2

In this section, we demonstrate the strategy in Section 2 for a chain of two reversible reactions modelling, for instance, reversible enzymes reactions. More precisely, we consider the enzyme reversible reaction of the form

$$A_1 + A_2 \leftrightharpoons A_3 \leftrightharpoons A_4 + A_5 \tag{4.1}$$

where all the reaction constants are assumed to be one. In [BCD07] and [BP10], this reaction were studied in the context of performing a quasi-steady-state-approximation, i.e. the releasing speeds from $A_3$ to $A_1 + A_2$ and from $A_3$ to $A_4 + A_5$ are infinitely fast.

As in the previous section, we assume the reaction to occur in a bounded domain $\Omega \subset \mathbb{R}^n$ with smooth boundary $\partial\Omega$. By applying the mass action law, the corresponding reaction-diffusion system of (4.1) reads as

$$\begin{cases} \partial_t c_1 - \mathrm{div}(d_1(x)\nabla c_1) = -c_1c_2 + c_3, & x\in\Omega, \quad t>0,\\ \partial_t c_2 - \mathrm{div}(d_2(x)\nabla c_2) = -c_1c_2 + c_3, & x\in\Omega, \quad t>0,\\ \partial_t c_3 - \mathrm{div}(d_3(x)\nabla c_3) = c_1c_2 + c_4c_5 - 2c_3, & x\in\Omega, \quad t>0,\\ \partial_t c_4 - \mathrm{div}(d_4(x)\nabla c_4) = -c_4c_5 + c_3, & x\in\Omega, \quad t>0,\\ \partial_t c_5 - \mathrm{div}(d_5(x)\nabla c_5) = -c_4c_5 + c_3, & x\in\Omega, \quad t>0,\\ \partial_\nu c_i = 0, & i=1,2,\ldots,5, \quad x\in\partial\Omega, \quad t>0,\\ c_i(0,x) = c_{i,0}(x), & i=1,2,\ldots,5, \quad x\in\Omega, \end{cases} \tag{4.2}$$

where $0 < d_{min} \le d_i(x) \le d_{max} < +\infty$ for all $x \in \Omega$ and $i = 1,2,\ldots,5$, are positive diffusion coefficients.

The rest of this section is organized as follows: We first derive the mass conservation laws for (4.2), which play an essential role in our strategy. Later, we show that (4.2) satisfies the assumptions (**A1**) and (**A2**). Finally, we apply the strategy in Section 2 to show the explicit convergence to equilibrium for (4.2). For the sake of convenience, we will denote by $\boldsymbol{c} = (c_1, c_2, c_3, c_4, c_5)$ and recall the spatial average

$$\overline{c_i} = \int_\Omega c_i(x)dx.$$

We begin with

**Lemma 4.1** (Conservation laws)**.** *For $i \in \{1,2\}$ and $j \in \{4,5\}$, we have*

$$\int_\Omega (c_i(x,t) + c_j(x,t) + c_3(x,t))dx = \int_\Omega (c_{i,0}(x) + c_{j,0}(x) + c_{3,0}(x))dx =: M_{i,j}, \tag{4.3}$$

*for all $t > 0$. Among these four conservation laws, there are exactly three linear independent laws.*

*Then, with respect to the general formulation, the matrix $\mathbb{Q}$ can be defined as*

$$\mathbb{Q} = \begin{pmatrix} 1 & 0 & 1 & 1 & 0\\ 1 & 0 & 1 & 0 & 1\\ 0 & 1 & 1 & 1 & 0 \end{pmatrix} \in \mathbb{R}^{3\times 5}.$$

**Remark 4.1.** *We denote by* $\mathbf{M} = (M_{1,4}, M_{1,5}, M_{2,4}, M_{2,5}) \in \mathbb{R}_+^4$ *the vector of initial mass. Note that* $\mathbf{M}$ *is fixed once three of its four coordinates are fixed. Hence, from now on, by a fixed initial mass* $\mathbf{M}$ *we mean that three of its coordinates are fixed.*

*It's also useful to notice that from the mass conservation laws* (4.3), *we obtain*

$$\int_\Omega (c_1(x,t) - c_2(x,t))dx = \int_\Omega (c_{1,0}(x) - c_{2,0}(x))dx =: N_{1,2}, \tag{4.4}$$

*and*

$$\int_\Omega (c_4(x,t) - c_5(x,t))dx = \int_\Omega (c_{4,0}(x) - c_{5,0}(x))dx =: N_{4,5}. \tag{4.5}$$

**Lemma 4.2** (Detailed balanced equilibrium)**.** *For any given positive initial mass* $\mathbf{M} \in \mathbb{R}_+^4$, *there exists a unique equilibrium* $\boldsymbol{c}_\infty = (c_{1,\infty}, c_{2,\infty}, \ldots, c_{5,\infty})$ *to* (4.2) *satisfying*

$$\begin{cases} c_{1,\infty}c_{2,\infty} = c_{3,\infty}, \\ c_{4,\infty}c_{5,\infty} = c_{3,\infty}, \\ c_{i,\infty} + c_{j,\infty} + c_{3,\infty} = M_{i,j}, \quad \forall i \in \{1,2\},\ \forall j \in \{4,5\}. \end{cases} \tag{4.6}$$

*Consequently, the system* (4.2) *satisfies the assumptions* (**A1**) *and* (**A2**).

To prove the convergence to equilibrium, we again consider the entropy

$$\mathcal{E}(\boldsymbol{c}) = \sum_{i=1}^5 \int_\Omega (c_i \log c_i - c_i + 1)dx \tag{4.7}$$

and its entropy dissipation

$$\mathcal{D}(\boldsymbol{c}) = \sum_{i=1}^5 \int_\Omega d_i(x)\frac{|\nabla c_i|^2}{c_i}dx + \int_\Omega \left((c_1c_2 - c_3)\log\frac{c_1c_2}{a_3} + (c_4c_5 - c_3)\log\frac{c_4c_5}{c_3}\right)dx. \tag{4.8}$$

*Proof of Theorem 1.2.* We follow the steps in the strategy in Section 2 to prove this Theorem.

- **Step 1 (Use of the Logarithmic Sobelev Inequality).** By using the additivity of the entropy we have

$$\begin{aligned} \mathcal{E}(\boldsymbol{c}) - \mathcal{E}(\boldsymbol{c}_\infty) &= (\mathcal{E}(\boldsymbol{c}) - \mathcal{E}(\overline{\boldsymbol{c}})) + (\mathcal{E}(\overline{\boldsymbol{c}}) - \mathcal{E}(\boldsymbol{c}_\infty)) \\ &= \sum_{i=1}^5 \int_\Omega c_i \log\frac{c_i}{\overline{c_i}}dx + \sum_{i=1}^5 \left(\overline{c_i}\log\frac{\overline{c_i}}{c_{i,\infty}} - \overline{c_i} + c_{i,\infty}\right). \end{aligned}$$

  It follows from the Logarithmic Sobolev Inequality that

$$\frac{1}{2}\mathcal{D}(\boldsymbol{c}) \geq \frac{1}{2}\min_{1\leq i\leq 5}\{C_{LSI}(d_i)\}(\mathcal{E}(\boldsymbol{c}) - \mathcal{E}(\overline{\boldsymbol{c}})).$$

  It remains to find $K_1 > 0$ such that

$$\frac{1}{2}\mathcal{D}(\boldsymbol{c}) \geq K_1(\mathcal{E}(\overline{\boldsymbol{c}}) - \mathcal{E}(\boldsymbol{c}_\infty)). \tag{4.9}$$

- **Step 2 (Transform terms into quadratic terms).** By the identification $\nabla\sqrt{f} = \frac{\nabla f}{2\sqrt{f}}$ and the inequality $(a-b)\log(a/b) \geq 4(\sqrt{a} - \sqrt{b})^2$ we have, with $C_i = \sqrt{c_i}$,

$$\frac{1}{2}\mathcal{D}(\boldsymbol{c}) \geq 2d_{min}\sum_{i=1}^5 \|\nabla C_i\|^2 + 2\|C_1C_2 - C_3\|^2 + 2\|C_4C_5 - C_3\|^2. \tag{4.10}$$

On the other hand, thanks to the function $\Phi(z) = (z\log z - z + 1)/(\sqrt{z}-1)^2$, we obtain

$$\mathcal{E}(\overline{\boldsymbol{c}}) - \mathcal{E}(\boldsymbol{c}_\infty) \le K_2 \sum_{i=1}^{5} \left(\sqrt{\overline{C_i^2}} - C_{i,\infty}\right)^2 \tag{4.11}$$

with

$$K_2 = \max_{1\le i\le 5}\left\{\Phi\left(\frac{K}{c_{i,\infty}}\right)\right\}.$$

From (4.10) and (4.11), we get (4.9) if

$$2d_{min}\sum_{i=1}^{5}\|\nabla C_i\|^2 + 2\|C_1C_2 - C_3\|^2 + 2\|C_4C_5 - C_3\|^2 \ge K_1K_2\sum_{i=1}^{5}\left(\sqrt{\overline{C_i^2}} - C_{i,\infty}\right)^2. \tag{4.12}$$

- **Step 3 (Reaction dissipation term and reaction dissipation term of averages).** By applying Lemma 2.6, there is an explicit constant $K_3 > 0$ such that

$$\begin{aligned}2d_{min}\sum_{i=1}^{5}\|\nabla C_i\|^2 &+ 2\|C_1C_2 - C_3\|^2 + 2\|C_4C_5 - C_3\|^2\\ &\ge K_3\left(\sum_{i=1}^{5}\|\nabla C_i\|^2 + \|\overline{C}_1\overline{C}_2 - \overline{C}_3\|^2 + \|\overline{C}_4\overline{C}_5 - \overline{C}_3\|^2\right)\end{aligned} \tag{4.13}$$

Therefore, (4.12) follows from (4.13) provided

$$\sum_{i=1}^{5}\|\nabla C_i\|^2 + \|\overline{C}_1\overline{C}_2 - \overline{C}_3\|^2 + \|\overline{C}_4\overline{C}_5 - \overline{C}_3\|^2 \ge \frac{K_1K_2}{K_3}\sum_{i=1}^{5}\left(\sqrt{\overline{C_i^2}} - C_{i,\infty}\right)^2. \tag{4.14}$$

- **Step 4 (Express averages in terms of the equilibrium).** We consider the ansatz

$$\overline{C_i^2} = C_{i,\infty}^2(1+\mu_i)^2 \tag{4.15}$$

for $\mu_i \in [-1; +\infty)$, and define the deviation to average

$$\delta_i(x) = C_i(x) - \overline{C_i}, \qquad \text{for } x \in \Omega, \tag{4.16}$$

for each $i = 1, 2, \ldots, 5$. It follows from $\|\delta_i\|^2 = \overline{C_i^2} - \overline{C_i}^2$ that

$$\overline{C_i} = C_{i,\infty}(1+\mu_i) - Q(C_i)\|\delta_i\|^2, \qquad \text{with} \qquad Q(C_i) = \frac{1}{\sqrt{\overline{C_i^2}} + \overline{C_i}}. \tag{4.17}$$

for all $i = 1, 2, \ldots, 5$. We see that $Q(C_i)$ becomes unbounded when $\overline{C_i^2}$ approaches zero. Therefore, we consider the following two cases when $\overline{C_i^2}$ is either "big" or "small". We choose two constants $\varepsilon > 0$ and $\eta > 0$ such that

$$\varepsilon^2 \le \frac{1}{4}\min\left\{M_{1,4}; M_{1,5}; M_{2,5}; \frac{M_{1,5}}{M_{2,4}+2}; \frac{M_{1,4}M_{1,5}}{4M_{2,4}}; \frac{M_{2,5}^2}{16}\right\} \tag{4.18}$$

and

$$\eta \le \frac{1}{8}\min\left\{M_{1,4}; M_{1,5}; M_{2,5}\right\}. \tag{4.19}$$

(i) $\overline{C_i^2} \ge \varepsilon^2$ for $i = 1, 2, \ldots, 5$.
In this case we have that $Q(C_i) \le 1/\varepsilon$ for all $i = 1, \ldots, 5$. By applying the Poincaré inequality $\|\nabla f\|^2 \ge C_P\|f - \overline{f}\|^2$, we bound the left hand side of (4.14) as follows,

with $\theta \in (0,1)$,

$$\begin{aligned}
\sum_{i=1}^{5}\|\nabla C_i\|^2 + \theta\left[(\overline{C}_1\overline{C}_2 - \overline{C}_3)^2 + (\overline{C}_4\overline{C}_5 - \overline{C}_3)^2\right]&\\
\geq C_P\sum_{i=1}^{5}\|\delta_i\|^2 &+ \theta(C_{1,\infty}C_{2,\infty}(1+\mu_1)(1+\mu_2) - C_{3,\infty}(1+\mu_3))^2\\
&+ \theta(C_{4,\infty}C_{5,\infty}(1+\mu_4)(1+\mu_5) - C_{3,\infty}(1+\mu_3))^2\\
&- \theta C(\varepsilon, M)\sum_{i=1}^{5}\|\delta_i\|^2\\
\geq \theta\Big[&(C_{1,\infty}C_{2,\infty}(1+\mu_1)(1+\mu_2) - C_{3,\infty}(1+\mu_3))^2\\
&\quad + (C_{4,\infty}C_{5,\infty}(1+\mu_4)(1+\mu_5) - C_{3,\infty}(1+\mu_3))^2\Big] \qquad (4.20)
\end{aligned}$$

for $\theta$ satisfying $\theta \leq \min\{1; C_P C(\varepsilon, M)^{-1}\}$.
Thanks to Lemma 4.3, there exists $\zeta > 0$ such that

$$\begin{aligned}
(C_{1,\infty}C_{2,\infty}(1+\mu_1)(1+\mu_2) - C_{3,\infty}(1+\mu_3))^2&\\
+\ (C_{4,\infty}C_{5,\infty}(1+\mu_4)(1+\mu_5) - C_{3,\infty}(1+\mu_3))^2&\\
\geq \zeta\sum_{i=1}^{5}\left(\sqrt{\overline{C_i^2}} - C_{i,\infty}\right)^2. &\qquad (4.21)
\end{aligned}$$

Then (4.14) follows from (4.20) and (4.21) by choosing

$$K_1 \leq \frac{\zeta\theta K_3}{K_2}. \qquad (4.22)$$

(ii) There exists $\overline{C_{i_0}^2} \leq \varepsilon^2$ for some $i_0 \in \{1, 2\ldots, 5\}$.
In this case, we will first bound the right hand side of (4.14) above as

$$\frac{K_1K_2}{K_3}\sum_{i=1}^{5}\left(\sqrt{\overline{C_i^2}} - C_{i,\infty}\right)^2 \leq \frac{10K_1K_2K}{K_3}. \qquad (4.23)$$

Then, we will bound the left hand side of (4.14) below. To do that, we will encounter two smaller cases due to the contribution of diffusion and reaction terms.

- (When the diffusion is dominant.)
  $\|\delta_{i^*}\|^2 \geq \eta$ for some $i^* \in \{1, 2, \ldots, 5\}$. We then can estimate

  $$\sum_{i=1}^{5}\|\nabla C_i\|^2 + (\overline{C}_1\overline{C}_2 - \overline{C}_3)^2 + (\overline{C}_4\overline{C}_5 - \overline{C}_3)^2 \geq C_P\eta.$$

  Hence, (4.14) follows from (4.23) if we choose

  $$K_1 \leq \frac{K_3C_P\eta}{10KK_2}. \qquad (4.24)$$

- (When the reaction is dominant.)
  $\|\delta_i\|^2 \leq \eta$ for all $i = 1, 2, \ldots, 5$. We recall $\overline{C_{i_0}^2} \leq \varepsilon^2$ for some $i_0 \in \{1, 2, \ldots, 5\}$ and remark that the roles of $C_1, C_2, C_4$ and $C_5$ in (4.14) are the same. Therefore, we investigate two situations: $i_0 = 1$ and $i_0 = 3$.

- ♦ When $i_0 = 1$, we imply first that $\overline{C}_1^2 \le \overline{C_1^2} \le \varepsilon^2$.
Then, from the mass conservation

$$\overline{C_1^2} + \overline{C_4^2} + \overline{C_3^2} = M_{1,4} \qquad \text{and} \qquad \overline{C_1^2} + \overline{C_5^2} + \overline{C_3^2} = M_{1,5},$$

we get

$$\overline{C_3^2} + \overline{C_4^2} \ge \underbrace{M_{1,4} - \varepsilon^2}_{=:\omega_1} \qquad \text{and} \qquad \overline{C_3^2} + \overline{C_5^2} \ge \underbrace{M_{1,5} - \varepsilon^2}_{=:\omega_2}. \tag{4.25}$$

Without loss of generality, we assume that $M_{1,4} \ge M_{1,5}$ thus $\omega_1 \ge \omega_2$. From (4.25) we have the following table

| Case | $\overline{C_3^2}$ | $\overline{C_4^2}$ | $\overline{C_5^2}$ |
|---|---|---|---|
| (I) | $\overline{C_3^2} \ge \frac{\omega_1}{2}$ | $\le \frac{\omega_1}{2}$ | $\le \frac{\omega_2}{2}$ |
| (II) | $\overline{C_3^2} \le \frac{\omega_2}{2}$ | $\ge \frac{\omega_1}{2}$ | $\ge \frac{\omega_2}{2}$ |
| (III) | $\frac{\omega_2}{2} \le \overline{C_3^2} \le \frac{\omega_1}{2}$ | $\ge \frac{\omega_1}{2}$ | $\le \frac{\omega_2}{2}$ |

In cases (I) and (III), we both have $\overline{C_3^2} \ge \frac{\omega_2}{2}$ and, thus

$$\overline{C}_3^2 = \overline{C_3^2} - \|\delta_3\|^2 \ge \frac{\omega_2 - 2\eta}{2} = \frac{M_{1,5} - \varepsilon^2 - 2\eta}{2}.$$

We can then estimate

$$\begin{aligned}
&\sum_{i=1}^{5} \|\nabla C_i\|^2 + (\overline{C}_1\overline{C}_2 - \overline{C}_3)^2 + (\overline{C}_4\overline{C}_5 - \overline{C}_3)^2 \\
&\qquad\qquad \ge (\overline{C}_1\overline{C}_2 - \overline{C}_3)^2 \ge \frac{1}{2}\overline{C}_3^2 - \overline{C}_1^2\overline{C}_2^2 \\
&\qquad\qquad \ge \frac{M_{1,5} - \varepsilon^2 - 2\eta}{2} - \varepsilon^2 M_{2,4} \ge \frac{M_{1,5}}{4}
\end{aligned} \tag{4.26}$$

thanks to (4.18) and (4.19).
In case (II), we have

$$\overline{C}_4^2 = \overline{C_4^2} - \|\delta_4\|^2 \ge \frac{M_{1,4} - \varepsilon^2 - 2\eta}{2},$$

and similarly

$$\overline{C}_5^2 \ge \frac{M_{1,5} - \varepsilon^2 - 2\eta}{2}.$$

We continue with

$$\begin{aligned}
&\sum_{i=1}^{5} \|\nabla C_i\|^2 + (\overline{C}_1\overline{C}_2 - \overline{C}_3)^2 + (\overline{C}_4\overline{C}_5 - \overline{C}_3)^2 \\
&\qquad\qquad \ge \frac{1}{2}\left(\overline{C}_1\overline{A}_2 - \overline{C}_4\overline{C}_5\right)^2 \ge \frac{1}{4}\overline{C}_4^2\overline{C}_5^2 - \frac{1}{2}\overline{C}_1^2\overline{C}_2^2 \\
&\qquad\qquad \ge \frac{(M_{1,4} - \varepsilon^2 - 2\eta)(M_{1,5} - \varepsilon^2 - 2\eta)}{4} - \frac{1}{2}\varepsilon^2 M_{2,4} \\
&\qquad\qquad \ge \frac{M_{1,4}M_{1,5}}{32}
\end{aligned} \tag{4.27}$$

thanks again to (4.18) and (4.19). Combining (4.26) and (4.27), we have

$$\begin{aligned}\sum_{i=1}^{5}\|\nabla C_i\|^2 + (\overline{C}_1\overline{C}_2 - \overline{C}_3)^2 + (\overline{C}_4\overline{C}_5 - \overline{C}_3)^2\\ \geq \min\left\{\frac{M_{1,5}}{4};\frac{M_{1,4}M_{1,5}}{32}\right\}\end{aligned} \tag{4.28}$$

in the case $i_0 = 1$.

- When $i_0 = 3$, we imply first that $\overline{C}_3^2 \leq \overline{C_3^2} \leq \varepsilon^2$.
Without loss of generality, we can assume that $M_{1,4}$ is the biggest component of $M$. Thus,
$$\overline{C_1^2} = \overline{C_2^2} + M_{1,4} - M_{2,4} \geq \overline{C_2^2},$$
and
$$\overline{C_4^2} = \overline{C_5^2} + M_{1,4} - M_{1,5} \geq \overline{C_5^2}.$$
By using the mass conservation $\overline{C_2^2} + \overline{C_3^2} + \overline{C_5^2} = M_{2,5}$, we get
$$\overline{C_2^2} + \overline{C_5^2} \geq M_{2,5} - \varepsilon^2,$$
hence
$$\overline{C_2^2} \geq \frac{M_{2,5}-\varepsilon^2}{2} \qquad \text{or} \qquad \overline{C_5^2} \geq \frac{M_{2,5}-\varepsilon^2}{2}.$$
If $\overline{C_2^2} \geq \frac{M_{2,5}-\varepsilon^2}{2}$ then $\overline{C_1^2} \geq \frac{M_{2,5}-\varepsilon^2}{2}$. It follows that
$$\overline{C}_1^2 = \overline{C_1^2} - \|\delta_1\|^2 \geq \frac{M_{2,5}-\varepsilon^2}{2} - \eta,$$
and
$$\overline{C}_2^2 = \overline{C_2^2} - \|\delta_2\|^2 \geq \frac{M_{2,5}-\varepsilon^2}{2} - \eta.$$
We then can estimate
$$\begin{aligned}\sum_{i=1}^{5}\|\nabla C_i\|^2 &+ (\overline{C}_1\overline{C}_2 - \overline{C}_3)^2 + (\overline{C}_4\overline{C}_5 - \overline{C}_3)^2\\ &\geq (\overline{C}_1\overline{C}_2 - \overline{C}_3)^2 \geq \frac{1}{2}\overline{C}_1^2\overline{C}_2^2 - \overline{C}_3^2\\ &\geq \frac{1}{2}\left(\frac{M_{2,5}-\varepsilon^2}{2} - \eta\right)^2 - \varepsilon^2 \geq \frac{M_{2,5}^2}{64}\end{aligned} \tag{4.29}$$
due to (4.18) and (4.19).
Similarly, if $\overline{C_5^2} \geq \frac{M_{2,5}-\varepsilon^2}{2}$ we can prove by using the same arguments above that
$$\sum_{i=1}^{5}\|\nabla C_i\|^2 + (\overline{C}_1\overline{C}_2 - \overline{C}_3)^2 + (\overline{C}_4\overline{C}_5 - \overline{C}_3)^2 \geq \frac{M_{2,5}^2}{64}. \tag{4.30}$$

Now from (4.28), (4.29) and (4.30), we get that if $\|\delta_i\|^2 \leq \eta$ for all $i = 1, 2, \ldots, 5$ then

$$\begin{aligned}\sum_{i=1}^{5}\|\nabla C_i\|^2 + (\overline{C}_1\overline{C}_2 - \overline{C}_3)^2 + (\overline{C}_4\overline{C}_5 - \overline{C}_3)^2\\ \geq \min\left\{\frac{M_{1,5}}{4};\frac{M_{1,4}M_{1,5}}{32};\frac{M_{2,5}^2}{64}\right\}.\end{aligned} \tag{4.31}$$

From (4.31) and (4.23) we obtain (4.14) by choosing

$$K_1 \le \frac{K_3}{10KK_2}\min\left\{\frac{M_{1,5}}{4}; \frac{M_{1,4}M_{1,5}}{32}; \frac{M_{2,5}^2}{64}\right\}. \tag{4.32}$$

At this point, we can conclude Step 4 by combining (4.22), (4.24) and (4.32),

$$K_1 \le \frac{K_2}{K_3}\min\left\{\zeta\theta;\ \frac{C_P\eta}{10K};\ \frac{1}{10K}\min\left\{\frac{M_{1,5}}{4}; \frac{M_{1,4}M_{1,5}}{32}; \frac{M_{2,5}^2}{64}\right\}\right\}.$$

□

**Lemma 4.3** (Proof of (4.21))**.** *Let $\mu_1, \ldots, \mu_5$ be defined as in (4.15). Then there exists an explicit constant $\zeta$ satisfying*

$$\begin{aligned}\big(C_{1,\infty}C_{2,\infty}(1+\mu_1)(1+\mu_2) - C_{3,\infty}(1+\mu_3)\big)^2&\\ + \big(C_{4,\infty}C_{5,\infty}(1+\mu_4)(1+\mu_5) - C_{3,\infty}(1+\mu_3)\big)^2&\\ \ge \zeta\sum_{i=1}^{5}\left(\sqrt{\overline{C_i^2}} - C_{i,\infty}\right)^2&.\end{aligned} \tag{4.33}$$

*Proof.* This inequality is similar to (3.39). However, as we mentioned, due to the different structure of mass conservation laws, we need to use a different proof.

We first prove that

$$\begin{aligned}\big((1+\mu_1)(1+\mu_2) - (1+\mu_3)\big)^2 + \big((1+\mu_4)(1+\mu_5) - (1+\mu_3)\big)^2&\\ \ge \frac{1}{4}\left((\mu_1-\mu_3)^2 + (\mu_3-\mu_5)^2\right)&.\end{aligned} \tag{4.34}$$

Since

$$\overline{C_1^2} - C_{1,\infty}^2 = \overline{C_2^2} - C_{2,\infty}^2 \tag{4.35}$$

we have

$$C_{1,\infty}^2(\mu_1^2 + 2\mu_1) = C_{2,\infty}^2(\mu_2^2 + 2\mu_2). \tag{4.36}$$

Due to $\mu_1, \mu_2 \in [-1, +\infty)$ it follows that $\mu_1$ and $\mu_2$ always have a same sign. Similarly, $\mu_4, \mu_5$ always have a same sign. From

$$\overline{C_1^2} + \overline{C_3^2} + \overline{C_5^2} = M_{15} = C_{1,\infty}^2 + C_{3,\infty}^2 + C_{5,\infty}^2 \tag{4.37}$$

we get

$$C_{1,\infty}^2(\mu_1^2 + 2\mu_1) + C_{3,\infty}^2(\mu_3^2 + 2\mu_3) + C_{5,\infty}^2(\mu_5^2 + 2\mu_5) = 0. \tag{4.38}$$

This relation helps us to determine the sign of $\mu_3$ via the signs of $\mu_1$ and $\mu_5$. We therefore consider four cases based on the signs of $\mu_1$ and $\mu_5$.

(i) $\mu_1 > 0$ and $\mu_5 > 0$. It follows that $\mu_2 > 0$, $\mu_4 > 0$ and from (4.38) that $-1 \le \mu_3 < 0$. Then

$$\begin{aligned}|(1+\mu_1)(1+\mu_2) - (1+\mu_3)| &\ge (1+\mu_1)(1+\mu_2) - (1+\mu_3)\\ &\ge (1+\mu_1) - (1+\mu_3) = \mu_1 - \mu_3 \ge 0,\end{aligned} \tag{4.39}$$

thus

$$[(1+\mu_1)(1+\mu_2) - (1+\mu_3)]^2 \ge (\mu_1-\mu_3)^2. \tag{4.40}$$

Similarly,

$$[(1+\mu_4)(1+\mu_5) - (1+\mu_3)]^2 \ge (\mu_3-\mu_5)^2. \tag{4.41}$$

Combining (4.40) and (4.41) leads to (4.34).

(ii) $-1 \le \mu_1 \le 0$ and $-1 \le \mu_5 \le 0$. In this case, we have $-1 \le \mu_2 \le 0$ and $-1 \le \mu_4 \le 0$. It follows from (4.38) that $\mu_3 \ge 0$. Thus, we can estimate

$$\begin{aligned} |(1+\mu_1)(1+\mu_2) - (1+\mu_3)| &\ge (1+\mu_3) - (1+\mu_1)(1+\mu_2) \\ &= (1+\mu_3) - (1+\mu_1) - \mu_2(1+\mu_1) \\ &\ge \mu_3 - \mu_1 \ge 0 \end{aligned} \tag{4.42}$$

and similarly

$$|(1+\mu_4)(1+\mu_5) - (1+\mu_3)| \ge \mu_3 - \mu_5 \ge 0. \tag{4.43}$$

From (4.42) and (4.43) we get (4.34).

(iii) $\mu_1 > 0$ and $-1 \le \mu_5 \le 0$. It follows that $\mu_2 > 0$ and $-1 \le \mu_4 \le 0$. However, from these we couldn't determine the sign of $\mu_3$. Hence, we have two consider two sub-cases.

- If $\mu_3 > 0$ then we get first (4.43). Secondly, the triangle inequality leads to

$$\begin{aligned} &|(1+\mu_1)(1+\mu_2) - \mu_3| + |(1+\mu_4)(1+\mu_5) - (1+\mu_3)| \\ &\ge |(1+\mu_1)(1+\mu_2) - (1+\mu_4)(1+\mu_5)| \\ &\ge (1+\mu_1)(1+\mu_2) - (1+\mu_4)(1+\mu_5) \\ &\ge (1+\mu_1) - (1+\mu_5) \\ &= \mu_1 - \mu_5 \ge 0. \end{aligned} \tag{4.44}$$

By combining this with (4.43), we get (4.34).

- If $-1 \le \mu_3 \le 0$ then we get (4.39) immediately. Similar to (4.44), we obtain

$$\begin{aligned} &|(1+\mu_1)(1+\mu_2) - \mu_3| + |(1+\mu_4)(1+\mu_5) - (1+\mu_3)| \\ &\qquad \ge \mu_5 - \mu_1 \ge 0. \end{aligned} \tag{4.45}$$

Hence (4.34) follows from (4.39) and (4.45).

(iv) $-1 \le \mu_1 \le 0$ and $\mu_5 > 0$. This case is similar to case (iii) thus we omit the proof.

We have proved (4.34), which means that the left hand side of (4.33) is bounded below by

$$\text{LHS of (4.33)} \ge \frac{1}{4} C_{3,\infty}^2 \left((\mu_1 - \mu_3)^2 + (\mu_3 - \mu_5)^2\right) \tag{4.46}$$

where we used the equilibrium criterion $C_{3,\infty} = C_{1,\infty}C_{2,\infty} = C_{4,\infty}C_{5,\infty}$. Hence, in order to show (4.33), it suffices to prove that

$$C_{3,\infty}^2 \left((\mu_1 - \mu_3)^2 + (\mu_3 - \mu_5)^2\right) \ge 4\zeta \sum_{i=1}^{5} C_{i,\infty}^2 \mu_i^2. \tag{4.47}$$

To prove (4.47), we first observe that, thanks the mass conservation laws $\overline{C_i^2} + \overline{C_3^2} + \overline{C_j^2} = M_{i,j}$ for $i \in \{1,2\}$, $j \in \{4,5\}$ and $\overline{C_i^2} = C_{i,\infty}^2(1+\mu_i)^2$, we get $\mu_i$ is bounded above

$$-1 \le \mu_i \le \mu_{i,max} < +\infty \quad \text{ for all } i = 1, \ldots, 5.$$

We then compute $\mu_2$ and $\mu_4$ in terms of $\mu_1$ and $\mu_5$ respectively to reduce the right hand side of (4.47) to an expression of $\mu_1$, $\mu_3$ and $\mu_5$. From the mass conservation (4.36) we have

$$\mu_2 = \left(\frac{C_{1,\infty}^2}{C_{2,\infty}^2} \frac{\mu_1 + 2}{\mu_2 + 2}\right) \mu_1 =: R(\mu_1, \mu_2)\mu_1 \tag{4.48}$$

where, by using $-1 \le \mu_i \le \mu_{i,max}$,

$$0 < C_{min} \le R(\mu_1, \mu_2) = \frac{C_{1,\infty}^2}{C_{2,\infty}^2} \frac{\mu_1 + 2}{\mu_2 + 2} \le C_{max} < +\infty$$

for some constants $C_{min}$ and $C_{max}$ which can be explicitly computed. Similarly,

$$\mu_4 = \left(\frac{C_{5,\infty}^2}{C_{4,\infty}^2}\frac{\mu_5+2}{\mu_4+2}\right)\mu_5 =: P(\mu_4,\mu_5)\mu_5 \tag{4.49}$$

with

$$0 < C_{min} \le P(\mu_4,\mu_5) = \frac{C_{5,\infty}^2}{C_{4,\infty}^2}\frac{\mu_5+2}{\mu_4+2} \le C_{max} < +\infty$$

Using (4.48) and (4.49), we can bound the right hand side of (4.47) above by

$$4\zeta\sum_{i=1}^{5} C_{i,\infty}^2\mu_i^2 \le \zeta_1(\mu_1^2+\mu_3^2+\mu_5^2) \tag{4.50}$$

with

$$\zeta_1 = 4\zeta\max\left\{C_{1,\infty}^2;\ C_{2,\infty}^2C_{max}^2;\ C_{3,\infty}^2;\ C_{4,\infty}C_{max}^2;\ C_{5,\infty}^2\right\}. \tag{4.51}$$

By using (4.50), it is sufficient to prove (4.47) provided

$$C_{3,\infty}^2\left((\mu_1-\mu_3)^2+(\mu_3-\mu_5)^2\right) \ge \zeta_1(\mu_1^2+\mu_3^2+\mu_5^2). \tag{4.52}$$

We now solve $\mu_3$ in terms of $\mu_1$ and $\mu_5$ from (4.38) as

$$\mu_3 = -\left(\frac{C_{1,\infty}^2}{C_{3,\infty}^2}\frac{\mu_1+2}{\mu_3+2}\right)\mu_1 - \left(\frac{C_{5,\infty}^2}{C_{3,\infty}^2}\frac{\mu_5+2}{\mu_3+2}\right)\mu_5 =: -Q_1(\mu_1,\mu_3)\mu_1 - Q_2(\mu_5,\mu_3)\mu_5 \tag{4.53}$$

in which

$$0 < C_{min} \le Q_1(\mu_1,\mu_3), Q_2(\mu_5,\mu_3) \le C_{max} < +\infty.$$

From (4.53), we estimate

$$\begin{aligned}
C_{3,\infty}^2\left((\mu_1-\mu_3)^2+(\mu_3-\mu_5)^2\right) &\ge \frac{C_{3,\infty}^2}{C_{max}^2}\left((Q_1\mu_1-Q_1\mu_3)^2+(Q_2\mu_3-Q_2\mu_5)^2\right)\\
&\ge \frac{C_{3,\infty}^2}{2C_{max}^2}\left((Q_1+Q_2)\mu_3-(Q_1\mu_1+Q_2\mu_5)\right)^2\\
&= \frac{C_{3,\infty}^2}{2C_{max}^2}(Q_1+Q_2+1)^2\mu_3^2\\
&\ge \frac{C_{3,\infty}^2(2C_{min}+1)^2}{2C_{max}^2}\mu_3^2.
\end{aligned}$$

Hence, the left hand side of (4.52) can be estimated as follows

$$\begin{aligned}
&C_{3,\infty}^2\left((\mu_1-\mu_3)^2+(\mu_3-\mu_5)^2\right)\\
&\ge \frac{C_{3,\infty}^2(2C_{min}+1)^2}{4C_{max}^2}\mu_3^2 + \frac{1}{2}C_{3,\infty}^2\left((\mu_1-\mu_3)^2+(\mu_3-\mu_5)^2\right)\\
&\ge \frac{1}{4}\min\left\{\frac{C_{3,\infty}^2(2C_{min}+1)^2}{6C_{max}^2};\ C_{3,\infty}^2\right\}\left(\mu_1^2+\mu_3^2+\mu_5^2\right).
\end{aligned} \tag{4.54}$$

That means we have proved (4.52) with

$$\zeta_1 = \frac{1}{4}\min\left\{\frac{C_{3,\infty}^2(2C_{min}+1)^2}{6C_{max}^2};\ C_{3,\infty}^2\right\},$$

thus from (4.50) and (4.51), we have proved (4.33) with

$$\zeta = \frac{\zeta_1}{4\max\left\{C_{1,\infty}^2;\ C_{2,\infty}^2C_{max}^2;\ C_{3,\infty}^2;\ C_{4,\infty}C_{max}^2;\ C_{5,\infty}^2\right\}}.$$

$\square$

## 5. Further Applications and Open Problems

5.1. **Further applications.** In this paper, we exploit the entropy method to show the convergence to equilibrium for chemical reaction networks of chemical substances reacting in a bounded domain $\Omega \subset \mathbb{R}^n$. More precisely, we propose a constructive method to prove an EED estimate, which is the main ingredient of the entropy method.

We point out that the proposed method works also for reaction networks where the chemical substances exist on different domains. For example, for a bounded domain $\Omega \subset \mathbb{R}^n$, we consider a reversible reaction

$$\alpha\mathcal{U} \leftrightharpoons \beta\mathcal{V}$$

where $\mathcal{U}$ is a domain-chemical substance inside $\Omega$ and $\mathcal{V}$ is a surface-chemical substance on $\partial\Omega$, and the reaction is assumed to happen on $\partial\Omega$. The corresponding (volume-surface) reaction-diffusion system reads as

$$\begin{cases} u_t - d_u\Delta u = 0, & x \in \Omega, \quad t > 0,\\ d_u\partial_\nu u = -\alpha(u^\alpha - v^\beta), & x \in \partial\Omega, \quad t > 0,\\ v_t - d_v\Delta_{\partial\Omega} v = \beta(u^\alpha - v^\beta), & x \in \partial\Omega, \quad t > 0,\\ u(0,x) = u_0(x), \quad v(0,x) = v_0(x), \end{cases} \tag{5.1}$$

in which $u : \Omega \times \mathbb{R}_+ \to \mathbb{R}_+$ is the volume-concentration of $\mathcal{U}$ and $v : \partial\Omega \times \mathbb{R}_+ \to \mathbb{R}_+$ is the surface-concentration of $\mathcal{V}$, and $\Delta_{\partial\Omega}$ is the Laplace-Beltrami operator which presents the diffusion of $\mathcal{V}$ along $\partial\Omega$. The system (5.1) possesses the mass conservation

$$\int_\Omega u(x,t)dx + \int_{\partial\Omega} v(x,t)dS = \int_\Omega u_0(x)dx + \int_\Gamma v_0(x)dS =: M > 0$$

and thus has a unique positive equilibrium $(u_\infty, v_\infty)$ satisfying

$$\begin{cases} u_\infty^\alpha = v_\infty^\beta,\\ |\Omega|u_\infty + |\Gamma|v_\infty = M. \end{cases}$$

To show the convergence to equilibrium for (5.1), we consider the entropy functional

$$\mathcal{E}(u,v) = \int_\Omega (u\log u - u + 1)dx + \int_\Gamma (v\log v - v + 1)dS$$

and its entropy dissipation

$$\mathcal{D}(u,v) = d_u\int_\Omega \frac{|\nabla u|^2}{u}dx + d_u\int_\Gamma \frac{|\nabla_\Gamma v|^2}{v}dS + \int_\Gamma (u^\alpha - v^\beta)\log\frac{u^\alpha}{v^\beta}dS.$$

The aim is to prove an EED estimate of the form

$$\mathcal{D}(u,v) \geq \lambda_M(\mathcal{E}(u,v) - \mathcal{E}(u_\infty, v_\infty)), \tag{5.2}$$

for all $(u,v)$ satisfying the mass conservation $\int_\Omega u(x)dx + \int_\Gamma v(x)dS = M$.

The EED estimate (5.2) can be proved by applying the method proposed in Section 2 with only few changes, e.g. the Poincaré inequality $\|\nabla f\|^2_{L^2(\Omega)} \geq C_P\|f - \overline{f}\|^2_{L^2(\Omega)}$ is replaced by the Trace inequality $\|\nabla f\|^2_{L^2(\Omega)} \geq C_T\|f - \overline{f}\|^2_{L^2(\partial\Omega)}$. The reader is referred to [FLT14] for more details.

5.2. **Open Problems.** There are many open problems connecting the problem considered in this paper. We list here the two problems we find the most interesting:

1. (How to choose the conservation laws in the general case?)
   As mentioned in the introduction, the conservation laws $\mathbb{Q}\,\overline{\mathbf{c}} = \mathbf{M}$ depends on the choice of the matrix $\mathbb{Q}$, which has rows forming a basis of $\ker(W)$, where $W$ is the Wegscheider matrix. The choice of $\mathbb{Q}$ is not unique and in fact, there are infinitely many matrices like $\mathbb{Q}$. The question is: can we have a procedure or a method to

choose such a matrix $\mathbb{Q}$, which is suitable for our method and allows to complete the proof of **step 4** in the general case?

2. (How to get optimal convergence rate?)
We made it clear in this paper (see Remark 2.3) that although we obtain an explicit bound for the convergence rate, the convergence rate in this work is non-optimal. The question of optimal convergence rate using the entropy method is left for future investigation.

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## References

[AMTU01] Arnold, A., Markowich, P., Toscani, G., Unterreiter, A.: On convex Sobolev inequalities and the rate of convergence to equilibrium for FokkerPlanck type equations. Commun. Part. Differ. Equ. **26** (2001) 43–100.

[BCD07] M. Bisi, F. Conforto and L. Desvillettes, *Quasi-steady-state approximation for reaction–diffusion equations*, Bull. Inst. Math. Acad. Sin. (N.S.) **2** (2007) 823– 850.

[BP10] D. Bothe and M. Pierre, *Quasi-steady-state approximation for a reaction-diffusion system with fast intermediate*, J. Math. Anal. Appl. **368** (2010) 120–132.

[CDF08] J.A. Carrillo, L. Desvillettes and K. Fellner, *Exponential decay towards equilibrium for the inhomogeneous Aizenman-Bak model*, Communications in Mathematical Physics, **278** (2008), 433-451.

[CDF08a] J.A. Carrillo, L. Desvillettes and K. Fellner, *Fast-Reaction Limit for the Inhomogeneous Aizenman-Bak Model,* Kinetic and Related Models **1** (2008) 127-137.

[CV03] J. Carrillo, J.L. Vazquez, *Fine asymptotics for fast diffusion equations,* Comm. Partial Differential Equations **28**, (2003), 1023–1056.

[CDSS09] G. Craciun, A. Dickenstein, A. Shiu, and B. Sturmfels. *Toric dynamical systems,* J. Symb. Comput., **44** (2009), 1551–1565.

[PD02] M. Del Pino, J. Dolbeault, *Best constants for Gagliardo-Nirenberg inequalities and applications to nonlinear diffusions,* J. Math. Pures Appl. **81**, **9** (2002), 847–875.

[DF06] L. Desvillettes, K. Fellner, *Exponential decay toward equilibrium via entropy methods for reaction-diffusion equations*, J. Math. Anal. Appl. **319**, (2006) 157 - 176.

[DF07] L. Desvillettes, K. Fellner, *Entropy methods for reaction-diffusion equations: degenerate diffusion*, Discrete. Cont. Dyn. Sys. Supplements Special (2007) 304 - 312.

[DF08] L. Desvillettes, K. Fellner, *Entropy methods for reaction-diffusion equations: slowly growing a-priori bounds*, Revista Matematica Iberoamericana. **24** (2008) 407 - 431.

[DF14] L. Desvillettes, K. Fellner, *Exponential Convergence to Equilibrium for a Nonlinear Reaction-Diffusion Systems Arising in Reversible Chemistry*, System Modelling and Optimization, IFIP AICT, **443** (2014) 96–104.

[DV00] L. Desvillettes, C. Villani, *On the spatially homogeneous Landau equation for hard potentials. II. $H$-theorem and applications,* Comm. Partial Differential Equations **25**, no. 1-2 (2000), 261–298.

[DV01] L. Desvillettes, C. Villani, *On the trend to global equilibrium in spatially inhomogeneous entropy-dissipating systems: the linear Fokker-Planck equation,* Comm. Pure Appl. Math. **54**, **1** (2001), 1–42.

[DV05] L. Desvillettes, C. Villani, *On the trend to global equilibrium for spatially inhomogeneous kinetic systems: the Boltzmann equation,* Inventiones Mathematicae. **159**, (2005) 245–316.

[FL] K. Fellner, E.-H. Laamri, *Exponential decay towards equilibrium and global classical solutions for nonlinear reaction-diffusion systems*, preprint.

[FLT14] K. Fellner, E. Latos and B.Q. Tang, *Well-posedness and exponential equilibration of a volume-surface reaction-diffusion system with nonlinear boundary coupling*, arXiv:1404.2809 [math.AP].

[FNS04] K. Fellner, L. Neumann, C. Schmeiser, *Convergence to global equilibrium for spatially inhomogeneous kinetic models of non-micro-reversible processes*, Monatsh. Math. **141**, (2004), 289–299.

[Fis15] J. Fischer, *Global existence of renormalized solutions to entropy-dissipating reaction-diffusion systems*, to appear in Arch. Ration. Mech. Anal., 2015.

[GGH96] A. Glitzky, K. Gröger, R. Hünlich, *Free energy and dissipation rate for reaction-diffusion processes of electrically charged species,* Appl. Anal. **60**, (1996), 201–217.

[GH97] A. Glitzky, R. Hünlich, *Energetic estimates and asymptotics for electro-reaction-diffusion systems,* Z. Angew. Math. Mech. **77** (1997), 823–832.

[Gro92] K. Gröger, *Free energy estimates and asymptotic behaviour of reaction-diffusion processes,* Preprint 20, Institut für Angewandte Analysis und Stochastik, Berlin, 1992.

[Pie10] Pierre, M., *Global existence in reactiondiffusion systems with control of mass: a survey.* Milan J. Math. **78** (2010), 417–455.

[MHM14] A. Mielke, J. Haskovec, P. A. Markowich, *On uniform decay of the entropy for reaction-diffusion systems*, to appear in J. Dyn. Diff. Eqs, 2014.

[Mur02] James D. Murray, *Mathematical Biology*, Springer, 2002.

[TV99] G. Toscani, C. Villani, *Sharp entropy dissipation bounds and explicit rate of trend to equilibrium for the spatially homogeneous Boltzmann equation,* Comm. Math. Phys. **203** (1999), 667–706.

[TV00] G. Toscani, C. Villani, *On the trend to equilibrium for some dissipative systems with slowly increasing a priori bounds,* J. Statist. Phys. **98** (2000), 1279–1309.

[Vil03] C. Villani, *Cercignani's conjecture is sometimes true and always almost true,* Comm. Math. Phys. **234** (2003), 455–490.

Bao Quoc Tang[1,2]

[1] Institute of Mathematics and Scientific Computing, University of Graz, Heinrichstra$\beta$e 36, 8010 Graz, Austria

[2] Faculty of Applied Mathematics and Informatics, Hanoi University of Sience and Technology, 1 Dai Co Viet, Hai Ba Trung, Hanoi, Vietnam

*E-mail address*: `quoc.tang@uni-graz.at`

Klemens Fellner

Institute of Mathematics and Scientific Computing, University of Graz, Heinrichstra$\beta$e 36, 8010 Graz, Austria

*E-mail address*: `klemens.fellner@uni-graz.at`