

CONVERGENCE TO THE COMPLEX BALANCED
EQUILIBRIUM FOR SOME CHEMICAL REACTION-DIFFUSION
SYSTEMS WITH BOUNDARY EQUILIBRIA

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ABSTRACT. In this paper we study the rate of convergence to the complex balanced equilibrium for some chemical reaction-diffusion systems with boundary equilibria. We first analyze a three-species system with boundary equilibria in some stoichiometric classes, and whose right hand side is bounded above by a quadratic nonlinearity in the positive orthant. We prove similar results on the convergence to the positive equilibrium for a fairly general two-species reversible reaction-diffusion network with boundary equilibria.

1. Introduction. The dynamical behavior of spatially homogeneous mass-action reaction systems has been the focus of much research over the last fifty years. These ODE systems are usually high-dimensional, non-linear, and depend on a large number of parameters, which makes them generally difficult to study. However, a fertile theory started fifty years ago with work of Horn, Jackson and Feinberg [15, 22, 23] has been successful in addressing questions of existence and stability of positive equilibria, and persistence (nonextinction) of variables. Their work shows that, surprisingly, the large class of *complex balanced* mass-action systems have unique positive equilibria which admit a global Lyapunov function, which makes them locally asymptotically stable independently of reaction rate constant values. This robustness is relevant in applications, where exact values of system parameters are typically unknown. Moreover, Horn conjectured that the unique equilibria are in fact globally asymptotically stable [23], a question known as the *Global Attractor Conjecture*. The conjecture stayed open until recent years, when new work fueled in

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part by advances in systems biology led to a series of partial results. It was shown that trajectories of complex balanced systems either converge to the positive equilibrium or go to boundary equilibria [32, 34], establishing that persistence implies global stability. A series of subsequent papers showed persistence for complex balanced systems in two variables and other classes of systems, and proved the Global Attractor Conjecture in two and three variables [1–3, 7, 8, 21, 28]. This work led to a proposed proof of the Global Attractor Conjecture in full generality [9].

Much less is known about the corresponding reaction-diffusion models, although a number of recent papers have focused on extending the results above in the PDE setting. A promising venue for relating the PDE and ODE models is by way of space discretization (the method of lines). As proof of concept, the network $A + B \rightleftharpoons C$ was considered in [27] where it was shown that solutions of the discretized system converge to the solution of the PDE system as the space discretization grows finer. Solutions of the reaction-diffusion system $A + B \rightleftharpoons C$ have been shown to approach a positive spatially homogeneous distribution [31] via semigroup theory. Newer work uses entropy techniques to prove global asymptotic stability for other systems, including dimerization networks $2A \rightleftharpoons B$ [10] and monomolecular networks [16].

For reversible complex balanced systems, recent work by Fischer established global existence of a certain notion of renormalized solutions [18]. Siegel and Mincheva showed that, with equal diffusion constants, ω -limit sets of general complex-balanced reaction-diffusion systems consist of constant functions corresponding to equilibria of the space-homogeneous ODEs [26]. Moreover, the unique positive equilibria are asymptotically stable. This is the analogous of the “persistence implies global stability” result from the ODE setting, albeit in the case of equal diffusion constants. Recent results by Desvillettes, Fellner and collaborators [12, 14, 17] removed the requirement of equal diffusion constants, and showed that in the absence of boundary equilibria, the positive equilibrium of a general complex balanced reaction-diffusion system attracts all solutions with positive initial data. These papers also considered special cases of networks with boundary equilibria, where a detailed analysis showed that positive solutions remain globally asymptotically stable. However, the general case of systems with boundary equilibria remains open, and the analysis of such systems is on a case-by-case basis.

A recent paper by Pierre et al [29] studies the general case of a reversible reaction; the authors prove that for nonnegative initial data in $L^1 \cap L \log L$, the solution will converge to some equilibrium. If the equilibrium happens to be the unique complex-balanced equilibrium in the given stoichiometric class (as opposed to a boundary equilibrium), then it is shown that the convergence is exponential. Furthermore, if the solution is globally (in time) essentially bounded, [29] also shows that the solution converges exponentially to the complex-balanced equilibrium.

Our paper studies two such special cases of complex balanced reaction networks with boundary equilibria, and uses the entropy method to show that in one spatial dimension under mild boundedness conditions on the initial data, solutions converge asymptotically to the unique positive equilibrium at explicit rates. Namely, we consider the three-species system $A + 2B \rightleftharpoons B + C$ (Theorem 1.1), and the two-species system $m_1 A + n_1 B \rightleftharpoons m_2 A + n_2 B$ (Theorem 1.2).

In the remainder of this introductory section we set up terminology and notation, we discuss some of the techniques used here and in previous work, and we state our main theorems. Sections 2 and 3 contain the proofs of the results for the three-species and two-species systems. We conclude with a few remarks and open

problems (Section 4), and with an appendix collecting a few technical results needed in the paper.

1.1. Terminology and previous results. Let us consider $0 < T \leq \infty$ and the semilinear parabolic system

$$\mathbf{c}_t - \mathcal{D}\Delta\mathbf{c} = R(\mathbf{c}) \text{ in } \Omega \times (0, T) \quad (1)$$

with initial data

$$\mathbf{c}(\cdot, 0) = \mathbf{c}_0 \text{ in } \Omega,$$

where $\mathbf{c} : \Omega \times [0, T] \rightarrow \mathbb{R}^n$ is the vector of concentrations at spatial position $x \in \Omega$ (an open subset of \mathbb{R}^d) and time $t \in [0, \infty)$, \mathcal{D} is a positive definite, diagonal $n \times n$ matrix, and $R : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is a vector field whose components are polynomials (determined by the chemical reactions under consideration). We exclusively consider Neumann boundary conditions throughout this work:

$$\nabla c_i \cdot \nu = 0 \text{ on } \partial\Omega \times (0, T), \quad i = 1, \dots, n,$$

where ν is the outer normal vector to the boundary. This system can be linear and “trivial” (at least in the sense that “enough” of its equations decouple), such as

$$\begin{aligned} a_t - d_a \Delta a &= -ka, \\ b_t - d_b \Delta b &= ka \text{ in } \Omega \times (0, T), \end{aligned}$$

(which corresponds to the reaction $A \rightarrow B$ with reaction rate $k > 0$), linear and nontrivial (weakly coupled) such as

$$\begin{aligned} a_t - d_a \Delta a &= -k_1 a + k_2 b, \\ b_t - d_b \Delta b &= k_1 a - k_2 b \text{ in } \Omega \times (0, T), \end{aligned}$$

(which corresponds to $A \xrightleftharpoons[k_2]{k_1} B$), or (as soon as a reaction includes two or more reactants) nonlinear in the zero order terms (semilinear). For example, the single reaction $A + B \xrightarrow{k} C$ yields

$$\begin{aligned} a_t - d_a \Delta a &= -kab, \\ b_t - d_b \Delta b &= -kab, \\ c_t - d_c \Delta c &= kab \text{ in } \Omega \times (0, T). \end{aligned}$$

We use this last system to illustrate, rather informally, some terminology and notation. Here A , B , and C are the three *species* of the network, and $A + B$ and C are its *complexes*. In general, complexes are formal linear combinations of species with non-negative integer coefficients, and sit on both sides of a reaction arrow. It is useful to think of complexes as vectors in a natural way, for example $A + B$ corresponds to $y = (1, 1, 0)$, and C to $y' = (0, 0, 1)$. The concentrations of A , B , C are non-negative functions of time and space and are collected in the *concentration vector* $\mathbf{c} = (a, b, c)$. The *reaction rate* of a reaction is given by mass-action, and is proportional to the concentration of each reactant species. This way, the reaction $A + B \xrightarrow{k} C$ has rate kab . The *reaction rate constant* k is a reaction-specific positive number. In general, the rate of a the reaction $y \xrightarrow{k} y'$ is given by

$$k\mathbf{c}^y = k \prod_{i=1}^n c_i^{y_i},$$

where n is the number of species, and complexes y and y' are viewed as vectors, as discussed above. The reaction rate kab enters with negative sign in the equations

for a_t and b_t (A and B are being consumed in the reaction), and with positive sign in the equation for c_t (C is being produced). Reaction rates are collected in the vector $R(\mathbf{c}) = (-kab, -kab, kab)$. In general, this is given by

$$R(\mathbf{c}) := \sum_{y \rightarrow y'} k_{y \rightarrow y'} \mathbf{c}^y (y' - y),$$

where $k_{y \rightarrow y'}$ is the rate constant of $y \rightarrow y'$ and the summation is over all reactions $y \rightarrow y'$ in the network. Finally, $\mathcal{D} = \text{diag}\{d_a, d_b, d_c\} \in M_{3 \times 3}(\mathbb{R})$ denotes the diagonal matrix of diffusion constants.

In the previous example the first two equations have the benefit of being decoupled, but that feature is lost as soon as we allow for reversibility; indeed, corresponding to $A + B \xrightleftharpoons[k_2]{k_1} C$ we have

$$\begin{aligned} a_t - d_a \Delta a &= -k_1 ab + k_2 c, \\ b_t - d_b \Delta b &= -k_1 ab + k_2 c, \\ c_t - d_c \Delta c &= k_1 ab - k_2 c \text{ in } \Omega \times (0, T). \end{aligned} \tag{2}$$

When it comes to basic questions on the existence, uniqueness, smoothness and non-negativity of solutions (if the initial data components are nonnegative), for linear systems the answers are provided in the (by now, classical) literature (see, e.g., [30]). However, complexity adds quickly as nonlinear reactions and more reactants enter the system.

In this paper we discuss examples of chemical reaction diffusion systems which have a specific structure relative to a *positive equilibrium*, i.e. a steady state solution with all positive components.

In general, we say that an equilibrium point c_0 of a *reaction system* (i.e. an equilibrium of the ODE system $\mathbf{c}_t = R(\mathbf{c})$; diffusion is removed) is a *complex balanced equilibrium* if for all complexes \bar{y} we have

$$\sum_{\bar{y} \rightarrow y} k_{\bar{y} \rightarrow y} c_0^{\bar{y}} = \sum_{y \rightarrow \bar{y}} k_{y \rightarrow \bar{y}} c_0^y.$$

In other words, the total chemical flux that exits the complex \bar{y} equals the total chemical flux that enters the complex \bar{y} (for any choice of \bar{y}). A reaction system is called *complex balanced* if it admits a positive complex balanced equilibrium. We call a reaction-diffusion system complex balanced if its corresponding reaction system is complex balanced. It was shown that all steady states of a complex balanced reaction-diffusion system are constant functions (do not depend on space), whose values equal the steady states of the corresponding complex balanced reaction system [26]. We can therefore identify the steady states (equilibria) of complex balanced reaction-diffusion systems with those of corresponding reaction systems.

Reaction systems often admit linear first integrals, called *conservation laws*; for example, the single reaction $A + B \rightarrow C$ has conservation laws $a + c = \text{const}$ and $b + c = \text{const}$. In this paper, an *accessible boundary equilibrium* of a reaction network is an equilibrium on the boundary of the positive orthant which gives the same values of the conservation laws as some phase point with strictly positive coordinates. These are the only equilibria that might be reachable from positive initial conditions, and the only ones relevant for positive solutions of the mass-action system. We note that not all equilibria on the boundary are accessible boundary equilibria. For example, $A + B \rightarrow A$ has one conservation law $a = \text{const}$. The positive a -axis $\{(a, 0) | a > 0\}$ consists of accessible boundary equilibria. On the other

hand, all points $\{(0, b) | b \geq 0\}$ on the non-negative b -axis are boundary equilibria which are not accessible (the conservation law $a = 0$ is not compatible with points in the positive orthant). The distinction between accessible boundary equilibria and inaccessible ones was relevant in previous work [14], although it was not made explicit. In that paper it was shown that for complex-balanced reaction-diffusion systems without accessible boundary equilibria, certain existence conditions imply convergence of solutions to positive equilibria. The reaction-diffusion systems we consider in this paper are complex-balanced with accessible boundary equilibria.

All systems arising from complex balanced reaction diffusion systems admit a “canonical” Lyapunov functional of the relative Boltzmann entropy type. Its general form (again, see, e.g., [14]), this logarithmic free relative energy functional reads

$$E(t) := \sum_{i=1}^n \int_{\Omega} \left[c_i(x, t) \log \frac{c_i(x, t)}{c_{i,\infty}} - c_i(x, t) + c_{i,\infty} \right] dx,$$

where $\mathbf{c}_{\infty} := (c_{1,\infty}, \dots, c_{n,\infty})$ is the constant vector denoting the positive complex balanced equilibrium. The entropy dissipation functional is computed by differentiating E along trajectories; that is, once all the time derivatives of concentrations are replaced by their equation specific expressions and the Neumann BC are used to integrate by parts wherever the Laplacian appears, one gets

$$D(t) := \sum_{i=1}^n d_i \int_{\Omega} \frac{|\nabla c_i(x, t)|^2}{c_i(x, t)} dx + \sum_{r=1}^{\rho} k_r c_{\infty}^{y_r} \int_{\Omega} \Phi \left(\frac{c^{y_r}}{c_{\infty}^{y_r}}; \frac{c^{y'_r}}{c_{\infty}^{y'_r}} \right) dx,$$

where ρ is the number of reactions and $\Phi(x, y) := x \log(x/y) - x + y$. Of course, one gets exponential decay to zero for E if one can prove that there exists a positive constant α such that

$$D(t) \geq \alpha E(t) \text{ for all } t \geq 0. \quad (3)$$

Naturally, $E(t)$ should not only be identically zero when $\mathbf{c}(t) = \mathbf{c}_{\infty}$, but it should also be bounded below by some increasing function of the distance (from some norm) between $\mathbf{c}(t)$ and \mathbf{c}_{∞} .

For complex balanced systems, in the spatially isotropic case ($\mathcal{D} = 0$, so the PDE’s are reduced to ODE’s) recent work by Craciun [9] answers in the affirmative a long standing conjecture on the convergence to the positive equilibrium in each stoichiometric class, called the Global Attractor Conjecture. This conjecture states that regardless of the existence of boundary equilibria, trajectories starting in the positive orthant converge to the unique positive equilibrium in the corresponding stoichiometric class. In the PDE case, the most general result concerns the case where there are no boundary equilibria. Very recently, Desvillettes, Fellner and Tang [14] showed that, contingent on the existence of suitable solutions (essentially, solutions that may not be classical but they are *renormalized* and do satisfy a weak entropy entropy-dissipation law), one obtains exponentially fast convergence to the equilibrium which lies in the same stoichiometric class as the initial data, which is merely assumed nonnegative and integrable over some bounded, C^2 domain in \mathbb{R}^d . This is also a remarkably general result in the sense that the initial concentrations are only assumed to lie in $L^1(\Omega)$. This improvement (over the previous works, where L^∞ -bounds were imposed on the initial data) is achieved via the use of the Log-Sobolev inequality (see, e.g., [14]) in order to establish the *entropy-entropy dissipation inequality* (EEDI) (3). In all the previous works, the EEDI follows from the standard zero-average Poincaré inequality applied to the square roots of the concentration functions, combined with their uniform L^∞ -bounds (in space-time);

these bounds need to be proved a priori. This uniform L^∞ -bound is key to the proofs of convergence to equilibrium in most of the works on this topic, (in fact, to our knowledge, the only exception comes when there are no boundary equilibria [14]) and the constant α from the EEDI (3) tends to vanish as the L^∞ -bound on the solution blows up. We note that (2) is one of the two systems studied in [10], and the authors use the uniform L^∞ -bound as available in the literature (for this particular system). In [27] the authors carry out the proof in some detail (adapted from a proof in [5]), and show that the properties of the Neumann Heat Kernel involved in it hold for the discrete Neumann Heat Kernel as well; as a consequence, one can emulate the proof in the continuous case to obtain uniform L^∞ bounds for the discretized problem. The main idea of the proof is a bootstrapping argument in which the bounds obtained on a and b in terms of c (from the first two equations of (2) we get $a_t - k_a \Delta a \leq k_2 c$ and $b_t - k_b \Delta b \leq k_2 c$) are fed into the inequality $c_t - k_c \Delta c \leq k_1 a b$ (from the third equation of (2)) to yield an L^∞ bound on c at some time $t \geq \delta > 0$ in terms of a sublinear function of the bound at times $t \leq \delta/2$. The success of this method relies on the right hand sides of the first two equations of (2) being bounded above in the positive orthant by a constant multiple of c . It therefore fails for systems where all complexes involve multiple species or multiple occurrences of the same species (such as $A + B \rightleftharpoons 2C$). These bounds are crucial to the proof of consistency and, ultimately, convergence [27].

Our method to prove these uniform L^∞ bounds seems confined to one-D, as it uses the stronger form of Poincaré's inequality on a bounded interval (where the essential sup norm of a Sobolev function is bounded in terms of its average and the L^1 norm of its Sobolev derivative). This leads to a uniform estimate (with respect to t) of the L^2 norm of the solutions in cylinders of type $(t, t+1) \times (0, 1)$, which, once more using $d = 1$, leads to a uniform in time L^∞ bound in the case where one of the right hand side polynomials is bounded above by a quadratic polynomial. It is an important improvement that we can deal with the quadratic case, since previous results (when accessible boundary equilibria are present) only dealt with two species reactions or, if at least three species are present, the right hand side of an equation from the system is dominated by a first-degree polynomial [10], [11], [12], [13], [16] etc.

1.2. The three-species system. A case not covered so far in the literature is $A + 2B \rightleftharpoons B + C$; this has accessible boundary equilibria in some (not all) stoichiometric classes, translates to a 3×3 system (2×2 being, in general, easier to treat via the standard maximum principle for the heat equation), and the right hand side is not bounded above (in the positive orthant) by a linear term. More precisely, the PDE system we are looking at is

$$\begin{cases} a_t - d_a \Delta a = -k_1 a b^2 + k_2 b c \\ b_t - d_b \Delta b = -k_1 a b^2 + k_2 b c \\ c_t - d_c \Delta c = k_1 a b^2 - k_2 b c \\ \nabla a \cdot \nu = \nabla b \cdot \nu = \nabla c \cdot \nu = 0 \\ a(\cdot, 0) = a_0, b(\cdot, 0) = b_0, c(\cdot, 0) = c_0 \end{cases} \quad \begin{array}{l} \text{in } \Omega \times (0, \infty) \\ \text{on } \partial\Omega \times (0, \infty) \\ \text{in } \Omega, \end{array} \quad (4)$$

where ν is the (outward) normal vector to $\partial\Omega$. We can, without loss of generality, assume that $k_1 = k_2 = 1$. Indeed, note that upon changing to $\tilde{a}(x, t) = \alpha a(x, \tau t)$, $\tilde{b}(x, t) = \alpha b(x, \tau t)$, $\tilde{c}(x, t) = \alpha c(x, \tau t)$ for $\alpha = k_1 k_2^{-1}$ and $\tau = k_1 k_2^{-2}$ we end up with (4) satisfied by \tilde{a} , \tilde{b} , \tilde{c} with $k_1 = k_2 = 1$, $d_{\tilde{a}} = \tau d_a$, $d_{\tilde{b}} = \tau d_b$, $d_{\tilde{c}} = \tau d_c$ and initial

conditions αa_0 , αb_0 , αc_0 . We assume $d = 1$ and (possibly after an affine spatial transformation, and without loss of generality) $\Omega = (0, 1)$. The restriction $d = 1$ is sufficient to obtain the uniform L^∞ bound on the solution, which is crucial to our analysis. We can (for the time being) only justify this uniform bound in the $d = 1$ case; note that only the estimates in subsection 2.1 are predicated on this restriction.

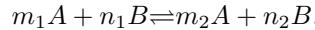
The conserved (in time) quantities here are $\bar{a} + \bar{c}$ and $\bar{b} + \bar{c}$, where \bar{f} denotes the average of the function f over Ω . If $b_\infty > 0$ we obviously can only have a boundary equilibrium at $(0, b_\infty, 0)$ (i.e. $a_\infty = c_\infty = 0$). The conservation of $\bar{a} + \bar{c}$ forces $a \equiv c \equiv 0$, the second equation of the system decouples into $b_t - d_b b_{xx} = 0$, and $b_\infty = \bar{b}_0$. This steady state cannot be approached from any initial state for which $\bar{a}_0 + \bar{c}_0 > 0$, so $(0, b_\infty, 0)$ is not an accessible boundary equilibrium. The other nontrivial type of steady states is given by $b_\infty = 0$ and $a_\infty + c_\infty = \bar{a}_0 + \bar{c}_0 > 0$. If $c_\infty = 0$, we get $b \equiv c \equiv 0$ (from the conservation of $\bar{b} + \bar{c}$); this is not an accessible boundary equilibrium either, and no initial data in the positive orthant will yield solutions which asymptotically converge to it. If, on the other hand, the initial data is on the b -axis (i.e. $a_0 \equiv c_0 \equiv 0$), then it is easy to see that (a, b, c) will converge exponentially to $(0, b_\infty, 0)$, where $b_\infty = \bar{b}_0$.

We are left with the accessible boundary equilibrium $(a_\infty, 0, c_\infty)$ for $a_\infty c_\infty > 0$. We do not know how to prove that $\bar{a}_0 \bar{b}_0 \bar{c}_0 > 0$ prevents convergence to such a steady state, but in this paper we will prove a slightly weaker statement, namely:

Theorem 1.1. *If $a_0, b_0, c_0 \in L^\infty(0, 1)$ are a.e. positive and such that $b_0 \geq \delta$ a.e. in $(0, 1)$ for some $\delta > 0$, then the (unique) global classical solution to (4) converges asymptotically exponentially fast (at an explicit rate) to the unique positive equilibrium in its stoichiometric class.*

The above theorem will be proved in Section 2.

1.3. The two-species system. Finally, in Section 3 we prove similar results on the convergence to the positive equilibrium for a two-species reversible reaction-diffusion network with accessible boundary equilibria:



Assume m_1, m_2, n_1, n_2 are nonnegative integers and let $\bar{m} := m_1 - m_2$, $\bar{n} := n_2 - n_1$. The 2×2 reaction-diffusion system is

$$\begin{cases} a_t - d_a \Delta a = \bar{m}(k_2 a^{m_2} b^{n_2} - k_1 a^{m_1} b^{n_1}) & \text{in } \Omega \times (0, \infty) \\ b_t - d_b \Delta b = \bar{n}(k_1 a^{m_1} b^{n_1} - k_2 a^{m_2} b^{n_2}) & \text{in } \Omega \times (0, \infty) \\ \nabla a \cdot \nu = \nabla b \cdot \nu = 0 & \text{on } \partial\Omega \times (0, \infty) \\ a(\cdot, 0) = a_0, b(\cdot, 0) = b_0 & \text{in } \Omega. \end{cases} \quad (5)$$

If $\bar{m} \neq \bar{n}$ we can, as in the three species system, change to $\tilde{a}(x, t) = \lambda a(x, \tau t)$, $\tilde{b}(x, t) = \lambda b(x, \tau t)$ for $\lambda = (k_1/k_2)^{1/(\bar{m}-\bar{n})}$ and $\tau = k_1 \lambda^{m_1+n_1-1}$. We end up with (5) satisfied by \tilde{a}, \tilde{b} with $k_1 = k_2 = 1$ (d_a and d_b get multiplied by positive constants). If $\bar{m} = \bar{n} = 0$ no rescaling is necessary, while for $\bar{m} = \bar{n} \neq 0$ we only rescale $\tilde{a}(x, t) = \lambda a(x, t)$ with $\lambda = (k_1/k_2)^{1/\bar{m}}$ to get the system (5) with $k_1 = k_2 = 1$, but where \bar{m} and \bar{n} are multiplied by two positive constants. Thus, it is enough to

study the system

$$\begin{cases} a_t - d_a \Delta a = \lambda_a \bar{m}(a^{m_2} b^{n_2} - a^{m_1} b^{n_1}) & \text{in } \Omega \times (0, \infty) \\ b_t - d_b \Delta b = \lambda_b \bar{n}(a^{m_1} b^{n_1} - a^{m_2} b^{n_2}) & \text{in } \Omega \times (0, \infty) \\ \nabla a \cdot \nu = \nabla b \cdot \nu = 0 & \text{on } \partial\Omega \times (0, \infty) \\ a(\cdot, 0) = a_0, b(\cdot, 0) = b_0 & \text{in } \Omega, \end{cases} \quad (6)$$

where λ_a, λ_b are positive constants.

Theorem 1.2. *Let Ω be a bounded domain of \mathbb{R}^d with a smooth boundary, for some integer $d \geq 1$. If $\bar{m}\bar{n} \geq 0$ and $0 < \alpha \leq a_0(x), b_0(x) \leq \beta < +\infty$ for a.e. x in Ω , then the (unique) global classical solution to (6) converges asymptotically exponentially (at an explicit rate) to the unique positive equilibrium in its stoichiometric class.*

Remarks. (1) The reason for the restriction $\bar{m}\bar{n} \geq 0$ is technical, as the estimates that follow after the conservation law (42) in subsection 3.2 only hold under this restriction.

(2) If initial data is on the b -axis (or, respectively, the a -axis), then the solution (a, b) will converge exponentially to $(0, b_\infty)$ (or, respectively, to $(a_\infty, 0)$). These are the only two types of boundary equilibria in this case, and are both accessible. Theorem 1.2 shows that if the initial condition is bounded away from zero and infinity componentwise, then the solution will not decay to any such boundary equilibrium.

2. Asymptotic decay for the three-species system. We consider the entropy functional $E(a, b, c)$ and the corresponding entropy dissipation (when computed along solutions) $D(a, b, c) = -\frac{d}{dt}E(a, b, c)$ associated to the system:

$$E(a, b, c) = \int_0^1 a(\ln a - 1)dx + \int_0^1 b(\ln b - 1)dx + \int_0^1 c(\ln c - 1)dx \quad (7)$$

and

$$\begin{aligned} D(a, b, c) = & 4d_a \int_0^1 |\partial_x \sqrt{a}|^2 dx + 4d_b \int_0^1 |\partial_x \sqrt{b}|^2 dx + 4d_c \int_0^1 |\partial_x \sqrt{c}|^2 dx \\ & + \int_0^1 (ab^2 - bc) \ln \left(\frac{ab^2}{bc} \right) dx. \end{aligned} \quad (8)$$

We would also like to record (for later use) the following *conservation laws*

$$\begin{aligned} \int_0^1 a(x, t)dx + \int_0^1 c(x, t)dx &= \int_0^1 a_0(x)dx + \int_0^1 c_0(x)dx =: M_1, \\ \int_0^1 b(x, t)dx + \int_0^1 c(x, t)dx &= \int_0^1 b_0(x)dx + \int_0^1 c_0(x)dx =: M_2, \end{aligned} \quad (9)$$

for all $t \geq 0$. Note that these are simply obtained by adding equations 1 and 3 (respectively, 2 and 3) and integrating in space over $[0, 1]$ by taking into account the boundary conditions. Note also that M_1 and M_2 are finite as long as $a_0, b_0, c_0 \in L^1(0, 1)$.

2.1. Local L^2 estimate (a priori estimate).

Proposition 2.1. *Let (a, b, c) be a solution for (4) with initial condition (a_0, b_0, c_0) such that $a_0 > 0$, $b_0 > 0$, $c_0 > 0$ a.e. in $[0, 1]$ and $a_0 \ln a_0, b_0 \ln b_0, c_0 \ln c_0 \in L^1(0, 1)$. Then there exists a real constant C such that*

$$\|a\|_{L^2([0,1] \times [\tau, \tau+1])}, \|b\|_{L^2([0,1] \times [\tau, \tau+1])}, \|c\|_{L^2([0,1] \times [\tau, \tau+1])} \leq C$$

for any $\tau > 0$.

Proof. We start with the obvious inequality (which holds for all $x \in [0, 1]$, $t > 0$)

$$\left| \sqrt{a(x, t)} - \int_0^1 \sqrt{a(y, t)} dy \right| \leq \int_0^1 |\partial_y \sqrt{a(y, t)}| dy,$$

then use Hölder's inequality to get

$$\begin{aligned} a(x, t) &\leq \left(\int_0^1 \sqrt{a(y, t)} dy + \int_0^1 |\partial_y \sqrt{a(y, t)}| dy \right)^2 \\ &\leq 2 \left(\int_0^1 \sqrt{a(y, t)} dy \right)^2 + 2 \left(\int_0^1 |\partial_y \sqrt{a(y, t)}| dy \right)^2 \\ &\leq 2 \int_0^1 a(y, t) dy + 2 \int_0^1 |\partial_y \sqrt{a(y, t)}|^2 dy. \end{aligned} \quad (10)$$

Obviously, the above inequalities also hold for b and c . Next we integrate the entropy dissipation in time to obtain

$$E(a(t), b(t), c(t)) + \int_0^t D(a(s), b(s), c(s)) ds = E(a_0, b_0, c_0),$$

where we have only displayed the dependence on time of the components of the solution vector. Since the last integrand in right hand side of (8) is nonnegative, we conclude

$$\begin{aligned} E(a(t), b(t), c(t)) + 4d_a \int_0^t \int_0^1 |\partial_x \sqrt{a}|^2 dx dt + 4d_b \int_0^t \int_0^1 |\partial_x \sqrt{b}|^2 dx dt + \\ 4d_c \int_0^t \int_0^1 |\partial_x \sqrt{c}|^2 dx dt \leq E(a_0, b_0, c_0). \end{aligned} \quad (11)$$

Since $x(\ln x - 1) \geq -1$ for all $x \geq 0$ (at $x = 0$ this holds in the limiting sense), we get

$$\begin{aligned} 4d_a \int_0^t \int_0^1 |\partial_x \sqrt{a}|^2 dx dt + 4d_b \int_0^t \int_0^1 |\partial_x \sqrt{b}|^2 dx dt + 4d_c \int_0^t \int_0^1 |\partial_x \sqrt{c}|^2 dx dt \\ \leq E(a_0, b_0, c_0) + 3, \end{aligned}$$

which implies

$$\begin{aligned} \|\partial_x \sqrt{a}\|_{L^2([0,1] \times [0,t])}^2 + \|\partial_x \sqrt{b}\|_{L^2([0,1] \times [0,t])}^2 + \|\partial_x \sqrt{c}\|_{L^2([0,1] \times [0,t])}^2 \\ \leq \frac{E(a_0, b_0, c_0) + 3}{4d} := C_1 \end{aligned}$$

for any $t \geq 0$, where $d := \min\{d_a, d_b, d_c\}$. Finally, we take into account (9) and (10) to estimate

$$\begin{aligned} \int_{\tau}^{\tau+1} \int_0^1 a^2 dx dt &\leq \int_{\tau}^{\tau+1} \|a(t)\|_{L^{\infty}[0,1]} \left(\int_0^1 a(x,t) dx \right) dt \\ &\leq 2M_1 \int_{\tau}^{\tau+1} \left(\int_0^1 a(x,t) dx + \int_0^1 |\partial_x \sqrt{a(x,t)}|^2 dx \right) dt \\ &\leq 2M_1 \int_{\tau}^{\tau+1} \left(M_1 + \int_0^1 |\partial_x \sqrt{a(x,t)}|^2 dx \right) dt \leq 2M_1^2 + 2M_1 C_1 =: C \end{aligned}$$

Similar inequalities hold for b and c , therefore we have finished the proof. \square

2.2. Uniform L^{∞} estimate. In this section we shall prove that a classical solution to (4) is bounded uniformly in time (and therefore, it also exists for all time). To achieve this, our goal is to place ourselves in the setting of Theorem 4.1 [19]. We shall refrain from transcribing the assumptions (H1)–(H3) from [19] here, as they are universally satisfied by CRDN systems with nonnegative and essentially bounded initial conditions. On the other hand, assumption (H4') is both specific to our case and nontrivial to verify. We state it below, as it refers to a general semilinear parabolic $m \times m$ system

$$u_{i,t} - \kappa_i \Delta u_i = f_i(x, t, u), \quad i = 1, \dots, m, \quad (12)$$

where $x \in \Omega$, $t > 0$, $u = (u_1, \dots, u_m)$. It reads:

There exist $K_1, K_2 > 0$, $1 \leq p < \infty$, $1 \leq r < 1 + \left[1 - \frac{d}{p(d+2)}\right] \frac{2p}{d+2}$ such that

for each $1 \leq j \leq m$ there exist $\alpha_{j,k}$, $1 \leq j \leq k$ with $\alpha_{j,j} = 1$ such that (13)

$$\sum_{k=1}^j \alpha_{j,k} f_j(x, t, v) \leq K_1 |v|^r + K_2 \text{ for all } v \text{ in the positive orthant of } \mathbb{R}^m.$$

The following result is a version of Theorem 4.1 [19] (see a sketch of proof in Appendix).

Theorem 2.2. *Suppose the initial data $u_{j,0} \in L^{\infty}(\Omega)$, $j = 1, \dots, m$, the generic assumptions (H1)–(H3) from [19] hold. Further assume (13) holds for some $1 \leq p < \infty$ and*

$$\|u\|_{L^p(\Omega \times (\tau, \tau+1); \mathbb{R}^m)} \leq M < \infty \text{ for all } \tau \geq 0. \quad (14)$$

Then

$$u \in L^{\infty}(\Omega \times [0, \infty); \mathbb{R}^m). \quad (15)$$

If we go back to (4) and denote by

$$u := (a, b, c), \quad f := (-ab^2 + bc, -ab^2 + bc, ab^2 - bc)$$

we see that (13) is satisfied with $\alpha_{1,1} = 1, \alpha_{2,1} = -1, \alpha_{2,2} = 1, \alpha_{3,1} = 0, \alpha_{3,2} = -1, \alpha_{3,3} = 1, r = 2, K_1 = k_2/2, K_2 = 0$. Thus, if we can find $1 \leq p < \infty$ such that (14) and the first inequality in (13) (the one bounding r in terms of p) are satisfied, we can apply Theorem 2.2 in order to obtain the uniform L^{∞} bound. But Proposition 2.1 shows that $p = 2$ does the job.

The same reference [19], Theorem 3.1 (checked, along with the preceding Lemma 3.1, to apply to bounded domains and Neumann BC) guarantees that the solution is classical, unique and nonnegative. Therefore, we have proved:

Theorem 2.3. *Let $a_0, b_0, c_0 \in L^\infty(0, 1)$ such that $a_0 > 0, b_0 > 0, c_0 > 0$ a.e. in $(0, 1)$ and $a_0 \ln a_0, b_0 \ln b_0, c_0 \ln c_0 \in L^1(0, 1)$. Then a unique classical solution to the system (4) exists for all time. Furthermore, the solution is uniformly (with respect to time) bounded in $L^\infty(0, 1)$, with bounds depending in a bounded way on the L^∞ norms of the initial data.*

Remark 1. If we approximate the initial data in $L^2(0, 1)$ by BC compatible initial $a_{0,n}, b_{0,n}, c_{0,n}$ which are uniformly bounded in $L^\infty(0, 1)$ by, say, $\eta := 2[\|a_0\|_\infty + \|b_0\|_\infty + \|c_0\|_\infty]$, then we can easily get the bound

$$\begin{aligned} & \|a_n(\cdot, t) - a(\cdot, t)\|_2^2 + \|b_n(\cdot, t) - b(\cdot, t)\|_2^2 + \|c_n(\cdot, t) - c(\cdot, t)\|_2^2 \\ & \leq e^{Ct} [\|a_{0,n} - a_0\|_2^2 + \|b_{0,n} - b_0\|_2^2 + \|c_{0,n} - c_0\|_2^2] \end{aligned}$$

for all $t \geq 0$, where $C = C(\eta) > 0$ is a finite constant. It follows that for any $t \geq 0$, $a_n(t, \cdot)$ converges in $L^2(0, 1)$ to $a(t, \cdot)$ (and likewise for b and c). Furthermore, note that if b_0 is bounded below by $2\delta > 0$, then the approximations $b_{0,n}$ above may also be chosen to satisfy the extra condition $b_{0,n} \geq \delta$ for all n . Via L^1 renormalization the approximations may also be chosen such that the approximating problem has the same complex-balanced equilibrium as the original one.

In the next subsection we use the Log-Sobolev and the Csizar-Kullback-Pinsker inequalities to first prove an entropy-entropy dissipation inequality which guarantees that the solution to (4) decays asymptotically to the complex balanced equilibrium at an explicit algebraic rate.

2.3. L^1 convergence. In view of Remark 1 we may assume a_0, b_0, c_0 to be smooth, positive on $[0, 1]$ and to satisfy the compatibility conditions (i.e. they have zero derivatives at the boundary). Indeed, if we replace the initial data with approximations as in Remark 1, then all the decay constants appearing below may be chosen independent of n . Further assume $\beta = \|\frac{1}{b_0}\|_{L^\infty[0,1]} < \infty$; because the classical solution is continuous on the cylinder $[0, \infty) \times [0, 1]$, there exists $t_1 > 0$ such that $\|\frac{1}{b(\cdot, t)}\|_{L^\infty[0,1]} < 10\beta$ for all $t \in [0, t_1]$. We next divide the second equation in (4) by $-b^2$ and use the uniform (in time) L^∞ boundedness of a to get

$$\partial_t \left(\frac{1}{b} \right) - d_b \Delta \left(\frac{1}{b} \right) = \frac{ab^2}{b^2} - \frac{bc}{b^2} - 2d_b \frac{|\nabla b|^2}{b^3} \leq a \leq k.$$

Using the maximum principle for the heat equation, we have that, for all $t \in [0, t_1]$,

$$\left\| \frac{1}{b(\cdot, t)} \right\|_{L^\infty[0,1]} \leq \left\| \frac{1}{b_0} \right\|_{L^\infty[0,1]} + kt = \beta + kt.$$

We can iterate this inequality in time to get

$$\tilde{b}(t) := \inf_{x \in [0,1]} b(x, t) \geq (\beta + kt)^{-1} \tag{16}$$

for all $t > 0$. Therefore, we now have an estimate on how fast b can decay to zero.

There exists a unique equilibrium with all positive components for (4) and by (4) and (9) we see that it is given by $v_\infty := (a_\infty, b_\infty, c_\infty)$, where its components are uniquely determined by

$$a_\infty b_\infty = c_\infty, \quad a_\infty + c_\infty = M_1, \quad b_\infty + c_\infty = M_2. \tag{17}$$

Now we introduce the *relative entropy*

$$\begin{aligned} E(a, b, c|a_\infty, b_\infty, c_\infty) &= \int_{[0,1]} \left(a \ln \frac{a}{a_\infty} - a + a_\infty \right) dx + \int_{[0,1]} \left(b \ln \frac{b}{b_\infty} - b + b_\infty \right) dx \\ &+ \int_{[0,1]} \left(c \ln \frac{c}{c_\infty} - c + c_\infty \right) dx \end{aligned} \quad (18)$$

and its corresponding *entropy dissipation*

$$\begin{aligned} D(a, b, c|a_\infty, b_\infty, c_\infty) &= d_a \int_{[0,1]} \frac{|\nabla a|^2}{a} dx + d_b \int_{[0,1]} \frac{|\nabla b|^2}{b} dx + d_c \int_{[0,1]} \frac{|\nabla c|^2}{c} dx \\ &+ a_\infty b_\infty^2 \int_{[0,1]} \Psi \left(\frac{ab^2}{a_\infty b_\infty^2}; \frac{bc}{b_\infty c_\infty} \right) dx + b_\infty c_\infty \int_{[0,1]} \Psi \left(\frac{bc}{b_\infty c_\infty}; \frac{ab^2}{a_\infty b_\infty^2} \right) dx, \end{aligned} \quad (19)$$

where

$$\Psi(x; y) = x \ln \left(\frac{x}{y} \right) - x + y. \quad (20)$$

At this point we introduce the notation

$$\bar{f} := \int_{[0,1]} f(x) dx \text{ for all essentially non-negative } f \in L^1(0, 1).$$

On the basis of the following identity

$$\int_{[0,1]} \left(a \ln \frac{a}{a_\infty} - a + a_\infty \right) dx = \int_{[0,1]} \left(a \ln \frac{a}{\bar{a}} - a + \bar{a} \right) dx + \int_{[0,1]} \left(\bar{a} \ln \frac{\bar{a}}{a_\infty} - \bar{a} + a_\infty \right) dx,$$

we get

$$E(a, b, c|a_\infty, b_\infty, c_\infty) = E(a, b, c|\bar{a}, \bar{b}, \bar{c}) + E(\bar{a}, \bar{b}, \bar{c}|a_\infty, b_\infty, c_\infty). \quad (21)$$

The Logarithmic Sobolev Inequality

$$\int_{[0,1]} \frac{|\nabla f|^2}{f} dx \geq C_{LSI} \int_{[0,1]} f \ln \frac{f}{\bar{f}} dx, \quad (22)$$

(where C_{LSI} only depends on the domain $[0, 1]$) yields

$$d_a \int_{[0,1]} \frac{|\nabla a|^2}{a} dx + d_b \int_{[0,1]} \frac{|\nabla b|^2}{b} dx + d_c \int_{[0,1]} \frac{|\nabla c|^2}{c} dx \geq C_2 E(a, b, c|\bar{a}, \bar{b}, \bar{c}) \quad (23)$$

for an explicit constant $C_2 = \min\{d_a, d_b, d_c\} \cdot C_{LSI}$. Next, we define two integrand functions:

$$\begin{aligned} S_1(a, b, c) &:= \left(a \ln \frac{a}{a_\infty} - a + a_\infty \right) + \left(b \ln \frac{b}{b_\infty} - b + b_\infty \right) + \left(c \ln \frac{c}{c_\infty} - c + c_\infty \right), \\ S_2(a, b, c) &:= \Psi \left(\frac{ab}{a_\infty b_\infty}; \frac{c}{c_\infty} \right) + \Psi \left(\frac{c}{c_\infty}; \frac{ab}{a_\infty b_\infty} \right) \end{aligned}$$

and set $S(a, b, c) := S_1(a, b, c) + S_2(a, b, c)$. From (19), (21), (23) and (16) we get

$$\begin{aligned}
D(a, b, c | a_\infty, b_\infty, c_\infty) &\geq C_2 E(a, b, c | \bar{a}, \bar{b}, \bar{c}) \\
&+ a_\infty b_\infty^2 \int_{[0,1]} \Psi\left(\frac{ab^2}{a_\infty b_\infty^2}; \frac{bc}{b_\infty c_\infty}\right) dx + b_\infty c_\infty \int_{[0,1]} \Psi\left(\frac{bc}{b_\infty c_\infty}; \frac{ab^2}{a_\infty b_\infty^2}\right) dx \\
&\geq C_2 [E(a, b, c | a_\infty, b_\infty, c_\infty) - E(\bar{a}, \bar{b}, \bar{c} | a_\infty, b_\infty, c_\infty)] \\
&+ a_\infty b_\infty \tilde{b}(t) \int_{[0,1]} \Psi\left(\frac{ab}{a_\infty b_\infty}; \frac{c}{c_\infty}\right) dx + c_\infty \tilde{b}(t) \int_{[0,1]} \Psi\left(\frac{c}{c_\infty}; \frac{ab}{a_\infty b_\infty}\right) dx \\
&\geq C_2 \int_{[0,1]} S_1(a, b, c) dx - C_2 \int_{[0,1]} S_1(\bar{a}, \bar{b}, \bar{c}) dx \\
&+ (\beta + kt)^{-1} \left[a_\infty b_\infty \int_{[0,1]} \Psi\left(\frac{ab}{a_\infty b_\infty}; \frac{c}{c_\infty}\right) dx + c_\infty \int_{[0,1]} \Psi\left(\frac{c}{c_\infty}; \frac{ab}{a_\infty b_\infty}\right) dx \right] \\
&\geq C_3(t) \left\{ \int_{[0,1]} [S_1(a, b, c) + S_2(a, b, c)] dx - S_1(\bar{a}, \bar{b}, \bar{c}) \right\} \\
&\geq C_3(t) [\hat{S}(\bar{a}, \bar{b}, \bar{c}) - S_1(\bar{a}, \bar{b}, \bar{c})],
\end{aligned} \tag{24}$$

where

$$C_3(t) := (\beta + kt)^{-1} \min\{\beta C_2, a_\infty b_\infty, c_\infty\}$$

and \hat{S} is the *convexification* of S , i.e. the supremum of all affine functions below S . The last inequality above holds due to Jensen's inequality and the unit volume of the spatial domain.

We next define the compatible class:

$$\begin{aligned}
C_{M_1, M_2} := \{v = (x, y, z) \in \mathbb{R}_{\geq 0}^3 : x + z = M_1, y + z = M_2, \\
E(x, y, z | a_\infty, b_\infty, c_\infty) \leq E(a_0, b_0, c_0 | a_\infty, b_\infty, c_\infty)\}.
\end{aligned}$$

In this class, the first two conditions are related to the conservation laws (9) while the last one follows from the decreasing relative entropy. Since we know $\hat{S} = \widehat{S_1 + S_2} \geq \hat{S}_1 + \hat{S}_2$, S_1 is convex and S_2 is non-negative, we have

$$(\hat{S} - S_1)(v) \geq (\hat{S}_1 + \hat{S}_2 - S_1)(v) \geq \hat{S}_2(v) \geq 0. \tag{25}$$

Furthermore, it is not hard to verify that

$$v \in C_{M_1, M_2} \quad \& \quad S_2(v) = 0 \text{ if and only if } v = (a_\infty, b_\infty, c_\infty). \tag{26}$$

It follows

$$\hat{S}_2(v) = 0 \text{ if and only if } v = (a_\infty, b_\infty, c_\infty).$$

Let

$$C_4 := \inf_{v \in C_{M_1, M_2}} \frac{(\hat{S} - S_1)(v)}{E(v | a_\infty, b_\infty, c_\infty)}.$$

By (25) and (26) we get C_4 can only be zero if there exists a sequence $\{v_n\}_n \subset C_{M_1, M_2}$ such that $v_n \rightarrow (a_\infty, b_\infty, c_\infty)$ as $n \rightarrow \infty$. This means

$$\liminf_{v \in C_{M_1, M_2}, v \rightarrow v_\infty} \frac{(\hat{S} - S_1)(v)}{E(v | a_\infty, b_\infty, c_\infty)} > 0 \text{ implies } C_4 > 0.$$

In order to show that the above limit inferior is positive we use the following lemma [25]:

Lemma 2.4. *There exists $\delta > 0$ such that for all $v \in B(v_\infty, \delta)$ (ball centered at v_∞ and of radius delta) $S(v)$ is locally convex in this ball.*

In particular, we get that $\hat{S} \equiv S$ in the ball centered at $(a_\infty, b_\infty, c_\infty)$ with radius δ . Let us now define

$$D_2(v) := a_\infty b_\infty^2 \Psi\left(\frac{ab^2}{a_\infty b_\infty^2}; \frac{bc}{b_\infty c_\infty}\right) + b_\infty c_\infty \Psi\left(\frac{bc}{b_\infty c_\infty}; \frac{ab^2}{a_\infty b_\infty^2}\right)$$

and consider the Taylor expansion of

$$\frac{D_2(v)}{E(v|a_\infty, b_\infty, c_\infty)}$$

around the unique positive equilibrium $(a_\infty, b_\infty, c_\infty)$. Since $a_\infty b_\infty = c_\infty$, we have $D_2(a_\infty, b_\infty, c_\infty) = \nabla D_2(a_\infty, b_\infty, c_\infty) = 0$ and quadratic term in the expansion is

$$D_2(v) = 2 \left[\frac{-(v_1 - a_\infty)}{a_\infty} + \frac{-(v_2 - b_\infty)}{b_\infty} + \frac{(v_3 - c_\infty)}{c_\infty} \right]^2.$$

Thus,

$$\liminf_{v \in C_{M_1, M_2}, v \rightarrow v_\infty} \frac{D_2(v)}{E(v|a_\infty, b_\infty, c_\infty)} = \inf_{v \in C_{M_1, M_2}} \frac{2 \left[\frac{-(x - a_\infty)}{a_\infty} + \frac{-(y - b_\infty)}{b_\infty} + \frac{(z - c_\infty)}{c_\infty} \right]^2}{\frac{(x - a_\infty)^2}{a_\infty} + \frac{(y - b_\infty)^2}{b_\infty} + \frac{(z - c_\infty)^2}{c_\infty}}$$

Since $v \in C_{M_1, M_2}$ (which means $x + z = a_\infty + c_\infty, y + z = b_\infty + c_\infty$), we get

$$-(x - a_\infty) = -(y - b_\infty) = z - c_\infty,$$

Then

$$\inf_{v \in C_{M_1, M_2}} \frac{2 \left[\frac{-(x - a_\infty)}{a_\infty} + \frac{-(y - b_\infty)}{b_\infty} + \frac{(z - c_\infty)}{c_\infty} \right]^2}{\frac{(x - a_\infty)^2}{a_\infty} + \frac{(y - b_\infty)^2}{b_\infty} + \frac{(z - c_\infty)^2}{c_\infty}} = 2 \left(\frac{1}{a_\infty} + \frac{1}{b_\infty} + \frac{1}{c_\infty} \right) > 0.$$

Also notice (by direct computation and using that $c_\infty = a_\infty b_\infty$) the identity $D_2(v) = bc_\infty S_2(v)$, which implies (in view of the above inequality)

$$\liminf_{v \in C_{M_1, M_2}, v \rightarrow v_\infty} \frac{S_2(v)}{E(v|a_\infty, b_\infty, c_\infty)} > 0.$$

Combining the above two steps, we have

$$\begin{aligned} & \liminf_{v \in C_{M_1, M_2}, v \rightarrow v_\infty} \frac{(\hat{S} - S_1)(v)}{E(v|a_\infty, b_\infty, c_\infty)} \\ &= \liminf_{v \in C_{M_1, M_2}, v \rightarrow v_\infty} \frac{S_2(v)}{E(v|a_\infty, b_\infty, c_\infty)} > 0. \end{aligned}$$

Therefore, in light of (24), we obtain

$$D(a, b, c|a_\infty, b_\infty, c_\infty) \geq C_3(t) C_4 E(a, b, c|a_\infty, b_\infty, c_\infty)$$

so,

$$D(a, b, c|a_\infty, b_\infty, c_\infty) \geq C_5(\beta + kt)^{-1} E(a, b, c|a_\infty, b_\infty, c_\infty),$$

where $C_5 = \min\{1, C_4\} \times \min\{\beta C_2, a_\infty b_\infty^2, b_\infty c_\infty\}$. Then Gronwall's lemma yields

$$E(a, b, c|a_\infty, b_\infty, c_\infty) \leq E(a_0, b_0, c_0|a_\infty, b_\infty, c_\infty) (\beta + kt)^{\frac{-C_5}{k}}$$

for all $t > 0$.

Now we need the following lemma [4]:

Lemma 2.5. *For all non-negative and measurable functions $a, b, c : [0, 1] \rightarrow \mathbb{R}$ and $\int_0^1 (a + c) = M_1, \int_0^1 (b + c) = M_2$. Then there exists a constant $C_K > 0$ depending boundedly only on M_1, M_2 such that:*

$$E(a, b, c | a_\infty, b_\infty, c_\infty) \geq C_K (\|a - a_\infty\|_1^2 + \|b - b_\infty\|_1^2 + \|c - c_\infty\|_1^2)$$

Therefore, we get

$$\|a(\cdot, t) - a_\infty\|_1^2 + \|b(\cdot, t) - b_\infty\|_1^2 + \|c(\cdot, t) - c_\infty\|_1^2 \leq C_6 (\beta + kt)^{\frac{-C_5}{k}} \text{ for all } t \geq 0,$$

where $C_6 = \frac{E(a_0, b_0, c_0 | a_\infty, b_\infty, c_\infty)}{C_K}$.

The above inequality shows that the solution stays away from the boundary equilibrium; in fact, its converges to the unique positive equilibrium in the L^1 norm. In order to show that the convergence rate is, in fact, exponential, we use the above inequality to conclude that there exists a time

$$T_\epsilon := \max \left\{ 1, \frac{1}{k} \left(\frac{2}{\min\{a_\infty, b_\infty, c_\infty\}} \right)^{2k/C_5} - \frac{\beta}{k} \right\}$$

such that

$$\|a(t)\|_1, \|b(t)\|_1, \|c(t)\|_1 > \epsilon^2 := \min\{a_\infty, b_\infty, c_\infty\}/2 > 0 \text{ for all } t > T_\epsilon. \quad (27)$$

We pause here briefly to comment on the fact that T_ϵ can also be taken independent of n if the initial data is as in Theorem 2.3 and is approximated as indicated in Remark 1. Thus, in view of Remark 1, we drop here the extra assumptions we made on the initial data in the beginning of this subsection.

2.4. Entropy entropy-dissipation estimate. In what follows we use the lower bound on the total mass of each species for $t \geq T_\epsilon$ to improve the algebraic rate to an explicit exponential decay rate. The Poincaré inequality for the square roots of the densities minus their averages, along with a few important algebraic inequalities proved in the Appendix and (27) help us obtain an EEDI of the type $D(t) \geq cE(t)$, where c is a positive real number (independent of time). Most of the algebraic intricacies involved are due to the special algebraic coupling of the equations of the system.

By using the inequality (45), Appendix, we obtain

$$\begin{aligned} D(a, b, c | a_\infty, b_\infty, c_\infty) &= d_a \int_{[0,1]} \frac{|\nabla a|^2}{a} dx + d_b \int_{[0,1]} \frac{|\nabla b|^2}{b} dx + d_c \int_{[0,1]} \frac{|\nabla c|^2}{c} dx \\ &+ a_\infty b_\infty^2 \int_{[0,1]} \Psi \left(\frac{ab^2}{a_\infty b_\infty^2}; \frac{bc}{b_\infty c_\infty} \right) dx + b_\infty c_\infty \int_{[0,1]} \Psi \left(\frac{bc}{b_\infty c_\infty}; \frac{ab^2}{a_\infty b_\infty^2} \right) dx \\ &\geq 4d_a \|\nabla \sqrt{a}\|_2^2 + 4d_b \|\nabla \sqrt{b}\|_2^2 + 4d_c \|\nabla \sqrt{c}\|_2^2 \\ &+ a_\infty b_\infty^2 \left\| \sqrt{\frac{ab^2}{a_\infty b_\infty^2}} - \sqrt{\frac{bc}{b_\infty c_\infty}} \right\|_2^2 + b_\infty c_\infty \left\| \sqrt{\frac{bc}{b_\infty c_\infty}} - \sqrt{\frac{ab^2}{a_\infty b_\infty^2}} \right\|_2^2 \\ &\geq C_7 \left(\|\nabla \sqrt{a}\|_2^2 + \|\nabla \sqrt{b}\|_2^2 + \|\nabla \sqrt{c}\|_2^2 + \left\| \sqrt{\frac{ab^2}{a_\infty b_\infty^2}} - \sqrt{\frac{bc}{b_\infty c_\infty}} \right\|_2^2 \right), \end{aligned} \quad (28)$$

where $C_7 := \min(4d_a, 4d_b, 4d_c, a_\infty b_\infty^2 + b_\infty c_\infty)$. Due to (9), we have $M := \max(M_1, M_2)$ such that $\overline{a(t)}, \overline{b(t)}, \overline{c(t)} < M$ for all $t \geq 0$. In what follows we drop the

dependence on t from the notation; each time we write \bar{a} or the likes we mean the spatial average of $a(t) = a(\cdot, t)$. Due to (47), we see that

$$\Psi(x, y) \leq \frac{\Psi(M, y)}{(\sqrt{M} - \sqrt{y})^2} (\sqrt{x} - \sqrt{y})^2 \text{ for all } x \leq M.$$

Since $0 < a_\infty, b_\infty, c_\infty < M$, we have

$$\begin{aligned} E(\bar{a}, \bar{b}, \bar{c} | a_\infty, b_\infty, c_\infty) &= \left(\bar{a} \ln \frac{\bar{a}}{a_\infty} - \bar{a} + a_\infty \right) + \left(\bar{b} \ln \frac{\bar{b}}{b_\infty} - \bar{b} + b_\infty \right) \\ &+ \left(\bar{c} \ln \frac{\bar{c}}{c_\infty} - \bar{c} + c_\infty \right) < \frac{\Psi(M, a_\infty)}{(\sqrt{M} - \sqrt{a_\infty})^2} (\sqrt{\bar{a}} - \sqrt{a_\infty})^2 \\ &+ \frac{\Psi(M, b_\infty)}{(\sqrt{M} - \sqrt{b_\infty})^2} (\sqrt{\bar{b}} - \sqrt{b_\infty})^2 + \frac{\Psi(M, c_\infty)}{(\sqrt{M} - \sqrt{c_\infty})^2} (\sqrt{\bar{c}} - \sqrt{c_\infty})^2 \\ &\leq C_8 [(\sqrt{\bar{a}} - \sqrt{a_\infty})^2 + (\sqrt{\bar{b}} - \sqrt{b_\infty})^2 + (\sqrt{\bar{c}} - \sqrt{c_\infty})^2], \end{aligned} \quad (29)$$

where

$$C_8 := \max \left\{ \frac{\Psi(M, a_\infty)}{(\sqrt{M} - \sqrt{a_\infty})^2}, \frac{\Psi(M, b_\infty)}{(\sqrt{M} - \sqrt{b_\infty})^2}, \frac{\Psi(M, c_\infty)}{(\sqrt{M} - \sqrt{c_\infty})^2} \right\}.$$

Next we claim that there exists a real constant C_9 such that

$$\begin{aligned} &\|\nabla \sqrt{a}\|_2^2 + \|\nabla \sqrt{b}\|_2^2 + \|\nabla \sqrt{c}\|_2^2 + \left\| \sqrt{\frac{ab^2}{a_\infty b_\infty^2}} - \sqrt{\frac{bc}{b_\infty c_\infty}} \right\|_2^2 \\ &> C_9 \left[\|\nabla \sqrt{a}\|_2^2 + \|\nabla \sqrt{b}\|_2^2 + \|\nabla \sqrt{c}\|_2^2 + \left(\frac{\sqrt{a}\sqrt{b}}{\sqrt{a_\infty b_\infty^2}} - \frac{\sqrt{b}\sqrt{c}}{\sqrt{b_\infty c_\infty}} \right)^2 \right]. \end{aligned} \quad (30)$$

In order to get the above estimate, we introduce the deviations from the mean, i.e. $\delta_a = \sqrt{a} - \bar{a}$, $\delta_b = \sqrt{b} - \bar{b}$, $\delta_c = \sqrt{c} - \bar{c}$. Now we make the decomposition

$$[0, 1] = D_L \cup D_L^c,$$

where $D_L = \{x \in [0, 1] : |\delta_a|, |\delta_b|, |\delta_c| \leq L\}$ for a fixed constant L . We expand

$$\sqrt{ab^2} = (\sqrt{a} + \delta_a)(\sqrt{b} + \delta_b)^2 = \sqrt{a}\sqrt{b}^2 + [\delta_a(\sqrt{b} + \delta_b)^2 + \sqrt{a}(2\sqrt{b}\delta_b + \delta_b^2)]$$

and

$$\sqrt{bc} = (\sqrt{b} + \delta_b)(\sqrt{c} + \delta_c) = \sqrt{b}\sqrt{c} + [\delta_b\sqrt{c} + \delta_c(\sqrt{b} + \delta_b)]$$

to see that on the set D_L one has

$$\begin{aligned} &\delta_a(\sqrt{b} + \delta_b)^2 + \sqrt{a}(2\sqrt{b}\delta_b + \delta_b^2) \\ &\leq (|\delta_a| + |\delta_b|) [(\sqrt{M_2} + L)^2 + \sqrt{M_1}(2\sqrt{M_2} + L)] = (|\delta_a| + |\delta_b|)R_1 \end{aligned}$$

and

$$\begin{aligned} &\delta_b\sqrt{c} + \delta_c(\sqrt{b} + \delta_b) \\ &\leq (|\delta_b| + |\delta_c|) [\sqrt{M_2} + (\sqrt{M_2} + L)] = (|\delta_b| + |\delta_c|)R_2, \end{aligned}$$

where $R_1 := (\sqrt{M_2} + L)^2 + \sqrt{M_1}(2\sqrt{M_2} + L)$ and $R_2 := \sqrt{M_2} + (\sqrt{M_2} + L)$. Thus,

$$\begin{aligned}
& \left\| \sqrt{\frac{ab^2}{a_\infty b_\infty^2}} - \sqrt{\frac{bc}{b_\infty c_\infty}} \right\|_{L^2(D_L)}^2 = \left\| \frac{\sqrt{a}\sqrt{b}}{\sqrt{a_\infty b_\infty^2}} - \frac{\sqrt{b}\sqrt{c}}{\sqrt{b_\infty c_\infty}} \right. \\
& \left. + \frac{[\delta_a(\sqrt{b} + \delta_b)^2 + \sqrt{a}(2\sqrt{b}\delta_b + \delta_b^2)]}{\sqrt{a_\infty b_\infty^2}} - \frac{[\delta_b\sqrt{c} + \delta_c(\sqrt{b} + \delta_b)]}{\sqrt{b_\infty c_\infty}} \right\|_{L^2(D_L)}^2 \\
& \geq \frac{1}{2} \left(\frac{\sqrt{a}\sqrt{b}}{\sqrt{a_\infty b_\infty^2}} - \frac{\sqrt{b}\sqrt{c}}{\sqrt{b_\infty c_\infty}} \right)^2 |D_L| - 2 \left\| |\delta_a| + |\delta_b| \right\|_{L^2(D_L)}^2 \frac{R_1^2}{a_\infty b_\infty^2} \\
& \quad - 2 \left\| |\delta_b| + |\delta_c| \right\|_{L^2(D_L)}^2 \frac{R_2^2}{b_\infty c_\infty} \\
& \geq \frac{1}{2} \left(\frac{\sqrt{a}\sqrt{b}}{\sqrt{a_\infty b_\infty^2}} - \frac{\sqrt{b}\sqrt{c}}{\sqrt{b_\infty c_\infty}} \right)^2 |D_L| - R(M_1, M_2, L) [\|\delta_a\|_{L^2(D_L)}^2 + \\
& \quad \|\delta_b\|_{L^2(D_L)}^2 + \|\delta_c\|_{L^2(D_L)}^2], \tag{31}
\end{aligned}$$

where $R(M_1, M_2, L) := \frac{4R_1^2}{a_\infty b_\infty^2} + \frac{4R_2^2}{b_\infty c_\infty}$.

On the set D_L^C , by using Poincaré's inequality, we get

$$\begin{aligned}
& \|\nabla \sqrt{a}\|_2^2 + \|\nabla \sqrt{b}\|_2^2 + \|\nabla \sqrt{c}\|_2^2 \\
& \geq C_P (\|\delta_a\|_{L^2(D_L^C)}^2 + \|\delta_b\|_{L^2(D_L^C)}^2 + \|\delta_c\|_{L^2(D_L^C)}^2) \\
& \geq C_P L^2 |D_L^C|.
\end{aligned}$$

Since

$$\left(\frac{\sqrt{a}\sqrt{b}}{\sqrt{a_\infty b_\infty^2}} - \frac{\sqrt{b}\sqrt{c}}{\sqrt{b_\infty c_\infty}} \right)^2 \leq \left(\frac{\sqrt{M_1}\sqrt{M_2}}{\sqrt{a_\infty b_\infty^2}} + \frac{\sqrt{M_2}\sqrt{M_1}}{\sqrt{b_\infty c_\infty}} \right)^2,$$

we infer

$$\|\nabla \sqrt{a}\|_2^2 + \|\nabla \sqrt{b}\|_2^2 + \|\nabla \sqrt{c}\|_2^2 \geq \tilde{R} \left(\frac{\sqrt{a}\sqrt{b}}{\sqrt{a_\infty b_\infty^2}} - \frac{\sqrt{b}\sqrt{c}}{\sqrt{b_\infty c_\infty}} \right)^2 |D_L^C|, \tag{32}$$

where

$$\tilde{R} := \frac{C_P L^2}{\left(\frac{\sqrt{M_1}\sqrt{M_2}}{\sqrt{a_\infty b_\infty^2}} + \frac{\sqrt{M_2}\sqrt{M_1}}{\sqrt{b_\infty c_\infty}} \right)^2}.$$

Pick $K > \frac{R+1}{\min\{1, C_P\}}$ and combine (31) and (32) to conclude

$$\begin{aligned}
& 3K(\|\nabla \sqrt{a}\|_2^2 + \|\nabla \sqrt{b}\|_2^2 + \|\nabla \sqrt{c}\|_2^2) + \left\| \sqrt{\frac{ab^2}{a_\infty b_\infty^2}} - \sqrt{\frac{bc}{b_\infty c_\infty}} \right\|_2^2 \\
& \geq K(\|\nabla \sqrt{a}\|_2^2 + \|\nabla \sqrt{b}\|_2^2 + \|\nabla \sqrt{c}\|_2^2) + K\tilde{R} \left(\frac{\sqrt{a}\sqrt{b}}{\sqrt{a_\infty b_\infty^2}} - \frac{\sqrt{b}\sqrt{c}}{\sqrt{b_\infty c_\infty}} \right)^2 |D_L^C| + \\
& \quad \left\{ \frac{1}{2} \left(\frac{\sqrt{a}\sqrt{b}}{\sqrt{a_\infty b_\infty^2}} - \frac{\sqrt{b}\sqrt{c}}{\sqrt{b_\infty c_\infty}} \right)^2 |D_L| - R(\|\delta_a\|_{L^2(D_L)}^2 + \|\delta_b\|_{L^2(D_L)}^2 + \|\delta_c\|_{L^2(D_L)}^2) \right\} \\
& \quad + K(\|\delta_a\|_{L^2(D_L)}^2 + \|\delta_b\|_{L^2(D_L)}^2 + \|\delta_c\|_{L^2(D_L)}^2)
\end{aligned}$$

$$\begin{aligned}
&\geq K(\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2 + \|\nabla\sqrt{c}\|_2^2) + \min\left\{K\tilde{R}, \frac{1}{2}\right\} \left(\frac{\sqrt{a}\sqrt{b}}{\sqrt{a_\infty b_\infty^2}} - \frac{\sqrt{b}\sqrt{c}}{\sqrt{b_\infty c_\infty}} \right)^2 \\
&+ (KC_P - R)(\|\delta_a\|_{L^2(D_L)}^2 + \|\delta_b\|_{L^2(D_L)}^2 + \|\delta_c\|_{L^2(D_L)}^2) \\
&\geq C_{K,R} \left[\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2 + \|\nabla\sqrt{c}\|_2^2 + \left(\frac{\sqrt{a}\sqrt{b}}{\sqrt{a_\infty b_\infty^2}} - \frac{\sqrt{b}\sqrt{c}}{\sqrt{b_\infty c_\infty}} \right)^2 \right].
\end{aligned}$$

where $C_{K,R} = \min\{K, K\tilde{R}, \frac{1}{2}, KC_P - R\} = \min\{K\tilde{R}, \frac{1}{2}\}$ (because $K - R > 1$). Therefore, (30) is proved with $C_9 = \frac{C_{K,R}}{3K}$.

It remains to show that there exists a constant C_{10} such that

$$\begin{aligned}
&\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2 + \|\nabla\sqrt{c}\|_2^2 + \left(\frac{\sqrt{a}\sqrt{b}}{\sqrt{a_\infty b_\infty^2}} - \frac{\sqrt{b}\sqrt{c}}{\sqrt{b_\infty c_\infty}} \right)^2 \geq \\
&C_{10} [(\sqrt{\bar{a}} - \sqrt{a_\infty})^2 + (\sqrt{\bar{b}} - \sqrt{b_\infty})^2 + (\sqrt{\bar{c}} - \sqrt{c_\infty})^2].
\end{aligned} \tag{33}$$

To this end, we introduce μ_a, μ_b, μ_c to parameterize $\sqrt{\bar{a}}, \sqrt{\bar{b}}, \sqrt{\bar{c}}$ with $\sqrt{\bar{a}} = \sqrt{a_\infty}(1 + \mu_a), \sqrt{\bar{b}} = \sqrt{b_\infty}(1 + \mu_b), \sqrt{\bar{c}} = \sqrt{c_\infty}(1 + \mu_c)$, where $-1 \leq \mu_a, \mu_b, \mu_c < \mu_k$ for $\mu_k = \frac{\sqrt{k}}{\min\{\sqrt{a_\infty}, \sqrt{b_\infty}, \sqrt{c_\infty}\}} - 1$. Since $\delta_a = \sqrt{a} - \sqrt{\bar{a}}$, we have

$$\begin{aligned}
\|\delta_a\|_2^2 &= \bar{a} - (\sqrt{\bar{a}})^2 = (\sqrt{\bar{a}} - \sqrt{a_\infty})(\sqrt{\bar{a}} + \sqrt{a_\infty}) \\
\implies \sqrt{\bar{a}} &= -\frac{\|\delta_a\|_2^2}{\sqrt{\bar{a}} + \sqrt{a_\infty}} + \sqrt{a_\infty} = \sqrt{a_\infty} - T(a)\|\delta_a\|_2^2,
\end{aligned}$$

where $T(a) = \frac{1}{\sqrt{\bar{a}} + \sqrt{a_\infty}} \leq \frac{1}{\epsilon}$; this inequality follows from $\bar{a} = \|a\|_1 > \epsilon^2 > 0$. Similarly,

$$\sqrt{\bar{b}} = \sqrt{\bar{b}} - T(b)\|\delta_b\|_2^2 \quad \& \quad \sqrt{\bar{c}} = \sqrt{\bar{c}} - T(c)\|\delta_c\|_2^2,$$

where $T(b) = \frac{1}{\sqrt{\bar{b}} + \sqrt{b_\infty}}, T(c) = \frac{1}{\sqrt{\bar{c}} + \sqrt{c_\infty}} \leq \frac{1}{\epsilon}$. And since

$$\epsilon^2 < \|b\|_1 \leq \|\sqrt{b}\|_\infty \|\sqrt{b}\|_1 \leq \sqrt{k} \|\sqrt{b}\|_1 \implies \sqrt{\bar{b}} \geq \frac{\epsilon^2}{\sqrt{k}},$$

due to this lower bound on $\sqrt{\bar{b}}$, we can factor out $(\frac{\sqrt{\bar{b}}}{\sqrt{b_\infty}})^2$ and reduce (4) to the system associated with the reversible reaction $A + B \rightleftharpoons C$ (which does not have accessible boundary equilibria). More precisely, we have

$$\begin{aligned}
&\left(\frac{\sqrt{a}\sqrt{b}}{\sqrt{a_\infty b_\infty^2}} - \frac{\sqrt{b}\sqrt{c}}{\sqrt{b_\infty c_\infty}} \right)^2 = \frac{(\sqrt{\bar{b}})^2}{b_\infty} \left(\frac{\sqrt{a}\sqrt{b}}{\sqrt{a_\infty b_\infty}} - \frac{\sqrt{c}}{\sqrt{c_\infty}} \right)^2 \\
&\geq \frac{\epsilon^4}{b_\infty k} \left\{ \frac{(\sqrt{\bar{a}} - T(a)\|\delta_a\|_2^2)(\sqrt{\bar{b}} - T(b)\|\delta_b\|_2^2)}{\sqrt{a_\infty b_\infty}} - \frac{\sqrt{\bar{c}} - T(c)\|\delta_c\|_2^2}{\sqrt{c_\infty}} \right\}^2 \\
&= \frac{\epsilon^4}{b_\infty k} \left\{ [1 + \mu_a - \frac{T(a)\|\delta_a\|_2^2}{\sqrt{a_\infty}}][1 + \mu_b - \frac{T(b)\|\delta_b\|_2^2}{\sqrt{b_\infty}}] - [1 + \mu_c - \frac{T(c)\|\delta_c\|_2^2}{\sqrt{c_\infty}}] \right\}^2
\end{aligned} \tag{34}$$

$$\begin{aligned}
&= \frac{\epsilon^4}{b_\infty k} \left\{ [(1 + \mu_a)(1 + \mu_b) - (1 + \mu_c)] + \frac{T(a)\|\delta_a\|_2^2 T(b)\|\delta_b\|_2^2}{\sqrt{a_\infty}} + \frac{T(c)\|\delta_c\|_2^2}{\sqrt{c_\infty}} \right. \\
&\quad \left. - \frac{T(a)\|\delta_a\|_2^2}{\sqrt{a_\infty}}(1 + \mu_b) - \frac{T(b)\|\delta_b\|_2^2}{\sqrt{b_\infty}}(1 + \mu_a) \right\}^2 \\
&\geq \frac{\epsilon^4}{b_\infty k} \left\{ \frac{1}{2} [(1 + \mu_a)(1 + \mu_b) - (1 + \mu_c)]^2 - \left[\frac{T(a)\|\delta_a\|_2^2 T(b)\|\delta_b\|_2^2}{\sqrt{a_\infty}} + \frac{T(c)\|\delta_c\|_2^2}{\sqrt{c_\infty}} \right. \right. \\
&\quad \left. - \frac{T(a)\|\delta_a\|_2^2}{\sqrt{a_\infty}}(1 + \mu_b) - \frac{T(b)\|\delta_b\|_2^2}{\sqrt{b_\infty}}(1 + \mu_a) \right]^2 \Big\} \\
&\geq \frac{\epsilon^4}{b_\infty k} \left\{ \frac{1}{2} [(1 + \mu_a)(1 + \mu_b) - (1 + \mu_c)]^2 - 4 \left[\frac{T(a)\|\delta_a\|_2^2 T(b)\|\delta_b\|_2^2}{\sqrt{a_\infty}} \right]^2 \right. \\
&\quad \left. - 4 \left[\frac{T(c)\|\delta_c\|_2^2}{\sqrt{c_\infty}} \right]^2 - 4 \left[\frac{T(a)\|\delta_a\|_2^2}{\sqrt{a_\infty}}(1 + \mu_b) \right]^2 - 4 \left[\frac{T(b)\|\delta_b\|_2^2}{\sqrt{b_\infty}}(1 + \mu_a) \right]^2 \right\}.
\end{aligned}$$

Since $\|\delta_a\|_2^2 = \bar{a} - (\sqrt{a})^2$, we get $\|\delta_a\|_2^2 \leq k$; similarly, $\|\delta_b\|_2^2, \|\delta_c\|_2^2 \leq k$. Combined with $T(a), T(b), T(c) \leq \frac{1}{\epsilon}$ and $0 \leq 1 + \mu_a, 1 + \mu_b, 1 + \mu_c \leq 1 + \mu_k$, (34) gives

$$\begin{aligned}
&\left(\frac{\sqrt{a}\sqrt{b}}{\sqrt{a_\infty b_\infty^2}} - \frac{\sqrt{b}\sqrt{c}}{\sqrt{b_\infty c_\infty}} \right)^2 \geq \frac{\epsilon^4}{b_\infty k} \left\{ \frac{1}{2} [(1 + \mu_a)(1 + \mu_b) - (1 + \mu_c)]^2 \right. \\
&\quad \left. - \frac{4k^3}{\epsilon^4 a_\infty} \|\delta_a\|_2^2 - \frac{4k}{\epsilon^2 c_\infty} \|\delta_c\|_2^2 - \frac{4k(1 + \mu_k)^2}{\epsilon^2 a_\infty} \|\delta_a\|_2^2 - \frac{4k(1 + \mu_k)^2}{\epsilon^2 b_\infty} \|\delta_b\|_2^2 \right\} \\
&\geq \frac{\epsilon^4}{2b_\infty k} [(1 + \mu_a)(1 + \mu_b) - (1 + \mu_c)]^2 - C_{11} (\|\delta_a\|_2^2 + \|\delta_b\|_2^2 + \|\delta_c\|_2^2),
\end{aligned}$$

where

$$C_{11} := \max \left\{ \frac{4k^2 + 4(1 + \mu_k)^2}{a_\infty b_\infty}, \frac{4(1 + \mu_k)^2}{b_\infty^2}, \frac{4(1 + \mu_k)^2}{b_\infty c_\infty} \right\}.$$

Poincaré's inequality reveals

$$\begin{aligned}
&\|\nabla \sqrt{a}\|_2^2 + \|\nabla \sqrt{b}\|_2^2 + \|\nabla \sqrt{c}\|_2^2 + \left(\frac{\sqrt{a}\sqrt{b}}{\sqrt{a_\infty b_\infty^2}} - \frac{\sqrt{b}\sqrt{c}}{\sqrt{b_\infty c_\infty}} \right)^2 \\
&\geq C_{12} [(1 + \mu_a)(1 + \mu_b) - (1 + \mu_c)]^2,
\end{aligned}$$

for $C_{12} := \frac{C_P \epsilon^4}{2b_\infty k C_{11}}$. On the other hand,

$$(\sqrt{\bar{a}} - \sqrt{a_\infty})^2 + (\sqrt{\bar{b}} - \sqrt{b_\infty})^2 + (\sqrt{\bar{c}} - \sqrt{c_\infty})^2 = a_\infty \mu_a^2 + b_\infty \mu_b^2 + c_\infty \mu_c^2,$$

so we would like to compare $[(1 + \mu_a)(1 + \mu_b) - (1 + \mu_c)]^2$ and $\mu_a^2 + \mu_b^2 + \mu_c^2$. The conservation laws (9) (applied to $\bar{a}, \bar{b}, \bar{c}$ and $a_\infty, b_\infty, c_\infty$) yield

$$\begin{aligned}
\frac{\bar{a}}{a_\infty} &= (1 + \mu_a), \quad \frac{\bar{b}}{b_\infty} = (1 + \mu_b), \quad \frac{\bar{c}}{c_\infty} = (1 + \mu_c), \\
\bar{a} + \bar{c} &= a_\infty + c_\infty = M_1, \quad \bar{b} + \bar{c} = b_\infty + c_\infty = M_2,
\end{aligned}$$

and so, $a_\infty \mu_a + c_\infty \mu_c = b_\infty \mu_b + c_\infty \mu_c = 0$. Thus, unless μ_a, μ_b, μ_c are all zero (trivial case!), we get $\mu_a \mu_c < 0$ and $\mu_b \mu_c < 0$. If $\mu_a, \mu_b > 0$ and $0 > \mu_c$, then

$$\begin{aligned}
&[(1 + \mu_a)(1 + \mu_b) - (1 + \mu_c)]^2 = (\mu_a \mu_b + \mu_a + \mu_b - \mu_c)^2 \\
&\geq (\mu_a \mu_b + \mu_a + \mu_b)^2 + (\mu_c)^2 > \mu_a^2 + \mu_b^2 + \mu_c^2.
\end{aligned}$$

Otherwise, if $\mu_a, \mu_b < 0$ and $0 < \mu_c$, then

$$\begin{aligned} [(1 + \mu_a)(1 + \mu_b) - (1 + \mu_c)]^2 &= (\mu_a \mu_b + \mu_a + \mu_b - \mu_c)^2 \\ &\geq (\mu_a + \mu_b - \mu_c)^2 + (\mu_a \mu_b)^2 > \mu_a^2 + \mu_b^2 + \mu_c^2. \end{aligned}$$

Therefore, in both cases we have

$$[(1 + \mu_a)(1 + \mu_b) - (1 + \mu_c)]^2 \geq \mu_a^2 + \mu_b^2 + \mu_c^2.$$

(Notice that when $\mu_a = \mu_b = \mu_c = 0$, both sides of the inequality are equal to zero.) Set

$$C_{10} := \frac{C_{12}}{\max(a_\infty, b_\infty, c_\infty)}$$

to conclude the proof of (33).

Proof of Theorem 1.1:

Proof. Finally, by (28), (29), (30) and (33), we obtain

$$\begin{aligned} D(a, b, c | a_\infty, b_\infty, c_\infty) &\geq C_7 C_9 C_{10} [(\sqrt{\bar{a}} - \sqrt{a_\infty})^2 + (\sqrt{\bar{b}} - \sqrt{b_\infty})^2 + (\sqrt{\bar{c}} - \sqrt{c_\infty})^2] \\ &\geq \frac{C_7 C_9 C_{10}}{C_8} E(\bar{a}, \bar{b}, \bar{c} | a_\infty, b_\infty, c_\infty). \end{aligned}$$

In view of the above inequality and (23), we discover

$$D(a, b, c | a_\infty, b_\infty, c_\infty) \geq C_{13} E(a, b, c | a_\infty, b_\infty, c_\infty),$$

where

$$C_{13} := \min\left(\frac{C_7 C_9 C_{10}}{C_8}, C_2\right).$$

In conclusion, we have proved that the solution decays exponentially to the positive equilibrium (with explicit rate). \square

3. Asymptotic decay for the two-species system. In this section we prove Theorem 1.2.

3.1. Uniform boundedness and global existence for the two-species system. To show the uniform boundedness for classical solutions to (6) we employ an invariant region approach. Note that here we do not need the assumptions from Theorem 1.2 on the signs of \bar{m} and \bar{n} .

Theorem 3.1. *Let f denote the two-dimensional mass-action vector field generated by the single reversible reaction $m_1 A + n_1 B \xrightleftharpoons[k_2]{k_1} m_2 A + n_2 B$, where $\bar{m} = m_1 - m_2$ and $\bar{n} = n_2 - n_1$ are nonzero. Then, for any compact set $K \subset \mathbb{R}_{>0}^2$ there exists a rectangle $R = [\alpha_1, \alpha_2] \times [\beta_1, \beta_2] \subset \mathbb{R}_{>0}^2$ such that $K \subset R$ and such that f points into the interior of R on ∂R .*

Proof. With the notation we have already introduced, a, b denote the concentrations of A and B , and $\bar{m} = m_1 - m_2$, $\bar{n} = n_2 - n_1$. The corresponding ODE system reads

$$\begin{pmatrix} \dot{a} \\ \dot{b} \end{pmatrix} = (k_1 a^{m_1} b^{n_1} - k_2 a^{m_2} b^{n_2}) \begin{pmatrix} -\lambda_a \bar{m} \\ \lambda_b \bar{n} \end{pmatrix},$$

so positive trajectories are confined to *stoichiometric classes* $(p + \text{span}(-\lambda_a \bar{m}, \lambda_b \bar{n}))^t \cap \mathbb{R}_{>0}^2$ (see Figure 1). The positive steady state manifold is the curve $a^{-\bar{m}} b^{\bar{n}} = k_1/k_2$,

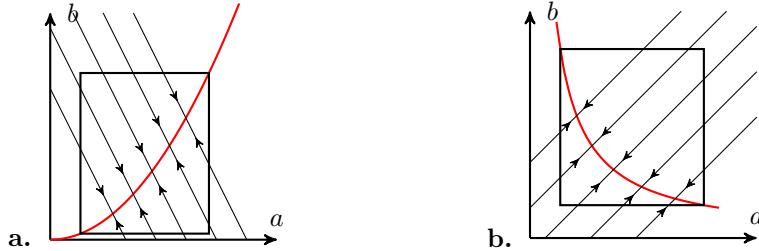


FIGURE 1. Construction of a rectangular invariant region for the reversible reaction $m_1A + n_1B \rightleftharpoons m_2A + n_2B$ for the cases **a.** $\bar{m} = m_1 - m_2$, $\bar{n} = n_2 - n_1$ nonzero and of the same sign; **b.** \bar{m}, \bar{n} nonzero and of different signs.

and it is easily checked that it intersects each stoichiometric class at precisely one point. It is also easy to see that the unique steady state in each stoichiometric class is globally asymptotically stable on that class. It follows that a rectangular region $R \subset \mathbb{R}_{>0}^2$ is invariant if and only if it contains the steady state on each stoichiometric class that intersects R . If $\bar{m}\bar{n} \neq 0$ this can be achieved by choosing opposite vertices of R on the steady state curve (Figure 1a, b.). \square

Now we use a less general (tailored to our needs) version of **Corollary 14.8** from [33].

Theorem 3.2. *Suppose that D is a $k \times k$ nonnegative definite diagonal matrix. Then any region of the form (invariant rectangle)*

$$\Sigma = \bigcap_{i=1}^k \{u : a_i \leq u_i \leq b_i\}$$

is invariant for the $k \times k$ reaction-diffusion system

$$v_t = Dv_{xx} + f(v, t)$$

provided that f points strictly into Σ on $\partial\Sigma$.

(1) By using the above two theorems we immediately conclude that if $\bar{m}\bar{n} \neq 0$, then the reaction-diffusion system (6) shares the same invariant regions with the corresponding reaction system. Thus, under the restrictions on a_0 and b_0 from the statement of Theorem 1.2, we get a uniform upper bound $0 < \omega < \infty$ for a and b ; this also implies the existence of a unique global classical solution.

(2) If $\bar{m} = \bar{n} = 0$, then we are dealing with two decoupled homogeneous Neumann heat problems on the same domain. It is known that the lower and upper bounds on a_0 , b_0 are preserved for all time. Both densities converge exponentially to the averages of the initial data.

(3) If only one of \bar{m} , \bar{n} is zero, say $\bar{m} = 0$, then the equation for a decouples and, as above, we have that a stays bounded globally in time between $\inf a_0$ and $\sup a_0$, and it converges exponentially to the average of a_0 . The equation for b becomes

$$b_t - d_b \Delta b = \lambda_b |\bar{n}| a^{m_1} b^p (1 - b^{|\bar{n}|}),$$

where $p := \min\{n_1, n_2\}$. The positive equilibrium is $b_\infty \equiv 1$. Now we use Theorem 3.2 with $k = 1$ and $f(b, t) := \lambda_b |\bar{n}| a^{m_1} b^p (1 - b^{|\bar{n}|})$; since a is bounded uniformly

away from zero and infinity, we conclude that at the boundary of any interval $[\delta, M]$, (where $0 < \delta < 1 < M < \infty$) f does, indeed, point strictly inside said interval.

In conclusion, if a_0, b_0 are bounded away from zero by α and from infinity by β (as in the statement of Theorem 1.2) we get explicit (depending only on α and β) global bounds (and global existence and uniqueness) on a, b in all cases. Let these bounds be ϵ^2, ω , so that

$$\begin{aligned} 0 < \epsilon^2 \leq \min\{a(x, t), b(x, t)\} &\leq \max\{a(x, t), b(x, t)\} \\ &\leq \omega < \infty \text{ for all } (x, t) \in \Omega \times [0, \infty). \end{aligned} \quad (35)$$

3.2. Convergence for the two-species system. We use the same entropy entropy dissipation method to obtain an explicit exponential convergence rate for the two species system in any dimension. Once again, the Log-Sobolev inequality, the Poincaré inequality for the square roots of the densities minus their averages, along with a few important algebraic inequalities proved in the Appendix help us obtain an EEDI of the type $D(t) \geq cE(t)$, where c is a positive real number (independent of time). Again we introduce the relative entropy

$$E(a, b|a_\infty, b_\infty) = \int_{\Omega} \left(a \ln \frac{a}{a_\infty} - a + a_\infty \right) dx + \int_{\Omega} \left(b \ln \frac{b}{b_\infty} - b + b_\infty \right) dx$$

and its corresponding entropy dissipation

$$\begin{aligned} D(a, b|a_\infty, b_\infty) &= d_a \int_{\Omega} \frac{|\nabla a|^2}{a} dx + d_b \int_{\Omega} \frac{|\nabla b|^2}{b} dx \\ &+ a_\infty^{m_1} b_\infty^{n_1} \int_{\Omega} \Psi \left(\frac{a^{m_1} b^{n_1}}{a_\infty^{m_1} b_\infty^{n_1}}; \frac{a^{m_2} b^{n_2}}{a_\infty^{m_2} b_\infty^{n_2}} \right) dx + a_\infty^{m_2} b_\infty^{n_2} \int_{\Omega} \Psi \left(\frac{a^{m_2} b^{n_2}}{a_\infty^{m_2} b_\infty^{n_2}}; \frac{a^{m_1} b^{n_1}}{a_\infty^{m_1} b_\infty^{n_1}} \right) dx. \end{aligned}$$

Due to the following identity

$$E(a, b|a_\infty, b_\infty) = E(a, b|\bar{a}, \bar{b}) + E(\bar{a}, \bar{b}|a_\infty, b_\infty)$$

and the Logarithmic Sobolev Inequality (22) we have

$$d_a \int_{\Omega} \frac{|\nabla a|^2}{a} dx + d_b \int_{\Omega} \frac{|\nabla b|^2}{b} dx \geq D_1 E(a, b|\bar{a}, \bar{b}), \quad (36)$$

where $D_1 = \min(d_a, d_b) \cdot C_{LSI}$.

From inequality (45) we get the following estimate

$$\begin{aligned} D(a, b|a_\infty, b_\infty) &= d_a \int_{\Omega} \frac{|\nabla a|^2}{a} dx + d_b \int_{\Omega} \frac{|\nabla b|^2}{b} dx \\ &+ a_\infty^{m_1} b_\infty^{n_1} \int_{\Omega} \Psi \left(\frac{a^{m_1} b^{n_1}}{a_\infty^{m_1} b_\infty^{n_1}}; \frac{a^{m_2} b^{n_2}}{a_\infty^{m_2} b_\infty^{n_2}} \right) dx + a_\infty^{m_2} b_\infty^{n_2} \int_{\Omega} \Psi \left(\frac{a^{m_2} b^{n_2}}{a_\infty^{m_2} b_\infty^{n_2}}; \frac{a^{m_1} b^{n_1}}{a_\infty^{m_1} b_\infty^{n_1}} \right) dx \\ &\geq 4d_a \|\nabla \sqrt{a}\|_2^2 + 4d_b \|\nabla \sqrt{b}\|_2^2 + 4d_c \|\nabla \sqrt{c}\|_2^2 \\ &+ a_\infty^{m_1} b_\infty^{n_1} \left\| \sqrt{\frac{a^{m_1} b^{n_1}}{a_\infty^{m_1} b_\infty^{n_1}}} - \sqrt{\frac{a^{m_2} b^{n_2}}{a_\infty^{m_2} b_\infty^{n_2}}} \right\|_2^2 + a_\infty^{m_2} b_\infty^{n_2} \left\| \sqrt{\frac{a^{m_2} b^{n_2}}{a_\infty^{m_2} b_\infty^{n_2}}} - \sqrt{\frac{a^{m_1} b^{n_1}}{a_\infty^{m_1} b_\infty^{n_1}}} \right\|_2^2 \\ &\geq D_2 \left(\|\nabla \sqrt{a}\|_2^2 + \|\nabla \sqrt{b}\|_2^2 + \|\nabla \sqrt{c}\|_2^2 + \left\| \sqrt{\frac{a^{m_1} b^{n_1}}{a_\infty^{m_1} b_\infty^{n_1}}} - \sqrt{\frac{a^{m_2} b^{n_2}}{a_\infty^{m_2} b_\infty^{n_2}}} \right\|_2^2 \right), \end{aligned} \quad (37)$$

where $D_2 = \min(4d_a, 4d_b, 4d_c, a_\infty^{m_1} b_\infty^{n_1} + a_\infty^{m_2} b_\infty^{n_2})$.

The global L^∞ bounds on a and b ensure that there exists N such that $\bar{a}, \bar{b} < N$. Thus, (47) (see Appendix) yields

$$\Psi(x, y) \leq \frac{\Psi(N, y)}{(\sqrt{N} - \sqrt{y})^2} (\sqrt{x} - \sqrt{y})^2 \text{ for all } x \leq N.$$

Since $0 < a_\infty, b_\infty < N$,

$$\begin{aligned} E(\bar{a}, \bar{b}|a_\infty, b_\infty) &= \left(\bar{a} \ln \frac{\bar{a}}{a_\infty} - \bar{a} + a_\infty \right) + \left(\bar{b} \ln \frac{\bar{b}}{b_\infty} - \bar{b} + b_\infty \right) \\ &< \frac{\Psi(N, a_\infty)}{(\sqrt{N} - \sqrt{a_\infty})^2} (\sqrt{\bar{a}} - \sqrt{a_\infty})^2 + \frac{\Psi(N, b_\infty)}{(\sqrt{N} - \sqrt{b_\infty})^2} (\sqrt{\bar{b}} - \sqrt{b_\infty})^2 \\ &\leq D_3 [(\sqrt{\bar{a}} - \sqrt{a_\infty})^2 + (\sqrt{\bar{b}} - \sqrt{b_\infty})^2], \end{aligned} \quad (38)$$

where

$$D_3 = \max \left\{ \frac{\Psi(N, a_\infty)}{(\sqrt{N} - \sqrt{a_\infty})^2}, \frac{\Psi(N, b_\infty)}{(\sqrt{N} - \sqrt{b_\infty})^2} \right\}.$$

Now we claim there exists a constant $D_4 > 0$ such that

$$\begin{aligned} \|\nabla \sqrt{a}\|_2^2 + \|\nabla \sqrt{b}\|_2^2 + \left\| \sqrt{\frac{a^{m_1} b^{n_1}}{a_\infty^{m_1} b_\infty^{n_1}}} - \sqrt{\frac{a^{m_2} b^{n_2}}{a_\infty^{m_2} b_\infty^{n_2}}} \right\|_2^2 \\ > D_4 \left\{ \|\nabla \sqrt{a}\|_2^2 + \|\nabla \sqrt{b}\|_2^2 + \left(\frac{\sqrt{a}^{m_1} \sqrt{b}^{n_1}}{\sqrt{a_\infty^{m_1} b_\infty^{n_1}}} - \frac{\sqrt{a}^{m_2} \sqrt{b}^{n_2}}{\sqrt{a_\infty^{m_2} b_\infty^{n_2}}} \right)^2 \right\}. \end{aligned} \quad (39)$$

Now we again introduce the deviations $\delta_a = \sqrt{a} - \bar{a}$, $\delta_b = \sqrt{b} - \bar{b}$ and make the decomposition

$$\Omega = D_L \cup D_L^C,$$

where $D_L := \{x \in \Omega : |\delta_a|, |\delta_b| \leq L\}$ with a fixed constant L . On the set D_L we get

$$\begin{aligned} \sqrt{a^{m_1} b^{n_1}} &= (\sqrt{\bar{a}} + \delta_a)^{m_1} (\sqrt{\bar{b}} + \delta_b)^{n_1} \\ &\leq \sqrt{\bar{a}}^{m_1} \cdot \sqrt{\bar{b}}^{n_1} + (|\delta_a| + |\delta_b|) R_1(|\delta_a|, |\delta_b|, \sqrt{\bar{a}}, \sqrt{\bar{b}}), \\ \sqrt{a^{m_2} b^{n_2}} &= (\sqrt{\bar{a}} + \delta_a)^{m_2} (\sqrt{\bar{b}} + \delta_b)^{n_2} \\ &\leq \sqrt{\bar{a}}^{m_2} \cdot \sqrt{\bar{b}}^{n_2} + (|\delta_a| + |\delta_b|) R_2(|\delta_a|, |\delta_b|, \sqrt{\bar{a}}, \sqrt{\bar{b}}), \end{aligned}$$

where R_1 and R_2 are finite due to the boundedness of $|\delta_a|, |\delta_b|, \sqrt{\bar{a}}, \sqrt{\bar{b}}$. Then we get

$$\begin{aligned} &\left\| \sqrt{\frac{a^{m_1} b^{n_1}}{a_\infty^{m_1} b_\infty^{n_1}}} - \sqrt{\frac{a^{m_2} b^{n_2}}{a_\infty^{m_2} b_\infty^{n_2}}} \right\|_{L^2(D_L)}^2 \\ &\geq \frac{1}{2} \left(\frac{\sqrt{a}^{m_1} \sqrt{b}^{n_1}}{\sqrt{a_\infty^{m_1} b_\infty^{n_1}}} - \frac{\sqrt{a}^{m_2} \sqrt{b}^{n_2}}{\sqrt{a_\infty^{m_2} b_\infty^{n_2}}} \right)^2 |D_L| - 2 \|\delta_a\|_{L^2(D_L)}^2 \frac{R_1^2}{a_\infty^{m_1} b_\infty^{n_1}} \\ &\quad - 2 \|\delta_b\|_{L^2(D_L)}^2 \frac{R_2^2}{a_\infty^{m_2} b_\infty^{n_2}} \\ &\geq \frac{1}{2} \left(\frac{\sqrt{a}^{m_1} \sqrt{b}^{n_1}}{\sqrt{a_\infty^{m_1} b_\infty^{n_1}}} - \frac{\sqrt{a}^{m_2} \sqrt{b}^{n_2}}{\sqrt{a_\infty^{m_2} b_\infty^{n_2}}} \right)^2 |D_L| - R(|\delta_a|, |\delta_b|, \sqrt{\bar{a}}, \sqrt{\bar{b}}) [\|\delta_a\|_{L^2(D_L)}^2 + \\ &\quad \|\delta_b\|_{L^2(D_L)}^2], \end{aligned}$$

where $R(|\delta_a|, |\delta_b|, \sqrt{a}, \sqrt{b}) = \frac{4R_1^2}{a_\infty^{m_1} b_\infty^{n_1}} + \frac{4R_2^2}{a_\infty^{m_2} b_\infty^{n_2}}$ is finite (depends on the choice of L and N).

On the set $D_L^{\mathfrak{C}}$, by using Poincaré's inequality, we get

$$\|\nabla \sqrt{a}\|_2^2 + \|\nabla \sqrt{b}\|_2^2 \geq C_P (\|\delta_a\|_{L^2(D_L^{\mathfrak{C}})}^2 + \|\delta_b\|_{L^2(D_L^{\mathfrak{C}})}^2) \geq C_P L^2 |D_L^{\mathfrak{C}}|.$$

Since

$$\left| \frac{\sqrt{a}^{m_1} \sqrt{b}^{n_1}}{\sqrt{a_\infty^{m_1} b_\infty^{n_1}}} - \frac{\sqrt{a}^{m_2} \sqrt{b}^{n_2}}{\sqrt{a_\infty^{m_2} b_\infty^{n_2}}} \right| \leq \frac{\sqrt{N}^{m_1+n_1}}{\sqrt{a_\infty^{m_1} b_\infty^{n_1}}} + \frac{\sqrt{N}^{m_2+n_2}}{a_\infty^{m_2} b_\infty^{n_2}},$$

we infer

$$\|\nabla \sqrt{a}\|_2^2 + \|\nabla \sqrt{b}\|_2^2 \geq \tilde{R} \left(\frac{\sqrt{a}^{m_1} \sqrt{b}^{n_1}}{\sqrt{a_\infty^{m_1} b_\infty^{n_1}}} - \frac{\sqrt{a}^{m_2} \sqrt{b}^{n_2}}{\sqrt{a_\infty^{m_2} b_\infty^{n_2}}} \right)^2 |D_L^{\mathfrak{C}}|,$$

where

$$\tilde{R} = C_P L^2 \left(\frac{\sqrt{N}^{m_1+n_1}}{\sqrt{a_\infty^{m_1} b_\infty^{n_1}}} + \frac{\sqrt{N}^{m_2+n_2}}{a_\infty^{m_2} b_\infty^{n_2}} \right)^{-2}.$$

We combine the above two parts, pick $K > \frac{R+1}{\min\{1, C_P\}}$ and have the following

$$\begin{aligned} 3K(\|\nabla \sqrt{a}\|_2^2 + \|\nabla \sqrt{b}\|_2^2) &+ \left\| \sqrt{\frac{a^{m_1} b^{n_1}}{a_\infty^{m_1} b_\infty^{n_1}}} - \sqrt{\frac{a^{m_2} b^{n_2}}{a_\infty^{m_2} b_\infty^{n_2}}} \right\|_2^2 \\ &\geq K(\|\nabla \sqrt{a}\|_2^2 + \|\nabla \sqrt{b}\|_2^2) + K\tilde{R} \left(\frac{\sqrt{a}^{m_1} \sqrt{b}^{n_1}}{\sqrt{a_\infty^{m_1} b_\infty^{n_1}}} - \frac{\sqrt{a}^{m_2} \sqrt{b}^{n_2}}{\sqrt{a_\infty^{m_2} b_\infty^{n_2}}} \right)^2 |D_L^{\mathfrak{C}}| \\ &+ \left\{ \frac{1}{2} \left(\frac{\sqrt{a}^{m_1} \sqrt{b}^{n_1}}{\sqrt{a_\infty^{m_1} b_\infty^{n_1}}} - \frac{\sqrt{a}^{m_2} \sqrt{b}^{n_2}}{\sqrt{a_\infty^{m_2} b_\infty^{n_2}}} \right)^2 |D_L| - R[\|\delta_a\|_{L^2(D_L)}^2 + \|\delta_b\|_{L^2(D_L)}^2] \right\} \\ &+ K C_P (\|\delta_a\|_{L^2(D_L)}^2 + \|\delta_b\|_{L^2(D_L)}^2) \\ &\geq C_{K,R} \left[\|\nabla \sqrt{a}\|_2^2 + \|\nabla \sqrt{b}\|_2^2 + \left(\frac{\sqrt{a}^{m_1} \sqrt{b}^{n_1}}{\sqrt{a_\infty^{m_1} b_\infty^{n_1}}} - \frac{\sqrt{a}^{m_2} \sqrt{b}^{n_2}}{\sqrt{a_\infty^{m_2} b_\infty^{n_2}}} \right)^2 \right], \end{aligned}$$

where $C_{K,R} := \min\{K\tilde{R}, \frac{1}{2}\}$. We can fix $L > 0$ and get the corresponding R , then pick sufficiently large K (e.g. $K > R+1$) such that we obtain (39) with $D_4 = \frac{C_{K,R}}{3K}$.

It remains to show that there exists a constant D_5 such that

$$\begin{aligned} \|\nabla \sqrt{a}\|_2^2 + \|\nabla \sqrt{b}\|_2^2 &+ \left(\frac{\sqrt{a}^{m_1} \sqrt{b}^{n_1}}{\sqrt{a_\infty^{m_1} b_\infty^{n_1}}} - \frac{\sqrt{a}^{m_2} \sqrt{b}^{n_2}}{\sqrt{a_\infty^{m_2} b_\infty^{n_2}}} \right)^2 \\ &> D_5 [(\sqrt{a} - \sqrt{a_\infty})^2 + (\sqrt{b} - \sqrt{b_\infty})^2]. \end{aligned} \tag{40}$$

We again introduce μ_a, μ_b to parameterize \sqrt{a}, \sqrt{b} with

$$\sqrt{a} = \sqrt{a_\infty}(1 + \mu_a), \quad \sqrt{b} = \sqrt{b_\infty}(1 + \mu_b), \tag{41}$$

where, in view of (35), we have $\mu_\epsilon \leq \mu_a, \mu_b < \mu_\omega$ with $\mu_\epsilon = \frac{\epsilon}{\max\{\sqrt{a_\infty}, \sqrt{b_\infty}\}} - 1$ and $\mu_\omega = \frac{\sqrt{\omega}}{\min\{\sqrt{a_\infty}, \sqrt{b_\infty}\}} - 1$. We have $\sqrt{a} = -\frac{\|\delta_a\|_2^2}{\sqrt{a} + \sqrt{a}} + \sqrt{a} = \sqrt{a} - T(a)\|\delta_a\|_2^2$, where $T(a) = \frac{1}{\sqrt{a} + \sqrt{a}}$. Similarly, $\sqrt{b} = \sqrt{b} - T(b)\|\delta_b\|_2^2$, where $T(b) = \frac{1}{\sqrt{b} + \sqrt{b}}$. Both $T(a), T(b)$ have uniform (in time) upper and lower bounds. Given the symmetry of (6), it suffices to discuss the case $\bar{m}, \bar{n} \geq 0$, so we make this assumption in what

follows; thus, we can factor out $\left(\frac{\sqrt{a}^{m_2}\sqrt{b}^{n_1}}{\sqrt{a_\infty}^{m_2}\sqrt{b_\infty}^{n_1}}\right)^2$ from the squared term in the left hand side of (40) to see that

$$\begin{aligned} & \left(\frac{\sqrt{a}^{m_1}\sqrt{b}^{n_1}}{\sqrt{a_\infty}^{m_1}\sqrt{b_\infty}^{n_1}} - \frac{\sqrt{a}^{m_2}\sqrt{b}^{n_2}}{\sqrt{a_\infty}^{m_2}\sqrt{b_\infty}^{n_2}}\right)^2 = \frac{(\sqrt{a}^{m_2}\sqrt{b}^{n_1})^2}{a_\infty^{m_2}b_\infty^{n_1}} \cdot \left(\frac{\sqrt{a}^{\bar{m}}}{\sqrt{a_\infty}^{\bar{m}}} - \frac{\sqrt{b}^{\bar{n}}}{\sqrt{b_\infty}^{\bar{n}}}\right)^2 \\ & \geq \frac{\epsilon^{2(m_2+n_1)}}{a_\infty^{m_2}b_\infty^{n_1}} \left[\left(1 + \mu_a - \frac{T(a)\|\delta_a\|_2^2}{\sqrt{a_\infty}}\right)^{\bar{m}} - \left(1 + \mu_b - \frac{T(b)\|\delta_b\|_2^2}{\sqrt{b_\infty}}\right)^{\bar{n}} \right]^2 =: A. \end{aligned}$$

Of course, if $\bar{m}, \bar{n} \leq 0$ we would factor out $\left(\frac{\sqrt{a}^{m_1}\sqrt{b}^{n_2}}{\sqrt{a_\infty}^{m_1}\sqrt{b_\infty}^{n_2}}\right)^2$ instead, which would replace the constant $\frac{\epsilon^{2(m_2+n_1)}}{a_\infty^{m_2}b_\infty^{n_2}}$ by $\frac{\epsilon^{2(m_1+n_2)}}{a_\infty^{m_1}b_\infty^{n_2}}$ and the proof would continue otherwise unchanged. We evaluate

$$\begin{aligned} A &= \frac{\epsilon^{2(m_2+n_1)}}{a_\infty^{m_2}b_\infty^{n_1}} \left\{ [(1 + \mu_a)^{\bar{m}} + \|\delta_a\|_2 S_1(\mu_a, \|\delta_a\|_2, T(a))] - [(1 + \mu_b)^{\bar{n}} \right. \\ &\quad \left. + \|\delta_b\|_2 S_2(\mu_b, \|\delta_b\|_2, T(b))] \right\}^2 \\ &\geq \frac{\epsilon^{2(m_2+n_1)}}{a_\infty^{m_2}b_\infty^{n_1}} \left\{ \frac{1}{2} [(1 + \mu_a)^{\bar{m}} - (1 + \mu_b)^{\bar{n}}]^2 - 2[\|\delta_a\|_2 S_1 - \|\delta_b\|_2 S_2]^2 \right\} \\ &\geq \frac{\epsilon^{2(m_2+n_1)}}{a_\infty^{m_2}b_\infty^{n_1}} \left\{ \frac{1}{2} [(1 + \mu_a)^{\bar{m}} - (1 + \mu_b)^{\bar{n}}]^2 - 4(\|\delta_a\|_2^2 + \|\delta_b\|_2^2)S \right\}, \end{aligned}$$

where $S = \max(|S_1|, |S_2|)$.

We have $\|\delta_a\|_2^2 = \bar{a} - (\sqrt{a})^2 \leq \omega$, similarly $\|\delta_b\|_2^2 \leq \omega$ and $T(a), T(b) \leq \frac{1}{\epsilon}$, $\mu_a, \mu_b < \mu_\omega$; so S is uniformly bounded and

$$\begin{aligned} & \left(\frac{\sqrt{a}^{m_1}\sqrt{b}^{n_1}}{\sqrt{a_\infty}^{m_1}\sqrt{b_\infty}^{n_1}} - \frac{\sqrt{a}^{m_2}\sqrt{b}^{n_2}}{\sqrt{a_\infty}^{m_2}\sqrt{b_\infty}^{n_2}}\right)^2 \\ & \geq \frac{\epsilon^{2(m_2+n_1)}}{2a_\infty^{m_2}b_\infty^{n_1}} [(1 + \mu_a)^{\bar{m}} - (1 + \mu_b)^{\bar{n}}]^2 - D_6(\|\delta_a\|_2^2 + \|\delta_b\|_2^2), \end{aligned}$$

where $D_6 = 4\frac{\epsilon^{2(m_2+n_1)}}{a_\infty^{m_2}b_\infty^{n_1}} \|S\|_\infty$. Poincaré's inequality yields

$$\begin{aligned} & \|\nabla \sqrt{a}\|_2^2 + \|\nabla \sqrt{b}\|_2^2 + \left(\frac{\sqrt{a}^{m_1}\sqrt{b}^{n_1}}{\sqrt{a_\infty}^{m_1}\sqrt{b_\infty}^{n_1}} - \frac{\sqrt{a}^{m_2}\sqrt{b}^{n_2}}{\sqrt{a_\infty}^{m_2}\sqrt{b_\infty}^{n_2}}\right)^2 \\ & > D_7[(1 + \mu_a)^{\bar{m}} - (1 + \mu_b)^{\bar{n}}]^2, \end{aligned}$$

where $D_7 = \frac{\epsilon^{2(m_2+n_1)}}{2a_\infty^{m_2}b_\infty^{n_1}} D_6^{-1}$. On the other hand,

$$(\sqrt{a} - \sqrt{a_\infty})^2 + (\sqrt{b} - \sqrt{b_\infty})^2 = a_\infty \mu_a^2 + b_\infty \mu_b^2,$$

so we need to compare $[(1 + \mu_a)^{\bar{m}} - (1 + \mu_b)^{\bar{n}}]^2$ with $\mu_a^2 + \mu_b^2$. First assume $\bar{m}\bar{n} > 0$, i.e. both \bar{m}, \bar{n} are positive integers. The conservation law for (6) reads

$$\lambda_b \bar{n} \bar{a}(t) + \lambda_a \bar{m} \bar{b}(t) = \lambda_b \bar{n} a_\infty + \lambda_a \bar{m} b_\infty \text{ for all } t \geq 0, \quad (42)$$

so (41) together with the nonnegativity of $\lambda_a, \lambda_b, \bar{m}, \bar{n}$ implies that either $\mu_a = \mu_b = 0$ (trivial case) or $\mu_a \mu_b < 0$. Recall that $\mu_a > -1, \mu_b > -1$ for all time. If $\mu_a > 0 > \mu_b$, then

$$[(1 + \mu_a)^{\bar{m}} - (1 + \mu_b)^{\bar{n}}]^2 \geq [(1 + \mu_a) - (1 + \mu_b)]^2 > \mu_a^2 + \mu_b^2.$$

Otherwise, if $\mu_b > 0 > \mu_a$,

$$[(1 + \mu_a)^{\bar{m}} - (1 + \mu_b)^{\bar{n}}]^2 = [(1 + \mu_b)^{\bar{n}} - (1 + \mu_a)^{\bar{m}}]^2 > \mu_a^2 + \mu_b^2,$$

so in all three cases we have that for all time $t \geq 0$

$$[(1 + \mu_a)^{\bar{m}} - (1 + \mu_b)^{\bar{n}}]^2 \geq \mu_a^2 + \mu_b^2.$$

Now, if $\bar{m} = \bar{n} = 0$, we get the decoupled heat equations case where $\mu_a = \mu_b = 0$ for all time t , so the inequality above is trivially satisfied. If $\bar{m} = 0$ and $\bar{n} > 0$, we get $\mu_a = 0$ for all time and it is easy to see that the inequality still holds because we can use $1 - (1 + \mu_b)^{\bar{n}} \geq -\mu_b$ if $\mu_b \leq 0$ and $(1 + \mu_b)^{\bar{n}} - 1 > \bar{n}\mu_b > \mu_b$ if $\mu_b > 0$.

Proof of Theorem 1.2:

Proof. Set $D_5 = \frac{D_7}{\max(a_\infty, b_\infty)}$ to see that (40) holds, and then combine (37), (38), (39) and (40) to reveal

$$D(a, b|a_\infty, b_\infty) \geq \frac{D_2 D_4 D_5}{D_3} E(\bar{a}, \bar{b}|a_\infty, b_\infty).$$

In view of (36), we get

$$D(a, b|a_\infty, b_\infty) \geq D_8 E(a, b|a_\infty, b_\infty)$$

for $D_8 = \min(\frac{D_2 D_4 D_5}{D_3}, D_1)$, which finally proves that the solution decays exponentially to the positive equilibrium at an explicit rate. \square

4. Remarks and open problems.

4.1. Generalized model. Here we indicate how to adapt the above analysis to get convergence to the complex-balanced equilibrium for the following model

$$A + (r+1)B \rightleftharpoons rB + C,$$

where $r > 0$. By the Gagliardo-Nirenberg interpolation inequality [35] (in spatial dimension 1), we know that

$$\|u\|_{L^\infty}^2 \leq C_1 \|\nabla u\|_{L^2}^2 \cdot \|u\|_{L^2}^2 + C_2 \|u\|_{L^2}^2,$$

where $u = \sqrt{a}, \sqrt{b}, \sqrt{c}$. The above inequality implies the following

$$\|a\|_{L^\infty} \lesssim \|\nabla a\|_{L^2}^2 \cdot \|a\|_{L^1}^2 + \|a\|_{L^1}^2 \lesssim \|\nabla a\|_{L^2}^2 + \|a\|_{L^1}^2;$$

the last inequality holds since $\|a\|_{L^1}^2$ has a uniform upper bound (due to the conservation law $a(\bar{t}) + c(\bar{t}) = \bar{a}_0 + \bar{c}_0$). Therefore, we have

$$\int_0^T \|a\|_{L^\infty} dt \lesssim \int_0^T \|\nabla a\|_{L^2}^2 dt + \|a\|_{L^1}^2 \cdot T \lesssim H_1 + \|a\|_{L^1}^2 \cdot T,$$

since $\int_0^\infty \|\nabla a\|_{L^2}^2 dt = H_1 < \infty$ (similarly as (11)). Thus, we get that $\int_0^T \|a\|_{L^\infty} dt$ has at most linear growth, and this estimate holds for b, c as well.

Now let us also make the assumption $\beta = \|\frac{1}{b_0}\|_{L^\infty[0,1]} < \infty$; because the classical solution is continuous, there exists $t_1 > 0$ such that $\|\frac{1}{b(\cdot, t)}\|_{L^\infty[0,1]} < 10\beta$ for all $t \in [0, t_1]$. We have the following equation for b :

$$\partial_t b - d_b \Delta b = b^r c - ab^{(r+1)}.$$

We next divide the above equation by $-b^{(r+1)}$ and get the following:

$$\partial_t \left(\frac{1}{b^r} \right) - d_b \Delta \left(\frac{1}{b^r} \right) = \frac{ab^{(r+1)}}{b^{(r+1)}} - \frac{b^r c}{b^{(r+1)}} - 2d_b r(r+2) \frac{|\nabla b|^2}{b^{(r+2)}} \leq a.$$

Using the maximum principle for the heat equation, we have that, for all $t \in [0, t_1]$,

$$\left\| \frac{1}{b^r(\cdot, t)} \right\|_{L^\infty[0,1]} \leq \left\| \frac{1}{b_0^r} \right\|_{L^\infty[0,1]} + \int_0^T \|a\|_{L^\infty} dt \lesssim \beta + \|a\|_{L^1}^2 \cdot t,$$

where $\beta = \|\frac{1}{b_0^r}\|_{L^\infty[0,1]} + H_1$. We can iterate this inequality in time to get

$$\tilde{b}(t) := \inf_{x \in [0,1]} b^r(x, t) \geq (\beta + \|a\|_{L^1}^2 t)^{-1} \quad (43)$$

for all $t > 0$. We conclude that b^r decays to zero at most linearly, and use the following inequality

$$\Psi\left(\frac{ab^{(r+1)}}{a_\infty b_\infty^{(r+1)}}; \frac{b^r c}{b_\infty^r c_\infty}\right) = \left(\frac{b}{b_\infty}\right)^r \Psi\left(\frac{ab}{a_\infty b_\infty}; \frac{c}{b_\infty c_\infty}\right) \geq \frac{\tilde{b}(t)}{b_\infty^r} \Psi\left(\frac{ab}{a_\infty b_\infty}; \frac{c}{b_\infty c_\infty}\right)$$

to get the L^1 convergence to the positive equilibrium by the same method as in the previous sections.

4.2. Future work. We believe this approach works to prove and quantify the decay rate to the complex balanced equilibrium for more general systems of the type

$$A_1 + A_2 + \dots + A_{n-1} + mA_n \rightleftharpoons A_n + A_{n+1}, \quad (44)$$

and even more complex systems such as

$$A_1 + A_2 + \dots + A_{n-1} + mA_n \rightleftharpoons A_n + A_{n+1} \rightleftharpoons B_1 + \dots + B_k + lA_n,$$

where $k \geq 1$ and $l, m \geq 2$ are integers. In fact, for the former the global essential boundedness of the solution can be proved exactly as for (4), via the method we adopted from [19]. The work [29] ensures that this global boundedness implies exponential decay to the complex-balanced equilibrium for reversible reactions. Albeit with no explicit rate of decay, we infer that if the initial data for (44) lie in $L^\infty(0, 1)$, then this system has a globally essentially bounded unique solution which converges exponentially in time to the its unique accessible complex-balanced equilibrium.

In order to obtain the uniform essential bound on the densities we used the L^∞ version of Poincaré's inequality, which is only available in 1D. Can we employ more refined techniques in order to prove the essential bounds in higher dimensions? These are some questions we plan to address in future work.

5. Appendix.

Lemma 5.1. *For any $x, y > 0$ we have*

$$\Psi(x, y) = x \ln \frac{x}{y} - x + y \geq (\sqrt{x} - \sqrt{y})^2. \quad (45)$$

Proof. The case $x = y$ is trivial. If $x > y > 0$ we use the Jensen inequality for the convex function $f(s) := [y + s(x - y)]^{-1}$ to get

$$\frac{\ln x - \ln y}{x - y} = \int_0^1 f(s) ds \geq f\left(\int_0^1 s ds\right) = \frac{2}{x + y}.$$

By using this inequality and $x + y > 2\sqrt{xy}$, we conclude

$$\begin{aligned} \Psi(x, y) &\geq x \frac{2(x - y)}{(x + y)} - x + y = x \left(2 - \frac{4y}{x + y}\right) - x + y \\ &> x \left(2 - \frac{4y}{2\sqrt{xy}}\right) - x + y = x - 2\sqrt{xy} + y = (\sqrt{x} - \sqrt{y})^2. \end{aligned}$$

Or suppose we have $y > x > 0$ and set $g(u) = e^u$, $u(s) = a + s(b - a)$, for $b > a$. Jensen's inequality shows

$$\frac{e^b - e^a}{b - a} = \int_0^1 g(u(s))ds \geq g\left(\int_0^1 u(s)ds\right) = e^{\frac{a+b}{2}}.$$

Let $b = \ln y$, $a = \ln x$ to deduce

$$\frac{x - y}{\ln x - \ln y} \geq \sqrt{xy}, \quad (46)$$

which implies

$$\frac{x - y}{\sqrt{xy}} \leq \ln\left(\frac{x}{y}\right).$$

It follows

$$\begin{aligned} \Psi(x, y) &\geq x \frac{(x - y)}{\sqrt{xy}} - x + y = \sqrt{\frac{x}{y}}x - \sqrt{xy} - x + y \\ &= \sqrt{\frac{x}{y}}x + \sqrt{xy} - 2\sqrt{xy} - x + y \geq 2x - 2\sqrt{xy} - x + y = (\sqrt{x} - \sqrt{y})^2. \end{aligned}$$

□

The second important tool is:

Lemma 5.2. *For each fixed $y > 0$,*

$$\psi(x, y) := \frac{\Psi(x, y)}{(\sqrt{x} - \sqrt{y})^2} \text{ is increasing in } x \in (0, \infty). \quad (47)$$

Proof. Suppose $x > y > 0$ and set $k = \sqrt{\frac{x}{y}} > 1$. We have

$$\begin{aligned} \frac{d\psi(x, y)}{dx} &= \frac{\ln\left(\frac{x}{y}\right)(\sqrt{x} - \sqrt{y})^2 - [x \ln\left(\frac{x}{y}\right) - x + y](\sqrt{x} - \sqrt{y})\frac{1}{\sqrt{x}}}{(\sqrt{x} - \sqrt{y})^4} \\ &= \frac{\ln\left(\frac{x}{y}\right)(\sqrt{x} - \sqrt{y}) - [x \ln\left(\frac{x}{y}\right) - x + y]\frac{1}{\sqrt{x}}}{(\sqrt{x} - \sqrt{y})^3} \\ &= \frac{[2(k-1)\ln k - (2k\ln k - k + \frac{1}{k})]\sqrt{y}}{(\sqrt{x} - \sqrt{y})^3} = \frac{(k - 2\ln k - \frac{1}{k})\sqrt{y}}{(\sqrt{x} - \sqrt{y})^3}. \end{aligned}$$

Since we have $k > 1$, we use (46) to obtain

$$\frac{k - \frac{1}{k}}{2\ln k} = \frac{k - \frac{1}{k}}{\ln k - \ln(\frac{1}{k})} \geq \sqrt{k \cdot \frac{1}{k}} \implies k - 2\ln k - \frac{1}{k} \geq 0.$$

Combine this with $\sqrt{x} - \sqrt{y} \geq 0$ and $y > 0$ to get

$$\frac{d\psi(x, y)}{dx} \geq 0.$$

We can use the same way to show this inequality is correct when $y > x > 0$. □

Sketch of proof of Theorem 2.2: In [19] the analysis is performed on the whole space $\Omega = \mathbb{R}^d$ and for more general elliptic operators (instead of the Laplacian). However, we argue here that Theorem 2.2 holds for the Laplacian with Neumann BC on bounded domains Ω as well. Indeed, our elliptic operator is the Laplacian

and on a bounded domain $\Omega \subset \mathbb{R}^d$ we have that the estimate (used to prove Lemma 2.1 in [19]) on the fundamental solution to the corresponding parabolic operator

$$0 < G(x, \xi, t, \tau) \leq c_1(T)(t - \tau)^{-d/2} \exp \left\{ -\frac{|x - \xi|^2}{c_2(T)(t - \tau)} \right\}$$

for $x, \xi \in \Omega$, $0 < \tau < t \leq T < \infty$ (where $c_1(T)$, $c_2(T)$ are bounded for finite T) holds for the Heat Kernel with Neumann BC on a bounded domain as well (see, e.g, inequality (1) [6]) with $c_1(t) = ce^t$, and $c_2(t) = C$, for some constants c , $C > 0$. It follows that for the homogeneous problem with initial value at $T \geq 0$, we also have the estimate [6]

$$0 < G_T(x, \xi, t) \leq c_1(t - T)(t - T)^{-d/2} \exp \left\{ -\frac{|x - \xi|^2}{c_2(t - T)(t - T)} \right\},$$

which is used to prove Lemma 4.1 [19]. The proof of Lemma 2.3 [19] requires no modification for the case of bounded domains and natural BC. In the proof of Lemma 2.2 [19] there is an estimate on solutions of the backward terminal value problem for the adjoint equation; [24] is given as a reference. We limit ourselves to noting that when the second order operator is the Laplacian, this backward terminal value problem is equivalent to a forward initial value problem for the right hand side $\tilde{\alpha}(t, x) := \alpha(x, T - t)$ (using the notation from [19], proof of Lemma 2.2); [24] does not cover the Neumann BC case on bounded domains. However, in [36] we do find the exact same estimate available in this case as well. These are the estimates one needs to check in order to convince oneself that Theorem 2.2 holds on a bounded domain $\Omega \subset \mathbb{R}^d$.

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