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Quantitative dynamics of irreversible enzyme reaction–diffusion systems*

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Abstract

In this work we investigate the convergence to equilibrium for mass action reaction–diffusion systems which model irreversible enzyme reactions. Using the standard entropy method in this situation is not feasible as the irreversibility of the system implies that the concentrations of the substrate and the complex decay to zero. The key idea we utilise in this work to circumvent this issue is to introduce a family of cut-off partial entropy-like functionals which, when combined with the dissipation of a mass like term of the substrate and the complex, yield an explicit exponential convergence to equilibrium. This method is also applicable in the case where the enzyme and complex molecules do not diffuse, corresponding to chemically relevant situation where these molecules are large in size.

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(Some figures may appear in colour only in the online journal)

1. Introduction

The focus of our work will be on the well known irreversible enzyme reaction system

$$E + S \underset{k_f}{\overset{k_r}{\leftrightarrows}} C \overset{k_c}{\to} E + P \tag{1.1}$$

where S represents the substrate of the system, E the enzymes, C the intermediate complex (which we will refer to as the complex for simplicity) and P the product.

1.1. The setting of the problem

Our study will concern itself with the inhomogeneous setting of (1.1) which manifests itself in the presence of diffusion of (some of) the system's elements. By applying Fick's law of diffusion and the law of mass action we find that the reaction–diffusion system that corresponds to (1.1) is given by

$$\begin{cases} \partial_t e(x,t) - d_e \Delta e(x,t) = -k_f e(x,t)s(x,t) + (k_r + k_c)c(x,t), & x \in \Omega, t > 0, \\ \partial_t s(x,t) - d_s \Delta s(x,t) = -k_f e(x,t)s(x,t) + k_r c(x,t), & x \in \Omega, t > 0, \\ \partial_t c(x,t) - d_c \Delta c(x,t) = k_f e(x,t)s(x,t) - (k_r + k_c)c(x,t), & x \in \Omega, t > 0, \\ \partial_t p(x,t) - d_p \Delta p(x,t) = k_c c(x,t), & x \in \Omega, t > 0, \\ d_e \partial_\nu e(x,t) = d_s \partial_\nu s(x,t) = d_c \partial_\nu c(x,t) = d_p \partial_\nu p(x,t) = 0, & x \in \partial\Omega, t > 0, \\ e(x,0) = e_0(x),\ s(x,0) = s_0(x),\ c(x,0) = c_0(x),\ p(x,0) = p_0(x), & x \in \Omega, \end{cases} \tag{1.2}$$

where $e(x,t), s(x,t), c(x,t), p(x,t)$ are the concentrations of E, S, C and P, respectively, at $x \in \Omega$ and $t > 0$. The homogeneous Neumann boundary condition indicates that the system is closed, and in order that the equations would make chemical sense we also require that the initial concentrations $e_0(x), s_0(x), c_0(x)$ and $p_0(x)$ are non-negative functions[5].

Looking at the system (1.2), one notices immediately that the equation that governs the concentration of P, $p(x,t)$, is decoupled from the rest of the system and is completely solvable once $c(x,t)$ has been found. Therefore, our main focus in the majority of this work will be on the dynamics of the sub-system of (1.2) which includes e, s and c alone.

[5] As the Neumann condition is connected to the diffusion of the concentration, we have elected to write it as

$$d_e \partial_\nu e(x,t) = d_s \partial_\nu s(x,t) = d_c \partial_\nu c(x,t) = d_p \partial_\nu p(x,t) = 0$$

to indicate that we do not require it when the diffusion coefficient is zero.

Much like many other reaction–diffusion systems in a bounded domain, one expects that the combination of the chemical reactions and the diffusion will result in a state of equilibrium that is composed of constant concentrations. Using the (formal) conservation laws

$$\int_{\Omega}(e(x,t)+c(x,t))\mathrm{d}x = M_0 := \int_{\Omega}(e_0(x)+c_0(x))\mathrm{d}x, \quad \forall\, t \geqslant 0, \tag{1.3}$$

$$\int_{\Omega}(s(x,t)+c(x,t)+p(x,t))\mathrm{d}x = M_1 := \int_{\Omega}(s_0(x)+c_0(x)+p_0(x))\mathrm{d}x, \quad \forall\, t \geqslant 0, \tag{1.4}$$

and under the assumption that $|\Omega| = 1$ for simplicity (which can always be achieved by a simple rescaling of the spatial variable) we find that if all elements in the system diffuse, i.e. if d_e, d_s, d_c and d_p are strictly positive, then the equations that determine the *constant* equilibrium concentrations $e_\infty, c_\infty, s_\infty$ and p_∞ are

$$\begin{cases} -k_f e_\infty s_\infty + (k_r + k_c)c_\infty = 0, \\ -k_f e_\infty s_\infty + k_r c_\infty = 0, \\ k_c c_\infty = 0 \\ e_\infty + c_\infty = M_0, \\ s_\infty + c_\infty + p_\infty = M_1, \end{cases}$$

from which we find that

$$e_\infty = M_0, \qquad c_\infty = 0, \qquad s_\infty = 0, \qquad p_\infty = M_1.$$

This equilibrium carries within it the chemical intuition of the process, as was expected: as time increases, the substrates get completely converted into product, the complex is used up, and the enzymes 'gobble up' whatever left overs remain in the system.

The above, however, is not the true equilibrium when essential parts of the system *do not diffuse*. In this case, we cannot *a priori* guarantee that an equilibrium states for these non-diffusing concentrations, if such exist, will be constant functions. This situation is chemically feasible, for instance when the molecules of the complex and the enzymes are large enough to deter diffusion. In terms of our system (1.2) this situation corresponds to the case where $d_e = d_c = 0$ and d_s and d_p are strictly positive. The lack of diffusion in the complex c is not very problematic, yet the lack of diffusion in the enzymes e complicates matter further. However, in this situation one can find another (formal) conservation law of the form[6]

$$e(x,t) + c(x,t) = e_0(x) + c_0(x), \tag{1.5}$$

which assists in balancing the system. With this in mind, we see that if an equilibrium of the form $e_\infty(x)$, $c_\infty(x)$ and s_∞ exists[7], then it must satisfy

$$\begin{cases} -k_f e_\infty(x) s_\infty + (k_r + k_c)c_\infty(x) = 0, \\ -k_f e_\infty(x) s_\infty + k_r c_\infty(x) = 0, \\ e_\infty(x) + c_\infty(x) = e_0(x) + c_0(x), \end{cases}$$

[6] In this case we have that $\partial_t\,(e(x,t)+c(x,t)) = 0$.

[7] The equilibrium for e and c could be a function of x, but s_∞ is still assumed to be constant due to the diffusion in s.

from which we find that $s_\infty = c_\infty(x) = 0$ and $e_\infty(x) = e_0(x) + c_0(x)$. The fact that $c_\infty(x) = 0$ would lead us to expect that $p(x, t)$ also converges to a constant p_∞ and due to (1.4) we conclude that the suspected equilibrium in this case is given by

$$e_\infty(x) = e_0(x) + c_0(x) \quad s_\infty = c_\infty(x) = 0, \quad p_\infty = M_1. \tag{1.6}$$

The main goal of our work is to explicitly and quantitatively explore the rate of convergence to equilibrium of the solutions to (1.2) in these two cases in the strongest form possible—the L^∞ norm.

1.2. Known results

The study of enzyme reactions goes back more than a century to the pioneering works of Henri [Hen03] and Michaelis and Menten [MM13] which gave rise to the so-called Michaelis–Menten kinetics—derived as a quasi steady state approximation of the mass action kinetics. Reaction–diffusion systems modelling enzyme reactions related to (1.1) have been investigated in many works, see e.g. [BMM93, GCB08, RKL17, TBP02], most of which revolved around the Michaelis–Menten kinetics. At the level of ODEs, this kinetic can be derived rigorously from the mass action kinetic. For the PDEs setting, on the other hand, only asymptotic derivation has been investigated (see e.g. [FLWW18]).

The study of the trend to equilibrium for *reversible* (bio-)chemical reaction–diffusion systems, which has witnessed significant progress in the last decades. The first results in this direction can be attributed to [GGH96, Grö83, Grö92] where the large time behaviour of two dimensional such systems was studied qualitatively. Quantitative results, i.e. explicit convergence rates and constants, have been provided in [DF06, DF08] for special systems, and have been extended later in [DFT17, MHM15] to more complicated ones. The most general equilibration results, which are currently feasible, are those found in [FT18, Mie17]. Reversible versions of (1.1) has also been investigated in [Eli18] where the author has managed to prove exponential convergence to equilibrium.

Despite these developments and advances, the *quantitative* large time behaviour of reaction–diffusion systems modelling *irreversible* reactions, of which (1.2) is a special case, to our knowledge, has not been investigated. The main reason, in our opinion, is the impact the irreversibility has on the *entropy method* which is commonly used to investigate quantitative long time behaviour. We shall address this point shortly, as our work will show how one can 'modify' this method to attain our claimed results. We believe that the method proposed in this work can be applied to more general systems featuring irreversible reactions. It is also remarked that the *qualitative* large time behaviour of (1.2) could be inferred from the vast literature of reaction–diffusion systems. For instance, the results in [PSY19] showed that the trajectory $\{(e(t), s(t), c(t))\}_{t\geqslant 0}$ is in fact relatively compact in $L^1(\Omega)$.

1.3. Main results

As was indicated in the end of section 1.1, our work is devoted to the investigation of two cases for the system (1.2). Our main results can be expressed by the following theorems:

Theorem 1.1. *Let $\Omega \subset \mathbb{R}^n$ be a bounded, open domain with $C^{2+\zeta}$, $\zeta > 0$, boundary, $\partial\Omega$. Assume that d_e, d_s, d_c and d_p are strictly positive constants and that the initial data $e_0(x), s_0(x), c_0(x)$ and $p_0(x)$ are all bounded non-negative functions. Then there exists a unique non-negative bounded classical solution to* (1.2)*. Moreover, there exists an explicit $\gamma > 0$ such* *that for any $\eta > 0$ there exists an explicit constant $\mathcal{C}_\eta$, depending only on geometric properties and the initial data which blows up as η goes to zero, such that*

$$\begin{aligned} \|c(t)\|_{L^\infty(\Omega)} + \|s(t)\|_{L^\infty(\Omega)} &\leqslant \mathcal{C}_\eta\, \mathrm{e}^{-\frac{2\gamma t}{n(1+\eta)}}, \\ \|e(t) - e_\infty\|_{L^\infty(\Omega)} &\leqslant \mathcal{C}_\eta\, \mathrm{e}^{-\frac{\gamma t}{n(1+\eta)}}. \end{aligned} \tag{1.7}$$

In addition for any $\varepsilon > 0$ and $\eta > 0$ with $n\,(1+\eta) \geqslant 4$ there exists an explicit constant $\mathcal{C}_{\eta,\varepsilon}$, depending only on geometric properties and the initial data which blows up as η or ε go to zero, such that

$$\|p(t) - p_\infty\|_{L^\infty(\Omega)} \leqslant \mathcal{C}_{\eta,\varepsilon}\left(1 + t^{\frac{4}{n(1+\eta)}\delta_{\frac{2d_p}{C_\mathrm{P}}(1-\varepsilon),\gamma}}\right)\mathrm{e}^{-\min\left(\frac{4d_p}{nC_\mathrm{P}(1+\eta)}(1-\varepsilon),\frac{2\gamma}{n(1+\eta)}\right)t} \tag{1.8}$$

where

$$\delta_{x,y} = \begin{cases} 1 & x = y \\ 0 & x \neq y \end{cases}$$

and C_P is the Poincaré constant associated to the domain Ω.

Theorem 1.2. *Let $\Omega \subset \mathbb{R}^n$ be a bounded, open domain with $C^{2+\zeta}, \zeta > 0$ boundary, $\partial\Omega$. Assume that d_s and d_p are strictly positive constants while $d_e = d_c = 0$. Assume in addition that the initial data $e_0(x)$, $s_0(x)$, $c_0(x)$ and $p_0(x)$ are all bounded non-negative functions and that there exists some $\beta > 0$ such that*

$$e_0(x) + c_0(x) \geqslant \beta \quad a.e.\ x \in \Omega. \tag{1.9}$$

Then there exists a unique non-negative bounded strong solution to (1.2). Moreover, there exists an explicit constant $\gamma > 0$ such that for any $\eta > 0$ there exists an explicit constant $\mathcal{C}_\eta$, depending only on geometric properties and the initial data which blows up as η goes to zero, such that

$$\begin{aligned} \|s(t)\|_{L^\infty(\Omega)} &\leqslant \mathcal{C}_\eta\, \mathrm{e}^{-\frac{2\gamma}{n(1+\eta)}t}, \\ \|e(x,t) - e_\infty(x)\|_{L^\infty(\Omega)} + \|c(t)\|_{L^\infty(\Omega)} &\leqslant \mathcal{C}_\eta\left(1 + t^{\delta_{k_r+k_c,\frac{2\gamma}{n(1+\eta)}}}\right)\mathrm{e}^{-\min\left(k_r+k_c,\frac{2\gamma}{n(1+\eta)}\right)t}. \end{aligned}$$

In addition for any $\varepsilon > 0$ and $\eta > 0$ with $n\,(1+\eta) \geqslant 4$ there exists an explicit constant $\mathcal{C}_{\eta,\varepsilon}$, depending only on geometric properties and the initial data which blows up as η or ε go to zero, such that

$$\|p(t) - p_\infty\|_{L^\infty(\Omega)} \leqslant \mathcal{C}_{\eta,\varepsilon}\left(1 + t^{\frac{4}{n(1+\eta)}\delta_{\frac{2d_p}{C_\mathrm{P}}(1-\varepsilon),\gamma}}\right)\mathrm{e}^{-\min\left(\frac{4d_p}{nC_\mathrm{P}(1+\eta)}(1-\varepsilon),\frac{2\gamma}{n(1+\eta)}\right)t}$$

Remark 1.3. Our notion of *strong solutions* to (1.2) is as follows: for any $p \in [1, \infty)$, any component of the solution belongs to $C([0,\infty);\ L^p(\Omega))$ and is absolutely continuous on $(0,\infty)$ with respect to $L^p(\Omega)$. Moreover, the time derivatives and the spatial derivatives up to second order of any concentration which is diffusing are in $L^p\left((\tau, T); L^p\left(\Omega\right)\right)$ for any $T > \tau > 0$, and the equations and boundary conditions are satisfied a.e. in $\Omega \times (0,T)$ and a.e. in $\partial\Omega \times (0,T)$ respectively, for any $T > 0$.

Remark 1.4. During our proofs we will be able to provide an explicit form to γ in each of the theorems. We will show that one can choose

$$\gamma = \min\left(\frac{\left(d_e C_{\mathrm{LSI}} - 6\left(\frac{(k_c+k_r)}{M_0} + k_f\right)\max(\varepsilon_c, \varepsilon_s)\right)}{\left(1 + \left(\log\left(1+\frac{M_1}{\varepsilon_s}\right) + \frac{k(2k_r+k_c)}{2k_r}\right)\frac{16(\varepsilon_s+M_1)}{(1-\log(2))M_0}\right)},\right.$$
$$\times \frac{\frac{kk_c}{2} - k_c - k_r - 2k_f\varepsilon_s}{\left(1 + k + \log\left(1+\frac{M_0}{\varepsilon_c}\right) + \left(\log\left(1+\frac{M_1}{\varepsilon_s}\right) + \frac{k(2k_r+k_c)}{2k_r}\right)\left(\frac{2k_r}{k_f M_0} + \frac{16(\varepsilon_s+M_1)}{(1-\log(2))M_0}\right)\right)},$$
$$\left.\times \frac{d_c d_s C_{\mathrm{LSI}}}{d_s + d_c\left(1 + \left(\log\left(1+\frac{M_1}{\varepsilon_s}\right) + \frac{k(2k_r+k_c)}{2k_r}\right)\right)}\right) \tag{1.10}$$

with

$$\varepsilon_c = \frac{C_{\mathrm{LSI}} M_0}{12\left(k_c + k_r + M_0 k_f\right)\max\left(1, \frac{k_r}{M_0 k_f}\right)}, \quad \varepsilon_s = \frac{k_r}{M_0 k_f}\varepsilon_c, \quad k = \frac{4\left(k_c + k_r + k_f \varepsilon_s\right)}{k_c}, \tag{1.11}$$

for theorem 1.1, where C_{LSI} is the log-Sobolev constant that is associated to the domain Ω, and

$$\gamma = \min\left(\frac{\frac{kk_c}{2} - k_f\varepsilon_s}{\left(1 + k + \log\left(1+\frac{k_r}{k_f\varepsilon_s}\right) + \left(\log\left(1+\frac{M_1}{\varepsilon_s}\right) + \frac{k(2k_r+k_c)}{2k_r}\right)\left(\frac{2k_r}{k_f\beta} + \frac{16(\varepsilon_s+M_1)}{(1-\log(2))\beta}\right)\right)}\right.$$
$$\left.\times \frac{d_s C_{\mathrm{LSI}}}{1 + \left(\log\left(1+\frac{M_1}{\varepsilon_s}\right) + \frac{k(2k_r+k_c)}{2k_r}\right)}\right), \tag{1.12}$$

with

$$\varepsilon_s \in (0, \infty), \qquad k = \frac{4k_f\varepsilon_s}{k_c}, \tag{1.13}$$

for theorem 1.2. These choices are clearly far from optimal. Optimal convergence rate is a subtle issue and remains open in most chemical reaction–diffusion systems. Some discussion about this issue in the case where all diffusion coefficients are strictly positive will be given in section 4.3.

Remark 1.5. In our analysis, the lower bound condition (1.9) is essential to be able to obtain the explicit exponential convergence to equilibrium. This condition is easily satisfied when we require that the initial enzyme concentration e_0 is present everywhere in Ω. In the case where (1.9) does not hold, numerical solutions suggest that convergence to equilibrium can still be expected as is indicated in figure 1 in section 4.4. A rigorous proof, however, remains an open problem.

A common method one employs to investigate the *quantitative* long time behaviour of chemical reaction–diffusion systems (and many other physically, chemically and biologically relevant equations) is the so-called *entropy method*: by considering the connection between a natural Lyapunov functional of the system, the *entropy*, and its dissipation, usually via a functional inequality, one recovers an explicit rate of convergence to equilibrium. This convergence rate can be boosted up to stronger norms in many situations, at least as long as the system has some smoothing effects.

This method has been extremely successful in dealing with reaction–diffusion systems which model *reversible* reactions, see e.g. [DF06, DFT17, FT18, MHM15] and references therein. A fundamental property of these systems which help facilitate the entropy method is the existence of a *strictly positive* equilibrium, which allows the consideration of natural entropies such as the Boltzmann entropy (to be defined shortly). This property, however, is not necessarily true in most open or irreversible reaction systems, precluding the consideration of the aforementioned entropies and, in our opinion, resulting in a relatively sparse study of the quantitative large time behaviour of such systems. The current work serves, to our knowledge, as the first study in this direction for the well known enzyme reaction (1.1), and we believe that the method introduced herein will be applicable to many other open and irreversible systems,

Let us delve deeper into the entropies one encounters in the study of chemical reaction–diffusion systems, the issues of a zero equilibrium, and how we propose to overcome it in this work.

A natural entropy to consider in many chemical reaction–diffusion systems is generated by the *Boltzmann entropy function*

$$\mathfrak{h}(x) = x \log x - x + 1, \quad x \geqslant 0. \tag{1.14}$$

In particular, one uses this entropy function to define a *relative entropy* functional that measures the 'entropic distance' between a solution to an equation, $f(x)$, and its equilibrium f_∞:

$$\mathcal{E}(f|f_\infty) = \int_\Omega h\left(f(x)|f_\infty\right) \mathrm{d}x \tag{1.15}$$

where

$$h\left(x|y\right) = x \log\left(\frac{x}{y}\right) - x + y = y\mathfrak{h}\left(\frac{x}{y}\right), \quad x, y > 0. \tag{1.16}$$

Both $\mathcal{E}$ and h are not well defined when $f_\infty = 0$ which is exactly the equilibrium we have (or suspect) for our substrate and complex concentrations s and c. Similar issues occur when the equilibrium is spatially inhomogeneous, i.e. $f_\infty = f_\infty(x)$, with

$$|\{x \in \Omega | f_\infty(x) = 0\}| > 0.$$

This situation can indeed occur, as was shown in [JR11] where one finds that f_∞ can be a sum of Dirac masses.

The first key idea and strategy that will guide us in showing our main results is to *modify* our Boltzmann entropy by defining a new relative entropy-like function that is 'cut' when the concentration becomes 'small enough':

$$h_\varepsilon\left(x|\varepsilon\right) = \begin{cases} x \log\left(\frac{x}{\varepsilon}\right) - x + \varepsilon & x \geqslant \varepsilon, \\ 0 & x < \varepsilon. \end{cases} \tag{1.17}$$

With this 'cut-off' entropy, we will consider a *partial* entropy-like functional

$$\mathscr{H}_{\varepsilon_c,\varepsilon_s}(e,s,c) = \int_\Omega h(e(x)|e_\infty)\mathrm{d}x + \int_\Omega h_{\varepsilon_c}(c(x)|\varepsilon_c)\mathrm{d}x + \int_\Omega h_{\varepsilon_s}(s(x)|\varepsilon_s)\mathrm{d}x,$$

where $\varepsilon_c, \varepsilon_s$ are to be chosen in a meaningful way. It is not clear if $\mathscr{H}_{\varepsilon_c,\varepsilon_s}$ is decreasing along the evolution of the system. Moreover, as we expect c and s to converge to zero, we expect $\mathscr{H}_{\varepsilon_c,\varepsilon_s}(e,s,c)$ to eventually become dependent only on e and e_∞ for any fixed ε_c and ε_s—the smallness of $\mathscr{H}_{\varepsilon_c,\varepsilon_s}(e,s,c)$ can only give us information on the convergence of e to e_∞.

This is the point where we introduce our second key idea: combine this partial entropy-like functional with a sum of masses from the substrate and complex which decreases and, together with the 'partial entropy', will drive these concentration to zero[8]. This sum of masses will be of the form

$$\mathscr{M}(s,c) = \int_\Omega (c(x) + \eta s(x))\mathrm{d}x$$

with a suitable choice of $\eta > 0$. The drive of the concentration towards zero by $\mathscr{M}(s,c)$ is expressed by the fact that we will find an explicit *mass density*, $\mathscr{d}_{\mathscr{M}}(x)$, such that

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{M}(s,c) = -\int_\Omega \mathscr{d}_{\mathscr{M}}(x)\mathrm{d}x \leqslant 0. \tag{1.18}$$

With $\mathscr{H}_{\varepsilon_c,\varepsilon_s}(e,s,c)$ and $\mathscr{M}(s,c)$ at hand we will define our *total* entropy-like functional to be

$$\mathscr{E}_{\varepsilon_c,\varepsilon_s,k}(e,s,c) = \mathscr{H}_{\varepsilon_c,\varepsilon_s}(e,s,c) + k\mathscr{M}(s,c)$$

for an appropriately chosen constant $k > 0$.

Showing the exponential convergence to equilibrium of $\mathscr{E}_{\varepsilon_c,\varepsilon_s,k}$ will take lead from ideas that govern the entropy method. Indeed, while $\mathscr{H}_{\varepsilon_c,\varepsilon_s}(e,s,c)$ might not be decreasing along the flow of (1.2), we will show that we could find a *'partial entropic' density*, $\mathscr{d}_{\varepsilon_c,\varepsilon_s}(x)$, such that

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}_{\varepsilon_c,\varepsilon_s,k}(e,s,c) \lesssim \begin{cases} -\int_\Omega \left(\mathscr{d}_{\varepsilon_c,\varepsilon_s}(x) + h(e(x)|\overline{e}) + \mathscr{d}_{\mathscr{M}}(x)\right)\mathrm{d}x & d_e, d_s, d_c > 0, \\ -\int_\Omega \left(\mathscr{d}_{\varepsilon_c,\varepsilon_s}(x) + \mathscr{d}_{\mathscr{M}}(x)\right)\mathrm{d}x & d_e = d_c = 0, \end{cases} \tag{1.19}$$

where $\overline{e} = \int_\Omega e(x)\mathrm{d}x$, and where the appropriate constant may depend on ε_c, ε_s and k. (1.19), together with the structure of $\mathscr{d}_{\varepsilon_c,\varepsilon_s}$ and $\mathscr{d}_{\mathscr{M}}$, will imply that for suitable choices for ε_c, ε_s and k we will get that

$$\begin{cases} -\int_\Omega \left(\mathscr{d}_{\varepsilon_c,\varepsilon_s}(x) + h(e(x)|\overline{e}) + \mathscr{d}_{\mathscr{M}}(x)\right)\mathrm{d}x & d_e, d_s, d_c > 0, \\ -\int_\Omega \left(\mathscr{d}_{\varepsilon_c,\varepsilon_s}(x) + \mathscr{d}_{\mathscr{M}}(x)\right)\mathrm{d}x & d_e = d_c = 0, \end{cases} \lesssim -\mathscr{E}_{\varepsilon_c,\varepsilon_s,k}(e,s,c),$$

from which the exponential decay of $\mathscr{E}_{\varepsilon_c,\varepsilon_s,k}$ follows. It is worth mentioning that the above inequality is a *purely functional inequality* that may be of interest in other related problems.

At this point it is important to note that while $\mathscr{E}_{\varepsilon_c,\varepsilon_s,k}$ is motivated from entropic considerations, the fact that it constructed from a truncated entropy density and a combination of mass

[8] One can think of this as a hypocoercivity idea.

terms excludes it from being a 'true' entropy in the physical sense. It is, nonetheless, a Lyapunov functional that is closely connected to using the *entropy method*. In the coming sections we shall abuse the notations of 'entropy' and 'entropy density' to simplify our presentation, yet we urge the reader to keep the above in mind.

With the decay of this entropy-like at hand, the boundedness of the solution to (1.2) will imply the desired L^∞ convergence in the regularising case of full diffusion fairly easily. As could be expected, the case where $d_e = d_c = 0$ is more complicated as it precludes regularisation for these concentration. However, as s still enjoys regularisation and its convergence can be boosted to an L^∞ one, the ODE nature of the equations for e and c together with the behaviour of s will give us the desired L^∞ estimation. As predicted, the explicit convergence of p to its equilibrium will follow immediately from our conservation law (1.4) and the long time behaviour of c.

We would like to mention that the idea of using a 'truncated entropy' functional has been used before, see for instance [BRZ20, GV10], yet to our knowledge this is the first time it has been used to attain *quantiative* convergence rates to equilibrium.

1.4. The structure of the work

In section 2 we will define our entropy-like functionals and will employ the ideas of the entropy method to achieve an exponential convergence to equilibrium in both our cases under the assumption of the existence of strong solutions. In section 3 we shall use the convergence of this 'entropy' and regularising properties of our system to conclude theorems 1.1 and 1.2. We will conclude with some final thoughts in section 4 which will be followed by an appendix A where we will consider a few technical lemmas and theorems that have been used along our work.

2. The modified entropy-like functional

The goal of this section is to define our entropy, which will comprise of 'cut off' Boltzmann entropy and a decreasing mass-like term, and to explore its evolution. We remind the reader that we assume throughout the presented work that $|\Omega| = 1$. Simple modification can be made to accommodate the general case.

Definition 2.1. For given non-negative functions $e(x)$, $c(x)$ and $s(x)$, strictly positive coefficients k_r, k_f and k_c, strictly positive constants ε_s and k, and strictly positive functions $\varepsilon_c(x)$ and $e_\infty(x)$, we define the partial mass function, $\mathscr{M}$, the Boltzmann entropy-like function, $\mathscr{H}_{\varepsilon_c,\varepsilon_s}$, and the entropy functional $\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}$ as

$$\mathscr{M}(c,s) := \int_\Omega \left(c(x) + \frac{1}{2}\left(\frac{2k_r + k_c}{k_r}\right) s(x)\right) \mathrm{d}x, \tag{2.1}$$

$$\mathscr{H}_{\varepsilon_c,\varepsilon_s}(e,c,s) := \int_\Omega h(e(x)|e_\infty(x))\mathrm{d}x + \int_\Omega h_{\varepsilon_c(x)}(c(x)|\varepsilon_c(x))\mathrm{d}x + \int_\Omega h_{\varepsilon_s}(s(x)|\varepsilon_s)\mathrm{d}x, \tag{2.2}$$

and

$$\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e,c,s) := \mathscr{H}_{\varepsilon_c,\varepsilon_s}(e,c,s) + k\mathscr{M}(c,s). \tag{2.3}$$

The subscripts of $\mathscr{H}_{\varepsilon_c,\varepsilon_s}$, ε_c and ε_s, correspond to the choice of entropic cut off we will perform. Their choices will be motivated by the *reversible* chemical reaction that the substrate and intermediate compound undergo. The additional parameter for the entropy $\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}$, k, corresponds to the ratio of the mass like element that we need to add to drive the convergence to equilibrium once we have reached our entropic threshold ε_c and ε_s.

The main theorem we will show in this section is the following:

Theorem 2.2. *Let $e(x,t), c(x,t)$ and $s(x,t)$ be non-negative bounded strong solutions to the irreversible enzyme system (1.2) with initial data $e_0(x), c_0(x)$ and $s_0(x)$. Then*

(*a*) *If d_e, d_s and d_c are strictly positive constants, and ε_c and ε_s are constants such that*

$$\frac{\varepsilon_c}{M_0\varepsilon_s} = \frac{k_f}{k_r}, \tag{2.4}$$

then for any γ such that

$$\begin{aligned}\gamma \leqslant \min\Bigg(&\frac{\left(d_e C_{\mathrm{LSI}} - 6\left(\frac{(k_c+k_r)}{M_0} + k_f\right)\max(\varepsilon_c,\varepsilon_s)\right)}{\left(1+\left(\log\left(1+\frac{M_1}{\varepsilon_s}\right)+\frac{k(2k_r+k_c)}{2k_r}\right)\frac{16(\varepsilon_s+M_1)}{(1-\log(2))M_0}\right)},\\ &\times \frac{\frac{kk_c}{2} - k_c - k_r - 2k_f\varepsilon_s}{\left(1+k+\log\left(1+\frac{M_0}{\varepsilon_s}\right)+\left(\log\left(1+\frac{M_1}{\varepsilon_c}\right)+\frac{k(2k_r+k_c)}{2k_r}\right)\left(\frac{2k_r}{k_f M_0}+\frac{16(\varepsilon_s+M_1)}{(1-\log(2))M_0}\right)\right)},\\ &\times \frac{d_c d_s C_{\mathrm{LSI}}}{d_s + d_c\left(1+\log\left(1+\frac{M_1}{\varepsilon_s}\right)+\frac{k(2k_r+k_c)}{2k_r}\right)}\Bigg),\end{aligned} \tag{2.5}$$

we have that

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e(t),c(t),s(t)) + \gamma\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e(t),c(t),s(t)) \leqslant 0, \tag{2.6}$$

and consequently

$$\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e(t),c(t),s(t)) \leqslant \mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0,c_0,s_0)e^{-\gamma t}. \tag{2.7}$$

(*b*) *If $d_e = d_c = 0$ and $d_s > 0$, and if there exists $\beta > 0$ such that*

$$e_\infty(x) = e_0(x) + c_0(x) \geqslant \beta, \quad a.e.\ x \in \Omega, \tag{2.8}$$

then for any strictly positive functions $\varepsilon_c(x)$ and constant ε_s such that

$$\frac{\varepsilon_c(x)}{e_\infty(x)} = \frac{k_f}{k_r}\varepsilon_s, \tag{2.9}$$

and any γ *such that*

$$\gamma \leqslant \min\left(\frac{\frac{kk_c}{2}-k_f\varepsilon_s}{\left(1+k+\log\left(1+\frac{k_r}{k_f\varepsilon_s}\right)+\left(\log\left(1+\frac{M_1}{\varepsilon_s}\right)+\frac{k(2k_r+k_c)}{2k_r}\right)\left(\frac{2k_r}{k_f\beta}+\frac{16(\varepsilon_s+M_1)}{(1-\log(2))\beta}\right)\right)}\right.$$
$$\left.\times\frac{d_sC_{\mathrm{LSI}}}{1+\log\left(1+\frac{M_1}{\varepsilon_s}\right)+\frac{k(2k_r+k_c)}{2k_r}}\right), \tag{2.10}$$

we have that (2.6) *and* (2.7) *are valid.*

Remark 2.3. Possible choices for ε_c, ε_s and k in (a) that give an explicit positive γ that equals the expression in the right-hand side of (2.5) are

$$\begin{aligned}\varepsilon_s &= \frac{d_eC_{\mathrm{LSI}}M_0}{12\left(k_c+k_r+M_0k_f\right)\max\left(1,\frac{M_0k_f}{k_r}\right)},\\ \varepsilon_c &= \frac{M_0k_f}{k_r}\varepsilon_s\\ k &= \frac{4\left(k_c+k_r+2k_f\varepsilon_s\right)}{k_c}.\end{aligned}$$

Similarly, for (b) one can choose

$$\varepsilon_s\in(0,\infty),$$
$$\varepsilon_c(x)=\frac{k_f\varepsilon_s}{k_r}e_\infty(x)=\frac{k_f\varepsilon_s}{k_r}\left(e_0(x)+c_0(x)\right)\geqslant\frac{k_f\varepsilon_s}{k_r}\beta>0$$
$$k=\frac{4k_f\varepsilon_s}{k_c}.$$

Remark 2.4. Condition (2.4) gives us one ingredient of how one chooses the thresholds for our substrate and intermediate compound. Note that it is strongly related to the reversible chemical reaction in (1.1), as was eluded before.

Looking at condition (2.9), on the other hand, one might wonder why ε_s is required to remain a constant while $\varepsilon_c(x)$ is allowed to be changed to a function. The fact that some change is needed is evident from the fact that our equilibrium state for e is no longer constant. However, when one differentiates the entropy $\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}$ with respect to time in the case where $d_e=d_c=0$ the only term that brings out a Laplacian, and as such requires additional integration by parts, is that which is induced from $h_{\varepsilon_s}\left(s(x)|\varepsilon_s\right)$. Keeping ε_s constant is a vital simplification to the estimation of the evolution of this term (as will be shown shortly).

In order to prove theorem 2.2 we will explore the dissipation properties of $\mathscr{M}$ and $\mathscr{H}_{\varepsilon_c,\varepsilon_s}$, starting with the simple mass-like term.

Lemma 2.5. *Let* $c(x,t)$ *and* $s(x,t)$ *be non-negative strong solutions to the irreversible enzyme system* (1.2). *Then*

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{M}(c(t),s(t))=-\frac{k_fk_c}{2k_r}\int_\Omega e(x,t)s(x,t)\mathrm{d}x-\frac{k_c}{2}\int_\Omega c(x,t)\mathrm{d}x. \tag{2.11}$$

Proof. As $c(x,t)$ and $s(x,t)$ are strong solutions to our system of equations we find that by integration by parts[9] one has that

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{M}(c(t),s(t)) = \int_\Omega \left(d_c\Delta c(x,t) + k_f e(x,t)s(x,t) - (k_r+k_c)\,c(x,t)\right) + \frac{1}{2}\left(\frac{2k_r+k_c}{k_r}\right)\left(d_s\Delta s(x,t) - k_f e(x,t)s(x,t) + k_r c(x,t)\right)\mathrm{d}x$$
$$= -\frac{k_f k_c}{2k_r}\int_\Omega e(x,t)s(x,t)\mathrm{d}x - \frac{k_c}{2}\int_\Omega c(x,t)\mathrm{d}x,$$

giving us the desired result. □

The investigation of the Boltzmann-like entropy is a bit more involved. To simplify the computations that will follow we define a few new functions that relate to the generators of $\mathscr{H}_{\varepsilon_c,\varepsilon_s}$ and its dissipation, as well as the generator of the dissipation of $\mathscr{M}$. To be able to do so we introduce another entropically relevant function, which makes its appearance in the entropic dissipation term:

$$\mathscr{h}(x) = x - \log x - 1, \quad x > 0. \tag{2.12}$$

Note that much like $\mathfrak{h}$, $\mathscr{h}$ is non-negative and $\mathscr{h}(x) = 0$ if and only if $x = 1$. We will also need a geometric constant for our definitions, C_{LSI}, which is the log-Sobolev constant of the domain Ω, i.e. the constant for which we have that

$$\int_\Omega \frac{|\nabla f(x)|^2}{f(x)}\,\mathrm{d}x \geqslant C_{\mathrm{LSI}}\int_\Omega h\left(f(x)|\overline{f}\right)\,\mathrm{d}x, \tag{2.13}$$

for any non-negative $f \in H^1(\Omega)$ where $\overline{f} = \int_\Omega f(x)\mathrm{d}x$. For more information on the above inequality we refer the reader to [DF14].

Definition 2.6. For a given non-negative functions $e(x)$, $c(x)$ and $s(x)$, strictly positive constants k_r, k_f and ε_s, and strictly positive functions $\varepsilon_c(x)$ and $e_\infty(x)$ we define the *mass density*

$$\mathscr{d}_{\mathscr{M}}(x) := \frac{k_f}{k_r}e(x)s(x) + c(x), \tag{2.14}$$

and the *partial entropy production density*

$$\mathscr{d}_{\varepsilon_c,\varepsilon_s}(x) := \begin{cases} k_f c(x)\mathbf{h}\left(\frac{e(x)s(x)}{c(x)}\middle|\frac{e_\infty(x)\varepsilon_s}{\varepsilon_c(x)}\right) + k_c e(x)h\left(\frac{c(x)}{e(x)}\middle|\frac{\varepsilon_c(x)}{e_\infty(x)}\right) \\ \quad +C_{\mathrm{LSI}}d_s h\left(s(x)|\overline{s_{\varepsilon_s}}\right) + C_{\mathrm{LSI}}d_c h\left(c(x)|\overline{c_{\varepsilon_c(x)}}\right) & x\in\Omega_1 \\ k_r c(x)\mathscr{h}\left(\frac{e(x)s(x)}{e_\infty(x)\varepsilon_s}\right) + k_c c(x)\mathscr{h}\left(\frac{e(x)}{e_\infty(x)}\right) \\ \quad +k_f h\left(e(x)s(x)|e_\infty(x)\varepsilon_s\right) + C_{\mathrm{LSI}}d_s h\left(s(x)|\overline{s_{\varepsilon_s}}\right) & x\in\Omega_2, \\ (k_r+k_c)\,e(x)h\left(\frac{c(x)}{e(x)}\middle|\frac{\varepsilon_c(x)}{e_\infty(x)}\right) + k_f c(x)s(x)h\left(\frac{e(x)}{c(x)}\middle|\frac{e_\infty(x)}{\varepsilon_c(x)}\right) \\ \quad +C_{\mathrm{LSI}}d_c h\left(c(x)|\overline{c_{\varepsilon_c(x)}}\right) & x\in\Omega_3 \\ k_f s(x)h\left(e(x)|e_\infty(x)\right) + (k_r+k_c)\,c(x)\mathscr{h}\left(\frac{e(x)}{e_\infty(x)}\right) & x\in\Omega_4 \end{cases}, \tag{2.15}$$

[9] More information about it is given in appendix A.

where

$$\Omega_1 = \{x \in \Omega | c(x) \geqslant \varepsilon_c(x),\ s(x) \geqslant \varepsilon_s\}, \qquad \Omega_2 = \{x \in \Omega | c(x) < \varepsilon_c(x),\ s(x) \geqslant \varepsilon_s\},$$
$$\Omega_3 = \{x \in \Omega | c(x) \geqslant \varepsilon_c(x),\ s(x) < \varepsilon_s\}, \qquad \Omega_4 = \{x \in \Omega | c(x) < \varepsilon_c(x),\ s(x) < \varepsilon_s\}, \tag{2.16}$$

$$\overline{f_\varepsilon} = \int_\Omega \max(f(x), \varepsilon)\, \mathrm{d}x, \tag{2.17}$$

and $\mathbf{h}(x|y) = (x - y)\log\left(\frac{x}{y}\right)$ for $x, y \geqslant 0$ with the value of ∞ when $y = 0$.

Remark 2.7. The appearance of the function $\mathscr{I}_{\varepsilon_c,\varepsilon_s}$ and its choice of name will become apparent when we will start differentiating $\mathscr{H}_{\varepsilon_c,\varepsilon_s}$. We would like to emphasise that its form is not surprising when considering the domain $\Omega_1, \Omega_2, \Omega_3$ and Ω_4. Indeed, intuitively speaking, in any domain where c or s are bigger than the threshold ε_c or ε_s respectively we find the relative entropy terms that push us towards the threshold, while if c or s are too small these terms are mostly replaced by linear terms in c or s that are very small.

With this auxiliary functions at hand we can state our first entropy inequality:

Theorem 2.8. *Let $e(x,t), c(x,t)$ and $s(x,t)$ be non-negative bounded strong solutions to the irreversible enzyme system (1.2). Then*

- *If all diffusion coefficients are strictly positive, then assuming that (2.4) is satisfied we have that*

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}_{\varepsilon_c,\varepsilon_s,k}(t) + \int_\Omega \left(\mathscr{I}_{\varepsilon_c,\varepsilon_s}(x,t) + \left(\frac{kk_c}{2} - k_c - k_r - 2k_f\varepsilon_s\right)\mathscr{I}_{\mathscr{M}}(x,t)\right)$$
$$+ \left(d_e C_{\mathrm{LSI}} - 6\left(\frac{(k_c + k_r)}{M_0} + k_f\right)\max(\varepsilon_c, \varepsilon_s)\right) h\left(e(x,t)|\overline{e(t)}\right)\mathrm{d}x \leqslant 0, \tag{2.18}$$

  where $\overline{f} = \int_\Omega f(x)\mathrm{d}x$.
- *If $d_e = d_c = 0$ and ε_s, $\varepsilon_c(x)$ and $e_\infty(x)$ satisfy (2.9) we have that*

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}_{\varepsilon_c,\varepsilon_s,k}(t) + \int_\Omega \mathscr{I}_{\varepsilon_c,\varepsilon_s}(x,t)\mathrm{d}x + \left(\frac{k_c k}{2} - k_f\varepsilon_s\right)\int_\Omega \mathscr{I}_{\mathscr{M}}(x,t)\mathrm{d}x \leqslant 0. \tag{2.19}$$

Remark 2.9. When all diffusion coefficients are strictly positive, we find that the suspected equilibrium of e is a constant e_∞, which satisfies

$$e_\infty = M_0 = \int_\Omega (e_0(x) + c_0(x))\,\mathrm{d}x = \int_\Omega (e(x,t) + c(x,t))\,\mathrm{d}x.$$

We see that in this case (2.4) is equivalent to

$$\frac{\varepsilon_c}{e_\infty\varepsilon_s} = \frac{k_f}{k_r},$$

which we will use in our proof.

One technical lemma we require to prove theorem 2.8 is the following:

Lemma 2.10. *Let Ω be a bounded domain with C^1 boundary and let $f \in H^2(\Omega)$ be a non-negative function such that $\nabla f(x) \cdot n(x) = 0$, where $n(x)$ is the outer normal to Ω at the point*

$x \in \partial\Omega$. Then for any $\varepsilon > 0$

$$-\int_{\Omega\cap\{x|f(x)\geqslant\varepsilon\}} \log\left(\frac{f(x)}{\varepsilon}\right)\Delta f(x)\mathrm{d}x \geqslant C_{\mathrm{LSI}}\int_{\Omega\cap\{x|f(x)\geqslant\varepsilon\}} h\left(f(x)|\overline{f_\varepsilon}\right)\mathrm{d}x, \tag{2.20}$$

where $\overline{f_\varepsilon}$ was defined in (2.17) and C_{LSI} is the log-Sobolev constant of the domain Ω.

Proof. We start by noticing that

$$\log\left(\frac{f(x)}{\varepsilon}\right)\chi_{\{z|f(z)\geqslant\varepsilon\}}(x) = \max\left(\log\left(\frac{f(x)}{\varepsilon}\right), 0\right).$$

Our next steps will be to assume that there exists $\eta > 0$ for which $f(x) \geqslant \eta$ in Ω, to prove the result in that case and to conclude from it the more general one. When f has this lower bound we find that

$$\left|\log\left(\frac{f(x)}{\varepsilon}\right)\right| \leqslant \left|\log\left(\frac{\eta}{\varepsilon}\right)\right| + \frac{f(x)}{\eta} \in L^2(\Omega),$$

and $\log\left(\frac{f(x)}{\varepsilon}\right)$ has a weak derivative[10] which satisfies

$$\left|\nabla\left(\log\left(\frac{f(x)}{\varepsilon}\right)\right)\right| = \frac{|\nabla f(x)|}{f(x)} \leqslant \frac{|\nabla f(x)|}{\eta} \in L^2(\Omega).$$

Thus $\log\left(\frac{f(x)}{\varepsilon}\right) \in H^1(\Omega)$ and we have that

$$\begin{aligned}-\int_{\Omega\cap\{x|f(x)\geqslant\varepsilon\}} \log\left(\frac{f(x)}{\varepsilon}\right)\Delta f(x)\mathrm{d}x &= \int_{\Omega}\max\left(\log\left(\frac{f(x)}{\varepsilon}\right), 0\right)\\ \times\Delta f(x)\mathrm{d}x &= -\int_{\{x|f(x)>\varepsilon\}}\nabla\log\left(\frac{f(x)}{\varepsilon}\right)\\ \times\nabla f(x)\mathrm{d}x &= \int_{\Omega\cap\{x|f(x)>\varepsilon\}}\frac{|\nabla f(x)|^2}{f(x)}\mathrm{d}x\end{aligned}$$

(see [LL01] for instance). Denoting by $f_\varepsilon(x) = \max(f(x), \varepsilon)$ we find (again, as in [LL01]) that since $f \in H^1(\Omega)$, so is f_ε and

$$\nabla f_\varepsilon(x) = \begin{cases}\nabla f(x) & f(x) > \varepsilon\\ 0 & f(x) \leqslant \varepsilon\end{cases}.$$

As such, the log-Sobolev inequality (2.13) and the above imply that

$$\begin{aligned}-\int_{\Omega\cap\{x|f(x)\geqslant\varepsilon\}} \log\left(\frac{f(x)}{\varepsilon}\right)\Delta f(x)\mathrm{d}x &= \int_{\Omega}\frac{|\nabla f_\varepsilon(x)|^2}{f_\varepsilon(x)}\mathrm{d}x\\ &\geqslant C_{\mathrm{LSI}}\int_{\Omega} h\left(f_\varepsilon(x)|\overline{f_\varepsilon}\right)\mathrm{d}x \geqslant C_{\mathrm{LSI}}\\ &\times\int_{\Omega\cap\{x|f(x)\geqslant\varepsilon\}} h\left(f_\varepsilon(x)|\overline{f_\varepsilon}\right)\\ &= C_{\mathrm{LSI}}\int_{\Omega\cap\{x|f(x)\geqslant\varepsilon\}} h\left(f(x)|\overline{f_\varepsilon}\right),\end{aligned}$$

[10] This is immediate from the fact that $\log(x)$ is C^∞ on $[\mu, \infty)$ and has bounded derivatives on this interval. See, for instance, [LL01],

which is the desired result.

We now turn our attention to the case where f is only non-negative on Ω.

For any $n \in \mathbb{N}$ we define

$$f_n(x) = f(x) + \frac{1}{n},$$

and notice that

$$-\int_{\Omega\cap\{x|f_n(x)\geqslant\varepsilon\}} \log\left(\frac{f_n(x)}{\varepsilon}\right)\Delta f_n(x)\mathrm{d}x = -\int_{\Omega\cap\{x|f_n(x)\geqslant\varepsilon\}} \log\left(\frac{f_n(x)}{\varepsilon}\right)\Delta f(x)\mathrm{d}x.$$

Since

$$\left|\log\left(\frac{f_n(x)}{\varepsilon}\right)\chi_{\{z|f_n(z)\geqslant\varepsilon\}}(x)\Delta f(x)\right| \leqslant \frac{|f_n(x)|}{\varepsilon}|\Delta f(x)| \leqslant \frac{|f(x)|+1}{\varepsilon}|\Delta f(x)| \in L^1(\Omega)$$

we conclude from the dominated convergence theory that[11]

$$\begin{aligned}\lim_{n\to\infty}&\left(-\int_{\Omega\cap\{x|f_n(x)\geqslant\varepsilon\}} \log\left(\frac{f_n(x)}{\varepsilon}\right)\Delta f_n(x)\mathrm{d}x\right)\\ &= \lim_{n\to\infty}\left(-\int_{\Omega\cap\{x|f_n(x)\geqslant\varepsilon\}} \log\left(\frac{f_n(x)}{\varepsilon}\right)\Delta f(x)\mathrm{d}x\right)\\ &= -\int_{\Omega\cap\{x|f(x)\geqslant\varepsilon\}} \log\left(\frac{f(x)}{\varepsilon}\right)\Delta f(x)\mathrm{d}x.\end{aligned} \tag{2.21}$$

On the other hand, since $h(x|y)$ is a non-negative function and

$$h\left(f_n(x)|\overline{(f_n)_\varepsilon}\right)\chi_{\{z|f_n(z)\geqslant\varepsilon\}}(x) \underset{n\to\infty}{\longrightarrow} h\left(f(x)|\overline{f_\varepsilon}\right)\chi_{\{z|f(z)\geqslant\varepsilon\}}(x)$$

pointwise[12], we can use Fatou's lemma to conclude that

$$\begin{aligned}C_{\mathrm{LSI}}\int_{\Omega\cap\{x|f(x)\geqslant\varepsilon\}} h\left(f(x)|\overline{f_\varepsilon}\right)\mathrm{d}x &\leqslant \liminf_{n\to\infty} C_{\mathrm{LSI}}\int_{\Omega\cap\{x|f_n(x)\geqslant\varepsilon\}} h\left(f_n(x)|\overline{(f_n)_\varepsilon}\right)\mathrm{d}x\\ &\leqslant \liminf_{n\to\infty}\left(-\int_{\Omega\cap\{x|f_n(x)\geqslant\varepsilon\}} \log\left(\frac{f_n(x)}{\varepsilon}\right)\Delta f_n(x)\mathrm{d}x\right)\\ &= -\int_{\Omega\cap\{x|f(x)\geqslant\varepsilon\}} \log\left(\frac{f(x)}{\varepsilon}\right)\Delta f(x)\mathrm{d}x\end{aligned}$$

where we have used (2.20) for $\{f_n\}_{n\in\mathbb{N}}$ and (2.21). The proof is thus complete. □

[11] Here we have used the fact that $f_n(x) \geqslant f(x)$ by definition. Thus, if $f(x) \geqslant \varepsilon$ then so are $f_n(x)$ for all n, while if $f(x) < \varepsilon$ then we know that for n large enough $f_n(x)$ satisfies the same. This shows that

$$\chi_{\{z|f_n(z)\geqslant\varepsilon\}}(x) \underset{n\to\infty}{\longrightarrow} \chi_{\{z|f(z)\geqslant\varepsilon\}}(x)$$

pointwise.

[12] Here we have also used the fact that $\overline{(f_n)_\varepsilon} \underset{n\to\infty}{\longrightarrow} \overline{f_\varepsilon}$ according to the dominated convergence theorem.

Proof of theorem 2.8. We shall use the abusive notation $\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(t)$ for $\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e(t), c(t), s(t))$ in this proof, as well as drop the x variable from $e_\infty(x)$ and $\varepsilon_c(x)$ for most of our estimations besides those where differences between the full diffusive and partial diffusive cases arise.

From the definition of $\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}$, lemma 2.5, and the fact that

$$\frac{\mathrm{d}}{\mathrm{d}x}h_\varepsilon(x|\varepsilon) = \begin{cases} \log\left(\dfrac{x}{\varepsilon}\right) & x \geqslant \varepsilon \\ 0 & x < \varepsilon. \end{cases}$$

we find that

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(t) &= \int_\Omega \log\left(\frac{e(x,t)}{e_\infty}\right)\partial_t e(x,t)\mathrm{d}x + \int_{\Omega\cap\{x|c(x,t)\geqslant\varepsilon_c\}} \log\left(\frac{c(x,t)}{\varepsilon_c}\right)\partial_t c(x,t)\mathrm{d}x \\
&\quad + \int_{\Omega\cap\{x|s(x,t)\geqslant\varepsilon_s\}} \log\left(\frac{s(x,t)}{\varepsilon_s}\right)\partial_t s(x,t)\mathrm{d}x + k\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{M}(c(t),s(t)) \\
&= \int_\Omega \left(d_e\Delta e(x,t) - k_f e(x,t)s(x,t) + (k_r+k_c)\,c(x,t)\right)\log\left(\frac{e(x,t)}{e_\infty}\right)\mathrm{d}x \\
&\quad + \int_{\Omega\cap\{x|c(x,t)\geqslant\varepsilon_c\}} \left(d_c\Delta c(x,t) + k_f e(x,t)s(x,t)\right. \\
&\quad \left. - (k_r+k_c)\,c(x,t)\right)\log\left(\frac{c(x,t)}{\varepsilon_c}\right)\mathrm{d}x \\
&\quad + \int_{\Omega\cap\{x|s(x,t)\geqslant\varepsilon_s\}} \left(d_s\Delta s(x,t) - k_f e(x,t)s(x,t) + k_r c(x,t)\right)\log\left(\frac{s(x,t)}{\varepsilon_s}\right)\mathrm{d}x \\
&\quad - \frac{k_f k_c k}{2k_r}\int_\Omega e(x,t)s(x,t)\mathrm{d}x - \frac{k_c k}{2}\int_\Omega c(x,t)\mathrm{d}x = \mathbf{I} + \mathbf{II} + \mathbf{III}
\end{aligned}$$

where

$$\begin{aligned}
\mathbf{I} &= \int_\Omega d_e\Delta e(x,t)\log\left(\frac{e(x,t)}{e_\infty}\right)\mathrm{d}x + \int_{\Omega\cap\{x|c(x,t)\geqslant\varepsilon_c\}} d_c\Delta c(x,t)\log\left(\frac{c(x,t)}{\varepsilon_c}\right)\mathrm{d}x \\
&\quad + \int_{\Omega\cap\{x|s(x,t)\geqslant\varepsilon_s\}} d_s\Delta s(x,t)\log\left(\frac{s(x,t)}{\varepsilon_s}\right)\mathrm{d}x,
\end{aligned}$$

$$\begin{aligned}
\mathbf{II} &= \int_\Omega \left(-k_f e(x,t)s(x,t) + (k_r+k_c)\,c(x,t)\right)\log\left(\frac{e(x,t)}{e_\infty}\right)\mathrm{d}x \\
&\quad + \int_{\Omega\cap\{x|c(x,t)\geqslant\varepsilon_c\}} \left(k_f e(x,t)s(x,t) - (k_r+k_c)\,c(x,t)\right)\log\left(\frac{c(x,t)}{\varepsilon_c}\right)\mathrm{d}x \\
&\quad + \int_{\Omega\cap\{x|s(x,t)\geqslant\varepsilon_s\}} \left(-k_f e(x,t)s(x,t) + k_r c(x,t)\right)\log\left(\frac{s(x,t)}{\varepsilon_s}\right)\mathrm{d}x
\end{aligned} \tag{2.22}$$

and

$$\mathbf{III} = -\frac{k_f k_c k}{2k_r}\int_\Omega e(x,t)s(x,t)\mathrm{d}x - \frac{k_c k}{2}\int_\Omega c(x,t)\mathrm{d}x = -\frac{kk_c}{2}\int_\Omega \mathscr{I}_{\mathcal{M}}(x)\mathrm{d}x. \tag{2.23}$$

As **III** is already a multiple of the integration of $\mathscr{d}_{\mathscr{M}}$, we are left with estimating **I** and **II**.

To simplify the coming integrals we will drop the t variable (even though the division to domains we will use in the estimation of **II** will depend on it via $c(x,t)$, $s(x,t)$ and $e(x,t)$). Using lemma 2.10 (whose conditions are satisfied according to the assumptions) when all diffusion constants are strictly positive (and thus e_∞ and ε_c are constants) we find that

$$\mathbf{I} \leqslant -d_e \int_\Omega \frac{|\nabla e(x)|^2}{e(x)}\,\mathrm{d}x - C_{\mathrm{LSI}} d_c \int_{\Omega\cap\{x|c(x)\geqslant\varepsilon_c\}} h\left(c(x)|\overline{c_{\varepsilon_c}}\right)\mathrm{d}x$$

$$-C_{\mathrm{LSI}} d_s \int_{\Omega\cap\{x|s(x)\geqslant\varepsilon_s\}} h\left(s(x)|\overline{s_{\varepsilon_s}}\right)\mathrm{d}x$$

from which we attain, using the log-Sobolev inequality on Ω (2.13)

$$\mathbf{I} \leqslant -C_{\mathrm{LSI}}\left(d_e\int_\Omega h(e(x)|\overline{e})\mathrm{d}x + d_c\int_{\Omega\cap\{x|c(x)\geqslant\varepsilon_c\}} h\left(c(x)|\overline{c_{\varepsilon_c}}\right)\mathrm{d}x\right.$$
$$\left. + d_s\int_{\Omega\cap\{x|s(x)\geqslant\varepsilon_s\}} h\left(s(x)|\overline{s_{\varepsilon_s}}\right)\mathrm{d}x\right), \tag{2.24}$$

where $\overline{e} = \int_\Omega e(x)\mathrm{d}x$. In the case $d_e = d_c = 0$ the above remains true as in this case

$$\mathbf{I} = \int_{\Omega\cap\{x|s(x,t)\geqslant\varepsilon_s\}} d_s \Delta s(x,t)\log\left(\frac{s(x,t)}{\varepsilon_s}\right)\mathrm{d}x,$$

and applying lemma 2.10 yields the desired result. It is important to note that we are allowed to use this lemma since ε_s is *a constant* (as was briefly discussed in remark 2.4).

The estimation of **II** is slightly more complicated and will require us to both divide the domain Ω into the subdomains $\Omega_1, \Omega_2, \Omega_3$ and Ω_4, defined in (2.16), and consider the two difference cases for ε_c and e_∞

$$\begin{array}{rll} e_\infty = M_0 & \varepsilon_c \text{ is a constant that satisfies (2.4)} & d_e, d_c, d_s > 0 \\ e_\infty(x) = e_0(x) + c_0(x) & \varepsilon_c \text{ is a function that satisfies (2.9)} & d_e = d_c = 0 \end{array}.$$

Writing $\mathbf{II} = \int_\Omega \mathfrak{r}(x)\mathrm{d}x$ with

$$\mathfrak{r}(x) = \left(-k_f e(x)s(x) + (k_r + k_c)\,c(x)\right)\log\left(\frac{e(x)}{e_\infty}\right)$$
$$+ \left(k_f e(x)s(x) - (k_r+k_c)\,c(x)\right)\chi_{\{z|c(z)\geqslant\varepsilon_c\}}(x)\log\left(\frac{c(x)}{\varepsilon_c}\right)$$
$$+ \left(-k_f e(x)s(x) + k_r c(x)\right)\chi_{\{z|s(z)\geqslant\varepsilon_s\}}(x)\log\left(\frac{s(x)}{\varepsilon_s}\right)$$

we see that:

For $x \in \Omega_1 = \{x | c(x) \geqslant \varepsilon_c,\ s(x) \geqslant \varepsilon_s\}$:

$$\imath(x) = -\left(k_f e(x)s(x) - k_r c(x)\right)\log\left(\frac{e(x)s(x)\varepsilon_c}{e_\infty \varepsilon_s c(x)}\right) + k_c c(x)\log\left(\frac{e(x)\varepsilon_c}{e_\infty c(x)}\right)$$

$$= -k_f c(x)\left(\frac{e(x)s(x)}{c(x)} - \frac{e_\infty \varepsilon_s}{\varepsilon_c}\right)\log\left(\frac{\frac{e(x)s(x)}{c(x)}}{\frac{e_\infty\varepsilon_s}{\varepsilon_c}}\right) - k_c c(x)\log\left(\frac{\frac{c(x)}{e(x)}}{\frac{\varepsilon_c}{e_\infty}}\right)$$

$$= -k_f c(x)\mathbf{h}\left(\frac{e(x)s(x)}{c(x)}\middle|\frac{e_\infty\varepsilon_s}{\varepsilon_c}\right) - k_c e(x) h\left(\frac{c(x)}{e(x)}\middle|\frac{\varepsilon_c}{e_\infty}\right) - k_c c(x) + k_c\varepsilon_c\frac{e(x)}{e_\infty}$$

$$= -\mathcal{d}_{\varepsilon_c,\varepsilon_s}(x) + C_{\mathrm{LSI}} d_s h\left(s(x)|\overline{s_{\varepsilon_s}}\right) + C_{\mathrm{LSI}} d_c h\left(c(x)|\overline{c_{\varepsilon_c}}\right) - k_c c(x) + k_c\varepsilon_c\frac{e(x)}{e_\infty}$$

where we have used condition (2.4) when all the diffusion coefficients are strictly positive and condition (2.9) when $d_e = d_c = 0$ together with the definition of $\mathcal{d}_{\varepsilon_c,\varepsilon_s}$, (2.15). The last term will be estimated for our two distinct cases.

- *All diffusion coefficients are strictly positive*. In this case we see that by using the inequality

$$x - 1 \leqslant 6\left(\sqrt{x} - 1\right)^2, \quad \forall\, x \geqslant 2, \tag{2.25}$$

and the fact that $c(x) \geqslant \varepsilon_c$ on Ω_1,

$$-k_c c(x) + k_c\varepsilon_c\frac{e(x)}{e_\infty} \leqslant \begin{cases} k_c\left(2\varepsilon_c - c(x)\right) & e(x) \leqslant 2e_\infty \\ k_c\varepsilon_c\left(\dfrac{e(x)}{e_\infty} - 1\right) & e(x) \geqslant 2e_\infty \end{cases}$$

$$\leqslant \begin{cases} k_c c(x) & e(x) \leqslant 2e_\infty \\ \dfrac{6k_c\varepsilon_c}{e_\infty}\left(\sqrt{e} - \sqrt{e_\infty}\right)^2 & e(x) \geqslant 2e_\infty \end{cases}.$$

Since

$$\overline{e} = \int_\Omega e(x)\mathrm{d}x \leqslant \int_\Omega \left(e(x) + c(x)\right)\mathrm{d}x = M_0 = e_\infty \tag{2.26}$$

we have that for $e(x) \geqslant e_\infty$

$$\left(\sqrt{e(x)} - \sqrt{e_\infty}\right)^2 \leqslant \left(\sqrt{e(x)} - \sqrt{\overline{e}}\right)^2.$$

Combining the above we see that

$$\begin{aligned} \imath(x) \leqslant{}& -\mathcal{d}_{\varepsilon_c,\varepsilon_s}(x) + C_{\mathrm{LSI}} d_s h\left(s(x)|\overline{s_{\varepsilon_s}}\right) + C_{\mathrm{LSI}} d_c h\left(c(x)|\overline{c_{\varepsilon_c}}\right) \\ &+ k_c c(x) + \frac{6k_c\varepsilon_c}{e_\infty}\left(\sqrt{e(x)} - \sqrt{\overline{e}}\right)^2, \quad \forall\, x \in \Omega_1 \end{aligned} \tag{2.27}$$

and as such

$$\int_{\Omega_1} \imath(x)\mathrm{d}x \leqslant \int_{\Omega_1} \left(-\mathscr{d}_{\varepsilon_c,\varepsilon_s}(x) + C_{\mathrm{LSI}} d_s h\left(s(x)|\overline{s_{\varepsilon_s}}\right) + C_{\mathrm{LSI}} d_c h\left(c(x)|\overline{c_{\varepsilon_c}}\right)\right)\mathrm{d}x$$
$$+ k_c \int_{\Omega_1} c(x)\mathrm{d}x + \frac{6k_c\varepsilon_c}{e_\infty}\int_{\Omega_1}\left(\sqrt{e(x)} - \sqrt{\overline{e}}\right)^2 \mathrm{d}x. \tag{2.28}$$

- $d_e = d_c = 0$. In this case we see that as

$$e(x) \leqslant e(x) + c(x) = e_0(x) + c_0(x) = e_\infty(x), \tag{2.29}$$

(the conservation law (1.5) holds for strong solutions) the fact that $c(x) \geqslant \varepsilon_c(x)$ on Ω_1 implies that

$$-k_c c(x) + k_c \varepsilon_c(x)\frac{e(x)}{e_\infty(x)} \leqslant 0$$

yielding the bound

$$\int_{\Omega_1} \imath(x)\mathrm{d}x \leqslant \int_{\Omega_1} \left(-\mathscr{d}_{\varepsilon_c,\varepsilon_s}(x) + C_{\mathrm{LSI}} d_s h\left(s(x)|\overline{s_{\varepsilon_s}}\right)\right)\mathrm{d}x. \tag{2.30}$$

For $x \in \Omega_2 = \{x \in \Omega | c(x) < \varepsilon_c,\ s(x) \geqslant \varepsilon_s\}$:

$$\begin{aligned}
\imath(x) &= \left(-k_f e(x)s(x) + k_r c(x)\right)\log\left(\frac{e(x)s(x)}{e_\infty\varepsilon_s}\right) + k_c c(x)\log\left(\frac{e(x)}{e_\infty}\right)\\
&= -k_f h\left(e(x)s(x)|e_\infty\varepsilon_s\right) - k_f e(x)s(x) + k_f e_\infty\varepsilon_s\\
&\quad - k_r c(x)\hbar\left(\frac{e(x)s(x)}{e_\infty\varepsilon_s}\right) + k_r c(x)\left(\frac{e(x)s(x)}{e_\infty\varepsilon_s} - 1\right)\\
&\quad - k_c c(x)\hbar\left(\frac{e(x)}{e_\infty}\right) + k_c c(x)\left(\frac{e(x)}{e_\infty} - 1\right).
\end{aligned} \tag{2.31}$$

Thus

$$\begin{aligned}
\imath(x) = -\mathscr{d}_{\varepsilon_c,\varepsilon_s}(x) + C_{\mathrm{LSI}} d_s h\left(s(x)|\overline{s_{\varepsilon_s}}\right) + \underbrace{(k_c + k_r)\, c(x)\left(\frac{e(x)}{e_\infty} - 1\right)}_{\mathbf{A}}\\
\underbrace{+k_r\frac{c(x)e(x)}{e_\infty}\left(\frac{s(x)}{\varepsilon_s} - 1\right) + k_f\varepsilon_s\left(e_\infty - \frac{e(x)s(x)}{\varepsilon_s}\right)}_{\mathbf{B}}.
\end{aligned} \tag{2.32}$$

Again, to estimate **A** and **B** we will consider our two cases.

- *All diffusion coefficients are strictly positive*. In this case we see that, much like the estimation on Ω_1

$$\mathbf{A} = (k_c + k_r)\, c(x) \left(\frac{e(x)}{e_\infty} - 1\right) \leqslant \begin{cases} (k_c + k_r)\, c(x) & e(x) \leqslant 2e_\infty \\ \dfrac{6\,(k_c + k_r)\, c(x)}{e_\infty}\left(\sqrt{e(x)} - \sqrt{e_\infty}\right)^2 & e(x) \geqslant 2e_\infty \end{cases}$$

$$\leqslant (k_c + k_r)\, c(x) + \frac{6\,(k_c + k_r)\,\varepsilon_c}{e_\infty}\left(\sqrt{e(x)} - \sqrt{\overline{e}}\right)^2,$$

where we have used the fact that $c(x) \leqslant \varepsilon_c$ on Ω_2. Using this fact again, together with the fact that $s(x) \geqslant \varepsilon_s$ on Ω_2 and condition (2.4), we find that

$$\mathbf{B} \leqslant k_r \varepsilon_c \frac{e(x)}{e_\infty}\left(\frac{s(x)}{\varepsilon_s} - 1\right) + k_f \varepsilon_s \left(e_\infty - \frac{e(x)s(x)}{\varepsilon_s}\right)$$

$$= k_f \varepsilon_s e(x)\left(\frac{s(x)}{\varepsilon_s} - 1\right) + k_f \varepsilon_s \left(e_\infty - \frac{e(x)s(x)}{\varepsilon_s}\right) = k_f \varepsilon_s\,(e_\infty - e(x))\,.$$

Thus

$$\int_{\Omega_2} \mathbf{B}\,\mathrm{d}x \leqslant k_f \varepsilon_s \int_{\Omega_2} ((e_\infty - \overline{e}) + (\overline{e} - e(x)))\,\mathrm{d}x$$

$$= \underbrace{k_f \varepsilon_s\,|\Omega_2| \int_\Omega c(x)\mathrm{d}x}_{\text{from (2.26)}} + k_f \int_{\Omega_2} \varepsilon_s\,(\overline{e} - e(x))\,\mathrm{d}x$$

$$\leqslant k_f \varepsilon_s \int_\Omega c(x)\mathrm{d}x + k_f \int_{\Omega_2 \cap \{x | e(x) \leqslant \overline{e} \leqslant 2e(x)\}} \varepsilon_s\,(\overline{e} - e(x))\,\mathrm{d}x + k_f \times \int_{\Omega_2 \cap \{x | \overline{e} \geqslant 2e(x)\}} \varepsilon_s\,(\overline{e} - e(x))\,\mathrm{d}x$$

$$\leqslant k_f \varepsilon_s \int_\Omega c(x)\mathrm{d}x + k_f \int_{\Omega_2 \cap \{x | e(x) \leqslant \overline{e} \leqslant 2e(x)\}} \varepsilon_s e(x)\mathrm{d}x + k_f \varepsilon_s \times \int_{\Omega_2 \cap \left\{x | \frac{\overline{e}}{e(x)} \geqslant 2\right\}} e(x)\left(\frac{\overline{e}}{e(x)} - 1\right)\mathrm{d}x$$

$$\leqslant k_f \varepsilon_s \int_\Omega c(x)\mathrm{d}x + k_f \int_{\Omega_2} e(x)s(x)\mathrm{d}x + 6k_f \varepsilon_s \int_{\Omega_2}\left(\sqrt{e(x)} - \sqrt{\overline{e}}\right)^2\mathrm{d}x,$$

where we have used the fact that $s(x) \geqslant \varepsilon_s$ again, as well as inequality (2.25).

Combining the estimations on **A** and **B** with (2.32) yields

$$\int_{\Omega_2} \mathfrak{r}(x)\mathrm{d}x \leqslant \int_{\Omega_2} \left(-\mathscr{d}_{\varepsilon_c,\varepsilon_s}(x) + C_{\mathrm{LSI}} d_s h\left(s(x)|\overline{s_{\varepsilon_s}}\right)\right) \mathrm{d}x$$
$$+ (k_c + k_r) \int_{\Omega_2} c(x)\mathrm{d}x + k_f \varepsilon_s \int_{\Omega} c(x)\mathrm{d}x + k_f \int_{\Omega_2} e(x)s(x)\mathrm{d}x$$
$$+ 6\left(k_f\varepsilon_s + \frac{(k_r + k_c)\,\varepsilon_c}{e_\infty}\right) \int_{\Omega_2} \left(\sqrt{e(x)} - \sqrt{\overline{e}}\right)^2 \mathrm{d}x. \qquad (2.33)$$

- $d_e = d_c = 0$. In this case we have that as $e(x) \leqslant e_\infty(x)$

$$\mathbf{A} = (k_c + k_r)\, c(x) \left(\frac{e(x)}{e_\infty(x)} - 1\right) \leqslant 0,$$

and using condition (2.9) together with the facts that $c(x) < \varepsilon_c(x)$ and $s(x) \geqslant \varepsilon_s$ we have that exactly like in the previous case

$$\mathbf{B} \leqslant k_f\varepsilon_s\,(e_\infty(x) - e(x)) = k_f\varepsilon_s c(x),$$

where we have used (2.29) in the last step. We conclude that in this case

$$\int_{\Omega_2} \mathfrak{r}(x)\mathrm{d}x \leqslant \int_{\Omega_2} \left(-\mathscr{d}_{\varepsilon_c,\varepsilon_s}(x) + C_{\mathrm{LSI}} d_s h\left(s(x)|\overline{s_{\varepsilon_s}}\right)\right) \mathrm{d}x + k_f\varepsilon_s \int_{\Omega_2} c(x)\mathrm{d}x. \qquad (2.34)$$

For $x \in \Omega_3 = \{x \in \Omega | c(x) \geqslant \varepsilon_c,\ s(x) < \varepsilon_s\}$:

$$\mathfrak{r}(x) = -(k_r + k_c)\, c(x) \log\left(\frac{\frac{c(x)}{e(x)}}{\frac{\varepsilon_c}{e_\infty}}\right) - k_f e(x)s(x) \log\left(\frac{\frac{e(x)}{c(x)}}{\frac{e_\infty}{\varepsilon_c}}\right)$$
$$= -(k_r + k_c)\, e(x) h\left(\frac{c(x)}{e(x)}\middle|\frac{\varepsilon_c}{e_\infty}\right) + \frac{k_r + k_c}{e_\infty}\left(\varepsilon_c e(x) - e_\infty c(x)\right) \qquad (2.35)$$
$$- k_f s(x)c(x) h\left(\frac{e(x)}{c(x)}\middle|\frac{e_\infty}{\varepsilon_c}\right) - \frac{k_f s(x)}{\varepsilon_c}\left(\varepsilon_c e(x) - e_\infty c(x)\right).$$

Thus

$$\mathfrak{r}(x) = -\mathscr{d}_{\varepsilon_c,\varepsilon_s}(x) + C_{\mathrm{LSI}} d_c h\left(c(x)|\overline{c_{\varepsilon_c}}\right) + \underbrace{\left(\frac{k_r + k_c}{e_\infty} - \frac{k_f s(x)}{\varepsilon_c}\right)\left(\varepsilon_c e(x) - e_\infty c(x)\right)}_{\mathbf{D}}. \qquad (2.36)$$

We will estimate **D** in our two distinct cases.

- *All diffusion coefficients are strictly positive*. In this case we see that if $\varepsilon_c e(x) - e_\infty c(x) \leqslant 0$ then since $s(x) \leqslant \varepsilon_s$ on Ω_3

$$-\frac{k_f s(x)}{\varepsilon_c}\left(\varepsilon_c e(x) - e_\infty c(x)\right) \leqslant -\frac{k_f\varepsilon_s}{\varepsilon_c}\left(\varepsilon_c e(x) - e_\infty c(x)\right)$$
$$= -\frac{k_r}{e_\infty}\left(\varepsilon_c e(x) - e_\infty c(x)\right),$$

where we have used (2.4). As such

$$\mathbf{D} \leqslant \frac{k_c}{e_\infty}\left(\varepsilon_c e(x) - e_\infty c(x)\right) \leqslant 0.$$

If, on the other hand, $\varepsilon_c e(x) - e_\infty c(x) \geqslant 0$ then

$$\mathbf{D} \leqslant \frac{k_r + k_c}{e_\infty}\left(\varepsilon_c e(x) - e_\infty c(x)\right)$$

i.e. for all $x \in \Omega_3$

$$\mathbf{D} \leqslant \max\left(\frac{k_r + k_c}{e_\infty}\left(\varepsilon_c e(x) - e_\infty c(x)\right), 0\right). \tag{2.37}$$

Using the fact that $c(x) \geqslant \varepsilon_c$ on Ω_3 we conclude that

$$\frac{k_r + k_c}{e_\infty}\left(\varepsilon_c e(x) - e_\infty c(x)\right) \leqslant (k_r + k_c)\,\varepsilon_c\left(\frac{e(x)}{e_\infty} - 1\right)$$

$$\leqslant \begin{cases} (k_r + k_c)\,\varepsilon_c & e(x) \leqslant 2e_\infty \\ \dfrac{6\,(k_r + k_c)\,\varepsilon_c}{e_\infty}\left(\sqrt{e(x)} - \sqrt{e_\infty}\right)^2 & e(x) \geqslant 2e_\infty \end{cases}$$

$$\leqslant (k_r + k_c)\,c(x) + \frac{6\,(k_r + k_c)\,\varepsilon_c}{e_\infty}\left(\sqrt{e(x)} - \sqrt{\overline{e}}\right)^2$$

where we once again used inequality (2.25) and a similar calculation to that we have performed when investigating Ω_1.

From the above, (2.36) and (2.37) we conclude that

$$\begin{aligned} \mathfrak{r}(x) \leqslant{}& -\mathfrak{d}_{\varepsilon_c,\varepsilon_s}(x) + C_{\mathrm{LSI}} d_c h\left(c(x)|\overline{c_{\varepsilon_c}}\right) \\ &+ (k_c + k_r)\,c(x) + \frac{6\,(k_c + k_r)\,\varepsilon_c}{e_\infty}\left(\sqrt{e(x)} - \sqrt{\overline{e}}\right)^2 \end{aligned} \tag{2.38}$$

and as such

$$\begin{aligned} \int_{\Omega_3} \mathfrak{r}(x)\mathrm{d}x \leqslant{}& \int_{\Omega_3}\left(-\mathfrak{d}_{\varepsilon_c,\varepsilon_s}(x) + C_{\mathrm{LSI}} d_c h\left(c(x)|\overline{c_{\varepsilon_c}}\right)\right)\mathrm{d}x \\ &+ (k_c + k_r)\int_{\Omega_3} c(x)\mathrm{d}x + \frac{6\,(k_r + k_c)\,\varepsilon_c}{e_\infty}\int_{\Omega_3}\left(\sqrt{e(x)} - \sqrt{\overline{e}}\right)^2\mathrm{d}x. \end{aligned} \tag{2.39}$$

- $d_e = d_c = 0$. In this case we see that since $\varepsilon_c(x) \leqslant c(x)$ and $e(x) \leqslant e_\infty(x)$

$$\varepsilon_c(x)e(x) - e_\infty(x)c(x) \leqslant 0.$$

Using condition (2.9) instead of (2.4) and following the same estimation that was shown in the previous case we find that

$$\mathbf{D} \leqslant \frac{k_c}{e_\infty(x)}\left(\varepsilon_c(x)e(x) - e_\infty c(x)\right) \leqslant 0.$$

We conclude that in this case

$$\int_{\Omega_3} \mathfrak{r}(x)\mathrm{d}x \leqslant -\int_{\Omega_3} \mathscr{d}_{\varepsilon_c,\varepsilon_s}(x)\mathrm{d}x. \tag{2.40}$$

For $x \in \Omega_4 = \{x \in \Omega | c(x) < \varepsilon_c,\ s(x) < \varepsilon_s\}$:

$$\begin{aligned} \mathfrak{r}(x) &= \left(-k_f e(x)s(x) + (k_r + k_c)\, c(x)\right) \log\left(\frac{e(x)}{e_\infty}\right) \\ &= -k_f s(x) h\left(e(x)|e_\infty\right) - k_f s(x)e(x) + k_f e_\infty s(x) \\ &\quad - (k_r + k_c)\, c(x) \hbar \left(\frac{e(x)}{e_\infty}\right) + \frac{(k_r + k_c)}{e_\infty} c(x)e(x) - (k_r + k_c)\, c(x). \end{aligned} \tag{2.41}$$

Thus

$$\mathfrak{r}(x) = -\mathscr{d}_{\varepsilon_c,\varepsilon_s}(x) + k_f s(x)\,(e_\infty - e(x)) + \frac{(k_r + k_c)\, c(x)}{e_\infty}\,(e(x) - e_\infty)\,. \tag{2.42}$$

Unsurprisingly, the last term will be estimated for our two distinct cases.

- *All diffusion coefficients are strictly positive*. In this case we notice that following similar ideas to those presented in the investigation of Ω_2 and the fact that $s(x) \leqslant \varepsilon_s$ on Ω_4 we find that

$$\int_{\Omega_4} k_f s(x)\,(e_\infty - e(x))\,\mathrm{d}x = k_f \underbrace{(e_\infty - \overline{e})}_{\geqslant 0} \int_{\Omega_4} s(x)\mathrm{d}x + k_f \int_{\Omega_4} s(x)\,(\overline{e} - e(x))\,\mathrm{d}x$$

$$\leqslant k_f \varepsilon_s\, |\Omega_4| \underbrace{\int_\Omega c(x)\mathrm{d}x}_{\text{from (2.26)}} + k_f \int_{\Omega_4 \cap \{x | e(x) \leqslant \overline{e} \leqslant 2e(x)\}} s(x)\,(\overline{e} - e(x))\,\mathrm{d}x$$

$$+ k_f \int_{\Omega_4 \cap \{x | \overline{e} \geqslant 2e(x)\}} s(x)\,(\overline{e} - e(x))\,\mathrm{d}x$$

$$\leqslant k_f \varepsilon_s \int_\Omega c(x)\mathrm{d}x + k_f \int_{\Omega_4} e(x)s(x)\mathrm{d}x + 6k_f \varepsilon_s \int_{\Omega_4} \left(\sqrt{e(x)} - \sqrt{\overline{e}}\right)^2 \mathrm{d}x.$$

  Moreover, much like previous estimations (for instance on Ω_3) we find that as $c(x) \leqslant \varepsilon_c$ on Ω_4

$$\frac{(k_r + k_c)\, c(x)}{e_\infty}\,(e(x) - e_\infty) \leqslant \begin{cases} (k_r + k_c)\, c(x) & e(x) \leqslant 2e_\infty \\ \dfrac{6\,(k_r + k_c)\,\varepsilon_c}{e_\infty}\left(\sqrt{e(x)} - \sqrt{e_\infty}\right)^2 & e(x) \geqslant 2e_\infty \end{cases}$$

$$\leqslant (k_r + k_c)\, c(x) + \frac{6\,(k_r + k_c)\,\varepsilon_c}{e_\infty}\left(\sqrt{e(x)} - \sqrt{\overline{e}}\right)^2.$$

These inequalities together with (2.42) yield

$$\int_{\Omega_4} \imath(x)\mathrm{d}x \leqslant -\int_{\Omega_4} \jmath_{\varepsilon_c,\varepsilon_s}(x)\mathrm{d}x + k_f\varepsilon_s \int_{\Omega} c(x)\mathrm{d}x + k_f \int_{\Omega_4} e(x)s(x)\mathrm{d}x + (k_c+k_r)\int_{\Omega_4} c(x)\mathrm{d}x + 6\left(\frac{(k_r+k_c)\,\varepsilon_c}{e_\infty} + k_f\varepsilon_s\right)\int_{\Omega_4}\left(\sqrt{e(x)}-\sqrt{\overline{e}}\right)^2\mathrm{d}x. \tag{2.43}$$

- $d_e = d_c = 0$. In this case, since $e(x) \leqslant e_\infty(x)$ and $s(x) \leqslant \varepsilon_s$ we find that due to (2.29)

$$k_f s(x)\left(e_\infty(x) - e(x)\right) + \frac{(k_r+k_c)\,c(x)}{e_\infty(x)}\left(e(x) - e_\infty(x)\right) \leqslant k_f s(x)c(x) \leqslant k_f\varepsilon_s c(x).$$

We conclude that in this case

$$\int_{\Omega_4} \imath(x)\mathrm{d}x \leqslant -\int_{\Omega_4} \jmath_{\varepsilon_c,\varepsilon_s}(x)\mathrm{d}x + k_f\varepsilon_s\int_{\Omega_4} c(x)\mathrm{d}x. \tag{2.44}$$

Using the fact that Ω_1, Ω_2, Ω_3 and Ω_4 are mutually disjoint with

$$\bigcup_{i=1}^{4}\Omega_i = \Omega, \quad \Omega_1\cup\Omega_2 = \left\{x|s(x)\geqslant\varepsilon_s\right\}, \quad \Omega_1\cup\Omega_3 = \left\{x|c(x)\geqslant\varepsilon_c\right\},$$

and the fact that

$$\mathbf{II} = \int_{\Omega_1}\imath(x)\mathrm{d}x + \int_{\Omega_2}\imath(x)\mathrm{d}x + \int_{\Omega_3}\imath(x)\mathrm{d}x + \int_{\Omega_4}\imath(x)\mathrm{d}x$$

we see that (2.28), (2.33), (2.39) and (2.43) imply that when all diffusion constants are strictly positive

$$\begin{aligned}\mathbf{II} \leqslant &-\int_{\Omega}\jmath_{\varepsilon_c,\varepsilon_s}(x)\mathrm{d}x + C_{\mathrm{LSI}}\int_{\Omega\cap\{x|s(x)\geqslant\varepsilon_s\}} d_s h\left(s(x)|\overline{s_{\varepsilon_s}}\right)\mathrm{d}x \\ &+ C_{\mathrm{LSI}}\int_{\Omega\cap\{x|c(x)\geqslant\varepsilon_c\}} d_c h\left(c(x)|\overline{c_{\varepsilon_c}}\right)\mathrm{d}x \\ &+ \left(k_c+k_r+2k_f\varepsilon_s\right)\int_{\Omega} c(x)\mathrm{d}x + k_f\int_{\Omega} e(x)s(x)\mathrm{d}x \\ &+ 6\left(\frac{(k_c+k_r)\,\varepsilon_c}{e_\infty} + k_f\varepsilon_s\right)\int_{\Omega}\left(\sqrt{e(x)}-\sqrt{\overline{e}}\right)^2\mathrm{d}x\end{aligned} \tag{2.45}$$

and (2.30), (2.34), (2.40) and (2.44) imply that when $d_e = d_c = 0$

$$\mathbf{II} \leqslant -\int_{\Omega}\jmath_{\varepsilon_c,\varepsilon_s}(x)\mathrm{d}x + C_{\mathrm{LSI}}\int_{\Omega\cap\{x|s(x)\geqslant\varepsilon_s\}} d_s h\left(s(x)|\overline{s_{\varepsilon_s}}\right)\mathrm{d}x + k_f\varepsilon_s\int_{\Omega} c(x)\mathrm{d}x. \tag{2.46}$$

Combining (2.45) with (2.23) and (2.24) and the fact that

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(t) = \mathbf{I} + \mathbf{II} + \mathbf{III}$$

yields the estimation

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(t) \leqslant & -\int_\Omega \mathcal{I}_{\varepsilon_c,\varepsilon_s}(x,t)\mathrm{d}x - d_e C_{\mathrm{LSI}}\int_\Omega h\left(e(x,t)|\overline{e(t)}\right)\mathrm{d}x \\ & + \left(k_c + k_r + 2k_f\varepsilon_s - \frac{k_c k}{2}\right)\int_\Omega c(x,t)\mathrm{d}x + \left(k_r - \frac{k_c k}{2}\right)\frac{k_f}{k_r}\int_\Omega e(x,t)s(x,t)\mathrm{d}x \\ & + 6\left(\frac{(k_c+k_r)\,\varepsilon_c}{e_\infty} + k_f\varepsilon_s\right)\int_\Omega \left(\sqrt{e(x,t)} - \sqrt{\overline{e(t)}}\right)^2 \mathrm{d}x\end{aligned}$$

when all diffusion coefficients are strictly positive which, together with the inequality $\left(\sqrt{x} - \sqrt{y}\right)^2 \leqslant h\left(x|y\right)$ and the definition of $\mathcal{I}_{\mathcal{M}}(x)$, shows that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(t) \leqslant & -\int_\Omega \mathcal{I}_{\varepsilon_c,\varepsilon_s}(x,t)\mathrm{d}x - \left(\frac{kk_c}{2} - k_c - k_r - 2k_f\varepsilon_s\right)\int_\Omega \mathcal{I}_{\mathcal{M}}(x,t) \\ & - \left(d_e C_{\mathrm{LSI}} - 6\left(\frac{(k_c+k_r)}{e_\infty} + k_f\right)\max\left(\varepsilon_c,\varepsilon_s\right)\right)\int_\Omega h\left(e(x,t)|\overline{e(t)}\right)\mathrm{d}x,\end{aligned}$$

which is the desired inequality in this case.

Similarly (2.46) will imply that when $d_e = d_c = 0$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(t) \leqslant -\int_\Omega \mathcal{I}_{\varepsilon_c,\varepsilon_s}(x,t)\mathrm{d}x + k_f\varepsilon_s\int_\Omega c(x)\mathrm{d}x - \frac{k_c k}{2}\int_\Omega \mathcal{I}_{\mathcal{M}}(x,t)\mathrm{d}x,$$

showing the second desired inequality. The proof is thus complete. □

We now have the tools to show our main theorem for this section.

Proof of theorem 2.2. Following from theorem 2.8 we see that when all diffusion coefficients are strictly positive (2.6) will follow immediately from (2.18) if

$$\begin{aligned}\gamma\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(t) \leqslant & \int_\Omega \left(\mathcal{I}_{\varepsilon_c,\varepsilon_s}(x,t) + \left(\frac{kk_c}{2} - k_c - k_r - 2k_f\varepsilon_s\right)\mathcal{I}_{\mathcal{M}}(x,t)\right. \\ & \left. + \left(d_e C_{\mathrm{LSI}} - 6\left(\frac{(k_c+k_r)}{M_0} + k_f\right)\max\left(\varepsilon_c,\varepsilon_s\right)\right)h\left(e(x,t)|\overline{e(t)}\right)\right)\mathrm{d}x. \end{aligned} \tag{2.47}$$

and when $d_e = d_c = 0$ (2.6) will follow immediately from (2.19) if

$$\gamma\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(t) \leqslant \int_\Omega \mathcal{I}_{\varepsilon_c,\varepsilon_s}(x,t)\mathrm{d}x + \left(\frac{k_c k}{2} - k_f\varepsilon_s\right)\int_\Omega \mathcal{I}_{\mathcal{M}}(x,t)\mathrm{d}x. \tag{2.48}$$

To show (2.47) and (2.48) we will use the definition of $\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}$,

$$\begin{aligned}\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}\left(e,c,s\right) = & \int_\Omega h(e(x)|e_\infty)\mathrm{d}x + \int_\Omega h_{\varepsilon_c}(c(x)|\varepsilon_c)\mathrm{d}x + \int_\Omega h_{\varepsilon_s}(s(x)|\varepsilon_s)\mathrm{d}x \\ & + k\int_\Omega \left(c(x) + \frac{1}{2}\left(\frac{2k_r + k_c}{k_r}\right)s(x)\right)\mathrm{d}x,\end{aligned}$$

and bound each term in the above expression by terms that appear in the right-hand side of (2.47) or (2.48).

Much like in the proof of theorem 2.8 we shall drop the t variable from our estimations, showing, as was mentioned in section 1.3, that the connection between the total entropy and an appropriate production term is of functional nature.

The term $h\left(e(x)|e_\infty\right)$:

- *All diffusion coefficients are strictly positive*. In this case $e_\infty = M_0$ and using the identity

$$h(x|y) = h(x|z) + x\ \log\left(\frac{z}{y}\right) + y - z \tag{2.49}$$

we see that

$$\begin{aligned}\int_\Omega h\left(e(x)|e_\infty\right)\mathrm{d}x &= \int_\Omega\left(h\left(e(x)|\overline{e}\right) + e(x)\log\left(\frac{\overline{e}}{e_\infty}\right) + e_\infty - \overline{e}\right)\mathrm{d}x \\ &\leqslant \int_\Omega h\left(e(x)|\overline{e}\right)\mathrm{d}x + (e_\infty - \overline{e}) = \int_\Omega h\left(e(x)|\overline{e}\right)\mathrm{d}x + \int_\Omega c(x)\mathrm{d}x \\ &\leqslant \int_\Omega h\left(e(x)|\overline{e}\right)\mathrm{d}x + \int_\Omega \ell_{\mathcal{M}}(x)\mathrm{d}x,\end{aligned}$$

where we have used the fact that $\overline{e} \leqslant e_\infty = \overline{e} + \int_\Omega c(x)\mathrm{d}x$.

- $d_e = d_c = 0$. In this case since $e(x) \leqslant e(x) + c(x) = e_0(x) + c_0(x) = e_\infty(x)$ we get that

$$h\left(e(x)|e_\infty(x)\right) = e(x)\log\left(\frac{e(x)}{e_\infty(x)}\right) - e(x) + e_\infty(x) \leqslant c(x)$$

and as such

$$\int_\Omega h\left(e(x)|e_\infty(x)\right)\mathrm{d}x \leqslant \int_\Omega c(x)\mathrm{d}x \leqslant \int_\Omega \ell_{\mathcal{M}}(x)\mathrm{d}x. \tag{2.51}$$

The term $h_{\varepsilon_c}\left(c(x)|\varepsilon_c\right)$:

- *All diffusion coefficients are strictly positive*. In this case using (2.49) again we find that

$$\int_\Omega h_{\varepsilon_c}\left(c(x)|\varepsilon_c\right)\mathrm{d}x = \int_{\{x|c(x)\geqslant\varepsilon_c\}} h\left(c(x)|\varepsilon_c\right)\mathrm{d}x$$

$$= \int_{\{x|c(x)\geqslant\varepsilon_c\}}\left(h\left(c(x)|\overline{c_{\varepsilon_c}}\right) + c(x)\log\left(\frac{\overline{c_{\varepsilon_c}}}{\varepsilon_c}\right) + \varepsilon_c - \overline{c_{\varepsilon_c}}\right)\mathrm{d}x.$$

Since

$$\varepsilon_c \leqslant \underbrace{\int_\Omega \max\left(c(x),\varepsilon_c\right)\mathrm{d}x}_{\overline{c_{\varepsilon_c}}} \leqslant \int_\Omega c(x)\mathrm{d}x + \varepsilon_c \leqslant M_0 + \varepsilon_c$$

we see that

$$\int_\Omega h_{\varepsilon_c}\left(c(x)|\varepsilon_c\right)\mathrm{d}x \leqslant \int_{\{x|c(x)\geqslant\varepsilon_c\}} h\left(c(x)|\overline{c_{\varepsilon_c}}\right)\mathrm{d}x + \log\left(1+\frac{M_0}{\varepsilon_c}\right)\int_{\{x|c(x)\geqslant\varepsilon_c\}} c(x)\mathrm{d}x$$
$$\leqslant \frac{1}{d_c C_{\mathrm{LSI}}}\int_\Omega \mathcal{I}_{\varepsilon_c,\varepsilon_s}(x)\mathrm{d}x + \log\left(1+\frac{M_0}{\varepsilon_c}\right)\int_\Omega \mathcal{I}_{\mathscr{M}}(x)\mathrm{d}x. \tag{2.52}$$

- $d_e = d_c = 0$. In this case we notice that as

$$c(x) \leqslant c(x) + e(x) = c_0(x) + e_0(x) = e_\infty(x)$$

and since (2.9) holds we have that

$$\frac{c(x)}{\varepsilon_c(x)} \leqslant \frac{e_\infty(x)}{\varepsilon_c(x)} = \frac{k_r}{k_f\varepsilon_s}.$$

Thus

$$\int_\Omega h_{\varepsilon_c}\left(c(x)|\varepsilon_c\right)\mathrm{d}x = \int_{\{x|c(x)\geqslant\varepsilon_c(x)\}}\left(c(x)\log\left(\frac{c(x)}{\varepsilon_c(x)}\right) - c(x) + \varepsilon_c(x)\right)\mathrm{d}x$$
$$\leqslant \int_{\{x|c(x)\geqslant\varepsilon_c(x)\}} c(x)\log\left(\frac{c(x)}{\varepsilon_c(x)}\right)\mathrm{d}x \leqslant \log\left(1+\frac{k_r}{k_f\varepsilon_s}\right)\int_\Omega c(x)\mathrm{d}x$$
$$\leqslant \log\left(1+\frac{k_r}{k_f\varepsilon_s}\right)\int_\Omega \mathcal{I}_{\mathscr{M}}(x)\mathrm{d}x. \tag{2.53}$$

The term $h_{\varepsilon_s}\left(s(x)|\varepsilon_s\right)$:
Similarly to our previous term we see that using the fact that[13]

$$\varepsilon_s \leqslant \underbrace{\int_\Omega \max\left(s(x),\varepsilon_s\right)\mathrm{d}x}_{=\overline{s_{\varepsilon_s}}} \leqslant \int_\Omega s(x)\mathrm{d}x + \varepsilon_s \leqslant M_1 + \varepsilon_s$$

we get that

$$\int_\Omega h_{\varepsilon_s}\left(s(x)|\varepsilon_s\right)\mathrm{d}x \leqslant \int_{\{x|s(x)\geqslant\varepsilon_s\}} h\left(s(x)|\overline{s_{\varepsilon_s}}\right)\mathrm{d}x + \log\left(1+\frac{M_1}{\varepsilon_s}\right)\int_\Omega s(x)\mathrm{d}x$$
$$\leqslant \frac{1}{d_s C_{\mathrm{LSI}}}\int_\Omega \mathcal{I}_{\varepsilon_c,\varepsilon_s}(x)\mathrm{d}x + \log\left(1+\frac{M_1}{\varepsilon_s}\right)\int_\Omega s(x)\mathrm{d}x. \tag{2.54}$$

In order to conclude the above estimation, and estimate the term that is connected to $\mathscr{M}(c,s)$ in $\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}$, we will now bound $\int_\Omega s(x)\mathrm{d}x$.

[13] The conservation of mass

$$\int_\Omega (s(x,t) + c(x,t) + p(x,t))\mathrm{d}x = M_1$$

is valid in both cases.

We start by noticing that if $x \geqslant 8y$ then

$$h(x|y) = x\left(\log(x) - \log(y) - 1\right) + y \geqslant x.$$

As such

$$\begin{aligned}\int_{\{x|s(x)\geqslant 8\overline{s_{\varepsilon_s}}\}} s(x)\mathrm{d}x &\leqslant \int_{\{x|s(x)\geqslant 8\overline{s_{\varepsilon_s}}\}} h\left(s(x)|\overline{s_{\varepsilon_s}}\right)\mathrm{d}x \\ &\leqslant \int_{\{x|s(x)\geqslant \varepsilon_s\}} h\left(s(x)|\overline{s_{\varepsilon_s}}\right)\mathrm{d}x \leqslant \frac{1}{d_s C_{\mathrm{LSI}}}\int_\Omega \mathscr{I}_{\varepsilon_c,\varepsilon_s}(x)\mathrm{d}x. \end{aligned} \tag{2.55}$$

To deal with the case where $s(x) \leqslant 8\overline{s_{\varepsilon_s}}$ we will need to consider our two cases separately.

- *All diffusion coefficients are strictly positive*. In this case we need to consider two options:
  - $*$ If $e(x) \leqslant \frac{e_\infty}{2}$ then as $h(x|y)$ is decreasing on $[0, y)$ we have that

$$\min_{x\in\left[0,\frac{y}{2}\right]} h(x|y) = h\left(\frac{y}{2}\Big| y\right) = \frac{(1-\log(2))\,y}{2}.$$

and as such

$$\begin{aligned}\int_{\left\{x|s(x)<8\overline{s_{\varepsilon_s}}\wedge e(x)\leqslant\frac{e_\infty}{2}\right\}} s(x)\mathrm{d}x &\leqslant \frac{16\overline{s_{\varepsilon_s}}}{(1-\log(2))\,e_\infty}\int_{\left\{x|s(x)<8\overline{s_{\varepsilon_s}}\wedge e(x)\leqslant\frac{e_\infty}{2}\right\}} h\left(e(x)|e_\infty\right)\mathrm{d}x \\ &\leqslant \frac{16\left(\varepsilon_s + M_1\right)}{(1-\log(2))\,e_\infty}\int_\Omega h\left(e(x)|e_\infty\right)\mathrm{d}x \\ &\leqslant \frac{16\left(\varepsilon_s + M_1\right)}{(1-\log(2))\,e_\infty}\left(\int_\Omega h\left(e(x)|\overline{e}\right)\mathrm{d}x + \int_\Omega \mathscr{I}_{\mathscr{M}}(x)\mathrm{d}x\right)\end{aligned} \tag{2.56}$$

where we have used (2.50).

  - $*$ If $e(x) > \frac{e_\infty}{2}$ then

$$\int_{\left\{x|s(x)<8\overline{s_{\varepsilon_s}}\wedge e(x)>\frac{e_\infty}{2}\right\}} s(x)\mathrm{d}x \leqslant \frac{2}{e_\infty}\int_{\left\{x|s(x)<8\overline{s_{\varepsilon_s}}\wedge e(x)>\frac{e_\infty}{2}\right\}} e(x)s(x) \leqslant \frac{2k_r}{k_f e_\infty}\int_\Omega \mathscr{I}_{\mathscr{M}}(x)\mathrm{d}x. \tag{2.57}$$

Thus

$$\begin{aligned}\int_\Omega s(x)\mathrm{d}x \leqslant{}& \frac{1}{d_s C_{\mathrm{LSI}}}\int_\Omega \mathscr{I}_{\varepsilon_c,\varepsilon_s}(x)\mathrm{d}x + \frac{16\left(\varepsilon_s + M_1\right)}{(1-\log(2))\,e_\infty}\int_\Omega h\left(e(x)|\overline{e}\right)\mathrm{d}x \\ &+ \left(\frac{2k_r}{k_f e_\infty} + \frac{16\left(\varepsilon_s + M_1\right)}{(1-\log(2))\,e_\infty}\right)\int_\Omega \mathscr{I}_{\mathscr{M}}(x)\mathrm{d}x. \end{aligned} \tag{2.58}$$

- $d_e = d_c = 0$. The same options as in the first case need to be considered. The exact same calculation, together with condition (2.8) and (2.51), show that[14]

$$\int_{\left\{x|s(x)<8\overline{s_{\varepsilon}}\wedge e(x)\leqslant \frac{e_\infty(x)}{2}\right\}} s(x)\mathrm{d}x \leqslant \frac{16\left(\varepsilon_s+M_1\right)}{\left(1-\log(2)\right)\beta}\int_\Omega h\left(e(x)|e_\infty(x)\right)\mathrm{d}x \leqslant \frac{16\left(\varepsilon_s+M_1\right)}{\left(1-\log(2)\right)\beta}\int_\Omega \mathscr{d}_{\mathscr{M}}(x)\mathrm{d}x. \tag{2.59}$$

and

$$\int_{\left\{x|s(x)<8\overline{s_{\varepsilon_s}}\wedge e(x)>\frac{e_\infty(x)}{2}\right\}} s(x)\mathrm{d}x \leqslant \frac{2}{\beta}\int_{\left\{x|s(x)<8\overline{s_{\varepsilon_s}}\wedge e(x)>\frac{\beta}{2}\right\}} e(x)s(x) \leqslant \frac{2k_r}{k_f\beta}\int_\Omega \mathscr{d}_{\mathscr{M}}(x)\mathrm{d}x, \tag{2.60}$$

from which we find that

$$\int_\Omega s(x)\mathrm{d}x \leqslant \frac{1}{d_s C_{\mathrm{LSI}}}\int_\Omega \mathscr{d}_{\varepsilon_c,\varepsilon_s}(x)\mathrm{d}x + \left(\frac{2k_r}{k_f\beta}+\frac{16\left(\varepsilon_s+M_1\right)}{\left(1-\log(2)\right)\beta}\right)\int_\Omega \mathscr{d}_{\mathscr{M}}(x)\mathrm{d}x. \tag{2.61}$$

Combining (2.50), (2.52), (2.54) and (2.58) with the definition of $\mathscr{E}_{\varepsilon_c,\varepsilon_s,k}$ and the facts that $e_\infty = M_0$ when all diffusion coefficients are strictly positive and $c(x) \leqslant \mathscr{d}_{\mathscr{M}}(x)$ we find that

$$\begin{aligned}\mathscr{E}_{\varepsilon_c,\varepsilon_s,k}\left(e,c,s\right) \leqslant &\left(1+\left(\log\left(1+\frac{M_1}{\varepsilon_s}\right)+\frac{k\left(2k_r+k_c\right)}{2k_r}\right)\frac{16\left(\varepsilon_s+M_1\right)}{\left(1-\log(2)\right)M_0}\right)\\ &\times\int_\Omega h\left(e(x)|\overline{e}\right)\mathrm{d}x\left(1+k+\log\left(1+\frac{M_0}{\varepsilon_c}\right)\right.\\ &+\left(\log\left(1+\frac{M_1}{\varepsilon_s}\right)+\frac{k\left(2k_r+k_c\right)}{2k_r}\right)\\ &\left.\times\left(\frac{2k_r}{k_f M_0}+\frac{16\left(\varepsilon_s+M_1\right)}{\left(1-\log(2)\right)M_0}\right)\right)\int_\Omega \mathscr{d}_{\mathscr{M}}(x)\mathrm{d}x\\ &+\frac{1}{C_{\mathrm{LSI}}}\left(\frac{1}{d_c}+\frac{1}{d_s}\left(1+\log\left(1+\frac{M_1}{\varepsilon_s}\right)+\frac{k\left(2k_r+k_c\right)}{2k_r}\right)\right)\int_\Omega \mathscr{d}_{\varepsilon_c,\varepsilon_s}(x)\mathrm{d}x\end{aligned}$$

when all diffusion coefficients are strictly positive, and similarly combining (2.51), (2.53), (2.54) and (2.61) yields

$$\begin{aligned}\mathscr{E}_{\varepsilon_c,\varepsilon_s,k}\left(e,c,s\right) \leqslant &\left(1+k+\log\left(1+\frac{k_r}{k_f\varepsilon_s}\right)+\left(\log\left(1+\frac{M_1}{\varepsilon_s}\right)\right.\right.\\ &\left.\left.+\frac{k\left(2k_r+k_c\right)}{2k_r}\right)\left(\frac{2k_r}{k_f\beta}+\frac{16\left(\varepsilon_s+M_1\right)}{\left(1-\log(2)\right)\beta}\right)\right)\int_\Omega \mathscr{d}_{\mathscr{M}}(x)\mathrm{d}x\\ &+\frac{1}{d_s C_{\mathrm{LSI}}}\left(1+\log\left(1+\frac{M_1}{\varepsilon_s}\right)+\frac{k\left(2k_r+k_c\right)}{2k_r}\right)\\ &\times\int_\Omega \mathscr{d}_{\varepsilon_c,\varepsilon_s}(x)\mathrm{d}x\end{aligned}$$

[14] When $e(x) \leqslant \frac{e_\infty(x)}{2}$ we have that

$$1 \leqslant \frac{2h\left(e(x)|e_\infty(x)\right)}{\left(1-\log\left(2\right)\right)e_\infty(x)} \leqslant \frac{2h\left(e(x)|e_\infty(x)\right)}{\left(1-\log\left(2\right)\right)\beta}$$

when $d_e = d_c = 0$.

Thus, (2.47) is satisfied when

$$\gamma \leqslant \frac{\left(d_e C_{\mathrm{LSI}} - 6\left(\frac{(k_c+k_r)}{M_0} + k_f\right)\max(\varepsilon_c, \varepsilon_s)\right)}{\left(1 + \left(\log\left(1 + \frac{M_1}{\varepsilon_s}\right) + \frac{k(2k_r+k_c)}{2k_r}\right)\frac{16(\varepsilon_s+M_1)}{(1-\log(2))M_0}\right)}$$

and

$$\gamma \leqslant \frac{\frac{kk_c}{2} - k_c - k_r - 2k_f\varepsilon_s}{\left(1 + k + \log\left(1 + \frac{M_0}{\varepsilon_c}\right) + \left(\log\left(1 + \frac{M_1}{\varepsilon_s}\right) + \frac{k(2k_r+k_c)}{2k_r}\right)\left(\frac{2k_r}{k_f M_0} + \frac{16(\varepsilon_s+M_1)}{(1-\log(2))M_0}\right)\right)}$$

and

$$\gamma \leqslant \frac{d_c d_s C_{\mathrm{LSI}}}{d_s + d_c\left(1 + \log\left(1 + \frac{M_1}{\varepsilon_s}\right) + \frac{k(2k_r+k_c)}{2k_r}\right)},$$

which yields the expression (2.5) and (2.48) is satisfied when

$$\gamma \leqslant \frac{\frac{kk_c}{2} - k_f\varepsilon_s}{\left(1 + k + \log\left(1 + \frac{k_r}{k_f\varepsilon_s}\right) + \left(\log\left(1 + \frac{M_1}{\varepsilon_s}\right) + \frac{k(2k_r+k_c)}{2k_r}\right)\left(\frac{2k_r}{k_f\beta} + \frac{16(\varepsilon_s+M_1)}{(1-\log(2))\beta}\right)\right)}$$

and

$$\gamma \leqslant \frac{d_s C_{\mathrm{LSI}}}{1 + \log\left(1 + \frac{M_1}{\varepsilon_s}\right) + \frac{k(2k_r+k_c)}{2k_r}},$$

which yields the expression (2.10). This completes the proof. □

With the entropic investigation complete, we can now turn our attention to the L^∞ convergence.

3. Convergence to equilibrium

In this section we will explore how one can use the properties of our system of equations, (1.2), to bootstrap the entropic convergence found in theorem 2.2 to a uniform one. To do so we start with a couple of theorems that guarantee an existence of non-negative bounded solutions to our system.

Theorem 3.1. *Assume that $\Omega \subset \mathbb{R}^n$ is a bounded, open domain with $C^{2+\zeta}, \zeta > 0$ boundary $\partial\Omega$. Assume in addition that all the diffusion coefficients, d_e, d_s, d_c, d_p, are strictly positive. Then for any non-negative, bounded initial data e_0, s_0, c_0 and p_0, there exists a unique global non-negative, classical solution to* (1.2) *which is uniformly bounded in time, i.e. there exists a constant $\mathcal{S} > 0$ such that*

$$\sup_{t\geqslant 0}\left(\|e(t)\|_{L^\infty(\Omega)} + \|c(t)\|_{L^\infty(\Omega)} + \|s(t)\|_{L^\infty(\Omega)} + \|p(t)\|_{L^\infty(\Omega)}\right) \leqslant \mathcal{S}.$$

Proof. The theorem follows from [MT20, theorem 1.2]. Indeed, we will check that all assumptions in [MT20, theorem 1.2] are satisfied. For the system (1.2), assumptions (A1) and (A2) are immediate, assumption (A3) is fulfilled with

$$h_e(e) = e, \qquad h_s(s) = s, \qquad h_c(c) = 2c, \qquad h_p(p) = p.$$

By using the lower triangle matrix

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

assumption (A4) is valid with a linear intermediate sum condition, i.e. $r = 1$. Finally, assumption (A5) is satisfied for $\mu = 2$. Since $r = 1$, condition (8) in [MT20, theorem 1.2] is satisfied for $p = 2$ thanks to [CzDF14, estimate (32)]. This guarantees the desired global result and uniform boundedness. □

Remark 3.2. The global existence of bounded solution to systems with triangular structure, such as that which is present in (1.2), has been investigated extensively with papers going back as early as the 80s in e.g. [HMP87, Mor89]. We refer the interested reader to the extensive review [Pie10] for more details.

Theorem 3.3. *Assume that $\Omega \subset \mathbb{R}^n$ is a bounded, open domain with $C^{2+\zeta}, \zeta > 0$ boundary $\partial\Omega$. Assume in addition that $d_s > 0, d_p > 0$ and $d_e = d_c = 0$. Then for any non-negative, bounded initial data e_0, s_0, c_0 and p_0, there exists a unique global non-negative, strong solution to (1.2) which is uniformly bounded in time, i.e. there exists a constant $\mathcal{S} > 0$ such that*

$$\sup_{t\geqslant 0}\left(\|e(t)\|_{L^\infty(\Omega)} + \|c(t)\|_{L^\infty(\Omega)} + \|s(t)\|_{L^\infty(\Omega)} + \|p(t)\|_{L^\infty(\Omega)}\right) \leqslant \mathcal{S}.$$

Proof. The proof is a fairly standard fixed point argument. As such, we defer it to appendix A. □

With these existence theorems at hand, we can now prove our main results: theorems 1.1 and 1.2. Before we do so, however, we shall state the following lemmas, whose proofs we leave to appendix A.

Lemma 3.4. *Assume that $\Omega \subset \mathbb{R}^n$, $n \geqslant 1$, is a bounded, open domain with $C^{2+\zeta}, \zeta > 0$, boundary. Let $u(x,t)$ be a strong solution to the inhomogeneous heat equation with Neumann conditions*

$$\begin{cases} \partial_t u(x,t) - d\Delta u(x,t) = f(x,t) & x \in \Omega,\ t > 0 \\ u(x,0) = u_0(x) & x \in \Omega \\ \partial_\nu u(x,t) = 0, & x \in \partial\Omega, t > 0. \end{cases}$$

Then, if there exists $p > \frac{n}{2}$ such that

$$\begin{aligned} &\max\left(\|u(t)\|_{L^p(\Omega)}, \|f(t)\|_{L^p(\Omega)}\right) \leqslant \mathcal{C}\, e^{-\delta t}, \\ &\sup_{t\in[0,1]} \|u(t)\|_{L^\infty(\Omega)} \leqslant \mathcal{S}, \end{aligned} \tag{3.1}$$

then there exist explicit constant $C_{d,n,p}$ that depends only on Ω, d, n and p such that

$$\|u(t)\|_{L^\infty(\Omega)} \leqslant e^{\delta} \max\left(\mathcal{S}, \mathcal{C}C_{d,n,p}\right) e^{-\delta t}. \tag{3.2}$$

Lemma 3.5. *Assume that $\Omega \subset \mathbb{R}^n$, $n \geqslant 1$, is a bounded, open domain with $C^{2+\zeta}, \zeta > 0$, boundary. Let $u(x,t)$ be a strong solution to the inhomogeneous heat equation with Neumann conditions*

$$\begin{cases} \partial_t u(x,t) - d\Delta u(x,t) = f(x,t) & x \in \Omega,\ t > 0 \\ u(x,0) = u_0(x) & x \in \Omega \\ \partial_\nu u(x,t) = 0, & x \in \partial\Omega, t > 0. \end{cases}$$

Then for any $\varepsilon > 0$ we have that

$$\|u(t) - \overline{u}(t)\|^2_{L^2(\Omega)} \leqslant \mathrm{e}^{-\frac{2d}{C_\mathrm{P}}(1-\varepsilon)t} \|u_0 - \overline{u_0}\|^2_{L^2(\Omega)} + \frac{C_\mathrm{P}\,\mathrm{e}^{-\frac{2d}{C_\mathrm{P}}(1-\varepsilon)t}}{2\mathrm{d}\varepsilon} \int_0^t \mathrm{e}^{\frac{2d}{C_\mathrm{P}}(1-\varepsilon)s} \left\|f(s) - \overline{f}(s)\right\|^2_{L^2(\Omega)} \mathrm{d}s, \tag{3.3}$$

where $\overline{g} = \int_\Omega g(x)\mathrm{d}x$ and C_P is the Poincaré constant associated to the domain, i.e. the positive constant for which

$$\left\|f - \overline{f}\right\|_{L^2(\Omega)} \leqslant C_\mathrm{P} \|\nabla f\|_{L^2(\Omega)}, \tag{3.4}$$

for any $f \in H^1(\Omega)$.

Proof of theorem 1.1. From theorems 3.1 and 2.2 we know that a unique non-negative bounded classical solution to (1.2) exists and satisfies

$$\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e(t), c(t), s(t)) \leqslant \mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0, c_0, s_0)\mathrm{e}^{-\gamma t},$$

for the parameters indicated in theorem 2.2. As was seen in remark 2.3, we can make the choices that correspond to (1.10) with (1.11).

Using the Csiszár–Kullback–Pinsker inequality

$$\|f - g\|_{L^1(\Omega)} \leqslant \sqrt{C_\mathrm{CPK} \int_\Omega h\left(f(x)|g(x)\right) \mathrm{d}x},$$

where C_CPK is a fixed known constant (see for instance [AMTU01]), together with the definition of $\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}$ we find that

$$\begin{aligned} \|c(t)\|_{L^1(\Omega)} &\leqslant \frac{\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e(t), c(t), s(t))}{k} \leqslant \frac{\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0, c_0, s_0)}{k}\mathrm{e}^{-\gamma t}, \\ \|s(t)\|_{L^1(\Omega)} &\leqslant \frac{2k_r\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e(t), c(t), s(t))}{k\,(2k_r + k_c)} \leqslant \frac{2k_r\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0, c_0, s_0)}{k\,(2k_r + k_c)}\mathrm{e}^{-\gamma t}, \\ \|e(t) - e_\infty\|_{L^1(\Omega)} &\leqslant \sqrt{C_\mathrm{CPK}\int_\Omega h\left(e(x,t)|e_\infty\right)\mathrm{d}x} \leqslant \sqrt{C_\mathrm{CPK}\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e(t), c(t), s(t))} \\ &\leqslant \sqrt{C_\mathrm{CPK}\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0, c_0, s_0)}\,\mathrm{e}^{-\frac{\gamma t}{2}}. \end{aligned} \tag{3.5}$$

Since for any $p \in [1, \infty)$

$$\|u\|_{L^p(\Omega)} \leqslant \|u\|_{L^\infty(\Omega)}^{1-\frac{1}{p}} \|u\|_{L^1(\Omega)}^{\frac{1}{p}}$$

we see that

$$\begin{aligned}
&\|c(t)\|_{L^p(\Omega)} \leqslant \mathcal{S}^{1-\frac{1}{p}} \left(\frac{\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0, c_0, s_0)}{k} \right)^{\frac{1}{p}} \mathrm{e}^{-\frac{\gamma t}{p}}, \\
&\|s(t)\|_{L^p(\Omega)} \leqslant \mathcal{S}^{1-\frac{1}{p}} \left(\frac{2k_r \mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0, c_0, s_0)}{k\,(2k_r + k_c)} \right)^{\frac{1}{p}} \mathrm{e}^{-\frac{\gamma t}{p}}, \\
&\|e(t) - e_\infty\|_{L^p(\Omega)} \leqslant (\mathcal{S} + M_0)^{1-\frac{1}{p}} \left(C_{\mathrm{CPK}} \mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0, c_0, s_0) \right)^{\frac{1}{2p}} \mathrm{e}^{-\frac{\gamma t}{2p}},
\end{aligned} \tag{3.6}$$

where $\mathcal{S}$ is given in theorem 3.1 and we have used the fact that $e_\infty = M_0$.

Denoting by

$$\begin{aligned}
&f_e(x,t) = -k_f e(x,t) s(x,t) + (k_r + k_c) c(x,t), \\
&f_s(x,t) = -k_f e(x,t) s(x,t) + k_r c(x,t), \\
&f_c(x,t) = k_f e(x,t) s(x,t) - (k_r + k_c) c(x,t),
\end{aligned}$$

we see that the first three equations of (1.2) can be rewritten as

$$\begin{cases}
\partial_t (e(x,t) - e_\infty) - d_e \Delta (e(x,t) - e_\infty) = f_e(x,t) & x \in \Omega, t > 0, \\
\partial_t s(x,t) - d_s \Delta s(x,t) = f_s(x,t) & x \in \Omega, t > 0, \\
\partial_t c(x,t) - d_c \Delta c(x,t) = f_c(x,t) & x \in \Omega, t > 0, \\
e(x,0) - e_\infty = e_0(x) - e_\infty,\ s(x,0) = s_0(x),\ c(x,0) = c_0(x), & x \in \Omega \\
\partial_\nu e(x,t) = \partial_\nu s(x,t) = \partial_\nu c(x,t) = 0, & x \in \partial\Omega, t > 0,
\end{cases}$$

and since (3.6) and theorem 3.1 imply that for any $p \in [1, \infty)$

$$\|e(t)s(t)\|_{L^p(\Omega)} \leqslant \mathcal{S}^{2-\frac{1}{p}} \left(\frac{2k_r \mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0, c_0, s_0)}{k\,(2k_r + k_c)} \right)^{\frac{1}{p}} \mathrm{e}^{-\frac{\gamma t}{p}}$$

we see that for $p = \frac{n(1+\eta)}{2}$ for any $\eta > 0$

$$\begin{aligned}
&\|f_e(t)\|_{L^{\frac{n}{2}(1+\eta)}(\Omega)} \leqslant \left(k_f \mathcal{S} + (k_r + k_c) \right) \mathcal{S}^{1-\frac{2}{n(1+\eta)}} \left(\frac{\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0, c_0, s_0)}{k} \right)^{\frac{2}{n(1+\eta)}} \mathrm{e}^{-\frac{2\gamma t}{n(1+\eta)}} \\
&\|f_s(t)\|_{L^{\frac{n}{2}(1+\eta)}(\Omega)} \leqslant \left(k_f \mathcal{S} + k_r \right) \mathcal{S}^{1-\frac{2}{n(1+\eta)}} \left(\frac{\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0, c_0, s_0)}{k} \right)^{\frac{2}{n(1+\eta)}} \mathrm{e}^{-\frac{2\gamma t}{n(1+\eta)}} \\
&\|f_c(t)\|_{L^{\frac{n}{2}(1+\eta)}(\Omega)} \leqslant \left(k_f \mathcal{S} + (k_r + k_c) \right) \mathcal{S}^{1-\frac{2}{n(1+\eta)}} \left(\frac{\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0, c_0, s_0)}{k} \right)^{\frac{2}{n(1+\eta)}} \mathrm{e}^{-\frac{2\gamma t}{n(1+\eta)}}
\end{aligned}$$

and as such

$$\max\left(\|s(t)\|_{L^{\frac{n}{2}(1+\eta)}(\Omega)}, \|c(t)\|_{L^{\frac{n}{2}(1+\eta)}(\Omega)}, \|f_s(t)\|_{L^{\frac{n}{2}(1+\eta)}(\Omega)}, \|f_c(t)\|_{L^{\frac{n}{2}(1+\eta)}(\Omega)}\right)$$

$$\leqslant \max\left(1, \left(k_f\mathcal{S} + (k_r + k_c)\right)\right)\mathcal{S}^{1-\frac{2}{n(1+\eta)}}\left(\frac{\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0, c_0, s_0)}{k}\right)^{\frac{2}{n(1+\eta)}}\mathrm{e}^{-\frac{2\gamma t}{n(1+\eta)}}$$

and

$$\max\left(\|e(t) - e_\infty\|_{L^{\frac{n}{2}(1+\eta)}(\Omega)}, \|f_e(t)\|_{L^{\frac{n}{2}(1+\eta)}(\Omega)}\right) \leqslant \max\left(1, \left(k_f\mathcal{S} + (k_r + k_c)\right)\right)$$

$$(\mathcal{S} + M_0)^{1-\frac{2}{n(1+\eta)}}\max\left(\sqrt{C_{\mathrm{CPK}}\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0, c_0, s_0)}, \left(\frac{\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0, c_0, s_0)}{k}\right)\right)^{\frac{2}{n(1+\eta)}}\mathrm{e}^{-\frac{\gamma t}{n(1+\eta)}}.$$

Applying lemma 3.4 we find that we can find explicit constants $\mathcal{C}_{e,\eta}$, $\mathcal{C}_{s,\eta}$ and $\mathcal{C}_{c,\eta}$ depending only geometric on properties, initial datum and η, that become unbounded as η goes to zero, such that

$$\begin{aligned}
\|c(t)\|_{L^\infty(\Omega)} &\leqslant \mathcal{C}_{c,\eta}\,\mathrm{e}^{-\frac{2\gamma t}{n(1+\eta)}},\\
\|s(t)\|_{L^\infty(\Omega)} &\leqslant \mathcal{C}_{s,\eta}\,\mathrm{e}^{-\frac{2\gamma t}{n(1+\eta)}},\\
\|e(t) - e_\infty\|_{L^\infty(\Omega)} &\leqslant \mathcal{C}_{e,\eta}\,\mathrm{e}^{-\frac{\gamma t}{n(1+\eta)}},
\end{aligned} \tag{3.7}$$

showing the desired result for $c(x, t)$, $s(x, t)$ and $e(x, t)$. To conclude the proof we consider the equation for $p(x, t)$

$$\begin{cases}
\partial_t p(x, t) - d_p\Delta p(x, t) = f_p(x, t) & x \in \Omega, t > 0,\\
p(x, 0) = p_0(x), & x \in \Omega\\
\partial_\nu p(x, t) = 0, & x \in \partial\Omega, t > 0,
\end{cases}$$

where $f_p(x, t) = k_c c(x, t)$. According to lemma 3.5 we see that for any $\varepsilon > 0$

$$\|p(t) - \overline{p}(t)\|^2_{L^2(\Omega)} \leqslant \mathrm{e}^{-\frac{2d_p}{C_p}(1-\varepsilon)t}\|p_0 - \overline{p_0}\|^2_{L^2(\Omega)} + \frac{C_{\mathrm{P}}\,\mathrm{e}^{-\frac{2d_p}{C_{\mathrm{P}}}(1-\varepsilon)t}}{2d_p\varepsilon}\int_0^t \mathrm{e}^{\frac{2d_p}{C_{\mathrm{P}}}(1-\varepsilon)s}\left\|f_p(s) - \overline{f_p}(s)\right\|^2_{L^2(\Omega)}\,\mathrm{d}s.$$

As

$$\|f_p(t)\|^2_{L^2(\Omega)} \leqslant \frac{k_c^2\mathcal{S}\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0, c_0, s_0)}{k}\cdot\mathrm{e}^{-\gamma t}$$

and

$$0 \leqslant \overline{f_p}(t) = k_c \overline{c}(t) = k_c \|c(t)\|_{L^1(\Omega)} \leqslant \frac{k_c \mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0, c_0, s_0)}{k} \, \mathrm{e}^{-\gamma t}$$

we can find an appropriate constant $C_{d,\delta,\gamma}$ such that

$$\|p(t) - \overline{p}(t)\|_{L^2(\Omega)} \leqslant C_{d,\varepsilon,\gamma} \left(1 + t^{\delta_{\frac{d_p}{C_\mathrm{P}}(1-\varepsilon),\frac{\gamma}{2}}}\right) \mathrm{e}^{-\min\left(\frac{d_p}{C_\mathrm{P}}(1-\varepsilon),\frac{\gamma}{2}\right)t},$$

where we have used the fact that

$$\mathrm{e}^{-\alpha t} \int_0^t \mathrm{e}^{(\alpha-\beta)s} \, \mathrm{d}s = \begin{cases} \dfrac{\mathrm{e}^{-\beta t} - \mathrm{e}^{-\alpha t}}{\alpha - \beta} & \alpha \neq \beta, \\ t\,\mathrm{e}^{-\beta t} & \alpha = \beta, \end{cases} \leqslant C_{\alpha,\beta} t^{\delta_{\alpha,\beta}} \, \mathrm{e}^{-\min(\alpha,\beta)t} \tag{3.8}$$

for

$$C_{\alpha,\beta} = \begin{cases} \dfrac{1}{|\alpha - \beta|} & \alpha \neq \beta \\ 1 & \alpha = \beta \end{cases}.$$

We also notice that

$$|p_\infty - \overline{p}(t)| = \left| M_1 - \int_\Omega p(x,t) \mathrm{d}x \right| = \int_\Omega (c(x,t) + s(x,t)) \, \mathrm{d}x$$

$$= \|c(t)\|_{L^1(\Omega)} + \|s(t)\|_{L^1(\Omega)} \leqslant \frac{2\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0, c_0, s_0)}{k} \, \mathrm{e}^{-\gamma t},$$

from which we see that

$$\|p(t) - p_\infty\|_{L^2(\Omega)} \leqslant \widetilde{C}_{d,\varepsilon} \left(1 + t^{\delta_{\frac{d_p}{C_\mathrm{P}}(1-\varepsilon),\frac{\gamma}{2}}}\right) \mathrm{e}^{-\min\left(\frac{d_p}{C_\mathrm{P}}(1-\varepsilon),\frac{\gamma}{2}\right)t}.$$

As $\|p(t) - p_\infty\|_{L^\infty(\Omega)} \leqslant \mathcal{S} + M_1$ according to Theorem 3.1 and since for any $p \geqslant 2$

$$\|u\|_{L^p(\Omega)} \leqslant \|u\|_{L^\infty(\Omega)}^{1-\frac{2}{p}} \|u\|_{L^2(\Omega)}^{\frac{2}{p}}$$

we can follow the same steps as those in our investigation of $c(x,t)$, $s(x,t)$ and $e(x,t)$ to conclude that

$$\|p(t) - p_\infty\|_{L^\infty(\Omega)} \leqslant \mathcal{C}_{p,\eta,\varepsilon} \left(1 + t^{\frac{4}{n(1+\eta)}\delta_{\frac{2d_p}{C_\mathrm{P}}(1-\varepsilon),\gamma}}\right) \mathrm{e}^{-\min\left(\frac{4d_p}{nC_\mathrm{P}(1+\eta)}(1-\varepsilon),\frac{2\gamma}{n(1+\eta)}\right)t}$$

when $\frac{n}{2}(1+\eta) \geqslant 2$. This completes the proof. □

Proof of theorem 1.2. Much like the proof of theorem 1.1 we use theorems 3.3 and 2.2 to show that[15]

$$\begin{aligned}
\|c(t)\|_{L^1(\Omega)} &\leqslant \frac{\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0,c_0,s_0)}{k}\,\mathrm{e}^{-\gamma t},\\
\|s(t)\|_{L^1(\Omega)} &\leqslant \frac{2k_r\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0,c_0,s_0)}{k\,(2k_r+k_c)}\mathrm{e}^{-\gamma t},\\
\|e(x,t)-e_\infty(x)\|_{L^1(\Omega)} &= \|c(t)\|_{L^1(\Omega)} \leqslant \frac{\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0,c_0,s_0)}{k}\,\mathrm{e}^{-\gamma t},
\end{aligned} \tag{3.9}$$

with γ satisfying (2.10). Note that to attain the last inequality we have used the conservation law (1.5)

$$e_\infty(x) = e(x,t) + c(x,t) = e_0(x) + c_0(x).$$

Again, using remark 2.3, we see that we can make the choices that correspond to (1.12) with (1.13).

Continuing as in the proof of theorem 1.1 we see that for any $p \geqslant 1$ we have that

$$\begin{aligned}
\|c(t)\|_{L^p(\Omega)} &\leqslant \mathcal{S}^{1-\frac{1}{p}}\left(\frac{\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0,c_0,s_0)}{k}\right)^{\frac{1}{p}}\mathrm{e}^{-\frac{\gamma t}{p}},\\
\|s(t)\|_{L^p(\Omega)} &\leqslant \mathcal{S}^{1-\frac{1}{p}}\left(\frac{2k_r\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0,c_0,s_0)}{k\,(2k_r+k_c)}\right)^{\frac{1}{p}}\mathrm{e}^{-\frac{\gamma t}{p}},\\
\|e(t)-e_\infty\|_{L^p(\Omega)} &= \|c(t)\|_{L^p(\Omega)} \leqslant \mathcal{S}^{1-\frac{1}{p}}\left(\frac{\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e_0,c_0,s_0)}{k}\right)^{\frac{1}{p}}\mathrm{e}^{-\frac{\gamma t}{p}}.
\end{aligned} \tag{3.10}$$

Since s satisfies

$$\partial_t s(x,t) - d_s\Delta s(x,t) = \underbrace{-k_f e(x,t)s(x,t) + k_r c(x,t)}_{f_s(x,t)}$$

and

$$\|f_s(t)\|_{L^p(\Omega)} \leqslant \mathcal{C}_s\,\mathrm{e}^{-\frac{\gamma t}{p}}$$

for an appropriate constant, we get from lemma 3.4 that for any $\eta > 0$ there exists a constant $\mathcal{C}_{s,\eta}$ that blows up as η goes to zero such that

$$\|s(t)\|_{L^\infty(\Omega)} \leqslant \mathcal{C}_{s,\eta}\,\mathrm{e}^{-\frac{2\gamma t}{n(1+\eta)}}.$$

Next we turn our attention to the convergence of c. As c satisfies the equation

$$\partial_t c(x,t) = k_f e(x,t)s(x,t) - (k_r+k_c)c(x,t)$$

we have that

$$c(x,t) = \mathrm{e}^{-(k_r+k_c)t}c_0(x) + k_f\int_0^t \mathrm{e}^{-(k_r+k_c)(t-\xi)}e(x,\xi)s(x,\xi)\mathrm{d}\xi.$$

[15] Remember that the entropy $\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e,c,s)$ is defined the same as in the full diffusion case, only with e_∞ and ε_c being functions that satisfy (2.9).

Since c is also non-negative we find that

$$\begin{aligned}\|c(t)\|_{L^\infty(\Omega)} &\leqslant \mathrm{e}^{-(k_r+k_c)t}\left(\|c_0\|_{L^\infty(\Omega)} + k_f\int_0^t \mathrm{e}^{(k_r+k_c)\xi}\|e(\xi)\|_{L^\infty(\Omega)}\|s(\xi)\|_{L^\infty(\Omega)}\,\mathrm{d}\xi\right)\\ &\leqslant \mathrm{e}^{-(k_r+k_c)t}\left(\|c_0\|_{L^\infty(\Omega)} + \mathcal{C}_{s,\eta}\mathcal{S}\int_0^t \mathrm{e}^{\left(k_r+k_c-\frac{2\gamma}{n(1+\eta)}\right)\xi} d\xi\right)\\ &\leqslant \mathcal{C}_{c,s,\eta}\left(1+t^{\delta_{k_r+k_c,\frac{2\gamma}{n(1+\eta)}}}\right)\mathrm{e}^{-\min\left(k_r+k_c,\frac{2\gamma}{n(1+\eta)}\right)t},\end{aligned}$$

where we have used (3.8). Using the conservation law (1.5) again we get that

$$\|e(x,t)-e_\infty(x)\|_{L^\infty(\Omega)} = \|c(t)\|_{L^\infty(\Omega)} \leqslant \mathcal{C}_{c,s,\eta}\left(1+t^{\delta_{k_r+k_c,\frac{2\gamma}{n(1+\eta)}}}\right)\mathrm{e}^{-\min\left(k_r+k_c,\frac{2\gamma}{n(1+\eta)}\right)t}.$$

The proof of the rate of convergence of $p(x,t)-p_\infty$ to zero is identical to that presented in the proof of theorem 1.1, and as such we conclude the proof of the theorem. □

With our main investigation complete, we now turn our attention to a few final remarks.

4. Final remarks

While some of the calculations presented in this work are quite technical, the true heart of proofs—the definition of a 'cut-off' entropy-like functional and the study of the interplay between it and a decreasing mass term—is simple and powerful enough that we believe it could be widely used in many other open and irreversible systems. We would like to end this study with a few remarks/observations.

4.1. The functional inequality

As was mentioned in our introduction section 1.3, showing the decay of our new entropy-like functional, $\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}$, heavily relied on a functional inequality of the form

$$\mathcal{E}_{\varepsilon_c,\varepsilon_s,k}(e,s,c) \lesssim \begin{cases}\displaystyle\int_\Omega \left(\mathcal{I}_{\varepsilon_c,\varepsilon_s}(x) + h(e(x)|\overline{e}) + \mathcal{I}_{\mathcal{M}}(x)\right)\mathrm{d}x & d_e,d_s,d_c>0,\\ \displaystyle\int_\Omega \left(\mathcal{I}_{\varepsilon_c,\varepsilon_s}(x) + \mathcal{I}_{\mathcal{M}}(x)\right)\mathrm{d}x & d_e=d_c=0\end{cases}.$$

While this inequality has not been stated explicitly as a lemma, proposition or a theorem, it is the sole ingredient of the proof of theorem 2.2, and its proof can be found there.

4.2. The case where $d_c = 0$ and $d_e > 0$

One can apply our techniques and find explicit exponential convergence to equilibrium for the L^∞ norms when all diffusion coefficients but d_c are strictly positive. In this case the equilibrium will be the same as that for when all diffusion coefficients were strictly positive. This situation, however, is not chemically relevant and as such we have elected to not treat it.

4.3. Optimal rate of convergence in the case where all diffusion coefficients are strictly positive

It is clear that the explicit rate of convergence given in remark 1.4 is not optimal. This stems from the multiple estimations we have made to achieve our results—estimations that are extremely hard to optimise simultaneously. Nevertheless, since we have shown exponential convergence to equilibrium we know that eventually (which can be expressed explicitly) the solution will be in a small neighbourhood of the equilibrium. This allows us to consider the linearised version of our equations and attain the optimal long time behaviour of the solutions, at least when this linear system indeed approximates the full nonlinear system of equations with respect to this behaviour.

Denoting by $\widetilde{y} = y - y_\infty$ for y which can be e, s, c or p, we find that the linearised system of equations around the equilibrium $(e_\infty, s_\infty, c_\infty, p_\infty)$ is given by

$$\begin{cases} \partial_t \widetilde{e}(x,t) - d_e\Delta\widetilde{e}(x,t) = -k_f e_\infty \widetilde{s}(x,t) + (k_r + k_c)\widetilde{c}(x,t), & x\in\Omega, t>0,\\ \partial_t \widetilde{s}(x,t) - d_s\Delta\widetilde{s}(x,t) = -k_f e_\infty \widetilde{s}(x,t) + k_r\widetilde{c}(x,t), & x\in\Omega, t>0,\\ \partial_t \widetilde{c}(x,t) - d_c\Delta\widetilde{c}(x,t) = k_f e_\infty \widetilde{s}(x,t) - (k_r + k_c)\widetilde{c}(x,t), & x\in\Omega, t>0,\\ \partial_t \widetilde{p}(x,t) - d_p\Delta\widetilde{p}(x,t) = k_c\widetilde{c}(x,t), & x\in\Omega, t>0, \end{cases} \tag{4.1}$$

with initial data $\widetilde{y}(x,0) = y_0(x) - y_\infty$ and homogeneous Neumann boundary conditions.

As before, we notice that the equation of $\widetilde{p}$ is decoupled from the rest of the equations.

Denoting by

$$0 = \lambda_0 < \lambda_1 < \lambda_2 \leqslant \lambda_3 \leqslant \ldots \to \infty$$

the eigenvalues of $-\Delta$ with homogeneous Neumann boundary condition in Ω, and by $\{\omega_j\}_{j\in\mathbb{N}\cup\{0\}}$ the corresponding orthonormal eigenfunctions basis of $L^2(\Omega)$ (see for instance [Tay11, section 5.7]), we claim the following.

Proposition 4.1. *The solution to the system* (4.1) *decays to zero in* $L^\infty(\Omega)$*-norm with the optimal rates*

$$\begin{aligned} &\|\widetilde{c}(t)\|_{L^\infty(\Omega)} + \|\widetilde{s}(t)\|_{L^\infty(\Omega)} \leqslant \mathcal{C}_{s,c}\, e^{-\mu_{\text{opt}} t},\\ &\|\widetilde{e}(t)\|_{L^\infty(\Omega)} \leqslant \mathcal{C}_{e,s,c} \left(1 + t^{\delta_{d_e\lambda_1,\mu_{\text{opt}}}}\right) \mathrm{e}^{-\min\left(d_e\lambda_1,\mu_{\text{opt}}\right)t},\\ &\|\widetilde{p}(t)\|_{L^\infty(\Omega)} \leqslant \mathcal{C}_{p,s,c} \left(1 + t^{\delta_{d_p\lambda_1,\mu_{\text{opt}}}}\right) \mathrm{e}^{-\min\left(d_p\lambda_1,\mu_{\text{opt}}\right)t}, \end{aligned} \tag{4.2}$$

where[16]

$$\mu_{\text{opt}} = \frac{1}{2}\left(k_f e_\infty + k_r + k_c - \sqrt{\left(k_f e_\infty - k_r - k_c\right)^2 + 4k_r k_f e_\infty}\right) > 0, \tag{4.3}$$

and

$$\delta_{x,y} = \begin{cases} 1 & x = y\\ 0 & x \neq y \end{cases}.$$

[16] Indeed

$$\begin{aligned} \mu_{\text{opt}} &= \frac{\left(k_f e_\infty + k_r + k_c\right)^2 - \left(k_f e_\infty - k_r - k_c\right)^2 - 4k_r k_f e_\infty}{2\left(k_f e_\infty + k_r + k_c + \sqrt{\left(k_f e_\infty - k_r - k_c\right)^2 + 4k_r k_f e_\infty}\right)}\\ &= \frac{4k_f e_\infty\left(k_r + k_c\right) - 4k_r k_f e_\infty}{2\left(k_f e_\infty + k_r + k_c + \sqrt{\left(k_f e_\infty - k_r - k_c\right)^2 + 4k_r k_f e_\infty}\right)} > 0. \end{aligned}$$

Remark 4.2. One notices from (4.2) and (4.3) that the optimal decay rates do not depend on the diffusion rate of s or c.

Proof. We give a formal proof to this proposition, and will not concern ourselves with discussing the existence and uniqueness of solutions, or other technical issues. Writing

$$\widetilde{y}(x,t) = \sum_{j=0}^{\infty} \widetilde{y}_j(t)\omega_j(x), \tag{4.4}$$

for y equals s or c, we see that the second and third equations of (4.1) (which are decoupled from the rest) are equivalent to the infinite system of ODEs

$$\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{X}_j(t) = A_j\widetilde{X}_j(t), \quad j \in \mathbb{N}\cup\{0\},$$

where

$$\widetilde{X}_j = \begin{pmatrix} \widetilde{s}_j \\ \widetilde{c}_j \end{pmatrix}, \qquad A_j = \begin{pmatrix} -d_s\lambda_j - k_f e_\infty & k_r \\ k_f e_\infty & -d_c\lambda_j - (k_r + k_c) \end{pmatrix}.$$

The eigenvalues of A_j are the solutions to the quadratic equation

$$\tau^2 + \left[(d_s + d_c)\lambda_j + k_f e_\infty + k_r + k_c\right]\tau + (d_s\lambda_j + k_f e_\infty)(d_c\lambda_j + k_r + k_c) - k_r k_f e_\infty = 0 \tag{4.5}$$

and consequently, the maximal eigenvalue, which determine the long time behaviour of the solution, is given by

$$\tau_{\max,j} = -\frac{(d_s + d_c)\,\lambda_j + k_f e_\infty + k_r + k_c - \sqrt{\triangle_j}}{2}$$

where

$$\triangle_j = \left(d_s\lambda_j + k_f e_\infty - (d_c\lambda_j + k_r + k_c)\right)^2 + 4k_r k_f e_\infty > 0.$$

Since for any $\alpha, \beta \in \mathbb{R}$ and $\gamma > 0$ we have that

$$\left|\frac{\mathrm{d}}{\mathrm{d}x}\sqrt{(\alpha x + \beta)^2 + \gamma}\right| = \frac{|\alpha|\,|(\alpha x + \beta)|}{\sqrt{(\alpha x + \beta)^2 + \gamma}} \leqslant |\alpha|$$

we see that for any $\delta > |\alpha|$

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\delta x - \sqrt{(\alpha x + \beta)^2 + \gamma}\right) \geqslant \delta - |\alpha| > 0.$$

Choosing $\delta = d_s + d_c$, $\alpha = d_s - d_c$, $\beta = k_f e_\infty - k_r - k_c$ and $\gamma = 4k_r k_f e_\infty$ in the above we conclude

$$\frac{\mathrm{d}}{\mathrm{d}\lambda_j}\tau_{\max,j} < 0$$

and since $\{\lambda_j\}_{j\in\mathbb{N}\cup\{0\}}$ is an increasing sequence we find that

$$\begin{aligned}\sup_{j\in\mathbb{N}} \tau_{\max,j} &= \tau_{\max,0}\\ &= \frac{-\left(k_f e_\infty + k_r + k_c\right) + \sqrt{\left(k_f e_\infty - k_r - k_c\right)^2 + 4k_r k_f e_\infty}}{2}\\ &= -\mu_{\text{opt}}.\end{aligned}$$

This implies that $\widetilde{s}$ and $\widetilde{c}$ decay with an exponential rate of μ_{opt}, which is optimal.

Next we turn our attention to $\widetilde{e}$ and $\widetilde{p}$. Using the same orthogonal decomposition (4.4) we find the following infinite set of ODEs:

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{e}_j(t) = -d_e\lambda_j\widetilde{e}_j(t) - k_f e_\infty \widetilde{s}_j(t) + (k_r + k_c)\widetilde{c}_j(t),\\ &\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{p}_j(t) = -d_p\lambda_j\widetilde{p}_j(t) + k_c\widetilde{c}_j(t).\end{aligned} \tag{4.6}$$

We will focus our attention on showing the convergence rate for $\widetilde{e}$. The convergence of $\widetilde{p}$ will be achieved in an identical way (by replacing d_e with d_p). Equation (4.6) implies that

$$\widetilde{e}_j(t) = \mathrm{e}^{-d_e\lambda_j t}\widetilde{e}_j(0) + \int_0^t \mathrm{e}^{-d_e\lambda_j(t-\xi)}\left(-k_f e_\infty \widetilde{s}_j(\xi) + (k_r + k_c)\widetilde{c}_j(\xi)\right)\mathrm{d}\xi. \tag{4.7}$$

Thus, using the known optimal decay rate for $\widetilde{c}_j$ and $\widetilde{s}_j$ we see that

$$|\widetilde{e}_j(t)| \leqslant \mathrm{e}^{-d_e\lambda_j t}\,|\widetilde{e}_j(0)| + \mathcal{C}_{s_j,c_j}\int_0^t \mathrm{e}^{-d_e\lambda_j(t-\xi)}\mathrm{e}^{-\mu_{\text{opt}}\xi}d\xi,$$

where $\mathcal{C}_{s_j,c_j}$ is a constant that depends only on

$$\widetilde{s}_j(0) = \langle s_0, \omega_j\rangle\,, \qquad \widetilde{c}_j(0) = \langle c_0, \omega_j\rangle$$

and k_f, k_r, k_c and e_∞. From this and (3.8) we conclude that

$$|\widetilde{e}_j(t)| \leqslant \left(|\widetilde{e}_j(0)| + \widetilde{\mathcal{C}}_{s_j,c_j}\right)\left(1 + t^{\delta_{d_e\lambda_j,\mu_{\text{opt}}}}\right)\mathrm{e}^{-\min\left(d_e\lambda_j,\mu_{\text{opt}}\right)t}. \tag{4.8}$$

Since $\{\lambda_j\}_{j\in\mathbb{N}}$ is an increasing sequence of numbers, we find that for any $j \geqslant 1$

$$|\widetilde{e}_j(t)| \leqslant \left(|\widetilde{e}_j(0)| + \widetilde{\mathcal{C}}_{s_j,c_j}\right)\left(1 + t^{\delta_{d_e\lambda_1,\mu_{\text{opt}}}}\right)\mathrm{e}^{-\min\left(d_e\lambda_1,\mu_{\text{opt}}\right)t}. \tag{4.9}$$

The above approach, however, is not useful when $j = 0$ as in this case $\lambda_j = 0$ and (4.8) yields only an upper bound. Instead we use the simple conservation law (much like in the full equation)

$$\int_\Omega \left(\widetilde{e}(x,t) + \widetilde{c}(x,t)\right)\mathrm{d}x = \int_\Omega (e(x,t) + c(x,t))\,\mathrm{d}x - M_0 = 0$$

and the fact that since $\omega_0(x) \equiv 1$ we have that

$$\widetilde{f}_0 = \left\langle \widetilde{f}, 1 \right\rangle = \int_\Omega \widetilde{f}(x)\mathrm{d}x,$$

to conclude that

$$|\widetilde{e}_0(t)| = |\widetilde{c}_0(t)| \leqslant \mathcal{C}_c\, \mathrm{e}^{-\mu_{\mathrm{opt}} t} \leqslant \mathcal{C}_c \left(1 + t^{\delta_{d_e\lambda_1,\mu_{\mathrm{opt}}}}\right) \mathrm{e}^{-\min\left(d_e\lambda_1,\mu_{\mathrm{opt}}\right)t}. \tag{4.10}$$

Combining (4.9) and (4.10) gives us the desired L^∞ bound on $\widetilde{e}(t)$. The treatment of $\widetilde{p}$ is exactly the same and uses of the second conservation law

$$\widetilde{s}_0(t) + \widetilde{c}_0(t) + \widetilde{p}_0(t) = \int_\Omega (s(x,t) + c(x,t) + p(x,t))\,\mathrm{d}x - M_1 = 0.$$

The proof is thus complete. □

4.4. Convergence to equilibrium without the lower bound condition on $e_0 + c_0$

As was mentioned in remark 1.5, and is clearer now from the proof of theorem 2.2, the lower bound (1.9) is essential to show and quantitatively estimate the convergence to equilibrium of the system (1.2) in the case where $d_e = d_c = 0$. Intuitively, however, we can still expect a strong convergence to equilibrium in situations where (1.9) is not fulfilled. Denoting the set

$$\Omega_{\mathrm{zero}} = \{x \in \Omega\, :\, e_0(x) + c_0(x) = 0\} = \{x \in \Omega\, :\, e_0(x) = c_0(x) = 0\}$$

we see that as the evolution of the concentration s is dominated by diffusion on Ω_{zero} at short times, s will diffuse away to $\Omega \backslash \Omega_{\mathrm{zero}}$ where it will get converted into product and complex and start a chain reaction that will lead to an eventual convergence to equilibrium. Proving this intuition rigorously, however, remains an interesting open problem. We would like to mention, however, that the tools we have developed in this work (mainly theorem 2.8) are sufficient to show *qualitative* convergence to equilibrium of the entropy-like functional even in this 'degenerate' case.

We end the main body of our work with figures of a numerical simulation that depict the case where $c_0 \equiv 0$, e_0 is not bounded away from zero, and $\mathrm{supp}\, e_0 \cap \mathrm{supp}\, s_0 = \emptyset$. More precisely, we considered

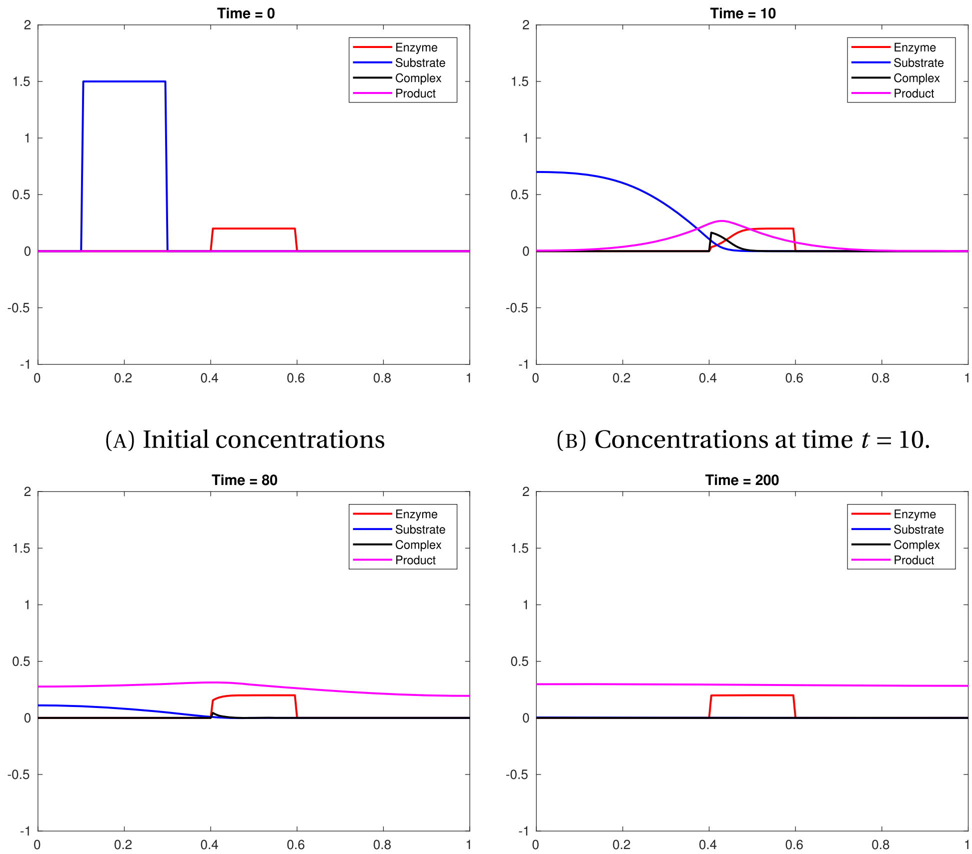
$$\Omega = (0,1), \qquad k_f = 100, \qquad k_r = k_c = 1, \qquad d_e = d_c = 0, \qquad d_s = d_p = 0.02,$$

$$e_0(x) = 0.2\chi_{(0.4,0.6)}(x), \qquad s_0(x) = 1.5\chi_{(0.1,0.3)}, \quad \text{and} \quad c_0(x) = p_0(x) = 0.$$

Under these assumptions we see that the equilibrium is given by

$$e_\infty(x) = 0.2\chi_{(0.4,0.6)}(x), \qquad s_\infty = c_\infty = 0, \qquad p_\infty = 0.3.$$

As expected, we see in figure 1(B) that when the substrate s diffuses to the region where the enzyme concentration is non-zero, it gets converted into the complex which subsequently produces the product. This procedure continues to dissolve the substrate, as seen in figure 1(C), and eventually converts it completely to the product while the enzyme returns to its initial configuration in figure 1(D).



(A) Initial concentrations

(B) Concentrations at time $t = 10$.

(C) Concentrations at time $t = 80$.

(D) Concentrations at time $t = 200$.

Figure 1. The evolution of enzyme, complex and substrate in the case where (1.9) is not fulfilled.

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Appendix A. Additional proofs

In this appendix we will show the proofs of several results which we elected to defer in order to not disrupt the flow of the presented work.

We start with the proof of theorem 3.3, which requires the following lemma:

Lemma A.1. *Assume that* $\Omega \subset \mathbb{R}^n$*,* $n \geqslant 1$*, is a bounded, open domain with* $C^{2+\zeta}, \zeta > 0$*, boundary. Assume that* $d, T > 0, u_0 \in L^{\infty}(\Omega)$ *and that the function* f *belongs to* $L^q(0, T; L^q(\Omega))$

for all $q \in [2, \infty)$. *Let*

$$u(x,t) = \mathrm{e}^{d\Delta t}u_0(x) + \int_0^t \mathrm{e}^{d\Delta(t-\xi)} f(x,\xi)\mathrm{d}\xi, \tag{A.1}$$

where $\mathrm{e}^{d\Delta t}$ *is the semigroup generated by the operator* $d\Delta$ *with homogeneous Neumann boundary conditions on* $L^q(\Omega)$. *Then* $u(x,t)$ *is a strong solution to*

$$\begin{cases} \partial_t u(x,t) - d\Delta u(x,t) = f(x,t) & x \in \Omega,\ t \in (0,T) \\ u(x,0) = u_0(x) & x \in \Omega \\ \partial_\nu u(x,t) = 0, & x \in \partial\Omega, t \in (0,T). \end{cases} \tag{A.2}$$

Proof. Denoting by

$$u_2(x,t) = \int_0^t \mathrm{e}^{d\Delta(t-\xi)} f(x,\xi)\mathrm{d}\xi$$

we see, according to [PS16, theorem 6.2.3], that for any $q \in [2, \infty)$ we have that

$$u_2 \in L^q((0,T); W^{2,q}(\Omega)) \cap W^{1,q}((0,T); L^q(\Omega)).$$

In particular, this implies that $u_2 \in C^0([0,T];\ L^q(\Omega))$ and that u_2 is a strong solution to (A.2) with $u_0 \equiv 0$.

To consider the general case we notice that we cannot use the same considerations for

$$u_1(x,t) = \mathrm{e}^{d\Delta t}u_0(x)$$

as u_0 does not necessarily belong to the right trace space. However, for every $t > 0$, we can use the regularisation properties of the semigroup to conclude that u_1 belongs to the space $C^0([0,T]; L^q(\Omega)) \cap C^1((0,T]; L^q(\Omega))$ and $u_1(\cdot,t) \in W^{2,q}(\Omega))$ for all positive t. This shows that u_1 is continuous with respect to $L^q(\Omega)$ and belongs to $L^q((\tau,T); W^{2,q}(\Omega)]) \cap W^{1,q}((\tau,T); L^q(\Omega))$ for every $\tau > 0$ and $q \in [2, \infty)$. Consequently, we obtain that u_1 is absolutely continuous as a $L^q(\Omega)$ valued function for positive times and is a strong solution to (A.2) with $f \equiv 0$. As $u = u_1 + u_2$ we conclude the desired result. □

Proof of theorem 3.3. The proof is based on a standard fixed point argument. For a fixed $T > 0$ we denote by

$$\begin{aligned} \mathcal{X} = \Big\{ &(e,s,c,p) \in (L^\infty([0,T]; L^\infty(\Omega)))^4 | (e(0), s(0), c(0), p(0)) = (e_0, s_0, c_0, p_0), \\ &\text{and} \quad \|(e,s,c,p)\|_{(L^\infty([0,T];L^\infty(\Omega)))^4} \leqslant \|(e_0,s_0,c_0,p_0)\|_{L^\infty(\Omega)} + 1 := M \Big\}, \end{aligned}$$

where

$$\|(f_1,f_2,f_3,f_4)\|_{(L^\infty([0,T];L^\infty(\Omega)))^4} = \sup_{t\in[0,T]} \sum_{i=1}^4 \|f_i\|_{L^\infty(\Omega)}.$$

We define a map $\mathcal{F}$ and $\mathcal{G}$ on $\mathcal{X}$ by

$$\begin{aligned}\mathcal{F}(e,s,c,p)(x,t) := \Bigg(& e_0(x) + \int_0^t \left(-k_f e(x,\xi)s(x,\xi) + (k_r+k_c)c(x,\xi)\right) \mathrm{d}\xi, \\ & \times e^{d_s\Delta t} s_0(x) + \int_0^t e^{d_s\Delta(t-\xi)} \left(-k_f e(x,\xi)s(x,\xi) + k_r c(x,\xi)\right) \mathrm{d}\xi, \\ & \times c_0(x) + \int_0^t \left(k_f e(x,\xi)s(x,\xi) - (k_r+k_c)c(x,\xi)\right) \mathrm{d}\xi, \\ & \times \mathrm{e}^{d_p\Delta t} p_0(x) + \int_0^t \mathrm{e}^{d_p\Delta(t-\xi)} k_c c(x,\xi) \mathrm{d}\xi \Bigg),\end{aligned}$$

and

$$\mathcal{G}(e,s,c,p)(x,t) := \mathcal{F}(e_+,s_+,c_+,p_+)(x,t),$$

where $f_+ := \max(f,0)$.

We will now prove that for T small enough, $\mathcal{F}$ is a contraction mapping from $\mathcal{X}$ into $\mathcal{X}$. This will show the existence of a unique bounded strong solution, at least on $(0,T)$. Moreover, by showing that $\mathcal{G}$ is also a contraction mapping $\mathcal{X}$ into $\mathcal{X}$ that admits a fixed point such that e, s, c and p are non-negative, we would be able conclude that this fixed point is in fact a fixed point for $\mathcal{F}$, and as such the strong solution we have found is in fact non-negative.

Clearly, $\mathcal{F}(e,s,c,p)(0) = \mathcal{G}(e,s,c,p)(0) = (e_0,s_0,c_0,p_0)$. Moreover, since

$$\|\mathrm{e}^{d\Delta t} f\|_{L^\infty(\Omega)} \leqslant \|f\|_{L^\infty(\Omega)} \tag{A.3}$$

and

$$\|f_+\|_{L^\infty(\Omega)} \leqslant \|f\|_{L^\infty(\Omega)} \tag{A.4}$$

we see that

$$\|\mathcal{F}(e,s,c,p)\|_{(L^\infty([0,T];L^\infty(\Omega)))^4} \leqslant \|(e_0,s_0,c_0,p_0)\|_{L^\infty(\Omega)} + \mathcal{C}_0\left(M^2+1\right)T$$

and

$$\|\mathcal{G}(e,s,c,p)\|_{(L^\infty([0,T];L^\infty(\Omega)))^4} \leqslant \|(e_0,s_0,c_0,p_0)\|_{L^\infty(\Omega)} + \mathcal{C}_0\left(M^2+1\right)T$$

for some constant $\mathcal{C}_0$ that is independent of M and T. Choosing T small enough so that

$$\mathcal{C}_0(M^2+1)T \leqslant 1$$

we conclude that $\mathcal{F}$ and $\mathcal{G}$ map $\mathcal{X}$ into $\mathcal{X}$ itself.

Next, using (A.3) again, we find that

$$\begin{aligned}&\|\mathcal{F}(e_1,s_1,c_1,p_1) - \mathcal{F}(e_2,s_2,c_2,p_2)\|_{(L^\infty([0,T];L^\infty(\Omega)))^4} \\ &\quad \leqslant \int_0^T \|-k_f(e_1(\xi)s_1(\xi) - e_2(\xi)s_2(\xi)) \\ &\qquad + (k_r+k_c)(c_1(\xi) - c_2(\xi))\|_{L^\infty(\Omega)} \mathrm{d}\xi + \int_0^T \|-k_f(e_1(\xi)s_1(\xi) - e_2(\xi)s_2(\xi)) \\ &\qquad + k_r(c_1(\xi) - c_2(\xi))\|_{L^\infty(\Omega)} \mathrm{d}\xi\end{aligned}$$

$$+\int_0^T \|k_f\,(e_1 s_1\,(\xi) - e_2\,(\xi)\,s_2\,(\xi)) - (k_r + k_c)\,(c_1\,(\xi) - c_2\,(\xi))\|_{L^\infty(\Omega)}\,\mathrm{d}\xi$$
$$+\int_0^T \|k_c\,(c_1\,(\xi) - c_2\,(\xi))\|_{L^\infty(\Omega)}\,\mathrm{d}\xi$$
$$\leqslant \mathcal{C}_1(M+1)T\|(e_1, s_1, c_1, p_1) - (e_2, s_2, c_2, p_2)\|_{(L^\infty([0,T];L^\infty(\Omega)))^4}$$

and

$$\|\mathcal{G}(e_1, s_1, c_1, p_1) - \mathcal{G}(e_2, s_2, c_2, p_2)\|_{(L^\infty([0,T];L^\infty(\Omega)))^4}$$
$$= \|\mathcal{F}(e_{1+}, s_{1+}, c_{1+}, p_{1+}) - \mathcal{F}(e_{2+}, s_{2+}, c_{2+}, p_{2+})\|_{(L^\infty([0,T];L^\infty(\Omega)))^4}$$
$$\leqslant \mathcal{C}_1(M+1)T\|(e_1, s_1, c_1, p_1) - (e_2, s_2, c_2, p_2)\|_{(L^\infty([0,T];L^\infty(\Omega)))^4}$$

for a constant $\mathcal{C}_1$ that is independent of M and T, where we have used the elementary inequality

$$|a_+ - b_+| \leqslant |a - b|.$$

Restricting T further so that

$$\mathcal{C}_1(M+1)T < 1$$

we see that $\mathcal{F}$ and $\mathcal{G}$ are contraction maps from $\mathcal{X}$ into $\mathcal{X}$, and therefore they each have a unique fixed point. We denote by $(\overline{e}, \overline{s}, \overline{c}, \overline{p})$ the fixed point of $\mathcal{G}$. According to lemma A.1 it is a local strong solution to the system of equations[17]

$$\begin{cases} \partial_t\overline{e}(x,t) = -k_f\overline{e}_+(x,t)\overline{s}_+(x,t) + (k_r + k_c)\overline{c}_+(x,t), & x \in \Omega, t > 0,\\ \partial_t\overline{s}(x,t) - d_s\Delta\overline{s}(x,t) = -k_f\overline{e}_+(x,t)\overline{s}_+(x,t) + k_r\overline{c}_+(x,t), & x \in \Omega, t > 0,\\ \partial_t\overline{c}(x,t) = k_f\overline{e}_+(x,t)\overline{s}_+(x,t) - (k_r + k_c)\overline{c}_+(x,t), & x \in \Omega, t > 0,\\ \partial_t\overline{p}(x,t) - d_p\Delta\overline{p}(x,t) = k_c\overline{c}_+(x,t), & x \in \Omega, t > 0,\\ \partial_\nu\overline{s}(x,t) = \partial_\nu\overline{p}(x,t) = 0, & x \in \partial\Omega, t > 0,\\ \overline{e}(x,0) = e_0(x),\ \overline{s}(x,0) = s_0(x),\ \overline{c}(x,0) = c_0(x),\ \overline{p}(x,0) = p_0(x), & x \in \Omega, \end{cases} \tag{A.5}$$

on $(0, T)$, where we have used the fact that e_0, s_0, c_0 and p_0 are non-negative. Let $T_{\max}$ be the maximal time of existence for the solution $(\overline{e}, \overline{s}, \overline{c}, \overline{p})$. To show that $(\overline{e}, \overline{s}, \overline{c}, \overline{p})$ is a global solution, i.e. $T_{\max} = +\infty$, it is enough to show that

$$\|(\overline{e}, \overline{s}, \overline{c}, \overline{p})\|_{(L^\infty([0,T];L^\infty(\Omega)))^4} \leqslant C(T) \tag{A.6}$$

for some continuous function $C(T) : [0, \infty) \to [0, \infty)$ (see, for instance, [Zhe04, theorem 2.5.5]). The proof of the existence of such function is intertwined with the non-negativity property of $(\overline{e}, \overline{s}, \overline{c}, \overline{p})$, which will also show that $(\overline{e}, \overline{s}, \overline{c}, \overline{p})$ is in fact a solution to (1.2).

[17] Note that by the definition of $\mathcal{X}$ and $\mathcal{F}$, the function f from (A.1) is in $L^\infty([0, T]; L^\infty(\Omega))$, and as such the conditions of the lemma are satisfied.

Denoting by $f_- = \max(0, -f) = (-f)_+$ the so-called negative part of f, we notice that when f is absolutely continuous with respect to t so is f_-, and a.e. in t

$$\frac{\mathrm{d}}{\mathrm{d}t} f_-^2(t) = 2f_-(t)\frac{\mathrm{d}}{\mathrm{d}t} f_-(t) = -2f_-(t)\frac{\mathrm{d}}{\mathrm{d}t} f(t).$$

As such, if $f(x,t)$ is a strong solution to

$$\begin{cases} \partial_t f(x,t) - d\Delta f(x,t) = g(t,x) - \alpha(x,t) f_+(x,t), & x \in \Omega, t > 0, \\ \mathrm{d}\partial_\nu f(x,t) = 0, & x \in \partial\Omega, t > 0 \end{cases} \tag{A.7}$$

where $g(x,t)$ and $\alpha(x,t)$ are non-negative functions. By multiplying the above with $-f_-(x,t) \leqslant 0$ we find that

$$\frac{1}{2}\partial_t f_-^2(x,t) + d\Delta f(x,t) f_-(x,t) = -g(t,x) f_-(x,t) \leqslant 0.$$

Integrating over $\Omega \times (0,t)$ gives[18]

$$\frac{1}{2}\|f_-(t)\|_{L^2(\Omega)}^2 + d\int_0^t \|\nabla f_-(\xi)\|_{L^2(\Omega)}^2 \,\mathrm{d}\xi \leqslant \frac{1}{2}\|f_-(0)\|_{L^2(\Omega)}^2,$$

where we have used the fact that $\nabla f \cdot \nabla f_- = -|\nabla f_-|^2$. This implies that if $f(0)$ is non-negative, i.e. $f_-(x,0) \equiv 0$ then $f_-(x,t) \equiv 0$ for any $t > 0$ for which f is a strong solution to (A.7). As the equations for $\overline{e}$, $\overline{c}$, $\overline{s}$ and $\overline{p}$ are of the form (A.7), we conclude the non-negativity of $\overline{e}$, $\overline{c}$, $\overline{s}$ and $\overline{p}$, and as such the fact that it is in fact a solution to (1.2).

Lastly, we shall show that (A.6) is valid for a constant function $C(T)$ which will show both the global existence and uniform boundedness, concluding the proof.

Indeed, using the definition of strong solution (Duhamel's formula, as is expressed in the definition of $\mathcal{F}$) and the non-negativity of $\overline{e}$ and $\overline{c}$ we see that

$$\begin{aligned} \max\left(|\overline{e}(x,t)|, |\overline{c}(x,t)|\right) &= \max\left(\overline{e}(x,t), \overline{c}(x,t)\right) \\ &\leqslant \overline{e}(x,t) + \overline{c}(x,t) \leqslant \|e_0\|_{L^\infty(\Omega)} + \|c_0\|_{L^\infty(\Omega)}. \end{aligned}$$

Thus, for any T for which $\overline{e}$ and $\overline{c}$ are strong solutions to (1.2) we have that

$$\sup_{t\leqslant T} \max\left(\|\overline{e}(t)\|_{L^\infty(\Omega)}, \|\overline{c}(t)\|_{L^\infty(\Omega)}\right) \leqslant \|e_0\|_{L^\infty(\Omega)} + \|c_0\|_{L^\infty(\Omega)}. \tag{A.8}$$

It remains to show the boundedness of $\overline{s}$ and $\overline{p}$. Summing $\overline{s}(t)$, $\overline{c}(t)$, $\overline{p}(t)$, and integrating over gives

$$\|\overline{s}(t)\|_{L^1(\Omega)} + \|\overline{c}(t)\|_{L^1(\Omega)} + \|\overline{p}(t)\|_{L^1(\Omega)} = \|s_0\|_{L^1(\Omega)} + \|c_0\|_{L^1(\Omega)} + \|p_0\|_{L^1(\Omega)} \quad \forall\, t \geqslant 0, \tag{A.9}$$

[18] According to the definition of strong solutions we find that v is absolutely continuous with respect to $L^2(\Omega)$). As the $L^2(\Omega)$ scalar product is bilinear and continuous, we can apply the product rule to find that

$$\frac{\mathrm{d}}{\mathrm{d}t}\|v(t)\|_{L^2(\Omega)}^2 = \frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega v(x,t)v(x,t)\mathrm{d}x = 2\int_\Omega \partial_t v(x,t)v(x,t)\mathrm{d}x$$

for almost all $t > 0$.

where we have used the non-negativity of the solution again. For any $q \geqslant 2$ we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\|\overline{s}(t)\|^q_{L^q(\Omega)} &= q\int_\Omega \overline{s}^{q-1}(x,t)\partial_t\overline{s}(x,t)\mathrm{d}x\\ &\leqslant -q(q-1)d_s\int_\Omega \overline{s}(x,t)^{q-2}|\nabla\overline{s}(x,t)|^2\mathrm{d}x + k_r q\int_\Omega \overline{s}(x,t)^{q-1}\overline{c}(x,t)\mathrm{d}x\\ &\leqslant -q(q-1)d_s\int_\Omega \overline{s}(x,t)^{q-2}|\nabla\overline{s}(x,t)|^2\mathrm{d}x + k_r q\|\overline{s}(t)\|^{q-1}_{L^q(\Omega)}\|\overline{c}(t)\|_{L^q(\Omega)}\\ &\leqslant -\frac{4(q-1)d_s}{q}\int_\Omega\left|\nabla\left(\overline{s}(x,t)^{\frac{q}{2}}\right)\right|^2\mathrm{d}x + k_r\left((q-1)\|\overline{s}(t)\|^q_{L^q(\Omega)} + \|\overline{c}(t)\|^q_{L^q(\Omega)}\right),\end{aligned}$$

where all the above differentiating and integrations are well defined and allowed due to the fact that $\overline{s}$ is a strong solution to our equation. Using the uniform bound of $\overline{c}$ from (A.8) we find that

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\overline{s}(t)\|^q_{L^q(\Omega)} + \frac{4(q-1)d_s}{q}\left\|\overline{s}(t)^{\frac{q}{2}}\right\|^2_{H^1(\Omega)} \leqslant qC_{c_0,e_0}\left(\|\overline{s}\|^q_{L^q(\Omega)} + 1\right). \tag{A.10}$$

Thanks to the continuous Sobolev embedding $H^1(\Omega) \hookrightarrow L^{n^*}(\Omega)$ with

$$n^* = \begin{cases} +\infty & \text{if } n = 1,\\ < +\infty \text{ arbitrary} & \text{if } n = 2,\\ \dfrac{2n}{n-2} & \text{if } n \geqslant 3.\end{cases}$$

we find that

$$\left\|\overline{s}^{\frac{q}{2}}\right\|^2_{H^1(\Omega)} \geqslant C_n\left\|\overline{s}^{\frac{q}{2}}\right\|^2_{L^{n^*}(\Omega)} = C_n\|\overline{s}\|^q_{L^{q_0}(\Omega)}, \tag{A.11}$$

where $q_0 = \frac{n^* q}{2} > q$. Using the interpolation inequality

$$\|f\|^q_{L^q(\Omega)} \leqslant \|f\|^{\theta q}_{L^{q_0}(\Omega)}\|f\|^{(1-\theta)q}_{L^1(\Omega)}$$

where $\theta \in (0,1)$ satisfies $\frac{1}{q} = \frac{\theta}{q_0} + \frac{1-\theta}{1}$, together with (A.9) and (A.11) we see that we can find $M_n > 0$ such that

$$\left\|\overline{s}^{\frac{q}{2}}\right\|^2_{H^1(\Omega)} \geqslant M_n\|\overline{s}\|^{\frac{q}{\theta}}_{L^q(\Omega)},$$

and consequently (A.10) implies that

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\overline{s}(t)\|^q_{L^q(\Omega)} + C_1\|\overline{s}(t)\|^{\frac{q}{\theta}}_{L^q(\Omega)} \leqslant C_2\left(\|\overline{s}(t)\|^q_{L^q(\Omega)} + 1\right),$$

for appropriate (dimension and initial datum dependent) constants $C_1, C_2 > 0$. Since $\theta \in (0, 1)$ the above implies that when

$$\|\overline{s}(t)\|^q_{L^q(\Omega)} \geqslant \max\left(1, \left(\frac{3C_2}{C_1}\right)^{\frac{\theta}{1-\theta}}\right)$$

we have that

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\overline{s}(t)\|^q_{L^q(\Omega)} \leqslant 2C_2\|\overline{s}(t)\|^q_{L^q(\Omega)} - C_1\|\overline{s}(t)\|^{\frac{q}{\theta}}_{L^q(\Omega)}$$

$$= \|\overline{s}(t)\|^q_{L^q(\Omega)}\left(2C_2 - C_1\|\overline{s}(t)\|^{\frac{(1-\theta)q}{\theta}}_{L^q(\Omega)}\right) \leqslant -C_2\|\overline{s}(t)\|^q_{L^q(\Omega)} \leqslant -C_2.$$

This is enough for us to conclude that

$$\sup_{t\geqslant 0}\|\overline{s}(t)\|_{L^q(\Omega)} < +\infty \tag{A.12}$$

for any $2 \leqslant q < +\infty$. Applying a simple variant of lemma 3.4 with $\delta = 0$, where the L^∞ bound is on $\left[0, \frac{T}{2}\right]$ instead of [0, 1], shows that[19]

$$\sup_{t\geqslant 0}\|\overline{s}(t)\|_{L^\infty(\Omega)} < +\infty.$$

The uniform bound of $\overline{p}$ follows in the exact same way. □

We conclude the appendix with the proofs of lemmas 3.4 and 3.5.

Proof of lemma 3.4. A known estimate on the kernel of the heat equation (see for instance [Dav90, theorem 3.2.9, page 90]) implies that the solution to the heat equation with homogeneous Neumann boundary condition and initial datum in $L^p(\Omega)$ satisfies

$$\|u(t)\|_{L^\infty(\Omega)} = \left\|\mathrm{e}^{d\Delta t}u_0\right\|_{L^\infty(\Omega)} \leqslant C_d t^{-\frac{n}{2p}}\|u_0\|_{L^p(\Omega)} \quad \forall\, 0 < t \leqslant 1, \tag{A.13}$$

for some fixed known constant that depends on Ω and the diffusion coefficient d.[20] As such, a solution to the equation

$$\begin{cases} \partial_t u(x,t) - d\Delta u(x,t) = f(x,t) & x \in \Omega,\ t > 0 \\ u(x,0) = 0 & x \in \Omega \\ \partial_\nu u(x,t) = 0, & x \in \partial\Omega, t > 0, \end{cases}$$

would satisfy, according to the Duhamel formula,

$$u(x,t+1) = \mathrm{e}^{d\Delta}u(x,t) + \int_0^1 \mathrm{e}^{d\Delta(1-s)}f(x,t+s)\mathrm{d}s, \quad t > 0$$

[19] The appropriate f in this case is $f = -k_f es + k_r c$ whose L^p bound follows from the uniform L^∞ bound on e and c and (A.12).

[20] One can easily extent (A.13) to $0 < t < T$ for any given $T > 0$. The constant C_d in that case will become dependent on T (and one should denote it by $C_{d,T}$).

which, together with (A.13), implies that

$$\|u(t+1)\|_{L^\infty(\Omega)} \leqslant C_d \left(\|u(t)\|_{L^p(\Omega)} + \int_0^1 \left(1 + (1-s)^{-\frac{n}{2p}}\right) \|f(t+s)\|_{L^p(\Omega)}\, \mathrm{d}s \right).$$

Using conditions (3.1) we find that

$$\|u(t+1)\|_{L^\infty(\Omega)} \leqslant \mathcal{C} C_d \left(1 + \int_0^1 \left(1 + (1-s)^{-\frac{n}{2p}}\right) \mathrm{e}^{-\delta s}\, \mathrm{d}s \right) \mathrm{e}^{-\delta t}.$$

If $p > \frac{n}{2}$ then

$$\int_0^1 (1-s)^{-\frac{n}{2p}} \mathrm{e}^{-\delta s}\, \mathrm{d}s \leqslant \int_0^1 (1-s)^{-\frac{n}{2p}} \mathrm{d}s = C_{n,p} < \infty,$$

and we conclude that for all $t \geqslant 1$

$$\|u(t)\|_{L^\infty(\Omega)} \leqslant \mathcal{C} C_d \left(2 + C_{n,p}\right) \mathrm{e}^{-\delta(t-1)}.$$

As for any $t \in [0, 1]$ we have that

$$\sup_{t\in[0,1]} \|u(t)\|_{L^\infty(\Omega)} \leqslant \mathcal{S} \leqslant \mathcal{S}\, \mathrm{e}^{\delta}\, \mathrm{e}^{-\delta t}$$

due to (3.1), we find that

$$\|u(t)\|_{L^\infty(\Omega)} \leqslant \mathrm{e}^{\delta} \max\left(\mathcal{S}, \mathcal{C} C_d \left(2 + C_{n,p}\right)\right) \mathrm{e}^{-\delta t},$$

which is the desired result. □

Proof of lemma 3.5. Defining the function $v(x,t) = u(x,t) - \overline{u}(t)$ we find that v solves the equation

$$\begin{cases} \partial_t v(x,t) - d\Delta v(x,t) = f(x,t) - \partial_t \overline{u}(t) & x \in \Omega, t > 0 \\ u(x,0) = u_0(x) - \overline{u_0} & x \in \Omega \\ \partial_\nu u(x,t) = 0, & x \in \partial\Omega.t > 0. \end{cases}$$

Denoting by $\widetilde{f}(x,t) = f(x,t) - \partial_t \overline{u}(t)$ and multiplying the first line of the equation by $v(x,t)$ and integrating over the domain yields the equality

$$\partial_t \|v(t)\|^2_{L^2(\Omega)} = -2d\|\nabla v(x,t)\|^2_{L^2(\Omega)} + 2\int_\Omega \widetilde{f}(x,t) v(x,t) \mathrm{d}x.$$

Thus, using the Poincaré inequality (3.4) and the fact that $\overline{v}(t) = 0$ we find that

$$\partial_t \|v(t)\|^2_{L^2(\Omega)} \leqslant -\frac{2d}{C_\mathrm{P}} \|v(t)\|^2_{L^2(\Omega)} + 2\left\|\widetilde{f}(t)\right\|_{L^2(\Omega)} \|v(t)\|_{L^2(\Omega)}$$

$$\leqslant -\frac{2d}{C_\mathrm{P}} (1-\varepsilon) \|v(t)\|^2_{L^2(\Omega)} + \frac{C_\mathrm{P} \left\|\widetilde{f}(t)\right\|^2_{L^2(\Omega)}}{2\, \mathrm{d}\varepsilon},$$

where we have used the fact that for any $\delta > 0$ and $a, b \geqslant 0$

$$2ab \leqslant \delta a^2 + \frac{b^2}{\delta}$$

and chose $\delta = \frac{2\,d_\varepsilon}{C_P}$. The result follows from a simple integration and the fact that by integrating our heat equation over Ω we find that

$$\partial_t \overline{u}(t) = \int_\Omega f(x,t)\mathrm{d}x = \overline{f}(t).$$

□

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