A FINITE ELEMENT METHOD FOR VOLUME-SURFACE REACTION-DIFFUSION SYSTEMS

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ABSTRACT. We consider the numerical simulation of coupled volume-surface reaction-diffusion systems having a detailed balance equilibrium. Based on the conservation of mass, an appropriate quadratic entropy functional is identified and an entropy-entropy dissipation inequality is proven. This allows us to show exponential convergence of solutions to equilibrium by the entropy method. We then investigate the discretisation of the system by finite element methods, including the domain approximation by polyhedral meshes, and an implicit time stepping scheme. Mass conservation and exponential convergence to equilibrium are established also on the discrete level by using arguments very similar to those on the continuous level. This allows us to establish convergence estimates for the discretisation error uniformly in time. Numerical tests are presented to illustrate the theoretical results. The analysis and numerical approximation are presented in detail for a simple model problem. Our arguments, however, can be applied also in a more general context. This is demonstrated by investigation of a biological volume-surface reaction-diffusion system modeling asymmetric stem cell division.

1. INTRODUCTION

Various physical phenomena in biology, material science, or chemical engineering are driven by reaction-diffusion processes in different compartments and by transfer between them. This may involve mass transfer between domains and interfaces or the boundary. In cell-biology, for instance, many phenomena are based on reaction-diffusion processes of proteins within the cell-body and on the cell cortex, see e.g. [19, 22]. Particular examples are systems modeling cell-biological signalling processes, see e.g. [21], or models for asymmetric stem cell division, which describe the localisation of so-called cell-fate determinants during mitosis, see e.g. [23, 25, 24].

As a simple model for a coupled volume-surface reaction-diffusion process, we consider the system

$$L_t - d_L \Delta L = 0, \qquad \text{on } \Omega, \tag{1a}$$

$$\ell_t - d_\ell \Delta_\Gamma \ell = \lambda L - \gamma \ell, \qquad \text{on } \Gamma. \tag{1b}$$

$$d_L \partial_\nu L = -\lambda L + \gamma \ell, \qquad \text{on } \Gamma, \tag{1c}$$

Here $\Gamma = \partial \Omega$ is the surface, Δ_Γ denotes the Laplace-Beltrami operator, and the parameters $d_L, d_\ell, \lambda, \gamma$ are positive constants. The equations are assumed to hold for all $t > 0$ and are complemented by appropriate initial conditions. The system (1a)–(1c) describe the diffusion of a substance with concentration L in the volume and concentration ℓ on the surrounding surface Γ, coupled by mass transfer between the two compartments. This problem may serve

as a starting point for considering more realistic adsorption/desorption processes but also as a reduced model for volume-surface reaction-diffusion processes arising in cell biology.

Despite its simplicity, the model problem (1a)–(1c) already features some interesting properties, which will be of main interest for our further considerations:

(i) The system preserves non-negativity of solutions and describes a conservation law, namely, the conservation of the total mass $M = \int_\Omega L dx + \int_\Gamma \ell ds$.

(ii) There exists a unique constant positive detailed balance equilibrium, which can be explicitly parametrised by the total conserved mass and the parameters λ and γ.

iii) The solutions are uniformly bounded and converge exponentially fast towards the equilibrium state with respect to any Lebesgue/Sobolev norm.

The first goal of our paper will be to establish these properties, in particular (iii), for the model problem (1a)–(1c). The second aim is to investigate the discretisation of the system by finite element methods. Our guideline is to preserve the key features of the model utilised for the analysis on the continuous level also on the discrete level. In particular, we establish the conservation of mass, the possibility for preserving non-negativity, the existence of a unique equilibrium, and the exponential convergence to equilibrium on the discrete level. The discretisation process involves domain approximations by polyhedral meshes, finite element approximation, and time stepping. The numerical analysis is based on arguments for the discretisation of evolution problems [16], on general ideas for the analysis of domain approximations [7, 10], and recent results results from [13], who considered a somewhat simpler elliptic volume-surface reaction-diffusion problem. A careful use of the entropy estimates and the convergence to equilibrium will allow us to establish order optimal convergence rates that are uniform in time.

The model problem (1a)–(1c) is simple enough to avoid complicated notation and therefore allows us to present our basic ideas in the most convenient way to the reader. To illustrate the application to more general problems, we consider also the following system in Section 7:

$$L_t - d_L \Delta L = -\beta L + \alpha P, \quad \text{on } \Omega, \tag{2a}$$

$$P_t - d_P \Delta P = \beta L - \alpha P, \quad \text{on } \Omega, \tag{2b}$$

$$\ell_t - d_\ell \Delta_\Gamma \ell = -d_L \partial_n L + \chi_{\Gamma_2}(-\sigma \ell + \kappa p), \quad \text{on } \Gamma, \tag{2c}$$

$$p_t - d_p \Delta_{\Gamma_2} = \sigma \ell - \kappa p - d_P \partial_n P, \quad \text{on } \Gamma_2. \tag{2d}$$

As before, $\Gamma = \partial \Omega$ denotes the boundary and $\Gamma_2 = \subset \Gamma$ is a proper part of it. The mass transfer between the domain and the surface is described by

$$d_L \partial_n L = -\lambda L + \gamma \ell, \quad \text{on } \Gamma, \tag{2e}$$

$$d_P \partial_n P = \chi_{\Gamma_2}(-\eta P + \xi p), \quad \text{on } \Gamma, \tag{2f}$$

$$d_p \partial_{n_{\Gamma_2}} p = 0, \quad \text{on } \partial \Gamma_2. \tag{2g}$$

The diffusion and reaction parameters are positive constants, and the equations are assumed to hold for $t > 0$ and to be complemented by appropriate initial conditions. This coupled volume-surface reaction-diffusion system models four conformations of the key protein Lgl during the mitosis of Drosophila SOP precursor stem-cells, see e.g. [23, 25, 8]. In particular, L and ℓ denote the concentrations of native Lgl within the cell cytoplasm and on the cell cortex, respectively, while P and p denote the corresponding phosphorylated Lgl conformations.

Let us point out that like the model problem (1a)–(1c), also the system (2a)–(2c) involves fully reversible reaction and mass transfer processes; see Figure 1 for a schematic sketch. This allows

$$L \qquad\qquad L \xleftrightharpoons[\alpha]{\beta} P$$

$$\lambda \mathbin{\Updownarrow} \gamma \qquad\qquad \lambda \mathbin{\Updownarrow} \gamma \qquad \eta \mathbin{\Updownarrow} \xi$$

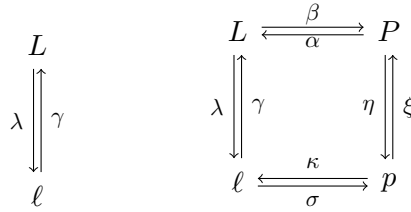$$\ell \qquad\qquad \ell \xleftrightharpoons[\sigma]{\kappa} p$$

FIGURE 1. The mass transfer dynamics for model (1) (left) and model (2) (right).

us to show that the key properties (i)–(iii) also hold for the system (2a)–(2c), i.e. solutions remain non-negative and the total mass is conserved, there exists a unique positive detailed balance equilibrium, and the solutions converge exponentially fast to the equilibrium state. These assertions can be verified by application of the arguments used for the model problem (1a)–(1c) to the more general system (2a)–(2g). As a consequence, also the discretization method can be extended straight forward yielding approximations of optimal order and uniform in time.

The remainder of the manuscript is organised as follows: Section 2 is devoted to the analysis of problem (1a)–(1c) on the continuous level. We establish global existence and non-negativity of solutions and show conservation of mass. The latter allows us to identify a unique constant equilibrium state and to define a quadratic entropy functional which serves as a Lyapunov functional. We establish entropy-dissipation and prove the essential entropy-entropy dissipation estimate, from which we directly obtain exponential convergence to equilibrium and uniform bounds for the solution and its derivatives. The relevant notations for the finite element discretization are introduced in Section 3, where we also recall some important results about domain approximations. In Section 4, we formulate the semi-discretization of the model problem by a finite element method. We establish existence and uniqueness of a discrete solution and establish the mass conservation. We then identify the discrete equilibrium and provide a simple error estimate. Based on the discrete equilibrium, we can formulate a discrete entropy functional and we establish entropy dissipation and the entropy-entropy dissipation inequality on the discrete level. As a consequence we obtain global in time existence and uniform bounds for the semi-discrete solution and exponential convergence to the discrete equilibrium. We then present a complete convergence analysis and establish order optimal convergence orders of the discretization error uniform in time. Section 5 is concerned with the time discretisation by the implicit Euler method. All important properties derived for the semi-discretisation can be preserved also on the fully discrete level and order optimal convergence is obtain with respect to both, the mesh size and the time step and, in particular, uniform in time. The validity of the theoretical results is illustrated by some numerical tests in Section 6. We then demonstrate the applicability of our arguments to more general volume-surface reaction-diffusion problems in Section 7, where we discuss in more detail the system (2a)–(2g) and show how our analysis and numerical methods can be extended naturally. The presentation closes with a short summary of our results and a discussion of open problems.

2. Analysis of the model problem

We start by introducing the relevant notation and basic assumptions, and recall the statement of our model problem. Next, we establish some basic properties, show existence and uniqueness of solutions, identify the unique equilibrium state and prove exponential convergence to equilibrium and uniform bounds.

2.1. **Preliminaries.** Let $\Omega \subset \mathbb{R}^n$ be a bounded domain with smooth boundary $\Gamma \in C^3$. We consider the coupled volume-surface reaction-diffusion system

$$L_t - d_L \Delta L = 0, \qquad x \in \Omega, \ t > 0, \tag{3a}$$

$$\ell_t - d_\ell \Delta_\Gamma \ell = \lambda L - \gamma \ell, \qquad x \in \Gamma, \ t > 0, \tag{3b}$$

subject to the boundary and initial conditions

$$d_L \partial_n L = \gamma \ell - \lambda L, \qquad x \in \Gamma, \ t > 0, \tag{3c}$$

$$L(0) = L_0, \quad x \in \Omega, \qquad \ell(0) = \ell_0, \quad x \in \Gamma. \tag{3d}$$

The diffusion coefficients d_L, d_ℓ and the reaction constants λ, γ are assumed to be positive. We use standard notation for function spaces [12] and, for brevity, we denote by $(\cdot, \cdot)_\Omega$ and $(\cdot, \cdot)_\Gamma$ the inner products and by $\|\cdot\|_\Omega$ and $\|\cdot\|_\Gamma$ the induced norms of $L^2(\Omega)$ and $L^2(\Gamma)$, respectively.

2.2. **Existence, uniqueness, and regularity.** In this section we will discuss the existence and uniqueness of weak solutions and their qualitative properties, which we shall need later on.

Definition 1 (Weak form). *Let $T \in (0, \infty]$ be a given constant, the time horizon, and define*

$$a(L, \ell; v, w) := d_L (\nabla L, \nabla v)_\Omega + d_\ell (\nabla_\Gamma \ell, \nabla_\Gamma w)_\Gamma + (\lambda L - \gamma \ell, v - w)_\Gamma, \tag{4}$$

as well as $c(L, \ell; v, w) = (L, v)_\Omega + (\ell, w)_\Gamma$. A pair of functions

$$(L, \ell) \in C([0, T]; L^2(\Omega) \times L^2(\Gamma)) \cap L^2(0, T; H^1(\Omega) \times H^1(\Gamma))$$

is called weak solution *of* (3a)–(3d)*, if $L(0) = L_0$, $\ell(0) = \ell_0$, and the identity*

$$\tfrac{d}{dt} c(L(t), \ell(t); v, w) + a(L(t), \ell(t); v, w) = 0, \tag{5}$$

holds for all $v \in H^1(\Omega)$ and $w \in H^1(\Gamma)$, and for a.e. $t > 0$.

The weak form is derived in the usual way by multiplying with appropriate test functions, integration-by-parts, and utilization of the boundary condition. Problem (5) fits within the framework of parabolic evolution equations as discussed, for instance, in [12, 17], and can be analysed with standard arguments. The main ingredient is the following

Lemma 2 (Gårding inequality). *There exists a constant $\eta > 0$ depending only on the parameters d_J, d_ℓ, γ, λ, and on the domain Ω, such that*

$$a(v, w; v, w) \geq \|v\|_{H^1(\Omega)}^2 + \|w\|_{H^1(\Gamma)}^2 - \eta(\|v\|_\Omega^2 + \|w\|_\Gamma^2)$$

for all functions $v \in H^1(\Omega)$ and $w \in H^1(\Gamma)$.

Proof. The result follows from the definition of a and the Cauchy-Schwarz inequality. □

Let us emphasize that the bilinear form a is not elliptic, which can easily be seen by choosing v and w as appropriate constants.

Theorem 3 (Existence of weak solutions). *For any initial data $L_0 \in L^2(\Omega)$ and $\ell_0 \in L^2(\Gamma)$, the problem* (3a)-(3d) *has a unique weak solution* (L, ℓ), *and*

$$\sup_{t \in (0,T)} (\|L(t)\|_{\Omega} + \|\ell(t)\|_{\Gamma}) + \int_0^T (\|L(t)\|_{H^1(\Omega)}^2 + \|\ell(t)\|_{H^1(\Gamma)}^2) \, dt \le C(T)(\|L_0\|_{\Omega} + \|\ell_0\|_{\Gamma}).$$

If the initial data are non-negative, then the solution remains non-negative for all time.

Proof. Existence and uniqueness of a global weak solution follow by standard results, see e.g., [17, Chapter XVIII], and positivity can be established by an iteration argument, see e.g. [8]. $\square$

From the abstract results, we obtain a constant $C(T)$ in the a-priori bound which increases with T. We will later show by entropy arguments, that the bounds are actually uniform in T. A basic ingredient for our analysis will be the fact, that the total mass is conserved during the evolution of our system.

Lemma 4 (Mass conservation). *Let* (L, ℓ) *denote a weak solution of* (3a)–(3d), *and denote by*

$$M(t) = (L(t), 1)_{\Omega} + (\ell(t), 1)_{\Gamma}$$

the total mass at time t. Then,

$$M(t) = M(0) =: M_0 \quad \text{for all} \quad t > 0.$$

Proof. Testing the weak form (5) with $v \equiv 1$ and $w \equiv 1$, we get

$$\frac{d}{dt} M(t) = \frac{d}{dt}(L(t), 1)_{\Omega} + \frac{d}{dt}(\ell(t), 1)_{\Gamma} = \frac{d}{dt} c(L(t), \ell(t); 1, 1) = -a(L(t), \ell(t); 1, 1) = 0,$$

and the result follows by integration with respect to time. $\square$

2.3. **Equilibrium system.** A reaction-diffusion system like (3a)–(3c) can be assumed to tend to a unique positive equilibrium on the long run. For the problem under consideration, the equilibrium concentrations L_{∞}, ℓ_{∞} have to satisfy

$$-d_L \Delta L_{\infty} = 0, \qquad\qquad\qquad \text{in } \Omega, \qquad\qquad (6a)$$
$$d_L \partial_n L_{\infty} = \gamma \ell_{\infty} - \lambda L_{\infty}, \qquad\qquad \text{on } \Gamma, \qquad\qquad (6b)$$
$$-d_\ell \Delta_\Gamma \ell_{\infty} = \lambda L_{\infty} - \gamma \ell_{\infty}, \qquad\qquad \text{on } \Gamma. \qquad\qquad (6c)$$

Because of the mass conservation law, one additionally knows that

$$(L_{\infty}, 1)_{\Omega} + (\ell_{\infty}, 1)_{\Gamma} = M_0, \qquad\qquad\qquad\qquad (6d)$$

where $M_0 = \int_{\Omega} L_0 + \int_{\Gamma} \ell_0$ is the total initial mass of the system. As we will see in a moment, this extra condition is also required to ensure the uniqueness of the equilibrium state.

Definition 5. *A pair of functions $L_{\infty} \in H^1(\Omega)$ and $\ell_{\infty} \in H^1(\Gamma)$ is called weak solution of the equilibrium system* (6a)–(6d), *if*

$$a(L_{\infty}, \ell_{\infty}; v, w) = 0, \qquad\qquad\qquad\qquad\qquad (7)$$

for all $v \in H^1(\Omega)$ and $w \in H^1(\Gamma)$, and the mass constraint (6d) *holds.*

For showing well-posedness of the equilibrium problem, we will utilize the following Poincaré-type inequality, which will also play a crucial role in our subsequent analysis.

Lemma 6 (Poincaré-type inequality)**.** *There exists a constant $C_P > 0$ depending only on the parameters d_L, d_ℓ, λ, γ, and on the domain Ω, such that*

$$\lambda\|L\|^2_{H^1(\Omega)} + \gamma\|\ell\|^2_{H^1(\Gamma)} \leq C_P\left(\lambda d_L\|\nabla L\|^2_\Omega + \gamma d_\ell\|\nabla_\Gamma\ell\|^2_\Gamma + \|\lambda L - \gamma\ell\|^2_\Gamma\right) \tag{8}$$

for all $L \in H^1(\Omega)$ and $\ell \in H^1(\Gamma)$ satisfying the mass constraint $(L,1)_\Omega + (\ell,1)_\Gamma = 0$.

Proof. The right hand side is zero if and only if L and ℓ are constants, and $L = \gamma/\lambda\ell$. Since $\gamma, \lambda > 0$, the mass constraint then yields $L = \ell = 0$. Therefore, the term in parenthesis on the right hand side of (8) defines a norm on $H^1(\Omega) \times H^1(\Gamma)$. The assertion then is a direct consequence of the *lemma of equivalent norms*; see e.g. [18, Ch. 11].   □

The choice of the norm on the right hand side of the Poincaré's inequality becomes clear from

Lemma 7 (Inf-sup stability)**.** *For any $v \in H^1(\Omega)$ and $w \in H^1(\Gamma)$ with $(v,1)_\Omega + (w,1)_\Gamma = 0$*

$$a(v,w;\lambda v,\gamma w) = \lambda d_L\|\nabla v\|^2_\Omega + \gamma d_\ell\|\nabla_\Gamma w\|_\Gamma + \|\lambda v - \gamma w\|^2_\Gamma, \tag{9}$$

Together with the Poincaré-type inequality, this stability condition already suffices to show the well-posedness of the weak form of the equilibrium problem. Since the right hand side in the weak formulation (7) is zero, the solution can however even be obtained explicitly here.

Lemma 8 (Equilibrium)**.** *The system (6a)–(6d) has a unique weak solution (L_∞, ℓ_∞) given by*

$$L_\infty = \frac{\gamma M_0}{\gamma|\Omega| + \lambda|\Gamma|} \qquad and \qquad \ell_\infty = \frac{\lambda}{\gamma}L_\infty. \tag{10}$$

Proof. One easily verifies that (L_∞, ℓ_∞) given by the formulas above is a solution satisfying the mass constraint. Now assume that L_*, ℓ_* is any other weak solution to (6a)–(6d). Then, the difference $(L_\infty - L_*, \ell_\infty - \ell_*)$ has zero mass, and

$$a(L_\infty - L_*, \ell_\infty - \ell_*; v, w) = 0 \tag{11}$$

for all $v \in H^1(\Omega)$ and $w \in H^1(\Gamma)$. By choosing $v = \lambda(L_\infty - L_*)$ and $w = \gamma(\ell_\infty - \ell_*)$, we get

$$\lambda d_L\|\nabla(L_\infty - L_*)\|^2_\Omega + \gamma d_\ell\|\nabla_\Gamma(\ell_\infty - \ell_*)\|^2_\Gamma + \|\lambda(L_\infty - L_*) - \gamma(\ell_\infty - \ell_*)\|^2_\Gamma = 0, \tag{12}$$

and Lemma 6 immediately implies that $L_\infty = L_*$ and $\ell_\infty = \ell_*$.   □

2.4. **Convergence to equilibrium.** We will now show that the solution $(L(t), \ell(t))$ converges to the equilibrium (L_∞, ℓ_∞) by using the entropy method. For a given constant equilibrium state (L_∞, ℓ_∞), we define the quadratic relative entropy functional

$$E(L,\ell) = \frac{1}{2}\left(\lambda\|L - L_\infty\|^2_\Omega + \gamma\|\ell - \ell_\infty\|^2_\Gamma\right), \tag{13}$$

which is just a scaled L^2-distance to the equilibrium on the product space $L^2(\Omega) \times L^2(\Gamma)$.

Lemma 9 (Entropy dissipation)**.** *Let (L,ℓ) denote a weak solution of (3a)–(3d) with corresponding constant equilibrium (L_∞, ℓ_∞). Then*

$$\frac{d}{dt}E(L(t),\ell(t)) = -d_L\lambda\|\nabla(L(t) - L_\infty)\|^2_\Omega - d_\ell\gamma\|\nabla_\Gamma(\ell(t) - \ell_\infty)\|^2_\Gamma \tag{14}$$
$$- \|\lambda(L(t) - L_\infty) - \gamma(\ell(t) - \ell_\infty)\|^2_\Gamma =: -D(L(t),\ell(t))$$

for all $t > 0$. The functional D is called the entropy dissipation.

Proof. By definition of E and elementary manipulations, we obtain

$$
\begin{aligned}
\tfrac{d}{dt}E(L(t),\ell(t)) &= \lambda(L_t(t),L(t)-L_\infty)_\Omega + \gamma(\ell_t(t),\ell(t)-\ell_\infty)_\Gamma \\
&= -a(L(t)-L_\infty,\ell(t)-\ell_\infty;\lambda(L(t)-L_\infty),\gamma(\ell(t)-\ell_\infty)) \\
&= -d_L\lambda\|\nabla(L-L_\infty)\|_\Omega^2 - d_\ell\gamma\|\nabla_\Gamma(\ell-\ell_\infty)\|_\Gamma^2 - \|\lambda(L-L_\infty)-\gamma(\ell-\ell_\infty)\|_\Gamma^2,
\end{aligned}
$$

which already yields the result. $\qquad\square$

From the Poincaré-type inequality established in Lemma 6, we directly deduce

Lemma 10 (Entropy-entropy dissipation inequality). *For functions $L \in H^1(\Omega)$ and $\ell \in H^1(\Gamma)$ satisfying $(L,1)_\Omega + (\ell,1)_\Gamma = M_0$, there holds*

$$
D(L,\ell) \geq c_0 E(L,\ell) \qquad with \quad c_0 = 2/C_P. \tag{15}
$$

A combination of the previous results now yields

Theorem 11 (Exponential convergence to equilibrium). *Let (L,ℓ) denote the weak solution of the system* (3a)–(3c) *and (L_∞,ℓ_∞) be the corresponding equilibrium. Then,*

$$
\|L(t)-L_\infty\|_\Omega^2 + \|\ell(t)-\ell_\infty\|_\Gamma^2 \leq Ce^{-c_0 t}\left(\|L_0-L_\infty\|_\Omega^2 + \|\ell_0-\ell_\infty\|_\Gamma^2\right)
$$

for all $t>0$ with constants $c_0, C>0$ depending only d_L, d_ℓ, λ, γ, and on the domain Ω.

Proof. As a direct consequence of Lemma 9 and 10, we get

$$
\tfrac{d}{dt}E(L(t),\ell(t)) \leq -c_0 E(L(t),\ell(t)) \quad \text{for all} \quad t>0.
$$

Therefore, the classic Gronwall inequality gives

$$
E(L(t),\ell(t)) \leq e^{-c_0 t}E(L_0,\ell_0).
$$

The desired result then follows from the fact that λ, γ are positive constants and therefore $E(L,\ell)$ is equivalent to the square of the L^2-norm distance to equilibrium. $\qquad\square$

The dependence of the constant c_0 on the parameters λ, γ, d_L, and d_ℓ and on certain geometric constants for the domain can be made more explicit; see [11, 26] for details also on non-linear problems. For linear problems, c_0 could alternatively be determined by computing a view eigenvalues of a generalized eigenvalue problem.

Remark 12. As a direct consequence of Theorem 11 we obtain uniform bounds for the solution in $L^\infty(0,\infty;L^2(\Omega)\times L^2(\Gamma))$. Since the problem (3a)–(3c) is linear and all coefficients are independent of time, one can obtain in the usual way also uniform bounds for (L,ℓ) and time derivatives $(\partial_t^j L, \partial_t \ell)$ in $L^p(0,\infty;H^k(\Omega)\times H^k(\Gamma))$, provided that the usual compatibility conditions hold; for details, see e.g., [12]. Since the growth of these regularity estimates is polynomial in time, an interpolation argument with the exponential convergence to equilibrium yields that all Sobolev norms decay in fact exponentially in time, see e.g. [11].

3. Basic notation and domain approximations

In this section, we introduce some basic notation needed for the formulation of the finite element approximation of our problem. In addition, we recall some basic results about domain approximation by polyhedral meshes from [10, 13]. For ease of presentation, we restrict our presentation to a two dimensional setting. All arguments however easily generalise to dimension three.

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with smooth boundary $\Gamma \in C^3$. We approximate Ω by a polygonal domain Ω_h for which a conforming triangulation $T^h = \{T\}$ is available. As usual, we denote by ρ_T and h_T the incircle radius and the diameter of the triangle T, respectively, and we call $h = \max_T h_T$ the meshsize. We further denote by $E^h = \{e\}$ the partition of Γ into edges e inherited from the triangulation T^h. Throughout, we make use of the following assumptions.

(A1) T^h is γ-shape-regular, i.e., there exists a constant $\gamma > 0$ such that
$$\rho_T \leq h_T \leq \gamma \rho_T, \qquad \text{for all } T \in T_h.$$

(A2) There exists a diffeomorphism $G_h : \Omega_h \to \Omega$ such that the estimates
$$\|G_h - id\|_{L^\infty(T)} \leq \beta h_T, \qquad \|DG_h - I\|_{L^\infty(T)} \leq \beta h_T,$$
$$\|DG_h^{-1}\|_{L^\infty(G_h(T))} \leq \beta, \qquad \|D^2 G_h\|_{L^\infty(T)} \leq \beta, \qquad \|D^2 G_h^{-1}\|_{L^\infty(G_h(T))} \leq \beta,$$
hold for all $T \in T_h$ with a constant β independent of the meshsize h. Morover, $G_h(T) = T$ for all elements T with $G(T) \cap \partial\Omega = \emptyset$.

An explicit construction of an appropriate domain mapping G_h can be found, for instance, in [13, Section 4.2]; for further details, see also [3, 7]. In order to be able to compare functions defined on Ω and Ω_h or the corresponding boundaries, we associate to any function $u : \Omega \to \mathbb{R}$ defined on the physical domain Ω a function
$$\widetilde{u} := u \circ G_h \tag{16}$$
defined on the discrete approximate domain Ω_h, which we call *restriction* of u to Ω_h. Using the properties of the mapping G_h, one easily obtains
$$c\|\widetilde{u}\|_{H^k(T)} \leq \|u\|_{H^k(G_h(T))} \leq c^{-1}\|\widetilde{u}\|_{H^k(T)}, \tag{17}$$
for all $u \in H^k(G_h(T))$ and $k \leq 2$ with a positive constant c that only depends on β. By restriction of G_h to the boundary of Ω_h, we may define
$$g_h : \Gamma_h \to \Gamma, \qquad g_h = G_h|_{\Gamma_h}. \tag{18}$$
which is piecewise smooth and invertible with $g_h^{-1} = G_h^{-1}|_\Gamma$. As a consequence of the properties of G_h, we obtain corresponding bounds for the derivatives of g_h and g_h^{-1}. In accordance with the above notation, we define for any function $p : \Gamma \to \mathbb{R}$ defined on the boundary Γ the restriction $\widetilde{p}$ to the boundary Γ_h of the discrete domain Ω_h by
$$\widetilde{p} := p \circ g_h. \tag{19}$$
By the chain rule and applications of the previous estimates, we then readily obtain
$$c\|\widetilde{p}\|_{H^k(e)} \leq \|p\|_{H^k(g_h(e))} \leq c^{-1}\|\widetilde{p}\|_{H^k(e)} \tag{20}$$
for all functions $p \in H^k(e)$ with $e \in E_h$ and integers $k \leq 2$.

4. Semi-discretisation in space

In this section, we investigate the semi-discretization of problem (3a)–(3c) in space by a finite element method. To this end, let

$$V^h = \{v^h \in C(\Omega_h) : v^h|_T \in P_1(T) \quad \text{for all } T \in T^h\}$$

be the space of piecewise linear continuous polynomials over Ω_h, and denote by

$$W^h = \{w^h : \Gamma_h \to \mathbb{R} : w^h = v^h|_{\Gamma_h} \quad \text{for some } v^h \in V^h\}$$

the space of piecewise linear polynomials over the surface Γ_h. Note that, by construction, W^h is the space of traces of functions in V^h, which we will use later on.

4.1. Finite element discretisation of the evolution problem.
As approximation of the volume-surface reaction-diffusion system (3a)–(3c), we then consider the following problem.

Problem 1 (Semi-discrete evolution problem). *Let us define*

$$a_h(L, \ell; v, w) = d_L(\nabla L, \nabla v)_{\Omega_h} + d_\ell(\nabla_{\Gamma_h} \ell, \nabla_{\Gamma_h} w)_{\Gamma_h} + (\lambda L - \gamma \ell, v - w)_{\Gamma_h}. \tag{21}$$

and $c_h(L, \ell; v, w) = (L, v)_{\Omega_h} + (\ell, w)_{\Gamma_h}$. *Find* $(L^h, \ell^h) \in H^1(0, T; V^h \times W^h)$ *such that*

$$(L^h(0), v^h)_{\Omega_h} = (\widetilde{L}_0, v^h)_{\Omega_h} \qquad \text{and} \qquad (\ell^h(0), w^h)_{\Gamma_h} = (\widetilde{\ell}_0, w^h)_{\Gamma_h},$$

for all $v^h \in V^h$, $w^h \in W^h$, *and such that*

$$\tfrac{d}{dt} c_h(L^h(t), \ell^h(t), v^h, w^h) + a_h(L^h, \ell^h; v^h, w^h) = 0 \tag{22}$$

holds for all $v^h \in V^h$ *and* $w^h \in W^h$, *and for all* $0 < t \le T$.

This semi-discrete problem has exactly the same structure as the weak form (5) of the continuous problem, which allows us to utilize similar arguments as in Section 2 for its analysis. By choice of a basis for the finite dimensional spaces V^h and W^h, Problem 1 can be recast as a linear system of ordinary differential equations. Existence and uniqueness of a solution then follow immediately from the Picard-Lindelöf theorem.

Lemma 13. *For any* $L_0 \in L^2(\Omega)$ *and* $\ell_0 \in L^2(\Gamma)$, *Problem 1 has a unique solution.*

As a next step, let us demonstrate that the total mass is conserved also on the discrete level. By using $v^h \equiv 1$ and $w^h \equiv 1$ as test functions in (22), we readily obtain

Lemma 14 (Mass conservation). *Let* L^h, ℓ^h *denote the solution of Problem 1. Then*

$$(L^h(t), 1)_{\Omega_h} + (\ell^h(t), 1)_{\Gamma_h} = (\widetilde{L}_0, 1)_{\Omega_h} + (\widetilde{\ell}_0, 1)_{\Gamma_h} =: M_0^h,$$

for all $t > 0$, *i.e., the total mass is conserved for all times also on the discrete level.*

4.2. The discretisation of the equilibrium problem.
For the approximation of the equilibrium system (6a)–(6d), we consider the following discrete variational problem.

Problem 2 (Discrete equilibrium problem). *Find* $L_\infty^h \in V^h$ *and* $\ell_\infty^h \in W^h$ *satisfying the conservation law constraint* $(L_\infty^h, 1)_{\Omega_h} + (\ell_\infty^h, 1)_{\Gamma_h} = M_0^h$ *such that for all* $(v^h, w^h) \in V^h \times W^h$ *there holds*

$$a_h(L_\infty^h, \ell_\infty^h; v^h, w^h) = 0. \tag{23}$$

In order to ensure the well-posedness of this problem, it suffices to show uniqueness, which readily follows from the following two results.

Lemma 15 (Discrete inf-sup stability). *For any $v \in H^1(\Omega_h)$ and $w \in H^1(\Gamma^h)$ satisfying the constraint $(v, 1)_{\Omega_h} + (w, 1)_{\Gamma_h} = 0$, there holds*

$$a_h(v, w; \lambda v, \gamma w) = \lambda d_L \|\nabla v\|_{\Omega_h}^2 + \gamma d_\ell \|\nabla_{\Gamma_h} w\|_{\Gamma_h}^2 + \|\lambda v - \gamma w\|_{\Gamma_h}^2. \tag{24}$$

Note that stability holds for all functions in $H^1(\Omega_h) \times H^1(\Gamma_h)$ defined on the discrete domain. The right hand side of (24) defines a norm on the subspace of functions with zero total mass, which follows by a Poincaré-type inequality. It will be important later on, that the equivalence constant can be chosen to be independent of the meshsize h.

Lemma 16. *For any $v \in H^1(\Omega_h)$ and $w \in H^1(\Gamma_h)$ with $(v, 1)_{\Omega_h} + (w, 1)_{\Gamma_h} = 0$ there holds*

$$\lambda d_L \|\nabla L\|_{\Omega_h}^2 + \gamma d_\ell \|\nabla_\Gamma \ell\|_{\Gamma_h}^2 + \|\lambda L - \gamma \ell\|_{\Gamma_h}^2 \geq C_P \left(\|L\|_{H^1(\Omega_h)}^2 + \|\ell\|_{H^1(\Gamma_h)}^2 \right) \tag{25}$$

with a constant C_P that only depends on the parameters d_L, d_ℓ, λ, and γ, on the domain Ω, and the constants in the estimates of G_h, but is otherwise independent of the meshsize h.

Proof. The proof follows from the Poincaré-type inequality stated in Lemma 6 by using the mapping G_h and the stability estimates (17) and (20). $\square$

Since the constant can be chosen independently of the meshsize, we deliberately use the same symbol C_P as on the continuous level here. By similar arguments as in Lemma 8, we then get

Proposition 17. *Problem 2 has a unique solution given by*

$$L_\infty^h = \frac{\gamma M_0^h}{\gamma |\Omega_h| + \lambda |\Gamma_h|} \qquad and \qquad \ell_\infty^h = \frac{\lambda}{\gamma} L_\infty^h. \tag{26}$$

Since the equilibrium solutions on the continuous and the discrete level are constants, we can give a very precise estimate for the discretization error.

Proposition 18. *Let (L_∞, ℓ_∞) and $(L_\infty^h, \ell_\infty^h)$ be the solutions of (7) and (23), respectively, and define $\widetilde{L} = L \circ G_h$ and $\widetilde{\ell} = \ell \circ g_h$. Then*

$$|\widetilde{L}_\infty - L_\infty^h| + |\widetilde{\ell}_\infty - \ell_\infty^h| \leq Ch^2.$$

with a constant C independent of the meshsize.

Proof. Using the explicit forms of L_∞ and L_∞^h in (10) and (26) we can write

$$|R_h L_\infty - L_\infty^h| = \left| \frac{\gamma M_0}{\lambda |\Omega| + \gamma |\Gamma|} - \frac{\gamma M_0^h}{\lambda |\Omega_h| + \gamma |\Gamma_h|} \right|$$

$$\leq c \left(\lambda |\Omega| |M_0 - M_0^h| + \gamma M_0 \left| \int_\Omega dx - \int_{\Omega_h} dx \right| \right)$$

The result for the volume term then follows from the properties of G_h, and that for the boundary component follows in a similar way. $\square$

4.3. **Convergence to discrete equilibrium.** Following our analysis on the continuous level, we define the discrete entropy functional

$$E^h(L^h, \ell^h) = \frac{1}{2} \left(\lambda \|L^h - L_\infty^h\|_{\Omega_h}^2 + \gamma \|\ell^h - \ell_\infty^h\|_{\Gamma_h}^2 \right). \tag{27}$$

With the same arguments as in the proof as on the continuous level, we then obtain

Lemma 19 (Discrete entropy dissipation). *Let (L^h, ℓ^h) denote the solution of discrete evolution Problem 1 and $(L_\infty^h, \ell_\infty^h)$ be the corresponding discrete equilibrium. Then,*

$$\frac{d}{dt} E^h(L^h(t), \ell^h(t)) = -d_L \lambda \|\nabla(L^h(t) - L_\infty^h)\|_{\Omega_h}^2 - d_\ell \gamma \|\nabla_\Gamma(\ell^h(t) - \ell_\infty^h)\|_{\Gamma_h}^2 \tag{28}$$
$$- \|\lambda(L^h(t) - L_\infty^h) - \gamma(\ell^h(t) - \ell_\infty^h)\|_{\Gamma_h}^2 =: -D^h(L^h(t), \ell^h(t)).$$

As a consequence of the discrete Poincaré-type inequality, we further get

Lemma 20 (Entropy-entropy dissipation inequality). *For any $v \in H^1(\Omega_h)$ and $w \in H^1(\Gamma_h)$ with $(v, 1)_{\Omega_h} + (w, 1)_{\Gamma_h} = (L_\infty^h, 1)_{\Omega_h} + (\ell_\infty^h, 1)_{\Gamma_h}$ there holds*

$$D^h(v, w) \geq c_0 E^h(v, w) \qquad with \quad c_0 = 2/C_P. \tag{29}$$

Note that c_0 can be chosen independent of h. Using the previous estimates, a Gronwall inequality, and the fact that the entropy is just a scaled L^2-norm distance, we finally obtain

Theorem 21 (Convergence to discrete equilibrium). *Let (L^h, ℓ^h) denote the solution to Problem 1 and $(L_\infty^h, \ell_\infty^h)$ be defined as in Proposition 17. Then*

$$\|L^h(t) - L_\infty^h\|_{\Omega_h}^2 + \|\ell^h(t) - \ell_\infty^h\|_{\Gamma_h}^2 \leq Ce^{-c_0 t} \left(\|\widetilde{L}_0 - L_\infty^h\|_{\Omega_h}^2 + \|\widetilde{\ell}_0 - \ell_\infty^h\|_{\Gamma_h}^2 \right), \tag{30}$$

where $C > 0$ and $c_0 > 0$ are independent of t and h.

Let us emphasize that up to perturbations that vanish with $h \to 0$, the constants C and c_0 are the same as on the continuous level. One can thus expect that the decay to equilibrium occurs at the same rate as on the continuous level. This is also what we observe in our numerical tests; see Section 6 for details.

4.4. **Geometric errors.** In order to be able to compare the continuous and discrete solutions, which are defined on different domains, we utilize the geometric transformations $G_h : \Omega_h \to \Omega$ and $g_h : \Gamma_h \to \Gamma$ and the restrictions

$$\widetilde{L} = L \circ G_h \qquad \text{and} \qquad \widetilde{\ell} = \ell \circ g_h,$$

as defined in Section 3. We then proceed with similar arguments as used in [7, 13], however, we work most of the time on the discrete domain Ω_h here, instead of Ω. We therefore define the restriction of the bilinear form a to the discrete domain Ω_h by

$$\widetilde{a}_h(\widetilde{L}, \widetilde{\ell}; \widetilde{v}, \widetilde{w}) := a(L, \ell; v, w) \quad \text{for all} \quad (L, \ell), (v, w) \in H^1(\Omega) \times H^1(\Gamma). \tag{31}$$

Using the transformation formulas for integrals and derivatives, we can express $\widetilde{a}_h$ directly by

$$\widetilde{a}_h(\widetilde{L}, \widetilde{\ell}; \widetilde{v}, \widetilde{w}) = d_L (A\nabla\widetilde{L}, \nabla\widetilde{v})_{\Omega_h} + d_\ell (B\nabla_{\Gamma_h}\widetilde{\ell}, \nabla_{\Gamma_h}\widetilde{w})_{\Gamma_h} + (C(\lambda\widetilde{L} - \gamma\widetilde{\ell}), \widetilde{v} - \widetilde{w})_{\Gamma_h}$$

with

$$A = (DG_h^\top DG_h)^{-1} \det(DG_h), \quad B = (Dg_h^\top Dg_h)^{-1} \det(Dg_h), \quad \text{and} \quad C = \det(Dg_h).$$

The bilinear form a_h used to define the finite element approximations can therefore be considered to be a non-conforming approximation of the true form $\widetilde{a}_h$. Similarly, we define

$$\widetilde{c}_h(\widetilde{L}, \widetilde{\ell}; \widetilde{v}, \widetilde{w}) := \int_{\Omega_h} \widetilde{L}v \det(DG_h)dx + \int_{\Gamma_h} \widetilde{\ell}_h w \det(Dg_h)dS = c(L, \ell; v, w).$$

The weak form (5) of Problem (3a)–(3c) can now be written equivalently as

$$\frac{d}{dt}\widetilde{c}_h(\widetilde{L}(t), \widetilde{\ell}(t); v, w) + \widetilde{a}_h(\widetilde{L}(t), \widetilde{\ell}(t); v, w) = 0 \tag{32}$$

for all $(v, w) \in H^1(\Omega_h) \times H^1(\Gamma_h)$, whereas the discrete variational problem has the form

$$\frac{d}{dt}c_h(L^h(t), \ell^h(t); v^h, w^h) + a_h(L^h(t), \ell^h(t); v^h, w^h) = 0 \tag{33}$$

for all $(v^h, w^h) \in V^h \times W^h$. The finite element problem, therefore, can be interpreted as a non-conforming approximation of the continuous problem over the discrete domain. The difference between the bilinear forms a_h and $\tilde{a}_h$ as well as $\widetilde{c}_h$ and c_h are however only due to "geometric errors", which can be quantified as follows.

Lemma 22. *For all $(L, \ell), (v, w) \in H^1(\Omega_h) \times H^1(\Gamma_h)$ there holds*

$$|a_h(L, \ell; v, w) - \widetilde{a}(L, \ell; v, w)| \le Ch\|(L, \ell)\|_{H^1(\Omega_h) \times H^1(\Gamma_h)}\|(v, w)\|_{H^1(\Omega_h) \times H^1(\Gamma_h)}. \tag{34}$$

with constant C independent of h. If $(L, \ell) \in H^2(\Omega) \times H^2(\Gamma)$, then one even has

$$|a_h(\widetilde{L}, \widetilde{\ell}; v, w) - \widetilde{a}(\widetilde{L}, \widetilde{\ell}; v, w)| \le Ch^2\|(L, \ell)\|_{H^2(\Omega) \times H^2(\Gamma)}\|(v, w)\|_{H^1(\Omega_h) \times H^1(\Gamma_h)}. \tag{35}$$

The same estimates hold for the difference in c_h and $\widetilde{c}_h$ with the regularity on the right hand side of the estimates reduced by one order.

Proof. The estimates follow from [13, Lemma 6.2] with minor modifications in the proofs. $\square$

4.5. **Error estimate.** The derivation of the error estimate now follows with standard arguments, see [16], but taking into account the additional geometric errors. An important step in our analysis will be the definition of an appropriate Ritz projection. For given functions (L, ℓ) in $H^1(\Omega) \times H^2(\Gamma)$, we define $R_h(L, \ell) \in V^h \times W^h$ by

$$a_h(R_h(\widetilde{L}, \widetilde{\ell}); v^h, w^h) + \eta c_h(R_h(\widetilde{L}, \widetilde{\ell}); v^h, w^h) = \widetilde{a}_h(\widetilde{L}, \widetilde{\ell}; v^h, w^h) + \eta c_h(\widetilde{L}, \widetilde{\ell}; v^h, w^h)$$

for all $(v^h, w^h) \in V^h \times W^h$. The following result states the basic properties of this construction.

Lemma 23 (Ritz projection)**.** *Let $\eta > 0$ be large enough. Then $R_h : H^1(\Omega_h) \times H^1(\Gamma_h) \to V^h \times W^h$ is a well-defined bounded linear operator and the following error estimates hold:*

$$\|(\widetilde{L}, \widetilde{\ell}) - R_h(\widetilde{L}, \widetilde{\ell})\|_{H^1(\Omega_h) \times H^1(\Gamma_h)} \le Ch\|(L, \ell)\|_{H^2(\Omega) \times H^2(\Gamma)}$$

and

$$\|(\widetilde{L}, \widetilde{\ell}) - R_h(\widetilde{L}, \widetilde{\ell})\|_{L^2(\Omega_h) \times L^2(\Gamma_h)} \le Ch^2\|(L, \ell)\|_{H^2(\Omega) \times H^2(\Gamma)},$$

for all $L \in H^2(\Omega)$ and $\ell \in H^2(\Gamma)$ with a constant C that is independent of the meshsize h. Moreover, $c_h(R_h(\widetilde{L}, \widetilde{\ell}); 1, 1) = c_h(\widetilde{L}, \widetilde{\ell}; 1, 1)$, i.e., R_h is mass preserving.

Proof. Note that for η large enough, the bilinear forms on both sides are elliptic. The Ritz projection therefore is the finite element approximation of an elliptic volume-surface reaction-diffusion problem. The error estimates then follow from the results in [13], and mass conservation follows directly from the definition of the bilinear forms. $\square$

We are now in the position to prove our first main error estimate.

Theorem 24. *Let (A1) and (A2) hold. Moreover, assume that the solution (L, ℓ) to (3a)–(3d) is sufficiently smooth. Then for all $t > 0$ we have the estimate*

$$\|\widetilde{L}(t) - L^h(t)\|_{\Omega_h} + \|\widetilde{\ell}(t) - \ell^h(t)\|_{\Gamma_h} \leq Ch^2,$$

with a constant C that is independent of t and h.

Proof. To improve the presentation of the proof, we will use the short-hand notation $U = (L, \ell)$, $\widetilde{U} = (\widetilde{L}, \widetilde{\ell})$, $U^h = (L^h, \ell^h)$, and $\Phi = (v, w)$. We further denote by $\mathcal{H}^h = L^2(\Omega_h) \times L^2(\Gamma_h)$ the tensor product space with inner product $(\cdot, \cdot)_{\mathcal{H}^h}$ and norm $\| \cdot \|_{\mathcal{H}^h}$. To prove the error estimate, we decompose the error in the usual manner into

$$U^h(t) - \widetilde{U}(t) = [\widetilde{U}(t) - R_h \widetilde{U}(t)] + [U^h(t) - R_h \widetilde{U}(t)] =: \rho(t) + \theta^h(t).$$

Using Lemma 23, we already have the desired estimate for the first component

$$\|\rho(t)\|_{L^2(\Omega_h) \times L^2(\Gamma_h)} \leq Ch^2 \|\widetilde{U}(t)\|_{H^2(\Omega_h) \times H^2(\Gamma_h)}.$$

To estimate the second term $\theta^h(t)$, observe that

$$
\begin{aligned}
c_h(\theta_t^h; &\Phi^h) + a_h(\theta^h; \Phi^h) \\
&= c_h(U_t^h; \Phi^h) - c_h(R_h \widetilde{U}_t; \Phi^h) + a_h(U^h; \Phi^h) - a_h(R_h \widetilde{U}; \Phi^h) \\
&= -c_h(R_h \widetilde{U}_t, \Phi^h) - \widetilde{a}_h(\widetilde{U}; \Phi^h) + \eta c_h(R_h \widetilde{U} - \widetilde{U}, \Phi^h) \\
&= c_h(\widetilde{U}_t - R_h \widetilde{U}_t; \Phi^h) + \left[c_h(\widetilde{U}_t, \Phi^h) - \widetilde{c}_h(\widetilde{U}_t, \Phi) \right] + \eta c_h(R_h \widetilde{U} - \widetilde{U}; \Phi^h) \\
&\leq \|\rho_t\|_{\mathcal{H}^h} \|\Phi^h\|_{\mathcal{H}^h} + \left| \widetilde{c}_h(\tilde{U}_t, \Phi^h) - (\widetilde{U}_t, \Phi^h) \right| + \eta \|\rho\|_{\mathcal{H}^h} \|\Phi^h\|_{\mathcal{H}^h}.
\end{aligned}
$$

By using Lemma 22, the properties of the mapping G_h, the estimate of the Ritz projection in Lemma 23 and the Cauchy-Schwarz inequality, it follows that

$$
\begin{aligned}
c_h(\theta_t^h, &\Phi^h) + a_h(\theta; \Phi^h) \\
&\leq Ch^2 \big(\|U_t\|_{H^2(\Omega) \times H^2(\Gamma)} \|\Phi\|_{L^2(\Omega^h) \times L^2(\Gamma^h)} + \|U\|_{H^2(\Omega) \times H^2(\Gamma)} \|\Phi\|_{H^1(\Omega_h) \times H^1(\Gamma_h)} \big).
\end{aligned}
$$

Now recall that $\theta^h(t) = (L^h(t) - \widetilde{L}_R(t), \ell^h(t) - \widetilde{\ell}_R(t))$, where $(\widetilde{L}_R, \widetilde{\ell}_R) := R_h \widetilde{U}$. We then choose the test function as $\Phi^h = (\lambda(L^h(t) - \widetilde{L}_R(t)), \gamma(\ell^h(t) - \widetilde{\ell}_R(t)))$, and we use the definition of the discrete entropy functional and the entropy dissipation in (27) and (28), to get

$$
\begin{aligned}
\frac{d}{dt} E^h(\theta^h) + D^h(\theta^h) &= c_h(\theta_t^h, \Phi^h) + a_h(\theta^h; \Phi^h) \\
&\leq Ch^2 \big(\|U_t\|_{H^2(\Omega) \times H^2(\Gamma)} \|\theta^h\|_{L^2(\Omega_h) \times L^2(\Gamma_h)} + \|U\|_{H^2(\Omega) \times H^2(\Gamma)} \|\theta^h\|_{H^1(\Omega_h) \times H^1(\Gamma_h)} \big).
\end{aligned}
$$

Since the total mass of $\theta^h(t) = U^h(t) - R_h \widetilde{U}(t)$ is zero, we obtain from Lemma 16

$$D^h(\theta^h) \geq c \|\theta^h\|_{H^1(\Omega_h) \times H^1(\Gamma_h)}^2 \geq c' E^h(\theta),$$

which allows us to absorb the terms containing θ^h via Young's inequality by the entropy dissipation, which finally leads to

$$\frac{d}{dt} E^h(\theta) + c_1 E^h(\theta) \leq C' h^4 \big(\|U_t\|_{H^2(\Omega) \times H^2(\Gamma)}^2 + \|U\|_{H^2(\Omega) \times H^2(\Gamma)}^2 \big)$$

The claim now follows by application of Gronwall's inequality and noting that the initial conditions are approximated with order h^2. □

5. TIME DISCRETISATION

5.1. Implicit backward Euler scheme.

For the time discretization of the semi-discrete problem, we consider the backward Euler method with a uniform time step. To be more precise, for a fixed time step $\tau > 0$, we denote by $t_n = n\tau$ for $n = 0, 1, 2, \ldots$, the time nodes. Given a sequence $\{u_n : n \geq 0\}$, we set as usual

$$\bar{\partial} u_n := \frac{u_n - u_{n-1}}{\tau} \tag{36}$$

The fully discrete approximation for the system (3a)–(3d) then reads

Problem 3 (Time Discretisation). *Define* $(L_0^h, \ell_0^h) \in V^h \times W^h$ *by*

$$(L_0^h, v^h)_{\Omega_h} = (\widetilde{L}_0, v^h)_{\Omega_h} \quad and \quad (\ell_0^h, w^h)_{\Gamma_h} = (\widetilde{\ell}_0, w^h)_{\Gamma_h} \tag{37}$$

for all $(v^h, w^h) \in V^h \times W^h$ *and for* $n = 1, 2, \ldots$, *find* $(L_n^h, \ell_n^h) \in V^h \times W^h$ *such that*

$$c_h(\bar{\partial} L_n^h, \bar{\partial}\ell^h; v^h, w_h) + a_h(L_n^h, \ell_n^h; v^h, w^h) = 0 \tag{38}$$

holds for all test functions $(v^h, w^h) \in V^h \times W^h$.

Note that the problem (38) can be written equivalently as

$$\tfrac{1}{\tau} c_h(L_n^h, \ell_n^h; v^h, w^h) + a_h(L_n^h, \ell_n^h; v^h, w^h) = \tfrac{1}{\tau} c_h(L_{n-1}^h, \ell_{n-1}^h; v^h, w^h). \tag{39}$$

As a consequence of the discrete inf-sup stability condition (24), the problems for the individual time-steps are uniquely solvable, and we obtain

Lemma 25. *For any time step* $\tau > 0$, *Problem 3 admits a unique solution* $(L_n^h, \ell_n^h)_{n \geq 0}$.

Further, by testing with $v^h \equiv 1$ and $w^h \equiv 1$, we directly obtain

Proposition 26 (Mass conservation). *Let* $M_0^h := (\widetilde{L}_0, 1)_\Omega + (\widetilde{\ell}_0, 1)_{\Gamma_h}$. *Then,*

$$(L_n^h, 1)_{\Omega_h} + (\ell_n^h, 1)_{\Gamma_h} = M_0^h \qquad for\ all\ n \geq 1, \tag{40}$$

i.e., the total mass is conserved for all time steps.

5.2. Convergence to discrete equilibrium.

To study the large time behavior, we again employ the discrete entropy of Section 4, which was defined as

$$E^h(L, \ell) = \frac{1}{2}\left(\lambda\|L - L_\infty^h\|_{\Omega_h}^2 + \gamma\|\ell - \ell_\infty^h\|_{\Gamma_h}^2\right). \tag{41}$$

As a replacement for the entropy dissipation stated in Lemma 19, we now have

Lemma 27 (Entropy dissipation). *For all* $n \geq 1$, *there holds*

$$\bar{\partial} E^h(L_n^h, \ell_n^h) \leq -\lambda d_L \|\nabla(L_n^h - L_\infty^h)\|_{\Omega_h}^2 - \gamma d_\ell \|\nabla_\Gamma(\ell_n^h - \ell_\infty^h)\|_{\Gamma_h}^2 \tag{42}$$
$$- \|\lambda(L_n^h - L_\infty^h) - \gamma(\ell_n^h - \ell_\infty^h)\|_\Gamma^2 = -D^h(L_n^h, \ell_n^h).$$

Proof. As one can see by direct computation, we have

$$\bar{\partial} E^h(L_n^h, \ell_n^h) \leq (\bar{\partial} L_n^h, \lambda(L_n^h - L_\infty^h))_{\Omega_h} + (\bar{\partial}\ell_n^h, \gamma(\ell_n^h - \ell_\infty^h))_{\Gamma_h}. \tag{43}$$

The rest follows along the lines of the proof of Lemma 19.   □

The convergence to equilibrium can now be established in a similar manner as on the semi-discrete level by using the previous lemma, the entropy-entropy dissipation inequality of Lemma 20, and a discrete Gronwall inequality. Summarizing, we obtain

Theorem 28 (Convergence to discrete equilibrium)**.** *For any $\tau > 0$ and $n \geq 0$, there holds*

$$\|L_n^h - L_\infty^h\|_{\Omega_h}^2 + \|\ell_n^h - \ell_\infty^h\|_{\Gamma_h}^2 \leq Ce^{-c_0\tau n}(\|L_0^h - L_\infty^h\|_{\Omega_h}^2 + \|\ell_0^h - \ell_\infty^h\|_{\Gamma_h}^2) \qquad (44)$$

with the same constants C and c_0 as in Theorem 21 independent of h and n.

5.3. **Error estimates.** For the derivation of error estimates for the full discretization, we again use standard arguments and appropriately take into account the geometric errors.

Theorem 29 (Convergence rate for time discretisation)**.** *Let (A1) and (A2) hold and assume that the solution (L, ℓ) of (3a)–(3d) is sufficiently smooth. Then, for all $n \geq 0$ we have*

$$\|L_n^h - \widetilde{L}(t_n)\|_{\Omega_h} + \|\ell_n^h - \widetilde{\ell}(t_n)\|_{\Gamma_h} \leq C(h^2 + \tau)$$

with a constant C that is independent of n, τ, and h.

Proof. To simplify the presentation, we again introduce the following short-hand notations $U_n^h = (L_n^h, \ell_n^h)$, $\widetilde{U} = (\widetilde{L}, \widetilde{\ell})$, and $\Phi = (v, w)$. As before, we write $R_h\widetilde{U} = (\widetilde{L}_R, \widetilde{\ell}_R)$ for the Ritz projection, and denote by $\mathcal{H}^h = L^2(\Omega_h) \times L^2(\Gamma_h)$ the tensor product space with inner product $(\cdot, \cdot)_{\mathcal{H}^h}$ and norm $\|\cdot\|_{\mathcal{H}^h}$. We then decompose the error into

$$U_n^h - \widetilde{U}(t_n) = [U_n^h - R_h\widetilde{U}(t_n)] + [R_h\widetilde{U}(t_n) - \widetilde{U}(t_n)] =: \theta_n^h + \rho_n.$$

Using the Ritz projection, ρ_n has the desired error estimate

$$\|\rho_n\|_{L^2(\Omega_h) \times L^2(\Gamma_h)} \leq Ch^2\|U(t_n)\|_{H^2(\Omega) \times H^2(\Gamma)}. \qquad (45)$$

To estimate the error in the second component, we consider the evolution of the discrete error

$$\begin{aligned}
c_h(\bar{\partial}\theta_n^h, \Phi^h) &+ a_h(\theta_n^h; \Phi^h) \\
&= c_h(\bar{\partial}U_n^h, \Phi^h) - c_h(\bar{\partial}R_h\widetilde{U}(t_n), \Phi^h) + a_h(U_n^h; \Phi^h) - a_h(R_h\widetilde{U}(t_n); \Phi^h) \\
&= c_h(\bar{\partial}\widetilde{U}(t_n) - R_h\bar{\partial}\widetilde{U}(t_n); \Phi^h) + \widetilde{c}_h(\bar{\partial}\widetilde{U}(t_n), \Phi^h) - c_h(\bar{\partial}\widetilde{U}(t_n); \Phi^h) \\
&\quad + \eta c_h(\widetilde{U}(t_n) - R_h\widetilde{U}(t_n); \Phi^h) + \widetilde{c}_h(\bar{\partial}\widetilde{U}(t_n) - \widetilde{U}_t(t_n); \Phi^h) \\
&= (i) + (ii) + (iii) + (iv).
\end{aligned}$$

The first three terms can now be estimated as in the proof of Theorem 24, and for the fourth term, we can use the explicit representation

$$\bar{\partial}\widetilde{U}(t_n) - \widetilde{U}_t(t_n) = \int_{t_{n-1}}^{t_n} \int_{t_{n-1}}^{t} U_{tt}(s)ds\, dt.$$

Using a suitable test function Φ^h, the discrete entropy and entropy dissipation, the Poincaré inequality, and the estimates for the Ritz projection finally leads to

$$\begin{aligned}
\bar{\partial}E^h(\theta_n^h) &+ c_1 E^h(\theta_n^h) \\
&\leq C'\big(h^4\|U_t(t_n)\|_{H^2(\Omega \times H^2(\Omega)}^2 + h^4\|U(t_n)\|_{H^2(\Omega \times H^2(\Omega)}^2 + \tau^2\|U_{tt}(\xi_n)\|_{L^2(\Omega) \times L^2(\Gamma)}^2\big)
\end{aligned}$$

for some positive constants $c_1, C' > 0$ and appropriate $\xi_n \in (t_{n-1}, t_n)$. The result then follows similarly as for the semi-discretization and by a discrete version of the Gronwall lemma. $\qquad \square$

Let us emphasize that our error estimates hold uniform in time. The basic tool that allowed us to obtain this was the exponential stability provided by the entropy estimates.

6. Numerics

For illustration of the theoretical results, we present in this section some numerical tests. For ease of presentation, we restrict ourselves again to two space dimensions and consider Ω to be the unit circle. In all simulations, we chose the parameters $d_L = 0.01$, $d_\ell = 0.02$, $\gamma = 2$, and $\lambda = 4$, and complement the system (1a)–(1c) with the initial data

$$L_0(x,y) = \frac{1}{2}(x^2 + y^2) \quad \text{and} \quad \ell_0(x,y) = \frac{1}{2}(1 + x).$$

We start by investigating the convergence of solutions for a sequence of uniformly refined meshes starting from an initial triangulation consisting of 258 elements, and we choose $T = 2$ as a final time and a time step of $\tau = 0.125$. As approximation for the error we use the difference of solutions obtained on two consecutive refinements, e.g., we use

$$L(T) - L_n^h(T) \approx L_n^{h/2}(T) - L_n^h(T) = \triangle L$$

to measure the various errors. In Table 6, we display the L^2 errors for L and ℓ, as well as the observed convergence rate. In addition, we display the error in the entropy and the errors in the H^1-norm. The results confirm the convergence rates that were predicted by Theorem 29.

elements	$\|\triangle L\|_{L^2}$	$\|\triangle \ell\|_{L^2}$	rate	$\triangle E(L,\ell)$	$(\triangle L, \triangle \ell)_{H^1 \times H^1}$
1032	5.62e-03	2.45e-03	-	1.38e-04	1.65e-01
4128	1.50e-03	6.06e-04	1.91	9.77e-06	8.22e-02
16512	3.86e-04	1.51e-04	1.96	6.41e-07	4.09e-02
66048	9.72e-05	3.78e-05	1.99	4.06e-08	2.04e-02
264192	2.43e-05	9.46e-06	2.00	2.55e-09	1.02e-02

Figure 2. Errors and rates for the numerical experiments depending on the number of triangles. The rate is calculated from two consecutive runs.

In a second test, we investigate the large time behavior of the system. To this end, we choose $T = 500$ and $\tau = 0.5$. We compute the discrete solutions for a sequence of uniformly refined meshes and evaluate the entropy, to be more precise, we compute

$$\widetilde{E}(L^h(t_n), \ell^h(t_n)) = \frac{1}{2}\big(\lambda \|L_n^h - L_\infty\|_{\Omega_h}^2 + \gamma \|\ell_n^h - \ell_\infty\|\big),$$

which measures the distance of the discrete solution to the exact equilibrium state. This allows us to evaluate at the same time the convergence to equilibrium and the approximation of the equilibrium state. The corresponding results are displayed in Figure 3. As predicted by our theoretical results, we observe exponential convergence. The numerical results also allow us to estimate the constant present in the exponential decay which is approximately $c_0 = 0.045$ here. Furthermore, we can see that for time approximately larger than $t = 250$, the discretisation error due to approximation of the equilibrium becomes dominant.
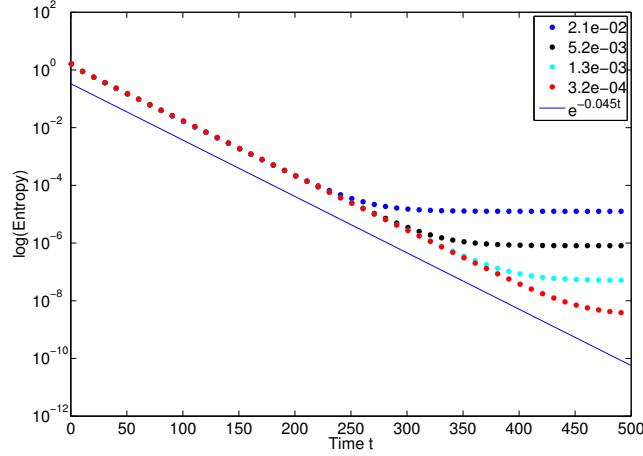
FIGURE 3. Convergence of modified entropy error $\widetilde{E}(L^h(t_n), \ell^h(t_n))$ for different mesh sizes. One can clearly see the exponential convergence with a mesh independent rate. For large time, the discretization error due to the approximation of the equilibrium state is dominant and leads to a saturation.

7. EXTENSION TO A SYSTEM ARISING IN ASYMMETRIC STEM CELL DIVISION

Let us now illustrate that the analysis and the discretisation presented for the model problem (3a)–(3c) can be extended more or less straight forward to more general volume-surface reaction-diffusion systems which have the same key properties: (i) a mass conservation law, (ii) a constant positive detailed balance equilibrium, and (iii) a quadratic entropy functional and an appropriate entropy-entropy dissipation estimate which allows to obtain exponential convergence to equilibrium.

We consider the following four species volume-surface reaction-diffusion system two volume concentrations L and P and two surface concentrations ℓ and p as mentioned in the introduction

$$L_t - d_L \Delta L = -\beta L + \alpha P, \qquad x \in \Omega, \ t > 0, \tag{46a}$$

$$P_t - d_P \Delta P = \beta L - \alpha P, \qquad x \in \Omega, \ t > 0, \tag{46b}$$

$$\ell_t - d_\ell \Delta_\Gamma \ell = -d_L \partial_n L + \chi_{\Gamma_2}(-\sigma \ell + \kappa p), \qquad x \in \Gamma, \ t > 0, \tag{46c}$$

$$p_t - d_p \Delta_{\Gamma_2} = \sigma \ell - \kappa p - d_P \partial_n P, \qquad x \in \Gamma_2, \ t > 0. \tag{46d}$$

As before, we assume Ω is a bounded domain in two or three space dimensions with a smooth boundary $\Gamma = \partial \Omega \in C^3$. We further assume that the boundary $\Gamma = \Gamma_1 \cup \Gamma_2$ divides into two disjoint subsets Γ_1 and Γ_2 where $\partial \Gamma_2$ is again smooth, and we denote by χ_{Γ_2} the characteristic function on Γ_2. The mass transfer between the volume and the surface is governed by the boundary conditions

$$d_L \partial_n L = -\lambda L + \gamma \ell, \qquad x \in \Gamma, \ t > 0, \tag{46e}$$

$$d_P \partial_n P = \chi_{\Gamma_2}(-\eta P + \xi p), \qquad x \in \Gamma, \ t > 0, \tag{46f}$$

$$d_p \partial_{n_{\Gamma_2}} p = 0, \qquad x \in \partial \Gamma_2, \ t > 0. \tag{46g}$$

The system (46a)–(46g) is again complemented by appropriate initial conditions.

This problem represents the mass transfer between the concentrations L, P, ℓ and p as visualised in the right diagram in Figure 1 in Section 1. A variant of system (46), where two of the reaction/desorption processes were considered irreversible with $\kappa = \eta = 0$, was studied recently in [8] in order to describe the asymmetric localisation of Lgl during the mitosis of SOP stem cells of Drosophila, [23, 25, 24]. The diffusion and reaction parameters are assumed to be positive constants and we further assume that the system has a detailed balance equilibrium, i.e. we require validity of the *detailed balance condition*

$$\frac{\alpha\lambda\sigma\xi}{\beta\gamma\kappa\eta} = 1. \tag{47}$$

Using this condition, one can show that the system (46a)–(46g) has very similar properties as the model problem (3a)–(3c), and, therefore, the analysis of the previous sections can be carried over to the system (46) almost verbatim. Let us sketch the necessary key steps in more detail:

(1) the system (46) has an inherent *mass conservation law*, i.e. the total mass is conserved for all time:

$$M(t) := \int_\Omega L(t) + P(t)dx + \int_\Gamma \ell(t)dS + \int_{\Gamma_2} p(t)dS = M(0) \qquad \text{for all } t > 0. \tag{48}$$

(2) Together with the detailed balance condition (47), one can show as for the model problem (3) that for any initial mass $M_0 > 0$ there exists a unique positive constant detailed balance equilibrium $(L_\infty, P_\infty, \ell_\infty, p_\infty)$. Again, analytic formulas depending only on the initial M_0 and the parameters α, β, λ, γ, σ, and κ can be derived.

(3) The system (46) also has a *quadratic relative entropy functional*, which has the form

$$E(L, P, \ell, p)(t) = \frac{1}{2}\left(\int_\Omega \frac{1}{L_\infty}|L(t) - L_\infty|^2 dx + \int_\Omega \frac{1}{P_\infty}|P(t) - P_\infty|^2 dx \right.$$
$$\left. + \int_\Gamma \frac{1}{\ell_\infty}|\ell(t) - \ell_\infty|^2 dS + \int_{\Gamma_2} \frac{1}{p_\infty}|p(t) - p_\infty|^2 dS\right). \tag{49}$$

Let us not that, up to scaling with a constant, also the entropy for the model problem (3a)–(3c) could be written in this way.

(4) The corresponding *entropy dissipation functional* reads

$$\frac{d}{dt}E(L, P, \ell, p)(t)$$
$$= -\frac{d_L}{L_\infty}\|\nabla L(t)\|_\Omega^2 - \frac{d_P}{P_\infty}\|\nabla P(t)\|_\Omega - \frac{d_\ell}{\ell_\infty}\|\nabla_\Gamma \ell(t)\|_\Gamma^2 - \frac{d_p}{p_\infty}\|\nabla_{\Gamma_2} p(t)\|_{\Gamma_2}^2$$
$$- \frac{1}{\beta L_\infty}\|\beta L(t) - \alpha P(t)\|_\Omega^2 - \frac{1}{\gamma\ell_\infty}\|\gamma\ell(t) - \lambda L(t))^2\|_\Gamma^2$$
$$- \frac{1}{\kappa p_\infty}\|\kappa p(t) - \sigma\ell(t)\,\Gamma_2^2 - \frac{1}{\eta P_\infty}\|\eta P(t) - \xi p(t)\|_{\Gamma_2}^2 =: -D(L, P, \ell, p).$$

(5) Similar to Lemma 6, one can show an *entropy-entropy dissipation estimate* of the form

$$D(L, P, \ell, p) \geq c_0\, E(L, P, \ell, p) \tag{50}$$

holds with a constant c_0 only depending on the parameters and the domain. The proof is again based on a Poincaré-type inequality.

Following the arguments of Section 2–Section 5 one can then establish the following results:

(i) The convergence to equilibrium for the continuous problem

$$\|L(t) - L_\infty\|_\Omega + \|P(t) - P_\infty\|_\Omega + \|\ell(t) - \ell_\infty\|_\Gamma + \|p(t) - p_\infty\|_{\Gamma_2} \leq Ce^{-c_0 t} \text{ for all } t > 0.$$

(ii) The convergence to the discrete equilibrium for semi-discrete solutions

$$\|L^h(t) - L^h_\infty\|_{\Omega_h} + \|P^h(t) - P^h_\infty\|_{\Omega_h} + \|\ell^h(t) - \ell^h_\infty\|_{\Gamma_h} + \|p^h(t) - p^h_\infty\|_{\Gamma^h_2} \leq Ce^{-c_0 t},$$

as well as for the fully discrete solutions

$$\|L^h_n - L^h_\infty\|_{\Omega_h} + \|P^h_n - P^h_\infty\|_{\Omega_h} + \|\ell^h_n - \ell^h_\infty\|_{\Gamma_h} + \|p^h_n - p^h_\infty\|_{\Gamma^h_2} \leq Ce^{-c_0 \tau n},$$

with constants c_0, C independent of the meshsize $h > 0$ and the time step $\tau > 0$.

(iii) Error estimates independent of time horizon and order optimal convergence under the assumption of sufficiently regular solutions, i.e.,

$$\|L^h(t) - \widetilde{L}(t)\|_{\Omega_h} + \|P^h(t) - \widetilde{P}(t)\|_{\Omega_h} + \|\ell^h(t) - \widetilde{\ell}(t)\|_{\Gamma_h} + \|p^h(t) - \widetilde{p}(t)\|_{\Gamma^h_2} \leq Ch^2$$

for the semi-deiscretization and

$$\|L^h_n - \widetilde{L}(t_n)\|_{\Omega_h} + \|P^h_n - \widetilde{P}(t_n)\|_{\Omega_h} + \|\ell^h_n - \widetilde{\ell}(t_n)\|_{\Gamma_h} + \|p^h_n - \widetilde{p}(t_n)\|_{\Gamma^h_2} \leq C(h^2 + \tau)$$

for the full discretization with a constant C that is independent of the time horizon, of the meshsize, and of the time step.

Some snapshot of the concentrations $P(t)$ and $L(t)$ are depicted in Figure 7.
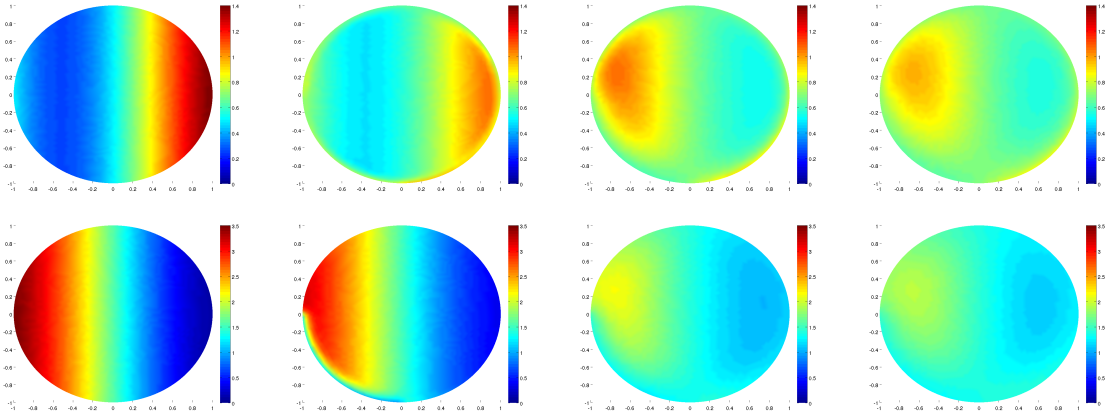

FIGURE 4. Snapshots for $L(t)$ and $P(t)$ at $t = 0, 0.13, 1.56, 3.0$. A mesh with 4064 triangles and $\tau = 0.01$ was used. The initial data were $L_0(x, y) = x\sin(x + 1) + 0.5$, $P_0(x, y) = (2 - x)\cos(x + 1) + 0.5$, $\ell_0(x, y) = 0.3(2 - y) + 1$, and $p_0(x, y) = 0.4y + 1$.

The evolution is driven by convergence to the constant equilibrium, but also some local effects due to the mass transfer with the boundary can be seen.

8. Summary

Volume-surface reaction-diffusion systems arise in many applications in chemistry, fluid dynamics, crystal growth, see e.g. [19, 20] and in particular in molecular-biology, where many current models aim to describe, for instance, signaling pathways, see e.g. [21], or the evolution of proteins, see e.g. [8].

As realistic models in biology are often large and the mathematical analysis accordingly cumbersome, our general aims is to develop methods, which are robust in the sense that they are based on a few fundamental properties, which are shared by many such models: i) conservation of mass and non-negativity of solutions, ii) a positive equilibrium, and ii) exponential convergence to equilibrium.

In this manuscript, we investigated volume-surface reaction-diffusion systems with a unique constant detailed balance equilibrium. We identified an appropriate quadratic entropy functional, characterized the entropy dissipation, and established an entropy-entropy dissipation inequality, which follows by a Poincaré-type inequality. Combining these ingredients allowed us to establish exponential convergence of solutions to the equilibrium.

For the discretization, we then investigated a finite element method and the implicit Euler scheme. The fact that the equilibrium was constant enabled us to carry over all arguments almost verbatim to the discrete level. In particular, exponential convergence to the discrete equilibrium could be established for the semi-discretization and the fully discrete approximations. In addition, we conducted a full error analysis, including domain approximations, and could establish convergence of optimal order uniform in time and with constants independent of the meshsize and the time step. The theoretical findings were confirmed in numerical tests.

Although we confined ourselves here to simple model problem, our general arguments, in particular the use of entropy estimates, can be applied to obtain similar results for a wide class of surface-volume reaction-diffusion problems having a constant equilibrium. Big parts of our analysis could even be extended to problems with non-constant equilibria. In particular, quadratic entropy functionals of the form (49) can be constructed for a much wider class of problems with linear reaction dynamics, but these cannot be applied so easily on the discrete level. Another possible direction of generalisation would be to consider complex balanced systems, such as weakly reversible reaction networks. Such systems still feature a positive equilibria and the entropy structure as well as exponential convergence to equilibrium, as recently established for general first order reaction-diffusion networks in [26]. The formulation of an appropriate discrete entropy and entropy dissipation will be direction of future research.

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