Applied Mathematics and Computation 336 (2018) 351–367

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Analysis and numerical solution of coupled volume-surface reaction-diffusion systems with application to cell biology

H. Egger[a,*], K. Fellner[b], J.-F. Pietschmann[c], B.Q. Tang[b,d]

[a] AG Numerical Analysis and Scientific Computing, Department of Mathematics, TU Darmstadt,Dolivostr, Darmstadt 15, 64293, Germany
[b] Institute of Mathematics and Scientific Computing, University of Graz, Heinrichstraße, Graz 36, 8010, Austria
[c] Institute for Applied Mathematics, Department of Mathematics and Computer Science, University of Münster, Orleansring, Münster 10,48149, Germany
[d] School of Applied Mathematics and Informatics, Hanoi University of Science and Technology,1 Dai Co Viet, Hai Ba Trung, Hanoi, Viet Nam

ARTICLE INFO

MSC:
35K57
65M60
35B40

Keywords:
Reaction-diffusion systems
Surface diffusion
Finite element method
Uniform error estimates
Entropy method
Asymmetric stem cell division

ABSTRACT

We consider the numerical solution 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 to equilibrium by the entropy method. We then investigate the discretization of the system by a finite element method and an implicit time stepping scheme including the domain approximation by polyhedral meshes. Mass conservation and exponential convergence to equilibrium are established on the discrete level by arguments similar to those on the continuous level and we obtain estimates of optimal order for the discretization error that hold uniformly in time. Some numerical tests are presented to illustrate these theoretical results. The analysis and the numerical approximation are discussed in detail for a simple model problem. The basic arguments however apply also in a more general context. This is demonstrated by investigation of a particular volume-surface reaction-diffusion system arising as a mathematical model for 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 different domains but also with domain interfaces or boundaries. In cell-biology, for instance, many phenomena are based on reaction-diffusion processes of proteins within the cell-body and on the cell cortex [21,22]. Particular examples are systems modeling cell-biological signaling processes [16] or models for asymmetric stem cell division that describe the localization of so-called cell-fate determinants during mitosis [2,20,27].

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

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

* Corresponding author.
E-mail addresses: egger@mathematik.tu-darmstadt.de (H. Egger), klemens.fellner@uni-graz.at (K. Fellner), pietschmann@mathematik.tu-darmstadt.de (J.-F. Pietschmann), quoc.tang@uni-graz.at (B.Q. Tang).

https://doi.org/10.1016/j.amc.2018.04.031
0096-3003/

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

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

which describes the diffusion of a substance with concentration L in the volume and concentration ℓ on the surrounding surface coupled by mass transfer between these two compartments. Here Ω is the volume domain, $\Gamma = \partial\Omega$ is the surface, Δ_Γ denotes the Laplace-Beltrami operator, and the model parameters d_L, d_ℓ, λ, γ are assumed to be positive constants. The equations are supposed to hold for all $t > 0$ and are complemented by appropriate initial conditions.

The system (1a)–(1c) may serve as a starting point for considering more realistic adsorption and desorption processes or as a reduced model for volume-surface reaction-diffusion processes arising in cell biology. But despite its simplicity, this model problem already features some interesting properties that will be of main interest for our further considerations:

(i) The system preserves non-negativity of solutions.
(ii) The total mass $M = \int_\Omega L dx + \int_\Gamma \ell ds$ is conserved for all time.
(iii) There exists a unique constant positive detailed balance equilibrium that can be parametrized explicitly by the total mass M and the model parameters λ and γ.
(iv) The solutions are uniformly bounded and converge exponentially fast toward the equilibrium state with respect to any reasonable Lebesgue or Sobolev norm.

The first goal of our paper will be to establish these properties, in particular (iii) and (iv), for the model problem (1a)–(1c). Based on this analysis, the second aim is then to investigate the systematic discretization of the system by finite elements and implicit time-stepping schemes. The guideline for the construction of the numerical approximation is to preserve and utilize the key features of the model as far as possible also for the analysis on the discrete level. In particular, we will establish the conservation of mass, prove the existence of a unique discrete equilibrium, and show the exponential convergence to equilibrium on the discrete level. We also comment briefly on the possibility for preserving the non-negativity of solutions.

Our arguments are closely related to the concepts of structure-preserving schemes, geometric integration, and compatible discretization that have been developed over the last decades. We refer the reader to the extensive survey [7] and the references therein. Several results concerning the preservation of entropic structures for discretization schemes have been obtained more recently, see e.g. [3,4,6,18,19]. This paper adds to this research by addressing the analysis and numerical solution of coupled volume-surface reaction-diffusion systems.

Apart from the entropy arguments, the numerical analysis is based on standard tools for the discretization of evolution problems [25,26], on previous work concerning the analysis of domain approximations [1,9–11], and on recent results from [13], who considered a somewhat simpler stationary volume-surface reaction-diffusion problem. The entropy estimates will allow us to establish order optimal convergence estimates with constants that are uniform in time.

The model problem (1a)–(1c) is simple enough to avoid complicated notation and to present our basic ideas in the most convenient way to the reader. To illustrate the applicability to more general problems, we consider in Section 7 the following system that models the evolution of four conformations of the key protein Lgl during the mitosis of Drosophila SOP precursor stem-cells [2,15,20].

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

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

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

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

Note that the last equation only holds on a part $\Gamma_2 \subseteq \Gamma$ of the boundary. The mass transfer between the domain and the surface is described by

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

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

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