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# A multiscale Galerkin approach for a class of nonlinear coupled reaction–diffusion systems in complex media

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ABSTRACT

A Galerkin approach for a class of multiscale reaction–diffusion systems with nonlinear coupling between the microscopic and macroscopic variables is presented. This type of models are obtained e.g. by upscaling of processes in chemical engineering (particularly in catalysis), biochemistry, or geochemistry. Exploiting the special structure of the models, the functions spaces used for the approximation of the solution are chosen as tensor products of spaces on the macroscopic domain and on the standard cell associated to the microstructure. Uniform estimates for the finite dimensional approximations are proven. Based on these estimates, the convergence of the approximating sequence is shown. This approach can be used as a basis for the numerical computation of the solution.


## 1. Introduction

One of the challenges of mathematics and modelling when dealing with processes in complex media (porous media, soil, biological tissue) is to derive effective descriptions at the macroscopic scale. Hereby, it is important that the system parameters can be calculated directly by solving microscopic cell problems, and thus including the contribution of the processes on the microscopic scale quantitatively. Starting from model equations at microscopic level, and using the techniques of multiscale analysis and homogenization, effective models could be derived and validated in a wealth of applications.

An important issue concerning the obtained effective (macroscopic) models is the quantitative evaluation of the solutions by means of numerical simulations. Many numerical methods have been recently developed for general systems involving multiple scales. E.g. the heterogeneous multiscale method, multiscale FEM, FEM$^2$, MAN, see [8,4,19,17], and the literature therein. However, if the systems exhibit special features, like those arising in homogenization theory, where a certain type of periodicity assumption is satisfied, exploiting the additional information leads to more robust and accurate numerical approaches. For the case of linear, elliptic equations, with periodically oscillating coefficients such approaches have been developed e.g. in [1], and [11]. However, there is not much progress in the development of multiscale approaches for nonlinear problems arising from homogenization theory. A contribution in this direction was given in [18], where a multiscale Galerkin approach was developed to investigate transport and nonlinear reaction in domains separated by membranes.

In the present paper, a class of two-scale reaction–diffusion systems with nonlinear micro-macro coupling is considered. Such systems are used to model the evolution and transfer of mass within different phases of a complex medium, and consist of a macroscopic system formulated on the macroscopic domain, coupled with a microscopic system, formulated

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on the standard cell associated to the microstructure. The coupling between these two systems is given on one hand by a sink/source term appearing in the macroscopic equation and involving an integral operator over the microscopic solution. On the other hand, by the boundary condition for the microscopic solution, which is a nonlinear Henry-type law involving the macroscopic concentration. Important applications are e.g. gas/liquid reactions in chemical engineering [14–16], extracellular/intracellular processes in biological tissue [10], processes in bulk and pellets for catalytic reactions [6].

The aim of this paper is to give an approach for the approximation of the solution, which exploits the special structure of the system and can be used as a basis for numerical computations. A Galerkin approach is chosen, and the functions spaces used for the approximation of the solution consist of tensor products of functions on the macroscopic domain and on the standard cell associated to the microstructure.

To show the convergence of the finite-dimensional approximates, we have to control the dependence of the cell solutions on the macroscopic variable. This is difficult because, on one hand we need strong $L^2$-convergence of the solutions and their traces to pass to the limit in the nonlinear terms. On the other hand, the macroscopic variable enters the cell problem just as a parameter, and therefore cannot be handled by standard methods. We remark that the techniques employed here are inspired by the analysis performed in [18].

This paper is organized as follows. In Section 2, the problem is stated and the assumptions on the data are formulated. In Section 3, we define the Galerkin approximations. Then, assuming stability of the projections on finite-dimensional subspaces with respect to appropriate norms, we prove estimates which guarantee the compactness of the finite-dimensional approximations. Finally, the convergence of the Galerkin approximations to a solution of the multiscale problem is shown. In Section 4, we prove uniqueness for the considered multiscale system. The positivity and boundedness of weak solutions are proved in Section 5.

## 2. Setting of the problem

To give a precise meaning to the variables in the reaction–diffusion system formulated in this section, we focus on the special case of gas-liquid reactions. Such reactions occur in a wealth of physicochemical processes in chemical engineering [2,3] or geochemistry [20], e.g. A minimal scenario for such reactions is the following: A chemical species $A_1$ penetrates an unsaturated porous material thorough the air-filled parts of the pores and dissolves in water along the interfaces between water and air. Once arrived in water, the species $A_1$ transforms into $A_2$ and diffuses then towards places occupied by another yet dissolved diffusing species $A_3$. As soon as $A_2$ and $A_3$ meet each other, they react to produce water and various products (typically salts). This reaction mechanism can be described as follows

$$\mathrm{A}_1 \leftrightharpoons \mathrm{A}_2 + \mathrm{A}_3 \xrightarrow{k} \mathrm{H_2O} + \text{products}. \tag{1}$$

For instance, the natural carbonation of stone follows the mechanism (1), where $\mathrm{A}_1 := \mathrm{CO_2(g)}$, $\mathrm{A}_2 := \mathrm{CO_2(aq)}$, and $\mathrm{A}_3 := \mathrm{Ca(OH)_2(aq)}$, while the product of reaction is in this case $\mathrm{CaCO_3(aq)}$.

Starting from a model at microscopic (pore) level, in [15] a two-scale description of gas-liquid reactions was derived by homogenization for the case when the transmission conditions at the gas/liquid interface is given by a linear Henry-type law. In this paper, we consider the case of nonlinear coupling between the microscopic and macroscopic problem. Our study is partly motivated by some remarks from [5] mentioning the occurrence of nonlinear mass-transfer effects at air/water interfaces, partly by the fact that there are still a number of incompletely understood fundamental issues concerning gas-liquid reactions, and hence, a greater flexibility in the choice of the micro-macro coupling may help to identify the precise mechanisms.

We assume that the microstructure consists of solid matrix and pores partially filled with water and partially filled with dry air; for details see Section 2.1. We assume the microstructure to be constant and wet, i.e. we do not account for any variations of the microstructure's boundaries. The wetness of the porous material is needed to host the chemical reaction (1). We assume the wet parts of the pore to be static so that they do not influence the microscopic transport. The local geometry of the porous media we are interested in is given by a standard cell.

### 2.1. Geometry of the domain

Let $\Omega$ and $\mathcal{Y}$ be connected domains in $\mathbb{R}^3$ with Lipschitz continuous boundaries. Here, $\Omega$ is the macroscopic domain, while $\mathcal{Y}$ denotes the standard pore associated with the microstructure within $\Omega$. We have that

$$\mathcal{Y} = Y \cup Y^g,$$

where $Y$ and $Y^g$ represent the wet region and the gas-filled part of the standard pore respectively. Let $Y$ and $Y^g$ be connected. The boundary of $Y$ is denoted by $\Gamma$, and consists of two parts

$$\Gamma = \Gamma_R \cup \Gamma_N,$$

where $\Gamma_R \cap \Gamma_N = \emptyset$, and $\lambda_y^2(\Gamma_R) \neq 0$. Note that $\Gamma_R$ is the gas/liquid interface along which the mass transfer occurs, and $\lambda_y^2$ denotes the surface measure on $\partial Y$. Furthermore, we denote by $\theta := |Y|$. A possible geometry for our standard pore is illustrated in Fig. 1.

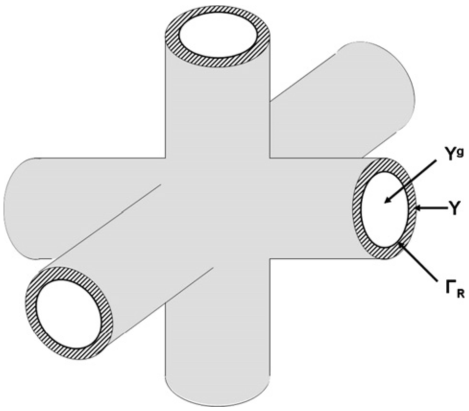


**Fig. 1.** Standard pore $\mathcal{Y}$. Typical shapes for $Y, Y^g \subset \mathcal{Y}$. $\Gamma_R$ is the interface between the gaseous part of the pore $Y^g$ and the wet region $Y$, along which the mass transfer occurs.

### *2.2. Setting of the equations*

Let us denote by $S$ the time interval $S = ]0, T[$ for a given $T > 0$. Let $U$, $u$ and $v$ denote the mass concentrations of the species $A_1$, $A_2$, and $A_3$ respectively, see (1). The mass-balance for the vector $(U, u, v)$ is described by the following two-scale system:

$$\theta \partial_t U(t,x) - D\Delta U(t,x) = -\int_{\Gamma_R} b\big(U(t,x) - u(t,x,y)\big)\, d\lambda_y^2 \quad \text{in } S \times \Omega, \tag{2}$$

$$\partial_t u(t,x,y) - d_1 \Delta_y u(t,x,y) = -k\eta\big(u(t,x,y), v(t,x,y)\big) \quad \text{in } S \times \Omega \times Y, \tag{3}$$

$$\partial_t v(t,x,y) - d_2 \Delta_y v(t,x,y) = -\alpha k\eta\big(u(t,x,y), v(t,x,y)\big) \quad \text{in } S \times \Omega \times Y, \tag{4}$$

with macroscopic non-homogeneous Dirichlet boundary condition

$$U(t,x) = U^{ext}(t,x) \quad \text{on } S \times \partial\Omega, \tag{5}$$

and microscopic homogeneous Neumann boundary conditions

$$\nabla_y u(t,x,y) \cdot n_y = 0 \quad \text{on } S \times \Omega \times \Gamma_N, \tag{6}$$

$$\nabla_y v(t,x,y) \cdot n_y = 0 \quad \text{on } S \times \Omega \times \Gamma. \tag{7}$$

The coupling between the micro- and the macro-scale is made by the following nonlinear Henry-type condition on $\Gamma_R$

$$-d_1 \nabla_y u(t,x,y) \cdot n_y = -b\big(U(t,x) - u(t,x,y)\big) \quad \text{on } S \times \Omega \times \Gamma_R. \tag{8}$$

The initial conditions

$$U(0,x) = U_I(x) \quad \text{in } \Omega, \tag{9}$$

$$u(0,x,y) = u_I(x,y) \quad \text{in } \Omega \times Y, \tag{10}$$

$$v(0,x,y) = v_I(x,y) \quad \text{in } \Omega \times Y, \tag{11}$$

close the system of mass-balance equations.

Note that the sink/source term $-\int_{\Gamma_R} b(U-u)\, d\lambda_y^2$ models the contribution in the effective equation (2) coming from mass transfer between air and water regions at microscopic level. The parameter $k$ is the reaction constant for the competitive reaction between the species $A_2$ and $A_3$, while $\alpha$ is the ratio of the molecular weights of these two species.

### *2.3. Assumptions on data and parameters*

For the transport coefficients, we assume that

(A1) $D > 0$, $d_1 > 0$, $d_2 > 0$.

Concerning the micro-macro transfer and the reaction terms, we suppose

(A2) The sink/source term $b:\mathbb{R}\to\mathbb{R}$ is globally Lipschitz continuous.
(A3) The reaction term $\eta:\mathbb{R}\times\mathbb{R}\to\mathbb{R}$ is globally Lipschitz continuous with respect to both variables.
Finally, $k,\alpha\in\mathbb{R}$, $k>0$, and $\alpha>0$.

For the initial and boundary functions, we assume

(A4) $U^{ext}\in H^1(S,H^2(\Omega))\cap H^2(S,L^2(\Omega))\cap L^\infty_+(S\times\Omega)$, $U_I\in H^2(\Omega)\cap L^\infty_+(\Omega)$, $U_I-U^{ext}(0,\cdot)\in H^1_0(\Omega)$, $u_I,v_I\in L^2(\Omega,H^2(Y))\cap L^\infty_+(\Omega\times Y)$.

Imposing additional structural conditions on the sink/source term $b$, and on the reaction term $\eta$, we are able to show also positivity and upper bounds for the solutions.

(B) Consider $b:\mathbb{R}\to\mathbb{R}_+$ with $b(z)=0$ if $z\leqslant 0$. This implies that it exists a constant $\hat{c}>0$ such that $b(z)\leqslant\hat{c}z$ if $z>0$. Furthermore, let $\eta:\mathbb{R}\times\mathbb{R}\to\mathbb{R}_+$ with $\eta(r,s)=0$ if $r\leqslant 0$ or $s\leqslant 0$.

The classical choice for $b$ in the literature on gas-solid reactions, see e.g. [3], is the linear one given by $b:\mathbb{R}\to\mathbb{R}_+$, $b(z)=\hat{c}z$ for $z>0$ and $b(z):=0$ for $z\leqslant 0$. However, there are applications, see e.g. [5], where extended Henry's Law models are required. Our assumptions on $b$ include self-limiting reactions, like e.g. Michaelis–Menten kinetics. Typical reaction rates satisfying (B) are power law reaction rates, sometimes also referred to as *generalized mass action laws*; see e.g. [2]. These laws have the form $\eta(r,s):=R(r)Q(s)$, with $R(r):=r^p$ and $Q(s):=s^q$, and $R(r)=0$ if $r\leqslant 0$, and $Q(s)=0$ if $s\leqslant 0$. The exponents $p\geqslant 1$ and $q\geqslant 1$ are called partial orders of reaction. However, to fulfill the Lipschitz condition (A3), for large values of the arguments the power laws have to replaced by Lipschitz functions.

### 2.4. Weak formulation

Our concept of weak solution is given in the following.

**Definition 1.** A triplet of functions $(U,u,v)$ with $(U-U^{ext})\in L^2(S,H^1_0(\Omega))$, $\partial_t U\in L^2(S\times\Omega)$, $(u,v)\in L^2(S,L^2(\Omega,H^1(Y)))^2$, $(\partial_t u,\partial_t v)\in L^2(S\times\Omega\times Y)^2$, is called a weak solution of (2)–(11) if for a.e. $t\in S$ the following identities hold

$$\int_\Omega \theta\partial_t U\varphi+\int_\Omega D\nabla U\nabla\varphi+\int_\Omega\int_{\Gamma_R} b(U-u)\varphi\,d\lambda_y^2\,dx=0, \tag{12}$$

$$\int_{\Omega\times Y}\partial_t u\phi+\int_{\Omega\times Y} d_1\nabla_y u\nabla_y\phi-\int_\Omega\int_{\Gamma_R} b(U-u)\phi\,d\lambda_y^2\,dx+k\int_{\Omega\times Y}\eta(u,v)\phi=0, \tag{13}$$

$$\int_{\Omega\times Y}\partial_t v\psi+\int_{\Omega\times Y} d_2\nabla_y v\nabla_y\psi+\alpha k\int_{\Omega\times Y}\eta(u,v)\psi=0, \tag{14}$$

for all $(\varphi,\phi,\psi)\in H^1_0(\Omega)\times L^2(\Omega;H^1(Y))^2$, and

$$U(0)=U_I\quad\text{in }\Omega,\qquad u(0)=u_I,\qquad v(0)=v_I\quad\text{in }\Omega\times Y.$$

### 2.5. Main result

The central result of our paper is summarized in the following theorem.

**Theorem 2.** *Let the assumptions* (A1)–(A4) *be satisfied. Assume further that the projection operators $P_x^N$, $P_y^N$ defined in* (18)–(20) *are stable with respect to the $L^2$-norm and $H^2$-norm. Let $(U_0^N,u^N,v^N)$ be the finite-dimensional approximations defined in* (21)–(23)*. Then, for $N\to\infty$, the sequence $(U_0^N+U^{ext},u^N,v^N)$ converges to the unique weak solution $(U,u,v)$ of problem* (2)–(11)*.*

The proof of this theorem is obtained by collecting the results from Theorem 6, Theorem 7, and Theorem 8.

## 3. Global existence of weak solutions

In this section, we define finite-dimensional approximations for the solutions of problem (2)–(11) by means of a multiscale Galerkin method. Our approach exploits the two-scale form of our system, and yields an ansatz for the numerical treatment of a more general class of multiscale problems. One important aspect is the choice of the bases which are used to define finite dimensional approximations of the solution. Here, the structure of the basis elements reflects the two-scale structure of the solution; the basis elements on the domain $\Omega \times Y$ are chosen as tensor products of basis elements on the macroscopic domain $\Omega$ and on the standard cell $Y$.

The convergence of the finite-dimensional approximations to the weak solution of problem (2)–(11) is shown, based on uniform estimates proved in Section 3.2. In order to be able to pass to the limit in the discretized problems, compactness for the finite-dimensional approximations, with respect to both, the microscopic and macroscopic variables, is needed. Since the macroscopic variable enters the cell problem just as a parameter, to get the required compactness is not straightforward and involves additional ideas.

### *3.1. Galerkin approximation. Global existence for the discretized problem*

We introduce the following Schauder bases: Let $\{\xi_i\}_{i\in\mathbb{N}}$ be a basis of $L^2(\Omega)$, with $\xi_j \in H_0^1(\Omega) \cap H^2(\Omega)$, forming an orthonormal system (say o.n.s.) with respect to $L^2(\Omega)$-norm. Furthermore, let $\{\zeta_{jk}\}_{j,k\in\mathbb{N}}$ be a basis of $L^2(\Omega \times Y)$, with

$$\zeta_{jk}(x, y) = \xi_j(x)\eta_k(y), \tag{15}$$

where $\{\eta_k\}_{k\in\mathbb{N}}$ is a basis of $L^2(Y)$, with $\eta_k \in H^2(Y)$, forming an o.n.s. with respect to $L^2(Y)$-norm.

Let us also define the projection operators on finite dimensional subspaces $P_x^N, P_y^N$ associated to the bases $\{\xi_j\}_{j\in\mathbb{N}}$, and $\{\eta_k,\}_{k\in\mathbb{N}}$ respectively. For $(\varphi, \psi)$ of the form

$$\varphi(x) = \sum_{j\in\mathbb{N}} a_j\xi_j(x), \tag{16}$$

$$\psi(x, y) = \sum_{j,k\in\mathbb{N}} b_{jk}\xi_j(x)\eta_k(y), \tag{17}$$

we define

$$\big(P_x^N\varphi\big)(x) = \sum_{j=1}^{N} a_j\xi_j(x), \tag{18}$$

$$\big(P_x^N\psi\big)(x, y) = \sum_{j=1}^{N}\sum_{k\in\mathbb{N}} b_{jk}\,\xi_j(x)\eta_k(y), \tag{19}$$

$$\big(P_y^N\psi\big)(x, y) = \sum_{j\in\mathbb{N}}\sum_{k=1}^{N} b_{jk}\,\xi_j(x)\eta_k(y). \tag{20}$$

The bases $\{\xi_j\}_{j\in\mathbb{N}}$, and $\{\eta_k\}_{k\in\mathbb{N}}$ are chosen such that the projection operators $P_x^N, P_y^N$ are stable with respect to the $L^2$-norm, and the $H^2$-norm; i.e. for a given function the $L^2$-norm and $H^2$-norm of the truncations by the projection operators can be estimated by the corresponding norms of the function.

Now, we look for finite-dimensional approximations of order $N \in \mathbb{N}$ for the functions $U_0 := U - U^{ext}, u$, and $v$, of the following form

$$U_0^N(t, x) = \sum_{j=1}^{N} \alpha_j^N(t)\xi_j(x), \tag{21}$$

$$u^N(t, x, y) = \sum_{j,k=1}^{N} \beta_{jk}^N(t)\xi_j(x)\eta_k(y), \tag{22}$$

$$v^N(t, x, y) = \sum_{j,k=1}^{N} \gamma_{jk}^N(t)\xi_j(x)\eta_k(y), \tag{23}$$

where the coefficients $\alpha_j^N, \beta_{jk}^N, \gamma_{jk}^N$, $j, k = 1, \ldots, N$ are determined by the following relations:

$$\int_\Omega \theta\partial_t U_0^N(t)\varphi\,dx + \int_\Omega D\nabla U_0^N(t)\nabla\varphi\,dx$$
$$= -\int_\Omega \bigg(\int_{\Gamma_R} b\big(\big(U_0^N + U^{ext} - u^N\big)(t)\big)\,d\lambda^2(y) + \theta\partial_t U^{ext}(t) - D\Delta U^{ext}(t)\bigg)\varphi\,dx, \tag{24}$$

$$\int_{\Omega\times Y} \partial_t u^N(t)\phi\,dx\,dy + \int_{\Omega\times Y} d_1 \nabla_y u^N(t)\nabla_y \phi\,dx\,dy$$
$$= \int_{\Omega}\int_{\Gamma_R} b\big(\big(U_0^N + U^{ext} - u^N\big)(t)\big)\phi\,d\lambda^2(y)\,dx - k\int_{\Omega\times Y} \eta\big(u^N(t), v^N(t)\big)\phi\,dy\,dx, \tag{25}$$

$$\int_{\Omega\times Y} \partial_t v^N(t)\psi\,dy\,dx + \int_{\Omega\times Y} d_2\nabla_y v^N(t)\nabla_y\psi\,dy\,dx = -\alpha k\int_{\Omega\times Y} \eta\big(u^N(t), v^N(t)\big)\psi\,dy\,dx \tag{26}$$

for all $\varphi \in \operatorname{span}\{\xi_j\colon\ j\in\{1,\dots,N\}\}$, and $\phi,\psi \in \operatorname{span}\{\zeta_{jk}\colon\ j,k\in\{1,\dots,N\}\}$, and

$$\alpha_j^N(0) := \int_{\Omega} \big(U_I - U^{ext}(0)\big)\xi_j\,dx, \tag{27}$$

$$\beta_{jk}^N(0) := \int_{\Omega}\int_{Y} u_I\zeta_{jk}\,dx\,dy, \tag{28}$$

$$\gamma_{jk}^N(0) := \int_{\Omega}\int_{Y} v_I\zeta_{jk}\,dx\,dy. \tag{29}$$

Taking in (24)–(26) as test functions $\varphi=\xi_j, \phi=\zeta_{jk}$, and $\psi=\zeta_{jk}$, for $j,k=1,\dots,N$, we obtain the following system of ordinary differential equations for the coefficients $\alpha^N = (\alpha_j^N)_{j=1,\dots,N}$, $\beta^N = (\beta_{jk}^N)_{\substack{j=1,\dots,N\\k=1,\dots,N}}$, and $\gamma^N = (\gamma_{jk}^N)_{\substack{j=1,\dots,N\\k=1,\dots,N}}$:

$$\partial_t\alpha^N(t) + \sum_{i=1}^N A_i\alpha_i^N(t) = F\big(\alpha^N(t),\beta^N(t)\big), \tag{30}$$

$$\partial_t\beta^N(t) + \sum_{i,l=1}^N B_{il}\beta_{il}^N(t) = \tilde F\big(\alpha^N(t),\beta^N(t)\big) + G\big(\beta^N(t),\gamma^N(t)\big), \tag{31}$$

$$\partial_t\gamma^N(t) + \sum_{i,l=1}^N C_{il}\gamma_{il}^N(t) = \alpha G\big(\beta^N(t),\gamma^N(t)\big), \tag{32}$$

where for $j,k,i,l = 1,\dots,N$ we have

$$(A_i)_j := \frac{1}{\theta}\int_{\Omega} D\nabla\xi_i(x)\nabla\xi_j(x)\,dx,$$

$$(B_{il})_{jk} := \int_{\Omega\times Y} d_1\nabla_y\zeta_{il}(x,y)\nabla\zeta_{jk}(x,y)\,dy\,dx,$$

$$(C_{il})_{jk} := \int_{\Omega\times Y} d_2\nabla_y\zeta_{il}(x,y)\nabla\zeta_{jk}(x,y)\,dy\,dx,$$

$$F_j := -\frac{1}{\theta}\int_{\Omega}\left(\int_{\Gamma_R} b\big(\big(U_0^N + U^{ext} - u^N\big)(t)\big)d\lambda_y^2 + \theta\partial_t U^{ext}(t) - D\Delta U^{ext}(t)\right)\xi_j(x)\,dx,$$

$$\tilde F_{jk} := \int_{\Omega}\int_{\Gamma_R} b\big(\big(U_0^N + U^{ext} - u^N\big)(t)\big)\zeta_{jk}(x,y)\,d\lambda^2(y)\,dx,$$

$$G_{jk} := k\int_{\Omega\times Y}\eta\big(u^N(t), v^N(t)\big)\zeta_{jk}\,dy\,dx.$$

Due to the assumptions (A2)–(A3) on $b$ and $\eta$, the functions $F, \tilde F$, and $G$ are globally Lipschitz continuous, and the Cauchy problem (27)-(32) has a unique solution $(\alpha^N, \beta^N, \gamma^N)$ in $C^1([0,T])^N \times C^1([0,T])^{N^2} \times C^1([0,T])^{N^2}$.

We conclude this section by proving the global Lipschitz property of $\tilde F$, the proof of the Lipschitz continuity of $F$ and $G$ is similar. Let $(U_0^N, u^N)$ and $(W_0^N, w^N)$ be of the form (21), (22), with coefficients $(\alpha_1^N, \beta_1^N), (\alpha_2^N, \beta_2^N) \in \mathbb{R}^N \times \mathbb{R}^{N^2}$. We have:

$$
\begin{aligned}
&\tilde F_{jk}\big(\alpha_1^N,\beta_1^N\big)-\tilde F_{jk}\big(\alpha_2^N,\beta_2^N\big)\\
&\quad=\int_\Omega\int_{\Gamma_R}\big[b\big(U_0^N+U^{ext}-u^N\big)(t)-b\big(W_0^N+U^{ext}-w^N\big)(t)\big]\zeta_{jk}\,d\lambda_y^2\,dx\\
&\quad\leqslant C\int_\Omega\int_{\Gamma_R}\big|\big(U_0^N-W_0^N\big)-\big(u^N-w^N\big)\big||\zeta_{jk}|\,d\lambda_y^2\,dx\\
&\quad=C\int_\Omega\int_{\Gamma_R}\left|\sum_{i=1}^N\big(\alpha_1^N(t)-\alpha_2^N(t)\big)_i\xi_i-\sum_{i=1}^N\sum_{\ell=1}^N\big(\beta_1^N(t)-\beta_2^N(t)\big)_{i\ell}\zeta_{i\ell}\right||\zeta_{jk}|\,d\lambda_y^2\,dx\\
&\quad\leqslant C\sum_{i=1}^N\big|\big(\alpha_1^N(t)-\alpha_2^N(t)\big)_i\big|\int_\Omega\int_{\Gamma_R}\big|\xi_i(x)\big|\big|\zeta_{jk}(x,y)\big|\,d\lambda_y^2\,dx\\
&\qquad+C\sum_{i=1}^N\sum_{\ell=1}^N\big|\big(\beta_1^N(t)-\beta_2^N(t)\big)_{i\ell}\big|\int_\Omega\int_{\Gamma_R}\big|\zeta_{i\ell}(x,y)\big|\big|\zeta_{jk}(x,y)\big|\,d\lambda_y^2\,dx\\
&\quad\leqslant C\max\{c_{ijk}\}\sum_{i=1}^N\big|\big(\alpha_1^N(t)-\alpha_2^N(t)\big)_i\big|+C\max\{c_{i\ell jk}\}\sum_{i=1}^N\sum_{\ell=1}^N\big|\big(\beta_1^N(t)-\beta_2^N(t)\big)_{i\ell}\big|,
\end{aligned}
$$

where the coefficients $c_{ijk}$ and $c_{i\ell jk}$ are given by

$$
\begin{aligned}
c_{ijk}&:=\int_\Omega\int_{\Gamma_R}\big|\xi_i(x)\big|\big|\zeta_{jk}(x,y)\big|\,d\lambda_y^2\,dx,\\
c_{i\ell jk}&:=\int_\Omega\int_{\Gamma_R}\big|\zeta_{i\ell}(x,y)\big|\big|\zeta_{jk}(x,y)\big|\,d\lambda_y^2\,dx
\end{aligned}
$$

for $i,l,j,k=1,\dots,N$. Thus, we obtain

$$
\big|\tilde F\big(\alpha_1^N,\beta_1^N\big)-\tilde F\big(\alpha_2^N,\beta_2^N\big)\big|\leqslant c(N)\big(\big|\alpha_1^N-\alpha_2^N\big|+\big|\beta_1^N-\beta_2^N\big|\big). \tag{33}
$$

**Remark 3.** In the representation of an element $\psi\in L^2(\Omega\times Y)$ with respect to the basis $\{\zeta_{jk}\}$, see e.g. (17), we make an abuse of notation when we let both indices $j$, and $k$ to vary from $1,\dots,N$. However, taking $j=1,\dots,N_1$, and $k=1,\dots,N_2$ would only overload the notation; the proofs in the article would not change.

### *3.2. Uniform estimates for the discretized problems*

In this section, we prove uniform estimates for the solutions to the finite-dimensional problems. Based on these estimates, in the next section, we are able to pass in (24)–(26) to the limit $N\to\infty$.

**Theorem 4.** *Assume that the projection operators $P_x^N$, $P_y^N$, defined in* (18)–(20)*, are stable with respect to the $L^2$-norm and $H^2$-norm, and that* (A1)–(A4) *are satisfied. Then there exists a constant $C>0$, independent of $N$, such that*

$$
\big\|U_0^N\big\|_{L^\infty(S,H^1(\Omega))}+\big\|\partial_tU_0^N\big\|_{L^2(S,L^2(\Omega))}\leqslant C, \tag{34}
$$

$$
\big\|u^N\big\|_{L^\infty(S,L^2(\Omega;H^1(Y)))}+\big\|\partial_tu^N\big\|_{L^2(S,L^2(\Omega;L^2(Y)))}\leqslant C, \tag{35}
$$

$$
\big\|v^N\big\|_{L^\infty(S,L^2(\Omega;H^1(Y)))}+\big\|\partial_tv^N\big\|_{L^2(S,L^2(\Omega;L^2(Y)))}\leqslant C. \tag{36}
$$

**Proof.** Let us first take $(\varphi,\phi,\psi)=(U_0^N,u^N,v^N)$ as test function in (24)–(26). Using the Lipschitz continuity of the reaction term $\eta$, we get

$$
\begin{aligned}
&\frac{\theta}{2}\frac{d}{dt}\big\|U_0^N(t)\big\|_{L^2(\Omega)}^2+\frac12\frac{d}{dt}\big\|u^N(t)\big\|_{L^2(\Omega\times Y)}^2+\frac12\frac{d}{dt}\big\|v^N(t)\big\|_{L^2(\Omega\times Y)}^2\\
&\quad+D\big\|\nabla U_0^N\big\|_{L^2(\Omega)}^2+d_1\big\|\nabla_yu^N\big\|_{L^2(\Omega\times Y)}^2+d_2\big\|\nabla_yv^N(t)\big\|_{L^2(\Omega\times Y)}^2\\
&\quad+\int_\Omega\int_{\Gamma_R}b\big(U_0^N+U^{ext}-u^N\big)\big(U_0^N-u^N\big)\,d\lambda_y^2\,dx+\int_\Omega\big(\theta\partial_tU^{ext}+\Delta U^{ext}\big)U_0^N
\end{aligned}
$$

$$
\begin{aligned}
&= -k \int_{\Omega\times Y} \eta\big(u^N, v^N\big)\big(u^N + \alpha v^N\big) \\
&\leqslant C \int_{\Omega\times Y} \big(1 + |u^N| + |v^N|\big)\big(|u^N| + |v^N|\big).
\end{aligned} \tag{37}
$$

To estimate the following term, we use the Lipschitz property of $b$ and the interpolation-trace inequality (2.21) from [12, p. 69].

$$
\begin{aligned}
&\int_\Omega \int_{\Gamma_R} b\big(U_0^N + U^{ext} - u^N\big)\big(U_0^N - u^N\big)\, d\lambda_y^2\, dx \\
&\quad \leqslant \hat{c} \int_\Omega \int_{\Gamma_R} \big|U_0^N + U_0^{ext} - u^N\big|\big|U_0^N - u^N\big|\, d\lambda_y^2\, dx \\
&\quad \leqslant C \int_\Omega \int_{\Gamma_R} \big(|U_0^N|^2 + |U^{ext}|^2 + |u^N|^2\big)\, d\lambda_y^2\, dx \\
&\quad \leqslant C\big(\|U_0^N\|^2_{L^2(\Omega)} + \|U^{ext}\|^2_{L^2(\Omega)}\big) + C\int_\Omega \|u^N\|_{H^1(Y)} \|u^N\|_{L^2(Y)} \\
&\quad \leqslant C\big(\|U_0^N\|^2_{L^2(\Omega)} + \|U^{ext}\|^2_{L^2(\Omega)}\big) + \epsilon \|\nabla_y u^N\|^2_{L^2(\Omega\times Y)} + C(\epsilon)\|u^N\|^2_{L^2(\Omega\times Y)}.
\end{aligned} \tag{38}
$$

Taking $\epsilon := \frac{d_1}{2}$ in (38), inserting (38) in (37), and using the regularity properties of $U^{ext}$, we obtain

$$
\begin{aligned}
&\frac{d}{dt}\|U_0^N(t)\|^2_{L^2(\Omega)} + \frac{d}{dt}\|u^N(t)\|^2_{L^2(\Omega\times Y)} + \frac{d}{dt}\|v^N(t)\|^2_{L^2(\Omega\times Y)} \\
&\qquad + \|\nabla U_0^N(t)\|^2_{L^2(\Omega)} + \|\nabla_y u^N\|^2_{L^2(\Omega\times Y)} + \|\nabla_y v^N\|^2_{L^2(\Omega\times Y)} \\
&\quad \leqslant C + \|U_0^N\|^2_{L^2(\Omega)} + \|u^N\|^2_{L^2(\Omega\times Y)} + \|v^N\|^2_{L^2(\Omega\times Y)}.
\end{aligned} \tag{39}
$$

Integrating with respect to time, and applying Gronwall's inequality yields the estimates

$$
\|U_0^N\|_{L^\infty(S,L^2(\Omega))} + \|\nabla U_0^N\|_{L^2(S,L^2(\Omega))} \leqslant c, \tag{40}
$$

$$
\|u^N\|_{L^\infty(S,L^2(\Omega\times Y)))} + \|\nabla_y u^N\|_{L^2(S,L^2(\Omega\times Y))} \leqslant c, \tag{41}
$$

$$
\|v^N\|_{L^\infty(S,L^2(\Omega\times Y)))} + \|\nabla_y v^N\|_{L^2(S,L^2(\Omega\times Y))} \leqslant c. \tag{42}
$$

To obtain $L^\infty$-estimates with respect to time of the gradients, and the estimates for the time derivatives, we differentiate with respect to time the weak formulation (24)–(26), and test with $(\varphi, \phi, \psi) = (\partial_t U_0^N, \partial_t u^N, \partial_t v^N)$. We obtain:

$$
\begin{aligned}
&\frac{1}{2}\frac{d}{dt}\int_\Omega \theta\big|\partial_t U_0^N(t)\big|^2 + \frac{1}{2}\frac{d}{dt}\int_{\Omega\times Y} \big|\partial_t u^N(t)\big|^2 + \frac{1}{2}\frac{d}{dt}\int_{\Omega\times Y} \big|\partial_t v^N(t)\big|^2 \\
&\qquad + D\int_\Omega \big|\nabla\partial_t U_0^N\big|^2 + d_1 \int_{\Omega\times Y} \big|\nabla_y \partial_t u^N\big|^2 + d_2 \int_{\Omega\times Y} \big|\nabla_y \partial_t v^N\big|^2 \\
&\qquad + \int_\Omega \int_{\Gamma_R} b'\big(U_0^N + U^{ext} - u^N\big)\big(\partial_t U_0^N + \partial_t U^{ext} - \partial_t u_t^N\big)\big(\partial_t U_0^N - \partial_t u_t^N\big)\, d\lambda_y^2 \\
&\quad = -\int_\Omega \theta \partial_{tt} U^{ext} \partial_t U_0^N + \int_\Omega D\Delta \partial_t U^{ext} \partial_t U_0^N \\
&\qquad + k\int_{\Omega\times Y} \big(\partial_u \eta\big(u^N, v^N\big)\partial_t u^N + \partial_v \eta\big(u^N, v^N\big)\partial_t v^N\big)\big(\partial_t u^N + \alpha\partial_t v^N\big).
\end{aligned} \tag{43}
$$

Integrating this expression with respect to time, using the Lipschitz properties of the nonlinear terms $b$ and $\eta$, and the regularity properties of $U^{ext}$, as well as the interpolation-trace inequality (2.21) from [12, p. 69], we obtain for all $t \in S$

$$\int_{\Omega} |\partial_t U_0^N(t)|^2 + \int_{\Omega\times Y} \left|\partial_t u^N(t)\right|^2 + \int_{\Omega\times Y} \left|\partial_t v^N(t)\right|^2 + \int_0^t \int_{\Omega\times Y} \left|\nabla \partial_t U_0^N\right|^2 \int_0^t \int_{\Omega\times Y} \left|\nabla_y \partial_t u^N\right|^2 + \int_0^t \int_{\Omega\times Y} \left|\nabla_y \partial_t v^N\right|^2$$
$$\leqslant \int_{\Omega} \left|\partial_t U_0^N(0)\right|^2 + \int_{\Omega\times Y} \left|\partial_t u^N(0)\right|^2 + \int_{\Omega\times Y} \left|\partial_t v^N(0)\right|^2$$
$$+ C\left(1 + \int_0^t \int_{\Omega} \left|\partial_t U_0^N(t)\right|^2 + \int_0^t \int_{\Omega\times Y} \left|\partial_t u^N\right|^2 + \int_0^t \int_{\Omega\times Y} \left|\partial_t v^N\right|^2\right). \tag{44}$$

To proceed, we have to estimate the norm of $(\partial_t U_0^N, \partial_t u^N, \partial_t v^N)$ at $t = 0$. For this purpose, we evaluate the weak formulation (24)–(26) at $t = 0$, and test with $(\partial_t U_0^N(0), \partial_t u^N(0), \partial_t v^N(0))$. We obtain

$$\int_{\Omega} \theta\left|\partial_t U_0^N(0)\right|^2 + \int_{\Omega} D\nabla U_0^N(0)\nabla \partial_t U_0^N(0)$$
$$= -\int_{\Omega}\int_{\Gamma_R} b\big(U_0^N(0) + U^{ext}(0) - u^N(0)\big)\partial_t U_0^N(0)\, d\lambda_y^2\, dx - \int_{\Omega} \theta \partial_t U^{ext}(0)\partial_t U_0^N(0) - \int_{\Omega} D\Delta U^{ext}(0)\partial_t U_0^N(0), \tag{45}$$

$$\int_{\Omega\times Y} \left|\partial_t u^N(0)\right|^2 + \int_{\Omega\times Y} \left|\partial_t v^N(0)\right|^2 + \int_{\Omega\times Y} d_1 \nabla_y u^N(0)\nabla_y \partial_t u^N(0) + \int_{\Omega\times Y} d_2 \nabla_y v^N(0)\nabla_y \partial_t v^N(0)$$
$$= \int_{\Omega}\int_{\Gamma_R} b\big(U_0^N(0) + U^{ext}(0) - u^N(0)\big)\partial_t u^N(0)\, d\lambda_y^2\, dx + k \int_{\Omega\times Y} \eta\big(u^N(0), v^N(0)\big)\big(\partial_t u^N(0) + \alpha \partial_t v^N(0)\big). \tag{46}$$

Integrating by parts in the higher order terms, and using the fact that $u^N$ satisfies the transmission condition (8) in a weak sense, we obtain

$$\int_{\Omega} \theta\left|\partial_t U_0^N(0)\right|^2 + \int_{\Omega\times Y} \left|\partial_t u^N(0)\right|^2 + \int_{\Omega\times Y} \left|\partial_t v^N(0)\right|^2$$
$$= \int_{\Omega} D\Delta U_0^N(0)\partial_t U_0^N(0) + \int_{\Omega\times Y} d_1 \Delta_y u^N(0)\partial_t u^N(0) + \int_{\Omega\times Y} d_2 \Delta_y v^N(0)\partial_t v^N(0)$$
$$- \int_{\Omega}\int_{\Gamma_R} b\big(U_0^N(0) + U^{ext}(0) - u^N(0)\big)\partial_t U_0^N(0)\, d\lambda_y^2\, dx - \int_{\Omega} \theta \partial_t U^{ext}(0)\partial_t U_0^N(0) - \int_{\Omega} D\Delta U^{ext}(0)\partial_t U_0^N(0)$$
$$+ k \int_{\Omega\times Y} \eta\big(u^N(0), v^N(0)\big)\big(\partial_t u^N(0) + \alpha \partial_t v^N(0)\big). \tag{47}$$

Now, the regularity properties of the initial and boundary data, together with the stability of the projection operators $P_x^N$ and $P_y^N$ with respect to the $H^2$-norm, yield the desired bounds on the time derivatives at $t = 0$:

$$\int_{\Omega} \left|\partial_t U_0^N(0)\right|^2 + \int_{\Omega\times Y} \left|\partial_t u^N(0)\right|^2 + \int_{\Omega\times Y} \left|\partial_t v^N(0)\right|^2 \leqslant c. \tag{48}$$

Inserting now (48) into (44), and using Gronwall's inequality, the estimates of the theorem are proved. □

The estimates proved in Theorem 4 still don't provide the compactness for the solutions $(U_0^N, u^N, v^N)$ needed to pass to the limit $N \to \infty$ in the nonlinear terms of the variational formulation (24)–(26). In the next theorem, additional regularity of the solutions $u^N, v^N$ with respect to the macroscopic variable $x$ is proved.

**Theorem 5.** *Assume that* (A1)–(A4) *are satisfied. Then there exists a constant* $c > 0$*, independent of* $N$*, such that the following estimates hold*

$$\left\|\nabla_x u^N\right\|_{L^\infty(S,L^2(\Omega\times Y))} + \left\|\nabla_x v^N\right\|_{L^\infty(S,L^2(\Omega\times Y))} \leqslant c, \tag{49}$$
$$\left\|\nabla_y \nabla_x u^N\right\|_{L^2(S,L^2(\Omega\times Y))} + \left\|\nabla_y \nabla_x v^N\right\|_{L^2(S,L^2(\Omega\times Y))} \leqslant c. \tag{50}$$

**Proof.** Let $\Omega'$ be an arbitrary compact subset of $\Omega$, and let $h \in ]0, dist(\Omega', \partial\Omega)[$. Denote by $D_i^h U_0^N$, $D_i^h u^N$, and $D_i^h v^N$ the difference quotients with respect to the variable $x_i$, for $i = 1, \dots, n$, of $U_0^N, u^N$, and $v^N$ respectively. For example,

$$D_i^h(t,x,y) := \frac{u^N(t, x + he_i, y) - u^N(t,x,y)}{h},$$

for all $t \in S$, $x \in \Omega'$, and $y \in Y$. Following the approach in [9], we fix an open set $G$ such that $\Omega' \subset\subset G \subset\subset \Omega$ and select a cutoff function $\vartheta \in C_0^\infty(\Omega)$ satisfying $\vartheta = 1$ on $\Omega'$, $\vartheta = 0$ on $\Omega \setminus G$, and $0 \leqslant \vartheta \leqslant 1$. We consider Eqs. (25)–(26), tested with $(\phi, \psi) := (-D_i^{-h}(\vartheta^2 D_i^h u^N), -D_i^{-h}(\vartheta^2 D_i^h v^N))$:

$$\begin{aligned}
&-\int_{\Omega\times Y} \partial_t u^N(t) D_i^{-h}\big(\vartheta^2 D_i^h u^N\big) - \int_{\Omega\times Y} d_1 \nabla_y u^N(t) \nabla_y\big(D_i^{-h}\big(\vartheta^2 D_i^h u^N\big)\big) \\
&\quad + \int_\Omega \int_{\Gamma_R} b\big(\big(U_0^N + U^{ext} - u^N\big)(t)\big) D_i^{-h}\big(\vartheta^2 D_i^h u^N\big)\, d\lambda^2(y) \\
&\quad = k \int_{\Omega\times Y} \eta\big(u^N(t), v^N(t)\big) D_i^{-h}\big(\vartheta^2 D_i^h u^N\big) \\
&\quad - \int_{\Omega\times Y} \partial_t v^N(t) D_i^{-h}\big(\vartheta^2 D_i^h v^N\big) - \int_{\Omega\times Y} d_2 \nabla_y v^N(t) \nabla_y\big(D_i^{-h}\big(\vartheta^2 D_i^h v^N\big)\big) \\
&\quad = \alpha k \int_{\Omega\times Y} \eta\big(u^N(t), v^N(t)\big) D_i^{-h}\big(\vartheta^2 D_i^h v^N\big).
\end{aligned}$$

Using the formula of integration by parts for difference quotients, see (16), Section 6.3 in [9], the Lipschitz property of the sink/source term $b$ and of the reaction term $\eta$, we obtain:

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}\int_{\Omega\times Y} \big|\vartheta D_i^h u^N\big|^2 + d_1 \int_{\Omega\times Y} \vartheta^2 \big|\nabla_y\big(D_i^h u^N\big)\big|^2 + \frac{1}{2}\frac{d}{dt}\int_{\Omega\times Y} \big|\vartheta D_i^h v^N\big|^2 + d_1 \int_{\Omega\times Y} \vartheta^2 \big|\nabla_y\big(D_i^h v^N\big)\big|^2 \\
&\quad = \int_\Omega \int_{\Gamma_R} D_i^h b\big(U_0^N + U^{ext} - u^N\big)\vartheta^2 D_i^h u^N d\lambda^2(y) + k \int_{\Omega\times Y} D_i^h \eta\big(u^N, v^N\big)\vartheta^2\big(D_i^h u^N + \alpha D_i^h v^N\big) \\
&\quad \leqslant C \int_\Omega \big(\big|\vartheta D_i^h U_0^N\big|^2 + \big|\vartheta D_i^h U^{ext}\big|^2\big) + \int_\Omega \int_{\Gamma_R} \big|\vartheta D_i^h u^N\big|^2 + C \int_{\Omega\times Y} \big(\big|\vartheta D_i^h u^N\big|^2 + \big|\vartheta D_i^h v^N\big|^2\big).
\end{aligned}$$

Using the regularity of the boundary term $U^{ext}$, the estimate (34) for $U_0^N$, as well as the interpolation-trace estimate (2.21) from [12, p. 69] to estimate the term on $\Gamma_R$, we obtain

$$\begin{aligned}
&\frac{d}{dt}\int_{\Omega\times Y} \big|\vartheta D_i^h u^N\big|^2 + \frac{d}{dt}\int_{\Omega\times Y} \big|\vartheta D_i^h v^N\big|^2 + d_1 \int_{\Omega\times Y} \vartheta^2 \big|\nabla_y\big(D_i^h u^N\big)\big|^2 + d_1 \int_{\Omega\times Y} \vartheta^2 \big|\nabla_y\big(D_i^h v^N\big)\big|^2 \\
&\quad \leqslant C + C \int_{\Omega\times Y} \big(\big|\vartheta D_i^h u^N\big|^2 + \big|\vartheta D_i^h v^N\big|^2\big). \qquad (51)
\end{aligned}$$

Integrating with respect to time in (51), and applying Gronwall's inequality and the stability of the projection operators with respect to the $H^1(\Omega)$-norm, yields for all $i = 1, \dots, n$, and $N \in \mathbb{N}$ the estimates

$$\big\|D_i^h u^N\big\|_{L^\infty(S, L^2(\Omega\times Y))} + \big\|D_i^h v^N\big\|_{L^\infty(S, L^2(\Omega\times Y))} \leqslant C, \qquad (52)$$

$$\big\|\nabla_y\big(D_i^h u^N\big)\big\|_{L^2(S, L^2(\Omega\times Y))} + \big\|\nabla_y\big(D_i^h v^N\big)\big\|_{L^2(S, L^2(\Omega\times Y))} \leqslant C \qquad (53)$$

with a constant $c$ independent of $i, h$, and $N$. Now applying the result on difference quotients from Lemma 7.24, in [7], the estimates (49)–(50) follow. □

### 3.3. Convergence of the Galerkin approximates

In this section, we prove the convergence of the Galerkin approximations $(U_0^N, u^N, v^N)$ to the weak solution of the two-scale problem (2)–(11). Based on the estimates proved in Section 3.2, we first derive the following convergence properties of the sequence of finite-dimensional approximations.

**Theorem 6.** *There exists a subsequence, again denoted by* $(U_0^N, u^N, v^N)$*, and a limit vector function* $(U_0, u, v) \in L^2(S; H^1(\Omega)) \times [L^2(S; L^2(\Omega; H^1(Y)))]^2$*, with* $(\partial_t U_0^N, \partial_t u^N, \partial_t v^N) \in L^2(S \times \Omega) \times [L^2(S \times \Omega \times Y)]^2$*, such that*

$$\big(U_0^N, u^N, v^N\big) \to (U_0, u, v) \quad \text{weakly in } L^2\big(S; H^1(\Omega)\big) \times \big[L^2\big(S; L^2\big(\Omega; H^1(Y)\big)\big)\big]^2, \tag{54}$$

$$\big(\partial_t U_0^N, \partial_t u^N, \partial_t v^N\big) \to (\partial_t U_0, \partial_t u, \partial_t v) \quad \text{weakly in } L^2, \tag{55}$$

$$\big(U_0^N, u^N, v^N\big) \to (U_0, u, v) \quad \text{strongly in } L^2, \tag{56}$$

$$u^N\big|_{\Gamma_R} \to u|_{\Gamma_R} \quad \text{strongly in } L^2\big(S \times \Omega, L^2(\Gamma_R)\big). \tag{57}$$

**Proof.** The estimates from Theorem 4 immediately imply (54) and (55). Since

$$\|U_0^N\|_{L^2(S,H^1(\Omega))} + \|\partial_t U_0^N\|_{L^2(S,L^2(\Omega))} \leqslant C,$$

Lions–Aubin's compactness theorem, see [13, Theorem 1, p. 58], implies that there exists a subset (again denoted by $U_0^N$) such that

$$U_0^N \longrightarrow U_0 \quad \text{strongly in } L^2(S \times \Omega).$$

To get the strong convergences for the cell solutions $u^N, v^N$, we need the higher regularity with respect to the variable $x$, proved in Theorem 5. We remark that the estimates (49)–(50) imply that

$$\|u^N\|_{L^2(S;H^1(\Omega,H^1(Y)))} + \|v^N\|_{L^2(S;H^1(\Omega,H^1(Y)))} \leqslant C.$$

Moreover, from Theorem 4, we have that

$$\|\partial_t u^N\|_{L^2(S\times\Omega\times Y)} + \|\partial_t v^N\|_{L^2(S\times\Omega\times Y)} \leqslant C.$$

Since the embedding

$$H^1\big(\Omega, H^1(Y)\big) \hookrightarrow L^2\big(\Omega, H^\beta(Y)\big)$$

is compact for all $\frac{1}{2} < \beta < 1$, it follows again from Lions–Aubin's compactness theorem that there exist subsequences (again denoted $u^N, v^N$), such that

$$\big(u^N, v^N\big) \longrightarrow (u, v) \quad \text{strongly in } L^2\big(S \times L^2\big(\Omega, H^\beta(Y)\big)\big), \tag{58}$$

for all $\frac{1}{2} < \beta < 1$. Now, (58) together with the continuity of the trace operator

$$H^\beta(Y) \hookrightarrow L^2(\Gamma_R), \quad \text{for } \frac{1}{2} < \beta < 1$$

yield the convergences (56) and (57). □

**Theorem 7.** *Let the assumptions* (A1)–(A4) *be satisfied. Assume further that the projection operators* $P_x^N, P_y^N$ *defined in* (18)–(20) *are stable with respect to the* $L^2$*-norm and* $H^2$*-norm. Let* $(U_0, u, v)$ *be the limit function obtained in Theorem* 6*. Then, the function* $(U_0 + U^{ext}, u, v)$ *is a weak solution of problem* (2)–(11)*.*

**Proof.** Using the convergence results in Theorem 6, and passing to the limit in (24)–(26), for $N \to \infty$, standard arguments lead to the variational formulation (12)–(14) for the function $(U, u, v) = (U_0 + U^{ext}, u, v)$. □

## 4. Uniqueness of weak solutions

Let us now show that problem (2)–(11) has a unique weak solution.

**Proposition 8.** *If* (A1)–(A4) *hold, then the weak solution to* (2)–(11) *is unique.*

**Proof.** Let $(U_i, u_i, v_i)$, $i \in \{1, 2\}$, be arbitrary weak solutions of problem (2)–(11). We subtract the weak formulation written for $(U_2, u_2, v_2)$ from that one written for $(U_1, u_1, v_1)$ and choose in the result as test function $(\varphi, \phi, \psi) := (U_2 - U_1, u_2 - u_1, v_2 - v_1) \in H_0^1(\Omega) \times [L^2(\Omega; H^1(Y))]^2$. We obtain:

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}\int_{\Omega}\theta|U_2-U_1|^2+\frac{1}{2}\frac{d}{dt}\int_{\Omega\times Y}|u_2-u_1|^2+\frac{1}{2}\frac{d}{dt}\int_{\Omega\times Y}|v_2-v_1|^2\\
&\quad+D\int_{\Omega}\left|\nabla(U_2-U_1)\right|^2+d_1\int_{\Omega\times Y}\left|\nabla_y(u_2-u_1)\right|^2+d_2\int_{\Omega\times Y}\left|\nabla_y(v_2-v_1)\right|^2\\
&\quad+k\int_{\Omega\times Y}\big(\eta(u_2,v_2)-\eta(u_1,v_1)\big)\big[(u_2-u_1)+\alpha(v_2-v_1)\big]\\
&\quad+\int_{\Omega}\int_{\Gamma_R}\big[b(U_2-u_2)-b(U_1-u_1)\big]\big[(U_2-U_1)-(u_2-u_1)\big]\,d\lambda_y^2\,dx=0.
\end{aligned}\tag{59}$$

The last two terms in (59), say $I_1$ and $I_2$, can be estimated as follows.

$$\begin{aligned}
I_1&\leqslant\left|k\int_{\Omega\times Y}\big(\eta(u_2,v_2)-\eta(u_1,v_1)\big)\big[(u_2-u_1)+\alpha(v_2-v_1)\big]\right|\\
&\leqslant C\int_{\Omega\times Y}\big(|u_2-u_1|^2+|v_2-v_1|^2\big).
\end{aligned}$$

We estimate $I_2$ as follows.

$$\begin{aligned}
I_2&\leqslant\left|\int_{\Omega}\int_{\Gamma_R}\big[b(U_2-u_2)-b(U_1-u_1)\big]\big[(U_2-U_1)-(u_2-u_1)\big]\,d\lambda_y^2\,dx\right|\\
&\leqslant C\int_{\Omega}\int_{\Gamma_R}|U_2-U_1|^2d\lambda_y^2\,dx+C\int_{\Omega}\int_{\Gamma_R}|u_2-u_1|^2\,d\lambda_y^2\,dx.
\end{aligned}\tag{60}$$

To estimate the second term in (60) we use the interpolation-trace inequality (2.21) from [12, p. 69]. We obtain

$$\begin{aligned}
\int_{\Omega}\int_{\Gamma_R}|u_2-u_1|^2d\lambda_y^2\,dx&\leqslant C\int_{\Omega}\big(\left\|\nabla_y(u_2-u_1)\right\|_{L^2(Y)}+\|u_2-u_1\|_{L^2(Y)}\big)\|u_2-u_1\|_{L^2(Y)}\\
&\leqslant\epsilon\int_{\Omega}\left\|\nabla_y(u_2-u_1)\right\|^2_{L^2(Y)}+c_\epsilon\int_{\Omega}\|u_2-u_1\|^2_{L^2(Y)}.
\end{aligned}$$

Choosing now $\epsilon=\frac{d_1}{2}$, and applying Gronwall's inequality, we conclude the statement of the proposition. □

## 5. Non-negativity and upper bounds of weak solutions

Assuming additional structural conditions for the sink/source term $b$, and the nonlinear reaction term $\eta$, we can show that weak solutions of problem (2)–(11) are non-negative and uniformly bounded. These results are proved in the following.

**Lemma 9.** *Assume that hypotheses* (A1)–(A4)*, and* (B) *hold, and that* $(U,u,v)$ *is a weak solution of problem* (2)–(11)*. Then, for a.e.* $(x,y)\in\Omega\times Y$ *and all* $t\in S$*, we have*

$$U(t,x)\geqslant 0,\qquad u(t,x,y)\geqslant 0,\qquad v(t,x,y)\geqslant 0.\tag{61}$$

**Proof.** We use here the notation $u^+:=\max\{0,u\}$ and $u^-:=\max\{0,-u\}$. Testing in (12)–(14) with $(\varphi,\phi,\psi):=(-U^-,-u^-,-v^-)$, we obtain

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}\int_{\Omega}\theta\left|U^-\right|^2+\frac{1}{2}\frac{d}{dt}\int_{\Omega\times Y}\left|u^-\right|^2+D\int_{\Omega}\left|\nabla U^-\right|^2+d_1\int_{\Omega\times Y}\left|\nabla_y u^-\right|^2\\
&\quad-k\int_{\Omega\times Y}\eta(u,v)u^-+\int_{\Omega}\int_{\Gamma_R}b(U-u)\big(u^--U^-\big)\,d\lambda_y^2\,dx=0,
\end{aligned}\tag{62}$$

$$\frac{1}{2}\frac{d}{dt}\int_{\Omega\times Y}\left|v^-\right|^2+d_2\int_{\Omega\times Y}\left|\nabla v^-\right|^2-\alpha k\int_{\Omega\times Y}\eta(u,v)v^-=0.\tag{63}$$

Note that by (A3) the last but one term of the r.h.s. of (62) and the last term of (63) vanish. We denote by $\mathcal{H}(\cdot)$ the Heaviside function and estimate the last term of (62) as follows:

$$\begin{aligned}
\int_\Omega\int_{\Gamma_R} b(U-u)\big(U^- - u^-\big)\,d\lambda_y^2\,dx &\leqslant \int_\Omega\int_{\Gamma_R} b(U-u)U^-\,d\lambda_y^2\,dx \\
&\leqslant \hat{c}\int_\Omega\int_{\Gamma_R} \mathcal{H}(U-u)(U-u)U^-\,d\lambda_y^2\,dx \\
&= \hat{c}\int_\Omega\int_{\Gamma_R} \mathcal{H}(U-u)\big[UU^- - u^+U^+ + u^-U^-\big]\,d\lambda_y^2\,dx \\
&\leqslant \hat{c}\lambda_y^2(\Gamma_R)\int_\Omega \big|U^-\big|^2 + \hat{c}\int_\Omega\int_{\Gamma_R} u^-U^-\,d\lambda_y^2\,dx \\
&\leqslant \hat{c}\lambda_y^2(\Gamma_R)\left(1+\frac{1}{2\epsilon}\right)\big\|U^-\big\|^2_{L^2(\Omega)} + \frac{\hat{c}\epsilon}{2}\int_\Omega\int_Y \big\|u^-\big\|^2_{H^1(Y)}. \qquad (64)
\end{aligned}$$

Now, we choose $\epsilon = \frac{d_1}{\hat{c}}$ and apply Gronwall's inequality in (62) and (63) to conclude the proof of the lemma. □

**Lemma 10.** *If the hypotheses* (A1)–(A4), *and* (B) *hold, and* $(U, u, v)$ *is a weak solution of problem* (2)–(11), *then for a.e.* $(x, y) \in \Omega \times Y$ *and all* $t \in S$, *we have*

$$U(t,x) \leqslant M_1, \qquad u(t,x,y) \leqslant M_2, \qquad v(t,x,y) \leqslant M_3, \qquad (65)$$

*where*

$$\begin{aligned}
M_1 &:= \max\big\{\big\|U^{ext}\big\|_{L^\infty(S\times\Omega)}, \|U_I\|_{L^\infty(\Omega)}\big\}, \\
M_2 &:= \max\big\{\|u_I\|_{L^\infty(\Omega\times Y)}, M_1\big\}, \\
M_3 &:= \|v_I\|_{L^\infty(\Omega\times Y)}.
\end{aligned}$$

**Proof.** Choosing in (12)–(14) the test functions $(\varphi, \phi, \psi) := ((U-M_1)^+, (u-M_2)^+, (v-M_3)^+)$, yields

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}\int_\Omega \theta\big|(U-M_1)^+\big|^2 + \frac{1}{2}\frac{d}{dt}\int_{\Omega\times Y}\big|(u-M_2)^+\big|^2 + D\int_\Omega\big|\nabla(U-M_1)^+\big|^2 \\
&\quad + d_1\int_{\Omega\times Y}\big|\nabla_y(u-M_2)^+\big|^2 + k\int_{\Omega\times Y}\eta(u,v)(u-M_2)^+ + \int_\Omega\int_{\Gamma_R} b(U-u)(U-M_1)^+\,d\lambda_y^2\,dx \\
&\quad = \int_\Omega\int_{\Gamma_R} b(U-u)(u-M_2)^+\,d\lambda_y^2\,dx \qquad (66)
\end{aligned}$$

and

$$\frac{1}{2}\frac{d}{dt}\int_{\Omega\times Y}\big|(v-M_3)^+\big|^2 + d_2\int_{\Omega\times Y}\big|\nabla_y(v-M_3)^+\big|^2 + \alpha k\int_{\Omega\times Y}\eta(u,v)(v-M_3)^+ = 0. \qquad (67)$$

Since the last two terms from the l.h.s of (66) and the last one from the l.h.s. of (67) are positive, the only term, which still needs to be estimated, is the term on the r.h.s of (66). We proceed as follows:

$$\begin{aligned}
&\int_\Omega\int_{\Gamma_R} b(U-u)(u-M_2)^+\,d\lambda_y^2\,dx \\
&\quad \leqslant \hat{c}\int_\Omega\int_{\Gamma_R}\mathcal{H}(U-u)(U-u)(u-M_2)^+\,d\lambda_y^2\,dx \\
&\quad \leqslant \hat{c}\int_\Omega\int_{\Gamma_R}\mathcal{H}(U-u)(U-M_1)(u-M_2)^+\,d\lambda_y^2\,dx - \hat{c}\int_\Omega\int_{\Gamma_R}\mathcal{H}(U-u)\big|(u-M_2)^+\big|^2\,d\lambda_y^2\,dx
\end{aligned}$$

$$\leqslant \hat{c}\int_\Omega\int_{\Gamma_R}\mathcal{H}(U-u)(U-M_1)^+(u-M_2)^+\,d\lambda_y^2\,dx-\hat{c}\int_\Omega\int_{\Gamma_R}\mathcal{H}(U-u)\left|(u-M_2)^+\right|^2 d\lambda_y^2\,dx$$

$$\leqslant \frac{\hat{c}}{2}\int_\Omega\int_{\Gamma_R}\mathcal{H}(U-u)\left|(U-M_1)^+\right|^2 d\lambda_y^2\,dx-\frac{\hat{c}}{2}\int_\Omega\int_{\Gamma_R}\mathcal{H}(U-u)\left|(u-M_2)^+\right|^2 d\lambda_y^2\,dx$$

$$\leqslant \frac{\hat{c}}{2}\lambda_y^2(\Gamma_R)\left\|(U-M_1)^+\right\|^2_{L^2(\Omega)}. \tag{68}$$

The desired estimates on the solution now follow from (66), (67), and (68) by Gronwall's inequality. □

Remark that, if the solution $(U, u, v)$ is sufficiently smooth, and (A1)–(A3) hold, then one can use the technique from Lemma 3.1 of [6] to prove that the system (2)–(11) satisfies the classical maximum principle.

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