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Analysis of a two-scale system for gas-liquid reactions
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by

A. Muntean, M. Neuss-Radu



Centre for Analysis, Scientific computing and Applications
Department of Mathematics and Computer Science
Eindhoven University of Technology
P.O. Box 513
5600 MB Eindhoven, The Netherlands
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ANALYSIS OF A TWO-SCALE SYSTEM FOR GAS-LIQUID REACTIONS WITH NON-LINEAR HENRY-TYPE TRANSFER

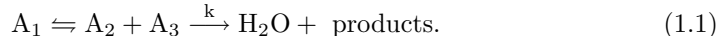
ADRIAN MUNTEAN* AND MARIA NEUSS-RADU†

Abstract. In this paper, we consider a coupled two-scale nonlinear reaction-diffusion system modelling gas-liquid reactions. The novel feature of the model is the nonlinear transmission condition between the microscopic and macroscopic concentrations, given by a nonlinear Henry-type transfer function. The solution is approximated by using a Galerkin method adapted to the multiscale form of the system. This approach leads to existence and uniqueness of the solution, and can also be used for numerical computations for a larger class of nonlinear multiscale problems.

Key words. non-linear reaction-diffusion systems, multiscale Galerkin approximation, structured porous media, gas-liquid reactions, Henry's law

AMS subject classifications. 35K57, 35B27, 65N30, 80A32, 76R50

1. Introduction. Gas-liquid reactions occur in a wealth of physicochemical processes in chemical engineering [2, 3] or geochemistry [15], e.g. A minimal reaction-diffusion 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



For instance, the natural carbonation of stone follows the mechanism (1.1), where $A_1 := \text{CO}_2(\text{g})$, $A_2 := \text{CO}_2(\text{aq})$, and $A_3 := \text{Ca}(\text{OH})_2(\text{aq})$, while the product of reaction is in this case $\text{CaCO}_3(\text{aq})$. This reaction mechanism is also encountered in catalysis, see [5] and references therein, or in civil engineering, e.g. in chemical corrosion scenarios as reported in [10, 11, 12].

This reaction-diffusion mechanism can be translated into a system of partial differential equations on the microscopic (pore) scale, together with transmission conditions at the interface separating the gas region from the region occupied by the liquid. Typical laws describing the mass transfer at these air-water interfaces are Henry-type laws.

When some information about the pore geometry is available, e.g. industrially produced porous media have periodic geometry, these microscopic models can be homogenized to obtain multiscale descriptions of the underlying processes. These consist of a macroscopic system formulated on the entire domain, coupled with a microscopic system, formulated 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

*CASA, Center for Analysis, Scientific computing and Applications, Department of Mathematics, Eindhoven Institute of Technology, PO Box 513, 5600 MB, Eindhoven, The Netherlands, (a.muntean@tue.nl).

†IWR, Heidelberg Graduate School of Mathematical and Computational Methods for the Sciences, University of Heidelberg, Im Neuenheimer Feld 294, D-69120 Heidelberg, Germany, (maria.neuss-radu@iwr.uni-heidelberg.de).

microscopic solution. On the other hand side by the boundary conditions for the microscopic solution, which is a (linear) Henry-type law involving the macroscopic concentration. For the derivation of such two-scale models (also called double porosity models) via homogenization techniques see e.g. [1, 7].

In our paper, we start from such a two-scale description of gas-liquid reactions in which the coupling between the microscopic and macroscopic problem is given by a nonlinear Henry-type law. Our study is partly motivated by some remarks from [4] 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 (1.1). 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.

The aim of the paper is to show that the two-scale model is well-posed, and to give an approach which can be used for the numerical computation of the solution. To this end, we use a Galerkin method to approximate the solutions of the two-scale system. We remark that this approach is of general interest for handling multiscale problems numerically.

To show the convergence of the finite-dimensional approximates, we prove estimates which guarantee the compactness of the approximate solutions. Here, the challenging feature is 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 very much inspired by the analysis performed in [13]. There a multiscale Galerkin approach was developed to investigate transport and nonlinear reaction in domains separated by membranes. Numerical tools for multiscale problems for linear diffusion processes were developed also in [8]. There, the aim was to construct a sparse finite element discretization for the high-dimensional multiscale problem.

The paper is organized as follows. We start with the statement of the problem and the assumptions on the data. The positivity and boundedness of weak solutions are proved in Sections 3 and 4. Next we show in Section 5 that there exists at most one weak solution of the considered multiscale system. In Section 6, we define the Galerkin approximations and show existence and uniqueness of the resulting systems of ordinary differential equations. The most delicate part of the paper is showing estimates which guarantee the compactness of the approximate solutions. Such estimates are proven assuming stability of the projections on finite dimensional subspaces with respect to appropriate norms. Finally, the convergence of the Galerkin approximates to the unique solution of the multiscale problem is shown.

2. Setting of the problem.

2.1. Geometry of the domain. Let Ω and \mathcal{Y} be connected domains in \mathbb{R}^3 with Lipschitz continuous boundaries. We denote by λ^k the k -dimensional Lebesgue measure ($k \in \{2, 3\}$), and assume that $\lambda^3(\Omega) \neq 0$ and $\lambda^3(\mathcal{Y}) \neq 0$. Here, Ω is the macroscopic domain, while \mathcal{Y} denotes the standard pore associated with the microstructure within Ω . We have that

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

where Y and Y^g represent the wet region and the air-filled part of the standard pore respectively. Let Y and Y^g be connected. The boundary of Y is denoted by Γ , 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 Γ_R is the gas/liquid interface along which the mass transfer occurs, and λ_y^2 denotes the surface measure on ∂Y . Furthermore, we denote by $\theta := \lambda^3(Y^g)$ the porosity of the medium. A possible geometry for our standard pore is illustrated in Figure 2.1.

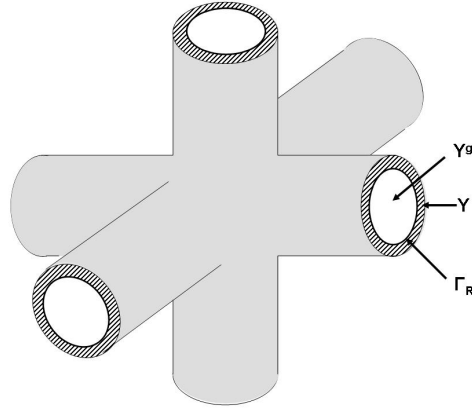


FIG. 2.1. Standard pore \mathcal{Y} . Typical shapes for $Y, Y^g \subset \mathcal{Y}$. Γ_R is the interface between the gaseous part of the pore Y^g and the wet region Y along which the mass transfer occurs.

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 (1.1). The mass-balance for the vector (U, u, v) is described by the following two-scale system:

$$\theta \partial_t U(t, x) - D \Delta U(t, x) = - \int_{\Gamma_R} b(U(t, x) - u(t, x, y)) d\lambda_y^2 \quad \text{in } S \times \Omega, \quad (2.1)$$

$$\partial_t u(t, x, y) - d_1 \Delta_y u(t, x, y) = -k\eta(u(t, x, y), v(t, x, y)) \quad \text{in } S \times \Omega \times Y, \quad (2.2)$$

$$\partial_t v(t, x, y) - d_2 \Delta_y v(t, x, y) = -\alpha k\eta(u(t, x, y), v(t, x, y)) \quad \text{in } S \times \Omega \times Y, \quad (2.3)$$

with macroscopic non-homogeneous Dirichlet boundary condition

$$U(t, x) = U^{ext}(t, x) \quad \text{on } S \times \partial\Omega, \quad (2.4)$$

and microscopic homogeneous Neumann boundary conditions

$$\nabla_y u(t, x, y) \cdot n_y = 0 \quad \text{on } S \times \Omega \times \Gamma_N, \quad (2.5)$$

$$\nabla_y v(t, x, y) \cdot n_y = 0 \quad \text{on } S \times \Omega \times \Gamma. \quad (2.6)$$

The coupling between the micro- and the macro-scale is made by the following non-linear Henry-type transmission condition on Γ_R

$$-\nabla_y u(t, x, y) \cdot n_y = -b(U(t, x) - u(t, x, y)) \quad \text{on } S \times \Omega \times \Gamma_R. \quad (2.7)$$

The initial conditions

$$U(0, x) = U_I(x) \quad \text{in } \Omega, \quad (2.8)$$

$$u(0, x, y) = u_I(x, y) \quad \text{in } \Omega \times Y, \quad (2.9)$$

$$v(0, x, y) = v_I(x, y) \quad \text{in } \Omega \times Y, \quad (2.10)$$

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 (2.1) 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 α 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

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

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

$$(A2) \quad \text{The sink/source term } b : \mathbb{R} \rightarrow \mathbb{R}_+ \text{ is globally Lipschitz, and } b(z) = 0 \text{ if } z \leq 0. \text{ This implies that it exists a constant } \hat{c} > 0 \text{ such that } b(z) \leq \hat{c}z \text{ if } z > 0.$$

$$(A3) \quad \eta : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}_+ \text{ is defined by } \eta(r, s) := R(r)Q(s), \text{ where } R, Q \text{ are globally Lipschitz continuous, with Lipschitz constants } c_R \text{ and } c_Q \text{ respectively. Furthermore, we assume that } R(r) > 0 \text{ if } r > 0 \text{ and } R(r) = 0 \text{ if } r \leq 0, \text{ and similarly, } Q(s) > 0 \text{ if } s > 0 \text{ and } Q(s) = 0 \text{ if } s \leq 0.$$

Finally, $k, \alpha \in \mathbb{R}, k > 0$, and $\alpha > 0$.

For the initial and boundary functions, we assume

$$(A4) \quad U^{ext} \in H^1(S, H^2(\Omega)) \cap H^2(S, L^2(\Omega)) \cap L_+^\infty(S \times \Omega), \quad U_I \in H^2(\Omega) \cap L_+^\infty(\Omega), \\ U_I - U^{ext}(0, \cdot) \in H_0^1(\Omega), \quad u_I, v_I \in L^2(\Omega, H^2(Y)) \cap L_+^\infty(\Omega \times Y).$$

The classical choice for b in the literature on gas-solid reactions, see e.g. [3], is the linear one given by $b : \mathbb{R} \rightarrow \mathbb{R}_+$, $b(z) = \hat{c}z$ for $z > 0$ and $b(z) := 0$ for $z \leq 0$. However, there are applications, see e.g. [4], 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 (A3) are power law reaction rates, sometimes also referred to as *generalized mass action laws*; see e.g. [2]. These laws have the form $R(r) := r^p$ and $Q(s) := s^q$, where the exponents $p \geq 1$ and $q \geq 1$ are called partial orders of reaction. However, to fulfill the Lipschitz condition, for large values of the arguments the power laws have to be replaced by Lipschitz functions.

2.4. Weak formulation. Our concept of weak solution is given in the following.

DEFINITION 2.1. *A triplet of functions (U, u, v) with $(U - U^{ext}) \in L^2(S, H_0^1(\Omega))$, $\partial_t U \in L^2(S \times \Omega)$, $(u, v) \in L^2(S, L^2(\Omega, H^1(Y)))^2$, $(\partial_t u, \partial_t v) \in L^2(S \times \Omega \times Y)^2$, is*

called a weak solution of (2.1)–(2.10) if for a.e. $t \in S$ the following identities hold

$$\frac{d}{dt} \int_{\Omega} \theta U \varphi + \int_{\Omega} D \nabla U \nabla \varphi + \int_{\Omega} \int_{\Gamma_R} b(U - u) \varphi d\lambda_y^2 dx = 0 \quad (2.11)$$

$$\begin{aligned} \frac{d}{dt} \int_{\Omega \times Y} u \phi + \int_{\Omega \times Y} d_1 \nabla_y u \nabla_y \phi - \int_{\Omega} \int_{\Gamma_R} b(U - u) \phi d\lambda_y^2 dx \\ + k \int_{\Omega \times Y} \eta(u, v) \phi = 0 \end{aligned} \quad (2.12)$$

$$\frac{d}{dt} \int_{\Omega \times Y} v \psi + \int_{\Omega \times Y} d_2 \nabla_y v \nabla_y \psi + \alpha k \int_{\Omega \times Y} \eta(u, v) \psi = 0, \quad (2.13)$$

for all $(\varphi, \phi, \psi) \in H_0^1(\Omega) \times L^2(\Omega; H^1(Y))^2$, and

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

3. Non-negativity of weak solutions. Let us first prove that weak solutions are non-negative.

LEMMA 3.1. *Assume that hypotheses (A1)–(A4) hold, and that (U, u, v) is a weak solution of problem (2.1)–(2.10). Then, for a.e. $(x, y) \in \Omega \times Y$ and all $t \in S$, we have*

$$U(t, x) \geq 0, \quad u(t, x, y) \geq 0, \quad v(t, x, y) \geq 0. \quad (3.1)$$

Proof. We use here the notation $u^+ := \max\{0, u\}$ and $u^- := \max\{0, -u\}$. Testing in (2.11)–(2.13) with $(\varphi, \phi, \psi) := (-U^-, -u^-, -v^-)$, we obtain

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} \theta |U^-|^2 + \frac{d}{dt} \int_{\Omega \times Y} |u^-|^2 + D \int_{\Omega} |\nabla U^-|^2 + d_1 \int_{\Omega \times Y} |\nabla_y u^-|^2 \\ - k \int_{\Omega \times Y} \eta(u, v) u^- + \int_{\Omega} \int_{\Gamma_R} b(U - u)(u^- - U^-) d\lambda_y^2 dx = 0 \end{aligned} \quad (3.2)$$

$$\frac{d}{dt} \int_{\Omega \times Y} |v^-|^2 d_2 \int_{\Omega \times Y} |\nabla v^-|^2 - \alpha k \int_{\Omega \times Y} \eta(u, v) v^- = 0. \quad (3.3)$$

Note that by (A3) the last but one term of the r.h.s. of (3.2) and the last term of (3.3) vanish. We denote by $\mathcal{H}(\cdot)$ the Heaviside function and estimate the last term of (3.2) as follows:

$$\begin{aligned} \int_{\Omega} \int_{\Gamma_R} b(U - u)(U^- - u^-) d\lambda_y^2 dx &\leq \int_{\Omega} \int_{\Gamma_R} b(U - u) U^- d\lambda_y^2 dx \\ &\leq \hat{c} \int_{\Omega} \int_{\Gamma_R} \mathcal{H}(U - u)(U - u) U^- d\lambda_y^2 dx \\ &= \hat{c} \int_{\Omega} \int_{\Gamma_R} \mathcal{H}(U - u)[U U^- - u^+ U^+ + u^- U^-] d\lambda_y^2 dx \\ &\leq \hat{c} \lambda_y^2(\Gamma_R) \int_{\Omega} |U^-|^2 + \hat{c} \int_{\Omega} \int_{\Gamma_R} u^- U^- d\lambda_y^2 dx \\ &\leq \hat{c} \lambda_y^2(\Gamma_R) \left(1 + \frac{1}{2\epsilon}\right) \|U^-\|_{L^2(\Omega)}^2 + \frac{\hat{c}\epsilon}{2} \int_{\Omega} \int_Y \|u^-\|_{H^1(Y)}^2. \end{aligned} \quad (3.4)$$

Now, we choose $\epsilon = \frac{d_1}{\hat{c}}$ and apply Gronwall's inequality in (3.2) and (3.3) to conclude the proof of the lemma. \square

4. Upper bounds for weak solutions. Next, we show that weak solutions are bounded.

LEMMA 4.1. *If the hypotheses (A1)–(A4) hold, and (U, u, v) is a weak solution of problem (2.1)–(2.10), then for a.e. $(x, y) \in \Omega \times Y$ and all $t \in S$, we have*

$$U(t, x) \leq M_1, \quad u(t, x, y) \leq M_2, \quad v(t, x, y) \leq M_3, \quad (4.1)$$

where

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

Proof. Choosing in (2.11)–(2.13) the test functions $(\varphi, \phi, \psi) := ((U - M_1)^+, (u - M_2)^+, (v - M_3)^+)$, yields

$$\begin{aligned} & \frac{d}{dt} \int_{\Omega} \theta |(U - M_1)^+|^2 + \frac{d}{dt} |(u - M_2)^+|^2 + D \int_{\Omega} |\nabla(U - M_1)^+|^2 \\ & + d_1 \int_{\Omega \times Y} |\nabla_y(u - M_2)^+|^2 + k \int_{\Omega \times Y} \eta(u, v)(u - M_2)^+ \\ & + \int_{\Omega} \int_{\Gamma_R} b(U - u)(U - M_1)^+ d\lambda_y^2 dx = \int_{\Omega} \int_{\Gamma_R} b(U - u)(u - M_2)^+ d\lambda_y^2 dx \quad (4.2) \end{aligned}$$

and

$$\begin{aligned} & \frac{d}{dt} \int_{\Omega \times Y} |(v - M_3)^+|^2 + d_2 \int_{\Omega \times Y} |\nabla_y(v - M_3)^+|^2 \\ & + \alpha k \int_{\Omega \times Y} \eta(u, v)(v - M_3)^+ = 0. \quad (4.3) \end{aligned}$$

Since the last two terms from the l.h.s of (4.2) and the last one from the l.h.s. of (4.3) are positive, the only term, which still needs to be estimated, is the term on the r.h.s of (4.2). We proceed as follows:

$$\begin{aligned} & \int_{\Omega} \int_{\Gamma_R} b(U - u)(u - M_2)^+ d\lambda_y^2 dx \leq \hat{c} \int_{\Omega} \int_{\Gamma_R} \mathcal{H}(U - u)(U - u)(u - M_2)^+ d\lambda_y^2 dx \\ & \leq \hat{c} \int_{\Omega} \int_{\Gamma_R} \mathcal{H}(U - u)(U - M_1)(u - M_2)^+ d\lambda_y^2 dx - \hat{c} \int_{\Omega} \int_{\Gamma_R} \mathcal{H}(U - u)|(u - M_2)^+|^2 d\lambda_y^2 dx \\ & \leq \hat{c} \int_{\Omega} \int_{\Gamma_R} \mathcal{H}(U - u)(U - M_1)^+(u - M_2)^+ d\lambda_y^2 dx - \hat{c} \int_{\Omega} \int_{\Gamma_R} \mathcal{H}(U - u)|(u - M_2)^+|^2 d\lambda_y^2 dx \\ & \leq \frac{\hat{c}}{2} \int_{\Omega} \int_{\Gamma_R} \mathcal{H}(U - u)|(U - M_1)^+|^2 d\lambda_y^2 dx - \frac{\hat{c}}{2} \int_{\Omega} \int_{\Gamma_R} \mathcal{H}(U - u)|(u - M_2)^+|^2 d\lambda_y^2 dx \\ & \leq \frac{\hat{c}}{2} \lambda_y^2(\Gamma_R) \|U - M_1\|_{L^2(\Omega)}^2. \quad (4.4) \end{aligned}$$

The desired estimates on the solution now follow from (4.2), (4.3), and (4.4) by Gronwall's inequality. \square

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 [5] to prove that the system (2.1)–(2.10) satisfies the classical maximum principle.

5. Uniqueness of weak solutions. Before starting with the proof of the existence of weak solutions for the problem (2.1)–(2.10), let us show that if they exist then weak solutions are unique.

PROPOSITION 5.1. *If (A1)–(A4) hold, then the weak solution to (2.1)–(2.10) is unique.*

Proof. Let (U_i, u_i, v_i) , $i \in \{1, 2\}$, be arbitrary weak solutions of the problem (2.1)–(2.10), thus satisfying for all $(\varphi, \phi, \psi) \in H_0^1(\Omega) \times [L^2(\Omega; H^1(Y))]^2$ the equalities

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} \theta U_i \varphi + \int_{\Omega} D \nabla U_i \nabla \varphi + \int_{\Omega} \int_{\Gamma_R} b(U_i - u_i) \varphi d\lambda_y^2 dx &= 0 \\ \frac{d}{dt} \int_{\Omega \times Y} u_i \phi + \int_{\Omega \times Y} d_1 \nabla_y u_i \nabla_y \phi - \int_{\Omega} \int_{\Gamma_R} b(U_i - u_i) \phi d\lambda_y^2 dx + k \int_{\Omega \times Y} \eta(u_i, v_i) \phi &= 0 \\ \frac{d}{dt} \int_{\Omega \times Y} v_i \psi + \int_{\Omega \times Y} d_2 \nabla_y v_i \nabla_y \psi + \alpha k \int_{\Omega \times Y} \eta(u_i, v_i) \psi &= 0. \end{aligned}$$

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:

$$\begin{aligned} & \frac{d}{dt} \int_{\Omega} \theta |U_2 - U_1|^2 + \frac{d}{dt} \int_{\Omega \times Y} |u_2 - u_1|^2 + \frac{d}{dt} \int_{\Omega \times Y} |v_2 - v_1|^2 \\ & + D \int_{\Omega} |\nabla(U_2 - U_1)|^2 + d_1 \int_{\Omega \times Y} |\nabla_y(u_2 - u_1)|^2 + d_2 \int_{\Omega \times Y} |\nabla_y(v_2 - v_1)|^2 \\ & + k \int_{\Omega \times Y} (\eta(u_2, v_2) - \eta(u_1, v_1)) [(u_2 - u_1) + \alpha(v_2 - v_1)] \\ & + \int_{\Omega} \int_{\Gamma_R} [b(U_2 - u_2) - b(U_1 - u_1)] [(U_2 - U_1) - (u_2 - u_1)] d\lambda_y^2 dx = 0 \end{aligned} \quad (5.1)$$

The last two terms in (5.1), say I_1 and I_2 , can be estimated as follows.

$$\begin{aligned} I_1 &\leq k \int_{\Omega \times Y} (\eta(u_2, v_2) - \eta(u_1, v_1)) [(u_2 - u_1) + \alpha(v_2 - v_1)] | \\ &\leq k \int_{\Omega \times Y} |Q(v_2)(R(u_2) - R(u_1)) [(u_2 - u_1) + \alpha(v_2 - v_1)]| \\ &\quad + k \int_{\Omega \times Y} |R(u_1)(Q(v_2) - Q(v_1)) [(u_2 - u_1) + \alpha(v_2 - v_1)]| \end{aligned}$$

Using the boundedness of the weak solutions and the Lipschitz continuity of the functions R and Q , we obtain

$$\begin{aligned} &\leq k Q_{\max} \int_{\Omega \times Y} |R(u_2) - R(u_1)| |(u_2 - u_1) + \alpha(v_2 - v_1)| \\ &+ k R_{\max} \int_{\Omega \times Y} |Q(v_2) - Q(v_1)| |(u_2 - u_1) + \alpha(v_2 - v_1)| \\ &\leq k(Q_{\max} c_R + R_{\max} c_Q) \max \left\{ \frac{3}{2}, \frac{\alpha^2}{2} + \alpha + \frac{1}{2} \right\} \int_{\Omega \times Y} (|u_2 - u_1|^2 + |v_2 - v_1|^2), \end{aligned}$$

where $R_{\max} := \max_{r \in [0, M_2]} R(r)$, and $Q_{\max} := \max_{s \in [0, M_3]} Q(s)$. We estimate I_2 as follows.

$$\begin{aligned} I_2 &\leq \left| \int_{\Omega} \int_{\Gamma_R} [b(U_2 - u_2) - b(U_1 - u_1)] [(U_2 - U_1) - (u_2 - u_1)] d\lambda_y^2 dx \right| \\ &\leq 2\hat{c} \int_{\Omega} \int_{\Gamma_R} |U_2 - U_1|^2 d\lambda_y^2 dx + 2\hat{c} \int_{\Omega} \int_{\Gamma_R} |u_2 - u_1|^2 d\lambda_y^2 dx. \end{aligned} \quad (5.2)$$

To estimate the second term in (5.2) we use the interpolation-trace inequality (5.3), see Proposition 5.2 below, with $\theta = \frac{1}{2}$. We obtain

$$\begin{aligned} &2\hat{c} \int_{\Omega} \int_{\Gamma_R} |u_2 - u_1|^2 \lambda_y^2 dx \\ &\leq C \int_{\Omega} (\|\nabla_y(u_2 - u_1)\|_{L^2(Y)} + \|u_2 - u_1\|_{L^2(Y)}) \|u_2 - u_1\|_{L^2(Y)}, \\ &\leq \epsilon \int_{\Omega} \|\nabla_y(u_2 - u_1)\|_{L^2(Y)}^2 + c_\epsilon \int_{\Omega} \|u_2 - u_1\|_{L^2(Y)}^2 \end{aligned}$$

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

PROPOSITION 5.2 (Theorem 5.9 in [14]). *Let Y be a bounded domain in \mathbb{R}^n with piecewise smooth Robin boundary Γ_R and let $u \in W^{1,p}(Y)$. The following inequality holds:*

$$\|u\|_{L^q(\Gamma_R)} \leq C (\|\nabla_y u\|_{L^p(Y)} + \|u\|_{L^\gamma(Y)})^\theta \|u\|_{L^r(Y)}^{1-\theta}, \quad (5.3)$$

where $\theta = \frac{p}{q} \frac{qn-r(n-1)}{p(n+r)-nr} \in]0, 1[$, $1 \leq \gamma < \infty$,

$$1 \leq r < \frac{np}{n-p} \text{ and } 1 \leq q < \frac{p(n-1)}{n-p} \text{ if } n > p$$

$$1 \leq r, q < \infty \text{ if } p = n \text{ or if } p > n.$$

6. Global existence of weak solutions. In this section, we prove existence of a global weak solution of problem (2.1)–(2.10) by using the Galerkin method. This method has to be adapted to 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 Ω and on the standard cell Y .

The most challenging aspect in the analysis of the discretized problems is to control the nonlinear sink/source integral term coupling the macroscopic and microscopic problems. More precisely, enough compactness for the finite-dimensional approximations, with respect to both, the microscopic and macroscopic variables, is needed in order to be able to pass to the limit in the discretized problems. This is not straightforward due to the fact that the macroscopic variable enters the cell problem just as a parameter.

In [13], a Galerkin approach for the approximation of a multiscale reaction-diffusion system with transmission conditions was developed. We will adapt the concepts used there to the structure of our actual problem. Numerical tools for elliptic linear multiscale problems were developed in [8]. There, the aim was to construct a sparse finite element discretization for the high-dimensional multiscale problem.

6.1. 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 $\xi_j \in H_0^1(\Omega)$, 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

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

where $\{\eta_k\}_{k \in \mathbb{N}}$ is a basis of $L^2(Y)$, with $\eta_k \in H^1(Y)$, 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 (φ, ψ) of the form

$$\begin{aligned} \varphi(x) &= \sum_{j \in \mathbb{N}} a_j \xi_j(x), \\ \psi(x, y) &= \sum_{j, k \in \mathbb{N}} b_{jk} \xi_j(x) \eta_k(y), \end{aligned}$$

we define

$$(P_x^N \varphi)(x) = \sum_{j=1}^N a_j \xi_j(x), \quad (6.1)$$

$$(P_x^N \psi)(x, y) = \sum_{j=1}^N \sum_{k \in \mathbb{N}} b_{jk} \sigma_j(x) \eta_k(y) \quad (6.2)$$

$$(P_y^N \psi)(x, y) = \sum_{j \in \mathbb{N}} \sum_{k=1}^N b_{jk} \sigma_j(x) \eta_k(y). \quad (6.3)$$

The bases $\{\sigma_j\}_{j \in \mathbb{N}}$, 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^∞ -norm and H^2 -norm; i.e. for a given function the L^∞ -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

$$U_0^N(t, x) = \sum_{j=1}^N \alpha_j^N(t) \xi_j(x), \quad (6.4)$$

$$u^N(t, x, y) = \sum_{j, k=1}^N \beta_{jk}^N(t) \xi_j(x) \eta_k(y), \quad (6.5)$$

$$v^N(t, x, y) = \sum_{j, k=1}^N \gamma_{jk}^N(t) \xi_j(x) \eta_k(y), \quad (6.6)$$

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

$$\int_{\Omega} \theta \partial_t U_0^N(t) \varphi dx + \int_{\Omega} D \nabla U_0^N(t) \nabla \varphi dx = \quad (6.7)$$

$$- \int_{\Omega} \left(\int_{\Gamma_R} b((U_0^N + U^{ext} - u^N)(t)) d\lambda^2(y) + \theta \partial_t U^{ext}(t) + D \Delta U^{ext}(t) \right) \varphi dx$$

$$\int_{\Omega \times Y} \partial_t u^N(t) \phi dx dy + \int_{\Omega \times Y} d_1 \nabla_y u^N(t) \nabla_y \phi dx dy = \quad (6.8)$$

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

$$\int_{\Omega \times Y} \partial_t v^N(t) \psi dy dx + \int_{\Omega \times Y} d_2 \nabla_y v^N(t) \nabla_y \psi dy dx = \quad (6.9)$$

$$- \alpha k \int_{\Omega \times Y} \eta(u^N(t), v^N(t)) \psi dy dx$$

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

$$\alpha_j^N(0) := \int_{\Omega} (U_I - U^{ext}(0)) \xi_j dx, \quad (6.10)$$

$$\beta_{jk}^N(0) := \int_{\Omega} \int_Y u_I \zeta_{jk} dx dy, \quad (6.11)$$

$$\gamma_{jk}^N(0) := \int_{\Omega} \int_Y v_I \zeta_{jk} dx dy. \quad (6.12)$$

Taking in (6.7)-(6.9) as test functions $\varphi = \xi_j, \phi = \xi_{jk}$, and $\psi = \xi_{jk}$, 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 $\gamma^N = (\gamma_{jk}^N)_{\substack{j=1, \dots, N \\ k=1, \dots, N}}$:

$$\partial_t \alpha^N(t) + \sum_{i=1}^N A_i \alpha_i^N(t) = F(\alpha^N(t), \beta^N(t)), \quad (6.13)$$

$$\partial_t \beta^N(t) + \sum_{i,l=1}^N B_{il} \beta_{il}^N(t) = \tilde{F}(\alpha^N(t), \beta^N(t)) + G(\beta^N(t), \gamma^N(t)), \quad (6.14)$$

$$\partial_t \gamma^N(t) + \sum_{i,l=1}^N C_{il} \gamma_{il}^N(t) = \alpha G(\beta^N(t), \gamma^N(t)), \quad (6.15)$$

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

$$\begin{aligned}
(A_i)_j &:= \int_{\Omega} D \nabla \xi_i(x) \nabla \xi_j(x) dx, \\
(B_{il})_{jk} &:= \int_{\Omega \times Y} d_1 \nabla \zeta_{il}(x, y) \nabla \zeta_{jk}(x, y) dy dx, \\
(C_{il})_{jk} &:= \int_{\Omega \times Y} d_2 \nabla \zeta_{il}(x, y) \nabla \zeta_{jk}(x, y) dy dx, \\
(C_{rm}^{\pm})_j &:= \frac{1}{2} D^{\pm} \int_{\Omega^{\pm}} \nabla \xi_{rm}^{\pm}(x) \nabla \xi_{j0}^{\pm}(x) dx, \\
F_j &:= -\frac{1}{\theta} \int_{\Omega} \left(\int_{\Gamma_R} b((U_0^N + U^{ext} - u^N)(t)) d\lambda_y^2 + \theta \partial_t U^{ext}(t) + D \Delta U^{ext}(t) \right) \xi_j(x) dx, \\
\tilde{F}_{jk} &:= \int_{\Omega} \int_{\Gamma_R} b((U_0^N + U^{ext} - u^N)(t)) \zeta_{jk}(x, y) d\lambda^2(y) dx, \\
G_{jk} &:= k \int_{\Omega \times y} \eta(u^N(t), v^N(t)) \zeta_{jk} dy dx.
\end{aligned}$$

Due to the assumptions (A2)–(A3) on b and η , the functions F, \tilde{F} , and G are globally Lipschitz continuous, and the Cauchy problem (6.10)–(6.15) 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 (6.4), (6.5), 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:

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

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

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

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

$$|\tilde{F}(\alpha_1^N, \beta_1^N) - \tilde{F}(\alpha_2^N, \beta_2^N)| \leq c(N) (|\alpha_1^N - \alpha_2^N| + |\beta_1^N - \beta_2^N|). \quad (6.16)$$

6.2. Uniform estimates for the discretized problems. In this section, we prove uniform estimates for the solutions to the finite-dimensional problems. Based on this estimates, in the next section, we are able to pass in (6.7)–(6.9) to the limit $N \rightarrow \infty$.

THEOREM 6.1. *Assume that the projection operators P_x^N, P_y^N , defined in (6.1)–(6.3), are stable with respect to the L^∞ -norm and H^2 -norm, and that (A1)–(A4) are satisfied. Then the following statements hold:*

(i) *The finite-dimensional approximations $U_0^N(t)$, $u^N(t)$, and $v^N(t)$ are positive and uniformly bounded. More precisely, we have for a.e. $(x, y) \in \Omega \times Y$, all $t \in S$, and all $N \in \mathbb{N}$*

$$0 \leq U_0^N(t, x) \leq m_1, \quad 0 \leq u^N(t, x, y) \leq m_2, \quad 0 \leq v^N(t, x, y) \leq m_3, \quad (6.17)$$

where

$$\begin{aligned} m_1 &:= 2\|U^{ext}\|_{L^\infty(S \times \Omega)} + \|U_I\|_{L^\infty(\Omega)}, \\ m_2 &:= \max\{\|u_I\|_{L^\infty(\Omega \times Y)}, m_1\}, \\ m_3 &:= \|v_I\|_{L^\infty(\Omega \times Y)}. \end{aligned}$$

(ii) *There exists a constant $c > 0$, independent of N , such that*

$$\|U_0^N\|_{L^\infty(S, H^1(\Omega))} + \|\partial_t U_0^N\|_{L^2(S, L^2(\Omega))} \leq c, \quad (6.18)$$

$$\|u^N\|_{L^\infty(S, L^2(\Omega; H^1(Y)))} + \|\partial_t u^N\|_{L^2(S, L^2(\Omega; L^2(Y)))} \leq c, \quad (6.19)$$

$$\|v^N\|_{L^\infty(S, L^2(\Omega; H^1(Y)))} + \|\partial_t v^N\|_{L^2(S, L^2(\Omega; L^2(Y)))} \leq c, \quad (6.20)$$

$$(6.21)$$

Proof. (i) We consider the function $U^N := U_0^N + U^{ext}$. Then (U^N, u^N, v^N) satisfies the equations

$$\begin{aligned} & \int_{\Omega} \theta \partial_t U^N(t) \varphi dx + \int_{\Omega} D \nabla U^N(t) \nabla \varphi dx = \\ & - \int_{\Omega} \int_{\Gamma_R} b((U^N - u^N)(t)) \varphi d\lambda^2(y) dx \end{aligned} \quad (6.22)$$

$$\int_{\Omega \times Y} \partial_t u^N(t) \phi dx dy + \int_{\Omega \times Y} d_1 \nabla_y u^N(t) \nabla_y \phi dx dy = \quad (6.23)$$

$$\int_{\Omega} \int_{\Gamma_R} b((U^N - u^N)(t)) \phi d\lambda^2(y) dx - k \int_{\Omega \times Y} \eta(u^N(t), v^N(t)) \phi dy dx$$

$$\begin{aligned} & \int_{\Omega \times Y} \partial_t v^N(t) \psi dy dx + \int_{\Omega \times Y} d_2 \nabla_y v^N(t) \nabla_y \psi dy dx = \\ & - \alpha k \int_{\Omega \times Y} \eta(u^N(t), v^N(t)) \psi dy dx \end{aligned} \quad (6.24)$$

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

$$U^N(0) = P_x^N(U_I - U^{ext}(0)) + U^{ext}(0) \text{ in } \Omega,$$

$$u^N(0) = P_x^N(P_y^N u_I) \text{ in } \Omega \times Y.$$

$$v^N(0) = P_x^N(P_y^N v_I) \text{ in } \Omega \times Y.$$

Using the stability of the projection operators with respect to the L^∞ -norm, the proof follows the lines of the proofs of Lemma 3.1 and Lemma 4.1.

(ii) Let us first take $(\varphi, \phi, \psi) = (U_0^N, u^N, v^N)$ as test function in (6.7)–(6.9). Using the positivity of the solution, we get

$$\frac{1}{2} \frac{d}{dt} \|v^N(t)\|_{L^2(\Omega \times Y)}^2 + d_2 \|\nabla_y v^N(t)\|_{L^2(\Omega \times Y)}^2 \leq 0, \quad (6.25)$$

$$\begin{aligned} & \frac{\theta}{2} \frac{d}{dt} \|U_0^N(t)\|_{L^2(\Omega)}^2 + \frac{1}{2} \frac{d}{dt} \|u^N(t)\|_{L^2(\Omega \times Y)}^2 \\ & + D \|\nabla U_0^N\|_{L^2(\Omega)}^2 + d_1 \|\nabla_y u^N\|_{L^2(\Omega \times Y)}^2 \\ & + \int_{\Omega} \int_{\Gamma_R} b(U_0^N + U^{ext} - u^N)(U_0^N - u^N) d\lambda_y^2 dx \\ & + \int_{\Omega} (\theta \partial_t U^{ext} + \Delta U^{ext}) U_0^N \leq 0. \end{aligned} \quad (6.26)$$

To estimate the following term, we use the Lipschitz property of b and the interpolation-trace inequality (5.3)

$$\begin{aligned} & \int_{\Omega} \int_{\Gamma_R} b(U_0^N + U^{ext} - u^N)(U_0^N - u^N) d\lambda_y^2 dx \\ & \leq \hat{c} \int_{\Omega} \int_{\Gamma_R} |U_0^N + U_0^{ext} - u^N| |U_0^N - u^N| d\lambda_y^2 dx \\ & \leq C \int_{\Omega} \int_{\Gamma_R} (|U_0^N|^2 + |U^{ext}|^2 + |u^N|^2) d\lambda_y^2 dx \\ & \leq C \left(\|U_0^N\|_{L^2(\Omega)}^2 + \|U^{ext}\|_{L^2(\Omega)}^2 \right) + C \int_{\Omega} \|u^N\|_{H^1(Y)} \|u^N\|_{L^2(Y)} \\ & \leq C \left(\|U_0^N\|_{L^2(\Omega)}^2 + \|U^{ext}\|_{L^2(\Omega)}^2 \right) + \epsilon \|\nabla_y u^N\|_{L^2(\Omega \times Y)}^2 + C(\epsilon) \|u^N\|_{L^2(\Omega \times Y)}^2. \end{aligned} \quad (6.27)$$

Taking $\epsilon := \frac{d_1}{2}$ in (6.27), inserting (6.27) in (6.26), and using the regularity properties of U^{ext} , we obtain

$$\begin{aligned} & \frac{d}{dt} \|U_0^N(t)\|_{L^2(\Omega)}^2 + \frac{d}{dt} \|u^N(t)\|_{L^2(\Omega \times Y)}^2 + \frac{d}{dt} \|v^N(t)\|_{L^2(\Omega \times Y)}^2 \\ & + \|\nabla U_0^N(t)\|_{L^2(\Omega)}^2 + \|\nabla_y u^N\|_{L^2(\Omega \times Y)}^2 + \|\nabla_y v^N\|_{L^2(\Omega \times Y)}^2 \\ & \leq C + \|U_0^N\|_{L^2(\Omega)}^2 + \|u^N\|_{L^2(\Omega \times Y)}^2. \end{aligned} \quad (6.28)$$

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

$$\|U_0^N\|_{L^\infty(S, L^2(\Omega))} + \|\nabla U_0^N\|_{L^2(S, L^2(\Omega))} \leq c, \quad (6.29)$$

$$\|u^N\|_{L^\infty(S, L^2(\Omega \times Y))} + \|\nabla_y u^N\|_{L^2(S, L^2(\Omega \times Y))} \leq c, \quad (6.30)$$

$$\|v^N\|_{L^\infty(S, L^2(\Omega \times Y))} + \|\nabla_y v^N\|_{L^2(S, L^2(\Omega \times Y))} \leq c. \quad (6.31)$$

To obtain L^∞ -estimates with respect to time of the gradients, and the estimates for the time derivatives, we differentiate with respect to time the weak formulation

(6.7)–(6.9), and test with $(\varphi, \phi, \psi) = (\partial_t U_0^N, \partial_t u^N, \partial_t v^N)$ and obtain:

$$\begin{aligned}
& \frac{1}{2} \frac{d}{dt} \int_{\Omega} \theta |\partial_t U_0^N(t)|^2 + \frac{1}{2} \frac{d}{dt} \int_{\Omega \times Y} |\partial_t u^N(t)|^2 + \frac{1}{2} \frac{d}{dt} \int_{\Omega \times Y} |\partial_t v^N(t)|^2 \\
& + D \int_{\Omega} |\nabla \partial_t U_0^N|^2 + d_1 \int_{\Omega \times Y} |\nabla_y \partial_t u^N|^2 + d_2 \int_{\Omega \times Y} |\nabla_y \partial_t v^N|^2 \\
& + \int_{\Omega} \int_{\Gamma_R} b'(U_0^N + U^{ext} - u^N) (\partial_t U_0^N + \partial_t U^{ext} - \partial_t u_t^N) (\partial_t U_0^N - \partial_t u_t^N) d\lambda_y^2 \\
& = - \int_{\Omega} \theta \partial_{tt} U^{ext} \partial_t U_0^N - \int_{\Omega} D \Delta \partial_t U^{ext} \partial_t U_0^N \\
& + k \int_{\Omega \times Y} R'(u^N) Q(v^N) (|u_t^N|^2 + \alpha u_t^N v_t^N) + k \int_{\Omega \times Y} R(u) Q'(v) (u_t^N v_t^N + \alpha |v_t^N|^2).
\end{aligned} \tag{6.32}$$

Integrating this expression with respect to time, using the Lipschitz properties of the nonlinear terms b and η , and the regularity properties of U^{ext} , as well as the interpolation-trace inequality (5.3), we obtain for all $t \in S$

$$\begin{aligned}
& \int_{\Omega} |\partial_t U_0^N(t)|^2 + \int_{\Omega \times Y} |\partial_t u^N(t)|^2 + \int_{\Omega \times Y} |\partial_t v^N(t)|^2 \\
& + \int_0^t \int_{\Omega \times Y} |\nabla \partial_t U_0^N|^2 + \int_0^t \int_{\Omega \times Y} |\nabla_y \partial_t u^N|^2 + \int_0^t \int_{\Omega \times Y} |\nabla_y \partial_t v^N|^2 \\
& \leq \int_{\Omega} |\partial_t U_0^N(0)|^2 + \int_{\Omega \times Y} |\partial_t u^N(0)|^2 + \int_{\Omega \times Y} |\partial_t v^N(0)|^2 \\
& + C \left(1 + \int_0^t \int_{\Omega} |\partial_t U_0^N(t)|^2 + \int_0^t \int_{\Omega \times Y} |\partial_t u^N|^2 + \int_0^t \int_{\Omega \times Y} |\partial_t v^N|^2 \right).
\end{aligned} \tag{6.33}$$

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 (6.7)–(6.9) at $t = 0$, and test with $(\partial_t U_0^N(0), \partial_t u^N(0), \partial_t v^N(0))$. We obtain

$$\begin{aligned}
& \int_{\Omega} \theta |\partial_t U_0^N(0)|^2 + \int_{\Omega} D \nabla U_0^N(0) \nabla \partial_t U_0^N(0) \\
& = - \int_{\Omega} \int_{\Gamma_R} b(U_0^N(0) + U^{ext}(0) - u^N(0)) \partial_t U_0^N(0) d\lambda_y^2 dx \\
& - \int_{\Omega} \theta \partial_t U^{ext}(0) \partial_t U_0^N(0) - \int_{\Omega} D \Delta U^{ext}(0) \partial_t U_0^N(0) \\
& \int_{\Omega \times Y} |\partial_t u^N(0)|^2 + \int_{\Omega \times Y} |\partial_t v^N(0)|^2 \\
& + \int_{\Omega \times Y} d_1 \nabla_y u^N(0) \nabla_y \partial_t u^N(0) + \int_{\Omega \times Y} d_2 \nabla_y v^N(0) \nabla_y \partial_t v^N(0) \\
& = \int_{\Omega} \int_{\Gamma_R} b(U_0^N(0) + U^{ext}(0) - u^N(0)) \partial_t u^N(0) d\lambda_y^2 dx \\
& + k \int_{\Omega \times Y} \eta(u^N(0), v^N(0)) (\partial_t u^N(0) + \alpha \partial_t v^N(0))
\end{aligned} \tag{6.34}$$

$$\begin{aligned}
& \int_{\Omega \times Y} |\partial_t u^N(0)|^2 + \int_{\Omega \times Y} |\partial_t v^N(0)|^2 \\
& + \int_{\Omega \times Y} d_1 \nabla_y u^N(0) \nabla_y \partial_t u^N(0) + \int_{\Omega \times Y} d_2 \nabla_y v^N(0) \nabla_y \partial_t v^N(0) \\
& = \int_{\Omega} \int_{\Gamma_R} b(U_0^N(0) + U^{ext}(0) - u^N(0)) \partial_t u^N(0) d\lambda_y^2 dx \\
& + k \int_{\Omega \times Y} \eta(u^N(0), v^N(0)) (\partial_t u^N(0) + \alpha \partial_t v^N(0))
\end{aligned} \tag{6.35}$$

Integrating by parts in the higher order terms, and using the fact that u^N satisfies

the transmission condition (2.7) in a weak sens, we obtain

$$\begin{aligned}
& \int_{\Omega} \theta |\partial_t U_0^N(0)|^2 + \int_{\Omega \times Y} |\partial_t u^N(0)|^2 + \int_{\Omega \times Y} |\partial_t v^N(0)|^2 \tag{6.36} \\
&= \int_{\Omega} D \Delta U_0^N(0) \partial_t U_0^N(0) + \int_{\Omega \times Y} d_1 \Delta_y u^N(0) \partial_t u^N(0) + \int_{\Omega \times Y} d_2 \Delta_y v^N(0) \partial_t v^N(0) \\
&- \int_{\Omega} \int_{\Gamma_R} b(U_0^N(0) + U^{ext}(0) - u^N(0)) \partial_t U_0^N(0) d\lambda_y^2 dx \\
&- \int_{\Omega} \theta \partial_t U^{ext}(0) \partial_t U_0^N(0) - \int_{\Omega} D \Delta U^{ext}(0) \partial_t U_0^N(0) \\
&+ k \int_{\Omega \times Y} \eta(u^N(0), v^N(0)) (\partial_t u^N(0) + \alpha \partial_t v^N(0))
\end{aligned}$$

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 $t = 0$:

$$\int_{\Omega} |\partial_t U_0^N(0)|^2 + \int_{\Omega \times Y} |\partial_t u^N(0)|^2 + \int_{\Omega \times Y} |\partial_t v^N(0)|^2 \leq c. \tag{6.37}$$

Inserting now (6.37) into (6.33), and using Gronwall's inequality, the estimates of the Theorem are proved. \square

The estimates proved in Theorem 6.1 still don't provide the compactness for the solutions (U_0^N, u^N, v^N) needed to pass to the limit $N \rightarrow \infty$ in the nonlinear terms of the variational formulation (6.7)–(6.9). In the next theorem, additional regularity of the solutions u^N, v^N with respect to the macroscopic variable x is proved.

THEOREM 6.2.

$$\|\nabla_x u^N\|_{L^\infty(S, L^2(\Omega \times Y))} + \|\nabla_x v^N\|_{L^\infty(S, L^2(\Omega \times Y))} \leq c \tag{6.38}$$

$$\|\nabla_y \nabla_x u^N\|_{L^2(S, L^2(\Omega \times Y))} + \|\nabla_y \nabla_x v^N\|_{L^2(S, L^2(\Omega \times Y))} \leq c \tag{6.39}$$

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

$$u_h^i(t, x, y) := \frac{u^N(t, x + h e_i, y) - u^N(t, x, y)}{h},$$

for all $t \in S$, $x \in \Omega'$, and $y \in Y$. We consider the following variational formulation

satisfied by these difference quotients, tested with $(\varphi, \phi, \psi) := (U_h^i, u_h^i, v_h^i)$:

$$\frac{d}{dt} \int_{\Omega} \theta |U_h^i|^2 + D \int_{\Omega} |\nabla U_h^i|^2 = \quad (6.40)$$

$$\begin{aligned} & - \int_{\Omega} \int_{\Gamma_R} \frac{1}{h} [b(U_0^N(t, x + he_i) + U^{ext}(x + he_i) - u^N(t, x + he_i, y)) \\ & - b(U_0^N(t, x) + U^{ext}(x) - u^N(t, x, y))] U_h^N d\lambda_y^2 dx, \\ & \frac{d}{dt} \int_{\Omega \times Y} |u_h^i|^2 + d_1 \int_{\Omega \times Y} |\nabla_y u_h^i|^2 = \quad (6.41) \end{aligned}$$

$$\begin{aligned} & \int_{\Omega} \int_{\Gamma_R} \frac{1}{h} [b(U_0^N(t, x + he_i) + U^{ext}(x + he_i) - u^N(t, x + he_i, y)) \\ & - b(U_0^N(t, x) + U^{ext}(x) - u^N(t, x, y))] u_h^i d\lambda_y^2 dx \\ & + k \int_{\Omega \times Y} \frac{1}{h} [\eta(u^N(t, x + he_i, y), v^N(t, x + he_i, y)) - \eta(u^N(t, x, y), v^N(t, x, y))] u_h^i, \\ & \frac{d}{dt} \int_{\Omega \times Y} |v_h^i|^2 + d_2 \int_{\Omega \times Y} |\nabla_y v_h^i|^2 = \quad (6.42) \\ & \alpha k \int_{\Omega \times Y} \frac{1}{h} [\eta(u^N(t, x + he_i, y), v^N(t, x + he_i, y)) - \eta(u^N(t, x, y), v^N(t, x, y))] v_h^i. \end{aligned}$$

Firstly, we add equations (6.40) and (6.41), and estimate the coupling terms using the Lipschitz property of b , the regularity of U^{ext} , and the interpolation-trace estimate (5.3) as follows.

$$\begin{aligned} & - \int_{\Omega} \int_{\Gamma_R} \frac{1}{h} [b(U_0^N(t, x + he_i) + U^{ext}(x + he_i) - u^N(t, x + he_i, y)) \\ & - b(U_0^N(t, x) + U^{ext}(x) - u^N(t, x, y))] (U_h^i - u_h^N) d\lambda_y^2 dx \quad (6.43) \\ & \leq \hat{c} \int_{\Omega} \int_{\Gamma_R} |U_h^i - u_h^i|^2 + |U_h^{ext,i}| |U_h^i - u_h^i| d\lambda_y^2 \\ & \leq c \int_{\Omega} \int_{\Gamma_R} (|U_h^i|^2 + |U_h^{ext,i}|^2 + |u_h^i|^2) d\lambda_y^2 dx \\ & \leq c \left(1 + \int_{\Omega} |U_h^i|^2 + C(\epsilon) \int_{\Omega} \int_Y |u_h^i|^2 \right) + \epsilon \int_{\Omega} \int_Y |\nabla_y u_h^i|^2. \end{aligned}$$

Next, we estimate the reaction term in the equation for u_h^i by using the Lipschitz properties of R and Q and the uniform boundedness of u^N and v^N as follows.

$$\begin{aligned} & \int_{\Omega \times Y} \frac{k}{h} [R(u^N(t, x + he_i, y))Q(v^N(t, x + he_i, y)) - R(u^N(t, x, y))Q(v^N(t, x, y))] u_h^i \\ & = \int_{\Omega \times Y} \left[\frac{R(u^N(t, x + he_i, y)) - R(u^N(t, x, y))}{h} Q(v^N(t, x + he_i, y)) \right. \\ & \left. + R(u^N(t, x, y)) \frac{Q(v^N(t, x + he_i, y)) - Q(v^N(t, x, y))}{h} \right] u_h^i \\ & \leq Q_{\max} c_R |u_h^i|^2 + R_{\max} c_Q u_h^N v_h^i \\ & \leq 2(Q_{\max} c_R + R_{\max} c_Q) (|u_h^i|^2 + |v_h^i|^2). \quad (6.44) \end{aligned}$$

The reaction term in the equation for v_h^i can be estimated analogously. Finally,

choosing $\epsilon := \frac{d_1}{2}$ in (6.43), and summarizing the above estimates, we get the inequality

$$\begin{aligned} & \frac{d}{dt} \int_{\Omega} |U_h^i|^2 + \frac{d}{dt} \int_{\Omega \times Y} |u_h^i|^2 + \frac{d}{dt} \int_{\Omega \times Y} |v_h^i|^2 \\ & + \int_{\Omega} |\nabla U_h^i|^2 + \int_{\Omega \times Y} |\nabla_y u_h^i|^2 + \int_{\Omega \times Y} |\nabla_y v_h^i|^2 \\ & \leq c \left(1 + \int_{\Omega} |U_h^i|^2 + \int_{\Omega \times Y} |u_h^i|^2 + \int_{\Omega \times Y} |v_h^i|^2 \right) \end{aligned} \quad (6.45)$$

Integrating with respect to time in (6.45), and applying Gronwall's inequality yields for all $i = 1, \dots, n$, and $N \in \mathbb{N}$ the estimates

$$\|u_h^i\|_{L^\infty(S, L^2(\Omega \times Y))} + \|v_h^i\|_{L^\infty(S, L^2(\Omega \times Y))} \leq c \quad (6.46)$$

$$\|\nabla_y u_h^i\|_{L^2(S, L^2(\Omega \times Y))} + \|\nabla_y v_h^i\|_{L^2(S, L^2(\Omega \times Y))} \leq c. \quad (6.47)$$

with a constant c independent on i, h , and N . Now applying the result on difference quotients from Lemma 7.24, in [6], the estimates (6.38)-(6.39) follow. \square

6.3. 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 (2.1)–(2.10). Based on the estimates proved in Section 6.2, we first derive the following convergence properties of the sequence of finite-dimensional approximations.

THEOREM 6.3. *There exists a subsequence, again denoted by (U_0^N, u^N, v^N) , and a limit $(U_0, u, v) \in L^2(S; H^1(\Omega)) \times [L^2(S; L^2(\Omega; H^1(Y)))]^2$, 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*

$$(U_0^N, u^N, v^N) \rightharpoonup (U_0, u, v) \text{ weakly in } L^2(S; H^1(\Omega)) \times [L^2(S; L^2(\Omega; H^1(Y)))]^2 \quad (6.48)$$

$$(\partial_t U_0^N, \partial_t u^N, \partial_t v^N) \rightharpoonup (\partial_t U_0, \partial_t u, \partial_t v) \text{ weakly in } L^2 \quad (6.49)$$

$$(U_0^N, u^N, v^N) \rightarrow (U_0, u, v) \text{ strongly in } L^2 \quad (6.50)$$

$$u^N|_{\Gamma_R} \rightarrow u|_{\Gamma_R} \text{ strongly in } L^2(S \times \Omega, L^2(\Gamma_R)) \quad (6.51)$$

Proof. The estimates from Theorem 6.1 immediately imply (6.48) and (6.49). Since

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

Lions-Aubin's compactness theorem, see [9], Theorem 1, page 58, implies that there exists a subset (again denoted by U_0^N) such that

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

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 6.2. We remark that the estimates (6.38)-(6.39) imply that

$$\|u^N\|_{H^1(\Omega, H^1(Y))} + \|v^N\|_{H^1(\Omega, H^1(Y))} \leq c.$$

Moreover, from Theorem 6.1, we have that

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

Since the embedding

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

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

$$(u^N, v^N) \longrightarrow (u, v) \text{ strongly in } L^2(S \times L^2(\Omega, H^\beta(Y))), \quad (6.52)$$

for all $\frac{1}{2} < \beta < 1$. Now, (6.52) 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 (6.50) and (6.51) \square

THEOREM 6.4. *Let the assumptions (A1)-(A4) be satisfied. Assume further that the projection operators P_x^N, P_y^N defined in (6.1)-(6.3) are stable with respect to the L^∞ -norm and H^2 -norm. Let (U_0, u, v) be the limit function obtained in Theorem 6.3. Then, the function $(U_0 + U^{ext}, u, v)$ is the unique weak solution of the problem (2.1)-(2.10).*

Proof. Using the convergence results in Theorem 6.3, and passing to the limit in (6.7)-(6.9), for $N \rightarrow \infty$, standard arguments lead to the variational formulation (2.11)-(2.13) for the function $(U, u, v) = (U_0 + U^{ext}, u, v)$. Furthermore, the uniqueness result from Proposition 5.1, yields the convergence of the whole sequence of Galerkin approximations. \square

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