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by

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Sulfate attack in sewer pipes: Derivation of a concrete corrosion model via two-scale convergence

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Abstract

We explore the homogenization limit and rigorously derive upscaled equations for a microscopic reaction-diffusion system modeling sulfate corrosion in sewer pipes made of concrete. The system, defined in a periodically-perforated domain, is semi-linear, partially dissipative and weakly coupled via a non-linear ordinary differential equation posed on the solid-water interface at the pore level. Firstly, we show the well-posedness of the microscopic model. We then apply homogenization techniques based on two-scale convergence for an uniformly periodic domain and derive upscaled equations together with explicit formulae for the effective diffusion coefficients and reaction constants. We use a boundary unfolding method to pass to the homogenization limit in the non-linear ordinary differential equation. Finally, besides giving its strong formulation, we also prove that the upscaled two-scale model admits a unique solution.

Key words: Sulfate corrosion of concrete, periodic homogenization, semi-linear partially dissipative system, two-scale convergence, periodic unfolding method, multiscale system.

1 Introduction

This paper treats the periodic homogenization of a semi-linear reaction-diffusion system coupled with a nonlinear differential equation arising in the modeling of the sulfuric acid attack in sewer pipes made of concrete. The concrete corrosion situation we are dealing with here strongly influences the durability of cement-based materials especially in hot environments leading to spalling of concrete and macroscopic fractures of sewer pipes. It is financially important to have a good estimate on the moment in time when such pipe systems need

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to be replaced, for instance, at the level of a city like Los Angeles. To get good such practical estimates, one needs on one side easy-to-use macroscopic corrosion models to be used for a numerical forecast of corrosion, while on the other side one needs to ensure the reliability of the averaged models by allowing them to incorporate a certain amount of microstructure information. The relevant question is: *How much of this oscillatory-type information is needed to get a sufficiently accurate description of the heterogeneous reality?* Due to the complexity of possible shapes of the microstructure, averaging concrete materials is far more difficult than averaging metallic composites with rigorously defined well-packed structure. In this paper, we imagine our concrete piece to be made of a periodically-distributed microstructure. Based on this assumption, we provide here a rigorous justification of the formal asymptotic expansion performed by us (in [1]) for this reaction-diffusion scenario. Note that in [1] upscaled models are derived for a more general situation involving a locally-periodic distribution of perforations [1]. Locally periodic geometries refer to a special case of x-dependent microstructures, where, inherently, the outer normals to (microscopic) inner interfaces are dependent on both spatial slow variable, say x, and fast variable, say y.

In the framework of this paper, we combine two-scale convergence concepts with the periodic unfolding of interfaces to pass to the homogenization limit (i.e. to $\varepsilon \to 0$, where ε is a small parameter linked to the relative size of the perforation) for the uniformly periodic case. Here, the outer normals to the inner interfaces are dependent only on the spatial fast variable. For more details on the mathematical modeling of sulfate corrosion of concrete, we refer the reader to [2,3] (a moving-boundary approach: numerics and formal matched asymptotics), [4] (a two-scale reaction-diffusion system modeling sulfate corrosion), as well as to [5], where a nonlinear Henry-law type transmission condition (modeling H_2S transfer across all air-water interfaces present in this sulfatation problem) is analyzed. Mathematical background on periodic homogenization can be found in e.g., [6–8], while a few relevant (remotely resembling) worked-out examples of this averaging methodology are explained, for instance, in [9–14]. It is worth noting that, since it deals with the homogenization of a linear Henry-law setting, the paper [11] is related to our approach. The major novelty here compared to [11] is that we now need to pass to the limit in a non-dissipative object, namely a nonlinear ordinary differential equation (ode). The ode is describing sulfatation reaction at the inner water-solid interface – place where corrosion localizes. This aspect makes a rigorous averaging challenging. For instance, compactness-type methods do not work in the case when the nonlinear ode is posed on ϵ-dependent surfaces. We circumvent this issue by "boundary unfolding" the ode. Thus we fix, as independent of ϵ, the reaction interface similarly as in [15], and only then we pass to the limit. Alternatively, one could use varifolds (cf. e.g. [16]), since this seems to

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[1] The word "perforation" is seen here as a synonym for "pore" or "microstructure".

be the natural framework for the rigorous passage to the limit when both the surface measure and the oscillating sequences depend on ϵ. However, we find the boundary unfolding technique easier to adapt to our scenario than the varifolds.

Note that here we approach the corrosion problem deterministically. However, we have reasons to expect that the uniform periodicity assumption can be relaxed by assuming instead a Birkhoff-type ergodicity of the microstructure shapes and positions, and hence, the natural averaging context seems to be the one offered by random fields; see ch. 1, sect. 6 in [17], ch. 8 and 9 in [18], or [19]. But, methodologically, how big is the overlap between homogenizing deterministically locally-periodic distributions of microstructures compared to working in the random fields context? We will treat these and related aspects elsewhere.

The paper is organized as follows: We start off in section 2 (and continue in section 3) with the analysis of the microscopic model. In section 4, we obtain the ε-independent estimates needed for the passage to the limit $\varepsilon \to 0$. Section 5 contains the main result of the paper: the set of the upscaled two-scal equations.

2 The microscopic model

In this section, we describe the geometry of our array of periodic microstructures and briefly indicate the most aggressive chemical reaction mechanism typically active in sewer pipes. Finally, we list the set of microscopic equations.

2.1 Basic geometry

Fig. 1 (i) shows a cross-section of a sewer pipe hosting corrosion. We assume that the geometry of the porous medium in question consists of a system of pores periodically distributed inside the three-dimensional cube $\Omega := [a,b]^3$ with $a, b \in \mathbb{R}$ and $b > a$. The exterior boundary of Ω consists of two disjoint, sufficiently smooth parts: Γ^N - the Neumann boundary and Γ^D - the Dirichlet boundary. The reference pore, say $Y := [0,1]^3$, has three pairwise disjoint connected domains Y^s, Y^w and Y^a with smooth boundaries Γ^{sw} and Γ^{wa}, as shown in Fig. 1 (iii). Moreover, $Y := \bar{Y}^s \cup \bar{Y}^w \cup \bar{Y}^a$.

Let ε be a sufficiently small scaling factor denoting the ratio between the characteristic length of the pore Y and the characteristic length of the domain Ω. Let χ^w and χ^a be the characteristic functions of the sets Y^w and Y^a, respectively. The shifted set Y_k^w is defined by

$$Y_k^w := Y + \Sigma_{j=0}^3 k_j e_j \text{ for } k = (k_1, k_2, k_3) \in \mathbb{Z}^3,$$

where e_j is the jth unit vector. The union of all shifted subsets of Y_k^w multiplied
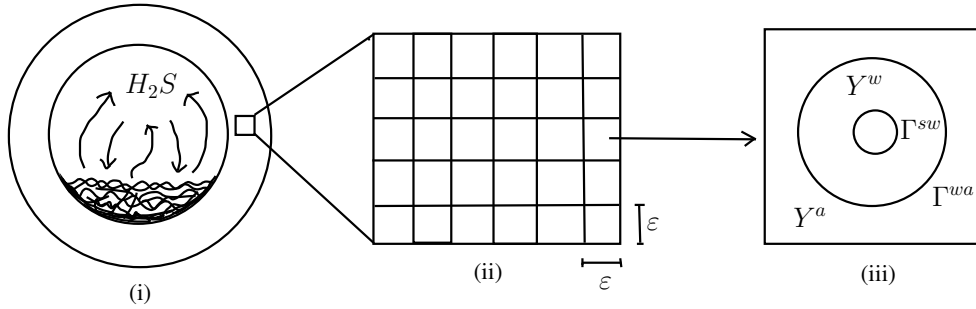
Fig. 1. Left: Cross-section of a sewer pipe and pointing out one region. Middle: Periodic approximation of the periodic rectangular domain. Right: Reference pore configuration.

by ε (and confined within Ω) defines the perforated domain Ω^ε, namely

$$\Omega^\varepsilon := \cup_{k \in \mathbb{Z}^3} \{\varepsilon Y_k^w \mid \varepsilon Y_k^w \subset \Omega\}.$$

Similarly, Ω_1^ε, Γ_ε^{sw}, and Γ_ε^{wa} denote the union of the shifted subsets (of Ω) Y_k^a, Γ_k^{sw}, and Γ_k^{wa} scaled by ε. Since usually the concrete in sewer pipes is not completely dry, we decide to take into account a partially saturated porous material[2]. We assume that every pore has three distinct non-overlapping parts: a solid part (grain) which is placed in the center of the pore, the water film which surrounds the solid part, and an air layer bounding the water film and filling the space of Y as shown in Fig. 1. The air connects neighboring pores to one another. The geometry defined above satisfies the following assumptions:

 (1) Neither solid nor water-filled parts touch the boundary of the pore.
 (2) All internal (air-water and water-solid) interfaces are sufficiently smooth and do not touch each other.

These geometrical restrictions imply that the pores are connected by air-filled parts only which is needed not only to give a meaning to functions defined across interfaces, but also to introduce the concept of extension as given, for instance, in [20]. Furthermore, there are no solid-air interfaces.
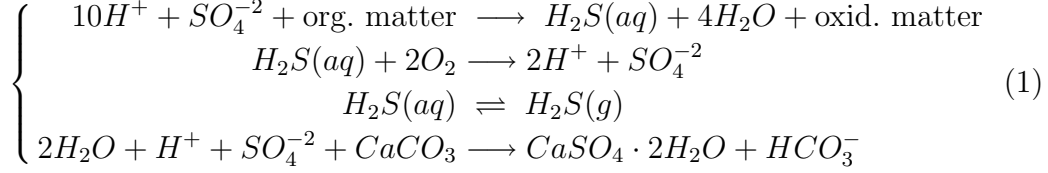
2.2 Description of the chemistry

There are many variants of severe attack to concrete in sewer pipes, we focus here on the most aggressive one – the sulfuric acid attack. The situation can be described briefly as follows: (The anaerobic bacteria in the flowing waste water release hydrogen sulfide gas (H_2S) within the air space of the pipe. These bacteria are especially active in hot environments. From the air space inside the pipe, $H_2S(g)$[3] enters the pores of the concrete matrix where it diffuses and then dissolves in the pore water. The aerobic bacteria catalyze some of the H_2S into sulfuric acid H_2SO_4. H_2S molecules can move between air-filled part and water-filled part the water-air interfaces [21]. We model this microscopic

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[2] The solid, water and air parts corresponds to Y^s, Y^w and Y^a, respectively.
[3] $H_2S(g)$ and $H_2S(aq)$ refer to gaseous, and respectively, aqueous H_2S.

interfacial transfer via Henry's law [22], (see the boundary conditions at Γ_ε^{wa} in (3) and (4)). H_2SO_4 being an aggressive acid reacts with the solid matrix [4] at the solid-water interface, which is made up of cement, sand, and aggregate, and produces gypsum (i.e. $CaSO_4 \cdot 2H_2O$). Here we restrict our attention to a minimal set of chemical reactions mechanisms as suggested in [2], namely.

$$\begin{cases} 10H^+ + SO_4^{-2} + \text{org. matter} \longrightarrow H_2S(aq) + 4H_2O + \text{oxid. matter} \\ H_2S(aq) + 2O_2 \longrightarrow 2H^+ + SO_4^{-2} \\ H_2S(aq) \rightleftharpoons H_2S(g) \\ 2H_2O + H^+ + SO_4^{-2} + CaCO_3 \longrightarrow CaSO_4 \cdot 2H_2O + HCO_3^- \end{cases} \tag{1}$$

We assume that reactions (1) do not interfere with the mechanics of the solid part of the pores. This is a rather strong assumption since it is known that (1) can actually produce local ruptures of the solid matrix [23]. For more details on the involved cement chemistry and connections to acid corrosion, we refer the reader to [24] (for a nice enumeration of the involved physicochemical mechanisms), [23] (standard textbook on cement chemistry), as well as to [25–27] and references cited therein. For a mathematical approach of a similar theme related to the conservation and restoration of historical monuments, we refer to the work by R. Natalini and co-workers (cf. e.g. [28]).

2.3 Setting of the equations

The data and unknown are given by

$u_{10}^\varepsilon : \Omega \longrightarrow \mathbb{R}_+$ - initial concentration of $H_2SO_4(aq)$

$u_{20}^\varepsilon : \Omega \longrightarrow \mathbb{R}_+$ - initial concentration of $H_2S(aq)$

$u_{30}^\varepsilon : \Omega \longrightarrow \mathbb{R}_+$ - initial concentration of $H_2S(g)$

$u_{40}^\varepsilon : \Omega \longrightarrow \mathbb{R}_+$ - initial concentration of moisture

$u_{50}^\varepsilon : \Omega \longrightarrow \mathbb{R}_+$ - initial concentration of gypsum

$u_3^D : \Gamma_D \times (0, T) \longrightarrow \mathbb{R}_+$ - exterior concentration (Dirichlet data) of $H_2S(g)$

$u_1^\varepsilon : \Omega^\varepsilon \times (0, T) \longrightarrow \mathbb{R}$ - concentration of $H_2SO_4(aq)$

$u_2^\varepsilon : \Omega^\varepsilon \times (0, T) \longrightarrow \mathbb{R}$ - concentration of $H_2S(aq)$

$u_3^\varepsilon : \Omega_1^\varepsilon \times (0, T) \longrightarrow \mathbb{R}$ - concentration of $H_2S(g)$

$u_4^\varepsilon : \Omega^\varepsilon \times (0, T) \longrightarrow \mathbb{R}$ - concentration of moisture

$u_5^\varepsilon : \Gamma_\varepsilon^{sw} \times (0, T) \longrightarrow \mathbb{R}$ - concentration of gypsum

All concentrations are viewed as mass concentrations. We consider the following system of mass-balance equations defined at the pore level. The mass-

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[4] The solid matrix is assumed here to consist of $CaCO_3$ only. This assumption can be removed in the favor of a more complex cement chemistry.

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balance equation for H_2SO_4 is

$$\partial_t u_1^\varepsilon + div(-d_1^\varepsilon \nabla u_1^\varepsilon) = -k_1^\varepsilon u_1^\varepsilon + k_2^\varepsilon u_2^\varepsilon, \quad x \in \Omega^\varepsilon, \ t \in (0,T)$$
$$u_1^\varepsilon(x,0) = u_{10}^\varepsilon(x), \quad x \in \Omega^\varepsilon$$
$$-n^\varepsilon \cdot d_1^\varepsilon \nabla u_1^\varepsilon = 0, \quad x \in \Gamma_\varepsilon^{wa}, \ t \in (0,T)$$
$$-n^\varepsilon \cdot d_1^\varepsilon \nabla u_1^\varepsilon = \varepsilon \eta(u_1^\varepsilon, u_5^\varepsilon), \quad x \in \Gamma_\varepsilon^{sw} \ t \in (0,T). \tag{2}$$

The mass-balance equation for $H_2S(aq)$ is given by

$$\partial_t u_2^\varepsilon + div(-d_2^\varepsilon \nabla u_2^\varepsilon) = k_1^\varepsilon u_1^\varepsilon - k_2^\varepsilon u_2^\varepsilon, \quad x \in \Omega^\varepsilon, \ t \in (0,T),$$
$$u_2^\varepsilon(x,0) = u_{20}^\varepsilon(x), \quad x \in \Omega^\varepsilon$$
$$-n^\varepsilon \cdot d_2^\varepsilon \nabla u_2^\varepsilon = \varepsilon(a^\varepsilon(x)u_3^\varepsilon - b^\varepsilon(x)u_2^\varepsilon), \quad x \in \Gamma_\varepsilon^{wa}, \ t \in (0,T)$$
$$-n^\varepsilon \cdot d_2^\varepsilon \nabla u_2^\varepsilon = 0, \quad x \in \Gamma_\varepsilon^{sw}, \ t \in (0,T). \tag{3}$$

The mass-balance equation for $H_2S(g)$ reads

$$\partial_t u_3^\varepsilon + div(-d_3^\varepsilon \nabla u_3^\varepsilon) = 0, \quad x \in \Omega_1^\varepsilon, \ t \in (0,T)$$
$$u_3^\varepsilon(x,0) = u_{30}^\varepsilon(x), \quad x \in \Omega_1^\varepsilon$$
$$-n^\varepsilon \cdot d_3^\varepsilon \nabla u_3^\varepsilon = 0, \quad x \in \Gamma^N, \ t \in (0,T)$$
$$u_3^\varepsilon(x,t) = u_3^D(x,t), \quad x \in \Gamma^D, \ t \in (0,T)$$
$$-n^\varepsilon \cdot d_3^\varepsilon \nabla u_3^\varepsilon = -\varepsilon(a^\varepsilon(x)u_3^\varepsilon - b^\varepsilon(x)u_2^\varepsilon), \quad x \in \Gamma_\varepsilon^{wa}, \ t \in (0,T). \tag{4}$$

The mass-balance equation for moisture follows

$$\partial_t u_4^\varepsilon + div(-d_4^\varepsilon \nabla u_4^\varepsilon) = k_1^\varepsilon u_1^\varepsilon, \quad x \in \Omega^\varepsilon, \ t \in (0,T)$$
$$u_4^\varepsilon(x,0) = u_{40}^\varepsilon(x), \quad x \in \Omega^\varepsilon$$
$$-n^\varepsilon \cdot d_4^\varepsilon \nabla u_4^\varepsilon = 0, \quad x \in \Gamma_\varepsilon^{wa}, \ t \in (0,T)$$
$$-n^\varepsilon \cdot d_4^\varepsilon \nabla u_4^\varepsilon = 0, \quad x \in \Gamma_\varepsilon^{sw}, \ t \in (0,T). \tag{5}$$

The mass-balance equation for the gypsum produced at the water-solid interface is

$$\partial_t u_5^\varepsilon = \eta(u_1^\varepsilon, u_5^\varepsilon), \quad x \in \Gamma_\varepsilon^{sw}, \ t \in (0,T)$$
$$u_5^\varepsilon(x,0) = u_{50}^\varepsilon(x), \quad x \in \Gamma_\varepsilon^{sw}, \ t \in (0,T). \tag{6}$$

3 Weak formulation and basic results

We begin this section with a list of notations and function spaces. Then we indicate our working assumptions and give the weak formulation of the microscopic problem; we bring reader's attention to the well-posedness of the system (2)–(6).

3.1 Notations and function spaces

We use $(\alpha, \beta)_{(0,T) \times \Omega^\varepsilon} := \int_0^T \int_{\Omega^\varepsilon} \alpha\beta dx dt$, $(\alpha, \beta)_{(0,T) \times \Gamma_\varepsilon} := \int_0^T \int_{\Gamma_\varepsilon} \alpha\beta d\sigma_x dt$. $\langle \cdot \rangle$, $|\cdot|$ and $\|\cdot\|$ denote the dual pairing of $H^1(\Omega^\varepsilon)$ and $H^{-1}(\Omega^\varepsilon)$, the norm in $L^2(\Omega^\varepsilon)$, and the norm in $H^1(\Omega^\varepsilon)$, respectively. φ^+ and φ^- will point out the

positive and respectively the negative part of the function φ. We denote by $C_\#^\infty(Y)$, $H_\#^1(Y)$, and $H_\#^1(Y)/\mathbb{R}$, the space of infinitely differentiable functions in $\mathbb{R}^n$ that are periodic of period Y, the completion of $C_\#^\infty(Y)$ with respect to H^1−norm, and the respective quotient space, respectively. Furthermore, $H_{\Gamma^D}^1(\Omega) := \{u \in H^1(\Omega)|u = 0 \text{ on } \Gamma^D\}$. The Sobolev space $H^\beta(\Omega)$ as a completion of $C^\infty(\Omega)$ is a Hilbert space equipped with a norm

$$\|\varphi\|_{H^\beta(\Omega)} = \|\varphi\|_{H^{[\beta]}(\Omega)} + \left(\int_\Omega \int_\Omega \frac{|\varphi(x) - \varphi(y)|^2}{|x-y|^{n+2(\beta-[\beta])}} dxdy \right)^{\frac{1}{2}}$$

and (cf. Theorem 7.57 in [29]) the embedding $H^\beta(\Omega) \hookrightarrow L^2(\Omega)$ is continuous. Since we deal with an evolution problem, we need typical Bochner spaces like $L^2(0,T;H^1(\Omega))$, $L^2(0,T;H^{-1}(\Omega))$, $L^2(0,T;H_{\Gamma^D}^1(\Omega))$, and $L^2((0,T)\times\Omega;H_\#^1(Y)/\mathbb{R})$. In the analysis of the microscopic model, we use frequently the following trace inequality for ε−dependent hypersurfaces Γ_ε^{wa}: For $\varphi_\varepsilon \in H^1(\Omega^\varepsilon)$, there exists a constant C^*, which is independent of ε, such that

$$\varepsilon|\varphi_\varepsilon|_{L^2(\Gamma_\varepsilon)}^2 \le C^*(|\varphi_\varepsilon|_{L^2(\Omega^\varepsilon)}^2 + \varepsilon^2|\nabla\varphi_\varepsilon|_{L^2(\Omega^\varepsilon)}^2). \tag{7}$$

The proof of (7) is given in Lemma 3 of [30]. For a function $\varphi^\varepsilon \in H^\beta(\Omega^\varepsilon)$ with $\beta \in (\frac{1}{2}, 1)$, the inequality (7) refines into

$$\varepsilon|\varphi_\varepsilon|_{L^2(\Gamma_\varepsilon)}^2 \le C_0^*(|\varphi_\varepsilon|_{L^2(\Omega^\varepsilon)}^2 + \varepsilon^{2\beta} \int_\Omega^\varepsilon \int_\Omega^\varepsilon \frac{|\varphi^\varepsilon(x) - \varphi^\varepsilon(y)|^2}{|x-y|^{n+2\beta}} dxdy), \tag{8}$$

where C_0^* is again a constant independent of ε. For proof of (8), see [15]. To simplify the writing of some of the estimates, we employ the next set of notations:

$$d_i := \min_{[0,T]\times\bar{\Omega}} |d_i^\varepsilon|, \ i \in \{1,2,3,4\}, \quad \tilde{d}_i := \min_{[0,T]\times\bar{\Omega}} |\tilde{d}_i^\varepsilon|,$$

$$D_m := \max_{[0,T]\times\Omega^\varepsilon} |\partial_t d_m^\varepsilon|, \ m \in \{1,2,3\}, \quad k_j := \min_{[0,T]\times\bar{\Omega}} |k_j^\varepsilon|, \ j \in \{1,2\}$$

$$K_j := \min_{[0,T]\times\bar{\Omega}} |\partial_t k_j^\varepsilon|, \quad \tilde{k}_j := \min_{[0,T]\times\bar{\Omega}} |\tilde{k}_j^\varepsilon|,$$

$$k_m^\infty := \sup_{(0,T)\times\Omega} |k_m^\varepsilon|, \quad \tilde{k}_m^\infty := \sup_{(0,T)\times\Omega} |\tilde{k}_m^\varepsilon|,$$

$$K_m^\infty := \sup_{(0,T)\times\Omega} |\partial_t k_m^\varepsilon|, \quad M_i := \sup_{(0,T)\times\Omega} |u_i^\varepsilon|, \ i \in \{1,2,3,4,5\},$$

$$A^\infty := \sup_{(0,T)\times\Gamma_\varepsilon^{wa}} |a_\varepsilon|, \ B^\infty := \sup_{(0,T)\times\Gamma_\varepsilon^{wa}} |b_\varepsilon|,$$

$$A^\infty := \sup_{(0,T)\times\Gamma_\varepsilon^{wa}} |\partial_t a_\varepsilon|, \ B^\infty := \sup_{(0,T)\times\Gamma_\varepsilon^{wa}} |\partial_t b_\varepsilon|,$$

$$\tilde{a}^\infty := \sup_{(0,T)\times\Gamma^{wa}} |\tilde{a}|, \ \tilde{b}^\infty := \sup_{(0,T)\times\Gamma^{wa}} |\tilde{b}|,$$

$$Q^\infty := \sup_{s\in(0,T)\times\Gamma_\varepsilon^{sw}} |Q(s)|, \quad \bar{\eta} := ||\eta||_\infty, \quad \hat{\eta} := ||\partial_t\eta||_\infty.$$

We consider the following restriction on the data and parameters:

(A1) $d_i \in L^\infty((0,T) \times Y)^{3\times3}$, $\partial_t d_i \in L^\infty((0,T) \times Y)^{3\times3}$, $\partial_{tt} d_i \in L^\infty((0,T) \times Y)^{3\times3}$, $(d_i(t,x)\xi, \xi) \geq d_{i0} \mid \xi \mid^2$ for $d_{i0} > 0$, for every $\xi \in \mathbb{R}^3$, $(t,x) \in (0,T) \times Y$, $i \in \{1,2,3,4\}$.

(A2) η is measurable w.r.t. t and x and $\eta(\alpha, \beta) = k_3^\varepsilon R(\alpha) Q(\beta)$, R is sub-linear and locally Lipschitz function and Q is bounded and locally Lipschitz function such that

$$R(\alpha) = \begin{cases} \text{positive,} & \text{if } \alpha \geq 0, \\ 0, & \text{otherwise} \end{cases} \qquad Q(\beta) = \begin{cases} \text{positive,} & \text{if } \beta < \beta_{max}, \\ 0, & \text{otherwise} \end{cases}$$

Additionally to (A2), we sometimes assume (A2)', that is

(A2)' $\partial_t \eta \leq \hat\eta$.

(A3) $u_{i0}^\varepsilon \in L^2(\Omega^\varepsilon) \cap L_+^\infty(\Omega^\varepsilon)$, $i \in \{1,2,4\}$, $u_{30}^\varepsilon \in L^2(\Omega_1^\varepsilon) \cap L_+^\infty(\Omega_1^\varepsilon)$, $u_{50}^\varepsilon \in L^2(\Gamma_\varepsilon^{sw}) \cap L_+^\infty(\Gamma_\varepsilon^{sw})$.

(A4) $a^\infty M_3 = b^\infty M_2$, $k_1^\infty M_1 = M_4$, $k_1 M_1 = k_2^\infty M_2$.

(A5) $a, b \in C^1([0,T]; C^{0,\alpha}(\Gamma^{wa})), a, b \geq 0$ in $[0,T] \times \Gamma^{wa}, \partial_t a, \partial_t b \in L^\infty((0,T) \times \Gamma^{wa})$.

(A6) $\partial_t u_3^D$, $\partial_{tt} u_3^D$ and $\nabla \partial_t u_3^D$ are bounded.

(A7) $k_3 \in C^1([0,T]; C^{0,\alpha}(\Gamma^{sw}))$ and $k_j \in C^1([0,T]; C^{0,\alpha}(\bar{Y}))$ for any $j \in \{1,2\}$ and $\alpha \in]0,1]$.

The assumptions (A1)–(A3), (A5), and (A6) are of technical nature. The first equality in (A4) points out an infinitely fast (equilibrium) Henry law, while the last two equalities remotely resemble a detailed balance in two of the involved chemical reactions.

3.3   Weak formulation of the microscopic model

Definition 1 *Assume (A1) and (A3). We call the vector $u^\varepsilon = (u_1^\varepsilon, u_2^\varepsilon, u_3^\varepsilon, u_4^\varepsilon, u_5^\varepsilon)$, a weak solution to (2)–(6) if $u_j^\varepsilon \in L^2(0,T; H^1(\Omega^\varepsilon)), \partial_t u_j^\varepsilon \in L^2(0,T; H^{-1}(\Omega^\varepsilon)), j \in \{1,2,4\}$, $u_3^\varepsilon \in u_3^D + L^2(0,T; H_{\Gamma^D}^1(\Omega_1^\varepsilon)), \partial_t u_3^\varepsilon \in u_3^D + L^2(0,T; H^{-1}(\Omega_1^\varepsilon)), u_5^\varepsilon \in L^\infty((0,T) \times \Gamma_\varepsilon^{sw}), \partial_t u_5^\varepsilon \in L^\infty((0,T) \times \Gamma_\varepsilon^{sw})$ such that the following identities hold*

$$\langle \partial_t u_1^\varepsilon, \varphi_1 \rangle_{(0,T)\times\Omega^\varepsilon} + (d_1 \nabla u_1^\varepsilon), \nabla \varphi_1)_{(0,T)\times\Omega^\varepsilon}$$
$$= -(k_1 u_1^\varepsilon, \varphi_1)_{(0,T)\times\Omega^\varepsilon} + (k_2 u_2^\varepsilon, \varphi_1)_{(0,T)\times\Omega^\varepsilon} \qquad (9)$$
$$- \varepsilon(\eta(u_1^\varepsilon, u_4^\varepsilon), \varphi_1)_{(0,T)\times\Gamma_\varepsilon^{sw}},$$

$$\langle \partial_t u_2^\varepsilon, \varphi_2 \rangle_{(0,T)\times\Omega^\varepsilon} + (d_2^\varepsilon \nabla u_2^\varepsilon), \nabla \varphi_2)_{(0,T)\times\Omega^\varepsilon}$$
$$= (k_1^\varepsilon u_1^\varepsilon, \varphi_2)_{(0,T)\times\Omega^\varepsilon} - (k_2^\varepsilon u_2^\varepsilon, \varphi_2)_{(0,T)\times\Omega^\varepsilon} \qquad (10)$$
$$+ \varepsilon(a_\varepsilon u_3^\varepsilon, \varphi_2)_{(0,T)\times\Gamma_\varepsilon^{wa}} - \varepsilon(a_\varepsilon u_2^\varepsilon, \varphi_2)_{(0,T)\times\Gamma_\varepsilon^{wa}},$$

$$\langle \partial_t u_3^\varepsilon, \varphi_3 \rangle_{(0,T) \times \Omega_1^\varepsilon} = -(d_3^\varepsilon \nabla u_3^\varepsilon), \nabla \varphi_3)_{(0,T) \times \Omega_1^\varepsilon}$$
$$- \varepsilon(a_\varepsilon u_3^\varepsilon, \varphi_3)_{(0,T) \times \Gamma_\varepsilon^{wa}} + \varepsilon(a_\varepsilon u_2^\varepsilon, \varphi_3)_{(0,T) \times \Gamma_\varepsilon^{wa}}, \tag{11}$$

$$\langle \partial_t u_4^\varepsilon, \varphi_4 \rangle_{(0,T) \times \Omega^\varepsilon} = -(d_4^\varepsilon \nabla u_4^\varepsilon), \nabla \varphi_4)_{(0,T) \times \Omega^\varepsilon} + (k_1^\varepsilon u_1^\varepsilon, \varphi_4)_{(0,T) \times \Omega^\varepsilon} \tag{12}$$

for all $\varphi_j \in L^2(0,T; H^1(\Omega^\varepsilon)), j \in \{1,2,4\}$ and $\varphi_3 \in L^2(0,T; H^1_{\Gamma^D}(\Omega_1^\varepsilon))$ together with the ode

$$\partial_t u_5^\varepsilon = \eta(u_1^\varepsilon, u_5^\varepsilon) \ a.e. \ on \ (0,T) \times \Gamma_\varepsilon^{ws} \tag{13}$$

and the initial conditions

$$
\begin{aligned}
u_i^\varepsilon(0,x) &= u_{i0}^\varepsilon(x) \ \ x \in \Omega^\varepsilon \ for \ all \ i \in \{1,2,4\}, \\
u_3^\varepsilon(0,x) &= u_{30}^\varepsilon(x) \ \ x \in \Omega_1^\varepsilon, \\
u_5^\varepsilon(0,x) &= u_{50}^\varepsilon(x) \ \ x \in \Gamma_\varepsilon^{ws}.
\end{aligned}
\tag{14}
$$

3.4   Basic results

Lemma 2 *(Positivity and L^∞-estimates) Assume (A1)-(A6), and let $t \in [0,T]$ be arbitrarily chosen. Then the following estimates hold:*

(i) $u_i^\varepsilon(t) \geq 0, \ \ i \in \{1,2,4\}$ a.e. in Ω^ε, $u_3^\varepsilon(t) \geq 0$ a.e. Ω_1^ε and $u_5^\varepsilon(t) \geq 0$ a.e. on Γ_ε^{ws}.

(ii) $u_i^\varepsilon(t) \leq M_i, \ i \in \{1,2\}$, $u_4^\varepsilon(t) \leq (t+1)M_4$ a.e. in Ω^ε , $u_3^\varepsilon(t) \leq M_3$ a.e. in Ω_1^ε and $u_5^\varepsilon(t) \leq M_5$ a.e. on Γ_ε^{ws}.

Proof (i). We test (9)-(12) with $\varphi = (-u_1^{\varepsilon-}, -u_2^{\varepsilon-}, -u_3^{\varepsilon-}, -u_4^{\varepsilon-})$ element of the space $[L^2(0,T; H^1(\Omega^\varepsilon))]^2 \times L^2(0,T; H^1_{\Gamma^D}(\Omega_1^\varepsilon)) \times L^2(0,T; H^1(\Omega^\varepsilon))$. We obtain the following inequality

$$\frac{1}{2}\partial_t |u_1^{\varepsilon-}|^2 + d_1 |\nabla u_1^{\varepsilon-}|^2 \leq -k_1 |u_1^{\varepsilon-}|^2 + k_2^\infty(u_1^{\varepsilon-}, u_2^{\varepsilon-})$$
$$- \varepsilon(\eta(u_1^\varepsilon, u_5^\varepsilon), -u_1^{\varepsilon-})_{\Gamma_\varepsilon^{sw}}. \tag{15}$$

Note that the first term on the r.h.s of (15) is negative, while the third term is zero because of (A2). We then get

$$\partial_t |u_1^{\varepsilon-}|^2 + 2d_1 |\nabla u_1^{\varepsilon-}|^2 \leq k_2^\infty \left(|u_1^{\varepsilon-}|^2 + |u_2^{\varepsilon-}|^2 \right). \tag{16}$$

On the other hand, (10) leads to

$$\frac{1}{2}\partial_t |u_2^{\varepsilon-}|^2 + d_2 |\nabla u_2^{\varepsilon-}|^2 \leq \frac{k_1^\infty}{2} \left(|u_1^{\varepsilon-}|^2 + |u_2^{\varepsilon-}|^2 \right)$$
$$+ \varepsilon a^\infty(u_2^{\varepsilon-}, u_3^{\varepsilon-})_{\Gamma_\varepsilon^{wa}} + \varepsilon b^\infty |u_2^{\varepsilon-}|^2_{\Gamma_\varepsilon^{wa}}.$$

By the trace inequality (7) (with $\varepsilon < 1$), we get

$$\partial_t |u_2^{\varepsilon-}|^2 + 2(d_2 - C^* b^\infty)|\nabla u_2^{\varepsilon-}|^2 \leq k_1^\infty \left(|u_1^{\varepsilon-}|^2 + |u_2^{\varepsilon-}|^2 \right)$$
$$+ 2C^* b^\infty |u_2^{\varepsilon-}|^2 + 2\varepsilon a^\infty(u_2^{\varepsilon-}, u_3^{\varepsilon-})_{\Gamma_\varepsilon^{wa}}. \tag{17}$$

(11) leads to

$$\partial_t |u_3^{\varepsilon-}|^2 + 2(d_3 - C^* a^\infty)|\nabla u_3^{\varepsilon-}|^2 \leq 2\varepsilon b^\infty (u_2^{\varepsilon-}, u_3^{\varepsilon-})_{\Gamma_\varepsilon^{wa}} + 2C^* a^\infty |u_3^{\varepsilon-}|^2, \quad (18)$$

while from (12), we see that

$$\partial_t |u_4^{\varepsilon-}|^2 + 2d_4 |\nabla u_5^{\varepsilon-}|^2 \leq k_1^\infty \left(|u_1^{\varepsilon-}|^2 + |u_5^{\varepsilon-}|^2 \right). \quad (19)$$

Adding up inequalities (16)-(19) gives

$$
\begin{aligned}
\partial_t \sum_{i=1}^4 |u_i^{\varepsilon-}|^2 &+ 2d_1 |\nabla u_1^{\varepsilon-}|^2 + 2(d_2 - C^* b^\infty)|\nabla u_2^{\varepsilon-}|^2 \\
&+ 2(d_3 - C^* a^\infty)|\nabla u_3^{\varepsilon-}|^2 + 2d_4 |\nabla u_4^{\varepsilon-}|^2 \\
&\leq (2k_1^\infty + k_2^\infty + 2C^* b^\infty + 2C^* a^\infty) \sum_{i=1}^4 |u_i^{\varepsilon-}|^2 \\
&+ 2\varepsilon (a^\infty + b^\infty)(u_2^{\varepsilon-}, u_3^{\varepsilon-})_{\Gamma_\varepsilon^{wa}},
\end{aligned}
\quad (20)
$$

and hence,

$$
\begin{aligned}
\partial_t \sum_{i=1}^4 |u_i^{\varepsilon-}|^2 &+ 2d_1 |\nabla u_1^{\varepsilon-}|^2 + 2(d_2 - C^* b^\infty)|\nabla u_2^{\varepsilon-}|^2 \\
&+ 2(d_3 - C^* a^\infty)|\nabla u_3^{\varepsilon-}|^2 + 2d_4 |\nabla u_5^{\varepsilon-}|^2 \\
&\leq (2k_1^\infty + k_2^\infty + C^*(a^\infty + b^\infty)) \sum_{i=1}^4 |u_i^{\varepsilon-}|^2 \\
&+ \varepsilon \left(a^\infty + b^\infty)(\delta |u_2^{\varepsilon-}|_{\Gamma_\varepsilon^{wa}}^2 + \frac{1}{\delta}|u_3^{\varepsilon-}|_{\Gamma_\varepsilon^{wa}}^2 \right).
\end{aligned}
\quad (21)
$$

Applying the trace inequality (7) to estimate the last term on the right side of (21), we finally get

$$
\begin{aligned}
\partial_t \sum_{i=1}^4 |u_i^{\varepsilon-}|^2 &+ 2d_1 |\nabla u_1^{\varepsilon-}|^2 + (2d_2 - 2C^* b^\infty - C^*\delta(a^\infty + b^\infty))|\nabla u_2^{\varepsilon-}|^2 \\
&+ (2d_3 - 2C^* a^\infty - \frac{C^* 2}{\delta}(a^\infty + b^\infty))|\nabla u_3^{\varepsilon-}|^2 + 2d_4 |\nabla u_4^{\varepsilon-}|^2 \\
&\leq C_1 \sum_{i=1}^4 |u_i^{\varepsilon-}|^2.
\end{aligned}
$$

Thus, we have

$$\partial_t \sum_{i=1}^4 |u_i^{\varepsilon-}|^2 \leq C_1 \sum_{i=1}^4 |u_i^{\varepsilon-}|^2.$$

where $C_1 := 2k_1^\infty + k_2^\infty + C^*(a^\infty + b^\infty) + C^*(\delta + \frac{1}{\delta})(a^\infty + b^\infty)$ and δ is chosen conveniently. Gronwall's inequality together with $[u_i^\varepsilon(0)]^- = 0$ gives now the desired result. Note that (A2) ensures automatically the positivity of u_5^ε.

(ii). We consider the test function

$$(\varphi_1, \varphi_2, \varphi_3, \varphi_4) = ((u_1^\varepsilon - M_1)^+, (u_2^\varepsilon - M_2)^+, (u_3^\varepsilon - M_3)^+, (u_4^\varepsilon - (t+1)M_4)^+).$$

Obviously, $\varphi \in [L^2(0, T; H^1(\Omega^\varepsilon))]^2 \times L^2(0, T; H^1_{\Gamma^D}(\Omega_1^\varepsilon) \times L^2(0, T; H^1(\Omega^\varepsilon)$ is allowed as test function. We obtain from (9) that

$$\frac{1}{2}\partial_t|(u_1^\varepsilon - M_1)^+|^2 + d_1|\nabla(u_1^\varepsilon - M_1)^+|^2 \leq -k_1|(u_1^\varepsilon - M_1)^+|^2$$
$$- (k_1 M_1, (u_1^\varepsilon - M_1)^+)$$
$$+ k_2^\infty((u_1^\varepsilon - M_1)^+, (u_2^\varepsilon - M_2)^+)$$
$$+ (k_2^\infty M_2, (u_1^\varepsilon - M_1)^+)$$
$$- \varepsilon(\eta(u_1^\varepsilon, u_5^\varepsilon), (u_1^\varepsilon - M_1)^+)_{\Gamma_\varepsilon^{sw}}.$$

Relying on (A4), we get the estimate

$$\partial_t|(u_1^\varepsilon - M_1)^+|^2 \leq k_2^\infty(|(u_1^\varepsilon - M_1)^+|^2 + |(u_2^\varepsilon - M_2)^+|^2). \tag{22}$$

(10) in combination with (A4) gives that

$$\partial_t|(u_2^\varepsilon - M_2)^+|^2 + 2(d_2 - C^*b^\infty)|\nabla(u_2^\varepsilon - M_2)^+|^2$$
$$\leq k_1^\infty(|(u_1^\varepsilon - M_1)^+|^2 + |(u_2^\varepsilon - M_2)^+|^2)$$
$$+ 2C^*b^\infty|(u_2^\varepsilon - M_2)^+|^2 \tag{23}$$
$$+ 2\varepsilon a^\infty((u_2^\varepsilon - M_2)^+, (u_3^\varepsilon - M_3)^+)_{\Gamma_\varepsilon^{wa}}.$$

By (11), we obtain

$$\partial_t|(u_3^\varepsilon - M_3)^+|^2 + 2(d_3 - C^*a^\infty)|\nabla(u_3^\varepsilon - M_3)^+|^2$$
$$\leq 2C^*a^\infty|\nabla(u_3^\varepsilon - M_3)^+|^2 \tag{24}$$
$$+ 2\varepsilon b^\infty((u_2^\varepsilon - M_2)^+, (u_3^\varepsilon - M_3)^+)_{\Gamma_\varepsilon^{wa}}.$$

Using again (A4), (12) yields

$$\partial_t|(u_4^\varepsilon - (t+1)M_4)^+|^2 \leq k_1^\infty(|(u_1^\varepsilon - M_1)^+|^2 + |(u_4^\varepsilon - (t+1)M_4)^+|^2). \tag{25}$$

Adding up (22)–(25) side by side, we get

$$\sum_{j=1}^3 \partial_t|(u_j^\varepsilon - M_j)^+|^2 + \partial_t|(u_4^\varepsilon - (t+1)M_4)^+|^2 + (2d_2 - 2C^*b^\infty)|\nabla(u_2^\varepsilon - M_2)^+|^2$$
$$+ (2d_3 - 2C^*a^\infty)|\nabla(u_3^\varepsilon - M_3)^+|^2$$
$$\leq (2k_2^\infty + k_1^\infty + 2C^*a^\infty + 2C^*b^\infty)(\sum_{j=1}^3 |(u_j^\varepsilon - M_j)^+|^2$$
$$+ |(u_4^\varepsilon - (t+1)M_4)^+|^2) + \varepsilon(a^\infty + b^\infty)(\delta|(u_2^\varepsilon - M_2)^+|^2_{\Gamma_\varepsilon^{wa}}$$
$$+ \frac{1}{\delta}|(u_3^\varepsilon - M_3)^+|^2_{\Gamma_\varepsilon^{wa}}).$$

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We use the trace inequality (7) (with $\varepsilon < 1$) to deal with the boundary terms in (26). Then Gronwall's inequality yields for all $t \in (0, T)$ the following estimate

$$u_j^\varepsilon(t) \leq M_j, \quad j \in \{1, 2, 5\} \ a. \ e. \ in \ \Omega^\varepsilon$$
$$u_3^\varepsilon(t) \leq M_3, \ a. \ e. \ in \ \Omega_1^\varepsilon$$
$$u_4^\varepsilon \leq (t + 1)M_4 \ a.e. \ in \ \Omega^\varepsilon.$$

Furthermore, by (A2) u_5^ε is bounded.

Proposition 3 *(Uniqueness) Assume (A1)–(A4). Then there exists at most one weak solution in the sense of Definition 1.*

Proof. We assume that $u^{j,\varepsilon} = (u_1^{j,\varepsilon}, u_2^{j,\varepsilon}, u_3^{j,\varepsilon}, u_4^{j,\varepsilon}, u_5^{j,\varepsilon}), j \in \{1, 2\}$ are two distinct weak solutions in the sense of Definition 1. We set $u_i^\varepsilon := u_i^{1,\varepsilon} - u_i^{2,\varepsilon}$ for all $i \in \{1, 2, 3, 4\}$. Firstly, we deal with (15). We obtain

$$\partial_t u_5^{1,\varepsilon} - \partial_t u_5^{2,\varepsilon} = \eta(u_1^{1,\varepsilon}, u_5^{1,\varepsilon}) - \eta(u_1^{2,\varepsilon}, u_5^{2,\varepsilon}). \tag{26}$$

Integrating (26) along (0,T) and using (A2), we get

$$|u_5^{1,\varepsilon} - u_5^{2,\varepsilon}| \leq k_3^\infty c_R c_Q M_1 \int_0^t |u_5^{1,\varepsilon} - u_5^{2,\varepsilon}| d\tau + k_3^\infty c_R Q^\infty \int_0^t |u_1^{1,\varepsilon} - u_1^{2,\varepsilon}| d\tau.$$

Gronwall's inequality implies

$$|u_5^{1,\varepsilon}(t) - u_5^{2,\varepsilon}(t)| \leq C_2 \int_0^t |u_1^{1,\varepsilon} - u_1^{2,\varepsilon}| d\tau \ \text{ for a.e. } t \in (0, T), \tag{27}$$

where $C_2 := k_3^\infty c_R Q^\infty (1 + C_3 t e^{C_3 t})$ and $C_3 := k_3^\infty c_R c_Q M_1$. We calculate

$$\frac{1}{2}\partial_t |u_1^\varepsilon|^2 + d_1 |\nabla u_1^\varepsilon|^2 \leq -k_1 |u_1^\varepsilon|^2 + k_2^\infty(u_1^\varepsilon, u_2^\varepsilon) + \varepsilon(\eta_1 - \eta_2, u_1^\varepsilon)_{\Gamma_\varepsilon^{sw}}, \tag{28}$$

where we denote $\eta_1 - \eta_2 := \eta(u_1^{1,\varepsilon}, u_5^{1,\varepsilon}) - \eta(u_1^{2,\varepsilon}, u_5^{2,\varepsilon})$. We can write

$$\begin{aligned}
\frac{1}{2}\partial_t |u_1^\varepsilon|^2 + d_1 |\nabla u_1^\varepsilon|^2 \leq{}& -k_1 |u_1^\varepsilon|^2 + \frac{k_2^\infty}{2}(|u_1^\varepsilon|^2 + |u_2^\varepsilon|^2) \\
&+ \varepsilon C_3 (u_5^{1,\varepsilon} - u_5^{2,\varepsilon}, u_1^\varepsilon)_{\Gamma_\varepsilon^{sw}} \\
&+ \varepsilon k_3^\infty c_R Q^\infty (u_1^{1,\varepsilon} - u_1^{2,\varepsilon}, u_1^\varepsilon)_{\Gamma_\varepsilon^{sw}}.
\end{aligned} \tag{29}$$

Now, inserting (27) in (29) yields

$$\begin{aligned}
\frac{1}{2}\partial_t |u_1^\varepsilon|^2 + d_1 |\nabla u_1^\varepsilon|^2 \leq{}& -k_1 |u_1^\varepsilon|^2 + \frac{k_2^\infty}{2}(|u_1^\varepsilon|^2 + |u_2^\varepsilon|^2) \\
&+ C_4 \varepsilon |u_1^\varepsilon|^2_{\Gamma_\varepsilon^{sw}} + \frac{\varepsilon C_3^2}{2\delta} \int_0^t |u_1^\varepsilon|^2_{\Gamma_\varepsilon^{sw}} d\tau,
\end{aligned} \tag{30}$$

where $C_4 := k_3^\infty c_R Q^\infty + \frac{C_3}{2\delta}$. Using (7), we estimate the last two terms in (30) to obtain the inequality

$$
\frac{1}{2}\partial_t|u_1^\varepsilon|^2 + d_1|\nabla u_1^\varepsilon|^2 \leq -k_1|u_1^\varepsilon|^2 + \frac{k_2^\infty}{2}(|u_1^\varepsilon|^2 + |u_2^\varepsilon|^2) + C^* C_4(|u_1^\varepsilon|^2
$$
$$
+ \varepsilon^2|\nabla u_1^\varepsilon|) + C^*\frac{C_3^2}{2\delta}\int_0^t (|u_1^\varepsilon|^2 + \varepsilon^2|\nabla u_1^\varepsilon|^2)d\tau. \tag{31}
$$

Note that the constant C^*, arising from in (31), stems from (7). Rearranging now the terms, we have

$$
\partial_t|u_1^\varepsilon|^2 + (2d_1 - 2C^*C_4\varepsilon^2)|\nabla u_1^\varepsilon|^2 + 2k_1|u_1^\varepsilon|^2 \leq (k_2^\infty + C^*C_4)(|u_1^\varepsilon|^2
$$
$$
+ |u_2^\varepsilon|^2) + C^*\frac{C_3^2}{2\delta}\int_0^t (|u_1^\varepsilon|^2 + \varepsilon^2|\nabla u_1^\varepsilon|^2)d\tau. \tag{32}
$$

Following the same line of arguments as before, we obtain from (10) that

$$
\partial_t|u_2^\varepsilon|^2 + 2d_2|\nabla u_2^\varepsilon|^2 \leq -2k_2|u_2^\varepsilon|^2 + k_1^\infty(|u_1^\varepsilon|^2 + u_2^\varepsilon|^2)
$$
$$
+ 2\varepsilon a^\infty(u_3^\varepsilon, u_2^\varepsilon)_{\Gamma_\varepsilon^{wa}} + 2\varepsilon b^\infty|u_2^\varepsilon|_{\Gamma_\varepsilon^{wa}}^2, \tag{33}
$$

while from (11), we deduce

$$
\partial_t|u_3^\varepsilon|^2 + 2d_3|\nabla u_3^\varepsilon|^2 \leq 2\varepsilon b^\infty(u_2^\varepsilon, u_3^\varepsilon)_{\Gamma_\varepsilon^{wa}} + 2\varepsilon a^\infty|u_3^\varepsilon|_{\Gamma_\varepsilon^{wa}}^2. \tag{34}
$$

Proceeding similarly, (12) yields

$$
\partial_t|u_4^\varepsilon|^2 + 2d_4|\nabla u_4^\varepsilon|^2 \leq k_2^\infty(|u_1^\varepsilon|^2 + |u_4^\varepsilon|^2). \tag{35}
$$

Putting together (32)–(35), we get

$$
\partial_t \Sigma_{i=1}^4 |u_i^\varepsilon|^2 + (2d_1 - C^*C_4\varepsilon^2)|\nabla u_1^\varepsilon|^2 + 2d_2|\nabla u_2^\varepsilon|^2 + 2d_3|\nabla u_3^\varepsilon|^2
$$
$$
+ 2d_4|\nabla u_4^\varepsilon|^2 + 2k_1|u_1^\varepsilon|^2
$$
$$
\leq (2k_1^\infty + k_2^\infty + C^*C_2)\, \Sigma_{i=1}^4 |u_i^\varepsilon|^2
$$
$$
+ C^*\frac{C_1^2}{2\delta}\int_0^t (|u_1^\varepsilon|^2 + \varepsilon^2|\nabla u_1^\varepsilon|^2)d\tau
$$
$$
+ 2\varepsilon b|u_2^\varepsilon|_{\Gamma_\varepsilon^{wa}}^2 + 2\varepsilon a|u_3^\varepsilon|_{\Gamma_\varepsilon^{wa}}^2
$$
$$
+ \varepsilon(a^\infty + b^\infty)(\delta|u_2^\varepsilon|_{\Gamma_\varepsilon^{wa}}^2 + \frac{1}{\delta}|u_3^\varepsilon|_{\Gamma_\varepsilon^{wa}}^2). \tag{36}
$$

Applying the trace inequality (7) to the boundary terms in (36), we get

$$
\partial_t \Sigma_{i=1}^4 |u_i^\varepsilon|^2 + (2d_1 - 2C^*C_4\varepsilon^2)|\nabla u_1^\varepsilon|^2
$$
$$
+ (2d_2 - 2C^*b^\infty\varepsilon^2 - C^*\delta\varepsilon^2(a^\infty + b^\infty))|\nabla u_2^\varepsilon|^2
$$
$$
+ (2d_3 - 2C^*a^\infty\varepsilon^2 - \frac{C^*\varepsilon^2}{\delta}(a^\infty + b^\infty))|\nabla u_3^\varepsilon|^2
$$
$$
+ 2d_4|\nabla u_4^\varepsilon|^2 + 2k_1|u_1^\varepsilon|^2 \leq C_5\Sigma_{i=1}^4 |u_i^\varepsilon|^2
$$

$$+ C^* \frac{C_1^2}{2\delta} \int_0^t (|u_1^\varepsilon|^2 + \varepsilon^2 |\nabla u_1^\varepsilon|^2) d\tau, \tag{37}$$

where $C_5 := 2k_1^\infty + k_2^\infty + C^* C_2 + 2C^*(a^\infty + b^\infty) + C^*(a^\infty + b^\infty)(\delta + \frac{1}{\delta})$. Let us choose ε and δ such that

$$\varepsilon \in \left] 0, \frac{2d_1}{C_1 C^*} \right[$$

$$\delta \in \left[\frac{C^* \varepsilon^2 (a^\infty + b^\infty)}{2d_3 - C^* a^\infty \varepsilon^2}, \frac{2d_2 - C^* b^\infty \varepsilon^2}{C^* \varepsilon^2 (a^\infty + b^\infty)} \right].$$

With this choice of (ε, δ), (37) takes the form

$$\partial_t \Sigma_{i=1}^4 |u_i^\varepsilon|^2 + \bar{C} |\nabla u_1^\varepsilon|^2 + \bar{C} |u_1^\varepsilon|^2 \leq C_6 (\Sigma_{i=1}^4 |u_i^\varepsilon|^2 + \int_0^t (|u_1^\varepsilon|^2 + \varepsilon^2 |\nabla u_1^\varepsilon|^2) d\tau),$$

where $C_6 := 2k_1^\infty + k_2^\infty + C^* C_2 + C^*(a^\infty + b^\infty) + C^* \frac{C_1^2}{2\delta}$ and $\bar{C} := \min\{2d_1 - 2C^* C_2 \varepsilon^2, 2k_1\}$. Taking in (37) the supremum along $t \in (0, T)$ and applying Gronwall's inequality, we obtain the following estimate

$$\Sigma_{i=1}^4 |u_i^\varepsilon|^2 + \bar{C} \int_0^T |\nabla u_1^\varepsilon|^2 dt + \bar{C} \int_0^T |u_1^\varepsilon|^2 dt \leq 0. \tag{38}$$

Thus, the proof of Proposition 3 is completed.

Theorem 4 *(Global Existence) Assume $(A1) - (A3)$. Then there exists at least a global-in-time weak solution in the sense of Definition 1.*

Proof. The proof is based on the Galerkin argument. Since the proof is rather standard, and here we wish to focus on the passage to the limit $\varepsilon \to 0$, we omit it.

4 *A priori* estimates for microscopic solutions

This section includes the $\varepsilon-$ independent estimates.

Lemma 5 *Assume (A1)-(A6). Then the weak solution of the microscopic model (9)-(14) satisfies the following* a priori *bounds:*

$$\| u_j^\varepsilon \|_{L^2(0,T;H^1(\Omega^\varepsilon))} \leq C, \ j \in \{1, 2, 3, 4\} \tag{39}$$
$$\| \nabla \partial_t u_2^\varepsilon \|_{L^2(0,T;L^2(\Omega^\varepsilon))} \leq C, \tag{40}$$
$$\| \partial_t u_j^\varepsilon \|_{L^2(0,T;L^2(\Omega^\varepsilon))} \leq C, \tag{41}$$
$$\| u_3^\varepsilon \|_{L^2(0,T;H^1(\Omega_1^\varepsilon))} \leq C, \tag{42}$$
$$\| \nabla \partial_t u_3^\varepsilon \|_{L^2(0,T;L^2(\Omega_1^\varepsilon))} \leq C, \tag{43}$$
$$\| \partial_t u_3^\varepsilon \|_{L^2(0,T;L^2(\Omega_1^\varepsilon))} \leq C, \tag{44}$$

$$\| u_5^\varepsilon \|_{L^\infty((0,T)\times\Gamma_\varepsilon^{sw})} \leq C, \tag{45}$$

$$\| \partial_t u_5^\varepsilon \|_{L^2((0,T)\times\Gamma_\varepsilon^{sw})} \leq C. \tag{46}$$

In (39)–(46), the generic constant C is independent of ε.

Proof. We test (9) with $\varphi_1 = u_1^\varepsilon$ to get

$$\begin{aligned}
\frac{1}{2}\partial_t |u_1^\varepsilon|^2 + d_1 |\nabla u_1^\varepsilon|^2 &\leq -k_1 |u_1^\varepsilon|^2 + k_2^\infty(u_1^\varepsilon, u_2^\varepsilon) - \varepsilon(\eta, u_1^\varepsilon)_{\Gamma_\varepsilon^{sw}}, \\
&\leq \frac{k_2^\infty}{2}(|u_1^\varepsilon|^2 + |u_2^\varepsilon|^2) + \varepsilon k_3^\infty Q^\infty c_R(u_1^\varepsilon, u_1^\varepsilon)_{\Gamma_\varepsilon^{sw}}.
\end{aligned} \tag{47}$$

After applying the trace inequality to the last term on r.h.s of (47), we get

$$\frac{1}{2}\partial_t |u_1^\varepsilon|^2 + d_1 |\nabla u_1^\varepsilon|^2 \leq \frac{k_2^\infty}{2}(|u_1^\varepsilon|^2 + |u_2^\varepsilon|^2) + C^* k_3^\infty Q^\infty c_R(|u_1^\varepsilon|^2 + \varepsilon^2 |\nabla u_1^\varepsilon|^2)_{\Gamma_\varepsilon^{sw}}.$$

$$\frac{1}{2}\partial_t |u_1^\varepsilon|^2 + (d_1 - \varepsilon^2 C^* k_3^\infty Q^\infty c_R)|\nabla u_1^\varepsilon|^2 \leq C_7(|u_1^\varepsilon|^2 + |u_2^\varepsilon|^2), \tag{48}$$

where $C_7 := \frac{k_2^\infty}{2} + C^* k_3^\infty Q^\infty c_R$. Taking $\varphi_2 = u_2^\varepsilon$ in (10), we get

$$\begin{aligned}
\frac{1}{2}\partial_t |u_2^\varepsilon|^2 + d_2 |\nabla u_2^\varepsilon|^2 &\leq \frac{k_1^\infty}{2}(|u_1^\varepsilon|^2 + |u_2^\varepsilon|^2) - k_2 |u_2^\varepsilon|^2 \\
&\quad + \varepsilon a^\infty(u_3^\varepsilon, u_2^\varepsilon)_{\Gamma_\varepsilon^{wa}} + \varepsilon b^\infty |u_2^\varepsilon|_{\Gamma_\varepsilon^{wa}}^2.
\end{aligned}$$

Application of the trace inequality (7) only to the last term leads to

$$\begin{aligned}
\frac{1}{2}\partial_t |u_2^\varepsilon|^2 + (d_2 - C^* b^\infty \varepsilon^2)|\nabla u_2^\varepsilon|^2 &\leq \frac{k_1^\infty}{2}(|u_1^\varepsilon|^2 + |u_2^\varepsilon|^2) + 2 \\
&\quad + \varepsilon a^\infty(u_3^\varepsilon, u_2^\varepsilon)_{\Gamma_\varepsilon^{wa}}.
\end{aligned} \tag{49}$$

We choose $\varphi_3 = u_3^\varepsilon$ as a test function in (11) to calculate

$$\frac{1}{2}\partial_t |u_3^\varepsilon|^2 + (d_3 - C^* a^\infty \varepsilon^2)|\nabla u_3^\varepsilon|^2 \leq \varepsilon b^\infty(u_3^\varepsilon, u_2^\varepsilon)_{\Gamma_\varepsilon^{wa}} + C^* a^\infty |u_3^\varepsilon|^2. \tag{50}$$

Setting $\varphi_4 = u_4^\varepsilon$ in (12), we are led to

$$\frac{1}{2}\partial_t |u_4^\varepsilon|^2 + d_4 |\nabla u_4^\varepsilon|^2 \leq \frac{k_1^\infty}{2}(|u_1^\varepsilon|^2 + |u_4^\varepsilon|^2). \tag{51}$$

Putting together (48)-(51), we obtain

$$\begin{aligned}
\frac{1}{2}\Sigma_{i=1}^4 \partial_t |u_i^\varepsilon|^2 &+ (d_1 - \varepsilon^2 C^* k_3^\infty Q^\infty c_R)|\nabla u_1^\varepsilon|^2 + d_4 |\nabla u_4^\varepsilon|^2 \\
&+ (d_2 - C^* b^\infty \varepsilon^2)|\nabla u_2^\varepsilon|^2 + (d_3 - C^* a^\infty \varepsilon^2)|\nabla u_3^\varepsilon|^2 \\
&\leq (k_1^\infty + \frac{k_2^\infty}{2} + C^* b^\infty + C^* a^\infty)\Sigma_{i=1}^4 |u_i^\varepsilon|^2 \\
&+ \varepsilon(a^\infty + b^\infty)(u_3^\varepsilon, u_2^\varepsilon)_{\Gamma_\varepsilon^{wa}}.
\end{aligned} \tag{52}$$

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Combing Young's inequality and the trace inequality to the boundary term, (52) turns out to be

$$\frac{1}{2}\Sigma_{i=1}^4\partial_t|u_i^\varepsilon|^2 + (d_1 - \varepsilon^2 C^* k_3^\infty Q^\infty c_R)|\nabla u_1^\varepsilon|^2$$

$$+ (d_2 - C^* b\varepsilon^2 - \frac{C^*\varepsilon^2\delta}{2}(a^\infty + b^\infty))|\nabla u_2^\varepsilon|^2$$

$$+ (d_3 - C^* a\varepsilon^2 - \frac{C^*\varepsilon^2}{2\delta}(a^\infty + b^\infty))|\nabla u_3^\varepsilon|^2 + d_4|\nabla u_4^\varepsilon|^2$$

$$\leq (k_1^\infty + \frac{k_2^\infty}{2} + C^*(a^\infty + b^\infty)(\delta + \frac{1}{\delta}))\Sigma_{i=1}^4|u_i^\varepsilon|^2.$$

Choosing ε small enough and δ conveniently such that the coefficients of the terms involving $|\nabla u_2^\varepsilon|^2$ and $|\nabla u_3^\varepsilon|^2$ stay positive, we are led to

$$\Sigma_{i=1}^4\partial_t|u_i^\varepsilon|^2 + d_1'|\nabla u_1^\varepsilon|^2 + d_2'|\nabla u_2^\varepsilon|^2 + d_3'|\nabla u_3^\varepsilon|^2 + 2d_4|\nabla u_4^\varepsilon|^2 \leq C_7\Sigma_{i=1}^4|u_i^\varepsilon|^2,$$

where

$$d_1' := 2(d_1 - \varepsilon^2 C^* k_3^\infty Q^\infty c_R),$$
$$d_2' := 2(d_2 - C^* b^\infty\varepsilon^2 - \frac{C^*\varepsilon^2\delta}{2}(a^\infty + b^\infty)),$$
$$d_3' := 2(d_3 - C^* a^\infty\varepsilon^2 - \frac{C^* b\varepsilon^2}{2\delta}(a^\infty + b^\infty)),$$

while the constant C is given by

$$C_8 := 2k_1^\infty + \frac{k_2^\infty}{2} + C^* a^\infty + C^* b^\infty + C^*(a^\infty + b^\infty)(\delta + \frac{1}{\delta}).$$

Summarizing, we have

$$\Sigma_{i=1}^4\partial_t|u_i^\varepsilon|^2 + d_0\Sigma_{j=1}^3|\nabla u_j^\varepsilon|^2 + d_0|\nabla u_3^\varepsilon|^2 \leq C\Sigma_{i=1}^4|u_i^\varepsilon|^2, \qquad (53)$$

where $d_0 := min\{d_1', d_2', d_3', d_4'\}$. By Gronwall's inequality, we have

$$\Sigma_{i=1}^4|u_i^\varepsilon|^2 \leq C\Sigma_{i=1}^4|u_i(0)|^2,$$

and hence,

$$\| u_j^\varepsilon \|_{L^2(0,T;L^2(\Omega^\varepsilon))} \leq C \text{ for all } i \in \{1,2,4\} \text{ and } \|u_3^\varepsilon\|_{L^2(0,T;L^2(\Omega_1^\varepsilon))} \leq C, \quad (54)$$

where C depends on initial data and model parameters but is independent of ε. Integrating (53) along $(0,T)$, we get

$$\| u_j^\varepsilon \|_{L^2(0,T;H^1(\Omega^\varepsilon))} \leq C, \ j \in \{1,2,4\},$$
$$\| u_3^\varepsilon \|_{L^2(0,T;H^1(\Omega_1^\varepsilon))} \leq C.$$
$$(55)$$

With the help of (A2) together with the boundedness of u_1^ε, we conclude from (13) that
$$\| u_5^\varepsilon \|_{L^\infty((0,T)\times\Gamma_\varepsilon^{sw})} \leq C.$$
Multiplying (13) by $\partial_t u_5^\varepsilon$ and using (A2), we get

$$\|\partial_t u_5^\varepsilon\|_{L^2((0,T)\times\Gamma_\varepsilon^{sw})} \leq C.$$

Now, we focus on obtaining $\varepsilon-$independent estimates on the time derivative of the concentrations. Firstly, we choose $\varphi_1 = \partial_t u_1^\varepsilon$ and get

$$
\int_0^t \int_{\Omega^\varepsilon} \partial_t u_1^\varepsilon \partial_t u_1^\varepsilon dx d\tau + \int_0^t \int_{\Omega^\varepsilon} d_1^\varepsilon \nabla u_1^\varepsilon \nabla \partial_t u_1^\varepsilon dx d\tau
$$
$$
= -\int_0^t \int_{\Omega^\varepsilon} k_1^\varepsilon u_1^\varepsilon \partial_t u_1^\varepsilon dx d\tau + \int_0^t \int_{\Omega^\varepsilon} k_2^\varepsilon u_2^\varepsilon \partial_t u_1^\varepsilon dx d\tau \quad (56)
$$
$$
- \varepsilon \int_0^t \int_{\Gamma_\varepsilon^{sw}} \eta \partial_t u_1^\varepsilon d\sigma_x d\tau.
$$

Consequently, it holds

$$
\int_0^t \int_{\Omega^\varepsilon} |\partial_t u_1^\varepsilon|^2 dx d\tau + \int_0^t \int_{\Omega^\varepsilon} \left(\frac{1}{2}\partial_t(d_1^\varepsilon|\nabla u_1^\varepsilon|^2) - (\partial_t d_1^\varepsilon)|\nabla u_1^\varepsilon|^2 \right) dx d\tau
$$
$$
\leq -\frac{k_1}{2}\int_0^t \int_{\Omega^\varepsilon} \partial_t|u_1^\varepsilon|^2 dx d\tau
$$
$$
+ \frac{k_2^\infty}{2}\int_0^t \int_{\Omega^\varepsilon} \left(\frac{1}{\delta}|u_2^\varepsilon|^2 + \delta|\partial_t u_1^\varepsilon|^2 \right) dx d\tau
$$
$$
- \varepsilon \int_0^t \int_{\Gamma_\varepsilon^{sw}} (\partial_t(\eta u_1^\varepsilon) - (\partial_t \eta)u_1^\varepsilon)d\sigma_x d\tau,
$$

$$
(1 - \frac{k_2^\infty \delta}{2}) \int_0^t \int_{\Omega^\varepsilon} |\partial_t u_1^\varepsilon|^2 dx d\tau \leq D_1 \int_0^t \int_{\Omega^\varepsilon} |\nabla u_1^\varepsilon|^2 dx d\tau
$$
$$
+ \frac{d_1^\infty}{2}\int_{\Omega^\varepsilon} |\nabla u_{10}|^2 dx + \frac{k_2^\infty}{2\delta}\int_0^t \int_{\Omega^\varepsilon} |u_2^\varepsilon|^2 dx d\tau
$$
$$
+ \frac{\varepsilon}{2}\int_{\Gamma_\varepsilon^{sw}} \left(|\eta|^2 + |u_1^\varepsilon|^2 + |\eta(0)|^2 + |u_1^\varepsilon(0)|^2 \right) d\sigma_x
$$
$$
+ \frac{\varepsilon}{2}\int_0^t \int_{\Gamma_\varepsilon^{sw}} \left(|\partial_t \eta|^2 + |u_1^\varepsilon|^2 \right) d\sigma_x d\tau,
$$
$$(57)$$
where $\eta(0) := \eta(u_1^\varepsilon(0), u_5^\varepsilon(0))$. Applying (7) and recalling (55), we have

$$
\int_0^t \int_{\Omega^\varepsilon} |\partial_t u_1^\varepsilon|^2 dx d\tau \leq C_9, \tag{58}
$$

where

$$
C_9 := D_1 \int_0^t \int_{\Omega^\varepsilon} |\nabla u_1^\varepsilon|^2 dx d\tau + \frac{k_1}{2}\int_{\Omega^\varepsilon} |u_1^\varepsilon(0)|^2 dx + \frac{d_1^\infty}{2}\int_{\Omega^\varepsilon} |\nabla u_{10}|^2 dx
$$

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$$+ \frac{k_2^\infty}{2\delta} \int_0^t \int_{\Omega^\varepsilon} |u_2^\varepsilon|^2 dxd\tau + \frac{\varepsilon}{2} \int_{\Gamma_\varepsilon^{sw}} (|\overline{\eta}|^2 + |\eta(0)|^2 + |\hat{\eta}|^2)$$

$$+ \frac{C^*}{2} \int_0^t \int_{\Omega^\varepsilon} (|u_1^\varepsilon|^2 + \varepsilon^2 |\nabla u_1^\varepsilon|^2) dxd\tau + \frac{C^*}{2} \int_{\Omega^\varepsilon} (|u_1^\varepsilon|^2 + \varepsilon^2 |\nabla u_1^\varepsilon|^2) dxd\tau,$$

and $\delta \in \left]0, \frac{2}{k_2^\infty}\right[$. Testing (10) with $\varphi_2 = \partial_t u_2^\varepsilon$ gives

$$\int_0^t \int_{\Omega^\varepsilon} |\partial_t u_2^\varepsilon|^2 dxd\tau + \int_0^t \int_{\Omega^\varepsilon} (\frac{1}{2} \partial_t (d_2^\varepsilon |\nabla u_2^\varepsilon|^2) - (\partial_t d_2^\varepsilon)|\nabla u_2^\varepsilon|^2) dxd\tau$$

$$\leq -\frac{k_2}{2} \int_0^t \int_{\Omega^\varepsilon} \partial_t |u_2^\varepsilon|^2 dxd\tau + \frac{k_1^\infty}{2} \int_0^t \int_{\Omega^\varepsilon} (\frac{1}{\delta} |u_1^\varepsilon|^2$$

$$+ \delta |\partial_t u_2^\varepsilon|^2) dxd\tau + \frac{\varepsilon a^\infty}{2} \int_0^t \int_{\Gamma_\varepsilon^{wa}} \left(|u_3^\varepsilon|^2 + |\partial_t u_2^\varepsilon|^2 \right) d\sigma_x d\tau$$

$$+ \frac{\varepsilon b^\infty}{2} \int_0^t \int_{\Gamma_\varepsilon^{wa}} \partial_t |u_2^\varepsilon|^2 d\sigma_x d\tau,$$

and hence,
$$\int_0^t \int_{\Omega^\varepsilon} |\partial_t u_2^\varepsilon|^2 dx\tau + \frac{d_2}{2} \int_{\Omega^\varepsilon} |\nabla u_2^\varepsilon|^2 dxd\tau$$

$$\leq \frac{d_2^\infty}{2} \int_{\Omega^\varepsilon} |\nabla u_2^\varepsilon(0)|^2 dx + D_2 \int_0^t \int_{\Omega^\varepsilon} |\nabla u_2^\varepsilon|^2 dxd\tau$$

$$+ \frac{k_1^\infty}{2} \int_0^t \int_{\Omega^\varepsilon} (\frac{1}{\delta} |u_1^\varepsilon|^2 + \delta |\partial_t u_2^\varepsilon|^2) dxd\tau$$

$$+ \frac{C^* a^\infty}{2} \int_0^t \int_{\Omega^\varepsilon} \left(|u_3^\varepsilon|^2 + \varepsilon^2 |\nabla u_3^\varepsilon|^2 + \varepsilon^2 |\nabla \partial_t u_2^\varepsilon|^2 \right) dxd\tau$$

$$+ \frac{\varepsilon b^\infty}{2} \int_{\Gamma_\varepsilon^{wa}} (|u_2^\varepsilon|^2 - |u_2^\varepsilon(0)|^2) d\sigma_x.$$

By (7) and (55), we get

$$\left(1 - \frac{C^* a^\infty}{2} - \frac{k_1^\infty \delta}{2} \right) \int_0^t \int_{\Omega^\varepsilon} |\partial_t u_2^\varepsilon|^2 dxd\tau \leq C_{10} \left(1 + \varepsilon^2 \int_0^t \int_{\Omega^\varepsilon} |\nabla \partial_t u_2^\varepsilon|^2 dxd\tau \right).$$

Consequently, choosing $\delta \in]0, \frac{2 - C^* a^\infty}{k_1^\infty}[$, we are led to

$$\int_0^t \int_{\Omega^\varepsilon} |\partial_t u_2^\varepsilon|^2 dxd\tau \leq C_{10}(1 + \varepsilon^2 \int_0^t \int_{\Omega^\varepsilon} |\nabla \partial_t u_2^\varepsilon|^2 dxd\tau), \qquad (59)$$

where

$$C_{10} := D_2 \int_0^t \int_{\Omega^\varepsilon} |\nabla u_1^\varepsilon|^2 dxd\tau + \frac{d_2^\infty}{2} \int_{\Omega^\varepsilon} |\nabla u^\varepsilon{}_2(0)|^2 dx + \frac{k_1^\infty}{2\delta} \int_0^t \int_{\Omega^\varepsilon} |u_2^\varepsilon|^2 dxd\tau$$

$$+ \frac{C^* b^\infty}{2} \int_{\Omega^\varepsilon} \left(|u_2^\varepsilon|^2 + \varepsilon^2 |\nabla u_2^\varepsilon|^2 + |u_2^\varepsilon(0)|^2 + \varepsilon^2 |\nabla u_2^\varepsilon(0)|^2 \right) dx$$

$$+ \frac{C^* a^\infty}{2} \int_0^t \int_{\Omega^\varepsilon} (|u_3^\varepsilon|^2 + \varepsilon^2 |\nabla u_3^\varepsilon|^2) dxd\tau.$$

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The initial data u_{30}^ε holding in Ω_1^ε and the Dirichlet data u_3^D acting on the exterior boundary of Ω_1^ε are considered here as restrictions of the respective functions defined on whole of $\overline{\Omega}$. Testing now (11) with $\varphi_3 = \partial_t(u_3^\varepsilon - u_3^D)$ leads to

$$
\int_0^t \int_{\Omega^\varepsilon} |\partial_t u_3^\varepsilon|^2 dx d\tau + \frac{d_3}{2} \int_{\Omega^\varepsilon} |\nabla u_3^\varepsilon|^2
$$
$$
\leq \frac{d_3}{2} \int_{\Omega^\varepsilon} |\nabla u_3^\varepsilon(0)|^2 + \frac{1}{2}(|\partial_t u_3^\varepsilon|^2 + |\partial_t u_3^D|^2)
$$
$$
+ D_3 \int_0^t \int_{\Omega^\varepsilon} |\nabla u_3^\varepsilon|^2 + \frac{d_3^\infty}{2} \int_0^t \int_{\Omega^\varepsilon} (|\nabla u_3^\varepsilon|^2 + |\nabla \partial_t u_3^D|^2)
$$
$$
+ \frac{\varepsilon a^\infty}{\delta} \int_0^t \int_{\Gamma_\varepsilon^{wa}} |u_3^\varepsilon|^2 + \frac{\varepsilon \delta}{2}(a^\infty + a^\infty) \int_0^t \int_{\Gamma_\varepsilon^{wa}} |\partial_t u_3^\varepsilon|^2
$$
$$
+ \frac{\varepsilon}{2}(a^\infty + b^\infty) \int_0^t \int_{\Gamma_\varepsilon^{wa}} |\partial_t u_3^D|^2 + \frac{\varepsilon b^\infty}{\delta} \int_0^t \int_{\Gamma_\varepsilon^{wa}} |u_2^\varepsilon|^2.
$$

Using (7) and (A6), we obtain

$$
\int_0^t \int_{\Omega^\varepsilon} |\partial_t u_3^\varepsilon|^2 dx d\tau \leq C_{11}(1 + \varepsilon^2 \delta \int_0^t \int_{\Omega^\varepsilon} |\nabla \partial_t u_3^\varepsilon|^2 dx d\tau), \tag{60}
$$

where $\delta \in]0, \frac{2}{C^*(a^\infty + b^\infty)}[$ and

$$
C_{11} := D_3 \int_0^t \int_{\Omega^\varepsilon} |\nabla u_3^\varepsilon|^2 dx d\tau + \frac{d_3}{2} \int_{\Omega^\varepsilon} |\nabla u_3^\varepsilon(0)|^2 dx + \frac{1}{2\delta} \int_0^t \int_{\Omega^\varepsilon} |\nabla u_3^D|^2
$$
$$
+ \frac{d_3^\infty}{2} \int_0^t \int_{\Omega^\varepsilon} (|\nabla u_3^\varepsilon|^2 + |\nabla \partial_t u_3^D|^2) + \frac{C^* a^\infty}{\delta} \int_0^t \int_{\Omega^\varepsilon} (|u_3^\varepsilon|^2 + \varepsilon^2 |\nabla u_3^\varepsilon|^2)
$$
$$
+ \frac{C^* b^\infty}{\delta} \int_0^t \int_{\Omega^\varepsilon} (|u_2^\varepsilon|^2 + \varepsilon^2 |\nabla u_2^\varepsilon|^2) dx d\tau
$$
$$
+ \frac{C^*(a^\infty + b^\infty)}{2} \int_0^t \int_{\Omega^\varepsilon} (|\partial_t u_3^D|^2 + \varepsilon^2 |\nabla \partial_t u_3^D|^2) dx d\tau.
$$

From (12), we get

$$
\int_0^t \int_{\Omega^\varepsilon} |\partial_t u_4^\varepsilon|^2 dx d\tau \leq C_{12}. \tag{61}
$$

In order to estimate (59) and (60), we proceed first with differentiating (10) with respect to time and then testing the result with $\partial_t u_2^\varepsilon$. Consequently, we derive

$$
\frac{1}{2} \int_{\Omega^\varepsilon} |\partial_t u_2^\varepsilon|^2 dx + d_2 \int_0^t \int_{\Omega^\varepsilon} |\nabla \partial_t u_2^\varepsilon|^2 dx d\tau \tag{62}
$$

$$+ \int_0^t \int_{\Omega^\varepsilon} \left(\frac{1}{2} (\partial_t d_2 |\nabla u_2{}^\varepsilon|^2 - (\partial_t \partial_t d_2)|\nabla u_2{}^\varepsilon|^2 \right)$$

$$\leq \frac{k_1^\infty}{2} \int_0^t \int_{\Omega^\varepsilon} (|\partial_t u_1^\varepsilon|^2 + |\partial_t u_2^\varepsilon|^2) + \frac{K_1^\infty}{2} \int_0^t \int_{\Omega^\varepsilon} (|u_1^\varepsilon|^2 + |\partial_t u_2^\varepsilon|^2)$$

$$- k_2 \int_0^t \int_{\Omega^\varepsilon} |\partial_t u_2^\varepsilon|^2 - \frac{K_2}{2} \int_0^t \int_{\Omega^\varepsilon} \partial_t |u_2^\varepsilon|^2$$

$$+ \frac{\varepsilon a^\infty}{2} \int_0^t \int_{\Gamma_\varepsilon^{wa}} (\frac{1}{\delta} |\partial_t u_2^\varepsilon|^2 + \delta |\partial_t u_3^\varepsilon|^2) d\sigma_x d\tau$$

$$+ \frac{\varepsilon b^\infty}{2} \int_0^t \int_{\Gamma_\varepsilon^{wa}} |\partial_t u_2^\varepsilon|^2 d\sigma_x d\tau + \frac{\varepsilon B}{2} \int_0^t \int_{\Gamma_\varepsilon^{wa}} \partial_t |u_2^\varepsilon|^2 d\sigma_x d\tau.$$

Using (7), it yields

$$\frac{1}{2} \int_{\Omega^\varepsilon} |\partial_t u_2^\varepsilon|^2 dx + \left(d_2 - \frac{C^* A^\infty \varepsilon^2}{2} - \frac{C^* B^\infty \varepsilon^2}{2} - \frac{C^* a^\infty \varepsilon^2}{2\delta} \right) \int_0^t \int_{\Omega^\varepsilon} |\nabla \partial_t u_2^\varepsilon|^2 dx d\tau$$

$$\leq C_{13} + \frac{C^* a^\infty \delta}{2} \int_0^t \int_{\Omega^\varepsilon} (|\partial_t u_3^\varepsilon|^2 + \varepsilon^2 |\nabla \partial_t u_3^\varepsilon|^2)$$

$$+ \left(\frac{k_1^\infty}{2} + \frac{K_1^\infty}{2} - k_2 + \frac{C^* A^\infty}{2} + \frac{C^* B^\infty \varepsilon^2}{2} + \frac{C^* a^\infty}{2\delta} \right) \int_0^t \int_{\Omega^\varepsilon} |\partial_t u_2^\varepsilon|^2,$$

$$(63)$$

where C_{13} depends on the bounded terms of r.h.s of (62). Differentiating now (11) with respect to time and then testing the result with $\partial_t (u_3^\varepsilon - u_3^D)$, we get

$$\frac{1}{2} \int_{\Omega^\varepsilon} |\partial_t u_3^\varepsilon|^2 dx + d_3 \int_0^t \int_{\Omega^\varepsilon} |\nabla \partial_t u_3{}^\varepsilon|^2 dx d\tau$$

$$+ \int_0^t \int_{\Omega^\varepsilon} \left(\frac{1}{2} (\partial_t d_3 |\nabla u_3{}^\varepsilon|^2 - (\partial_t \partial_t d_3)|\nabla u_3{}^\varepsilon|^2 \right)$$

$$\leq \frac{D_3}{2} \int_0^t \int_{\Omega^\varepsilon} |\nabla u_3{}^\varepsilon|^2 dx d\tau + \frac{d_3^\infty}{2} \int_0^t \int_{\Omega^\varepsilon} |\nabla \partial_t u_3{}^\varepsilon|^2 dx d\tau$$

$$+ \frac{d_3^\infty + D_3}{2} \int_0^t \int_{\Omega^\varepsilon} |\nabla \partial_t u_3{}^D|^2 dx d\tau + \frac{\varepsilon A^\infty}{2} \int_0^t \int_{\Gamma_\varepsilon^{wa}} \partial_t |u_3{}^\varepsilon|^2 dx d\tau$$

$$+ \varepsilon a^\infty \int_0^t \int_{\Gamma_\varepsilon^{wa}} |\partial_t u_3{}^\varepsilon|^2 dx d\tau + \frac{\varepsilon A^\infty}{2} \int_0^t \int_{\Gamma_\varepsilon^{wa}} (|u_3{}^\varepsilon|^2 + |\partial_t u_3{}^D|^2) dx d\tau$$

$$+ \frac{\varepsilon a^\infty}{2} \int_0^t \int_{\Gamma_\varepsilon^{wa}} (|\partial_t u_3{}^\varepsilon|^2 + |\partial_t u_3{}^D|^2) dx d\tau$$

$$+ \frac{\varepsilon B^\infty}{2} \int_0^t \int_{\Gamma_\varepsilon^{wa}} (|u_2{}^\varepsilon|^2 + |\partial_t u_3{}^\varepsilon|^2 + |u_2{}^\varepsilon|^2 + |\partial_t u_3{}^D|^2) dx d\tau$$

$$+ \frac{\varepsilon b^\infty}{2} \int_0^t \int_{\Gamma_\varepsilon^{wa}} (\frac{1}{\delta} |\partial_t u_2{}^\varepsilon|^2 + \delta |\partial_t u_3{}^\varepsilon|^2 + |\partial_t u_2{}^\varepsilon|^2 + |\partial_t u_3{}^D|^2) dx d\tau.$$

Using (7) to deal with the boundary terms, we obtain

$$\frac{1}{2} \int_{\Omega^\varepsilon} |\partial_t u_3^\varepsilon|^2 dx + \left(d_3 - \frac{d_3^\infty}{2} - \frac{C^* \varepsilon^2}{2} (3a^\infty + B^\infty + b^\infty + a^\infty \delta) \right) \int_0^t \int_{\Omega^\varepsilon} |\nabla \partial_t u_3{}^\varepsilon|^2 dx d\tau$$

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$$\leq C_{14} + C_{15} \int_0^t \int_{\Omega^\varepsilon} |\partial_t u_3{}^\varepsilon|^2 dx d\tau \tag{64}$$

$$+ C^* b^\infty \int_0^t \int_{\Omega^\varepsilon} (|\partial_t u_3{}^\varepsilon|^2 + \varepsilon^2 |\nabla \partial_t u_3{}^\varepsilon|^2) dx d\tau \tag{65}$$

Adding (63) and (64) and using (59) and (60) to get the desired result.

4.1 Extension step

Since we deal here with an oscillating system posed in a perforated domain, the natural next step is to extend all concentrations to the whole Ω. We do this by following a two-steps procedure: In Step 1, we rely on the standard extension results indicated in section 4.2 to extend all active concentrations u_ℓ^ε ($\ell \in \{1, \ldots, 4\}$) to Ω. In step 2, we unfold the ode for u_5^ε such that the unfolded concentration is defined on the fixed boundary Γ; see section 5.1.

4.2 Extension lemmas

Since all the concentrations are defined in Ω^ε and Ω_1^ε, to get macroscopic equations we need to extend them into Ω.

Remark 6 *Take $\varphi^\varepsilon \in L^2(0, T; H^1(\Omega^\varepsilon))$. Note that since our microscopic geometry is sufficiently regular, we can speak in terms of extensions. Recall the linearity of the extension operator*

$$\mathcal{P}^\varepsilon : L^2(0, T; H^1(\Omega^\varepsilon)) \to L^2(0, T; H^1(\Omega))$$

defined by $\mathcal{P}^\varepsilon \varphi^\varepsilon = \tilde{\varphi}^\varepsilon$. To keep notation simple, we denote the extension $\tilde{\varphi}^\varepsilon$ again by φ^ε.

Lemma 7 *(Extension) Consider the geometry described in Section 2.1. There exists an extension $\tilde{u}^\varepsilon$ of u^ε such that*

(1) $\| \tilde{u}^\varepsilon \|_{L^2(Y)} \leq \hat{C} \| u^\varepsilon \|_{L^2(Y^w)}$, for $u^\varepsilon \in L^2(Y^w)$
(2) $\| \nabla \tilde{u}^\varepsilon \|_{L^2(Y)} \leq \hat{C} \| \nabla u^\varepsilon \|_{L^2(Y^w)}$, for $\nabla u^\varepsilon \in L^2(Y^w)$
(3) $\| \tilde{u}^\varepsilon \|_{H^1(\Omega)} \leq \hat{C} \| u^\varepsilon \|_{H^1(\Omega^\varepsilon)}$, for $u^\varepsilon \in H^1(\Omega^\varepsilon)$

Proof. For the proof of this Lemma, see Section 2 in [20] or compare Lemma 5, p.214 in [30].

Definition 8 *(Two-scale convergence cf. [31,32]) Let $\{u^\varepsilon\}$ be a sequence of functions in $L^2((0, T) \times \Omega)$ (Ω being an open set of $\mathbb{R}^N$) where ε being a*

sequence of strictly positive numbers that tends to zero. $\{u^\varepsilon\}$ is said to two-scale converge to a unique function $u_0(t, x, y) \in L^2((0, T) \times \Omega \times Y)$ if and only if for any $\psi \in C_0^\infty((0, T) \times \Omega, C_\#^\infty(Y))$, we have

$$lim_{\varepsilon \to 0} \int_0^T \int_\Omega u^\varepsilon \psi(t, x, \frac{x}{\varepsilon}) dx dt = \int_\Omega \int_Y u_0(t, x, y) \psi(t, x, y) dy dx dt. \qquad (66)$$

We denote (66) by $u^\varepsilon \xrightarrow{2} u_0$.

Theorem 9 *(i) From each bounded sequence $\{u^\varepsilon\}$ in $L^2((0, T) \times \Omega)$, one can extract a subsequence which two-scale converges to $u_0(t, x, y) \in L^2((0, T) \times \Omega \times Y)$.*

(ii) Let $\{u^\varepsilon\}$ be a bounded sequence in $H^1((0, T) \times \Omega)$, which converges weakly to a limit function $u_0(t, x, y) \in H^1((0, T) \times \Omega \times Y)$. Then there exists $\tilde{u} \in L^2(\Omega; H_\#^1(Y)/\mathbb{R})$ such that up to a subsequence $\{u^\varepsilon\}$ two-scale converges to $u_0(t, x, y)$ and $\nabla u^\varepsilon \xrightarrow{2} \nabla_x u_0 + \nabla_y \tilde{u}$.

(iii) Let $\{u^\varepsilon\}$ and $\{\varepsilon \nabla u^\varepsilon\}$ be bounded sequences in $L^2((0, T) \times \Omega)$, then there exists $u_0 \in L^2((0, T) \times \Omega; H_\#^1(Y))$ such that up to a subsequence u^ε and $\varepsilon \nabla u^\varepsilon$ two-scale converge to $u_0(t, x, y)$ and $\nabla_y u_0(t, x, y)$ respectively.

Definition 10 *(Two-scale convergence for $\varepsilon-$periodic hypersurfaces [33]) A sequence of functions $\{u^\varepsilon\}$ in $L^2((0, T) \times \Gamma_\varepsilon)$ is said to two-scale converge to a limit $u_0 \in L^2((0, T) \times \Omega \times \Gamma)$ if and only if for any $\psi \in C_0^\infty((0, T) \times \Omega, C_\#^\infty(\Gamma))$ we have*

$$lim_{\varepsilon \to 0} \varepsilon \int_0^T \int_{\Gamma_\varepsilon} u^\varepsilon \psi(t, x, \frac{x}{\varepsilon}) d\sigma_x dt = \int_\Omega \int_\Gamma u_0(t, x, y) \psi(t, x, y) d\sigma_y dx dt.$$

Theorem 11 *(i) From each bounded sequence $\{u^\varepsilon\} \in L^2((0, T) \times \Gamma_\varepsilon)$, one can extract a subsequence u^ε which two-scale converges to a function $u_0 \in L^2((0, T) \times \Omega \times \Gamma)$.*

(ii) If a sequence of functions $\{u^\varepsilon\}$ is bounded in $L^\infty((0, T) \times \Gamma_\varepsilon)$, then u^ε two-scale converges to a function $u_0 \in L^\infty((0, T) \times \Omega \times \Gamma)$.

Proof. For proof of (i), see [33] and the one for (ii), see [15].

Lemma 12 *Assume the hypotheses of Lemma 5 and Lemma 7 to hold. The a priori estimates lead to the following convergence results:*

(a) $u_i^\varepsilon \rightharpoonup u_i$ in $L^2(0, T; H^1(\Omega)$ for all $i \in \{1, 2, 3, 4\}$,

(b) $u_i^\varepsilon \xrightarrow{*} u_i$ in $L^\infty((0, T) \times \Omega)$,

(c) $\partial_t u_i^\varepsilon \rightharpoonup \partial_t u_i$ in $L^2((0, T) \times \Omega)$,

(d) $u_i^\varepsilon \to u_i$ in $L^2(0, T; H^\beta(\Omega))$ for $\frac{1}{2} < \beta < 1$, also $\| u_i^\varepsilon - u_i \|_{L^2((0,T) \times \Gamma_\varepsilon)} \to 0$ as $\varepsilon \to 0$,

(e) $u_i^\varepsilon \xrightarrow{2} u_i, \nabla u_i^\varepsilon \xrightarrow{2} \nabla_x u_i + \nabla_y u_{i1}, u_{i1} \in L^2((0, T) \times \Omega; H_\#^1(Y)/\mathbb{R})$,

(f) $u_5^\varepsilon \xrightarrow{2} u_5$, and $u_5 \in L^\infty((0, T) \times \Omega \times \Gamma^{sw})$,

(g) $\partial_t u_5^\varepsilon \xrightarrow{2} \partial_t u_5$, and $u_5 \in L^2((0, T) \times \Omega \times \Gamma^{sw})$.

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Proof. (a) and (b) are obtained as a direct consequence of the fact that u_i^ε is bounded in $L^2(0, T; H^1(\Omega)) \cap L^\infty((0, T) \times \Omega)$; up to a subsequence (still denoted by u_i^ε) u_i^ε converges weakly to u_i in $L^2(0, T; H^1(\Omega)) \cap L^\infty((0, T) \times \Omega)$. A similar argument gives (c). To get (d), we use the compact embedding $H^{\beta'}(\Omega) \hookrightarrow H^\beta(\Omega)$, for $\beta \in (\frac{1}{2}, 1)$ and $0 < \beta < \beta' \le 1$ (since Ω has Lipschitz boundary). We have

$$W := \{u_i \in L^2(0, T; H^1(\Omega)) \text{ and } \partial_t u_i \in L^2((0, T) \times \Omega) \text{ for all } i \in \{1, 2, 3, 4\}\}$$

For a fixed ε, W is compactly embedded in $L^2(0, T; H^\beta(\Omega))$ by the Lions-Aubin Lemma; cf. e.g. [34]. Using the trace inequality (8)

$$\begin{aligned}
\| u_i^\varepsilon - u_i \|_{L^2((0,T) \times \Gamma_\varepsilon)} &\le C_0^* \| u_i^\varepsilon - u_i \|_{L^2(0,T; H^\beta(\Omega^\varepsilon))}, \\
&\le C \| u_i^\varepsilon - u_i \|_{L^2(0,T; H^\beta(\Omega))},
\end{aligned}$$

where $\| u_i^\varepsilon - u_i \|_{L^2(0,T; H^\beta(\Omega))} \to 0$ as $\varepsilon \to 0$. To investigate (e), (f) and (g), we use the notion of two-scale convergence as indicated in Definition 8 and 10. Since u_i^ε are bounded in $L^2(0, T; H^1(\Omega))$, up to a subsequence $u_i^\varepsilon \overset{2}{\rightharpoonup} u_i$ in $L^2((0, T) \times \Omega \times Y)$, and $\nabla u_i^\varepsilon \overset{2}{\rightharpoonup} \nabla_x u_i + \nabla_y \tilde{u}_i$, $\tilde{u}_i \in L^2((0, T) \times \Omega; H^1_\#(Y)/\mathbb{R})$. By Theorem 11, u_5^ε in $L^\infty((0, T) \times \Omega \times \Gamma)$ converges two-scale to u_5 in the same space and $\partial_t u_5^\varepsilon$ converges two-scale to $\partial_t u_5$ in $L^2((0, T) \times \Omega \times \Gamma)$. Due to the presence of the non-linear reaction rate on the interface Γ_ε^{sw}, the convergences listed in Lemma 12 are still not sufficient to pass to the limit $\varepsilon \to 0$ in the microscopic model. To be more precise, we can pass to $\varepsilon \to 0$ in the pde's, but not in the ode.

4.3 Cell problems

In order to be able to formulate the upscaled equations, we define two classes of *cell problems* very much in the spirit of [9]. One class of problems will refer to the water-filled parts of the pore, while the second class will refer to the air-filled part of the pores.

Definition 13 *(Cell problems) The cell problems in water-filled part are given by*

$$-\nabla_y.(D_\ell(t, y) \nabla_y \chi_i) = \sum_{k=1}^3 \partial_{y_k} D_{\ell k i}(t, y), \ \ in \ Y^w,$$

$$-D_\ell(t, y) \frac{\partial \chi_i}{\partial n} = \sum_{k=1}^3 D_{\ell k i}(t, y) n_k \ \ on \ \Gamma^{sw},$$

$$-D_\ell(t, y) \frac{\partial \chi_i}{\partial n} = \sum_{k=1}^3 D_{\ell k i}(t, y) n_k \ \ on \ \Gamma^{wa},$$

for all $i, \ell \in \{1, 2, 4\}$ and χ_i are Y-periodic in y. The <u>cell problems in air-filled part</u> are given by

$$-\nabla_y.(D_3(t, y)\nabla_y \varsigma_i) = \sum_{k=1}^{3} \partial_{y_k} D_{3ki}(t, y), \ \ in \ Y^a,$$

$$-D_3(t, y)\frac{\partial \varsigma_i}{\partial n} = \sum_{k=1}^{3} D_{3ki}(t, y)n_k \ \ on \ \Gamma^{wa},$$

$$-D_3(t, y)\frac{\partial \varsigma_i}{\partial n} = \sum_{k=1}^{3} D_{3ki}(t, y)n_k \ \ on \ \partial Y^a - \Gamma^{wa},$$

for all $i \in \{1, 2, 3\}$ and ς_i are Y-periodic in y.

5 Two-scale limit equations

Theorem 14 *The sequences of the solutions of the weak formulation (9)-(13) converges to the weak solution $u_i, i \in \{1, 2, 3, 4, 5\}$ as $\varepsilon \to 0$ such that $u_i \in H^1(0, T; L^2(\Omega)) \cap L^2(0, T; H^1(\Omega)) \cap L^\infty((0, T) \times \Omega)$ and $u_5 \in H^1(0, T; L^2(\Omega \times \Gamma)) \cap L^\infty((0, T) \times \Omega \times \Gamma))$. The weak formulation of the two-scale limit equations is given by*

$$\int_0^T \int_\Omega \partial_t u_i(t, x)\phi_i(t, x)dxdt + \int_0^T \int_\Omega \tilde{d}_i(t)\nabla u_i(t, x)\nabla \phi_i dxdt \qquad (67)$$

$$= \int_0^T \int_\Omega F_i(u)\phi_i dxdt \ for \ all \ i \in \{1, 2, 3, 4\},$$

where

$$F_1(u) := -\tilde{k}_1(t)u_1(t, x) + \tilde{k}_2(t)u_2(t, x)$$
$$- \frac{1}{|Y|} \int_\Gamma k_3(t, y)R(u_1(t, x))Q(u_5(t, x, y))d\sigma_y,$$
$$F_2(u) := \tilde{k}_1(t)u_1(t, x) - \tilde{k}_2(t)u_2(t, x) + \tilde{a}(t)u_3(t, x) - \tilde{b}(t)u_2(t, x),$$
$$F_3(u) := -\tilde{a}(t)u_3(t, x) + \tilde{b}(t)u_2(t, x),$$
$$F_4(u) := \tilde{k}_1(t)u_1(t, x),$$

with the initial values $u_i(0, x) = u_{i0}(x)$ for $x \in \Omega$, and

$$\int_0^T \int_{\Omega \times \Gamma} \partial_t u_5(t, x, y)\phi_5(t, x, y)dtdxd\sigma_y$$

$$= \int_0^T \int_{\Omega \times \Gamma} k_3(t, y)R(u_1(t, x))Q(u_5(t, x, y))\phi_5(t, x, y)dtdxd\sigma_y, \qquad (68)$$

with $u_5(0, x, y) = u_{50}(x, y)$ for $x \in \Omega$, $y \in \Gamma^{sw}$. Also $\phi := (\phi_1, \phi_2, \phi_3, \phi_4) \in [C^\infty((0, T) \times \Omega)]^4$, $\psi := (\psi_1, \psi_2, \psi_3, \psi_4) \in [C^\infty((0, T) \times \Omega); C^\infty_\#(Y)]^4$,

$$\tilde{k}_j(t) := \frac{1}{|Y|} \int_Y k_j(t,y) dy, \ j \in \{1,2\}, \tag{69}$$

$$\tilde{a}(t) := \frac{1}{|Y|} \int_{\Gamma^{wa}} a(t,y) d\sigma_y, \tag{70}$$

$$\tilde{b}(t) := \frac{1}{|Y|} \int_{\Gamma^{wa}} b(t,y) d\sigma_y, \tag{71}$$

$$\tilde{d}_{\ell ij} := \sum_{k=1}^{3} \int_Y (d_{\ell ij}(t,y) + d_{\ell ik}(t,y)(\delta_{n\ell} \partial_{y_k} \chi_j + \delta_{3\ell} \partial_{y_k} \varsigma_j)) dy, \tag{72}$$
$$\ell \in \{1,2,3,4\}, \ n \in \{1,2,4\}$$

with χ_j, ς_j being solutions of the cell problems defined in Definition 13, while δ denotes here the Kronecker's symbol.

Proof. We apply two-scale convergence techniques together with Lemma 12 to get macroscopic equations. We take test functions incorporating the following oscillating behavior $\varphi_i(t,x) = \phi_i(t,x) + \varepsilon \psi_i(t,x,\frac{x}{\varepsilon})$, $\phi_i \in C^\infty((0,T) \times \Omega)$, $\phi_i \in C^\infty((0,T) \times \Omega, ; C^\infty_\#(Y))$, $i \in \{1,2,3,4\}$. Applying two-scale convergence yields

$$|Y| \int_0^T \int_\Omega \partial_t u_i \phi_i(t,x) dx dt + \int_0^T \int_\Omega \int_Y d_i(t,y)(\nabla_x u_i(t,x)$$
$$+ \nabla_y \tilde{u}_i(t,x,y))(\nabla_x \phi_i(t,x) + \nabla_y \psi_i(t,x,\frac{x}{\varepsilon})) dy dx dt$$
$$= \int_0^T \int_\Omega f_i(u) \phi_i(t,x) dx dt. \tag{73}$$

$$\int_0^T \int_\Omega f_1(u) \quad \phi_1(t,x) dx dt = -\lim_{\varepsilon \to 0} \int_0^T \int_{\Omega^\varepsilon} k_1^\varepsilon u_1^\varepsilon (\phi_1(t,x) + \varepsilon \psi_1(t,x,\frac{x}{\varepsilon})) dx dt$$
$$+ \lim_{\varepsilon \to 0} \int_0^T \int_{\Omega^\varepsilon} k_2^\varepsilon u_2^\varepsilon (\phi_1(t,x) + \varepsilon \psi_1(t,x,\frac{x}{\varepsilon})) dx dt$$
$$- \lim_{\varepsilon \to 0} \varepsilon \int_0^T \int_{\Gamma_\varepsilon^{sw}} \eta(R(u_1^\varepsilon), Q(u_5^\varepsilon))(\phi_1(t,x) + \varepsilon \psi_1(t,x,\frac{x}{\varepsilon})) d\sigma_x dt.$$

Using Lemma 12, we have

$$\int_0^T \int_\Omega f_1(u) \phi_1(t,x) dx dt = -\int_0^T \int_\Omega \int_Y k_1(t,y) u_1(t,x) \phi_1(t,x) dy dx dt$$
$$+ \int_0^T \int_\Omega \int_Y k_2(t,y) u_2(t,x) \phi_1(t,x) dy dx dt$$
$$- \lim_{\varepsilon \to 0} \varepsilon \int_0^T \int_{\Gamma_\varepsilon^{sw}} \partial_t u_5^\varepsilon (\phi_1(t,x) + \varepsilon \psi_1(t,x,\frac{x}{\varepsilon})) d\sigma_x dt.$$

$$\int_0^T \int_\Omega f_1(u)\phi_1(t,x)dxdt = -|Y| \int_0^T \int_\Omega \tilde{k}_1(t)u_1(t,x)\phi_1(t,x)dxdt$$
$$+|Y| \int_0^T \int_\Omega \tilde{k}_2(t)u_2(t,x)\phi_1(t,x)dxdt$$
$$-\int_0^T \int_\Omega \int_\Gamma \partial_t u_5 \phi_1(t,x)d\sigma_y dxdt.$$

$$\int_0^T \int_\Omega f_2(u)\phi_2(t,x)dxdt = \lim_{\varepsilon \to 0} \int_0^T \int_{\Omega^\varepsilon} k_1^\varepsilon u_1^\varepsilon(\phi_2(t,x) + \varepsilon\psi_2(t,x,\frac{x}{\varepsilon}))dxdt$$
$$-\lim_{\varepsilon \to 0} \int_0^T \int_{\Omega^\varepsilon} k_2^\varepsilon u_2^\varepsilon(\phi_2(t,x) + \varepsilon\psi_2(t,x,\frac{x}{\varepsilon}))dxdt$$
$$+\lim_{\varepsilon \to 0} \varepsilon \int_0^T \int_{\Gamma_\varepsilon^{wa}} a_\varepsilon u_3^\varepsilon(\phi_2(t,x) + \varepsilon\psi_2(t,x,\frac{x}{\varepsilon}))d\sigma_x dt$$
$$-\lim_{\varepsilon \to 0} \varepsilon \int_0^T \int_{\Gamma_\varepsilon^{wa}} b_\varepsilon u_2^\varepsilon(\phi_2(t,x) + \varepsilon\psi_2(t,x,\frac{x}{\varepsilon}))d\sigma_x dt.$$

$$\int_0^T \int_\Omega f_2(u)\phi_2(t,x)dxdt = |Y| \int_0^T \int_\Omega \tilde{k}_1(t)u_1(t,x)\phi_2(t,x)dxdt$$
$$-|Y| \int_0^T \int_\Omega \tilde{k}_2(t)u_2(t,x)\phi_2(t,x)dxdt$$
$$+|Y| \int_0^T \int_\Omega \tilde{a}(t)u_3(t,x)\phi_2(t,x)dxdt$$
$$-|Y| \int_0^T \int_\Omega \tilde{b}(t)u_2(t,x)\phi_2(t,x)dxdt.$$

We also have

$$\int_0^T \int_\Omega f_3(u)\phi_3(t,x)dxdt = -|Y| \int_0^T \int_\Omega \tilde{a}(t)u_3(t,x)\phi_3(t,x)dxdt$$
$$+|Y| \int_0^T \int_\Omega \tilde{b}(t)u_2(t,x)\phi_3(t,x)dxdt$$

and

$$\int_0^T \int_\Omega f_4(u)\phi_4(t,x)dxdt = |Y| \int_0^T \int_\Omega \tilde{k}_1(t)u_1(t,x)\phi_4(t,x)dxdt.$$

We set $\phi_i = 0, i \in \{1,2,3,4\}$ in (73) to calculate the expression of the known function $\tilde{u}_1$ and obtain

$$\int_0^T \int_\Omega \int_Y d_i(t,y)(\nabla_x u_i(t,x) + \nabla_y \tilde{u}_i(t,x,y))\nabla_y \psi_i(t,x,\frac{x}{\varepsilon})dydxdt = 0, \text{ forall } \psi_i.$$

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Since $\tilde{u}_1$ depends linearly on $\nabla_x u_1$, it can be defined as

$$\tilde{u}_i := \sum_{j=1}^3 \partial_{x_j} u_i (\delta_{in} \chi_j(t,y) + \delta_{3i} \varsigma_j(t,y)) \text{ for } n \in \{1,2,4\}$$

where the function χ_j, ς_j are the unique solutions of the cell problems defined in Definition 13. Setting $\psi_i = 0$ in (73), we get

$$\int_0^T \int_\Omega \int_Y \sum_{j,k=1}^3 d_{ijk}(t,y)(\partial_{x_k} u_i(t,x)$$
$$+ \sum_{m=1}^3 (\delta_{in} \partial_{y_k} \chi_m + \delta_{3i} \partial_{y_k} \varsigma_m) \partial_{x_m} u_i(t,x)) \partial_{x_j} \phi_k(t,x) dy dx dt$$
$$= |Y| \int_0^T \int_\Omega \sum_{j,k=1}^3 \tilde{d}_{ijk} \partial_{x_k} u_i(t,x) \partial_{x_j} \phi_i(t,x) dx dt.$$

Hence, the coefficients (entering the effective diffusion tensor) are given by

$$\tilde{d}_{ijk} := \frac{1}{|Y|} \sum_{k=1}^3 \int_Y (d_{\ell ij}(t,y) + d_{\ell ik}(t,y)(\delta_{in} \partial_{y_k} \chi_j + \delta_{3i} \partial_{y_k} \varsigma_j)) dy. \qquad (74)$$

$i \in \{1,2,3,4\}$, $n \in \{1,2,4\}$ and $j,k \in \{1,2,3\}$.

5.1 Passing to the limit $\varepsilon \to 0$ in (13)

It is not yet possible to pass to the limit $\varepsilon \to 0$ with the convergence results stated in Lemma 12. To overcome this difficulty, we use the notion of periodic unfolding. It si worth mentioning that there is an intimate link between the two-scale convergence and weak convergence of the unfolded sequences; see [35,15]. The key idea is: Instead of getting strong convergence for u_5^ε, obtain strong convergence for the periodic unfolding of u_5^ε.

Definition 15 *For $\varepsilon > 0$, the boundary unfolding of a measurable function φ posed on oscillating surface Γ_ε is defined by*

$$T_\varepsilon^b \varphi(x,y) = \varphi(\varepsilon y + \varepsilon k), \quad y \in \Gamma, x \in \Omega$$

where $k := \left[\frac{x}{\varepsilon}\right]$ denotes the unique integer combination $\Sigma_{j=1}^3 k_j e_j$ of the periods such that $x - \left[\frac{x}{\varepsilon}\right]$ belongs to Y. Note that the oscillation due to the perforations are shifted into the second variable y which belongs to fixed surface Γ.

Lemma 16 *If u_ε converges two-scale to u and $T_b^\varepsilon u_\varepsilon$ converges weakly to u^* in $L^2((0,T) \times \Omega; L_\#^2(\Gamma))$, then $u = u^*$ a.e. in $(0,T) \times \Omega \times \Gamma$.*
Proof. The proof details for this statement can be found in Lemma 4.6 of [15].

Lemma 17 *If $\varphi \in L^2((0,T) \times \Gamma^\varepsilon)$, then the following identity holds*

$$\frac{1}{|Y|}\|T_b^\varepsilon \varphi\|_{L^2((0,T)\times\Omega\times\Gamma)} = \varepsilon\|\varphi\|_{L^2((0,T)\times\Gamma^\varepsilon)}.$$

Proof. Consider
$$\frac{1}{|Y|}|T_b^\varepsilon\varphi|^2_{L^2(\Omega\times\Gamma)} = \frac{1}{|Y|}\int_{\Omega\times\Gamma}|T_b^\varepsilon\varphi|^2 dxd\sigma_y = \frac{1}{|Y|}\int_{\Omega\times\Gamma}T_b^\varepsilon\varphi^2 dxd\sigma_y,$$
$$= \frac{1}{|Y|}\Sigma_{k=1}^3\int_{\varepsilon(Y+k)}\int_\Gamma T_b^\varepsilon\varphi^2 dxd\sigma_y = \frac{1}{|Y|}\Sigma_{k=1}^3\int_{\varepsilon(Y+k)}dx\int_\Gamma\varphi^2 d\sigma_y,$$
$$= \Sigma_{k=1}^3\varepsilon^3\int_\Gamma\varphi^2 d\sigma_y.$$

Changing variable $z = \varepsilon(y+k)$, where $k = [\frac{x}{\varepsilon}]$, we get

$$\frac{1}{|Y|}|T_b^\varepsilon\varphi|^2_{L^2(\Omega\times\Gamma)} = \Sigma_{k=1}^3\varepsilon^3\int_\Gamma\varphi^2 d\sigma_y = \Sigma_{k=1}^3\varepsilon\int_{\varepsilon(\Gamma+k)}\varphi^2 d\sigma_z = \varepsilon\int_{\Gamma^\varepsilon}\varphi^2 d\sigma_z.$$

This completes the proof of (17).

Lemma 18 *If $\varphi \in L^2(\Omega)$, then $T_b^\varepsilon\varphi \to \varphi$ as $\varepsilon \to 0$ strongly in $L^2(\Omega \times \Gamma)$.*

Proof. See in [36,37] for proof details.

Using the boundary unfolding operator T_b^ϵ, we unfold the ode (13). Changing the variable, $x = \varepsilon y + \varepsilon k$ (for $x \in \Gamma_\varepsilon^{sw}$) to the fixed domain $(0,T) \times \Omega \times \Gamma$, we have

$$\partial_t T_b^\epsilon u_5^\epsilon(t,x,y) = \eta(T_b^\epsilon u_1^\epsilon(t,x,y), T_b^\epsilon u_5^\epsilon(t,x,y)). \tag{75}$$

In the remainder of this section, we prove that $T_b^\varepsilon u_5^\varepsilon$ converges strongly to u_5 in $L^2(\Omega \times \Gamma)$. From the two-scale convergence of u_5^ϵ, we obtain weak convergence of $T^\epsilon u_5^\epsilon$ to u_5 in $L^\infty((0,T) \times \Omega; L^2_{per}(\Gamma))$. We start with showing that $\{T_b^\varepsilon u_5^\varepsilon\}$ is a Cauchy sequence in $L^2(\Omega \times \Gamma)$. To this end, we choose $m,n \in \mathbb{N}$ with $n > m$ arbitrary. Writing down (75) for the two different choices of ε (i.e. $\varepsilon_i = \varepsilon_n$ and $\varepsilon_i = \varepsilon_m$), we obtain after subtracting the corresponding equations that

$$\partial_t \int_{\Omega\times\Gamma}|T_b^{\epsilon_n}u_5^{\epsilon_n} - T_b^{\epsilon_m}u_5^{\epsilon_m}|^2 d\sigma_y dx$$
$$= \int_{\Omega\times\Gamma}[k_3^\varepsilon R(T_b^{\epsilon_n}u_1^{\epsilon_n})Q(T_b^{\epsilon_n}u_5^{\epsilon_n}) - k_3^\varepsilon R(T_b^{\epsilon_m}u_1^{\epsilon_m})Q(T_b^{\epsilon_m}u_5^{\epsilon_m}))$$
$$\times (T_b^{\epsilon_n}u_5^{\epsilon_n} - T_b^{\epsilon_m}u_5^{\epsilon_m})d\sigma_y dx,$$
$$\leq k_3^\infty c_R(\frac{Q^\infty}{2} + c_Q sup_{\Omega\times\Gamma}|T_b^{\epsilon_n}u_1^{\epsilon_n}|)\int_{\Omega\times\Gamma}|T_b^{\epsilon_n}u_5^{\epsilon_n} - T_b^{\epsilon_m}u_5^{\epsilon_m}|^2 d\sigma_y dx$$
$$+ \frac{k_3^\infty c_R Q^\infty}{2}\int_{\Omega\times\Gamma}|T_b^{\epsilon_n}u_1^{\epsilon_n} - T_b^{\epsilon_m}u_1^{\epsilon_m}|^2 d\sigma_y dx. \tag{76}$$

To get (76), we have used the uniform boundedness of $T_b^{\epsilon_n} u_1^{\epsilon_n}$. We consider now

$$\int_{\Omega \times \Gamma} |T_b^{\epsilon_n} u_1^{\epsilon_n} - T_b^{\epsilon_n} u_1^{\epsilon_m}|^2 d\sigma_y dx$$

$$\leq \int_{\Omega \times \Gamma} (|T_b^{\epsilon_n} u_1^{\epsilon_n} - T_b^{\epsilon_m} u_1|^2 + |T_b^{\epsilon_n} u_1 - u_1|^2) d\sigma_y dx$$

$$+ \int_{\Omega \times \Gamma} (|T_b^{\epsilon_m} u_1 - u_1|^2 + |T_b^{\epsilon_m} u_1^{\epsilon_m} - T_b^{\epsilon_m} u_1|^2) d\sigma_y dx. \tag{77}$$

Since u_1 is constant w.r.t. y, we have that $T_b^{\epsilon_m} u_1 \to u_1$ strongly in $L^2((0,T) \times \Omega \times \Gamma)$ as $\varepsilon \to 0$. From Lemma 17, we conclude that

$$\int_{\Omega \times \Gamma} |T_b^\epsilon u_1^\epsilon - T_b^\epsilon u_1|^2 d\sigma_y dx \leq \varepsilon \int_{\Gamma^\varepsilon} |u_1^\epsilon - u_1|^2 d\sigma_y dx \leq \varepsilon C.$$

(77) turns out to be

$$\int_{\Omega \times \Gamma} |T_b^{\epsilon_n} u_1^{\epsilon_n} - T_b^{\epsilon_n} u_1^{\epsilon_m}|^2 d\sigma_y dx dt \leq C(\varepsilon_n + \varepsilon_m),$$

while (76) becomes

$$\partial_t \int_{\Omega \times \Gamma} |T_b^{\epsilon_n} u_5^{\epsilon_n} - T_b^{\epsilon_m} u_5^{\epsilon_m}|^2 d\sigma_y dx \leq C_{15} \int_{\Omega \times \Gamma} |T_b^{\epsilon_n} u_5^{\epsilon_n} - T_b^{\epsilon_m} u_5^{\epsilon_m}|^2 d\sigma_y dx + \frac{C_{16}}{n},$$

where $C_{15} := k_3^\infty c_R(\frac{Q^\infty}{2} + c_Q sup_{\Omega \times \Gamma}|T_b^{\epsilon_n} u_1^{\epsilon_n}|)$ and $C_{16} := \frac{k_3^\infty c_R Q^\infty}{2} C$. The Gronwall's inequality gives

$$\| T_b^{\epsilon_n} u_5^{\epsilon_n} - T_b^{\epsilon_m} u_5^{\epsilon_m} \|_{L^2(\Omega \times \Gamma)} \leq \frac{C_{16}}{n}. \tag{78}$$

By (78), $\{T_b^\epsilon u_5^\epsilon\}$ is a Cauchy sequence. Now, we take the two-scale limit in the ode (75) to get

$$\lim_{\varepsilon \to 0} \varepsilon \int_0^T \int_{\Gamma_\varepsilon^{sw}} \partial_t T_b^\epsilon u_5^\varepsilon \phi_1(t, x, \frac{x}{\varepsilon}) d\sigma_x dt = \lim_{\varepsilon \to 0} \varepsilon \int_0^T \int_{\Gamma_\varepsilon^{sw}} \eta(T_b^\epsilon u_1^\varepsilon, T_b^\epsilon u_5^\varepsilon) \phi_1(t, x, \frac{x}{\varepsilon}) d\sigma_x dt.$$

Consequently, we have

$$\int_0^T \int_{\Omega \times \Gamma^{sw}} \partial_t u_5 \phi_5(t, x, y) dx d\sigma_y dt$$

$$= \lim_{\varepsilon \to 0} \varepsilon \int_0^T \int_{\Gamma_\varepsilon^{sw}} T_b^\epsilon k_3^\varepsilon R(T_b^\epsilon u_1^\varepsilon) Q(u_5^\varepsilon) \phi_5(t, x, \frac{x}{\varepsilon}) d\sigma_x dt,$$

$$= \lim_{\varepsilon \to 0} \varepsilon \int_0^T \int_{\Gamma_\varepsilon^{sw}} T_b^\epsilon k_3^\varepsilon R(T_b^\epsilon u_1^\varepsilon) Q(u_5) \phi_5(t, x, \frac{x}{\varepsilon}) d\sigma_x dt$$

$$+ \lim_{\varepsilon \to 0} \varepsilon \int_0^T \int_{\Gamma_\varepsilon^{sw}} T_b^\epsilon k_3^\varepsilon R(T_b^\epsilon u_1^\varepsilon)(Q(T_b^\epsilon u_5^\varepsilon) - Q(u_5)) \phi_5(t, x, \frac{x}{\varepsilon}) d\sigma_x dt. \tag{79}$$

By (A2) and the strong convergence of u_1^ε, the first term on the right hand side of (79) converges two-scale to

$$\int_0^T \int_\Omega \int_{\Gamma^{sw}} k_3(t,y) R(u_1) Q(u_5) \phi_5(t,x,y) d\sigma_y dx dt,$$

while the second integral of (79)

$$\varepsilon \int_0^T \int_{\Gamma_\varepsilon^{sw}} T_b^\epsilon k_3^\varepsilon R(T_b^\epsilon u_1^\varepsilon)(Q(T_b^\epsilon u_5^\varepsilon) - Q(u_5))\phi_5(t,x,\frac{x}{\varepsilon}) d\sigma_x dt$$

$$\leq \varepsilon \left(\int_0^T \int_{\Gamma_\varepsilon^{sw}} |T_b^\epsilon k_3^\varepsilon R(T_b^\epsilon u_1^\varepsilon) \phi_5(t,x,\frac{x}{\varepsilon})|^2 d\sigma_x dt \right)^{\frac{1}{2}} \cdot$$

$$\cdot \left(\int_0^T \int_{\Gamma_\varepsilon^{sw}} |Q(T_b^\epsilon u_5^\varepsilon) - Q(u_5)|^2 d\sigma_x dt \right)^{\frac{1}{2}},$$

$$\to 0 \text{ as } \varepsilon \to 0.$$

At this point, we have used again (A2) in combination with the strong convergence of $T_b^\epsilon u_5^\varepsilon$. So, as result of passing to the limit $\varepsilon \to 0$ in (13) we get (68).

It is worth noting that the weak solution to the two-scale model inherits a.e. the positivity and boundedness properties from the corresponding properties of the weak solution of the microscopic model. Now, it only remains to ensure the uniqueness of weak solutions to the upscaled model.

Lemma 19 *(Uniqueness of solutions of (67)-(68) Assume (A1)-(A6). There exists at most one weak solution to the two-scale limit problem (67) and (68).*
Proof. Suppose there are two weak solutions to the two-scale limit problem $(u_1^j, u_2^j, u_3^j, u_4^j, u_5^j)$ with $j \in \{1,2\}$. We denote $u_\ell = u_\ell^1 - u_\ell^2$, $\ell \in \{1,2,3,4\}$ and choose as test function $\phi_\ell = u_\ell$. After straightforward calculations, we have from (68)

$$|u_5^1 - u_5^2| \leq C \int_0^t |u_1^1 - u_1^2| d\tau. \tag{80}$$

Take $\phi_1 = u_1$ in (67) to obtain

$$\frac{1}{2} \int_0^t \int_\Omega \partial_t |u_1|^2 dx dt + \tilde{d}_1 \int_0^t \int_\Omega |\nabla u_1|^2 dx dt$$

$$\leq -\tilde{k}_1 \int_0^t \int_\Omega \partial_t |u_1|^2 dx dt + \frac{\hat{k}_2^\infty}{2} \int_0^t \int_\Omega (|u_1|^2 + |u_2|^2) dx dt$$

$$+ \frac{k_3^\infty}{|Y|} c_R c_Q M_1 \int_0^t \int_{\Omega \times \Gamma^{sw}} (u_5^1 - u_5^2) u_1 dx d\sigma_y dt$$

$$+ \frac{k_3^\infty}{|Y|} c_R Q^\infty \int_0^t \int_{\Omega \times \Gamma^{sw}} |u_1|^2 dx d\sigma_y dt. \tag{81}$$

Using (80) together with the trace inequality for fixed domains, see section 5.5 Theorem 1 in [38] and also the fact that u_1 is independent of y in (81), we get

$$\int_0^t \int_\Omega \partial_t |u_1|^2 dx dt + (2\tilde{d}_1 - k_3^\infty c_R C^*(\delta M_1 + Q^\infty)) \int_0^t \int_\Omega |\nabla u_1|^2 dx d\tau$$

$$+ 2\tilde{k}_1 \int_0^t \int_\Omega \partial_t |u_1|^2 dx d\tau$$

$$\leq (\tilde{k}_2^\infty + k_3^\infty c_R C^*(\delta M_1 + Q^\infty)) \int_0^t \int_\Omega (|u_1|^2 + |u_2|^2) dx d\tau$$

$$+ k_3^\infty \delta c_R c_Q M_1 C^* \int_0^t \int_\Omega \int_0^\tau (|u_1|^2 + |\nabla u_1|^2) ds dx d\tau.$$

For suitable choice of $\delta \in]0, \frac{2d_1 - k_3^\infty c_R C^* Q^\infty}{k_3^\infty c_R C^* M_1}[$, we have

$$\int_0^T \int_\Omega \partial_t |u_1|^2 dx dt + \tilde{d}_1 \int_0^T \int_\Omega |\nabla u_1|^2 dx d\tau + 2\tilde{k}_1 \int_0^T \int_\Omega \partial_t |u_1|^2 dx d\tau$$

$$\leq (\tilde{k}_2^\infty + k_3^\infty c_R C^*(\delta M_1 + Q^\infty)) \int_0^T \int_\Omega (|u_1|^2 + |u_2|^2) dx d\tau$$

$$+ \frac{k_3^\infty}{\delta} c_R c_Q M_1 C^* \int_0^T \int_\Omega \int_0^\tau (|u_1|^2 + |\nabla u_1|^2) ds dx d\tau. \quad (82)$$

Take $\phi_2 = u_2$ in (67), we get

$$\frac{1}{2} \int_0^t \int_\Omega \partial_t |u_2|^2 dx d\tau + \tilde{d}_2 \int_0^t \int_\Omega |\nabla u_2|^2 dx d\tau$$

$$\leq -\tilde{k}_2 \int_0^t \int_\Omega \partial_t |u_2|^2 dx d\tau + \frac{\tilde{k}_1^\infty}{2} \int_0^t \int_\Omega (|u_1|^2 + |u_2|^2) dx d\tau$$

$$+ \tilde{a}^\infty \int_0^t \int_\Omega u_2 u_3 dx dt - \tilde{b} \int_0^T \int_\Omega |u_2|^2 dx d\tau.$$

$$\int_0^t \int_\Omega \partial_t |u_2|^2 dx d\tau + \tilde{d}_2 \int_0^t \int_\Omega |\nabla u_2|^2 dx d\tau$$

$$\leq (\tilde{k}_1^\infty + \tilde{a}^\infty) \int_0^t \int_\Omega (|u_1|^2 + |u_2|^2 + |u_3|^2) dx d\tau. \quad (83)$$

Similarly, we obtain from (67)

$$\int_0^t \int_\Omega \partial_t |u_3|^2 dx d\tau + \tilde{d}_3 \int_0^t \int_\Omega |\nabla u_3|^2 dx d\tau \leq \tilde{b}^\infty \int_0^t \int_\Omega (|u_2|^2 + |u_3|^2) dx d\tau \quad (84)$$

$$\int_0^t \int_\Omega \partial_t |u_4|^2 dx d\tau + \tilde{d}_4 \int_0^t \int_\Omega |\nabla u_4|^2 dx d\tau \leq \tilde{k}_1^\infty \int_0^T \int_\Omega (|u_1|^2 + |u_3|^2) dx d\tau \quad (85)$$

Adding side by side (82)-(85) and applying Gronwall's inequality to the corresponding result, we receive

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$$\Sigma_{i=1}^4 \int_\Omega |u_i|^2 dx + \hat{d}\Sigma_{i=1}^4 \int_0^t \int_\Omega |\nabla u_i|^2 dx d\tau + \hat{d} \int_0^t \int_\Omega |u_1|^2 dx d\tau \leq 0. \qquad (86)$$

In (86), we have $\hat{d} := min\{\tilde{d}_1, \tilde{d}_2, \tilde{d}_3, \tilde{d}_4, \tilde{k}_1\} > 0$. Taking in (87) supremum over $(0, T)$, we obtain

$$\Sigma_{i=1}^4 \int_\Omega |u_i|^2 dx + \hat{d}\Sigma_{i=1}^4 \int_0^T \int_\Omega |\nabla u_i|^2 dx d\tau \leq 0, \qquad (87)$$

which concludes the proof of the Lemma.

Lemma 20 *(Strong formulation of the two-scale limit equations) Assume the hypothesis of Lemma 12 to hold. Then the strong formulation of the two-scale limit equations (for all $t \in (0, T)$) reads*

$$\partial_t u_1(t, x) + \nabla \cdot (-\tilde{d}_1 \nabla u_1(t, x))$$
$$= -\tilde{k}_1(t)u_1(t, x) + \tilde{k}_2(t)u_2(t, x)$$
$$- \frac{1}{|Y|} \int_{\Gamma^{sw}} k_3(t, y) R(u_1(t, x)) Q(u_5(t, x, y)) d\sigma_y, \ x \in \Omega$$
$$u_1(0, x) = u_{10}(x), \ x \in \bar{\Omega},$$
$$n \cdot (-\tilde{d}_1 \nabla u_1(t, x)) = 0, \ x \in \partial\Omega$$
$$\tag{88}$$

$$\partial_t u_2(t, x) + \nabla \cdot (-\tilde{d}_2 \nabla u_2(t, x)) = \tilde{k}_1(t)u_1(t, x) - \tilde{k}_2(t)u_2(t, x)$$
$$+ \tilde{a}(t)u_3(t, x) - \tilde{b}(t)u_2(t, x), \ x \in \Omega,$$
$$u_2(0, x) = u_{20}(x), \ x \in \bar{\Omega},$$
$$n \cdot (-\tilde{d}_2 \nabla u_2(t, x)) = 0, \ x \in \partial\Omega,$$
$$\tag{89}$$

$$\partial_t u_3(t, x) + \nabla \cdot (-\tilde{d}_3 \nabla u_3(t, x)) = -\tilde{a}(t)u_3(t, x) + \tilde{b}(t)u_2(t, x), \ x \in \Omega,$$
$$u_3(0, x) = u_{30}(x), \ x \in \bar{\Omega},$$
$$u_3(t, x) = u_3^D(x), \ x \in \Gamma^D,$$
$$n \cdot (-\tilde{d}_3 \nabla u_3(t, x)) = 0, \ x \in \Gamma^N$$
$$\tag{90}$$

$$\partial_t u_4(t, x) + \nabla \cdot (-\tilde{d}_4 \nabla u_4(t, x)) = \tilde{k}_1(t)u_1(t, x), \ x \in \Omega,$$
$$u_4(0, x) = u_{40}(x), \ x \in \bar{\Omega},$$
$$n \cdot (-\tilde{d}_4 \nabla u_4(t, x)) = 0, \ x \in \partial\Omega$$
$$\tag{91}$$

$$\partial_t u_5(t, x, y) = k_3(t, y) R(u_1(t, x)) Q(u_5(t, x, y)), \ x \in \Omega, y \in \Gamma^{sw},$$
$$u_5(0, x, y) = u_{50}(x, y) \ x \in \bar{\Omega}, y \in \Gamma^{sw},$$
$$\tag{92}$$

where $\tilde{d}_i, i \in \{1, 2, 3, 4\}$ and $\tilde{k}_j, j \in \{1, 2\}$ are defined in Theorem 14.

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