INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 5, Supp , Pages 109–125

A NOTE ON THE CONSTRUCTION OF FUNCTION SPACES FOR DISTRIBUTED-MICROSTRUCTURE MODELS WITH SPATIALLY VARYING CELL GEOMETRY

SEBASTIAN MEIER AND MICHAEL BÖHM

Abstract. We construct Lebesgue and Sobolev spaces of functions defined on a continuous distribution of domains $\{Y_x \subset \mathbb{R}^m : x \in \Omega\}$. The resulting spaces can be viewed as a generalisation of the Bochner spaces $L_p(\Omega; W^l_q(Y))$ for the case that Y depends on $x \in \Omega$. Furthermore, we introduce a Lebesgue space of functions defined on the boundaries $\{\partial Y_x : x \in \Omega\}$. The latter construction relies on a uniform Lipschitz parametrisation of the above collection of boundaries, interpreted as a higher-dimensional manifold. The results are applied to prove existence, uniqueness and upper and lower bounds for a distributed-microstructure model of reactive transport in a heterogeneous porous medium.

Key Words. Lebesgue spaces, Sobolev spaces, distributed-microstructure model, direct integral, reaction–diffusion, homogenisation.

1. Introduction

Transport in porous media is governed by at least two highly different spatial scales: the *pore scale* and the *macroscopic scale*, the latter of which is usually of interest in applications. In cases where two or more transport processes happen simultaneously on highly different time scales, it has been shown by periodic homogenisation that *distributed-microstructure models* (or *two-scale models*) are appropriate [3, 2]. Such models consist of averaged equations describing the fast transport processes and of local microscopic cell problems accounting for the slow transport. The most studied example is flow in fissured media [1, 25].

¿From a mathematical point of view, these models are interesting due to the non-standard coupling of the equations and the unusual choice of solution spaces. In [25], the authors show that the variational formulation of a distributed-microstructure model with a cell geometry that varies at different points of the medium naturally leads to function spaces of the form $L_2(\Omega; H^1(Y_x))$ where Y_x is another domain depending on $x \in \Omega$. The construction of such spaces and particularly of their trace spaces is quite intricate and it is the major aim of this paper.

We briefly recall the model from [25] and how a variational formulation is derived. If $\Omega \subset \mathbb{R}^n$ is the macroscopic flow region, then at each $x \in \Omega$ the local geometry is described by a solid matrix block $Y_x \subset Y \subset \mathbb{R}^n$ surrounded by the pore $Y \setminus \overline{Y}_x$. The domain Y_x can depend on the macroscopic space coordinate $x \in \Omega$ in order to account for a heterogeneous medium. For $x \in \Omega$, $y \in Y_x$ and $t \geq 0$, let $u(x, t)$ be the fluid density in the pore space and $U(x, y, t)$ that in the matrix blocks. The

2000 *Mathematics Subject Classification.* 46E30, 46E35, 35K57, 35B27.

model equations consist of the (averaged) mass balance of fluid within the pores[1]

(1a)
$$\frac{\partial}{\partial t}(a(x)u) - \operatorname{div}_x(A(x)\nabla_x u) = \frac{1}{|Y|}\int_{\partial Y_x} k(\gamma_x U(x,y,t) - u(x,t)) \cdot \nu \, d\sigma_y, \quad x \in \Omega,\ t > 0,$$

where $\gamma_x U(t,x,y)$ denotes the trace of U at $y \in \partial Y_x$, and a family of local mass balances in the matrix blocks parameterised by $x \in \Omega$,

(1b)
$$\frac{\partial}{\partial t}(b(x)U) - \operatorname{div}_y(B(x)\nabla_y U) = 0, \qquad x \in \Omega,\ y \in Y_x,\ t > 0.$$

The exchange condition reads

(1c)
$$-B(x)\nabla_y U \cdot \nu_x = k(\gamma_x U(x,y,t) - u(x,t)), \qquad x \in \Omega,\ y \in \partial Y_x,\ t > 0.$$

Following [25], a variational formulation of (1) is given as follows. Let $V := L_2(\Omega; H^1(Y_x))$ be an anisotropic Sobolev space (see Def. 4). We look for a pair of functions $u \in L_2(0,T; H^1(\Omega))$ and $U \in L_2(0,T; V)$ satisfying (1a) in the usual weak sense and

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega\int_{Y_x} bU\Psi \, dy \, dx + \int_\Omega\int_{Y_x} B\nabla_y U \cdot \nabla_y \Psi \, dy \, dx + \int_\Omega\int_{\partial Y_x} k(\gamma_x U - u)\, \gamma_x \Psi \, d\sigma_y \, dx = 0 \qquad \forall \Phi \in V.$$

In [25], the authors prove that the system (1) is wellposed in the above sense. However, a systematic discussion of the properties spaces of the form $L_2(\Omega; H^1(Y_x))$ is missing. Moreover, the cell boundaries Γ_x need to have some regularity with respect to $x \in \Omega$ in order to justify terms of the form

$$\int_\Omega\int_{\partial Y_x} \gamma_x U \, \gamma_x \Psi \, d\sigma_y \, dx.$$

It is the aim of this paper to fill this gap by constructing general spaces $L_p(\Omega; W^l_q(Y_x))$ and $L_p(\Omega; L_q(\partial Y_x))$ and proving some elementary properties of them like separability and reflexivity. While for the former space, it is sufficient that the higher-dimensional set $Q := \cup_{x\in\Omega}(\{x\} \times Y_x)$ is Lebesgue measurable, it turns out that for the latter space of functions defined on a family of cell *boundaries*, the situation is more intricate. We construct a uniform parametrisation of the cell boundaries ∂Y_x under quite general conditions on the geometry. With this framework at hand, objects like the *distributed trace operator* $\gamma U(x,y) := \gamma_x U(x,\cdot)(y)$ are easily constructed. Afterwards, the results are applied to a semilinear two-scale reaction–diffusion system, which has also been discussed in [17] under stronger restrictions on the cell geometry. Modifying techniques from [14, 9], we prove boundedness, existence and uniqueness of weak solutions.

We mention some related work for constant microstructure: The analysis of a similar two-scale reaction–diffusion system has been shown in [10]. Homogenisation results for a general diffusion–convection–reaction–adsorption system can be found in [12, 13]. For numerical approaches to two-scale models, see [21, 1, 18]. A huge list of further references is also given in [11]. We emphasise that in the present paper and in all of the above cited work, a change of the microstructure *w.r.t. time* is not considered. For homogenisation and two-scale models with evolving microstructure, we refer to [22, 16].

This paper is organised as follows. In section 2, we discuss function spaces on cell *domains*. Function spaces on the cell *boundaries* are treated in section 3. In

[1]The model (1) corresponds to the *regularised-microstructure* case in [25].

section 4, we apply the results to prove well-posedness of a two-scale model for reactive transport.

2. Spaces of functions defined in the cell

We construct spaces $L_p(\Omega; L_q(Y_x))$ and $L_p(\Omega; W_q^l(Y_x))$ of functions defined on a family of bounded domains $\{Y_x \subset \mathbb{R}^m : x \in \Omega \subset \mathbb{R}^n\}$. As our basic tool, we use the $(n+m)$-dimensional Lebesgue measure of the domain $Q = \cup_{x\in\Omega}(\{x\} \times Y_x)$. The corresponding spaces of Bochner integrable functions are recovered as special cases if $Y_x \equiv Y$. For general information on the Bochner integral, see [28, 15].

Some of the following results are well-known for the special case that $\Omega = [0, T]$ and x is the time variable. In this case, these spaces are widely used when dealing with free-boundary problems or PDEs on noncylindrical domains. See [19] for similar definitions and further references.

2.1. The Lebesgue space $L_p(\Omega; L_q(Y_x))$.

Let $\Omega \subset \mathbb{R}^n$ and $Y \subset \mathbb{R}^m$ be bounded domains. For each $x \in \Omega$, let $Y_x \subset Y \subset \mathbb{R}^m$ be another domain such that

$$Q := \Omega \times Y_x := \bigcup_{x\in\Omega} (\{x\} \times Y_x) \subset \mathbb{R}^{n+m}$$

is measurable with respect to the $(n+m)$-dimensional Lebesgue measure. If no further restrictions are given, then $p \in [1, \infty]$ and $q \in [1, \infty)$ are given exponents and p' and q' are the dual exponents defined by $1/p + 1/p' = 1$ and $1/q + 1/q' = 1$. The case $q = \infty$ is not considered in this paper.

Definition 1 (The space $L_{p,q}(Q)$)**.**

(1) We define the Banach space

$$\begin{aligned} L_{p,q}(Q) &\equiv L_p(\Omega; L_q(Y_x)) \\ &:= \{u \in L_p(\Omega; L_q(Y)) : \ u(x, \cdot) = 0 \text{ on } Y \setminus Y_x \quad \text{for a.e. } x \in \Omega\} \end{aligned}$$

with the norm

$$\|u\|_{L_{p,q}(Q)} := \begin{cases} (\int_\Omega \|U(x)\|^p_{L_q(Y_x)}\, dx)^{1/p}, & p < \infty, \\ \operatorname{ess\,sup}_{x\in\Omega} \|U(x)\|_{L_q(Y_x)}, & p = \infty. \end{cases}$$

(2) In the case $p = q = 2$, we define the Hilbert space $L_{2,2}(Q)$ with the scalar product

$$(u,\, v)_{L_{2,2}(Q)} := \int_\Omega (u(x),\, v(x))_{L_2(Y_x)}\, dx.$$

Remark. Since $q < \infty$, the function $x \mapsto \|u(x, \cdot)\|_{L_q(Y_x)}$ is measurable by Fubini's theorem. Thus, the space $L_{p,q}(Q)$ is well-defined. As a closed subspace of $L_p(\Omega; L_q(Y))$, it is also complete.

Proposition 2 (Properties of the space $L_{p,q}(Q)$)**.**

(1) (Hlder's inequality) For all $u \in L_p(\Omega; L_q(Y_x))$ and $v \in L_{p'}(\Omega; L_{q'}(Y_x))$, it holds

$$\int_\Omega \int_{Y_x} u(x, y) v(x, y)\, dy\, dx \le \|u\|_{L_{p,q}(Q)} \|v\|_{L_{p',q'}(Q)}.$$

(2) Let $p < \infty$. Then $L_{p,p}(Q)$ is isometrically isomorph to $L_p(Q)$.

(3) Let $p < \infty$. Then the simple functions as well as the continuous functions on $\overline{Q}$ are dense in $L_{p,q}(Q)$. In particular, $L_{p,q}(Q)$ is separable.

Proof. Part (1) is obtained straightforwardly from the standard Hlder's inequalities in the spaces $L_p(\Omega)$ and $L_q(Y_x)$.

Part (2) follows via extension by zero from the corresponding fact for the Bochner space $L_p(\Omega; L_p(Y))$. A proof of the latter result can be found in [8], pp. 196ff.

(3) By definition, $f \in L_{p,q}(Q)$ is Bochner-integrable as a function $f : \Omega \to L_q(Y)$. Therefore we can approximate f by simple functions $f_k : \Omega \to L^q(Y)$ via

$$f_k(x) := \sum_{i=1}^{m_k} \alpha_i^k \mathbb{1}_{E_i^k}(x), \quad \alpha_i^k \in L^q(Y),\ E_i^k \subset \Omega \text{ measurable for } i, k \in \mathbb{N},$$

such that $f_k \to f$ in $L_p(\Omega; L_q(Y))$ for $k \to \infty$. Moreover, each α_i^k can be approximated by

$$\alpha_i^{kl}(y) := \sum_{j=1}^{n_l} \beta_{ij}^{kl} \mathbb{1}_{D_{ij}^{kl}}(y), \quad \beta_{ij}^{kl} \in \mathbb{R}, \quad D_{ij}^{kl} \subset Y \text{ measurable for } j, l \in \mathbb{N}.$$

Then one easily verifies that the simple functions on Q given by

$$f^{kl}(x,y) := \sum_{i=1}^{m_k} \sum_{j=1}^{n_l} \beta_{ij}^{kl} \mathbb{1}_{E_i^k \times (D_{ij}^{kl} \cap Y_x)}(x,y)$$

approximate f in $L^{p,q}(Q)$ for $k, l \to \infty$. In order to prove the density of $C(\overline{Q})$ in $L_{p,q}(Q)$, it suffices to approximate simple functions $f : Q \to \mathbb{R}$. Thus, we can assume that $f \in L^r(Q)$ for every $r \geq 1$. Since $C(\overline{Q})$ is dense in $L_{\max\{p,q\}}(Q)$, the result follows. □

Proposition 3 (Characterisation of the dual space)**.** Let $p \in [1, \infty)$ and $q \in (1, \infty)$. The operator

$$\langle J(f),\, g\rangle := \int_\Omega \int_{Y_x} f(x,y) g(x,y)\, dy\, dx, \qquad g \in L_{p,q}(Q),\ f \in L_{p',q'}(Q),$$

is an isometric isomorphism $J : L_{p',q'}(Q) \to [L_{p,q}(Q)]'$. In particular, $L_{p,q}(Q)$ is reflexive for $p > 1$.

Remark. The case $q = 1$ is not covered since the space $L_{p',\infty}(Q)$ has not been defined.

Proof. Let $f \in L_{p',q'}(Q)$. By Hlder's inequality, $J(f)$ is well-defined and $\|J(f)\| \leq \|f\|_{p',q'}$. Moreover, by the fundamental lemma of calculus of variations, J is injective.

Let $F \in [L_{p,q}(Q)]'$ be given. We have to show that an $f \in L_{p',q'}(Q)$ exists with

$$F = J(f) \qquad \text{and} \qquad \|f\|_{p',q'} \leq \|F\|.$$

We reduce the statement to the cylindrical situation in the following way: Define

$$\tilde{J} : L_{p'}(\Omega; L_{q'}(Y)) \to [L_p(\Omega; L_q(Y))]', \qquad \langle \tilde{J}(f),\, g\rangle := \int_\Omega \int_Y f g\, dy\, dx.$$

In this case, it is known that $\tilde{J}$ is an isometric isomorphism. The proof, which is very similar to the real-valued case $L_p(\Omega)$, can be found in [4]. Define $\lambda_{p,q} : L_p(\Omega; L_q(Y)) \to L_{p,q}(Q)$ to be the linear restriction operator and let $\lambda'_{p,q}$ be its dual. Both operators have norm 1, and the right-inverse of $\lambda_{p,q}$ is the extension by zero, which we denote by $\gamma_{p,q} : L_{p,q}(Q) \to L_p(\Omega; L_q(Y))$. Hence, $\gamma_{p,q} \circ \lambda_{p,q} = \text{id}$. Let

$$f := \lambda_{p',q'} \circ \tilde{J}^{-1} \circ \lambda'_{p,q} \circ F \in L_{p',q'}(Q).$$

Then $\|f\|_{p',q'} \leq \|F\|$ and, for any $g \in L_{p,q}(Q)$,

$$\begin{aligned}\langle J(f), g\rangle &= \left\langle J \circ \lambda_{p',q'} \circ \tilde{J}^{-1} \circ \lambda'_{p,q} \circ F, g\right\rangle \\ &= \int_\Omega \int_{Y_x} (\lambda_{p',q'} \circ \tilde{J}^{-1} \circ \lambda'_{p,q} \circ F)\, g\, dy\, dx \\ &= \int_\Omega \int_Y (\tilde{J}^{-1} \circ \lambda'_{p,q} \circ F)\, \gamma_{p,q} g\, dy\, dx \\ &= \left\langle \lambda'_{p,q} \circ F, \gamma_{p,q} \circ g\right\rangle \\ &= \left\langle F, (\lambda_{p,q} \circ \gamma_{p,q}) g\right\rangle \\ &= \langle F, g\rangle.\end{aligned}$$

Hence $J(f) = F$, which proves the Proposition. □

2.2. The Sobolev space $L_p(\Omega; W^l_q(Y_x))$. In the following, let $l \in \mathbb{N}$. For a multi-index $\alpha \in \{0, \dots, l\}^m$, let $\partial_\alpha u(x, y)$ denote the α-th derivative w.r.t. y.

Definition 4. We define the Banach space

$$W^{0,l}_{p,q}(Q) \equiv L_p(\Omega; W^l_q(Y_x)) := \{u \in L_{p,q}(Q) : \ \partial^\alpha u \in L_{p,q}(Q)\ \forall |\alpha| \leq l\}$$

with the norm

$$\|u\|_{W^{0,l}_{p,q}(Q)} := \sum_{|\alpha| \leq l} \|\partial_\alpha u\|_{L_{p,q}(Q)}.$$

In the case $p = q = 2$, $W^{0,l}_{2,2}(Q)$ is a Hilbert space with the scalar product

$$(u, v)_{W^{0,l}_{2,2}(Q)} := \sum_{|\alpha| \leq l} (\partial_\alpha u, \partial_\alpha v)_{L_{2,2}(Q)}\,.$$

Remark. The proof that $W^{0,l}_{p,q}(Q)$ is complete reduced to the completeness of $L_{p,q}(Q)$ by the analogous argument as for standard Sobolev spaces.

Proposition 5 (Properties of $W^{0,l}_{p,q}(Q)$)**.** The space $W^{0,l}_{p,q}(Q)$ is separable if $p < \infty$ and reflexive if $p, q \in (1, \infty)$.

Proof. In order to prove separability, define the linear bounded operator

$$T : X := W^{0,l}_{p,q}(Q) \to \prod_{|\alpha| \leq l} L_{p,q}(Q), \qquad f \mapsto (\partial_\alpha f)_{|\alpha| \leq l}.$$

Then $T(f)$ can be estimated from above and below by the norm $\|f\|_X$. Thus, X is isomorph to $T(X)$. Since $C(\overline{Q})$ is dense in $L_{p,q}(Q)$ for $p < \infty$, the subspace $T(X)$ is separable and, hence, also X.

Finally, for $p, q \in (1, \infty)$, $L_{p,q}(Q)$ is reflexive by Prop. 3. Since X is a Banach space, $T(X)$ is a closed subspace of $L_{p,q}(Q)$ and is therefore also reflexive. □

Remark. As already mentioned in [25], for the special case $q = 2$ and $p < \infty$, the space $W^{0,l}_{p,2}(Q)$ can alternatively be constructed as a *direct integral of Hilbert spaces*. See [7, 26] for abstract definitions, or [6] for the special case that $n = 1$ and $\Omega = (a, b)$. For details on how the construction works for the space $W^{0,l}_{p,2}(Q)$, the reader is referred to [16].

3. Spaces of functions defined on the cell boundary

In order to give a meaning to integrals of the form $\int_\Omega \int_{\partial Y_x} u(x,y)\, d\sigma_y\, dx$, we need to define spaces of functions defined on the cell boundary ∂Y_x. Here the situation is more complicated since we need to parameterise the whole collection of cell boundaries $\{\Gamma_x : x \in \Omega\}$. For a concise presentation, we exclude some (degenerate) geometries that could perhaps be treated with more technical effort.

3.1. Parametrisation of the cell boundaries. We assume that the Lebesgue measure of the cells $Y_x \subset \mathbb{R}^m$ is uniformly bounded from below, i.e., there exists a constant $c > 0$ such that $|Y_x| \geq c$ for all $x \in \Omega$. Let us introduce a parametrisation of

$$\Sigma := \overline{\Omega} \times \partial Y_x := \bigcup_{x \in \overline{\Omega}} (\{x\} \times \partial Y_x) \subset \partial Q.$$

Note that ∂Q is not smoother than Lipschitz, even if Y_x and Ω have smooth boundaries. In general, the normal will be multi-valued at points $(x,y) \in \partial\Omega \times \partial Y_x$. In order to avoid technicalities, we therefore assume that Q can be extended to a bounded Lipschitz domain $Q_1 \supset Q$ (cf. figure 2 on the left) and construct a parameterisation of $\Sigma_1 := \partial Q_1 \supset \Sigma$.

We recall the definition of a Lipschitz boundary (cf. [27], e.g.). At any given point $(x_0, y_0) \in \Sigma_1$, there exists a neighbourhood U of (x_0, y_0) such that, after an Euclidean coordinate transform, $\Sigma_1 \cap U$ is the graph of a (locally) Lipschitz continuous function $g : \mathbb{R}^{n+m-1} \to \mathbb{R}$ and $Q_1 \cap U$ lies on one side of the graph. See figure 1. More precisely, there exists an orthonormal basis $\{v_j\}_{j=1,\dots,n+m}$, a number $r > 0$, such that with the notation $\xi' = (\xi_1, \dots, \xi_{n+m-1})$, the bijective coordinate transform

$$\Psi^{-1} : \mathbb{R}^{n+m} \to \mathbb{R}^{n+m}, \quad \xi \mapsto (x,y) = (x_0, y_0) + \sum_{i=1}^{n+m-1} \xi_j v_j + (\xi_{n+m} + g(\xi')) v_{n+m},$$

the cube $W^{n+m} = (-r, r)^{n+m}$, $r > 0$, and the open set

$$U = \Psi^{-1}(W^{n+m}) \subset \mathbb{R}^{n+m},$$

it holds for all $(x,y) \in U$

$$(2) \qquad (x,y) \in U \cap \Sigma_1 \quad \Longleftrightarrow \quad \xi_{n+m} = g(\xi'),$$

$$(3) \qquad (x,y) \in U \cap Q_1 \quad \Longleftrightarrow \quad 0 < \xi_{n+m} - g(\xi') < r,$$

$$(4) \qquad (x,y) \in U \setminus \overline{Q_1} \quad \Longleftrightarrow \quad -r < \xi_{n+m} - g(\xi') < 0.$$

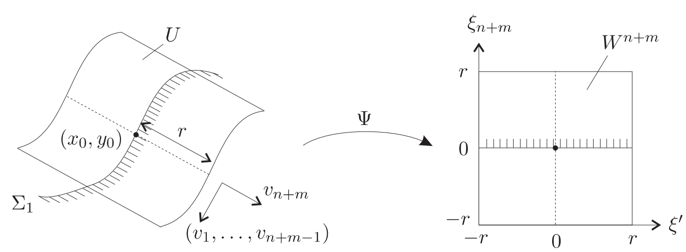

FIGURE 1. Parametrisation of the $(n+m-1)$-dimensional manifold Σ_1.

The set of unit normal vectors directed outward is defined (independently of the parametrisation) as

$$(5)\quad \nu_\Sigma(x,y) := (1+|\nabla_{\xi'} g(\xi')|^2)^{-1/2} \left(\sum_{j=1}^{n+m-1} \partial_j g(\xi') v_j - v_{n+m} \right), \qquad (x,y) \in \Sigma_1.$$

Here, $\partial_j g$ and $\nabla_{\xi'} g$ can be multi-valued and refer to the Clarke gradient (see [5]). In general, at some given point $(x,y) \in \Sigma_1$ the normal $\nu_\Sigma(x,y)$ is a convex set of vectors, but for almost every (x,y) it is a singleton.

We recall how the integral over the $(n+m-1)$-dimensional manifold Σ is defined. Since Σ is compact, there exist finitely many of such parameterisations (x_0^k, y_0^k), U^k, g^k, $\{v_j^k\}_{j=1,\dots,n+m}$ such that $\Sigma \subset \cup_{k=1}^N U^k$. Let $(\eta^k)_{k=1,\dots,N}$ be a partition of unity subordinated to the U^k. We define the integral of a function $f : \Sigma \to \mathbb{R}$ to be

$$\int_\Sigma f \, d\sigma_{x,y} := \sum_{k=1}^N \int_{W^{n+m-1}} (\eta^k f) \left((\Psi^k)^{-1}(\xi', 0) \right) \sqrt{1 + |\nabla_{\xi'} g^k(\xi')|^2} \, d\xi'.$$

Note that the integral is single-valued, as the set of points where the g^k are not differentiable is of measure zero (Rademacher's theorem).

Next we construct a parametrisation of the cell boundaries $\{\partial Y_x : x \in \Omega\}$ from the above one. Cf. figure 2 in the center, we define the normal ν_x at the cell boundary ∂Y_x to be the (normalised) projection P_y of ν_Σ onto the subspace $\{x = 0\}$ spanned by the vectors $e_{n+1}, \dots, e_{n+m}$, with other words,

$$(6)\qquad \nu_x(y) := \frac{\mathrm{P}_y \nu_\Sigma(x,y)}{|\mathrm{P}_y \nu_\Sigma(x,y)|}, \qquad (x,y) \in \Sigma.$$

For this definition to make sense, it is necessary that the projection is nonzero. It can be shown that this condition is also *sufficient* for constructing a parametrisation of the cell boundaries. This is the purpose of the following Lemma.

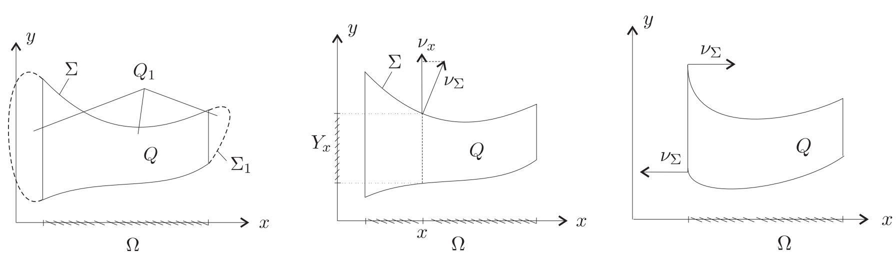

FIGURE 2. Left: The extension Σ_1 of the boundary. Center: Unit normal ν_Σ at Σ and cell normal ν_x. Right: Example of a geometry that does *not* satisfy condition (7).

Lemma 6. Assume that

$$\mathrm{P}_y \nu_\Sigma(x,y) \not\ni 0 \qquad \forall (x,y) \in \Sigma. \tag{7}$$

Then the cells Y_x are bounded Lipschitz domains with unit normals at ∂Y_x given by (6) and the parametrisation in each point $(x_0, y_0) \in \Sigma$ can be chosen such that

$$v_j = e_j, \qquad j = 1, \dots, n.$$

Moreover, there exist positive constants c and C such that

$$c \le |Y_x|, |\partial Y_x| \le C \qquad \text{for all } x \in \Omega. \tag{8}$$

Remark. It is important that (7) is valid for all (x,y) in the *closed* set $\Sigma = \overline{\Omega} \times \partial Y_x$. By this assumption, we exclude some degenerate cases; see figure 2 on the right.

Proof. Let $(x_0, y_0) \in \Sigma$ be an arbitrary point and assume that a local parametrisation in a neighbourhood U is given as above. We construct a new parametrisation as required. We write (2) in (x,y)-coordinates:

$$v_{n+m} \cdot (x,y) = g(v_1 \cdot (x,y), \dots, v_{n+m-1} \cdot (x,y)) \qquad \forall (x,y) \in U \cap \Sigma_1,$$

or

$$G(x,y) := g(v_1 \cdot (x,y), \dots, v_{n+m-1} \cdot (x,y)) - v_{n+m} \cdot (x,y) = 0 \qquad \forall (x,y) \in U \cap \Sigma_1.$$

We have, according to (5) and (7),

$$\begin{aligned} \nabla_y G(x,y) &= \sum_{j=1}^{n+m-1} \partial_j g(\xi') \mathrm{P}_y v_j - \mathrm{P}_y v_{n+m} \\ &= (1 + |\nabla_{\xi'} g(\xi')|)^2)^{1/2} \; P_y \nu_\Sigma(x,y) \;\not\ni 0 \qquad \forall (x,y) \in U \cap \Sigma_1. \end{aligned}$$

We can therefore apply the implicit function theorem (see [5] for a Lipschitz version) and resolve the equation near (x_0, y_0) with respect to a vector lying in the subspace $\{x = 0\}$ spanned by $e_{n+1}, \dots, e_{n+m}$. More precisely, there exists an ONB $w_1, \dots, w_n$ of $\mathbb{R}^n$ and a (possibly smaller) cube $\tilde{W}^{n+m} = (-\tilde{r}, \tilde{r})^{n+m}$ and a Lipschitz continuous function $\tilde{g} : \mathbb{R}^{n+m-1} \to \mathbb{R}$ such that, with the coordinate transform

$$\Psi^{-1} : \tilde{W}^{n+m} \to \mathbb{R}^{n+m}, \qquad (x, \zeta) \mapsto (x_0, y_0) + \left(x, \sum_{i=1}^{m-1} \zeta_i w_i + (\zeta_m + \tilde{g}(x, \zeta')) w_m \right),$$

(where $\zeta' := (\zeta_1, \dots, \zeta_{n-1})$), it holds for all $(x,y) \in \Psi^{-1}(\tilde{W}^{n+m}) = \tilde{U}$,

$$\zeta_m = \tilde{g}(x, \zeta'), \qquad \Longleftrightarrow \qquad (x,y) \in \Sigma_1 \cap \tilde{U},$$

with other words, since $\tilde{U} = (x_0 - r, x_0 + r) \times \tilde{U}_x$, where $\tilde{U}_x$ is a neighbourhood of $y_0 \in \partial Y_x$,

$$\zeta_m = \tilde{g}(x, \zeta'), \qquad \Longleftrightarrow \qquad y \in \partial Y_x \cap \tilde{U}_x.$$

It follows that, with $\tilde{g}_x(y) := \tilde{g}(x,y)$, $(x,y) \in \Omega \times W^m$, and the new transformation

$$\tilde{\Psi}_x^{-1} = \tilde{\Psi}^{-1}(x, \cdot) : W^m \to \tilde{U}_x, \qquad \zeta \mapsto y_0 + \sum_{i=1}^{m-1} \zeta_i w_i + (\zeta_m + \tilde{g}_x(\zeta')) w_m$$

we have found a parametrisation of ∂Y_x. If the neighbourhood $\tilde{U}$ has been chosen small enough, then the corresponding conditions (2)–(4) are satisfied.

The estimates (8) are now obvious since, due to the compactness of Σ, the whole collection of cells can be covered by a finite number of maps Ψ^k, $k = 1, \dots, N$. $\square$

Motivated by the preceding Lemma, we define:

Definition 7 (Regular family of cells)**.** The family $\{(Y_x, \Gamma_x):\ x \in \Omega\}$ is called a regular family of cells if $\Omega \subset \mathbb{R}^n$ is a bounded Lipschitz domain and it holds:

(1) For each $x \in \Omega$, $Y_x \subset \mathbb{R}^m$ is a bounded domain such that $Q := \Omega \times Y_x \subset \mathbb{R}^{n+m}$ is measurable. There exists a constant $c > 0$ such that $|Y_x| \geq c$ for all $x \in \Omega$.
(2) For each $x \in \Omega$, Γ_x is a measurable subset of ∂Y_x.
(3) $\Sigma := \partial Q \subset \mathbb{R}^{n+m}$ can be extended to a boundary of a Lipschitz domain $Q_1 \supset Q$ in $\mathbb{R}^{n+m}$, such that the convex set of unit normals ν_Σ at ∂Q_1 satisfies

$$\mathrm{P}_y \nu_\Sigma(x, y) \not\ni 0 \qquad \forall (x, y) \in \Sigma.$$

Let $\{(Y_x, \Gamma_x):\ x \in \Omega\}$ be a regular family of cells. Remember that we want to define the integral of a function over Γ_x such that it is measurable w.r.t. x. W.l.o.g., we assume that the parametrisation $\{x_0^k, y_0^k, U^k, g^k\}_{k=1,\dots,N}$ has already the form as constructed in the proof of Lemma 6. We define the corresponding transformations Ψ^k such that $\Sigma \subset \cup_{k=1}^N U^k$. Clearly, the x-intersections $U_x^k \subset \mathbb{R}^m$ cover Γ_x for every $x \in \Omega$ and the $\eta_x^k = \eta^k(x, \cdot)$ can be chosen as a partition of unity subordinated to the U_x^k. Thus, we can define:

Definition 8 (Integral over Γ_x)**.** Let $\{(Y_x, \Gamma_x):\ x \in \Omega\}$ be a regular family of cells. For a function $f: \Sigma \to \mathbb{R}$ which is integrable with respect to the $(n+m-1)$-dimensional Lebesgue measure, we define, for almost every $x \in \Omega$,

$$\int_{\Gamma_x} f(x, y) d\sigma_y := \sum_{k=1}^N \int_{W^{m-1}} (\eta^k f)\left(x, (\Psi_x^k)^{-1}(\zeta')\right) \sqrt{1 + |\nabla_{\zeta'} g_x^k(\zeta')|^2}\, d\zeta'.$$

Remark.

(1) By our assumption on the geometry, jumps in the cell structure along the x-coordinate are excluded. We can account for at least finitely many jumps by a simple modification: Assume that Ω is decomposed into $M \geq 1$ disjoint domains such that $\bar{\Omega} = \cup_{i=1}^M \bar{\Omega}_i$. We now adopt the Lipschitz and geometric conditions for each of the domains Ω_i. The integral is then constructed as the sum of all integrals over Ω_i.
(2) An important special case is given if $\Omega = (a, b)$ is one-dimensional and $t := x \in (a, b)$ represents the time variable. Then the cells $\{Y_t:\ t \in (a, b)\}$, describe a time-dependent domain. In this case, the normal velocity of the interface at $(t, y) \in Q = (a, b) \times \Gamma_t$ is given by

$$w_\Gamma(t, y) = \frac{\mathrm{P}_t \nu_\Sigma(t, y)}{|\mathrm{P}_y \nu_\Sigma(t, y)|}, \qquad \text{for a.e. } t \in (a, b),\ y \in Y_t,$$

where P_t is the projection to $\{y = 0\}$. See also figure 2 in the center. The condition that $\{(Y_t, \Gamma_t):\ t \in (a, b)\}$ is a regular family of cells guarantees that w_Γ is well-defined almost everywhere.

3.2. The space $L_p(\Omega; L_q(\Gamma_x))$. In what follows, let $\{(Y_x, \Gamma_x) : x \in \Omega\}$ be a regular family of cells.

Proposition 9. The space

$$L_{p,q}(\Sigma) \equiv L_p(\Omega; L_q(\Gamma_x)) := \{u : \Sigma \to \mathbb{R} \text{ measurable such that } u(x) \in L_q(\Gamma_x) \text{ for a.e. } x \in \Omega \text{ and } \|u\|_{L_p(\Omega;L_q(\Gamma_x))} < \infty\Big\}$$

is a Banach space with the norm

$$\|u\|_{L_{p,q}(\Sigma)} := \begin{cases} (\int_\Omega \|u(x)\|^p_{L_q(\Gamma_x)}\, dx)^{1/p}, & p < \infty, \\ \operatorname{ess\,sup}_{x\in\Omega} \|u(x)\|_{L_q(\Gamma_x)}, & p = \infty. \end{cases}$$

and a Hilbert space in case of $p = q = 2$ with the obvious scalar product.

Proof. It is clear by construction that $u(x, \cdot) : \Gamma_x \to \mathbb{R}$ is a measurable function and the norm $\|u(x, \cdot)\|_{L_q(\Gamma_x)}$ is measurable in x. Hence, the space above is well-defined. The proof of completeness is obtained by slight modification of the usual Fischer-Riesz type arguments. See [16] for details. □

Proposition 10. Let $p < \infty$. Then the space $L_{p,p}(\Sigma)$ is equivalent to $L_p(\Sigma)$. In general, both spaces are *not* isometric isomorph.

Proof. Let $f \in L_{p,p}(\Sigma)$. Then, by Fubini's theorem, the mapping $x \mapsto \int_{\Gamma_x} f(x, y)\, d\sigma_y$ is measurable and

(9)

$$\begin{aligned} \|f\|^p_{L_{p,p}(\Sigma)} &= \int_\Omega \int_{\Gamma_x} |f(x, y)|^p\, d\sigma_y\, dx \\ &= \sum_{k=1}^N \int_\Omega \int_{W^{m-1}} (\eta^k |f|^p) \left(x, (\Psi^k_x)^{-1}(\zeta', 0)\right) \sqrt{1 + |\nabla_{\zeta'} g^k_x(\zeta')|^2}\, d\zeta'\, dx. \end{aligned}$$

Moreover, by construction, the integral of f over Σ can be written as

(10)

$$\begin{aligned} &\|f\|^p_{L_p(\Sigma)} = \int_\Sigma |f(x, y)|^p\, d\sigma_{x,y} \\ &= \sum_{k=1}^N \int_{W^{n+m-1}} (\eta^k |f|^p) \left((\Psi^k)^{-1}(\xi', 0)\right) \sqrt{1 + |\nabla_{\xi'} g^k(\xi')|^2}\, d\xi' \\ &= \sum_{k=1}^N \int_\Omega \int_{W^{m-1}} (\eta^k |f|^p) \left(x, (\Psi^k_x)^{-1}(\zeta', 0)\right) \sqrt{1 + |\nabla_x g^k(x, \zeta')|^2 + |\nabla_{\zeta'} g^k_x(\zeta')|^2}\, d\zeta'\, dx. \end{aligned}$$

The norm equivalence follows now from the fact that the surface elements in (9) and (10), namely

$$\sqrt{1 + |\nabla_{\zeta'} g^k_x(\zeta')|^2} \qquad \text{and} \qquad \sqrt{1 + |\nabla_x g^k(x, \zeta')|^2 + |\nabla_{\zeta'} g^k_x(\zeta')|^2},$$

are essentially bounded from above and below, uniformly w.r.t. x.

A counterexample that the spaces are not isometric isomorph is given as follows: Let $n = m = 1$, $\Omega = (a, b)$, $b > a > 0$, and $Y_x := (-x, x)$. If we integrate 1 over Γ_x, we obtain 2 in each cell. Therefore, the integration (9) gives $\int_\Omega \int_{\Gamma_x} d\sigma_y\, dx = 2(b-a)$ whereas an integration over the one-dimensional surface measure according to (10) gives the value $2(b - a)\sqrt{2}$.

□

Next we construct the connection between the spaces $W^{0,1}_{p,q}$ and $L_{p,q}(\Sigma)$ via the *distributed trace*.

Proposition 11. Let $p < \infty$ and $\gamma_x : W^1_q(Y_x) \to L_q(\Gamma_x)$ be the continuous trace operator. Then $\|\gamma_x\|$ is uniformly bounded in $x \in \Omega$ and the distributed trace

$$\gamma : W^{0,1}_{p,q}(Q) \to L_{p,q}(\Sigma), \qquad \gamma(u)(x) = \gamma_x(u(x)),$$

is a bounded linear operator.

Proof. By construction, γ_x is measurable and the norm $\|\gamma_x\|$ is bounded uniformly w.r.t. x. (See [16] for details and for an estimation of $\|\gamma_x\|$ in terms of the parametrisation.) The boundedness of the distributed trace follows then from the estimate

$$\|\gamma u\|^p_{L_{p,q}(\Sigma)} = \int_\Omega \|\gamma_x u(x)\|^p_{L_q(\Gamma_x)}\, dx \le \sup_{x\in\Omega} \|\gamma_x\|^p \cdot \int_\Omega \|u(x)\|^q_{W^1_q(Y_x)}\, dx.$$

□

Remark. Higher order trace estimates in $W^l_q(Y_x)$, $l > 1$, can also be formulated. The only technical difficulty is the higher regularity needed for the boundary Γ_x. The parametrisation has to be adapted to the case where the geometry is smoother with respect to y than w.r.t. x. We do not follow this direction.

4. Application to reactive transport in porous media

Making use of the space constructions in the previous sections, we can now define a variational formulation of a distributed-microstructure system for reactive transport in a heterogeneous porous medium and prove its wellposedness.

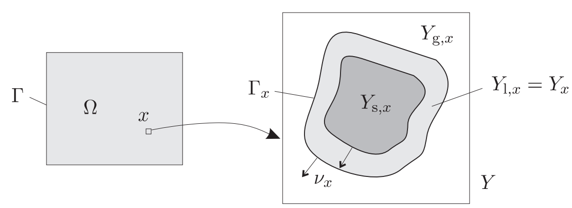

Figure 3. Geometry of the distributed microstructure model (11).

4.1. The problem. We consider an unsaturated porous medium, in which the distribution of pore water is assumed completely known and transport of water is at rest. Let $S = [0, T]$ be a bounded time interval and $\Omega \subset \mathbb{R}^n$ be a bounded Lipschitz domain with boundary $\Gamma = \partial\Omega$, representing the macroscopic domain filled by the medium.

Let $Y := (0, l)^n$ denote the n-dimensional cuboid with side length $l > 0$. For each $x \in \Omega$, assume we are given bounded domains $Y_{s,x}, Y_x \subset Y$ representing the solid and the liquid phase near x such that $Y_{s,x} \cap Y_x = \emptyset$. We assume that the pore air is connected, whereas the liquid domains Y_x are individually isolated, i.e., $\overline{Y}_x \subset Y$. An example of such a geometry is depicted in figure 3. In typical applications, this corresponds to a *low* humidity of the medium. We then denote the interface between the gaseous and the liquid phase by $\Gamma_x := \partial Y_x \setminus \partial Y_{s,x} \neq \emptyset$ and assume that the family $\{(Y_x, \Gamma_x) : x \in \Omega\}$ is a regular distribution of cells in the sense of Def. 7.

We consider a substance A that diffuses *slowly* as a solute in the pore water and *fast* as a gas in the pore air. At the gas–liquid interfaces, exchange of A occurs in both directions. In the pore water, A is subjected to one or more chemical reactions. The setting is motivated by carbonation of concrete; see [24, 18]. The mass balance for the concentration $u = u(t, x)$ of A in the pore air is effectively described by an averaged diffusion equation of the form

$$\partial_t(\theta(x)u(t,x)) - \operatorname{div}(d(x)\nabla u) = -f(t,x), \qquad t \in S,\ x \in \Omega, \tag{11a}$$

where $\theta(x) = |Y_{\mathrm{g},x}|/|Y|$ is the volume fraction of the pore air, $d(x) \in \mathbb{R}^{n\times n}$ is the effective diffusion tensor and $f(t, x)$ is the amount of A that gets absorbed in the pore water. The structure of f will be derived below. At $\Gamma = \partial\Omega$ we impose the Robin condition

$$-d\nabla u(t,x) \cdot \nu(x) = b(x)(u - u^{\mathrm{e}}(t,x))), \qquad t \in S,\ x \in \Gamma, \tag{11b}$$

with the unit normal $\nu(x)$ (directed outward), an exchange coefficient $b(x)$ and a given external concentration $u^{\mathrm{e}}(t, x)$.

The slower transport of A in the pore water is described at the micro scale. Let $U = U(t, x, y)$ be the concentration of A at time $t \in S$, macroscopic coordinate $x \in \Omega$ and microscopic coordinate $y \in Y_x$. Then the microscopic (not-averaged!) mass balance reads

$$\partial_t U(t,x,y) - \operatorname{div}_y(D\nabla_y U) = g(t,x,y,U), \qquad t \in S,\ x \in \Omega,\ y \in Y_x, \tag{11c}$$

where $D > 0$ is the microscopic diffusivity and $g(t, x, y, U)$ is the production or consumption of A by chemical reactions. Note that all spatial derivatives in (11c) are taken with respect to the microscopic coordinate y, such that x is effectively a parameter in (11c). We indicate this by the lower index y. In contrast, the symbols "∇" and "div" without lower index stand for differentiation w.r.t. x.

For a function $w : Y_x \to \mathbb{R}$, let $\gamma_x w := w|_{\Gamma_x}$ be its trace at the boundary Γ_x. Then the boundary conditions for U read

$$-D\nabla_y U(t,x,y) \cdot \nu_x = k(\gamma_x U(t,x,y) - Hu(t,x)), \qquad t \in S,\ x \in \Omega,\ y \in \Gamma_x, \tag{11d}$$

where ν_x is the unit normal to ∂Y_x (directed outward), k is an exchange coefficient and H is the equilibrium constant between u and U (*Henry constant*), and

$$-D\nabla_y U(t,x,y) \cdot \nu_x = 0 \qquad t \in S,\ x \in \Omega,\ y \in \partial Y_x \setminus \Gamma_x. \tag{11e}$$

Now the *total amount of A crossing the interface* Γ_x at a given time $t \in S$ and a given point $x \in \Omega$ is

$$f(t,x) = \frac{1}{|Y|}\int_{\Gamma_x} k(Hu - \gamma_x U)\, d\sigma_y, \qquad t \in S,\ x \in \Omega, \tag{11f}$$

which completes the mass balance (11a) for u. Finally, the initial conditions are

$$u(0,x) = u_0(x), \qquad U(0,x,y) = U_0(x,y), \qquad x \in \Omega,\ y \in Y_x. \tag{11g}$$

The system (11) is a semilinear, weakly coupled system of two parabolic PDEs. It is conceptually similar to the *regularised microstructure model* introduced in [25] for flow in fissured media.

4.2. Variational formulation. Let $\theta \in L_\infty(\Omega)$ be bounded away from zero, i.e. $\theta(x) \geq \theta_0 > 0$ for a.e. $x \in \Omega$. Let $d : \Omega \to \mathbb{R}^{n\times n}$ be measurable and uniformly elliptic, i.e. there exist constants $c, C > 0$ such that

$$c\,|\xi|^2 \leq \sum_{k,l} d_{k,l}(x)\xi_k\xi_l \leq C\,|\xi|^2 \qquad \forall \xi \in \mathbb{R}^n,\ \text{a.e. } x \in \Omega.$$

Let $b \in L^\infty(\partial\Omega)$ be nonnegative and let k, H and D be positive constants. For the initial and external values we assume that $u_0 \in L^\infty(\Omega)$, $U_0 \in L^\infty(\Omega \times Y_x)$ and $u^{\mathrm{e}} \in L^\infty(S \times \partial\Omega)$ such that for a positive constant C_U it holds

$$0 \leq Hu_0(x), U_0(x,y), Hu^{\mathrm{e}}(t,x) \leq C_U \quad \text{a.e.} \tag{12}$$

The reaction term has the structure

$$g(t,x,y,U) = -M_1(t,x,y)\eta_1(U) + M_2(t,x,y)\eta_2(U), \tag{13}$$

where $M_1, M_2 \in L_\infty(S\times\Omega\times Y_x)$ are nonnegative functions and $\eta_1, \eta_2 : \mathbb{R} \to [0,\infty)$ are locally Lipschitz and satisfy

$$\eta_1(U) = 0 \quad \text{for } U \leq 0 \qquad \text{and} \qquad \eta_2(U) \leq 1 + |U| \quad \text{for } U \in \mathbb{R}. \tag{14}$$

Note that (14) actually implies that the production rate η_2 is *globally* Lipschitz on $[0,\infty)$.

We denote by H_θ the usual space $L_2(\Omega)$, equipped with the equivalent scalar product

$$(u,\,v)_{H_\theta} := \int_\Omega \theta(x)u(x)v(x)\,dx, \qquad u,v \in H_\theta,$$

and introduce

$$\begin{aligned} V &:= H^1(\Omega) \times L_2(\Omega; H^1(Y_x)),\\ H &:= H_\theta \times L_2(\Omega; L_2(Y_x)),\\ \mathcal{V} &:= L_2(S;V), \quad \mathcal{V}' := L_2(S;V'). \end{aligned}$$

Then, by Def. 4 and Prop. 5, V and H are separable Hilbert spaces and the embeddings $V \hookrightarrow H \hookrightarrow V'$ are continuous and dense. Moreover, if $\gamma_x : H^1(Y_x) \to L_2(\Gamma_x)$ is the usual trace map on the cell boundary, then from Prop. 11 we obtain that the *distributed trace* $\gamma : L_2(\Omega; H^1(Y_x)) \to L_2(\Omega; L_2(\Gamma_x))$ is a bounded linear operator. We introduce the notation

$$(u,\,v)_{\Omega\times\Gamma_x} := \int_\Omega\int_{\Gamma_x} uv\,d\sigma_y dx, \qquad u,v \in L_2(\Omega; L_2(\Gamma_x)), \tag{15}$$

and $(\cdot,\,\cdot)_{\Omega\times Y_x}$, $(\cdot,\,\cdot)_\Omega$, etc., analogously. Note that (15) is *not* equal to the integral over the $(2n-1)$-dimensional manifold $\Omega \times \Gamma_x$ (cf. Prop. 10).

Definition 12 (Weak upper and lower solutions)**.** A pair of essentially bounded functions $[u,U] \in \mathcal{V}$ is called a weak lower (upper) solution of problem (11) if $[u(0), U(0)] \leq (\geq)\,[u_0, U_0]$, and for all $[\varphi,\Psi] \in V$ with $[\varphi,\Psi] \geq 0$ a.e., it holds

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}t}\left([u,U],\,[\varphi,\Psi]\right)_H + (d\nabla u,\,\nabla\varphi)_\Omega + (D\nabla_y U,\,\nabla_y\Psi)_{\Omega\times Y_x} + (b(u-u^{\mathrm{e}}),\,\varphi)_\Gamma \\ &\quad + \big(k(Hu-\gamma U),\,|Y|^{-1}\varphi - \gamma\Psi\big)_{\Omega\times\Gamma_x} \leq (\geq)\ (g(\cdot,U),\,\Psi)_{\Omega\times Y_x} \qquad \text{for a.e. } t \in S. \end{aligned} \tag{16}$$

If $[u,U]$ is both a lower and an upper weak solution, then it is called a weak solution.

Remark. The system for u, U is *quasi-monotone increasing* in the sense of [20]. We modify the technique of weak upper and lower solutions and the comparison principle from [14, 9].

Proposition 13 (Comparison Principle)**.** Assume that g is globally Lipschitz in U. Let $[\underline{u},\underline{U}]$ and $[\overline{u},\overline{U}]$ be lower and upper weak solutions, resp., corresponding to different data satisfying $\underline{u}_0, \le \overline{u}_0$, $\underline{U}_0 \le \overline{U}_0$ and $\underline{u}^{\mathrm{e}} \le \overline{u}^{\mathrm{e}}$ a.e. Then

$$\underline{u}(t,x) \le \overline{u}(t,x),\ \underline{U}(t,x,y) \le \overline{U}(t,x,y) \qquad \text{for a.e. } t \in S,\ x \in \Omega,\ y \in Y_x.$$

Proof. Let $\beta = (H|Y|)^{-1}$ and denote $u = \underline{u} - \overline{u}$, $u_0 = \underline{u}_0 - \overline{u}_0$, etc. Subtracting both inequalities (16) for $[\underline{u},\underline{U}]$ and for $[\overline{u},\overline{U}]$ and testing with

$$[\varphi, \Psi](t) = [u^+(t), \beta U^+(t)], \qquad t \in S,$$

gives with standard arguments for $\tau \in (0,T]$

$$\begin{aligned}\frac{1}{2}\|[u^+(\tau), \beta U^+(\tau)]\|_H^2 &+ \int_0^\tau \big(d\nabla u,\, \nabla u^+\big)_\Omega + \int_0^\tau \big(D\nabla_y U,\, \beta\nabla_y U^+\big)_{\Omega\times Y_x} \\ &+ \int_0^\tau \big(bu,\, u^+\big)_\Gamma + \int_0^\tau \big(k(Hu - \gamma U),\, \beta(Hu^+ - \gamma U^+)\big)_{\Omega\times\Gamma_x} \\ &\le \frac{1}{2}\|[u_0^+, \beta U_0^+]\|_H^2 + \int_0^\tau \big(bu^{\mathrm{e}},\, u^+\big)_\Gamma + \int_0^\tau \big(g(\cdot,\underline{U}) - g(\cdot,\overline{U}),\, \beta U^+\big)_{\Omega\times Y_x}.\end{aligned}$$

Since the cut-off function $(\cdot)^+ : \mathbb{R} \to \mathbb{R}^{\ge 0}$ is monotone, it holds

$$\int_0^\tau \big(k(Hu - \gamma U),\, \beta(Hu^+ - \gamma U^+)\big)_{\Omega\times\Gamma_x} \ge 0.$$

Since g is globally Lipschitz in U, it follows that

$$\begin{aligned}\frac{1}{2}\|[u^+(\tau), \beta U^+(\tau)]\|_H^2 &+ c\int_0^\tau \|\nabla u^+\|_\Omega^2 + A\beta\int_0^\tau \|\nabla_y U^+\|_{\Omega\times Y_x}^2 \\ &\le \frac{1}{2}\|[u_0^+, \beta U_0^+]\|_H^2 + \frac{1}{2}\int_0^\tau \|\sqrt{b}(u^{\mathrm{e}})^+\|_\Gamma^2 + C\int_0^\tau \|U^+\|_{\Omega\times Y_x}^2.\end{aligned}$$

By Gronwall's inequality one obtains

$$\begin{aligned}\|[(\underline{u} - \overline{u})^+, (\underline{U} - \overline{U})^+]\|_{L_\infty(S;H)} &+ \|[(\underline{u} - \overline{u})^+, (\underline{U} - \overline{U})^+]\|_{L_2(S;V)} \\ &\le C\Big(\|(\underline{u}^{\mathrm{e}} - \overline{u}^{\mathrm{e}})^+\|_{L_2(S\times\Gamma)} + \|[(\underline{u}_0 - \overline{u}_0)^+, (\underline{U}_0 - \overline{U}_0)^+]\|_H\Big).\end{aligned}$$

Now the result follows immediately. □

By similar arguments, we obtain an energy estimate for the system.

Proposition 14 (Energy estimate)**.** There exists a constant $C > 0$ such that every weak solution $[u,U] \in \mathcal{V}$ satisfies

$$\|[u,U]\|_{L_\infty(S;H)} + \|[u,U]\|_{L_2(S;V)} \le \Big(C(1 + \|u^{\mathrm{e}}\|_{L_2(S\times\Gamma)} + \|[u_0,U_0]\|_H\Big) \tag{17}$$

and

$$\|[u',U']\|_{L_2(S;V')} \le C\Big(\|[u,U]\|_{L_2(S;V)} + \|u^{\mathrm{e}}\|_{L_2(S\times\Gamma)} + \|g(\cdot,U)\|_{L_2(S\times\Omega\times Y_x)}\Big). \tag{18}$$

Remark. Due to assumption (14), global Lipschitz continuity of g is *not* needed for the result. However, if either g is globally Lipschitz in U or if an a-priori L_∞-bound for U is known, then the *a-posteriori* estimate (18) for the time derivative can be turned into an *a-priori* estimate using (17).

4.3. Boundedness, existence and uniqueness. First, we are looking for candidates for upper and lower solutions.

Proposition 15 (**Positivity and boundedness**)**.** Let $\overline{U} \in C^1(S)$ be a solution of the ODE

$$\partial_t \overline{U} = \|M_2\|_\infty \eta_2(\overline{U}), \qquad t \in S,$$

satisfying $\overline{U}(0) \geq C_U$ where C_U and M_2 are given from (12) and (13). Then each solution $[u, U]$ satisfies

$$0 \leq u(t,x) \leq H^{-1}\overline{U}(t), \quad 0 \leq U(t,x,y) \leq \overline{U}(t) \qquad \text{for a.e. } t \in S,\ x \in \Omega,\ y \in Y_x.$$

Proof. Let $[u, U]$ be a solution. Since by definition $[u, U]$ is essentially bounded, we can replace η_1 w.l.o.g by a cut-off function. So g can be assumed *globally* Lipschitz in U. Hence, Prop. 13 can be applied. Now the nonnegativity result follows from the fact that by (14) $g(\cdot, 0) \geq 0$ and therefore $[0, 0]$ is a weak lower solution.

Denote $\overline{u} := H^{-1}\overline{U}$. Then one has to check that $[\overline{u}, \overline{U}]$ is a weak upper solution: By (12) we have

$$[\overline{u}(0), \overline{U}(0)] = [H^{-1}\overline{U}(0), \overline{U}(0)] \geq [u_0, U_0]$$

and also $b(\overline{u} - u^{\mathrm{e}}) \geq 0$ a.e. Finally, for nonnegative test functions $[\varphi, \Psi] \in V$, we have

$$\begin{aligned} \big([\overline{u}', \overline{U}'],\, [\varphi, \Psi]\big)_H &= \big(\theta \overline{u}',\, \varphi\big)_\Omega + \big(\overline{U}',\, \Psi\big)_{\Omega \times Y_x} \\ &\geq 0 + \big(\|M_2\|_\infty \eta_2(U),\, \Psi\big)_{\Omega \times Y_x} \\ &\geq \big(g(U),\, \Psi\big)_{\Omega \times Y_x}. \end{aligned}$$

This gives the inequality (16) for $[\overline{u}, \overline{U}]$. □

Remark. Note that the cutoff argument works only for the *negative* reaction term η_1. The crucial point is that, after cutting off the function η_1 for values above $M > 0$, say, we are able to prove L_∞-bounds for U that are *independent* of M. This is not possible for the positive part η_2.

Theorem 16 (Existence and uniqueness)**.** There exists a unique weak solution of problem (11).

Proof. We use Banach's fixed point theorem with the weighted-norm space

$$X = C(S; H), \qquad \|u\|_X = \max_{t \in S}\{e^{-\lambda t}\|u(t)\|_H\}, \qquad \lambda > 0.$$

For $[\tilde{u}, \tilde{U}] \in X$ given, we consider the linearised problem (16) for $[u, U]$, in which the right-hand side is replaced by $\Big(g(\cdot, \tilde{U}),\, \Psi\Big)_{\Omega \times Y_x}$. By Prop. 14, we can w.l.o.g. assume g to be globally Lipschitz. By a standard result on evolution equations (see, e.g., [23], Thm. 10.3), there exists a unique solution $[u, U] \in L_2(S; V) \cap H^1(S; V') \hookrightarrow X$.

Now we define a fixed point operator as

$$T : X \to X, \qquad T([\tilde{u}, \tilde{U}]) = [u, U],$$

and consider solutions $[u, U]$, $[v, V]$ corresponding to different data $[\tilde{u}, \tilde{U}]$ and $[\tilde{v}, \tilde{V}]$. By similar arguments as in Prop. 13, we obtain, for $\tau \in (0, T]$, the estimate

$$\begin{aligned}\|[u(\tau) - v(\tau), U(\tau) - V(\tau)]\|_H^2 &\le C \int_0^\tau \|[\tilde{u}(t) - \tilde{v}(t), \tilde{U}(t) - \tilde{V}(t)]\|_H^2 \, dt \\ &\le C \int_0^\tau e^{\lambda t} \, dt \max_{t \in [0,\tau]} \left\{ e^{-\lambda t} \|[\tilde{u}(t) - \tilde{v}(t), \tilde{U}(t) - \tilde{V}(t)]\|_H^2 \right\} \\ &\le C \frac{e^{\lambda \tau}}{\lambda} \|[\tilde{u} - \tilde{v}, \tilde{U} - \tilde{V}]\|_X^2.\end{aligned}$$

It follows that

$$\|[u - v, U - V]\|_X \le \sqrt{\frac{C}{\lambda}} \|[\tilde{u} - \tilde{v}, \tilde{U} - \tilde{V}]\|_X,$$

and, hence, for λ chosen small enough, $T : X \to X$ is strictly contractive. □

Remark.

(1) Note that the embedding $V \hookrightarrow H$ is *not compact.* For this reason, we have chosen a technique of proving existence that does not need any compactness arguments.

(2) Uniqueness can alternatively be obtained by the analogous estimate as in the proof of Prop. 13, applied to two solutions and omitting the cut-off functions. This procedure yields also continuous dependence of the solutions on the initial and boundary data.

Acknowledgments

The authors would like to express their gratitude to the state of Bremen for funding this work via the PhD program *Scientific Computing in Engineering (SCiE)* as well as to the German National Science Foundation (DFG) for a grant through the special priority program 1122 *Prediction of the Course of Physicochemical Damage Processes Involving Mineral Materials.*

References

[1] T. Arbogast. Analysis of the simulation of single phase flow through a naturally fractured reservoir. *SIAM J. Numer. Anal.*, 26(1):12–29, 1989.

[2] T. Arbogast, J. Douglas, Jr., and U. Hornung. Deriving the double porosity model of single phase flow via homogenization theory. *SIAM J. Math. Anal.*, 21:823–863, 1990.

[3] T. Arbogast, J. Douglas, Jr., and U. Hornung. Modeling of naturally fractured reservoirs by formal homogenization techniques. In R. Dautray, editor, *Frontiers in Pure and Applied Mathematics*, pages 1–19. Elsevier, 1991.

[4] A. Benedek and R. Panzone. The space L^p, with mixed norm. *Duke Math. J.*, 28:301–324, 1961.

[5] F. H. Clarke, Yu. S. Ledyaev, R. J. Stern, and P. R. Wolenski. *Nonsmooth Analysis and Control Theory.* Springer, 1998.

[6] R. Dautray and J.-L. Lions. *Spectral theory and applications*, volume 3 of *Mathematical analysis and numerical methods for science and technology.* Springer, 1992.

[7] J. Dixmier. *Von Neumann algebras.* North-Holland, 1981.

[8] N. Dunford and J. T. Schwartz. *Linear operators I.* Interscience Publishers, 1971.

[9] A. Friedman and P. Knabner. A transport model with micro- and macrostructure. *J. Differ. Equations*, 98(2):328–354, 1992.

[10] A. Friedman and A. T. Tzavaras. A quasilinear parabolic system arising in modeling of catalytic reactors. *J. Differ. Equations*, 70:167–196, 1987.

[11] U. Hornung, editor. *Homogenization and Porous Media.* Springer, 1997.

[12] U. Hornung and W. Jäger. Diffusion, convection, adsorption, and reactions of chemicals in porous media. *J. Differ. Equations*, 92:199–225, 1991.

[13] U. Hornung, W. Jäger, and A. Mikelić. Reactive transport through an array of cells with semi-permeable membranes. *RAIRO Modél. Math. Anal. Numér.*, 28(1):59–94, 1994.

[14] P. Knabner. *Mathematische Modelle für Transport und Sorption gelöster Stoffe in porösen Medien.* Verlag Peter Lang, 1991.
[15] A. Kufner, O. John, and S. Fuçík. *Function Spaces.* Academia, Publishing house of the Czecholovak Academy of Sciences, 1977.
[16] S. A. Meier. *Two-scale models of reactive transport and evolving microstructure.* PhD thesis, University of Bremen, 2008.
[17] S. A. Meier and M. Böhm. On a micro-macro system arising in diffusion–reaction problems in porous media. In M. Fila et al., editors, *Proceedings of the Equadiff 11 (Bratislava, 2005)*, pages 259–263, 2005.
[18] S. A. Meier, M. A. Peter, and M. Böhm. A two-scale modelling approach to reaction-diffusion processes in porous materials. *Comp. Mat. Sci.*, 39:29–34, 2007.
[19] M. Milla Miranda and J. Límaco Ferrel. The Navier-Stokes equation in noncylindrical domain. *Mat. Apl. Comput.*, 16(3):247–265, 1997.
[20] C. V. Pao. *Nonlinear Parabolic and Elliptic Equations.* Plenum Press, 1992.
[21] M. Peszyńska. *Flow through fissured media. Mathematical analysis and numerical approach.* PhD thesis, University of Augsburg, 1992.
[22] M. A. Peter. Homogenisation in domains with evolving microstructure. *C. R. Mécanique*, 335(7):357–362, 2007.
[23] M. Renardy and R. C. Rogers. *An introduction to partial differential equations.* Springer, 1996.
[24] A. V. Saetta, B. A. Schrefler, and R. V. Vitaliani. The carbonation of concrete and the mechanism of moisture, heat and carbon dioxide flow through porous materials. *Cem. Conc. Res.*, 23(4):761–772, 1993.
[25] R. E. Showalter and N. J. Walkington. Micro-structure models of diffusion in fissured media. *J. Math. Anal. Appl.*, 155:1–20, 1991.
[26] M. Takesaki. *Theory of operator algebras.* Springer, 2003.
[27] J. Wloka. *Partielle Differentialgleichungen.* Teubner, 1982.
[28] K. Yosida. *Functional analysis.* Springer, 1978.

Centre for Industrial Mathematics, University of Bremen, Postfach 330 440, 28334 Bremen, Germany

E-mail: sebam@math.uni-bremen.de and mbohm@math.uni-bremen.de

URL: http://www.math.uni-bremen.de/zetem/modpde/indexmod.html