Proceedings of Equadiff-11
2005, pp. 259–263

ON A MICRO-MACRO SYSTEM ARISING IN DIFFUSION-REACTION PROBLEMS IN POROUS MEDIA

SEBASTIAN A. MEIER* AND MICHAEL BÖHM†

Abstract. In this note we describe a model of a reaction-diffusion process in a heterogeneous medium. The model resolves processes on the macro-scale as well as on the micro-scale by imposing a continuous family of local cell problems at each point of the medium. We list the model equations and derive a variational formulation in terms of special Sobolev spaces, constructed as direct integrals of Hilbert spaces. This construction modifies the concept of *distributed-microstructure models* of single-phase flow in fissured media, presented by Showalter et al. [1, 2]. The basic results on existence and uniqueness of weak solutions are given, and their proofs are sketched.

Key words. reaction-diffusion, porous medium, coupled system, micro-macro, cell problem, distributed microstructure

AMS subject classifications. 35K50, 35K57, 80A20, 35K99

1. Introduction.

In this note we investigate a coupled micro-macro model of a reaction-diffusion process in a heterogeneous medium. We confine ourselves to a simply structured problem that can serve as a prototype for various applications. One possible scenario can be the following: Let Ω be a porous medium consisting of a solid matrix and a pore space that is partially saturated with water. We assume that a substance diffuses in the air phase in

*Centre for Industrial Mathematics, FB 3, University of Bremen, Postfach 330 440, 28334 Bremen, Germany, 49421-2189173 (sebam@math.uni-bremen.de). Partially supported by the PhD program *Scientific Computing in Engineering*.

†Centre for Industrial Mathematics, FB 3, University of Bremen, Postfach 330 440, 28334 Bremen, Germany, 49421-2189141 (mbohm@math.uni-bremen.de)

gaseous form, and diffuses and reacts in the liquid phase as a solute. On the phase boundary inside the pores, some exchange occurs. We consider the effective diffusivity in the gas phase to be much greater than the one in the liquid, which is a typical scenario for real-world applications such as chemical degradation processes of concrete. Therefore, the bulk transport is happening in the gaseous phase, and the diffusion-reaction process in the liquid phase is restricted to a local neighbourhood of a given "macroscopic point" $x \in \Omega$. The present model is directly adapted to this situation by proposing a coupled system of parabolic equations for the two concentrations: a macroscopic equation for the gaseous phase (u), and a family of microscopic equations (*cell problems*) for the liquid phase (U), one at each point x. By employing a Lipschitz transformation (assumption (G_2)), the microscopic geometry is allowed to vary in space.

Such *distributed-microstructure models* have been proposed and analysed by Showalter et al. [1, 2] in the context of single-phase flow in fissured media. Other applications include capacitance of micro-circuits [3] and heat flow in heterogeneous media [4, 5]. For a spatially constant micro-structure, such models can also arise as homogenisation limits of classical microscopic models [6].

2. The distributed-microstructure model. Let $\Omega \subset \mathbb{R}^n$ be a bounded Lipschitz domain. For each $x \in \Omega$, let $Y_x^l \subset \mathbb{R}^n$ also be a Lipschitz domain completely contained in a fixed, bounded domain $Y \subset \mathbb{R}^n$ as depicted in FIG. 2.1. The fixed domain Y is usually chosen as the unit cell, $Y = (0,1)^n$. Let the phase boundary ∂Y_x^l be divided into two measurable parts, $\partial Y_x^l = \Gamma_x^s \cup \Gamma_x^l$, such that $\overset{\circ}{\Gamma}{}_x^s \cap \overset{\circ}{\Gamma}{}_x^l = \emptyset$, and Γ_x^l has positive measure. In typical applications, Γ_x^l and Γ_x^s are phase boundaries of the liquid phase with a gaseous and a solid phase, respectively.

We consider a system of PDEs for the two concentrations $u : \overline{\Omega \times S} \to \mathbb{R}$ and $U : \overline{\Omega \times Y_x^l \times S} \to \mathbb{R}$. We refer to $x \in \Omega$ as the *macroscopic* spatial variable and to y as the *microscopic* spatial variable. The gradient with respect to x is denoted by ∇ and that with respect to y by ∇_y; the same applies for the divergences, div and div_y.

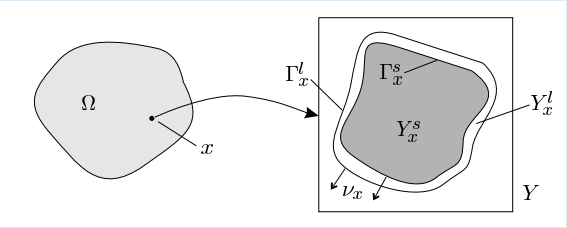

FIG. 2.1. *Typical model geometry, including three phases at the micro-scale.*

The macroscopic system is given by

$$\theta(x)\partial_t u(x,t) - \operatorname{div}(a(x)\nabla u) = -\frac{1}{|Y|}\int_{\Gamma_x^l} k(\beta u - U)\,\mathrm{d}s, \qquad x \in \Omega,\ t > 0, \tag{2.1a}$$

$$a(s)\nabla u(s,t)\cdot\nu = b((u^{\mathrm{e}}(t) - u), \qquad s \in \partial\Omega,\ t > 0, \tag{2.1b}$$

$$u(x,0) = u_0(x), \qquad x \in \Omega, \tag{2.1c}$$

and the cell problem in each point $x \in \Omega$ is

$$\partial_t U(x,y,t) - \operatorname{div}_y(A\nabla_y U) = f(U), \qquad y \in Y_x^l,\ t > 0, \tag{2.1d}$$

$$A\nabla_y U(x,s,t)\cdot\nu_x = k(\beta u - U), \qquad s \in \Gamma_x^l,\ t > 0, \tag{2.1e}$$

$$A\nabla_y U(x,s,t)\cdot\nu_x = 0, \qquad s \in \Gamma_x^s,\ t > 0, \tag{2.1f}$$

$$U(x,y,0) = U_0(x,y), \qquad y \in Y_x^l. \tag{2.1g}$$

For a fixed U, eq. (2.1a)–(2.1c) constitute a linear diffusion-adsorption problem for the concentration u; while, for a fixed u, a nonlinear diffusion-reaction problem for U is given at each $x \in \Omega$ by eq. (2.1d)–(2.1g). The coupling of both systems is given by the linear volume term in (2.1a) and by the linear boundary condition (2.1e).

3. Variational formulation. We present the main results of the mathematical analysis of the model (2.1) using variational methods. To our knowledge, mathematical analyses of diffusion-reaction systems with a similar micro-macro coupling have been performed only for cell geometries *independent* of x [7, 8, 9]. We focus our attention on the allowance of a heterogeneous (i.e. x-dependent) microstructure that can be of low regularity. The key feature of our model formulation is that the x-dependence of the microscopic domains Y_x^l is incorporated into the function spaces. This treatment is based on appropriate modifications of the ideas in [1, 2], where a comparable system (without reactions terms) is investigated. The advantage of this formulation is that, initially, there is no need to transform the cell problems on Y_x^l to a fixed domain. Nevertheless, the existence of such a transformation is currently postulated for proving the existence of a solution; see assumption (G_2) below.

Let $S = (0, T)$ be a bounded time interval. By $\Omega \times Y_x^l$, we denote the product domain $\bigcup_{x\in\Omega}(\{x\} \times Y_x^l) \subset \mathbb{R}^{n+n}$. We make the following assumptions:

(G_1) There exists a (globally) Lipschitz continuous function $f : \Omega \times Y \to \mathbb{R}$ such that the $(2n-1)$-dimensional boundary $\Omega \times \Gamma_x^l$ of $\Omega \times Y_x^l$ is given by

$$f(x, y) = 0 \quad \Longleftrightarrow \quad (x, y) \in \Omega \times \Gamma_x^l.$$

Moreover, the Clarke gradient $\partial_y f(x, y)$ is *regular*[1] for all $(x, y) \in \Omega \times Y$, and the measures $|Y_x^l|$ are uniformly bounded away from zero.

(R) The reaction rate is given by $f = -f_1 + f_2$, where $f_1, f_2 \geq 0$ are locally Lipschitz and $f_1(U) = 0$ if $U \leq 0$ and $f_2(U) \leq R_1 U + R_2$ if $U \geq 0$,

(D_1) k, β, b, A are positive constants, and $\theta, a \in L^\infty(\Omega)$ are uniformly bounded away from zero.

(D_2) $u_0 \in L^\infty(\Omega)$, $U_0 \in L^\infty(\Omega \times Y_x^l)$, and $u^e \in L^\infty(S)$ are non-negative functions.

Assumption (D_1) yields the non-degeneracy of the problem, while (D_2) and (R) guarantee that its solutions are global, bounded, and non-negative.

[1] See, e.g., [10], pp. 133ff.

Assumption (G_1) is employed in the construction of the *distributed trace spaces*. For this purpose, let us identify the space $L^2(\Omega; L^2(Y_x^l))$ with the usual Hilbert space $L^2(\Omega \times Y_x^l)$. Note that (G_1) implies that the measures $|\Gamma_x^l|$ and $|Y_x^l|$ are uniformly bounded w.r.t. $x \in \Omega$. Therefore the following *direct integrals of Hilbert spaces*

$$L^2(\Omega; H^1(Y_x^l)) := \left\{U \in L^2(\Omega; L^2(Y_x^l)) : \ \nabla_y U \in L^2(\Omega; L^2(Y_x^l))\right\}$$

and

$$L^2(\Omega; L^2(\Gamma_x^l)) := \left\{U : \Omega \times \Gamma_x^l \to \mathbb{R} \text{ measurable such that } \int_\Omega \|U(x)\|^2_{L^2(\Gamma_x^l)} \,\mathrm{d}x < \infty\right\}$$

are well-defined, separable Hilbert spaces. We refer to [11] for further details on the construction of these spaces. If the usual trace map on the cell boundary is denoted by $\gamma_x : H^1(Y_x^l) \to L^2(\Gamma_x^l)$, the *distributed trace*,

$$(\gamma U)(x,s) := (\gamma_x U(x))(s), \qquad x \in \Omega, \ s \in \Gamma_x^l, \ U \in L^2(\Omega; H^1(Y_x^l)),$$

is a bounded linear operator $\gamma : L^2(\Omega; H^1(Y_x^l)) \to L^2(\Omega; L^2(\Gamma_x^l))$.

Define $L^2_\theta(\Omega)$ as the usual Lebesgue space, equipped with the (equivalent) scalar product $(u|v)_{L^2_\theta(\Omega)} := \int_\Omega \theta uv \,\mathrm{d}x$. Define the Hilbert spaces

$$V := H^1(\Omega) \times L^2(\Omega; H^1(Y_x^l)), \qquad H := L^2_\theta(\Omega) \times L^2(\Omega; L^2(Y_x^l)).$$

It can easily be seen that the spaces V and H form a Gelfand triple $V \hookrightarrow H \hookrightarrow V'$. Note that the embeddings are *not* compact.

The weak formulation of problem (2.1), denoted by (P), can now be written as follows:

Find $[u, U] \in L^2(S; V) \cap H^1(S, V')$ *such that* $[u, U](0) = [u_0, U_0]$, *and it holds*

$$\frac{\mathrm{d}}{\mathrm{d}t}([u,U]|[\phi,\Phi])_H + \int_\Omega a\nabla u \nabla\phi \,\mathrm{d}x + \int_\Omega \int_{Y_x^l} A\, \nabla_y U \nabla_y \Phi \,\mathrm{d}y \,\mathrm{d}x$$
$$+ \int_\Omega \int_{\Gamma_x^l} k(\beta u - U)(|Y|^{-1}\phi - \Phi) \,\mathrm{d}s \,\mathrm{d}x + \int_{\partial\Omega} b(u - u^{\mathrm{e}})\phi \,\mathrm{d}s = \int_\Omega \int_{Y_x^l} f(U)\Phi \,\mathrm{d}y \,\mathrm{d}x \quad (3.1)$$

for all $[\phi, \Phi] \in V$.

4. Wellposedness of the problem. First we prove that solutions of (P) are a-priori positive and bounded.

PROPOSITION 4.1. *Every solution* $[u, U]$ *of* (P) *satisfies*

$$0 \le \beta u(x,t), U(x,y,t) \le K(t) \quad \text{a.e. } x \in \Omega,\ y \in Y_x^l,\ \forall t \in S,$$

where

$$K(t) = \begin{cases} \sup\{\beta u_0, \beta u^{\mathrm{e}}, U_0\} + R_2 t, & \text{if } R_1 = 0, \\ \mathrm{e}^{R_1 t}(\sup\{\beta u_0, \beta u^{\mathrm{e}}, U_0\} + \frac{R_2}{R_1}(1 - e^{-R_1 t})), & \text{otherwise} \end{cases}$$

The proof of PROPOSITION 4.1 is obtained by choosing appropriate cut-off functions as test functions in (3.1). In the subsequent analysis, PROPOSITION 4.1 is used extensively in order to handle the nonlinear reaction term $f(U)$. In most of the proofs, f can be replaced w.l.o.g. by a globally bounded and Lipschitz continuous function.

Applying a-priori estimates of the usual energy-type to (3.1), we obtain the following result.

PROPOSITION 4.2 (Uniqueness). *Let* $[u, U]$ *and* $[v, V]$ *be solutions corresponding to initial values* $[u_0, U_0], [v_0, V_0] \in H$ *and external data* $u^{\mathrm{e}}, v^{\mathrm{e}} \in \mathrm{L}^2(S)$, *respectively. Then there exists a constant* $C > 0$ *depending on* T *and on the data such that*

$$\|[u - v, U - V]\|^2_{\mathrm{L}^2(S;V)} + \|[(u - v)', (U - V)']\|_{\mathrm{L}^2(S;V')} \le C(\|u^{\mathrm{e}} - v^{\mathrm{e}}\|^2_{\mathrm{L}^2(S)} + \|[u_0 - v_0, U_0 - V_0]\|^2_H). \quad (4.1)$$

In particular, solutions of (P) *are unique and depend continuously on the initial and exterior data.*

To show the *existence of a weak solution*, we apply a standard fixed-point argument based on Schauder's theorem, similar to [8]. For demonstrating the continuity of the operators involved, the cell problems on Y_x^l need to be transformed to a fixed reference domain Z by a Lipschitz map, uniformly in x. The existence of such a transformation is postulated as an additional assumption on the geometry:

(G_2) There exist bounded Lipschitz domains Z^l, Z with $\bar{Z}^l \subset\subset Z \subset \mathbb{R}^n$ and a mapping $\psi \in C(\bar{\Omega}, C^{0,1}(\bar{Z}, \bar{Y}))$ such that $\psi_x(Z^l) = Y_x^l$ for each $x \in \Omega$.
Moreover, for each $x \in \Omega$, the mapping $\psi_x := \psi(x, \cdot) : Z \to Y$ is bijective, the transformation determinant $\det \nabla_y \psi(x, y)$ (in the Clarke sense) is uniformly bounded from above and below, and the inverse mapping $x \mapsto \psi_x^{-1}(x, \cdot)$ is in $C(\bar{\Omega}, C^{0,1}(\bar{Y}, \bar{Z}))$.

In the following, the application of the transformation ψ_x in the existence proof is sketched. For details see [11]. First we prove that for fixed $x \in \Omega$, $\bar{u}(x, \cdot)$, each cell problem (2.1d)–(2.1g) has a unique solution $U(x, \cdot, \cdot)$. By transforming the weak formulations of the cell problems to the fixed domain Z^l, it can be shown that U depends continuously on x and $\bar{u}$. Vice versa, for a fixed family of cell solutions $\bar{U}$, there exists a solution u of the macroscopic system (2.1a)–(2.1c). This yields a continuous fixed point operator $F : \bar{u} \mapsto U =: \bar{U} \mapsto u$. By the Lions-Aubin lemma, F is compact in the corresponding Bochner spaces. Hence, the classical Schauder's fixed point theorem gives a solution $[u, U]$ of problem (P).

THEOREM 4.3 (Existence of a weak solution). *Assume that* (G_2) *holds. Then there exists a unique weak solution* $[u, U] \in L^2(S; V) \cap H^1(S; V')$ *of* (P).

We conclude with the remark that actually more regularity can be shown for the solutions. For details, we again refer to [11].

REFERENCES

[1] R. E. Showalter and N. J. Walkington, *Micro-structure models of diffusion in fissured media*, Journal of Mathematical Analysis and Applications, **155** (1991), 1–20.
[2] R. E. Showalter and N. J. Walkington, *Diffusion of fluid in a fissured medium with microstructure*, SIAM Journal of Mathematical Analysis, **22**(6) (1991), 1702–1722.

[3] B. L. Hollingsworth and R. E. Showalter, *Semilinear degenerate parabolic systems and distributed capitance models*, Discrete and Continuous Dynamical Systems, **1**(1) (1995), 59–76.
[4] R. E. Showalter and D. B. Visarraga, *Absorption-delay models of heat transport*, Mathematical Models and Methods in Applied Sciences, **13**(5) (2002), 645–660.
[5] R. E. Showalter and D. B. Visarraga, *Double diffusion models from a highly-heterogeneous medium*, Journal of Mathematical Analysis and Applications, **295** (2004), 191–210.
[6] G. W. Clark and R. E. Showalter, *Two-scale convergence of a model for flow in a partially fissured medium*, Electronic Journal of Differential Equations, **2** (1999), 1–20.
[7] A. Friedman and P. Knabner, *A Transport Model with Micro- and Macro-structure*, Journal of Differential Equations, **98** (1992), 328–354.
[8] A. Friedman and A. T. Tzavaras, *A quasilinear parabolic system arising in modeling of catalytic reactors*, Journal of Differential Equations, **70** (1987), 167–196.
[9] W. Desch and J. Prüss, *Dynamical behaviour of a two-phase chemically reacting system including mass transfer*, Differential and Integral Equations, **7** (1994), 767–793.
[10] F. H. Clarke, Yu. S. Ledyaev, R. J. Stern, and P. R. Wolenski, *Nonsmooth Analysis and Control Theory*, Springer, 1998.
[11] S. A. Meier, *Two-scale models of reactive transport in porous media involving microstructural changes*, Ph.D. thesis, University of Bremen, 2007, in preparation.