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by

T.L. van Noorden, A. Muntean



Centre for Analysis, Scientific computing and Applications
Department of Mathematics and Computer Science
Eindhoven University of Technology
P.O. Box 513
5600 MB Eindhoven, The Netherlands
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Homogenization of a locally-periodic medium with areas of low and high diffusivity

T. L. VAN NOORDEN¹ and A. MUNTEAN^{1,2}

¹ *Department of Mathematics and Computer Science, Technische Universiteit Eindhoven, P.O. Box 513, 5600 MB Eindhoven, The Netherlands*

² *Institute of Complex Molecular Systems (ICMS), Technische Universiteit Eindhoven, P.O. Box 513, 5600 MB Eindhoven, The Netherlands*

We aim at understanding transport in porous materials including regions with both high and low diffusivities. For such scenarios, the transport becomes structured (here: *micro-macro*). The geometry we have in mind includes regions of low diffusivity arranged in a locally-periodic fashion. We choose a prototypical advection-diffusion system (of minimal size), discuss its formal homogenization (the heterogeneous medium being now assumed to be made of zones with circular areas of low diffusivity of x -varying sizes), and prove the weak solvability of the limit two-scale reaction-diffusion model. A special feature of our analysis is that most of the basic estimates (positivity, L^∞ -bounds, uniqueness, energy inequality) are obtained in x -dependent Bochner spaces.

Keywords: Heterogeneous porous materials, homogenization, micro-macro transport, two-scale model, reaction-diffusion system, weak solvability

1 Introduction

We consider transport in heterogeneous media presenting regions with high and low diffusivities. Examples of such media are concrete and scavenger packaging materials. For the scenario we have in mind, the old classical idea to replace the heterogeneous medium by a homogeneous equivalent representation (see [1, 2, 5, 22] and references therein) that gives the average behaviour of the medium submitted to a macroscopic boundary condition is not working anymore. Specifically, now the transport becomes structured (here: *micro-macro*¹) [3, 14].

The geometry we have in mind includes space-dependent perforations² arranged in a locally-periodic fashion. We refer the reader to section 2 (in particular to Fig. 1), where we explain our concept of local periodicity. Our approach is based on the one developed in [24, 25] and is conceptually related to, e.g., [6, 11]. When periodicity is lacking, the typical strategy would be to tackle the matter from the percolation theory perspective

¹ “Micro” refers here to a continuum description of a porous subdomain at a separated (lower) spatial scale compared to the “macro” one.

² By “space-dependent perforations”, we mean that at each spatial position x , our model will allow us to zoom in a x -dependent pore space, or subject to a more general interpretation, a x -dependent porous subdomain, called here perforation.

(see e.g. chapter 2 in [12] and references cited therein³) or to reformulate the oscillating problem in terms of stochastic homogenization (see e.g. [4]). In this paper, we stay within a deterministic framework by deviating in a controlled manner (made precise in section 2) from the purely periodic homogenization.

We show our working methodology for a prototypical diffusion system of minimal size. To keep presentation simple, our scenario does not include chemistry. With minimal effort, both our asymptotic technique and analysis can be extended to account for volume and surface reaction production terms and other linear micro-macro transmission conditions. We only emphasize the fact that if chemical reactions take place, then most likely that they will be hosted by the micro-structures of the low-diffusivity regions. We discuss the microscale model for the particular case in which the heterogenous medium is only composed of zones with circular areas of low diffusivity of x -varying sizes. This assumption on the geometry should not be seen as a restriction. We only use it for ease of presentations and it does not play a role in our formal and analytical results. Our asymptotic strategy is based on a suitable expansion (remotely resembling the boundary unfolding operator [7]) of the boundary of the perforations in terms of level-set functions. In particular, we can treat in a quite similar way situations when free-interfaces travel the microstructure; we refer the reader to [24] for a dissolution precipitation free-boundary problem and [20] for a fast-reaction slow-diffusion scenario where we addressed the matter.

The results of our paper are twofold:

- (i) We develop a strategy to deal (formally) with the asymptotics $\epsilon \rightarrow 0$ for a locally periodic medium (where $\epsilon > 0$ is the microstructure width) and derive a macroscopic equation and x -dependent effective transport coefficients (porosity, permeability, tortuosity) for the species undergoing fast transport (i.e. that one living in high diffusivity areas), while we preserve the precise geometry of the microstructure and corresponding balance equation. The result of this homogenization procedure is a distributed-microstructure model in the terminology of R. E. Showalter, which we refer here as *two-scale model*.
- (ii) We analyze the solvability of the resulting two-scale model. Solutions of the two-scale model are elements of x -dependent Bochner spaces. Our approach benefits from previous work on two-scale models by, e.g., Showalter and Walkington [23], Eck [9], and Meier and Böhm [17, 18]. A special feature of our analysis is that most of the basic estimates (positivity, L^∞ -bounds, uniqueness, energy inequality) are obtained in the x -dependent Bochner spaces. Our existence proof is constructed using a Schauder fixed-point argument and is an alternative to [23], where the situation is formulated as a Cauchy problem in Hilbert spaces and then resolved by holomorphic semigroups, or to [17], where a Banach-fixed point argument for the problem stated in transformed domains (i.e. x -independent) is employed.

Note that (i) and (ii) are preliminary results preparing the framework for rigorously

³ Fig. 2.3 (a) from [12], p. 39 illustrates a computer simulation of the consolidation of spherical grains showing regions with high and low porosities corresponding to high and low diffusivity areas.

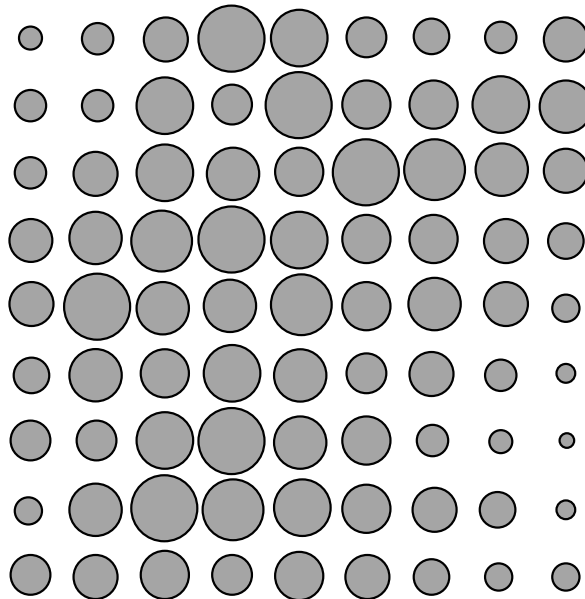


FIGURE 1. Schematic representation of a locally-periodic heterogeneous medium. The centers of the gray circles are on a grid with width ϵ . These circles represent the areas of low diffusivity and their radii may vary.

proving a convergence rate for the asymptotics $\epsilon \rightarrow 0$; we will address this convergence issue elsewhere.

The paper is organized in the following fashion: Section 2 contains the description of the model equations at the micro scale together with the precise geometry of our x -dependent microstructure for the particular case of circular perforations. The homogenization procedure is detailed in section 3. The main result of this part of the paper is the two-scale model equations as well as a couple of effective coefficients reported in section 4. The second part of the paper focusses on the analysis of the two-scale model; see section 5. The main result, i.e. Theorem 5.11, ensures the global-in-time existence of weak solutions to our two-scale model and appears at the end of section 5.3. A brief discussion section concludes the paper.

2 Model equations

We consider a heterogeneous medium consisting of areas of high and low diffusivity. The medium is in the present paper represented by a two dimensional domain. We denote the two dimensional bounded domain by $\Omega \subset \mathbb{R}^2$, with boundary Γ , and for ease of presentation we suppose in this section that the areas of the medium with low diffusivity are circles. We do not use this restriction in later sections; there the areas with low diffusivity can have different shapes, as long as neighboring areas do not touch each other.

Let the centers of the circles B_{ij} with low diffusivity, with radius $R_{ij} < \epsilon/2$, be located in a equidistant grid with nodes at $(\epsilon i, \epsilon j)$, where ϵ is a small dimensionless length scale.

We assume that there is given a function $r(x) : \Omega \rightarrow [0, 1/2)$ such that the radii R_{ij} of the circles B_{ij} are given by $R_{ij} = \epsilon r(x_{ij})$, where $x_{ij} = (\epsilon i, \epsilon j)$. We define the area of low diffusivity Ω_l^ϵ , which is the collection of the circles of low diffusivity, as $\Omega_l^\epsilon := \cup B_{ij}$ and we define the area of high diffusivity Ω_h^ϵ , which is the complement of Ω_l^ϵ in Ω , as $\Omega_h^\epsilon := \Omega \setminus \Omega_l^\epsilon$. The boundary between high and low diffusivity areas is denoted by Γ^ϵ , which is given by $\Gamma^\epsilon := \partial\Omega_l^\epsilon$. It is important to note that we assume that the circles of low diffusivity do not touch each other, so that $\Gamma_{ij} \cap \Gamma_{kl} = \emptyset$ if $i \neq k$ or $j \neq l$, where $\Gamma_{ij} := \partial B_{ij}$, and we also assume that the area of low permeability does not intersect the outer boundary of the domain Ω , so that $\Gamma \cap \Gamma_{ij} = \emptyset$ for all i, j .

We denote the tracer concentration in the high diffusivity area by u^ϵ , the concentration in the low diffusivity area by v^ϵ , the velocity of the fluid phase by q^ϵ and the pressure by p^ϵ . All these unknowns are dimensionless. In the high diffusivity area we assume for the fluid flow a Darcy-like law and incompressibility, while we neglect fluid flow in the low diffusivity area. The diffusion coefficient in the low diffusivity area is assumed to be of the order of $O(\epsilon^2)$, while all the remaining coefficients are of the order of $O(1)$ in ϵ . We assume continuity of concentration and of fluxes across the boundary between the high and low diffusivity areas.

The model is now given by

$$\begin{cases} u_t^\epsilon = \nabla \cdot (D_h \nabla u^\epsilon - q^\epsilon u^\epsilon) \\ q^\epsilon = -\kappa \nabla p^\epsilon \\ \nabla \cdot q^\epsilon = 0 \end{cases} \quad \text{in } \Omega_h^\epsilon, \quad (2.1)$$

$$\begin{cases} v_t^\epsilon = \epsilon^2 \nabla \cdot (D_l \nabla v^\epsilon) \end{cases} \quad \text{in } \Omega_l^\epsilon, \quad (2.2)$$

$$\begin{cases} \nu^\epsilon \cdot (D_h \nabla u^\epsilon) = \epsilon^2 \nu^\epsilon \cdot (D_l \nabla v^\epsilon) \\ u^\epsilon = v^\epsilon \\ q^\epsilon = 0 \end{cases} \quad \text{on } \Gamma^\epsilon, \quad (2.3)$$

$$\begin{cases} u^\epsilon(x, t) = u_b(x, t) \\ q^\epsilon(x, t) = q_b(x, t) \end{cases} \quad \text{on } \Gamma, \quad (2.4)$$

$$\begin{cases} u^\epsilon(x, 0) = u_I^\epsilon(x) & \text{in } \Omega_h^\epsilon, \\ v^\epsilon(x, 0) = v_I^\epsilon(x) & \text{in } \Omega_l^\epsilon, \end{cases} \quad (2.5)$$

where D_h denotes the diffusion coefficient in the high diffusivity region, D_l the diffusion coefficient in the low diffusivity regions, κ denotes the permeability in the Darcy law for the flow in the high diffusivity region, ν^ϵ denotes the unit normal to the boundary $\Gamma^\epsilon(t)$, where q_b and u_b denote the Dirichlet boundary data for the concentration u^ϵ and Darcy velocity q^ϵ and where u_I^ϵ and v_I^ϵ denote initial value data for the concentration u^ϵ and v^ϵ .

3 Formal homogenization

In addition to the macroscopic variable x , we introduce a periodic unit cube U with microscopic variable y :

$$y = (y_1, y_2), \text{ and } U := \{y \in \mathbb{R}^2 \mid -1/2 \leq y_i \leq 1/2 \text{ for } i = 1, 2\}. \quad (3.1)$$

For the formal homogenization we assume the following formal asymptotic expansions for u^ϵ , v^ϵ , q^ϵ and p^ϵ :

$$\begin{aligned} u^\epsilon(x, t) &= u_0(x, x/\epsilon, t) + \epsilon u_1(x, x/\epsilon, t) + \epsilon^2 u_2(x, x/\epsilon, t) + \dots \\ v^\epsilon(x, t) &= v_0(x, x/\epsilon, t) + \epsilon v_1(x, x/\epsilon, t) + \epsilon^2 v_2(x, x/\epsilon, t) + \dots \\ q^\epsilon(x, t) &= q_0(x, x/\epsilon, t) + \epsilon q_1(x, x/\epsilon, t) + \epsilon^2 q_2(x, x/\epsilon, t) + \dots \\ p^\epsilon(x, t) &= p_0(x, x/\epsilon, t) + \epsilon p_1(x, x/\epsilon, t) + \epsilon^2 p_2(x, x/\epsilon, t) + \dots \end{aligned}$$

where $u_k(\cdot, y, \cdot)$, $v_k(\cdot, y, \cdot)$, $q_k(\cdot, y, \cdot)$ and $p_k(\cdot, y, \cdot)$ are 1-periodic in $y = \frac{x}{\epsilon}$. The gradient of a function $f(x, \frac{x}{\epsilon})$, depending on x and $y = \frac{x}{\epsilon}$ is given by

$$\nabla f = \nabla_x f + \frac{1}{\epsilon} \nabla_y f|_{y=\frac{x}{\epsilon}}, \quad (3.2)$$

where ∇_x and ∇_y denote the gradients with respect to the first and second variables of f .

3.1 Level set formulation of the perforations boundary

Since the location of the interfaces between the low and the high diffusivity regions also depends on ϵ , we need an ϵ -dependent parametrization of these interfaces. A convenient way to parameterize the interfaces is to use a level set function, which we denote by $S^\epsilon(x)$:

$$x \in \Gamma^\epsilon \Leftrightarrow S^\epsilon(x) = 0.$$

Since we allow the size and shape of the perforations to vary with the macroscopic variable x , we might use the following characterization of S^ϵ :

$$S^\epsilon(x) = S(x, x/\epsilon) \quad (3.3)$$

where $S : \Omega \times U \rightarrow \mathbb{R}$ is 1-periodic in its second variable, and is independent of ϵ . In this section we show, using the example of a grid of circles with varying sizes, that this characterization of S^ϵ is not sufficient to characterize all locally-periodic sequences of perforation geometries. In fact, we need to expand S^ϵ as

$$S^\epsilon(x) = S_0(x, x/\epsilon) + \epsilon S_1(x, x/\epsilon) + \epsilon^2 S_2(x, x/\epsilon) + \dots \quad (3.4)$$

where the $S_i : \Omega \times U \rightarrow \mathbb{R}$ are 1-periodic in their second variable, for $i = 0, 1, 2, \dots$ and are independent of ϵ .

In order to find an explicit expression for $S^\epsilon(x)$ in this particular case, i.e. the case of circular domains with radius $r(x)$ (see Fig. 1), we define $P(x)$ to be the periodic extension of the function $x \rightarrow |x|$ and $Q(x)$ to be the periodic extension of the function $x \rightarrow x$,

both defined on the square $[-\frac{1}{2}, \frac{1}{2}] \times [-\frac{1}{2}, \frac{1}{2}]$, given by

$$\begin{aligned} P(x) &= P(x_1, x_2) = \sqrt{[x_1 + 1/2]^2 + [x_2 + 1/2]^2}, \\ Q(x) &= Q(x_1, x_2) = ([x_1 + 1/2], [x_2 + 1/2]), \end{aligned}$$

where $\lfloor a \rfloor := \max\{n \in \mathbb{Z} \mid n \leq a\}$ denotes the floor of a (rounding down). We can write $S^\epsilon(x)$ as follows:

$$S^\epsilon(x) = r(x - \epsilon Q(x/\epsilon)) - P(x/\epsilon). \quad (3.5)$$

Interestingly, the expression (3.5) plays the same role as the boundary unfolding operator (cf., for instance, [7] Definition 5.1). Note that S^ϵ is not a continuous function, it jumps when x_1 or x_2 cross a multiple of ϵ . Whenever we assume that $r(x, t) < 1/2$, this is not a problem, since in this case S^ϵ is continuous and smooth in a neighborhood of its zero level set, which is what we are interested in.

To check that the zero level set of S^ϵ consists indeed of circles around x_{ij} with radius $\epsilon r(x_{ij})$, we consider a curve, which without loss of generality can be parametrized in the square with sides ϵ around x_{ij} by $x_{ij} + \gamma(s)$. For this curve to be a zero level set, it should hold that

$$r(x_{ij} + \gamma(s) - \epsilon Q(\epsilon^{-1}(x_{ij} + \gamma(s)))) = P(\epsilon^{-1}(x_{ij} + \gamma(s))).$$

Using that $x_{ij} = (\epsilon i, \epsilon j)$, with $\epsilon i, \epsilon j \in \epsilon \mathbb{Z} \cap \Omega$, we obtain

$$r((\epsilon i, \epsilon j) + \gamma(s) - \epsilon Q((i, j) + \epsilon^{-1}\gamma(s))) = P((i, j) + \gamma(s)),$$

and using the periodicity of P and Q we get

$$r(x_{ij}) = |\gamma(s)|,$$

which means that $\gamma(s)$ should be a circle with radius $r(x_{ij})$.

Now we can write the level set function S^ϵ formally as the expansion

$$S^\epsilon(x) = S_0(x, x/\epsilon) + \epsilon S_1(x, x/\epsilon) + \epsilon^2 S_2(x, x/\epsilon) + O(\epsilon^3),$$

where $S_k(\cdot, y, \cdot)$, for $k = 0, 1, 2, \dots$, are 1-periodic in $y = \frac{x}{\epsilon}$, and are independent of ϵ . In order to find the terms in this expansion, we assume that r is sufficiently smooth and so that we can use the Taylor series of r around x :

$$r(x - \epsilon Q(x/\epsilon)) = r(x) - \epsilon Q(x/\epsilon) \cdot \nabla r(x) + \frac{\epsilon^2}{2} Q(x/\epsilon) \cdot \mathcal{D}^2 r(x) Q(x/\epsilon) + O(\epsilon^3),$$

where $\mathcal{D}^2 r$ denotes the Hessian of r w.r.t. x . This suggests the following definition of the terms in the expansion of S^ϵ :

$$\begin{aligned} S_0(x, x/\epsilon) &:= r(x) - P(x/\epsilon), \\ S_1(x, x/\epsilon) &:= -Q(x/\epsilon) \cdot \nabla r(x), \\ S_2(x, x/\epsilon) &:= \frac{1}{2} Q(x/\epsilon) \cdot \mathcal{D}^2 r(x) Q(x/\epsilon), \\ &\vdots \end{aligned}$$

3.2 Interface conditions

In (2.3₁) we have used the superscript ϵ for the normal vector ν^ϵ in the interface conditions for v^ϵ and u^ϵ . The reason is that the normal vector depends on the geometry of the different regions, and this in turn depends on ϵ . In order to perform the steps of formal homogenization, we have to expand ν^ϵ in a power series in ϵ . This can be done in terms of the level set function S^ϵ :

$$\nu^\epsilon = \frac{\nabla S^\epsilon(x, x/\epsilon)}{|\nabla S^\epsilon(x, x/\epsilon)|} \text{ at } x \in \Gamma^\epsilon. \quad (3.6)$$

First we expand $|\nabla S^\epsilon|$. Using the chain rule (3.2) (see also [12]), the expansion of S^ϵ and the Taylor series of the square-root function, we obtain

$$|\nabla S^\epsilon| = \frac{1}{\epsilon} |\nabla_y S_0| + O(\epsilon^0). \quad (3.7)$$

In the same fashion, we get

$$\nu^\epsilon = \nu_0 + \epsilon \nu_1 + O(\epsilon^2),$$

where

$$\nu_0 := \frac{\nabla_y S_0}{|\nabla_y S_0|}$$

and

$$\nu_1 := \frac{\nabla_x S_0 + \nabla_y S_1}{|\nabla_y S_0|} - \frac{(\nabla_x S_0 \cdot \nabla_y S_0 + \nabla_y S_0 \cdot \nabla_y S_1)}{|\nabla_y S_0|^2} \frac{\nabla_y S_0}{|\nabla_y S_0|}.$$

If we introduce the normalized tangential vector τ_0 , with $\tau_0 \perp \nu_0$, we can rewrite ν_1 as

$$\nu_1 = \tau_0 \frac{\tau_0 \cdot (\nabla_x S_0 + \nabla_y S_1)}{|\nabla_y S_0|}. \quad (3.8)$$

Now we focus on the interface conditions posed at Γ^ϵ . In order to obtain interface conditions in the auxiliary problems, we substitute the expansions of u^ϵ , q^ϵ , and ν^ϵ into (2.3). This is not so straight-forward as it may seem, since the interface conditions (2.3) are enforced at the oscillating interface Γ^ϵ , i.e. at every x where $S^\epsilon(x) = 0$. For formulating the upscaled model it would be convenient to have boundary conditions enforced at

$$\Gamma_0(x) := \{y \mid S_0(x, y) = 0\}. \quad (3.9)$$

To obtain them, we suppose that we can parametrize the part of the boundary Γ_{ij}^ϵ that surrounds the sphere B_{ij} with $k^\epsilon(s)$, so that holds

$$S^\epsilon(k^\epsilon(s)) = 0,$$

and we assume that we can expand $k^\epsilon(s)$ using the formal asymptotic expansion

$$k^\epsilon(s) = x_{ij} + \epsilon k_0(s) + \epsilon^2 k_1(s) + O(\epsilon^3). \quad (3.10)$$

Using the expansion for S^ϵ , the periodicity of S_i in y , and the Taylor series of S_0 and S_1 around (x, k_0) , we obtain

$$S_0(x, k_0) + \epsilon(S_1(x, k_0) + k_0 \cdot \nabla_x S_0(x, k_0) + k_1 \cdot \nabla_y S_0(x, k_0)) + O(\epsilon^2) = 0.$$

Collecting terms with the same order of ϵ , we see that $k_0(s)$ parametrizes locally the zero level set of S_0 :

$$S_0(x, k_0) = 0.$$

For k_1 , we have the equation

$$S_1(x, k_0) + k_0 \cdot \nabla_x S_0(x, k_0) + k_1 \cdot \nabla_y S_0(x, k_0) = 0. \quad (3.11)$$

It suffices to seek for k_1 that is aligned with ν_0 , so that we write

$$k_1(s) = \lambda(s)\nu_0(s) = \lambda \frac{\nabla_y S_0}{|\nabla_y S_0|}, \quad (3.12)$$

where, using (3.11), λ is given by

$$\lambda := -\frac{S_1}{|\nabla_y S_0|} - \frac{k_0 \cdot \nabla_x S_0}{|\nabla_y S_0|}. \quad (3.13)$$

Each of the boundary conditions in (2.3) admits the structural form

$$K(x, x/\epsilon) = 0 \text{ for all } x \in \Gamma^\epsilon,$$

where K is a suitable linear combination of u^ϵ , ∇u^ϵ , q^ϵ , p^ϵ , v^ϵ , and ∇v^ϵ . Using (3.10) and the Taylor series of K around (x, k_0) , we obtain

$$\begin{aligned} K(x, k_0) + \epsilon(k_0 \cdot \nabla_x K(x, k_0) + k_1 \cdot \nabla_y K(x, k_0)) \\ + \frac{\epsilon^2}{2}(k_0, k_1) \cdot (\mathcal{D}^2 K(x, k_0))(k_0, k_1) + \epsilon^3(\dots) = 0, \end{aligned} \quad (3.14)$$

where $\mathcal{D}^2 K$ denotes the Hessian of K w.r.t. x and y . Substituting (3.12) into (3.14), we can restate (3.14) in the following way:

$$\begin{aligned} K(x, y) + \epsilon(y \cdot \nabla_x K(x, y) + \lambda \nu_0 \cdot \nabla_y K(x, y)) \\ + \frac{\epsilon^2}{2}(y, \lambda \nu_0) \cdot (\mathcal{D}^2 K(x, y))(y, \lambda \nu_0) + O(\epsilon^3) = 0 \text{ for all } y \in \Gamma_0(x). \end{aligned} \quad (3.15)$$

In order to proceed further, we make use of the following technical lemmas. Their proofs can be found in [24].

Lemma 3.1 Let $g(x, y)$ be a scalar function such that $g(x, y) = 0$ for all $y \in \Gamma_0(x)$, $x \in \Omega$ and $t \geq 0$. Then it holds that

$$\nabla_x g = \frac{\nu_0 \cdot \nabla_y g}{|\nabla_y S_0|} \nabla_x S_0, \text{ for } x \in \Omega, y \in \Gamma_0(x, t).$$

Lemma 3.2 Let $F(x, y)$ be a vector valued function such that $\nabla_y \cdot F(x, y) = 0$ on $Y_0(x) := \{y \mid S_0(x, y) > 0\}$ and $\nu_0 \cdot F(x, y) = 0$ on $\Gamma_0(x)$ for all $x \in \Omega$. Then it holds that

$$\int_{\Gamma^0(x)} \frac{\tau_0 \cdot \nabla_y S_1}{|\nabla_y S_0|} \tau_0 \cdot F - \frac{S_1}{|\nabla_y S_0|} \nu_0 \cdot \nabla_y (\nu_0 \cdot F) d\sigma = 0, \text{ for } x \in \Omega.$$

3.3 Flow equations

Substituting the asymptotic expansions of q^ϵ and p^ϵ into (2.1_{2,3}), we obtain

$$q_0 = -\kappa \frac{1}{\epsilon} \nabla_y p_0 - \kappa \nabla_y p_1 - \kappa \nabla_x p_0 + O(\epsilon), \quad (3.16)$$

$$\frac{1}{\epsilon} \nabla_y \cdot q_0 + \nabla_x \cdot q_0 + \nabla_y \cdot q_1 + O(\epsilon) = 0. \quad (3.17)$$

Substituting the asymptotic expansion of q^ϵ into the boundary condition (2.3₃), and using (3.15), gives

$$q_0 + \epsilon \left(q_1 + (\nabla_x q_0)^T y + \lambda (\nabla_y q_0)^T \nu_0 \right) + O(\epsilon^2) = 0, \quad \text{for all } y \in \Gamma_0(x). \quad (3.18)$$

The ϵ^{-1} -term in (3.16) indicates that $\nabla_y p_0 = 0$, so that we conclude that p_0 is independent of y . Furthermore, we obtain, after collecting ϵ^0 -terms from (3.16) and (3.18) and ϵ^{-1} -terms from (3.17), the equations for q_0 and p_1 :

$$\begin{cases} q_0 = -\kappa \nabla_y p_1 - \kappa \nabla_x p_0 & \text{in } Y_0(x), \\ \nabla_y \cdot q_0 = 0 & \text{in } Y_0(x), \\ q_0 = 0 & \text{on } \Gamma_0(x), \\ q_0 \text{ and } p_0 \text{ } y\text{-periodic,} \end{cases} \quad (3.19)$$

where

$$Y_0(x) := \{y \mid S_0(x, y) > 0\}. \quad (3.20)$$

These equations (together with boundary conditions on the outer boundary $\partial\Omega$) determine the averaged velocity field given by

$$\bar{q}(x) = \int_{Y_0(x)} q_0(x, y) dy.$$

Now we compute the divergence of \bar{q} (where we use the ϵ^0 -terms from (3.17))

$$\begin{aligned} \nabla_x \cdot \bar{q} &= \nabla_x \cdot \int_{Y_0(x)} q_0 dy = \int_{Y_0(x)} \nabla_x \cdot q_0 dy - \int_{\Gamma_0(x)} \frac{\nabla_x S_0}{|\nabla_y S_0|} \cdot q_0 d\sigma \\ &= - \int_{Y(x)} \nabla_y \cdot q_1 dy = - \int_{\Gamma_0(x)} \nu_0 \cdot q_1 d\sigma \\ &= \int_{\Gamma_0(x)} -\nu_0 \cdot \left((\nabla_x q_0)^T y + \lambda (\nabla_y q_0)^T \nu_0 \right) d\sigma \\ &= -I_1 - I_2, \end{aligned}$$

with

$$\begin{aligned} I_1 &:= \int_{\Gamma_0(x)} \nu_0 \cdot \left((\nabla_x q_0)^T y - \frac{y \cdot \nabla_x S_0}{|\nabla_y S_0|} (\nabla_y q_0)^T \nu_0 \right) d\sigma, \\ I_2 &:= - \int_{\Gamma_0(x)} \nu_0 \cdot \left(\frac{S_1}{|\nabla_y S_0|} (\nabla_y q_0)^T \nu_0 \right) d\sigma. \end{aligned}$$

We apply Lemma 3.1 with $g = \nu_0 \cdot q_0$, and obtain

$$\nabla_x (\nu_0 \cdot q_0) = \frac{\nu_0 \cdot \nabla_y (\nu_0 \cdot q_0)}{|\nabla_y S_0|} \nabla_x S_0, \quad \text{on } \Gamma_0(x, t).$$

Since $q_0 = 0$ on $\Gamma_0(x)$ it follows that $(\nabla_x q_0)^T \nu_0 = \frac{\nu_0 \cdot (\nabla_y q_0)^T \nu_0}{|\nabla_y S_0|} \nabla_x S_0$, so that $I_1 = 0$. Next we apply Lemma 3.2 with $F = q_0$, and get consequently

$$\int_{\Gamma_0(x)} \frac{\tau_0 \cdot \nabla_y S_1}{|\nabla_y S_0|} \tau_0 \cdot q_0 - \frac{S_1}{|\nabla_y S_0|} \nu_0 \cdot \nabla_y (\nu_0 \cdot q_0) d\sigma = 0.$$

Again using $q_0 = 0$ on $\Gamma_0(x)$, it follows that $I_2 = 0$, so that we have

$$\nabla_x \cdot \bar{q} = 0. \quad (3.21)$$

3.4 Diffusion equation in the low diffusivity areas

Substituting the asymptotic expansion of v^ϵ into (2.2), we obtain

$$\partial_t v_0 = D_l \nabla_y v_0 + O(\epsilon). \quad (3.22)$$

Similarly expanding the boundary condition (2.3₂), we get

$$0 = u_0 - v_0 + O(\epsilon) \quad \text{on } \Gamma^\epsilon,$$

which, after substitution into (3.15), becomes

$$0 = u_0 - v_0 + O(\epsilon) \quad \text{on } \Gamma_0(x).$$

Collecting the lowest order terms, and using that u_0 does not depend on y , we obtain the boundary condition

$$v_0(x, y, t) = u_0(x, t) \quad \text{for all } y \in \Gamma_0(x), x \in \Omega. \quad (3.23)$$

3.5 Convection-diffusion equation in the high diffusivity area

Substituting the asymptotic expansion of u^ϵ into (2.1₁), we obtain

$$\begin{aligned} \partial_t u_0 &= \frac{1}{\epsilon^2} D_h \Delta_y u_0 + \frac{1}{\epsilon} (\nabla_y \cdot F_h + \nabla_x \cdot (D_h \nabla_y u_0)) \\ &\quad + \nabla_y \cdot (D_h (\nabla_y u_2 + \nabla_x u_1) - q_1 u_0 - q_0 u_1) + \nabla_x \cdot F_h \\ &\quad + O(\epsilon), \end{aligned} \quad (3.24)$$

where

$$F_h := D_h (\nabla_x u_0 + \nabla_y u_1) - q_0 u_0. \quad (3.25)$$

Using the expansions for u^ϵ , v^ϵ and ν^ϵ , we first expand (2.3₁):

$$\begin{aligned} 0 &= \nu^\epsilon \cdot (D_h \nabla u^\epsilon) - \epsilon^2 \nu^\epsilon \cdot (D_l \nabla v^\epsilon) \\ &= \frac{1}{\epsilon} \nu_0 \cdot (D_h \nabla_y u_0) + \nu_0 \cdot (D_h (\nabla_x u_0 + \nabla_y u_1)) + \nu_1 \cdot (D_h \nabla_y u_0) \\ &\quad + \epsilon \left(\nu_0 \cdot (D_h (\nabla_x u_1 + \nabla_y u_2)) + \nu_1 \cdot (D_h (\nabla_x u_0 + \nabla_y u_1)) + \nu_2 \cdot (D_h \nabla_y u_0) - \nu_0 \cdot (D_l \nabla_y v_0) \right) \\ &\quad + O(\epsilon^2), \quad \text{for all } x \in \Gamma^\epsilon \text{ and } y = \frac{x}{\epsilon}. \end{aligned}$$

Next we substitute this expansion into (3.15), and thus obtain

$$\begin{aligned}
0 &= \frac{1}{\epsilon} \nu_0 \cdot (D_h \nabla_y u_0) \\
&+ \nu_0 \cdot (D_h(\nabla_x u_0 + \nabla_y u_1)) + \nu_1 \cdot (D_h \nabla_y u_0) + y \cdot \nabla_x(\nu_0 \cdot (D_h \nabla_y u_0)) + \lambda \nu_0 \cdot \nabla_y(\nu_0 \cdot (D_h \nabla_y u_0)) \\
&+ \epsilon \left(\nu_0 \cdot (D_h(\nabla_x u_1 + \nabla_y u_2)) + \nu_1 \cdot D_h(\nabla_x u_0 + \nabla_y u_1) + \nu_2 \cdot (D_h \nabla_y u_0) \right. \\
&\quad \left. - \nu_0 \cdot (D_l \nabla_y v_0) + y \cdot \nabla_x(\nu_0 \cdot (D_h(\nabla_x u_0 + \nabla_y u_1)) + \nu_1 \cdot (D_h \nabla_y u_0)) \right. \\
&\quad \left. + \lambda \nu_0 \cdot \nabla_y(\nu_0 \cdot (D_h(\nabla_x u_0 + \nabla_y u_1)) + \nu_1 \cdot (D_h \nabla_y u_0)) \right. \\
&\quad \left. + \frac{1}{2}(y, \lambda \nu_0) \cdot (\mathcal{D}^2(\nu_0 \cdot (D_h \nabla_y u_0)))(y, \lambda \nu_0) \right) \\
&+ O(\epsilon^2), \text{ for } y \in \Gamma_0(x). \tag{3.26}
\end{aligned}$$

Now we collect the ϵ^{-2} -term from (3.24) and the ϵ^{-1} -term from (3.26). Hence we obtain for u_0 the equations

$$\begin{cases} \Delta_y u_0 = 0 & \text{in } Y_0(x), \\ \nu_0 \cdot \nabla_y u_0 = 0 & \text{on } \Gamma_0(x), \\ u_0 \text{ } y\text{-periodic,} \end{cases} \tag{3.27}$$

where $Y_0(x)$ is given by (3.20). This means that u_0 is determined up to a constant and does not depend on y , so that $\nabla_y u_0 = 0$. Collecting the ϵ^{-1} terms from (3.24), the ϵ^0 -terms from (3.26), and using that $\nabla_y u_0 = 0$, we get for u_1 the equations

$$\begin{cases} \nabla_y \cdot (D_h \nabla_y u_1 - q_0 u_0) = 0 & \text{in } Y_0(x), \\ \nu_0 \cdot (D_h(\nabla_x u_0 + \nabla_y u_1)) = 0 & \text{on } \Gamma_0(x), \\ u_1 \text{ } y\text{-periodic.} \end{cases} \tag{3.28}$$

Collecting the ϵ^0 -terms from (3.24) and the ϵ^1 -terms from (3.26), we obtain

$$\begin{cases} \partial_t u_0 = \nabla_y \cdot (D_h(\nabla_y u_2 + \nabla_x u_1) - q_1 u_0 - q_0 u_1) + \nabla_x \cdot F_h & \text{in } Y_0(x), \\ \nu_0 \cdot (D_h(\nabla_x u_1 + \nabla_y u_2)) = -\nu_1 \cdot (D_h(\nabla_x u_0 + \nabla_y u_1)) \\ \quad + \nu_0 \cdot (D_l \nabla_y v_0) - y \cdot \nabla_x(\nu_0 \cdot (D_h(\nabla_x u_0 + \nabla_y u_1))) & \\ \quad - \lambda \nu_0 \cdot \nabla_y(\nu_0 \cdot (D_h(\nabla_x u_0 + \nabla_y u_1))) & \text{on } \Gamma_0(x), \\ u_2 \text{ } y\text{-periodic.} \end{cases} \tag{3.29}$$

Integrating (3.29₁) over $Y_0(x)$ and using the boundary conditions (3.19₃) and (3.29₂) yields

$$\begin{aligned}
|Y_0(x)| \partial_t u_0 &= \int_{Y_0(x)} \nabla_y \cdot (D_h(\nabla_x u_1 + \nabla_y u_2) - q_1 u_0 - q_0 u_1) dy + \int_{Y_0(x)} \nabla_x \cdot F_h dy \\
&= \int_{\Gamma_0(x)} -\nu_1 \cdot F_h + \nu_0 \cdot (D_l \nabla_y v_0) - y \cdot \nabla_x(\nu_0 \cdot F_h) - \lambda \nu_0 \cdot \nabla_y(\nu_0 \cdot F_h) d\sigma \\
&\quad + \nabla_x \cdot \int_{Y_0(x)} F_h dy + \int_{\Gamma_0(x)} \frac{\nabla_x S_0}{|\nabla_y S_0|} \cdot F_h d\sigma.
\end{aligned}$$

Using (3.8), (3.13), and the boundary conditions (3.19₃) and (3.28₂), this can be rewritten as

$$\begin{aligned} |Y_0(x)|\partial_t u_0 &= \nabla_x \cdot \int_{Y_0(x)} (D_h(\nabla_y u_1 + \nabla_x u_0) - q_0 u_0) dy \\ &\quad + \int_{\Gamma_0(x)} \nu_0 \cdot (D_l \nabla_y v_0) dy - I_1 - I_2, \end{aligned}$$

where

$$\begin{aligned} I_1 &:= \int_{\Gamma_0(x)} y \cdot \nabla_x g - \frac{y \cdot \nabla_x S_0}{|\nabla_y S_0|} \nu_0 \cdot \nabla_y g d\sigma, \\ I_2 &:= \int_{\Gamma_0(x)} \frac{\tau_0 \cdot \nabla_y S_1}{|\nabla_y S_0|} \tau_0 \cdot F_h - \frac{S_1}{|\nabla_y S_0|} \nu_0 \cdot \nabla_y (\nu^0 \cdot F_h) d\sigma, \end{aligned}$$

with $g := \nu_0 \cdot F_h$. The boundary conditions (3.19₃) and (3.28₂) give us $g(x, y, t) = 0$ for $y \in \Gamma_0(x, t)$. Now invoking Lemma 3.1 leads to $\nabla_x g = \frac{\nu_0 \cdot \nabla_y g}{|\nabla_y S_0|} \nabla_x S_0$. So $I_1 = 0$. For the integral I_2 we invoke Lemma 3.2 to obtain $I_2 = 0$. As a last step, we use the divergence theorem and interface condition (3.23) to obtain

$$\partial_t \left(|Y_0(x)|u_0 + \int_{Y_0^C(x)} v_0 dy \right) = \nabla_x \cdot \int_{Y_0(x)} (D_h(\nabla_y u_1 + \nabla_x u_0) - q_0 u_0) dy, \quad (3.30)$$

where $Y_0^C(x)$ is the complement of $Y_0(x)$ in U given by $Y_0^C(x) := U \setminus Y_0(x) = \{S_0(x) < 0\}$.

Remark 3.3 Note that in this section we have not used any assumptions of the shape of the perforations. They may have any shape as long as their limiting shape is described by the level set function S_0 .

4 Upscaled equations

The equations for lowest order terms of q^ϵ and p^ϵ , (3.19) and (3.21), v^ϵ , (3.22), u^ϵ , (3.30), and the coupling conditions (3.23) together constitute the upscaled model. In this section we collect these equations for the case discussed in Section 2, i.e. for circular perforations. For this purpose we return to a formulation in terms of $r(x, t)$, where we use

$$\begin{aligned} \Gamma_0(x) &= \{y \in U \mid |y| = r(x)\}, \\ Y_0(x) &= \{y \in U \mid |y| > r(x)\}, \\ Y_0^C(x) &= \{y \in U \mid |y| < r(x)\}. \end{aligned}$$

We write the solutions of equations (3.28) and (3.19) in terms of the solutions of the following two cell problems (see, e.g. [12])

$$\begin{cases} \Delta_y v_j(x, y) = 0 & \text{for all } x \in \Omega, y \in U, |y| > r(x), \\ \nu_0 \cdot \nabla_y v_j(x, y) = -\nu_0 \cdot e_j & \text{for all } x \in \Omega, |y| = r(x), \\ v_j(x, y) \text{ } y\text{-periodic,} \end{cases} \quad (4.1)$$

and

$$\begin{cases} w_j(x, y) = \nabla_y \pi_j(x, y) + e_j & \text{for all } x \in \Omega, y \in U, |y| > r(x), \\ \nabla_y \cdot w_j(x, y) = 0 & \text{for all } x \in \Omega, y \in U, |y| > r(x), \\ w_j = 0 & \text{for all } x \in \Omega, |y| = r(x), \\ w_j(x, y) \text{ and } \pi_j(x, y) \text{ } y\text{-periodic,} \end{cases} \quad (4.2)$$

for $j = 1, 2$. The use of these cell problems allows us to write the results of the formal homogenization procedure in the form of the following distributed-microstructure model

$$\begin{cases} \partial_t v_0(x, y, t) = D_l \Delta_y v_0(x, y, t) & \text{for } |y| < r(x), x \in \Omega, \\ \partial_t \left(\theta(x) u_0 + \int_{|y| < r(x)} v_0 dy \right) = \\ \quad \nabla_x \cdot (D_h \mathcal{A}(x) \nabla_x u_0 - \bar{q} u_0) & \text{for } x \in \Omega, \\ \bar{q} = -\kappa \mathcal{K}(x) \nabla_x p_0 & \text{for } x \in \Omega, \\ \nabla_x \cdot \bar{q} = 0 & \text{for } x \in \Omega, \end{cases} \quad (4.3)$$

$$\begin{cases} v_0(x, y, t) = u_0(x, t) & \text{for } |y| = r(x), \\ u_0(x, t) = u_b(x, t) & \text{for } x \in \Gamma, \\ \bar{q}(x, t) = q_b(x, t) & \text{for } x \in \Gamma, \end{cases} \quad (4.4)$$

$$\begin{cases} u_0(x, 0) = u_I(x) & \text{for } x \in \Omega, \\ v_0(x, y, 0) = v_I(x, y) & \text{for } |y| < r(x), x \in \Omega. \end{cases} \quad (4.5)$$

where the porosity $\theta(x)$ of the medium is given by

$$\theta(x) := 1 - \pi r^2(x),$$

while the effective diffusivity $\mathcal{A}(x) := (a_{ij}(x))_{i,j}$ and the effective permeability $\mathcal{K}(x) := (k_{ij}(x))_{i,j}$ are defined by

$$a_{ij}(x) := \int_{\{y \in U \mid |y| > r(x)\}} \delta_{ij} + \partial_{y_i} v_j(x, y, t) dy,$$

and

$$k_{ij}(x) := \int_{\{y \in U \mid |y| > r(x)\}} w_{ji}(x, y, t) dy.$$

5 Analysis of upscaled equations

In this section we investigate the solvability of the upscaled equations (4.3)-(4.5). Note that the equations (4.3_{3,4}) for \bar{q} and p_0 , together with the boundary condition (4.4₃) are decoupled from the other equations. We may assume that we can solve these equations for \bar{q} and p_0 such that $q \in L^\infty(\Omega; \mathbb{R}^2)$ (see Assumption 2 below). Standard arguments from the theory of partial differential equations justify this assumption if the data q_b and r are suitable, see [13] for a closely related scenario. With this assumption the equations

(4.3)-(4.5) reduce to the following problem

$$(P) \begin{cases} \theta(x)\partial_t u - \nabla_x \cdot (D(x)\nabla_x u - qu) = - \int_{\partial B(x)} \nu_y \cdot (D_l \nabla_y v) d\sigma & \text{in } \Omega, \\ \partial_t v - D_l \Delta_y v = 0 & \text{in } B(x), \\ u(x, t) = v(x, y, t) & \text{at } (x, y) \in \Omega \times \partial B(x), \\ u(x, t) = u_b(x, t) & \text{at } x \in \partial\Omega, \\ u(x, 0) = u_I(x) & \text{in } \bar{\Omega}, \\ v(x, y, 0) = v_I(x, y) & \text{at } (x, y) \in \bar{\Omega} \times \overline{B(x)}, \end{cases}$$

where $B(x) := Y_0(x)$, where Y_0 is defined in (3.20). Notice that in this section we again do not restrict ourselves to circular perforations. The perforations may have any shape as long as they are described by the level set S_0 . In the following sections we discuss the existence and uniqueness of weak solutions to problem (P).

5.1 Functional setting and weak formulation

For notational convenience we define the following spaces:

$$V_1 := H_0^1(\Omega), \quad (5.1)$$

$$V_2 := L^2(\Omega; H^2(B(x))), \quad (5.2)$$

$$H_1 := L_\theta^2(\Omega), \quad (5.3)$$

$$H_2 := L^2(\Omega; L^2(B(x))). \quad (5.4)$$

The spaces H_2 and V_2 make sense if, for instance, we assume (like in [18]):

Assumption 1 The function $S_0 : \Omega \times U \rightarrow \mathbb{R}$, which defines $B(x) := Y_0(x)$ in (3.20), and which also defines the 1-dimensional boundary $\Omega \times \partial B(x)$ of $\Omega \times B(x)$ as

$$(x, y) \in \Omega \times \partial B(x) \text{ if and only if } S_0(x, y) = 0,$$

is an element of $C^2(\bar{\Omega} \times \bar{U})$. Assume additionally that the Clarke gradient $\partial_y S_0(x, y)$ is regular for all choices of $(x, y) \in \bar{\Omega} \times \bar{U}$.

Following the lines of [18] and [23], Assumption 1 implies in particular that the measures $|\partial B(x)|$ and $|B(x)|$ are bounded away from zero (uniformly in x). Consequently, the following direct Hilbert integrals (cf. [8] (part II, chapter 2), e.g.)

$$L^2(\Omega; H^1(B(x))) := \{u \in L^2(\Omega; L^2(B(x))) : \nabla_y u \in L^2(\Omega; L^2(B(x)))\}$$

$$L^2(\Omega; H^1(\partial B(x))) := \{u : \Omega \times \partial B(x) \rightarrow \mathbb{R} \text{ measurable such that } \int_{\Omega} \|u(x)\|_{L^2(\partial B(x))}^2 < \infty\}$$

are well-defined separable Hilbert spaces and, additionally, the *distributed trace*

$$\gamma : L^2(\Omega; H^1(B(x))) \rightarrow L^2(\Omega, L^2(\partial B(x)))$$

given by

$$\gamma u(x, s) := (\gamma_x U(x))(s), \quad x \in \Omega, s \in \partial B(x), u \in L^2(\Omega; H^1(B(x))) \quad (5.5)$$

is a bounded linear operator. For each fixed $x \in \Omega$, the map γ_x , which is arising in (5.5), is the standard trace operator from $H^1(B(x))$ to $L^2(\partial B(x))$. We refer the reader to [17] for more details on the construction of these spaces and to [19] for the definitions of their duals as well as for a less regular condition (compared to Assumption 1) allowing to define these spaces in the context of a certain class of anisotropic Sobolev spaces.

Furthermore we assume

Assumption 2

$$\begin{cases} \theta, D \in L_+^\infty(\Omega), \\ q \in L^\infty(\Omega; \mathbb{R}^d) \text{ with } \nabla \cdot q = 0, \\ u_b \in L_+^\infty(\Omega \times S) \cap H^1(S; L^2(\Omega)), \\ \partial_t u_b \leq 0 \text{ a.e. } (x, t) \in \Omega \times S, \\ u_I \in L_+^\infty(\bar{\Omega}) \cap H_1, \\ v_I(x, \cdot) \in L_+^\infty(B(x)) \cap H_2 \text{ for a.e. } x \in \bar{\Omega}. \end{cases}$$

We also define the following constants for later use:

$$M_1 := \max\{\|u_I\|_{L^\infty(\Omega)}, \|u_b\|_{L^\infty(\Omega)}\}, \quad (5.6)$$

$$M_2 := \max\{\|v_I\|_{L^\infty(\Omega)}, M_1\}. \quad (5.7)$$

Note that M_1 and M_2 depend on the initial and boundary data, but not on the final time T . Let us introduce the evolution triple $(\mathbb{V}, \mathbb{H}, \mathbb{V}^*)$, where

$$\mathbb{V} := \{(\phi, \psi) \in V_1 \times V_2 \mid \phi(x) = \psi(x, y) \text{ for } x \in \Omega, y \in \partial B(x)\}, \quad (5.8)$$

$$\mathbb{H} := H_1 \times H_2, \quad (5.9)$$

Denote $U := u - u_b$ and notice that $U = 0$ at $\partial\Omega$.

Definition 5.1 Assume Assumptions 1 and 2. The pair (u, v) , with $u = U + u_b$ and where $(U, v) \in \mathbb{V}$, is a weak solution of the problem (P) if the following identities hold

$$\begin{aligned} \int_{\Omega} \theta \partial_t (U + u_b) \phi \, dx + \int_{\Omega} (D \nabla_x (U + u_b) - q(U + u_b)) \cdot \nabla_x \phi \, dx = \\ - \int_{\Omega} \int_{\partial B(x)} \nu_y \cdot (D_l \nabla_y v) \phi \, d\sigma \, dx, \end{aligned} \quad (5.10)$$

$$\int_{\Omega} \int_{B(x)} \partial_t v \psi \, dy \, dx + \int_{\Omega} \int_{B(x)} D_l \nabla_y \cdot \nabla_y \psi \, dy \, dx = \int_{\Omega} \int_{\partial B(x)} \nu_y \cdot (D_l \nabla_y v) \phi \, d\sigma \, dx, \quad (5.11)$$

for all $(\phi, \psi) \in \mathbb{V}$ and $t \in S$.

As a last item in this section on the functional framework, we mention for reader's convenience the following lemma by Lions and Aubin [16], which we will need later on:

Lemma 5.2 (Lions-Aubin) Let $B_0 \hookrightarrow B \hookrightarrow B_1$ be Banach spaces such that B_0 and B_1

are reflexive and the embedding $B_0 \hookrightarrow B$ is compact. Fix $p, q > 0$ and let

$$W = \left\{ z \in L^p(S; B_0) : \frac{dz}{dt} \in L^q(S; B_1) \right\}$$

with

$$\|z\|_W := \|z\|_{L^p(S; B_0)} + \|\partial_t z\|_{L^q(S; B_1)}.$$

Then $W \hookrightarrow L^p(S; B)$.

5.2 Estimates and uniqueness

In this section we establish the positivity and boundedness of the concentrations. Furthermore, we prove an energy inequality and ensure the uniqueness of weak solutions to problem (P).

Lemma 5.3 Let Assumptions 1 and 2 be satisfied. Then any weak solution (u, v) of problem (P) has the following properties:

- (i) $u \geq 0$ for a.e. $x \in \Omega$ and for all $t \in S$;
- (ii) $v \geq 0$ for a.e. $(x, y) \in \Omega \times B(x)$ and for all $t \in S$;
- (iii) $u \leq M_1$ for a.e. $x \in \Omega$ and for all $t \in S$;
- (iv) $v \leq M_2$ for a.e. $(x, y) \in \Omega \times B(x)$ and for all $t \in S$;
- (v) The following energy inequality holds:

$$\begin{aligned} & \|u\|_{L^2(S; V_1) \cap L^\infty(S; H_1)}^2 + \|v\|_{L^2(S; L^2(\Omega, V_2)) \cap L^\infty(S; H_2)}^2 \\ & + \|\nabla_x u\|_{L^2(S; H_1)}^2 + \|\nabla_y v\|_{L^2(S \times \Omega \times B(x))}^2 \leq c_1 \end{aligned} \quad (5.12)$$

where M_1 and M_2 are given in (5.6) and (5.7), and where c_1 is a constant independent of u and v .

Proof We prove (i) and (ii) simultaneously. Similar arguments combined with corresponding suitable choices of test functions lead in a straightforward manner to (iii), (iv), and (v). We omit the proof details. Choosing in the weak formulation as test functions $(\varphi, \psi) := (-U^-, -v^-) \in \mathbb{V}$, we obtain:

$$\begin{aligned} & \frac{1}{2} \int_{\Omega} \phi(\partial_t U^-)^2 + \frac{1}{2} \int_{\Omega} \int_{B(x)} \partial_t (v^-)^2 + \int_{\Omega} D|\nabla U^-|^2 + \int_{\Omega} \int_{B(x)} D_\ell |\nabla_y v^-|^2 \\ & = \int_{\Omega} \phi \partial_t u_b U^- + \int_{\Omega} D \nabla u_b \nabla U^- - \int_{\Omega} \nabla \cdot (q(U + u_b)) \nabla U^- \\ & \leq \int_{\Omega} D \nabla u_b \nabla U^- - \int_{\Omega} q(\nabla U + \nabla u_b) \nabla U^- - \int_{\Omega} (U + u_b) \operatorname{div} q \nabla U^- \\ & = \min_{\bar{\Omega}} q \int_{\Omega} |\nabla U^-|^2 + \int_{\Omega} U^- \operatorname{div} q \nabla U^- \\ & - \int_{\Omega} U^+ \operatorname{div} q \nabla U^- + \int_{\Omega} (D \nabla u_b - u_b \operatorname{div} q) \nabla U^-. \end{aligned} \quad (5.13)$$

Note that, excepting the last two terms, the right-hand side of (5.13) has the right sign. Assuming, additionally, a compatibility relation between the data q, u_b , for instance, of the type $D\nabla u_b = u_b \operatorname{div} q$ a.e. in $\Omega \times S$, makes the last term of the r.h.s. of (5.13) vanish. The key observation in estimating the last by one term is the fact that the sets $\{x \in \Omega : U(x) \geq 0\}$ and $\{x \in \Omega : U(x) \leq 0\}$ are Lebesgue measurable. This allow to proceed as follows:

$$\int_{\Omega} U^+ \operatorname{div} q \nabla U^- = \int_{\{x \in \Omega : U(x) \geq 0\}} U^+ \operatorname{div} q \nabla U^- + \int_{\{x \in \Omega : U(x) \leq 0\}} U^+ \operatorname{div} q \nabla U^- = 0. \quad (5.14)$$

$$(5.15)$$

After applying the inequality between the arithmetic and geometric means applied to the second term for the right hand-side of (5.13), the conclusion of both (i) and (ii) follows via the Gronwall's inequality. \square

Proposition 5.4 (Uniqueness) Problem (P) admits at most one weak solution.

Proof Let (u_i, v_i) , with $i \in \{1, 2\}$, be two distinct arbitrarily chosen weak solutions. Then for the pair $(\rho, \theta) := (u_2 - u_1, v_2 - v_1)$ we have

$$\begin{aligned} \int_{\Omega} \phi \partial_t \rho \varphi + \int_{\Omega} D \nabla \rho \nabla \varphi - \int_{\Omega} q \rho \nabla \varphi \\ + \int_{\Omega} \int_{B(x)} \partial_t \theta \psi + \int_{\Omega} \int_{B(x)} D_{\ell} \nabla_y \theta \nabla_y \psi = 0 \end{aligned} \quad (5.16)$$

for all $(\varphi, \psi) \in \mathbb{V}$.

Choosing now as test functions $(\varphi, \psi) := (\rho, \theta) \in \mathbb{V}$, we reformulate the latter identity as:

$$\int_{\Omega} \frac{\phi}{2} (\partial_t \rho)^2 + \int_{\Omega} \int_{B(x)} \frac{1}{2} (\partial_t \theta)^2 + \int_{\Omega} D |\nabla \rho|^2 + \int_{\Omega} \int_{B(x)} D_{\ell} |\nabla_y \theta|^2 = \int_{\Omega} q \rho \nabla \rho. \quad (5.17)$$

Noticing that for any $\epsilon > 0$ we can find a constant $c_{\epsilon} \in]0, \infty[$ such that

$$\int_{\Omega} q \rho \nabla \rho \leq \epsilon \int_{\Omega} |\nabla \rho|^2 + c_{\epsilon} \|q\|_{\infty}^2 \int_{\Omega} |\rho|^2,$$

then (5.17) yields:

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \int_{\Omega} \phi |\rho|^2 + \frac{1}{2} \frac{d}{dt} \int_{\Omega} \int_{B(x)} |\theta|^2 + \int_{\Omega} (D - \epsilon) |\nabla \rho|^2 \\ + \int_{\Omega} \int_{B(x)} D_{\ell} |\nabla_y \theta|^2 \leq c_{\epsilon} \|q\|_{\infty}^2 \int_{\Omega} |\rho|^2. \end{aligned} \quad (5.18)$$

Choose

$$\epsilon \in \left] 0, \frac{\min_{\Omega \times B(x)} D}{\|q\|_{\infty}^2} \right]. \quad (5.19)$$

Since for all $x \in \overline{\Omega}$ and $y \in \overline{B(x)}$ we have $\theta(x, y, 0) = \rho(x, 0) = 0$, (5.18) together with (5.19) allow for the direct application of Gronwall's inequality. Consequently, the solutions (u_i, v_i) with $i \in \{1, 2\}$ must coincide a.e. in space and for all $t \in S$. \square

Remark 5.5 At the technical level, the merit of the basic estimates enumerated in this section is that they are derived in the x -dependent framework and not in a fixed-domain formulation. Note also that the proof of uniqueness does not rely on the use of L^∞ - and positivity estimates on concentrations.

5.3 Existence of weak solutions

In this section, we prove existence of weak solutions of problem (P) . We will do this using the Schauder fixed-point argument. The operator, for which we seek a fixed point, maps the space $L^2(S; L^2(\Omega))$ into itself, and consists of a composition of three other operators. In order to define these operators, we need the following functional framework:

$$X_1 := L^2(S; L^2(\Omega)), \quad (5.20)$$

$$X_2 := L^2(S; H_0^1(\Omega)) \cap H^1(S; L^2(\Omega)), \quad (5.21)$$

$$X_3 := L^2(S; V_2) \cap H^1(S; L^2(\Omega; L^2(B(x)))). \quad (5.22)$$

The first operator T_1 maps a $f \in X_1$ to the solution $w \in X_2$ of

$$\int_{\Omega} \theta \partial_t (U + u_b) \phi \, dx + \int_{\Omega} (D \nabla_x (U + u_b) - q(U + u_b)) \cdot \nabla_x \phi \, dx = - \int_{\Omega} f \phi \, dx, \quad (5.23)$$

for all $\phi \in H_0^1(\Omega)$.

The second operator T_2 maps a $w \in X_2$ to a solution $v \in X_3$ of

$$\begin{aligned} \int_{\Omega} \int_{B(x)} \partial_t (V + w) \psi \, dy dx + \int_{\Omega} \int_{B(x)} D_l \nabla_y (V + w) \cdot \nabla_y \psi \, dy dx = \\ \int_{\Omega} \int_{\partial B(x)} \nu_y \cdot (D_l \nabla_y (V + w)) \psi \, d\sigma dx, \end{aligned} \quad (5.24)$$

for all $\psi \in V_2$ and $t \in S$.

The third operator T_3 maps a $v \in X_3$ to $f \in X_1$ by

$$f = \int_{\partial B(x)} \nu_y \cdot \nabla_y v \, d\sigma. \quad (5.25)$$

The operator $T : X_1 \rightarrow X_1$ of which a fixed point corresponds to a weak solution of problem (P) is now given by

$$T := T_3 \circ T_2 \circ T_1. \quad (5.26)$$

Lemma 5.6 The operator T is well-defined and continuous.

Proof Since the auxiliary problem (obtained by fixing f) is well-posed (see e.g. chapter 3 in [15]), we easily see that T_1 is well-defined. Furthermore, by standard arguments we can ensure the stability of the weak solution to the latter problem with respect to initial and boundary data and especially with respect to the choice of the r.h.s. f , that is T_1 maps continuously X_1 into X_2 .

Analogously, same arguments lead to the well-definedness of T_2 and to its continuity

from X_2 to $\hat{X}_2 \subset X_3$. The fact that the linear PDE (5.24) and its weak solution depend (continuously) on the fixed parameter $x \in \Omega$ is not "disturbing" at this point⁴.

Since for any $v \in X_3$ the gradient $\nabla_y v$ has a trace on $\partial B(x)$, the well-definedness and continuity of T_3 is ensured. \square

Furthermore we need for the fixed-point argument that the operator T is compact. It is enough that one of the operators T_1, T_2 and T_3 is compact. Here we will show that T_2 maps X_2 compactly into X_3 .

Lemma 5.7 (Compactness) The operator $T_3 \circ T_2$ is compact.

Proof We will first reformulate (5.24) by mapping the x -dependent domains for the y -coordinate to the referential domain $B(0)$ so that the transformed solution \hat{v} is in $L^2(S; L^2(\Omega; L^2(B(0)))) \cap H^1(S; L^2(\Omega; L^2(B(0))))$

This transformation is a mapping $\Psi : \Omega \times B(0) \rightarrow \Omega \times B(x)$. We call Ψ a *regular C^2 -motion* if $\Psi \in C^2(\Omega \times B(0))$ with the property that for each $x \in \Omega$

$$\Psi(x, \cdot) : B(0) \rightarrow B(x) := \Psi(x, B(0)) \quad (5.27)$$

is bijective, and if there exist constants $c, C > 0$ such that

$$c \leq \det \nabla_y \Psi(x, y) \leq C, \quad (5.28)$$

for all $(x, y) \in \Omega \times B(0)$. The existence of such a mapping is ensured by the fact that $S_0 \in C^2(\bar{\Omega} \times \bar{U})$, by Assumption 1.

If Ψ is a regular C^2 -motion, then the quantities

$$F := \nabla_y \Psi \text{ and } J := \det F \quad (5.29)$$

are continuous functions of x and y . Furthermore, we have the following calculation rules:

$$\begin{aligned} \nabla_y v &= F^{-T} \nabla_{\hat{y}} \hat{v}, \\ \partial_t v &= \partial_t \hat{v}, \\ \int_{\partial B(x)} \nu_y \cdot j \, d\sigma &= \int_{\Gamma_0} J F^{-T} \hat{\nu}_{\hat{y}} \cdot \hat{j} \, d\sigma. \end{aligned}$$

The transformed version of (5.24) is now written as: let $w \in X_2$ be given, find $\hat{V} \in L^2(S; L^2(\Omega; H_0^1(B(0)))) \cap H^1(S; L^2(\Omega; L^2(B(0))))$

$$\begin{aligned} \int_{\Omega} \int_{B(0)} \partial_t(\hat{V} + w) \psi J \, dy dx + \int_{\Omega} \int_{B(0)} J F_{-1}^{-T} D_t F^{-T} \nabla_y(\hat{V} + w) \cdot \nabla_y \psi \, dy dx = \\ \int_{\Omega} \int_{\Gamma_0} \hat{\nu}_y \cdot (J F^{-1} D_t F^{-T} \nabla_y(\hat{V} + w)) \psi \, d\sigma dx, \quad (5.30) \end{aligned}$$

for all $\psi \in L^2(\Omega; H_0^1(B(0)))$ and $t \in S$.

Denote by Γ_0 the boundary of $B(0)$.

⁴ Note however that this x -dependence will play a crucial role in getting (at a later stage) the compactness of T_2 .

Claim 5.8 Γ_0 is C^2 .

Proof of claim The conclusion of the Lemma is a straightforward consequence of the regularity of S_0 , by Assumption 1. \square

Claim 5.9 (Interior and boundary H^2 -regularity) Assume Assumptions 1 and 2 and take $\hat{V}_I \in L^2(\Omega, H^1(B(0)))$. Then

$$\hat{V} \in L^2(S; L^2(\Omega; H_{loc}^2(B(0)) \cap H_0^1(B(0))))). \quad (5.31)$$

Since Γ_0 is C^2 , we have

$$\hat{V} \in L^2(S; L^2(\Omega; H^2(B(0)) \cap H_0^1(B(0))))). \quad (5.32)$$

Proof of claim The proof idea follows closely the lines of Theorem 1 and Theorem 4 (cf. [10], sect. 6.3) \square

Claim 5.10 (Additional two-scale regularity) Assume the hypotheses of Lemma 5.9 to be satisfied. Then

$$\hat{V} \in L^2(S; H^1(\Omega; H^2(B(0)) \cap H_0^1(B(0))))). \quad (5.33)$$

Proof of claim Let us take $\emptyset \neq \Omega' \subset \Omega$ arbitrary such that $h := \text{dist}(\Omega', \partial\Omega) > 0$. At this point, we wish to show that

$$\hat{V} \in L^2(S; H^1(\Omega'; H^2(B(0)) \cap H_0^1(B(0))))). \quad (5.34)$$

The extension to $L^2(S; H^1(\Omega; H^2(B(0)) \cap H_0^1(B(0))))$ can be done with help of a cutoff function as in [10] (see e.g. Theorem 1 in sect. 6.3). We omit this step here and refer the reader to *loc. cit.* for more details on the way the cutoff enters the estimates. To simplify the writing of this proof, instead of \hat{V} (and other functions derived from \hat{V}) we write V (without the hat). Furthermore, since here we focus on the regularity w.r.t. x of the involved functions, we omit to indicate the dependence of U on t and of V on y and t . For all $t \in S$, $x \in \Omega'$ and $Y \in Y_0$, we denote by U_h^i and V_h^i the following difference quotients with respect to the variable x :

$$\begin{aligned} U_h^i(x, t) &:= \frac{U(x + he_i, t) - U(x, t)}{h}, \\ V_h^i(x, y, t) &:= \frac{V(x + he_i, y, t) - V(x, y, t)}{h}. \end{aligned}$$

We have for all $\psi \in L^2(\Omega', H_0^1(B(0)))$ the following identities:

$$\begin{aligned} & \int_{\Omega' \times B(0)} J(x + he_i) \partial_t (V(x + he_i) + U(x + he_i)) \psi + \int_{\Omega' \times B(0)} S(x + he_i) \nabla_y V(x + he_i) \nabla_y \psi \\ & - \int_{\Omega' \times \Gamma_0} \nu_y \cdot (S(x + he_i) D_\ell \nabla_y V(x + he_i)) \psi d\sigma = 0 \end{aligned} \quad (5.35)$$

and

$$\begin{aligned} & \int_{\Omega' \times B(0)} J(x) \partial_t (V(x) + U(x)) \psi + \int_{\Omega' \times B(0)} S(x) \nabla_y V(x) \nabla_y \psi \\ & - \int_{\Omega' \times \Gamma_0} \nu_y \cdot (S(x) D_\ell \nabla_y V(x)) \psi d\sigma = 0. \end{aligned} \quad (5.36)$$

Subtracting the latter two equations, dividing the result by $h > 0$ and choosing then as test function $\psi := V_h^i$ yields the expression

$$A_1 + A_2 + A_3 = 0,$$

where

$$\begin{aligned} A_1 &:= \int_{\Omega' \times B(0)} V_h^i [J(x + he_i) \partial_t (V(x + he_i) + U(x + he_i)) - J(x) \partial_t (V(x) + U(x))] \frac{1}{h} \\ &= \int_{\Omega' \times B(0)} V_h^i (\partial_t V_h^i + \partial_t U_h^i) J(x) + \int_{\Omega' \times B(0)} (\partial_t V(x + he_i) + \partial_t U(x + he_i)) J_h^i(x) V_h^i \\ A_2 &:= \int_{\Omega' \times B(0)} \frac{1}{h} [S(x + he_i) \nabla_y V(x + he_i) - S(x) \nabla_y V(x)] \nabla_y V_h^i \\ &= \int_{\Omega' \times B(0)} S \nabla_y V_h^i \nabla_y V_h^i + \int_{\Omega' \times B(0)} S_h^i \nabla_y V(x + he_i) \nabla_y V_h^i \\ A_3 &:= - \int_{\Omega' \times \Gamma_0} \frac{1}{h} \nabla_y \cdot [S(x + he_i) \nabla_y V(x + he_i) - S(x) \nabla_y V(x)] V_h^i \\ &= - \int_{\Omega' \times \Gamma_0} \nu_y \cdot (S_h^i \nabla_y V(x + he_i) + S \nabla_y V_h^i V_h^i). \end{aligned}$$

Re-arranging conveniently the terms, we obtain the following inequality:

$$\begin{aligned} & \frac{1}{2} \int_{\Omega' \times B(0)} (V_h^i)^2 |J(x)| + \int_{\Omega' \times B(0)} |S(x)| (\nabla_y V_h^i)^2 \leq \int_{\Omega' \times B(0)} |V_h^i \partial_t U_h^i J(x)| \\ & \quad + \int_{\Omega' \times B(0)} |(\partial_t V(x + he_i) + \partial_t U(x + he_i)) J_h^i(x) V_h^i| \\ & \quad + \int_{\Omega' \times B(0)} |S_h^i \nabla_y V(x + he_i) \nabla_y V_h^i| \\ & \quad + \int_{\Omega' \times \Gamma_0} |\nu_y \cdot (S \nabla_y V_h^i) V_h^i| + \int_{\Omega' \times \Gamma_0} |\nu_y \cdot (S_h^i \nabla_y V(x + he_i) V_h^i)| \\ & = \sum_{\ell=1}^5 I_\ell. \end{aligned} \quad (5.37)$$

To estimate the terms I_ℓ we make use of Cauchy-Schwarz and Young inequalities, the inequality between the arithmetic and geometric means, and of the trace inequality. We get

$$|I_1| \leq \frac{\|J\|_{L^\infty(\Omega' \times B(0))}^2}{2} \|V_h^i\|_{L^2(\Omega' \times B(0))} + \frac{1}{2} \|\partial_t U_h^i\|_{L^2(\Omega' \times B(0))}, \quad (5.38)$$

$$|I_2| \leq \frac{\|J\|_{L^\infty(\Omega' \times B(0))}^2}{2} 2 (\|\partial_t V(x + he_i)\|_{L^2(\Omega' \times B(0))} + \|\partial_t U(x + he_i)\|_{L^2(\Omega' \times B(0))}) + \|V_h^i\|_{L^2(\Omega' \times B(0))}, \quad (5.39)$$

$$|I_3| \leq \epsilon \|\nabla_y V_h^i\|_{L^2(\Omega' \times B(0))}^2 + c_\epsilon \|S_h^i\|_{L^\infty(\Omega' \times B(0))}^2 \|\nabla_y V(x + he_i)\|_{L^2(\Omega' \times B(0))}^2, \quad (5.40)$$

$$\begin{aligned} \int_{\Omega' \times \Gamma_0} |\nu_y \cdot (S \nabla_y V_h^i) V_h^i| &\leq \|S\|_{L^\infty(\Omega' \times \Gamma_0)} \|V_h^i\|_{L^\infty(\Omega' \times \Gamma_0)} \int_{\Omega' \times \Gamma_0} |\nu_y \cdot \nabla_y V_h^i| \\ &\leq |B(0)|^{\frac{1}{2}} \|S\|_{L^\infty(\Omega' \times \Gamma_0)} \|V_h^i\|_{L^\infty(\Omega' \times \Gamma_0)} \|V_h^i\|_{L^1(\Omega'; H^2(B(0)))}, \end{aligned} \quad (5.41)$$

and

$$\int_{\Omega' \times \Gamma_0} |\nu_y \cdot (S \nabla_y V(x + he_i)) V_h^i| \leq |B(0)|^{\frac{1}{2}} \|S\|_{L^\infty(\Omega' \times \Gamma_0)} \|V_h^i\|_{L^\infty(\Omega' \times \Gamma_0)} \|V\|_{L^1(\Omega'; H^2(B(0)))}. \quad (5.42)$$

Note that all terms $|I_\ell|$ are bounded from above. To get their boundedness we essentially rely on the energy estimates for V , U , U_h^i as well as on the L^∞ -estimates on V and V_h^i on sets like $\Omega' \times B(0)$ and $\Omega' \times \Gamma_0$. The conclusion of this proof follows by applying Gronwall's inequality. \square

Using the claims above, we are now able to finish the proof of Lemma 5.7, by noting that $T_3 \circ T_2 : L^2(S; H^1(\Omega; H^2 \cap H_0^1(B_0))) \rightarrow L^2(S; H^1(\Omega))$ is continuous and compact via applying Lemma 5.2 with $B_0 = H^1(\Omega)$ and $B = B_1 = L^2(\Omega)$. \square

Putting now together the above results, we are able to formulate the main result of section 5, namely:

Theorem 5.11 *Problem (P) admits at least a global-in-time weak solution in the sense of Definition 5.1.*

6 Discussion

The remaining challenge is to make the asymptotic homogenization step (the passage $\epsilon \rightarrow 0$) rigorous. Due to the x -dependence of the microstructure the existing rigorous ways of passing to the limit seem to fail [3, 14, 21]. As next step, we hope to be able to marry successfully the philosophy of the corrector estimates analysis by Checkin and Piatnitski [6] with the intimate two-scale structure of our model.

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