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Homogenisation of a locally periodic medium with areas of low and high diffusivity

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We aim at understanding transport in porous materials consisting of regions with both high and low diffusivities. We apply a formal homogenisation procedure to the case where *the heterogeneities are not arranged in a strictly periodic manner*. The result is a two-scale model formulated in x-dependent Bochner spaces. We prove the weak solvability of the limit two-scale model for a prototypical advection–diffusion system of minimal size. 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.

Key words: Heterogeneous porous materials; Locally periodic homogenisation; 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 [2–4, 8, 24] 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]) [6, 16].

The homogenisation of these 'high-contrast' media is well developed (see, e.g. [4, 6] and the references therein), but in this paper we relax the strictly periodic setting that is considered in the cited papers. We value this an important issue since a real heterogeneous medium is almost never periodic. The geometric arrangement of the heterogeneities that we allow in this paper is such that the spacing of the low diffusive areas is still periodic, but their shape and size need not be identical. We call this a locally periodic[2] medium and we refer the reader to Section 2 (in particular to Figure 1), where we explain our

[1] 'Micro' refers here to a continuum description of a porous sub-domain at a separated (lower) spatial scale compared to the 'macro' one.
[2] The terminology 'local periodicity' is taken form [9].

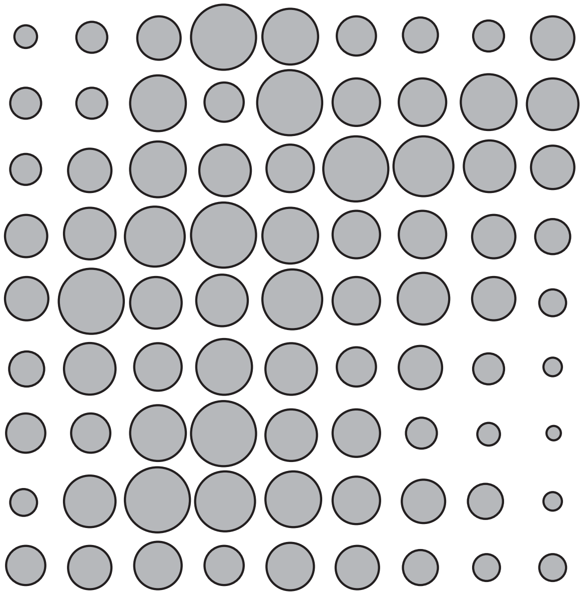

FIGURE 1. Schematic representation of a locally periodic heterogeneous medium. For a given $\epsilon > 0$, the low-diffusivity areas might look like the grey areas in the figure. The centres of the grey areas are on a grid with width ϵ, but their shape and size may vary.

concept of local periodicity. To avoid confusion, we find it important to mention, already at this early stage, that here we tackle locally periodic arrays of micro-structures, which is much more challenging than simply considering locally periodic coefficients in PDEs posed in fixed or eventually periodically perforated domains (see, e.g. [5]).

The two-scale convergence concept (see, e.g. [1, 28]) fails to be directly applicable to the locally periodic setting in this paper. When periodicity is lacking, the typical strategy would be to tackle the matter from the percolation theory perspective (see, e.g. chapter 2 in [14] and references cited therein[3]) or to reformulate the oscillating problem in terms of stochastic homogenisation/random fields (see, e.g. [7]). In this paper, we wish to stay within a deterministic framework by deviating in a controlled manner (made precise in Section 2) from the purely periodic homogenisation. On this way, we prepare the justification of the formal asymptotic homogenisation performed in [13] for a reaction–diffusion scenario modelling the slow chemical corrosion of concrete materials.

The results of our paper are twofold:

(i) We adapt existing strategies to deal (formally) with the asymptotics $\epsilon \to 0$ for a locally periodic medium (where $\epsilon > 0$ is the micro-structure width) and derive a macroscopic equation and *x-dependent* effective transport coefficients (porosity, permeability, tortuosity) for the species undergoing fast transport (i.e. one living in highly diffusive areas), while we preserve the precise (x-dependent) geometry of the micro-structure

[3] Figure 2.3(a) in [14], 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.

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and corresponding balance equation. The result of this homogenisation procedure is a distributed-micro-structure model in the terminology of R. E. Showalter, which we refer here as *two-scale model*.

(ii) We analyse the solvability of the resulting two-scale model with perfectly matched micro–macro boundary condition. As a consequence of the presence of x-dependent micro-structures, the (weak) solutions of the two-scale model are elements of x-dependent Bochner spaces. Our approach benefits from previous works on two-scale models by, e.g. Showalter and Walkington [25], Eck [11] and Meier and Böhm [19,20]. 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 [25], where the situation is formulated as a Cauchy problem in Hilbert spaces and then resolved by holomorphic semigroups, or to [19], where a Banach fixed-point argument for the problem stated in transformed domains (i.e. x-independent) is employed. Our construction of the fixed point operator seems to be new.

We illustrate here our working methodology for a prototypical diffusion system of minimal size. Having this tool now available allows us to address elsewhere the practical situation described in [13]. 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 (see Remark 5.12). We only emphasise the fact that if chemical reactions take place, then most likely they will be hosted by the micro-structures of the low-diffusivity regions. In particular, as far as the formal homogenisation approach is concerned, we can treat in a quite similar way situations where free-interfaces travel the micro-structure; we refer the reader to [26] for a dissolution/precipitation free-boundary problem and [22] for a fast-reaction–slow-diffusion scenario where we addressed the matter.

The formal asymptotics approach we choose here builds upon the one used in [26,27] and is conceptually related to the (locally periodic) formal asymptotics and corresponding rigorous justifications as performed by Belyaev, Chechkin, Piatnitskii, Friedman and co-workers during the last 10–15 years (see, for instance the corresponding papers cited in [9,13]).

The paper is organised 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 micro-structure. The homogenisation 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 conclusions section concludes the paper.

2 Model equations

We consider a heterogenous 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

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two-dimensional bounded domain by $\Omega \subset \mathbb{R}^2$, with boundary Γ. A convenient way to parameterise the interface Γ^ϵ between the high- and low-diffusivity areas 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 use the following characterisation of S^ϵ:

$$S^\epsilon(x) = S_0(x, x/\epsilon) + \epsilon S_1(x, x/\epsilon + \epsilon^2 S_2(x, x/\epsilon) + \ldots, \tag{2.1}$$

where $S_i : \Omega \times U \to \mathbb{R}$, for $i = 0, 1, 2, \ldots$, are 1-periodic in their second variable, with U the unit square defined by

$$U := \{y \in \mathbb{R}^2 \mid -1/2 \leqslant y_i \leqslant 1/2 \text{ for } i = 1, 2\}), \tag{2.2}$$

and where S is independent of ϵ.

We call a medium of which the geometry is specified with a level set function of the type that is given in (2.1) a locally periodic medium [9]. In Figure 1, a schematic picture is given of how such a medium might look like for a given $\epsilon > 0$.

We define the area of low diffusivity Ω_l^ϵ by

$$\Omega_h^\epsilon := \{x \in \Omega \mid S^\epsilon(x) > 0\},$$

and we define the area of high diffusivity Ω_h^ϵ by

$$\Omega_h^\epsilon := \{x \in \Omega \mid S^\epsilon(x) > 0\}.$$

The boundary between high- and low-diffusivity areas Γ^ϵ is now given by

$$\Gamma^\epsilon := \{x \in \Omega \mid S^\epsilon(x) = 0\}.$$

We assume that $S_0(x, 0) <$ const. < 0 and $S_0(x, y)|_{y \in \partial U} >$ const. > 0 for all $x \in \Omega$ and that the S_i, for $i = 0, 1, 2, \ldots$, are bounded so that in the limit $\epsilon \to 0$ the areas of low diffusivity in each unit cell do not touch each other.

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 fluxes across the boundary between the high- and low-diffusivity areas.

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The model is now given by

$$\begin{cases} u_t^\epsilon = \nabla \cdot (D_h \nabla u^\epsilon - q^\epsilon u^\epsilon) \\ q^\epsilon = -\kappa \nabla p^\epsilon \\ \nabla \cdot q^\epsilon = 0 \end{cases} \quad \text{in } \Omega_h^\epsilon, \tag{2.3}$$

$$\left\{ v_t^\epsilon = \epsilon^2 \nabla \cdot (D_l \nabla v^\epsilon) \quad \text{in } \Omega_l^\epsilon, \right. \tag{2.4}$$

$$\begin{cases} v^\epsilon \cdot (D_h \nabla u^\epsilon) = \epsilon^2 v^\epsilon \cdot (D_l \nabla v^\epsilon) \\ u^\epsilon = v^\epsilon \\ q^\epsilon = 0 \end{cases} \quad \text{on } \Gamma^\epsilon, \tag{2.5}$$

$$\begin{cases} u^\epsilon(x,t) = u_b(x,t) \\ q^\epsilon(x,t) = q_b(x,t) \end{cases} \quad \text{on } \Gamma, \tag{2.6}$$

$$\begin{cases} u^\epsilon(x,0) = u_I^\epsilon(x) & \text{in } \Omega_h^\epsilon, \\ v^\epsilon(x,0) = v_I^\epsilon(x) & \text{in } \Omega_l^\epsilon, \end{cases} \tag{2.7}$$

where D_h denotes the diffusion coefficient in the high-diffusivity region, D_l denotes the diffusion coefficient in the low-diffusivity regions, κ denotes the permeability in the Darcy law for the flow in the high-diffusivity region, v^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 homogenisation

For the formal homogenisation, 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

$$\nabla f = \nabla_x f + \frac{1}{\epsilon} \nabla_y f|_{y=\frac{x}{\epsilon}}, \tag{3.1}$$

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

3.1 Interface conditions

In (2.5_1), we have used the superscript ϵ for the normal vector v^ϵ in the interface conditions for v^ϵ and u^ϵ. The reason is that the normal vector depends on the geometry

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of the different regions, and this, in turn, depends on ϵ. In order to perform the steps of formal homogenisation, we have to expand v^ϵ in a power series in ϵ. This can be done in terms of the level set function S^ϵ:

$$v^\epsilon = \frac{\nabla S^\epsilon(x, x/\epsilon)}{|\nabla S^\epsilon(x, x/\epsilon)|} \text{ at } x \in \Gamma^\epsilon. \tag{3.2}$$

First, we expand $|\nabla S^\epsilon|$. Using the chain rule (3.1) (see also [14]), the expansion (2.1) of S^ϵ and the Taylor series of the square-root function, we obtain

$$|\nabla S^\epsilon| = \frac{1}{\epsilon}|\nabla_y S_0| + O(\epsilon^0). \tag{3.3}$$

In the same fashion, we get

$$v^\epsilon = v_0 + \epsilon v_1 + O(\epsilon^2),$$

where

$$v_0 := \frac{\nabla_y S_0}{|\nabla_y S_0|}$$

and

$$v_1 := \frac{\nabla_x S_0 + \nabla_y S_1}{|\nabla_y S_0|} - \frac{(\nabla_x S_0 \cdot \nabla_y S_0 + \nabla_y S_0 \cdot \nabla_y S_1)}{|\nabla_y S_0|^2}\frac{\nabla_y S_0}{|\nabla_y S_0|}.$$

If we introduce the normalised tangential vector τ_0, with $\tau_0 \perp v_0$, we can rewrite v_1 as

$$v_1 = \tau_0 \frac{\tau_0 \cdot (\nabla_x S_0 + \nabla_y S_1)}{|\nabla_y S_0|}. \tag{3.4}$$

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 v^ϵ into (2.5). This is not so straightforward as it may seem, since the interface conditions (2.5) 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

$$\Gamma_0(x) := \{y \,|\, S_0(x, y) = 0\}. \tag{3.5}$$

To obtain them, we suppose that we can parameterise 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

$$k^\epsilon(s) = x_{ij} + \epsilon k_0(s) + \epsilon^2 k_1(s) + O(\epsilon^3). \tag{3.6}$$

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 $k_0(s)$ parameterises locally the zero level set of S_0:

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

For k_1, we have equation

$$S_1(x,k_0) + k_0 \cdot \nabla_x S_0(x,k_0) + k_1 \cdot \nabla_y S_0(x,k_0) = 0. \tag{3.7}$$

It suffices to seek for k_1 that is aligned with v_0 so that we write

$$k_1(s) = \lambda(s))v_0(s) = \lambda \frac{\nabla_y S_0}{|\nabla_y S_0|}, \tag{3.8}$$

where, using (3.7), λ is given by

$$\lambda := -\frac{S_1}{|\nabla_y S_0|} - \frac{k_0 \cdot \nabla_x S_0}{|\nabla_y S_0|}. \tag{3.9}$$

Each of the boundary conditions in (2.5) 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 (3.6) and the Taylor series of K around (x, k_0), we obtain

$$K(x,k_0) + \epsilon(k_0 \cdot \nabla_x K(x,k_0) + k_1 \cdot \nabla_y K(x,k_0)) + \frac{\epsilon^2}{2}(k_0,k_1) \cdot (\mathscr{D}^2 K(x,k_0))(k_0,k_1) + \epsilon^3(\ldots) = 0, \tag{3.10}$$

where $\mathscr{D}^2 K$ denotes the Hessian of K with respect to x and y. Substituting (3.8) into (3.10), we can re-state (3.10) in the following way:

$$K(x,y) + \epsilon(y \cdot \nabla_x K(x,y) + \lambda v_0 \cdot \nabla_y K(x,y)) + \frac{\epsilon^2}{2}(y, \lambda v_0) \cdot (\mathscr{D}^2 K(x,y))(y, \lambda v_0) + O(\epsilon^3) = 0 \text{ for all } y \in \Gamma_0(x). \tag{3.11}$$

In order to proceed further, we make use of the following technical lemmas. Their proofs can be found in [26].

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 $t \geqslant 0$. Then, it holds that*

$$\nabla_x g = \frac{v_0 \cdot \nabla_y g}{|\nabla_y S_0|} \nabla_x S_0, \quad \textit{for } x \in \Omega, \; y \in \Gamma_0(x,t).$$

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

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

3.2 Flow equations

Substituting the asymptotic expansions of q^ϵ and p^ϵ into $(2.3_{2,3})$, we obtain

$$q_0 = -\kappa \frac{1}{\epsilon} \nabla_y p_0 - \kappa \nabla_y p_1 - \kappa \nabla_x p_0 + O(\epsilon), \tag{3.12}$$

$$\frac{1}{\epsilon} \nabla_y \cdot q_0 + \nabla_x \cdot q_0 + \nabla_y \cdot q_1 + O(\epsilon) = 0. \tag{3.13}$$

Substituting the asymptotic expansion of q^ϵ into the boundary condition (2.5_3), and using (3.11), gives

$$q_0 + \epsilon\big(q_1 + (\nabla_x q_0)^T y + \lambda (\nabla_y q_0)^T \nu_0\big) + O(\epsilon^2) = 0, \ \text{ for all } y \in \Gamma_0(x). \tag{3.14}$$

The ϵ^{-1}-term in (3.12) 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 (3.12) and (3.14) and ϵ^{-1}-terms from (3.13), equations for q_0 and p_1 as follows:

$$\begin{cases} q_0 = -\kappa \nabla_y p_1 - \kappa \nabla_x p_0 & \text{in } \ Y_0(x), \\ \nabla_y \cdot q_0 = 0 & \text{in } \ Y_0(x), \\ q_0 = 0 & \text{on } \ \Gamma_0(x), \\ q_0 \text{ and } p_0 \ y\text{-periodic}, & \end{cases} \tag{3.15}$$

where

$$Y_0(x) := \{y \,|\, S_0(x, y) > 0\}. \tag{3.16}$$

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 (3.13))

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

with

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

$$I_2 := - \int_{\Gamma_0(x)} \nu_0 \cdot \left(\frac{S_1}{|\nabla_y S_0|} (\nabla_y q_0)^T \nu_0 \right) d\sigma.$$

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

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

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

$$\nabla_x \cdot \bar{q} = 0. \tag{3.17}$$

3.3 Diffusion equation in the low-diffusivity areas

Substituting the asymptotic expansion of v^ϵ into (2.4), we obtain

$$\partial_t v_0 = D_l \nabla_y v_0 + O(\epsilon). \tag{3.18}$$

Similarly expanding the boundary condition (2.5$_2$), we get

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

which, after substitution into (3.11), becomes

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

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

$$v_0(x, y, t) = u_0(x, t) \text{ for all } y \in \Gamma_0(x),\ x \in \Omega. \tag{3.19}$$

3.4 Convection–diffusion equation in the high-diffusivity area

Substituting the asymptotic expansion of u^ϵ into (2.3$_1$), we obtain

$$\partial_t u_0 = \frac{1}{\epsilon^2} D_h \Delta_y u_0 + \frac{1}{\epsilon} (\nabla_y \cdot F_h + \nabla_x \cdot (D_h \nabla_y u_0)) + \nabla_y \cdot (D_h(\nabla_y u_2 + \nabla_x u_1) - q_1 u_0 - q_0 u_1)$$
$$+ \nabla_x \cdot F_h \quad + O(\epsilon), \tag{3.20}$$

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where

$$F_h := D_h(\nabla_x u_0 + \nabla_y u_1) - q_0 u_0. \tag{3.21}$$

Using the expansions for u^ϵ, v^ϵ and v^ϵ, we first expand (2.5_1):

$$\begin{aligned}
0 &= v^\epsilon \cdot (D_h \nabla u^\epsilon) - \epsilon^2 v^\epsilon \cdot (D_l \nabla v_\epsilon) \\
&= \frac{1}{\epsilon} v_0 \cdot (D_h \nabla_y u_0) + v_0 \cdot (D_h(\nabla_x u_0 + \nabla_y u_1)) + v_1 \cdot (D_h \nabla_y u_0) \\
&\quad + \epsilon\big(v_0 \cdot (D_h(\nabla_x u_1 + \nabla_y u_2)) + v_1 \cdot (D_h(\nabla_x u_0 + \nabla_y u_1)) + v_2 \cdot (D_h \nabla_y u_0) - v_0 \cdot (D_l \nabla_y v_0)\big) \\
&\quad + O(\epsilon^2), \text{ for all } x \in \Gamma^\epsilon \text{ and } y = \frac{x}{\epsilon}.
\end{aligned}$$

Next, we substitute this expansion into (3.11) and thus obtain

$$\begin{aligned}
0 = &\frac{1}{\epsilon} v_0 \cdot (D_h \nabla_y u_0) \\
&+ v_0 \cdot (D_h(\nabla_x u_0 + \nabla_y u_1)) + v_1 \cdot (D_h \nabla_y u_0) + y \cdot \nabla_x (v_0 \cdot (D_h \nabla_y u_0)) + \lambda v_0 \cdot \nabla_y (v_0 \cdot (D_h \nabla_y u_0)) \\
&+ \epsilon\big(v_0 \cdot (D_h(\nabla_x u_1 + \nabla_y u_2)) + v_1 \cdot D_h(\nabla_x u_0 + \nabla_y u_1) + v_2 \cdot (D_h \nabla_y u_0) \\
&- v_0 \cdot (D_l \nabla_y v_0) + y \cdot \nabla_x (v_0 \cdot (D_h(\nabla_x u_0 + \nabla_y u_1)) + v_1 \cdot (D_h \nabla_y u_0)) \\
&+ \lambda v_0 \cdot \nabla_y (v_0 \cdot (D_h(\nabla_x u_0 + \nabla_y u_1)) + v_1 \cdot (D_h \nabla_y u_0)) \\
&+ \frac{1}{2}(y, \lambda v_0) \cdot (\mathscr{D}^2(v_0 \cdot (D_h \nabla_y u_0)))(y, \lambda v_0)\big) + O(\epsilon^2), \quad \text{for } y \in \Gamma_0(x).
\end{aligned} \tag{3.22}$$

Now, we collect the ϵ^{-2}-term from (3.20) and the ϵ^{-1}-term from (3.22). Hence, we obtain for u_0 the equations

$$\begin{cases}
\Delta_y u_0 = 0 & \text{in } Y_0(x), \\
v_0 \cdot \nabla_y u_0 = 0 & \text{on } \Gamma_0(x), \\
u_0 \ y\text{-periodic},
\end{cases} \tag{3.23}$$

where $Y_0(x)$ is given by (3.16). 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 (3.20), the ϵ^0-terms from (3.22), and using that $\nabla_y u_0 = 0$, we get for u_1 the equations

$$\begin{cases}
\nabla_y \cdot (D_h \nabla_y u_1 - q_0 u_0) = 0 & \text{in } Y_0(x), \\
v_0 \cdot (D_h(\nabla_x u_0 + \nabla_y u_1)) = 0 & \text{on } \Gamma_0(x), \\
u_1 \ y\text{-periodic}.
\end{cases} \tag{3.24}$$

Collecting the ϵ^0-terms from (3.20) and the ϵ^1-terms from (3.22), we obtain

$$\begin{cases}
\partial_t u_0 = \nabla_y \cdot (D_h(\nabla_y u_2 + \nabla_x u_1) - q_1 u_0 - q_0 u_1) + \nabla_x \cdot F_h & \text{in } Y_0(x), \\
v_0 \cdot (D_h(\nabla_x u_1 + \nabla_y u_2)) = -v_1 \cdot (D_h(\nabla_x u_0 + \nabla_y u_1)) \\
\qquad + v_0 \cdot (D_l \nabla_y v_0) - y \cdot \nabla_x (v_0 \cdot (D_h(\nabla_x u_0 + \nabla_y u_1))) \\
\qquad - \lambda v_0 \cdot \nabla_y (v_0 \cdot (D_h(\nabla_x u_0 + \nabla_y u_1))) & \text{on } \Gamma_0(x), \\
u_2 \ y\text{-periodic}.
\end{cases} \tag{3.25}$$

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Integrating (3.25_1) over $Y_0(x)$ and using the boundary conditions (3.15_3) and (3.25_2) yields

$$
\begin{aligned}
|Y_0(x)|\partial_t u_0 &= \int_{Y_0(x)} \nabla_y \cdot (D_h(\nabla_x u_1 + \nabla_y u_2) - q_1 u_0 - q_0 u_1)\, dy + \int_{Y_0(x)} \nabla_x \cdot F_h\, dy \\
&= \int_{\Gamma_0(x)} -v_1 \cdot F_h + v_0 \cdot (D_l \nabla_y v_0) - y \cdot \nabla_x (v_0 \cdot F_h) - \lambda v_0 \cdot \nabla_y (v_0 \cdot F_h)\, d\sigma \\
&\quad + \nabla_x \cdot \int_{Y_0(x)} F_h\, dy + \int_{\Gamma_0(x)} \frac{\nabla_x S_0}{|\nabla_y S_0|} \cdot F_h\, d\sigma.
\end{aligned}
$$

Using (3.4), (3.9) and the boundary conditions (3.15_3) and (3.24_2), this can be re-written as

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

where

$$
\begin{aligned}
I_1 &:= \int_{\Gamma_0(x)} y \cdot \nabla_x g - \frac{y \cdot \nabla_x S_0}{|\nabla_y S_0|} v_0 \cdot \nabla_y g\, d\sigma, \\
I_2 &:= \int_{\Gamma_0(x)} \frac{\tau_0 \cdot \nabla_y S_1}{|\nabla_y S_0|} \tau_0 \cdot F_h - \frac{S_1}{|\nabla_y S_0|} v_0 \cdot \nabla_y (v^0 \cdot F_h)\, d\sigma,
\end{aligned}
$$

with $g := v_0 \cdot F_h$. The boundary conditions (3.15_3) and (3.24_2) give us $g(x, y, t) = 0$ for $y \in \Gamma_0(x, t)$. Now, invoking Lemma 3.1 leads to $\nabla_x g = \frac{v_0 \cdot \nabla_y g}{|\nabla_y S_0|} \nabla_x S_0$. 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 (3.19) to obtain

$$
\partial_t \left(|Y_0(x)| u_0 + \int_{Y_0^C(x)} v_0\, dy \right) = \nabla_x \cdot \int_{Y_0(x)} (D_h(\nabla_y u_1 + \nabla_x u_0) - q_0 u_0)\, dy, \tag{3.26}
$$

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

Equations for lowest order terms of q^ϵ and p^ϵ, (3.15) and (3.17), v^ϵ, (3.18), u^ϵ, (3.26), and the coupling conditions (3.19) together constitute the upscaled model. In this section, we collect these equations. We write the solutions of (3.24) and (3.15) in terms of the

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solutions of the following two cell problems (see, e.g. [14])

$$\begin{cases} \Delta_y v_j(x,y) = 0 & \text{for all } x \in \Omega,\ y \in Y_0(x), \\ v_0 \cdot \nabla_y v_j(x,y) = -v_0 \cdot e_j & \text{for all } x \in \Omega,\ y \in \Gamma_0(x), \\ v_j(x,y) \ y\text{-periodic}, \end{cases} \tag{4.1}$$

and

$$\begin{cases} w_j(x,y) = \nabla_y \pi_j(x,y) + e_j & \text{for all } x \in \Omega,\ y \in Y_0(x), \\ \nabla_y \cdot w_j(x,y) = 0 & \text{for all } x \in \Omega,\ y \in Y_0(x), \\ w_j = 0 & \text{for all } x \in \Omega,\ y \in \Gamma_0(x), \\ w_j(x,y) \text{ and } \pi_j(x,y) \ y\text{-periodic}, \end{cases} \tag{4.2}$$

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

$$\begin{cases} \partial_t v_0(x,y,t) = D_l \Delta_y v_0(x,y,t) & \text{for } x \in \Omega,\ y \in Y_0^C(x), \\ \partial_t \left(\theta(x) u_0 + \int_{|y|<r(x)} v_0 \, dy \right) & \\ \quad = \nabla_x \cdot (D_h \mathscr{A}(x) \nabla_x u_0 - \bar{q} u_0) & \text{for } x \in \Omega, \\ \bar{q} = -\kappa \mathscr{K}(x) \nabla_x p_0 & \text{for } x \in \Omega, \\ \nabla_x \cdot \bar{q} = 0 & \text{for } x \in \Omega, \end{cases} \tag{4.3}$$

$$\begin{cases} v_0(x,y,t) = u_0(x,t) & \text{for } x \in \Omega,\ y \in \Gamma_0(x), \\ u_0(x,t) = u_b(x,t) & \text{for } x \in \Gamma, \\ \bar{q}(x,t) = q_b(x,t) & \text{for } x \in \Gamma, \end{cases} \tag{4.4}$$

$$\begin{cases} u_0(x,0) = u_I(x) & \text{for } x \in \Omega, \\ v_0(x,y,0) = v_I(x,y) & \text{for } x \in \Omega,\ y \in Y_0^C(x). \end{cases} \tag{4.5}$$

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

$$\theta(x) := |Y_0(x)|,$$

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

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

and

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

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5 Analysis of upscaled equations

In this section, we investigate the solvability of the upscaled equations (4.3)–(4.5). Note that ($4.3_{3,4}$) for $\bar{q}$ and p_0, together with the boundary condition (4.4_3) 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 form the theory of partial differential equations justify this assumption if the data q_b and r are suitable (see [15] for a closely related scenario). With this assumption, (4.3)–(4.5) reduce to the following problem:

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

where $B(x) := Y_0(x)$, where Y_0 is defined in (3.16). 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:

$$V_1 := H_0^1(\Omega), \tag{5.1}$$
$$V_2 := L^2(\Omega; H^2(B(x))), \tag{5.2}$$
$$H_1 := L_\theta^2(\Omega), \tag{5.3}$$
$$H_2 := L^2(\Omega; L^2(B(x))). \tag{5.4}$$

The *x-dependent Bochner spaces* H_2 and V_2 make sense , for instance we assume (like in [20]) the following.

Assumption 1 *The function $S_0 : \Omega \times U \to \mathbb{R}$, which defines $B(x) := Y_0(x)$ in* (3.16)*, and which also defines the one-dimensional boundary $\Omega \times \partial B(x)$ of $\Omega \times B(x)$ as*

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

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

Following the lines of [20] and [25], Assumption 1 implies in particular that the measures $|\partial B(x)|$ and $|B(x)|$ are bounded away from zero (uniformly in x). Consequently,

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the following direct Hilbert integrals (cf. [10] (part II, chapter 2))

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

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

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

given by

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

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 [19] for more details on the construction of these spaces and to [21] 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

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

where $S = (0, T]$.

We also define the following constants for later use:

$$M_1 := \max\{\|u_I\|_{L^\infty(\Omega)}, \|u_b\|_{L^\infty(\Omega)}\}, \tag{5.6}$$
$$M_2 := \max\{\|v_I\|_{L^\infty(\Omega)}, M_1\}. \tag{5.7}$$

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

$$\mathbb{V} := \{(\phi, \psi) \in V_1 \times V_2 \,|\, \phi(x) = \psi(x,y) \text{ for } x \in \Omega,\ y \in \partial B(x)\}, \tag{5.8}$$
$$\mathbb{H} := H_1 \times H_2, \tag{5.9}$$

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

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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:*

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

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

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 [18], 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, $W \hookrightarrow\hookrightarrow L^p(S; B)$.

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) $u \geqslant 0$ *for a.e.* $x \in \Omega$ *and for all* $t \in S$*;*

(ii) $v \geqslant 0$ *for a.e.* $(x, y) \in \Omega \times B(x)$ *and for all* $t \in S$*;*

(iii) $u \leqslant M_1$ *for a.e.* $x \in \Omega$ *and for all* $t \in S$*;*

(iv) $v \leqslant M_2$ *for a.e.* $(x, y) \in \Omega \times B(x)$ *and for all* $t \in S$*;*

(v) *The following energy inequality holds:*

$$\|u\|^2_{L^2(S;V_1)\cap L^\infty(S;H_1)} + \|v\|^2_{L^2(S;L^2(\Omega,V_2))\cap L^\infty(S;H_2)} + \|\nabla_x u\|^2_{L^2(S;H_1)} + \|\nabla_y v\|^2_{L^2(S\times\Omega\times B(x))} \leqslant c_1, \tag{5.12}$$

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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

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

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 $D\nabla u_b = u_b\mathrm{div}q$ a.e. in $\Omega \times S$, makes the last term of the right-hand side of (5.13) vanish. The key observation in estimating the last by one term is the fact that the sets $\{x \in \Omega : U(x) \geqslant 0\}$ and $\{x \in \Omega : U(x) \leqslant 0\}$ are Lebesque measurable. This allow to proceed as follows:

$$\int_\Omega U^+\mathrm{divq}\nabla U^- = \int_{\{x\in\Omega:U(x)\geqslant 0\}} U^+\mathrm{div}q\nabla U^- + \int_{\{x\in\Omega:U(x)\leqslant 0\}} U^+\mathrm{div}q\nabla U^- = 0. \tag{5.14}$$

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. □

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

$$\int_\Omega \phi\partial_t\rho\varphi + \int_\Omega D\nabla\rho\nabla\varphi - \int_\Omega q\rho\nabla\varphi + \int_\Omega\int_{B(x)} \partial_t\theta\psi + \int_\Omega\int_{B(x)} D_\ell\nabla_y\theta\nabla_y\psi = 0 \tag{5.15}$$

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

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

$$\int_\Omega \frac{\phi}{2}(\partial_t \rho)^2 + \int_\Omega \int_{B(x)} \frac{1}{2}(\partial_t \theta)^2 + \int_\Omega D|\nabla \rho|^2 + \int_\Omega \int_{B(x)} D_\ell |\nabla_y \theta|^2 = \int_\Omega q\rho\nabla\rho. \tag{5.16}$$

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

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

then (5.16) yields

$$\frac{1}{2}\frac{d}{dt}\int_\Omega \phi|\rho|^2 + \frac{1}{2}\frac{d}{dt}\int_\Omega \int_{B(x)} |\theta|^2 + \int_\Omega (D - \epsilon)|\nabla\rho|^2 + \int_\Omega \int_{B(x)} D_\ell |\nabla_y \theta|^2 \leqslant c_\epsilon ||q||_\infty^2 \int_\Omega |\rho|^2. \tag{5.17}$$

Choose

$$\epsilon \in \left]0, \min_{\Omega \times B(x)} D\right[. \tag{5.18}$$

Since for all $x \in \overline{\Omega}$ and $y \in \overline{B(x)}$, we have $\theta(x, y, 0) = \rho(x, 0) = 0$, (5.17) together with (5.18) 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 $t \in S$. □

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:

$$X_1 := L^2(S; L^2(\Omega)), \tag{5.19}$$

$$X_2 := L^2(S; H_0^1(\Omega)) \cap H^1(S; L^2(\Omega)), \tag{5.20}$$

$$X_3 := L^2(S; V_2) \cap H^1(S; L^2(\Omega; L^2(B(x)))). \tag{5.21}$$

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

$$\int_\Omega \theta\partial_t(U + u_b)\phi\, dx + \int_\Omega (D\nabla_x(U + u_b) - q(U + u_b)) \cdot \nabla_x \phi\, dx = -\int_\Omega f\phi\, dx, \tag{5.22}$$

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

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

$$\int_\Omega \int_{B(x)} \partial_t (V + w)\psi \, dy dx + \int_\Omega \int_{B(x)} D_l \nabla_y (V + w) \cdot \nabla_y \psi \, dy dx = \int_\Omega \int_{\partial B(x)} \nu_y \cdot (D_l \nabla_y (V + w))\psi \, d\sigma dx, \tag{5.23}$$

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

$$f = \int_{\partial B(x)} \nu_y \cdot \nabla_y v \, d\sigma. \tag{5.24}$$

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

$$T := T_3 \circ T_2 \circ T_1. \tag{5.25}$$

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 [17]), 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 right-hand side 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 (5.23) and its weak solution depend (continuously) on the fixed parameter $x \in \Omega$ is not 'disturbing' at this point[4].

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 are ensured. □

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 re-formulate (5.23) 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 $\Psi : \Omega \times B(0) \to \Omega \times B(x)$. We call Ψ a *regular C^2-motion* if $\Psi \in C^2(\Omega \times B(0))$ with the property that for each $x \in \Omega$

$$\Psi(x, \cdot) : B(0) \to B(x) := \Psi(x, B(0)) \tag{5.26}$$

[4] However, note that this x-dependence will play a crucial role in getting (at a later stage) the compactness of T_2.

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

$$c \leqslant \det \nabla_y \Psi(x, y) \leqslant C, \tag{5.27}$$

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

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

$$F := \nabla_y \Psi \text{ and } J := \det F \tag{5.28}$$

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

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

The transformed version of (5.23) is now written as follows: let $w \in X_2$ be given, find $\hat{V} \in L^2(S; L^2(\Omega; H_0^1(B(0)))) \cap H^1(S; L^2(\Omega; L^2(B(0)))) * **$

$$\int_\Omega \int_{B(0)} \partial_t(\hat{V} + w)\psi J \, dy dx + \int_\Omega \int_{B(0)} J F_{-1} D_l F^{-T} \nabla_y(\hat{V} + w) \cdot \nabla_y \psi \, dy dx$$
$$= \int_\Omega \int_{\Gamma_0} \hat{v}_y \cdot (J F^{-1} D_l F^{-T} \nabla_y(\hat{V} + w))\psi \, d\sigma dx, \tag{5.29}$$

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

Denote by Γ_0 the boundary of $B(0)$.

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. □

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,*

$$\hat{V} \in L^2(S; L^2(\Omega; H^2_{loc}(B(0)) \cap H_0^1(B(0)))). \tag{5.30}$$

Since Γ_0 is C^2, we have

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

Proof of claim The proof idea follows closely the lines of Theorems 1 and 4 (cf. [12], Section 6.3) □

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

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

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

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

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 [12] (see, e.g. Theorem 1 in Section 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 with respect to x of the involved functions, we omit to indicate the dependence of U on t and 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:

$$\begin{aligned} &\int_{\Omega' \times B(0)} J(x+he_i)\partial_t(V(x+he_i) + U(x+he_i))\psi + \int_{\Omega' \times B(0)} S(x+he_i)\nabla_y V(x+he_i)\nabla_y \psi \\ &\quad - \int_{\Omega' \times \Gamma_0} v_y \cdot (S(x+he_i)D_\ell \nabla_y V(x+he_i))\psi d\sigma = 0 \end{aligned} \tag{5.34}$$

and

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

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

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

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where

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

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

$$\begin{aligned}\frac{1}{2}\int_{\Omega'\times B(0)} (V_h^i)^2|J(x)| + \int_{\Omega'\times B(0)} |S(x)|(\nabla_y V_h^i)^2 \leqslant \int_{\Omega'\times B(0)} |V_h^i\partial_t U_h^i J(x)| \\ + \int_{\Omega'\times B(0)} |(\partial_t V(x+he_i) + \partial_t U(x+he_i))J_h^i(x)V_h^i| \\ + \int_{\Omega'\times B(0)} |S_h^i\nabla_y V(x+he_i)\nabla_y V_h^i| \\ + \int_{\Omega'\times\Gamma_0} |v_y\cdot(S\nabla_y V_h^i)V_h^i| + \int_{\Omega'\times\Gamma_0} |v_y\cdot(S_h^i\nabla_y V(x+he_i)V_h^i)| \\ = \sum_{\ell=1}^{5} I_\ell. \end{aligned} \tag{5.36}$$

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

$$|I_1| \leqslant \frac{||J||^2_{L^\infty(\Omega'\times B(0))}}{2}||V_h^i||_{L^2(\Omega'\times B(0))} + \frac{1}{2}||\partial_t U_h^i||_{L^2(\Omega'\times B(0))}, \tag{5.37}$$

$$\begin{aligned}|I_2| \leqslant \frac{||J||^2_{L^\infty(\Omega'\times B(0))}}{2}2\left(||\partial_t V(x+he_i)||_{L^2(\Omega'\times B(0))} + ||\partial_t U(x+he_i)||_{L^2(\Omega'\times B(0))}\right) \\ + ||V_h^i||_{L^2(\Omega'\times B(0))},\end{aligned} \tag{5.38}$$

$$|I_3| \leqslant \epsilon||\nabla_y V_h^i||^2_{L^2(\Omega'\times B(0))} + c_\epsilon||S_h^i||^2_{L^\infty(\Omega'\times B(0))}||\nabla_y V(x+he_i)||^2_{L^2(\Omega'\times B(0))}, \tag{5.39}$$

$$\begin{aligned}\int_{\Omega'\times\Gamma_0} |v_y\cdot(S\nabla_y V_h^i)V_h^i| \leqslant ||S||_{L^\infty(\Omega'\times\Gamma_0)}||V_h^i||_{L^\infty(\Omega'\times\Gamma_0)}\int_{\Omega'\times\Gamma_0}|v_y\cdot\nabla_y V_h^i| \\ \leqslant |B(0)|^{\frac{1}{2}}||S||_{L^\infty(\Omega'\times\Gamma_0)}||V_h^i||_{L^\infty(\Omega'\times\Gamma_0)}||V_h^i||^2_{L^1(\Omega';H^2(B(0)))},\end{aligned} \tag{5.40}$$

and

$$\int_{\Omega'\times\Gamma_0} |v_y \cdot (S\nabla_y V(x+he_i))V_h^i| \leqslant |B(0)|^{\frac{1}{2}}||S||_{L^\infty(\Omega'\times\Gamma_0)}||V_h^i||_{L^\infty(\Omega'\times\Gamma_0)}||V||^2_{L^1(\Omega';H^2(B(0)))}. \tag{5.41}$$

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. □

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

Putting now together the above results, we are able to formulate the main result of section 5, as given below.

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

Remark 5.12 It is worthwhile to note that the methods of proof used in this section can also deal with volume and surface nonlinear (Lipschitz) reaction rates as well as monotone transport operators. These extensions of the analysis of the problem give some freedom to the modelling of the situation. From the perspective of the formal asymptotics, there are no such limitations in the choice of non-linearities.

6 Conclusions

In this paper, we have derived an effective, two-scale model for transport in heterogeneous porous media using a formal, locally periodic asymptotic method. In this way, we have relaxed the strictly periodic setting that is usual in the existing literature. Furthermore, we have proved existence and uniqueness of weak solutions of the resulting two-scale model, which is defined on x-dependent Bochner spaces.

The remaining challenge is to make the asymptotic homogenisation step (the passage $\epsilon \to 0$) rigorous. Due to the x-dependence of the micro-structure, the existing rigorous ways of passing to the limit seem to fail [6, 16, 23]. As next step, we hope to be able to marry successfully the philosophy of the corrector estimates analysis by Chechkin and Piatnitski [9] with the intimate two-scale structure of our model.

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