SCALINGS IN HOMOGENISATION OF REACTION, DIFFUSION AND INTERFACIAL EXCHANGE IN A TWO-PHASE MEDIUM

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Abstract. We consider the homogenisation of a coupled system of parabolic partial differential equations in a heterogeneous two-phase medium and study various choices of scaling of the material parameters with powers of the homogenisation parameter. The system may be regarded as modelling a reaction–diffusion problem, the Stokes problem of single-phase flow of a slightly compressible fluid or as a heat conduction problem (with or without interfacial resistance). A proper nondimensionalisation shows that, depending on the ratio of the characteristic diffusion times of the different species, different scalings of the diffusivities and the interfacial-exchange coefficient with the scale parameter ε appear reasonable. It is shown that, starting with the same type of problem on the microscopic scale, different choices of scaling of the diffusion coefficients (resp. permeability or conductivity) and the interfacial-exchange coefficient lead to different types of macroscopic systems of equations in the limit. In a unified approach, the limit problems are classified for a whole range of scaling parameters. New limit problems arise and well-known results from the literature are recovered as special cases for certain scalings such as the models of Barenblatt $et.\ al$ and Arbogast $et.\ al$ for single-phase flow.

Key words. Homogenisation, micro-macro, reaction-diffusion

AMS subject classifications. 35B27, 35B30, 35K50, 35K57, 80A20, 80M40.

1. Introduction. In this note, the homogenisation of a coupled system of two partial differential equations given on the microscopic scale is investigated, i.e. we are interested in obtaining the system of equations describing the effective behaviour on the macroscopic scale. The specific setting is such that we are looking at a two-phase medium (a porous medium, for example) made up of two distinct parts (solid matrix and voids, for example) and each equation describes the behaviour of an unknown, such as a concentration or the temperature, e.g., in one part of the medium. The two equations are coupled by an exchange across the internal boundary separating the two parts. The system of equations we are considering can be used to model different physical processes such as a reaction—diffusion problem, the Stokes problem of single-phase flow of a slightly compressible fluid or a heat conduction problem, also cf. (2.1).

More specifically, we consider a material body $\Omega \subset \mathbb{R}^n, n \geq 2$, with Lipschitz-continuous boundary which is made up of two finely interwoven parts, Ω^p and Ω^s . To fix ideas, Ω is assumed to be a porous medium (motivating the superscripts p and s) although any two-phase material can be imagined. It is assumed that Ω is periodic with respect to a representative cell $Y = (0,1)^n$, scaled by the factor $\varepsilon > 0$, which contains a solid particle Z^s (with Lipschitz-continuous boundary) surrounded by void (pore) space Z^p , i.e. we have $\Omega^p_{\varepsilon} = \Omega \cap \bigcup_k \varepsilon \overline{Z}^p_k$ and $\Omega^s_{\varepsilon} = \Omega \cap \bigcup_k \varepsilon \overline{Z}^s_k$ where the subscript k denotes translation of the set by $k \in \mathbb{Z}^n$ and the subscript ε indicates the ε -periodic geometry of the domain. It can be noted that Z^s may or may not be completely contained in Y so that Ω^s may either be connected or not. However, Ω^p_{ε} is assumed connected and, for n = 2, this implies that Ω^s_{ε} may not be connected. The Lipschitz-continuous interface

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separating Ω_{ε}^{p} from Ω_{ε}^{s} is denoted by Γ_{ε} (i.e. $\Gamma_{\varepsilon} = \Omega \cap \bar{\Omega}_{\varepsilon}^{p} \cap \bar{\Omega}_{\varepsilon}^{s}$) and its unit normal ν_{ε} is directed into Ω_{ε}^{s} . Moreover, the reference time interval is S = (0, T) with T > 0.

Before beginning with the homogenisation analysis, a proper nondimensionalisation is carried out. Depending on the ratio of the characteristic diffusion times of the different species, different scalings of the diffusivities and the interfacial-exchange coefficient with the scale parameter ε appear reasonable. We remark that most authors considering similar problems omit the nondimensionalisation.

While the (possibly approximate) value of ε is given by the underlying geometry of the medium, the idea of homogenisation theory (cf. [6, 17, 8], for example) is to examine the limit as ε approaches zero in order to obtain averaged problems defined in all of Ω which are easier to treat numerically and which give useful information about macroscopically observable processes. Depending on the particular scaling of the diffusivities and the interfacial-exchange coefficient, different types of limit problems are obtained from the same type of micromodel.

This note is organised as follows. After formulating the problem in its dimensional form, we perform a nondimensionalisation which results in a system of equations where powers of the scaling parameter ε appear in the diffusion and interfacial-exchange terms. A-priori estimates and existence of solutions of the problem can be proven for each given ε . The method of two-scale convergence can then be extended to allow the determination of the limit problems depending on the choice of powers of ε . For certain choices, well-known results from the literature are recovered while for others, new limit problems arise (cf. Section 4, especially Subsection 4.2)

2. The problem. Introduce a characteristic macroscopic length scale L (the diameter of Ω , e.g.) and a characteristic microscopic length scale ℓ (a typical pore diameter, e.g.) and write $\varepsilon = \ell/L$. It is clear that we then have $\varepsilon \ll 1$. Denoting the unknowns by $u_{\varepsilon}^{\rm s}$ and $u_{\varepsilon}^{\rm s}$, respectively, we consider the following problem,

$$\partial_t u_{\varepsilon}^{\mathbf{p}}(x,t) - \nabla \cdot (D_{\varepsilon}^{\mathbf{p}} \nabla u_{\varepsilon}^{\mathbf{p}}) = \hat{f}_{\varepsilon}^{\mathbf{p}}, \quad x \in \Omega_{\varepsilon}^{\mathbf{p}}, \ t \in S,
\partial_t u_{\varepsilon}^{\mathbf{s}}(x,t) - \nabla \cdot (D_{\varepsilon}^{\mathbf{s}} \nabla u_{\varepsilon}^{\mathbf{s}}) = \hat{f}_{\varepsilon}^{\mathbf{s}}, \quad x \in \Omega_{\varepsilon}^{\mathbf{s}}, \ t \in S,$$
(2.1a)

$$-(D_{\varepsilon}^{p} \nabla u_{\varepsilon}^{p}) \cdot \nu_{\varepsilon} = -(D_{\varepsilon}^{s} \nabla u_{\varepsilon}^{s}) \cdot \nu_{\varepsilon}, \qquad x \in \Gamma_{\varepsilon}, \ t \in S,$$

$$-(D_{\varepsilon}^{p} \nabla u_{\varepsilon}^{p}) \cdot \nu_{\varepsilon} = a_{\varepsilon} (C^{H} u_{\varepsilon}^{p} - u_{\varepsilon}^{s}), \qquad x \in \Gamma_{\varepsilon}, \ t \in S.$$

$$(2.1b)$$

The positive constant C^H describes the ratio of u_{ε}^s and u_{ε}^p in equilibrium and $\hat{f}_{\varepsilon}^{\alpha}$, $\alpha \in \{p, s\}$, describes any internal sources or sinks. The system is completed by initial conditions and boundary conditions at the exterior boundary. We choose homogeneous Neumann conditions for simplicity in what follows although other types of boundary conditions could be prescribed.

A typical situation where a system like (2.1) arises is when modelling the degradation of concrete structures induced by *carbonation*. A main sub-process of the carbonation process is that of atmospheric carbon dioxide entering the concrete through the air-filled pores and getting dissolved in the pore water. There it reacts with dissolved constituents of the cement paste in a reaction of the form

$$aA(aq) + bB(aq) \rightarrow cC(aq) + \dots$$

In this problem, the unknowns u_{ε}^{p} and u_{ε}^{s} are the concentrations of carbon dioxide in pore air and pore water, respectively, and Ω is actually made up of three different phases (where one phase, the solid matrix, does not need to be considered).

2.1. Nondimensionalisation. In order to avoid technicalities, we assume D_{ε}^{p} , D_{ε}^{s} and a_{ε} to equal positive constants D^{p} , D^{s} and a, respectively. However, the following considerations could also be carried out with positive tensors D_{ε}^{p} , D_{ε}^{s} and a_{ε} being bounded from above and away from zero. In this case, D^{p} , D^{s} and a, need to be taken as the respective L^{∞} -bounds in the nondimensionalisation.

Introduce the following dimensionless concentrations,

$$\tilde{u}_{\varepsilon}^{\mathrm{p}} := u_{\varepsilon}^{\mathrm{p}} C^{\mathrm{H}} / u_{\mathrm{ref}}^{\mathrm{p}}, \qquad \tilde{u}_{\varepsilon}^{\mathrm{s}} := u_{\varepsilon}^{\mathrm{s}} / u_{\mathrm{ref}}^{\mathrm{s}},$$

$$(2.2)$$

where u_{ref}^{α} , $\alpha \in \{p, s\}$, are some reference concentrations representing upper bounds on the concentrations. These may be given from physical considerations or maximum estimates, e.g. For each concentration, define a characteristic diffusion time,

$$T^{\mathbf{p}} := \ell^k L^{2-k} / D^{\mathbf{p}}, \qquad T^{\mathbf{s}} := \ell^l L^{2-l} / D^{\mathbf{s}},$$
 (2.3)

where $k,l \in [0,2]$ are to be specified later (cf. Subsection 2.2). Making use of the characteristic length scales introduced earlier, let $\tilde{x} := x/L$ and $\tilde{t}^{\alpha} := t/T^{\alpha}$ be the nondimensional (macroscopic) space and time variables and write $\tilde{u}^{\alpha}(\tilde{x},\tilde{t}^{\alpha}) := u^{\alpha}(\tilde{x}L,\tilde{t}^{\alpha}T^{\alpha})$. Note that the corresponding time intervals are then given by $\tilde{S}^{\rm P} := S/T^{\rm P}$ and $\tilde{S}^{\rm S} := S/T^{\rm S}$. Moreover, we introduce the parameter $m \in \mathbb{R}$ related to the speed of the interfacial exchange (also cf. Subsection 2.2, in particular after (2.8)). Dropping the tildes again and assuming nondimensional variables in what follows, (2.1) transforms to

$$\partial_{t^{\mathrm{p}}} u_{\varepsilon}^{\mathrm{p}} - \varepsilon^{k} \Delta u_{\varepsilon}^{\mathrm{p}} = \frac{T^{\mathrm{p}} C^{\mathrm{H}}}{u_{\mathrm{ref}}^{\mathrm{p}}} \hat{f}_{\varepsilon}^{\mathrm{p}}, \qquad x \in \Omega_{\varepsilon}^{\mathrm{p}},$$

$$\partial_{t^{\mathrm{s}}} u_{\varepsilon}^{\mathrm{s}} - \varepsilon^{l} \Delta u_{\varepsilon}^{\mathrm{s}} = \frac{T^{\mathrm{s}}}{u_{\mathrm{ref}}^{\mathrm{s}}} \hat{f}_{\varepsilon}^{\mathrm{s}}, \qquad x \in \Omega_{\varepsilon}^{\mathrm{s}},$$

$$(2.4a)$$

$$-\varepsilon^{k} \nabla u_{\varepsilon}^{p} \cdot \nu_{\varepsilon} = \varepsilon^{m} \ell^{-m} L^{m-1} T^{p} a(u_{\varepsilon}^{p} - u_{\varepsilon}^{s} u_{\text{ref}}^{s} / u_{\text{ref}}^{p}), \quad x \in \Gamma_{\varepsilon},$$

$$-\varepsilon^{l} \nabla u_{\varepsilon}^{s} \cdot \nu_{\varepsilon} = \varepsilon^{m} \ell^{-m} L^{m-1} T^{s} a(u_{\varepsilon}^{p} u_{\text{ref}}^{p} / u_{\text{ref}}^{s} - u_{\varepsilon}^{s}), \quad x \in \Gamma_{\varepsilon},$$

$$(2.4b)$$

where $t^{\alpha} \in S^{\alpha}$, $\alpha \in \{p, s\}$, and we have $t^{s} = t^{p}T^{p}/T^{s}$ in (2.4b). From a physical point of view, conditions (2.4b) motivate the assumption that both concentrations tend toward the equilibrium $u_{ref}^{p}u_{\varepsilon}^{p} = u_{ref}^{s}u_{\varepsilon}^{s}$. Therefore, it is reasonable to take $u_{ref}^{s} = u_{ref}^{p} =: u_{ref}$, which makes the problem less technical. Note that this simplification is not necessary, however. Introducing the following dimensionless combinations,

$$C_{\text{ex}}^{\text{p}} := \ell^{-m} L^{m-1} T^{\text{p}} a, \quad C_{\text{ex}}^{\text{s}} := \ell^{-m} L^{m-1} T^{\text{s}} a,$$
 (2.5)

$$R^{\rm p} := \frac{T^{\rm p}C^{\rm H}}{u_{\rm ref}}, \quad R^{\rm s} := \frac{T^{\rm s}}{u_{\rm ref}},$$
 (2.6)

and writing $f_{\varepsilon}^{\alpha} := R^{\alpha} \hat{f}_{\varepsilon}^{\alpha}$, the system simplifies to

$$\partial_{t^{p}} u_{\varepsilon}^{p} - \varepsilon^{k} \Delta u_{\varepsilon}^{p} = f_{\varepsilon}^{p}, \qquad x \in \Omega_{\varepsilon}^{p}, \ t^{p} \in S^{p},$$

$$\partial_{t^{s}} u_{\varepsilon}^{s} - \varepsilon^{l} \Delta u_{\varepsilon}^{s} = f_{\varepsilon}^{s}, \qquad x \in \Omega_{\varepsilon}^{s}, \ t^{s} \in S^{s},$$

$$(2.7a)$$

$$-\varepsilon^{k} \nabla u_{\varepsilon}^{p} \cdot \nu_{\varepsilon} = \varepsilon^{m} C_{\text{ex}}^{p} (u_{\varepsilon}^{p} - u_{\varepsilon}^{s}), \qquad x \in \Gamma_{\varepsilon}, -\varepsilon^{l} \nabla u_{\varepsilon}^{s} \cdot \nu_{\varepsilon} = \varepsilon^{m} C_{\text{ex}}^{s} (u_{\varepsilon}^{p} - u_{\varepsilon}^{s}), \qquad x \in \Gamma_{\varepsilon}.$$

$$(2.7b)$$

2.2. Choice of k, l and m. System (2.7) contains three parameters, k, l and m, introduced by the nondimensionalisation. From the nondimensionalisation we get a suggestion which choice of parameters is reasonable: It is desirable (especially from a numerical point of view) that all processes happen on the same time scale. Therefore, k and l need to be chosen such that the characteristic times of diffusion of both species are equal and about one, $T_1 = T_2 \approx 1$. Note that this implies $S^p = S^s =: S$ and $C^p_{\text{ex}} = C^s_{\text{ex}} =: C^{\text{ex}}$. System (2.7) then simplifies to

$$\partial_t u_{\varepsilon}^{\mathbf{p}} - \varepsilon^k \Delta u_{\varepsilon}^{\mathbf{p}} = f_{\varepsilon}^{\mathbf{p}}, \qquad x \in \Omega_{\varepsilon}^{\mathbf{p}}, \ t \in S,
\partial_t u_{\varepsilon}^{\mathbf{s}} - \varepsilon^l \Delta u_{\varepsilon}^{\mathbf{s}} = f_{\varepsilon}^{\mathbf{s}}, \qquad x \in \Omega_{\varepsilon}^{\mathbf{s}}, \ t \in S,$$
(2.8a)

$$-\varepsilon^{k} \nabla u_{\varepsilon}^{p} \cdot \nu_{\varepsilon} = \varepsilon^{m} C^{ex} (u_{\varepsilon}^{p} - u_{\varepsilon}^{s}), \qquad x \in \Gamma_{\varepsilon}, \ t \in S,$$

$$-\varepsilon^{l} \nabla u_{\varepsilon}^{s} \cdot \nu_{\varepsilon} = \varepsilon^{m} C^{ex} (u_{\varepsilon}^{p} - u_{\varepsilon}^{s}), \qquad x \in \Gamma_{\varepsilon}, \ t \in S.$$

$$(2.8b)$$

The parameter m is to be chosen such that $C^{\rm ex} \approx 1$. Note that this corresponds to $a \approx \varepsilon^m L/T_1$, i.e. m needs to be chosen small (or even negative) if a is large and large and positive if a is small.

For future reference, we state the weak form of problem (2.8). We denote the $L^2(\Omega_{\varepsilon}^{\alpha})$ -scalar product by $(\cdot | \cdot)_{\Omega_{\varepsilon}^{\alpha}}$ and define

$$V(\Omega) := L^2(S; W^{1,2}(\Omega)) \quad \text{and} \quad \mathcal{V}(\Omega) := \{ u \in V(\Omega) \mid \partial_t u \in L^2(\Omega \times S) \}. \tag{2.9}$$

The weak form of problem (2.8) then reads as follows. Find $(u_{\varepsilon}^{\mathbf{p}}, u_{\varepsilon}^{\mathbf{s}}) \in \mathcal{V}(\Omega_{\varepsilon}^{\mathbf{p}}) \times \mathcal{V}(\Omega_{\varepsilon}^{\mathbf{s}})$ such that $u_{\varepsilon}^{\alpha}(0) = u_{0}^{\alpha} \in L^{2}(\Omega)$ for $\alpha \in \{\mathbf{p}, \mathbf{s}\}$ and

$$(\partial_{t}u_{\varepsilon}^{\mathbf{p}}(t) | \phi(t))_{\Omega_{\varepsilon}^{\mathbf{p}}} + \varepsilon^{k} (\nabla u_{\varepsilon}^{\mathbf{p}}(t) | \nabla \phi(t))_{\Omega_{\varepsilon}^{\mathbf{p}}}$$

$$= (f_{\varepsilon}^{\mathbf{p}}(t) | \phi(t))_{\Omega_{\varepsilon}^{\mathbf{p}}} - \varepsilon^{m} (f_{\varepsilon}^{\mathbf{ex}}(t) | \phi(t))_{\Gamma_{\varepsilon}},$$

$$(2.10a)$$

$$(\partial_t u_{\varepsilon}^{\mathrm{s}}(t) | \psi(t))_{\Omega_{\varepsilon}^{\mathrm{s}}} + \varepsilon^l (\nabla u_{\varepsilon}^{\mathrm{s}}(t) | \nabla \psi(t))_{\Omega_{\varepsilon}^{\mathrm{s}}}$$

$$= (f_{\varepsilon}^{\mathrm{s}}(t) | \psi(t))_{\Omega_{\varepsilon}^{\mathrm{s}}} + \varepsilon^m (f_{\varepsilon}^{\mathrm{ex}}(t) | \psi(t))_{\Gamma_{\varepsilon}}$$

$$(2.10b)$$

for all $(\phi, \psi) \in V(\Omega_{\varepsilon}^{p}) \times V(\Omega_{\varepsilon}^{s})$ and a.e. $t \in S$ where the interfacial-exchange term has been abbreviated by $f_{\varepsilon}^{\text{ex}}$,

$$f_{\varepsilon}^{\text{ex}}(x,t) = C^{\text{ex}}(u_{\varepsilon}^{\text{p}}(x,t) - u_{\varepsilon}^{\text{s}}(x,t)), \tag{2.11}$$

for ease of notation. Problem (2.10) is of a suitable form for a homogenisation analysis. We remark that most authors *start* with this form omitting the proper nondimensionalisation.

3. A-priori estimates, convergence and literature remarks. We use the method of two-scale convergence [13, 1, 2] together with some extensions [16] to determine the limit problems associated with (2.10) as ε approaches zero.

In addition to the assumptions made in the previous section, we further require that the sequences $f_{\varepsilon}^{\alpha}(x,t)$, $\alpha \in \{p,s\}$, are bounded independently of ε in $L^{2}(\Omega_{\varepsilon}^{\alpha} \times S)$ and therefore have two-scale limits denoted by $f^{\alpha}(x,y,t)$.

Under these assumptions, the following theorem is obtained by variational techniques where the notation

$$|u(t)|_{\Omega}^{2} = (u(t) | u(t))_{\Omega} \text{ and } |u|_{\Omega,t}^{2} = \int_{0}^{t} (u(s) | u(s))_{\Omega} ds$$
 (3.1)

is used.

THEOREM 3.1. For fixed $\varepsilon > 0$, there exists a solution $(u_{\varepsilon}^{\mathrm{p}}, u_{\varepsilon}^{\mathrm{s}}) \in \mathcal{V}(\Omega_{\varepsilon}^{\mathrm{p}}) \times \mathcal{V}(\Omega_{\varepsilon}^{\mathrm{s}})$ of problem (2.10) such that

$$|u_{\varepsilon}^{\mathrm{p}}(t)|_{\Omega_{\varepsilon}^{\mathrm{p}}} + \varepsilon^{k/2} |\nabla u_{\varepsilon}^{\mathrm{p}}|_{\Omega_{\varepsilon}^{\mathrm{p}},t} + |u_{\varepsilon}^{\mathrm{s}}(t)|_{\Omega_{\varepsilon}^{\mathrm{s}}} + \varepsilon^{l/2} |\nabla u_{\varepsilon}^{\mathrm{s}}|_{\Omega_{\varepsilon},t} + \varepsilon^{m/2} |u_{\varepsilon}^{\mathrm{p}} - u_{\varepsilon}^{\mathrm{s}}|_{\Gamma_{\varepsilon},t} \leq C_{1}(3.2a)$$

for a.e. $t \in S$. Furthermore, if we have $m \ge 1$ or $u_0^p = u_0^s$ on Γ_{ε} , we also have

$$|\partial_t u_{\varepsilon}^{\mathbf{p}}(t)|_{\Omega_{\varepsilon}^{\mathbf{p}}} + |\partial_t u_{\varepsilon}^{\mathbf{s}}(t)|_{\Omega_{\varepsilon}^{\mathbf{s}}} \le C_2 \tag{3.2b}$$

for a.e. $t \in S$. The constants C_1, C_2 depend on the data appearing in (2.10) and the initial values but not on ε .

For the determination of the two-scale limits of the terms in (2.10), the method of two-scale convergence needs to be extended. A detailed presentation of these results also including the case k > 2 or l > 2 can be found in [16] and will also be presented in a forthcoming publication.

At this point, we would like to point out that the results for *some* choices of the parameters can be found in the literature. We briefly discuss a selection of contributions. For example, the distributed-microstructure model of Arbogast $et\ al.$ [3] modelling the flow of a slightly compressible fluid in a fissured medium is obtained for $k=0,\ l=2,$ m=0. The parallel-flow model for the same physical application (the macromodel of which has been suggested by Barenblatt $et\ al.$ [5]) is obtained for $k=0,\ l=0,$ $m=1,\ cf.$ [10] for the homogenisation of the stationary case. The problem of miscible displacement in a porous medium has been considered by Hornung [11] where also a Robin-type transmission condition at the pore-matrix interface is assumed. Here, the choice of scaling was also $k=0,\ l=2,\ m=1.$

Moreover, similar problems focusing on the different choices of scaling have been discussed. In particular, for k=l=0 and varying m, similar problems have been studied quite extensively. Auriault and Ene [4] seem to be the first to examine different choices of m by formal techniques. Most notably, we would like to mention the works of Canon and Pernin [7] who considered the stationary case with k=l=0 varying m and both subdomains connected and Pankratov et al. [15] who considered the case k=0 varying l with a matched boundary condition on Γ_{ε} and $\Omega_{\varepsilon}^{\rm s}$ disconnected. It should also be pointed out that the case k,l=0 and $\Omega_{\varepsilon}^{\rm s}$ disconnected is not covered in [16], the treatment of which can be found in [12, 9] by different techniques for the stationary case. We would also like to mention the book by Panfilov [14] who investigates the influence of scalings when modelling flow in porous media.

4. The macroscopic limit problems. The macroscopic limit problems of problem (2.10) are now stated. Obviously, different choices of the scaling exponents k, l and m need to be distinguished. Moreover, we assume Ω_s^s connected if l = 0.

To ease notation, when referring to the limit function u^{α} , $\alpha \in \{p,s\}$, the scaling exponent is denoted by λ , i.e. $\lambda = k$ if $\alpha = p$ and $\lambda = l$ if $\alpha = s$. Moreover, if $k \neq l$, we assume k < l. Note that this does cause any restriction of generality owing to the symmetry of the problem.

In order to be able to write the macroscopic limit equations in a simple way, two factors are introduced:

$$\theta(\lambda) := \begin{cases} 1, & \lambda = 0 \text{ or } \lambda = 2, \\ 0, & 0 < \lambda < 2, \end{cases} \qquad \sigma^{\alpha}(m) := \begin{cases} -1, & \alpha = p, \ m = 1, \\ 1, & \alpha = s, \ m = 1, \\ 0, & \alpha \in \{p, s\}, \ m \neq 1. \end{cases}$$
 (4.1)

It is useful to distinguish the cases $m \geq 1$ and m < 1 as these correspond to particularly different limit behaviours. Note that independently of the choice of m, u^{α} is independent of the spatial variable y if $\lambda < 2$.

4.1. The case $m \geq 1$. In this case, the limit functions u^p and u^s need to be considered separately. Therefore, it suffices to discuss the limit problem associated with one unknown u^{α} . The total limit problem of (2.10) is then given by the respective equations for $\alpha = p$ and $\alpha = s$. The solutions of two cell problems are required. For $\alpha \in \{p, s\}$, let ς_j^{α} , $j = 1, \ldots, n$, be the Y-periodic solution of the cell problem

$$-\nabla_y \cdot (\nabla_y \varsigma_i^{\alpha}(y) + e_j) = 0, \quad y \in Z^{\alpha}, \tag{4.2}$$

the weak form of which is given by

$$(\nabla_y \varsigma_i^{\alpha} + e_j \,|\, \nabla_y \phi)_{Z^{\alpha}} = 0 \tag{4.3}$$

for all Y-periodic test functions ϕ . The vector e_j is the jth unit vector in n-dimensional Euclidean space. This allows the definition of the tensors $P^{\alpha} = [p_{jk}^{\alpha}]_{jk}$ via

$$p_{jk}^{\alpha} = \int_{Z^{\alpha}} \delta_{jk} + \partial_{y_j} \varsigma_k^{\alpha}(y) \, \mathrm{d}y, \tag{4.4}$$

where δ_{jk} is the Kronecker delta. These tensors turn out to be the diffusion tensors in the macroscopic limit problems. They are symmetric and positive definite (cf. [8], for example).

In order to be able to formulate the macroscopic limit equations in a simple way, the limit of the interfacial-exchange term is written as

$$f^{\text{ex}}(x, y, t) = C^{\text{ex}}(u^{\text{p}}(x, y, t) - u^{\text{s}}(x, y, t)). \tag{4.5}$$

The limit problems can now be stated. If $0 \le \lambda < 2$, the macroscopic limit problem of problem (2.10) is given by

$$|Z^{\alpha}|(\partial_{t}u^{\alpha}(t))|\phi(t))_{\Omega} + \theta(\lambda) (P^{\alpha}(t)\nabla u^{\alpha}(t)|\nabla\phi(t))_{\Omega}$$

$$= (\int_{Z^{\alpha}} f^{\alpha}(\cdot, y, t) dy |\phi(t)|_{\Omega} + \sigma^{\alpha}(m) (\int_{\Gamma} f^{\text{ex}}(\cdot, y, t) d\sigma_{y} |\phi(t)|_{\Omega})^{(4.6)}$$

for all $\phi \in V(\Omega)$ and a.e. $t \in S$. If $\lambda = 2$, the macroscopic limit problem of problem (2.10) is given by

$$(\partial_t u^{\alpha}(t) | \psi(t))_{\Omega \times Z^{\alpha}} + (\nabla_y u^{\alpha}(t) | \nabla_y \psi(t))_{\Omega \times Z^{\alpha}}$$

$$= (f^{\alpha}(t) | \psi(t))_{\Omega \times Z^{\alpha}} + \sigma^{\alpha}(m)(f^{\text{ex}}(t) | \psi(t))_{\Omega \times \Gamma}$$

$$(4.7)$$

for all $\psi \in \mathcal{W}(Z^{\alpha}) := L^2(S; L^2(\Omega; W^{1,2}_{\#}(Z^{\alpha})))$ and a.e. $t \in S$.

4.2. The case m < 1. In this case, the limit functions satisfy $u^{p}(x, y, t) = u^{s}(x, y, t)$ for a.e. $x \in \Omega$, $y \in \Gamma$, $t \in S$. It therefore makes sense to define

$$u(x, y, t) = \chi^{P}(y)u^{P}(x, y, t) + \chi^{S}(y)u^{S}(x, y, t), \tag{4.8}$$

where $\chi^{\rm p}$ and $\chi^{\rm s}$ are the characteristic functions of $Z^{\rm p}$ and $Z^{\rm s}$, respectively, and look for the single equation satisfied by u. For ease of notation, we also define

$$f(x, y, t) = \chi^{P}(y)f^{P}(x, y, t) + \chi^{s}(y)f^{s}(x, y, t).$$
(4.9)

For m < 1, an additional assumption is necessary if $k \neq l$ and $m \leq k - 1$. In this case, let

$$\varepsilon^{(k-1)/2} |u_{\varepsilon}^{\mathbf{p}}|_{\Gamma_{\varepsilon}} + \varepsilon^{(k-1)/2} |u_{\varepsilon}^{\mathbf{s}}|_{\Gamma_{\varepsilon}} \le C \tag{4.10}$$

additionally be satisfied. Note that this condition cannot be obtained without making further assumptions. Moreover, the solutions of the following cell problems are needed: For l=0, let $\zeta_j^{m,l}$, $j=1,\ldots,n$, be the Y-periodic solution of the cell problem

$$-\nabla_y \cdot (\nabla_y \varsigma_i^{m,l}(y) + e_j) = 0, \quad y \in Z^p \cup Z^s, \tag{4.11a}$$

subject to the following boundary conditions on Γ ,

$$-(\nabla_{y}(\varsigma_{j}^{m,l})^{\alpha}(y) + e_{j}) \cdot \nu = 0, \quad \text{if } m > -1,$$

$$-(\nabla_{y}(\varsigma_{j}^{m,l})^{\alpha}(y) + e_{j}) \cdot \nu - C^{\text{ex}}[(\varsigma_{j}^{m,l})^{p}(y) - (\varsigma_{j}^{m,k,l})^{s}(y)] = 0, \quad \text{if } m = -1,$$

$$(\varsigma_{j}^{m,l})^{p}(y) - (\varsigma_{j}^{m,l})^{s}(y) = 0,$$

$$(\nabla_{y}(\varsigma_{j}^{m,l})^{p}(y) + e_{j}) \cdot \nu - (\nabla_{y}(\varsigma_{j}^{m,l})^{s}(y) + e_{j}) \cdot \nu = 0,$$

$$if m < -1.$$

$$(4.11b)$$

For l > 0, let $\zeta_j^{m,l}$, $j = 1, \ldots, n$, be the Y-periodic solution of the cell problem

$$-\nabla_y \cdot (\nabla_y \varsigma_j^{m,l}(y) + e_j) = 0, \quad y \in Z^{\mathcal{P}}, \tag{4.12a}$$

subject to to the following boundary conditions on Γ ,

$$-(\nabla_{y}\varsigma_{j}^{m,l}(y) + e_{j}) \cdot \nu = 0, \quad \text{if } m > -1,$$

$$-(\nabla_{y}\varsigma_{j}^{m,l}(y) + e_{j}) \cdot \nu + C^{\text{ex}}(\varsigma_{j}^{m,l}(y) + (y \mid \nabla u)) = 0, \quad \text{if } m = -1, \quad (4.12b)$$

$$\varsigma_{j}^{m,l}(y) = 0, \quad \text{if } m < -1.$$

This allows the definition of the tensors $P^{m,l} = [p_{ij}^{m,l}]_{ij}$ via

$$p_{ij}^{m,l} = \begin{cases} \int_{Y} \delta_{ij} + \partial_{y_i} \varsigma_j^{m,l}(y) \, \mathrm{d}y, & \text{if } l = 0, \\ \int_{Y} \delta_{ij} + \partial_{y_i} \varsigma_j^{m,l}(y) \, \mathrm{d}y, & \text{if } l \neq 0. \end{cases}$$
(4.13)

Note that in the case l > 0 and m = -1, this tensor is dependent on ∇u .

The limit problems can now be stated. If $0 \le k, l < 2$, the macroscopic limit problem of problem (2.10) is given by

$$(\partial_t u(t) \mid \phi(t))_{\Omega} + \theta(k) \left(P^{m,l}(t) \nabla u(t) \mid \nabla \phi(t) \right)_{\Omega} = \left(\int_Y f(\cdot, y, t) \, \mathrm{d}y \mid \phi(t) \right)_{\Omega} \tag{4.14}$$

for all $\phi \in V(\Omega)$, if k = 0, and $\phi \in L^2(\Omega \times S)$, if k > 0, and a.e. $t \in S$. If k, l = 2, the macroscopic limit problem is given by

$$(\partial_t u(t) \mid \psi(t))_{\Omega \times Y} + (\nabla_y u(t) \mid \nabla_y \psi(t))_{\Omega \times Z^{\mathcal{P}}} + (\nabla_y u(t) \mid \nabla_y \psi(t))_{\Omega \times Z^{\mathcal{S}}} = (f(t) \mid \psi(t))_{\Omega \times Y}$$

$$(4.15)$$

for all $\psi \in \{\psi = \chi^p \psi^p + \chi^s \psi^s \mid \psi^\alpha \in \mathcal{W}(Z^\alpha), \psi^p = \psi^s \text{ on } \Gamma\}$ and a.e. $t \in S$ where $\psi = 0$

on Γ if $k \neq l$. If k < 2 and l = 2, the limit problem is given by

$$|Z^{\mathbf{p}}|(\partial_{t}u^{\mathbf{p}}(t) | \phi(t))_{\Omega} + \theta(k) (P^{m,l}(t)\nabla u^{\mathbf{p}}(t) | \nabla \phi(t))_{\Omega}$$

$$= \theta(l) \left(\int_{\Gamma} \nabla_{y} u^{\mathbf{s}}(\cdot, y, t) \cdot \nu \, d\sigma_{y} | \phi(t) \right)_{\Omega} + \left(\int_{Z^{\mathbf{p}}} f^{\mathbf{p}}(\cdot, y, t) \, dy | \phi(t) \right)_{\Omega}$$

$$(4.16a)$$

$$(\partial_t u^{\mathbf{s}}(t) \mid \psi(t))_{\Omega \times Z^{\mathbf{s}}} + \theta(l)(\nabla_y u^{\mathbf{s}}(t) \mid \nabla_y \psi(t))_{\Omega \times Z^{\mathbf{s}}} = (f^{\mathbf{s}} \mid \nabla_y \psi(t))_{\Omega \times Z^{\mathbf{s}}}$$
(4.16b)

for all $(\phi, \psi) \in V(\Omega) \times \mathcal{W}(Z^{s})$, where $\psi = 0$ on Γ , and a.e. $t \in S$, together with $u^{p} = u^{s}$ on Γ . Note that the tensor $P^{m,l}$ only appears in the above equations if k = 0.

REFERENCES

- G. Allaire, Homogenization and two-scale convergence, SIAM J. Math. Anal. 23(6) (1992), 1482– –1518.
- [2] G. Allaire, A. Damlamian and U. Hornung Two-scale convergence on periodic surfaces and applications, In: Proceedings of the international conference on mathematical modelling of flow through porous media (ed. by A. P. Bourgeat, C. Carasso, S. Luckhaus and A. Mikelic), pp. 15–25, World Scientific, 1995.
- [3] T. Arbogast, J. Douglas Jr. and U. Hornung, Derivation of the double porosity model of single phase flow via homogenization theory, SIAM J. Math. Anal. 21(4) (1990), 823–836.
- [4] J.-L. Auriault and H. I. Ene, Macroscopic modelling of heat transfer in composites with interfacial thermal barrier, Int. J. Heat Mass Transfer 37(18) (1994), 2885–2892.
- [5] G. I. Barenblatt, I. P. Zheltov and I. N. Kochina, Basic concepts in the theory of seepage of homogeneous liquids in fissured rocks, J. Appl. Math. Mech. 24 (1960), 1286–1303.
- [6] A. Bensoussan, J.-L. Lions, and G. Papanicolaou, Asymptotic analysis for periodic structures. North-Holland, 1978.
- [7] É. Canon and J.-N. Pernin, Homogenization of diffusion in composite media with interfacial barrier, Rev. Roumaine Math. Pures Appl. 44(1), (1999), 23–36.
- [8] D. Cioranescu and P. Donato, An introduction to homogenization. Oxford University Press, 1999.
- [9] P. Donato and S. Monsurrò, Homogenization of two heat conductors with an interfacial contact barrier, Anal. Appl. 2(3) (2004), 247–273.
- [10] H. I. Ene and D. Poliševski, Model of diffusion in partially fissured media, Z. angew. Math. Phys. 53 (2002), 1052–1059.
- [11] U. Hornung (ed.), Homogenization and porous media. Springer, 1997.
- [12] S. Monsurrò, Homogenization of a two-component composite with interfacial thermal barrier, Adv. Math. Sci. Appl. 13(1) (2003), 44-63.
- [13] G. Nguetseng, A general convergence result for a functional related to the theory of homogenization, SIAM J. Math. Anal. 20 (1989), 608–629.
- [14] M. Panfilov, Macroscale models of flow through highly heterogeneous porous media. Kluwer, 2000.
- [15] L. Pankratov, A. Piatnitskii and V. Rybalko, Homogenized model of reaction-diffusion in a porous medium, C. R. Mecanique 331 (2003), 253–258.
- [16] M. A. Peter, Coupled reaction-diffusion systems and evolving microstructure: mathematical modelling and homogenisation, PhD dissertation, University of Bremen, 2006. Also: Logos Verlag Berlin, 2007
- [17] E. Sanchez-Palencia, Non-homogeneous media and vibration theory. Springer, 1980.