

HOMOGENIZATION OF SECONDARY-FLUX MODELS OF PARTIALLY FISSURED MEDIA

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Abstract. Fully-saturated and partially fissured media, in which supplementary flow and transport arise from direct cell-to-cell diffusion paths, have been described accurately over a wide range of scales by discrete *secondary-flux models*. These models were constructed as an extension of classical double-porosity models for totally fissured media by two-scale modeling considerations. There is some substantial literature on the analysis of continuously distributed secondary-flux models, and the corresponding discrete models have been proven to give efficient and accurate simulations when compared to recently available experimental data. These are particularly effective in the presence of advection. In this note, a summary description is given for the two-scale convergence of the discrete secondary-flux model to the corresponding continuous double-porosity secondary-flux model.

Key Words. secondary-flux, partially fissured porous media, homogenization, multiscale flow and transport.

1. Introduction

Problems of flow and transport through porous media lead to initial-boundary-value problems for a coupled elliptic-parabolic system of partial differential equations of elliptic and parabolic type. The fluid flow is described by an elliptic equation, and its solution provides the velocity for a parabolic equation with advection for the concentration u of a dissolved chemical transported by that flow. When the process takes place in a non-homogeneous medium, the coefficients vary on such a small scale that computation of the solution is very intensive and an upscaled model is needed. We shall consider the generic case of the single parabolic equation in a periodic medium of very small period $\varepsilon > 0$. This provides an indication of the corresponding results for the full system of flow and transport.

The locally representative unit cell is given in the two parts, $Y = Z^f \cup Z^s$, and then it is scaled to εY in the ε -periodic structure. In the classical case of the diffusion equation for transport, the diffusion coefficient varies between two constants, D^f on the *fast region* Z^f and D^s on the *slow region* Z^s of the unit cell Y . We denote the fine-scale coefficient in this situation by $D_\varepsilon(x) = [D^f, D^s; \varepsilon]$. The system is homogenized by taking the two-scale limit as $\varepsilon \rightarrow 0$, and the limit of its solution $u_\varepsilon(x, t)$ is the solution $u(x, t)$ of an equation of the same form but with the constant effective coefficient \tilde{D} . The formulae for \tilde{D} show that the fast and slow regions are *flux coupled* through the gradient of the solution on the two regions. The gains of this homogenized model are that the fine-scale geometry is averaged out, so it is computationally straightforward, and it provides a good approximation of the real situation in the low-contrast cases when ε is small. See [7]

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for detailed expositions of various approaches and background in homogenization of porous media.

However, such models do not recover the tailing effects that are observed in experiments or in simulations when the contrast D^f/D^s is large, for then there are consequential memory effects due to the relatively slower release of the solute stored in the small cells. A very special situation is the *obstacle problem* which corresponds to the extreme case of $D^s = 0$. We denote the corresponding effective coefficient by \tilde{D}^0 . Here, of course, there are no such memory effects, as there is no secondary storage, and this situation is described well by the preceding classical case. It is the cases of intermediate contrast that require better modeling.

The situation of highly-heterogeneous media in which the contrast between fast and slow regions is *very high* can be described as above but with the diffusion coefficient $D_\varepsilon(x) = [D^f, \varepsilon^2 D^s; \varepsilon]$ scaled as indicated in the slow region. Here the contrast is balanced with the cell size to maintain the two-way coupling of concentration and flux between the slow cells and the fast surrounding region. The limit leads to a *system* whose structure is quite different from the original single equation, namely, a macro-equation for an unknown $u(x, t)$ given on the macroscopic medium and a family of micro-equations for unknowns $U(x, y, t)$ given in the local reference cell at each point x of the macroscopic region. The cell solution provides the *source term* or input $q(x, t) = \int_{\partial Z^s} D^s \nabla_y U \cdot \nu \, d\sigma$ back into the macro-equation, while the macro-variable enters the cell problem through the boundary condition

$$(1) \quad U(x, y, t) = u(x, t), \quad y \in \partial Z^s.$$

This is the *double-porosity model* of Arbogast, Douglas & Hornung [2]. It is a large fully-coupled system, with a local diffusion problem at each point in the medium, but the structure is highly parallel and amenable to computation. It is *value* or *concentration coupled* into the cells and *gradient* or *flux coupled* into the macro-equation. The gain of this model includes the additional *secondary-storage* via the coupling of the fast and slow components and some of the resultant tailing effects and memory effects observed in experiments but unattainable with the classical model. The assumptions depend on the critical contrast ε^2 between coefficients. It was observed in [9] that the coefficients in the macro-equation are precisely those of the corresponding obstacle problem.

The double-porosity model completely misses any advective effects at the cell level, since the input to the cell (1) is constant on the local boundary. In order to couple the cells more tightly to the surrounding medium, the boundary condition (1) was replaced with the *affine* constraint

$$(2) \quad U(x, y, t) = u(x, t) + \nabla u(x, t) \cdot (y - y_0), \quad y \in \partial Z^s,$$

by Peszyńska & Showalter [9]. Their objective was to include the local advective contributions and accurately model the full range of contrasts that were reported in the extensive experiments [13]. They showed the source term $q(x, t)$ needs to be altered to maintain conservation of mass, and this leads to the *secondary-flux* term. With the affine coupling into the cells, this model captures advection effects and contributes both the secondary-storage and the secondary-flux which are added back through the source term to the macro-equation. With this tighter coupling through both values and gradients, this model can cover a wide range of contrasts and accurately reproduce the break-through curves throughout the entire range of contrasts. See [9] for further discussion.

Since $D_\varepsilon = [D^f, D^s; \varepsilon]$ suits the very-low-contrast case while $D_\varepsilon = [D^f, \varepsilon^2 D^s; \varepsilon]$ describes the very-high-contrast case well, it is tempting to expect that an intermediate choice, *e.g.*, $D_\varepsilon = [D^f, \varepsilon D^s; \varepsilon]$, might be appropriate for the intermediate contrast. This is untrue, however, because, in this intermediate-contrast situation, advective effects become important [13]. These can not be captured by microscopic models describing diffusive transport only, cf. [11, 10]. The cell variable U needs to see the gradient of the macro-variable, ∇u , in order to account for an additional advection. This is accomplished by a condition of the type (2).

Discrete models of secondary-flux type were recently introduced in [9], although the continuous analogues were developed in [5] and [6] without any justification. The affine constraint (2) had been introduced earlier in the numerical work of Arbogast [3]. His *viscous* dual-porosity model used this pressure gradient to substantially improve the simulations of recovery at later times. These had been inadequate with only the pressure coupling of (1), and it was recognized that some modification of the source term $q(x, t)$ in the macro-equation was needed. We shall show here that the continuous model is not *ad hoc*, but is obtained as the two-scale limit of the corresponding exact microproblem of discrete type introduced in [9]. The detailed analysis of the problem will be presented in a forthcoming publication.

2. Statement of the problem

Let $Y = (0, 1)^n$ be the reference cell, made up of two distinct parts Z^f and Z^s where $\overline{Z^s} \subset Y$, and let $\Gamma = \partial Z^s$. Given the open bounded Lipschitz-domain $\Omega \in \mathbb{R}^n$ and $\varepsilon > 0$, we define $\Omega_\varepsilon^\alpha = \Omega \cap \text{int} \bigcup_k \varepsilon \overline{Z}_k^\alpha$, $\alpha \in \{f, s\}$, where the subscript k denotes translation of the set by the n -tuple of integers $k \in \mathbb{Z}^n$. Similarly, $\Gamma_\varepsilon = \Omega \cap \bigcup_k \varepsilon \Gamma_k$. The time interval under consideration is $S = (0, T)$ where $T > 0$.

Let $[x]_Y$ denote the unique integer combination $\sum_{i=1}^n k_i e_i$ of the periods such that $\{x\}_Y = x - [x]_Y$ belongs to $[0, 1)^n$. The vector e_j is the j th unit vector in n -dimensional Euclidean space. Note that we have $x = \varepsilon([x/\varepsilon]_Y + \{x/\varepsilon\}_Y)$ for any $x \in \mathbb{R}^n$.

Let $\mathcal{T}_\varepsilon: L^p(\Omega) \rightarrow L^p(\Omega \times Y)$, $p \in [1, \infty]$, be the periodic unfolding operator [4], *i.e.* for $u \in L^p(\Omega)$, extended by zero outside of Ω , we define

$$(3) \quad \mathcal{T}_\varepsilon(u)(x, y) = u(\varepsilon[x/\varepsilon]_Y + \varepsilon y) \text{ for } x \in \Omega \text{ and } y \in Y.$$

We define $z_\varepsilon(x)$ to be the function mapping each x to its part in εY translated by y_0 ,

$$(4) \quad z_\varepsilon(x) = (\{x/\varepsilon\}_Y - y_0),$$

where y_0 is the centroid of the interior region of the unit cell, Z^s . Moreover, we denote the mean value of a $u \in W^{1,2}(\Omega_\varepsilon^f)$ on each $\varepsilon \Gamma_k$ by $m_0(u)$,

$$(5) \quad m_0(u) = \frac{1}{|\Gamma|} \int_\Gamma \mathcal{T}_\varepsilon(u)(x, y) d\sigma_y,$$

and the mean value of a vector-valued $v \in [L^2(\Omega_\varepsilon^f)]^n$ in each εZ_k^f by $m_1(v)$,

$$(6) \quad m_1(v) = \frac{1}{|Z^f|} \int_{Z^f} \mathcal{T}_\varepsilon(v)(x, y) dy.$$

Notice that m_0 and m_1 are constant in each cell εY_k .

All source terms are combined in the functions $f_\varepsilon^\alpha = f_\varepsilon^\alpha(x, t) = f^\alpha(x, x/\varepsilon, t)$, $\alpha \in \{f, s\}$, whose extensions by zero to all of Ω are assumed bounded independently of ε in $L^2(\Omega \times S)$. The coefficient functions $D_\varepsilon^\alpha = D_\varepsilon^\alpha(x, t) = D^\alpha(x, x/\varepsilon, t)$ are assumed bounded from above and away from zero by $D_0^\alpha > 0$ independently of

$\varepsilon, \alpha \in \{f, s\}$, and they are supposed to be admissible test functions in two-scale-convergence sense [1].

The micro-problem under consideration is given by

$$\begin{aligned}
(7a) \quad & \partial_t u_\varepsilon^f(x, t) - \nabla \cdot (D_\varepsilon^f(x, t) \nabla u_\varepsilon^f(x, t)) = f_\varepsilon^f(x, t), \quad x \in \Omega_\varepsilon^f, \quad t \in S, \\
(7b) \quad & \partial_t u_\varepsilon^s(x, t) - \nabla \cdot (\varepsilon^2 D_\varepsilon^s(x, t) \nabla u_\varepsilon^s(x, t)) = f_\varepsilon^s(x, t), \quad x \in \Omega_\varepsilon^s, \quad t \in S, \\
(7c) \quad & m_0(u_\varepsilon^f) + \beta m_1(\nabla u_\varepsilon^f) \cdot z_\varepsilon = u_\varepsilon^s(x, t), \quad x \in \Gamma_\varepsilon, \quad t \in S, \\
(7d) \quad & -D_\varepsilon^f(x, t) \nabla u_\varepsilon^f(x, t) \cdot \nu_\varepsilon^f = \varepsilon^2 \frac{1}{|\Gamma|} \int_\Gamma \mathcal{T}_\varepsilon(D_\varepsilon^s \nabla u_\varepsilon^s \cdot \nu_\varepsilon^s)(x, y) \, d\sigma_y \\
& + \beta \varepsilon^2 \frac{1}{|Z^f|} \int_\Gamma \mathcal{T}_\varepsilon(D_\varepsilon^s \nabla u_\varepsilon^s \cdot \nu_\varepsilon^s z_\varepsilon)(x, y) \, d\sigma_y \cdot \nu_\varepsilon^f, \quad x \in \Gamma_\varepsilon, \quad t \in S. \\
(7e) \quad & u_\varepsilon^f(x, t) = 0, \quad x \in \partial\Omega_\varepsilon^f \cap \partial\Omega, \quad t \in S, \\
(7f) \quad & u_\varepsilon^f(x, 0) = u_0^f, \quad u_\varepsilon^s(x, 0) = u_0^s, \quad x \in \Omega.
\end{aligned}$$

Note that, in particular, condition (7d) ensures that we have flux conservation across Γ_ε , since

$$\begin{aligned}
(8) \quad & - \int_{\Gamma_\varepsilon} D_\varepsilon^f(x, t) \nabla u_\varepsilon^f(x, t) \cdot \nu_\varepsilon^f \, d\sigma_x = \varepsilon^2 \frac{1}{|\Gamma|} \int_{\Gamma_\varepsilon} \int_\Gamma \mathcal{T}_\varepsilon(D_\varepsilon^s \nabla u_\varepsilon^s \cdot \nu_\varepsilon^s)(x, y) \, d\sigma_y \, d\sigma_x \\
& = \int_{\Gamma_\varepsilon} \varepsilon^2 D_\varepsilon^s(x, t) \nabla u_\varepsilon^s(x, t) \cdot \nu_\varepsilon^s \, d\sigma_x,
\end{aligned}$$

where we have used the norm identity

$$(9) \quad \int_{\Gamma_\varepsilon} v(x) \, d\sigma_x = \frac{1}{|\Gamma|} \int_{\Gamma_\varepsilon \times \Gamma} \mathcal{T}_\varepsilon(v)(x, y) \, d\sigma_y \, d\sigma_x.$$

For the weak formulation, the following function space is used,

$$\begin{aligned}
(10) \quad \mathcal{V}_\varepsilon(\Omega) = & \{(u_\varepsilon^f, u_\varepsilon^s) \in L^2(0, T; W^{1,2}(\Omega_\varepsilon^f)) \times L^2(0, T; W^{1,2}(\Omega_\varepsilon^s)) \mid \\
& u_\varepsilon^f = 0 \text{ on } \partial\Omega_\varepsilon^f \cap \partial\Omega \text{ and } m_0(u_\varepsilon^f) + \beta m_1(\nabla u_\varepsilon^f) \cdot z_\varepsilon = u_\varepsilon^s \text{ on } \Gamma_\varepsilon\},
\end{aligned}$$

and we write $u(t) = u(\cdot, t)$,

$$(11) \quad (u(t) | v(t))_{\Omega_\varepsilon^\alpha} = \int_{\Omega_\varepsilon^\alpha} u(x, t) v(x, t) \, dx, \quad (u | v)_{\Omega_\varepsilon^\alpha, t} = \int_0^t (u(s) | v(s))_{\Omega_\varepsilon^\alpha} \, ds.$$

A weak form of problem (7) is defined as follows: find $(u_\varepsilon^f, u_\varepsilon^s) \in \mathcal{V}_\varepsilon(\Omega)$ with $(u_\varepsilon^f(0), u_\varepsilon^s(0)) = (u_0^f, u_0^s)$ such that

$$\begin{aligned}
(12) \quad & (\partial_t u_\varepsilon^f(t) | \phi^f(t))_{\Omega_\varepsilon^f} + (\partial_t u_\varepsilon^s(t) | \phi^s(t))_{\Omega_\varepsilon^s} + (D_\varepsilon^f(t) \nabla u_\varepsilon^f(t) | \nabla \phi^f(t))_{\Omega_\varepsilon^f} \\
& + \varepsilon^2 (D_\varepsilon^s(t) \nabla u_\varepsilon^s(t) | \nabla \phi^s(t))_{\Omega_\varepsilon^s} = (f_\varepsilon^f(t) | \phi^f(t))_{\Omega_\varepsilon^f} + (f_\varepsilon^s(t) | \phi^s(t))_{\Omega_\varepsilon^s}
\end{aligned}$$

for all $(\phi^f, \phi^s) \in \mathcal{V}_\varepsilon(\Omega)$ and a.e. $t \in S$.

The following proposition ensures that (12) is an appropriate weak form of (7), the proof of which makes extensive use of (9) and the fact that for a function $\phi^f \in C_0^\infty(\Omega_\varepsilon^f \times S)$, we have

$$(13) \quad m_1(\nabla \phi^f) = \frac{1}{|Z^f|} \int_{Z^f} \mathcal{T}_\varepsilon(\nabla \phi^f)(x, y) \, dy = \frac{1}{|Z^f|} \int_\Gamma \mathcal{T}_\varepsilon(\phi^f \nu_\varepsilon^f)(x, y) \, d\sigma_y.$$

Proposition 2.1. *Let $(u_\varepsilon^f, u_\varepsilon^s) \in \mathcal{V}_\varepsilon(\Omega)$ be a solution of (12). If the pair of functions $(u_\varepsilon^f, u_\varepsilon^s)$ also belongs to the space $C^1([0, T]; C^2(\overline{\Omega_\varepsilon^f})) \times C^1([0, T]; C^2(\overline{\Omega_\varepsilon^s}))$, it satisfies problem (7).*

Rather than the extra assumed smoothness of the solution, one can use the *abstract Green's theorem* [12, Proposition II.5.3] to characterize the strong form of the problem.

3. Macroscopic limit problems

We state the macroscopic limit problem satisfied by the limit functions of the sequences of solutions of (7) as $\varepsilon \rightarrow 0$. The limit functions of u_ε^f and u_ε^s are denoted by u^f and u^s , respectively. An outline of how these limit problems are obtained is given in §4.

The solution of a cell problem is required. Let ς_j , $j = 1, \dots, n$, be the Y -periodic solution of the cell problem

$$(14) \quad \begin{aligned} -\nabla_y \cdot (D^f(x, y, t)(\nabla_y \varsigma_j(x, y, t) + e_j)) &= 0, & y \in Z^f, x \in \Omega, t \in S, \\ -D^f(x, y, t)(\nabla_y \varsigma_j(x, y, t) + e_j) \cdot \nu^f &= 0, & y \in \Gamma, x \in \Omega, t \in S, \end{aligned}$$

the weak form of which is given by

$$(15) \quad (D^f(x, \cdot, t)(\nabla_y \varsigma_j(x, \cdot, t) + e_j) | \nabla_y \phi)_{Z^f} = 0$$

for all Y -periodic test functions ϕ . This allows the definition of the tensor $P^f = [p_{ij}^f]$ via

$$(16) \quad p_{ij}^f(x, t) = \int_{Z^f} D^f(x, y, t)(\delta_{ij} + \partial_{y_i} \varsigma_j(x, y, t)) \, dy,$$

where δ_{ij} is the Kronecker delta. This turns out to be the effective tensor in the macroscopic limit problem. It is symmetric and positive definite, since D^f is bounded away from zero.

The limit problem reads as follows:

$$(17a) \quad \begin{aligned} |Z^f| \partial_t u^f(x, t) - \nabla \cdot (P^f(x, t) \nabla u^f(x, t)) \\ = \int_{Z^f} f^f(x, y, t) \, dy - \int_{\Gamma} f^{\text{int}}(x, y, t) \, d\sigma_y + \nabla \cdot \int_{\Gamma} \beta f^{\text{int}}(x, y, t)(y - y_0) \, d\sigma_y, \end{aligned} \quad x \in \Omega, t \in S,$$

$$(17b) \quad u^f(x, t) = 0, \quad x \in \partial\Omega, t \in S,$$

$$(17c) \quad \partial_t u^s(x, y, t) - \nabla_y \cdot (D^s(x, y, t) \nabla_y u^s(x, y, t)) = f^s(x, y, t), \quad x \in \Omega, y \in Z^s, t \in S,$$

$$(17d) \quad u^f(x, t) + \beta \nabla u^f(x, t) \cdot (y - y_0) = u^s(x, y, t), \quad x \in \Omega, y \in \Gamma, t \in S,$$

$$(17e) \quad u^f(x, 0) = u_0^f, \quad u^s(x, y, 0) = u_0^s, \quad x \in \Omega, y \in Z^s.$$

The weak form of problem (17) is: find $(u^f, u^s) \in L^2(0, T; W_0^{1,2}(\Omega)) \times [(u^f + \beta \nabla u^f \cdot (y - y_0)) + L^2(0, T; (L^2(\Omega); W_0^{1,2}(Z^s)))]$ with $(u^f(0), u^s(0)) = (u_0^f, u_0^s)$ such that

$$(18a) \quad \begin{aligned} |Z^f| (\partial_t u^f(t) | \phi(t))_\Omega + (P^f(t) \nabla u^f(t) | \nabla \phi(t))_\Omega &= \left(\int_{Z^f} f^f(\cdot, y, t) \, dy | \phi(t) \right)_\Omega \\ &\quad - \left(\int_{\Gamma} f^{\text{int}}(\cdot, y, t) \, dy | \phi(t) \right)_\Omega - \left(\int_{\Gamma} \beta f^{\text{int}}(\cdot, y, t)(y - y_0) \, dy | \nabla \phi(t) \right)_\Omega, \end{aligned}$$

$$(18b) \quad (\partial_t u^s(t) | \psi(t))_{\Omega \times Z^s} + (D^s(t) \nabla_y u^s(t) | \nabla_y \psi(t))_{\Omega \times Z^s} = (f^s(t) | \psi(t))_{\Omega \times Z^s}$$

for all $(\phi, \psi) \in L^2(0, T; W_0^{1,2}(\Omega)) \times L^2(0, T; (L^2(\Omega); W_0^{1,2}(Z^s)))$ and a.e. $t \in S$, where the interface term f^{int} is given by

$$(19) \quad f^{\text{int}}(x, y, t) = D^s(x, y, t) \nabla_y u^s(x, y, t) \cdot \nu^s, \quad x \in \Omega, y \in \Gamma, t \in S.$$

It is interesting to note that the limit problem would have been the same if we chose an average over Z^f instead of Γ in the definition of m_0 (cf. (5)).

4. Existence of solutions, a-priori estimates, convergence

We briefly summarize the steps of the homogenization analysis. The following theorem follows by standard techniques.

Theorem 4.1. *For fixed $\varepsilon > 0$, there exists a solution $(u_\varepsilon^f, u_\varepsilon^s) \in \mathcal{V}_\varepsilon(\Omega)$ of problem (12) such that*

$$(20) \quad |u_\varepsilon^f(t)|_{\Omega_\varepsilon^f} + |\nabla u_\varepsilon^f|_{\Omega_\varepsilon^f, t} + |u_\varepsilon^s(t)|_{\Omega_\varepsilon^s} + \varepsilon |\nabla u_\varepsilon^s|_{\Omega_\varepsilon^s, t} \leq C,$$

for a.e. $t \in S$, where the constant C depends on T and the data but not on ε .

We use elements of two-scale convergence [8, 1] and periodic unfolding [4] in order to investigate the convergence of the sequences of solutions of (7) as $\varepsilon \rightarrow 0$. A key element in this analysis is the following proposition, which deals with the convergence of the terms $m_0(u_\varepsilon^f)$ and $m_1(\nabla u_\varepsilon^f)$.

Proposition 4.2. *The following convergence results hold:*

- (a) $m_0(u_\varepsilon^f) \rightarrow u^f$ strongly in $L^2(\Omega)$.
- (b) $m_1(\nabla u_\varepsilon^f) \rightarrow \nabla u^f$ in two-scale sense.

The limit problems associated with the limits of sequences of solution of the microproblem need to be identified. This is performed in two steps: the identification of the boundary condition (17c) and of equations (18a) and (18b). Particular attention needs to be paid to the recovery of the secondary-flux term in (18a). The main result can be summarized as follows:

Theorem 4.3. *The limit functions as $\varepsilon \rightarrow 0$ associated with a sequence of solutions of the microproblem (12) satisfy the macroproblem (18).*

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