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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, $Y = Z^{\mathrm{f}} \cup Z^{\mathrm{s}}$, 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 $D_\varepsilon(x) = [D^{\mathrm{f}}, D^{\mathrm{s}}; \varepsilon]$. The system is homogenized by taking the two-scale limit as $\varepsilon \to 0$, 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 $D^{\mathrm{f}}/D^{\mathrm{s}}$ 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 $D^{\mathrm{s}} = 0$. 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 $D_\varepsilon(x) = [D^{\mathrm{f}}, \varepsilon^2 D^{\mathrm{s}}; \varepsilon]$ 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 $q(x,t) = \int_{\partial Z^{\mathrm{s}}} D^{\mathrm{s}} \nabla_y U \cdot \nu \, \mathrm{d}\sigma$ back into the macro-equation, while the macro-variable enters the cell problem through the boundary condition

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

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

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

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.