NUMERICAL UPSCALED MODEL OF TRANSPORT WITH NON-SEPARATED SCALE

Son-Young Yi∗, Małgorzata Peszyńska† and Ralph E. Showalter†

∗The University of Texas at El Paso (UTEP)
El Paso, TX 79968, USA
e-mail: syi@utep.edu

† Oregon State University
Corvallis, OR 97331, USA
e-mail: {mpesz,show}@math.oregonstate.edu

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Summary. We study numerically a new model describing the multiscale flow of a single-phase incompressible fluid and transport of a dissolved chemical by advection and diffusion through a heterogeneous porous medium without the usual assumptions of scale separation. The new model includes as special cases the classical homogenized model as well as the double porosity models, but it is characterized by the presence of additional memory terms which describe the effects of local advective transport as well as diffusion. We discuss numerical discretizations and present numerical results to show the quantitative significance of each memory term in different regimes of flow and transport.

1 INTRODUCTION

Let Ω be a two-dimensional heterogeneous porous medium containing two disjoint flow regimes. The subscripts f and s are associated with the fast and slow regions Ω_f and Ω_s, respectively. The region Ω_f is connected, but Ω_s = \bigcup_{i=1}^{N_{incl}} Ω_{is} is a union of disjoint connected regions Ω_{is}.

Assume that Ω is covered by a union of rectangular subdomains Ω_i, i = 1, . . . , N_{incl}, with each Ω_i containing exactly one inclusion Ω_{is}. Let Ω_{if} = Ω_i ∩ Ω_f be the fast part surrounding Ω_{is} and let Γ_i = \partial Ω_{is} ∩ \partial Ω_{if} denote the local interfaces so that Ω_i = Ω_{is} ∪ Ω_{if} ∪ Γ_i. Let us assume that each Ω_i is congruent to a generic cell Ω_0 which contains the fast flow region Ω_{0f} surrounding the slow flow region Ω_{0s}. We also denote the volume fraction of the fast part by θ_f = |Ω_{0f}| / |Ω_0| and analogously θ_s = |Ω_{0s}| / |Ω_0| = 1 − θ_f.

Now we describe the microscopic model of the flow and solute transport in the heterogeneous porous medium, with porosity and permeability discontinuous across the interface
The flow is described by conservation of mass and Darcy’s law:

$$
\nabla \cdot \mathbf{v}_f = 0, \quad \mathbf{v}_f = -\mathbf{K}_f \nabla p_f, \quad x \in \Omega_f,
$$

$$
\nabla \cdot \mathbf{v}_i = 0, \quad \mathbf{v}_i = -\mathbf{K}_s \nabla p_i, \quad x \in \Omega_{is}, \ i = 1, \ldots, N_{incl},
$$

$$
p_i = p_f, \quad \mathbf{v}_i \cdot \mathbf{n} = \mathbf{v}_f \cdot \mathbf{n}, \quad x \in \Gamma_i,
$$

where $\mathbf{v}$ and $p$ are the velocity and the pressure of the flow, respectively. The coefficient $\mathbf{K}$ is the permeability of the porous medium. The solute transport equation is an advection-diffusion-dispersion equation as follows:

$$
\phi_f \frac{\partial c_f}{\partial t} - \nabla \cdot (\mathbf{D}_f \nabla c_f - \mathbf{v}_f c_f) = 0, \quad x \in \Omega_f,
$$

$$
\phi_i \frac{\partial c_i}{\partial t} - \nabla \cdot (\mathbf{D}_i \nabla c_i - \mathbf{v}_i c_i) = 0, \quad x \in \Omega_{is}, \ i = 1, \ldots, N_{incl},
$$

$$
c_i = c_f, \quad (\mathbf{D}_f \nabla c_f - \mathbf{v}_f c_f) \cdot \mathbf{n} = (\mathbf{D}_i \nabla c_i - \mathbf{v}_i c_i) \cdot \mathbf{n}, \quad x \in \Gamma_i.
$$

Here, $c$ is the solute concentration and $\phi$ is the porosity of the medium. The diffusion-dispersion tensor is given by

$$
\mathbf{D} = \mathbf{D}(\mathbf{v}) \equiv \phi [d_{mol} \mathbf{I} + |\mathbf{v}| (d_l \mathbf{E}(\mathbf{v}) + d_t (\mathbf{I} - \mathbf{E}(\mathbf{v})))].
$$

Here $d_{mol}, d_l, d_t$ are coefficients of molecular diffusivity, longitudinal and transversal dispersivity, respectively, and the dispersion tensor $\mathbf{E}(\mathbf{v}) = \frac{1}{|\mathbf{v}|^2} \mathbf{v}_i \mathbf{v}_j$ is a rank two tensor.

## 2 THE UPSCALED COUPLED FLOW-ADVECTION-DIFFUSION MODEL WITH MEMORY TERMS

We shall describe the discrete version of the double-porosity model with various memory terms for the coupled flow-transport equation as developed in [1]. To describe the upscaled flow equation, we first define the upscaled permeability tensor $\mathbf{K}^*$ as follows:

$$
(K^*)_{jk} = \frac{1}{|\Omega_0|} \int_{\Omega_{of}} (K_f)_{jm}(\mathbf{y}) (\delta_{mk} + \partial_m \omega_k(\mathbf{y})) \, dA,
$$

where the $\Omega_0$-periodic function $\omega_k(\mathbf{y})$ is defined as the solution of the periodic cell problem

$$
\begin{cases}
-\nabla \cdot \nabla \omega_j(\mathbf{y}) = 0, & \mathbf{y} \in \Omega_{of} \\
\nabla \omega_j(\mathbf{y}) \cdot \mathbf{n} = -\mathbf{e}_j \cdot \mathbf{n}, & \mathbf{y} \in \Gamma_{fs}.
\end{cases}
$$

The discrete double-porosity model that we employ here uses a local affine approximation on the interfaces which enables the model to capture the effects of advection and secondary diffusion. The upscaled flow model can be described by the following system of equations using a coefficient $\mathbf{K}^* = \mathbf{K}^* + \theta_s \mathbf{K}_s$. 

### 2.1 Upscaled Flow Model

The upscaled flow equation is given by

$$
\nabla \cdot \mathbf{v}_f^* = 0, \quad \mathbf{v}_f^* = -\mathbf{K}^* \nabla p_f^*, \quad x \in \Omega_f,
$$

$$
\nabla \cdot \mathbf{v}_i^* = 0, \quad \mathbf{v}_i^* = -\mathbf{K}_s \nabla p_i^*, \quad x \in \Omega_{is}, \ i = 1, \ldots, N_{incl},
$$

$$
p_i^* = p_f^*, \quad \mathbf{v}_i^* \cdot \mathbf{n} = \mathbf{v}_f^* \cdot \mathbf{n}, \quad x \in \Gamma_i.
$$

### 2.2 Upscaled Transport Model

The upscaled solute transport equation is given by

$$
\phi_f \frac{\partial c_f^*}{\partial t} - \nabla \cdot (\mathbf{D}_f^* \nabla c_f^* - \mathbf{v}_f^* c_f^*) = 0, \quad x \in \Omega_f,
$$

$$
\phi_i \frac{\partial c_i^*}{\partial t} - \nabla \cdot (\mathbf{D}_i^* \nabla c_i^* - \mathbf{v}_i^* c_i^*) = 0, \quad x \in \Omega_{is}, \ i = 1, \ldots, N_{incl},
$$

$$
c_i^* = c_f^*, \quad (\mathbf{D}_f^* \nabla c_f^* - \mathbf{v}_f^* c_f^*) \cdot \mathbf{n} = (\mathbf{D}_i^* \nabla c_i^* - \mathbf{v}_i^* c_i^*) \cdot \mathbf{n}, \quad x \in \Gamma_i.
$$
\begin{align*}
\nabla \cdot \mathbf{v}^* = 0, & \quad \mathbf{v}^* = -K^* \nabla p^*, \quad \mathbf{x} \in \Omega, \quad (6a) \\
\nabla \cdot \mathbf{v}_i^* = 0, & \quad \mathbf{v}_i^* = -\mathbf{K}_s \nabla p_i^*, \quad \mathbf{y} \in \Omega_i, \ i = 1, \cdots, N_{incl}, \quad (6b) \\
\left. p_i^* \right|_{r_i} = (\Pi_1 (p^*))_i, & \quad (6c)
\end{align*}

where the operator \( \Pi_1 \) is the local affine approximation.

To describe the upscaled transport system with memory terms in a convolution form, we define auxiliary functions as follows: for every \( i = 1, \cdots, N_{incl} \),

\begin{align*}
\phi_i \frac{\partial r_i^0}{\partial t} - \nabla \cdot (D_i \nabla r_i^0 - \mathbf{v}_i^* r_i^0) = 0, & \quad \mathbf{y} \in \Omega_{is}, \quad (7a) \\
r_i^0(\mathbf{y}, 0) = 0, & \quad \mathbf{y} \in \Omega_{is}, \quad (7b) \\
r_i^0(\mathbf{y}, 0) = 1, & \quad \mathbf{y} \in \Gamma_i. \quad (7c)
\end{align*}

and for \( k = 1, 2, \ i = 1, \cdots, N_{incl} \),

\begin{align*}
\phi_i \frac{\partial r_i^k}{\partial t} - \nabla \cdot (D_i \nabla r_i^k - \mathbf{v}_i^* r_i^k) = 0, & \quad \mathbf{y} \in \Omega_{is}, \quad (8a) \\
r_i^k(\mathbf{y}, 0) = 0, & \quad \mathbf{y} \in \Omega_{is}, \quad (8b) \\
r_i^k(\mathbf{y}, 0) = (\mathbf{y} - \mathbf{x}_{0i}^k), & \quad \mathbf{y} \in \Gamma_i. \quad (8c)
\end{align*}

Here \( \mathbf{x}_{0i}^k \) the centroid of \( \Omega_{is} \).

We use kernels arising from various averages of \( r^k \). First, we use the averages of rate of change in time

\[
\mathcal{T}_{i}^{k_0}(t) \equiv \frac{1}{|\Omega_i|} \int_{\Omega_{is}} \phi_i \frac{\partial r_i^k}{\partial t}(\mathbf{y}, t) \, dA, \quad k = 0, 1, 2
\]

Next, the kernels \( \mathcal{T}_{i}^{k1}, \mathcal{T}_{i}^{k2} \) arising from the components of the first moments of \( r_i^k, k = 0, 1, 2 \), are defined by

\[
\mathcal{T}_{i}^{k_j}(t) \equiv \frac{1}{|\Omega_i|} \int_{\Omega_{is}} \phi_i \frac{\partial r_i^k}{\partial t}(\mathbf{y}, t)(\mathbf{y} - (\mathbf{x}_{0i}^k))_j \, dA, \quad j = 1, 2; \ k = 0, 1, 2.
\]

Finally, for each \( r_i^k, k = 0, 1, 2 \) we set

\[
\mathcal{S}_i^k(t) \equiv \frac{1}{|\Omega_i|} \int_{\Omega_{is}} (D_i \nabla r_i^k(\mathbf{y}, t) - \mathbf{v}_i^* r_i^k(\mathbf{y}, t)) \, dA.
\]
Let \( N_{incl} \) be large and let us suppress the dependence of the kernels on \( i \). Then the limiting model of the transport systems with memory terms in convolution form is

\[
\phi^* \frac{\partial c^*}{\partial t} + T^{00} \ast \frac{\partial c^*}{\partial t} + (T^{10}, T^{20}) \ast \nabla \frac{\partial c^*}{\partial t} - \nabla \cdot \left( (T^{01}, T^{02}) \ast \frac{\partial c^*}{\partial t} - \nabla \cdot \left( (S^{01}, S^{02}) \ast \frac{\partial c^*}{\partial t} \right) \right) - \nabla \cdot \left( (S^{11}, S^{12}) \ast \frac{\partial c^*}{\partial t} \right) - \nabla \cdot \left( (D^1 \nabla c^* - v^* c^*) \right) = 0,
\]

where the effective porosity \( \phi^* = \theta_f \phi_f \). After we collect similar terms, the above equation (12) can be written in the compact form

\[
\phi^* \frac{\partial c^*}{\partial t} + T^{00} \ast \frac{\partial c^*}{\partial t} + M \ast \nabla \frac{\partial c^*}{\partial t} - \nabla \cdot \left( M \ast \frac{\partial c^*}{\partial t} \right) - \nabla \cdot \left( (D^1 \nabla c^* - v^* c^*) \right) = 0,
\]

where \( M : (0, \infty) \to \mathbb{R}^2, M : (0, \infty) \to \mathbb{R}^{2 \times 2} \) are time dependent vector and matrix valued memory kernels.

### 3 NUMERICAL DISCRETIZATION

In this section, we describe the Locally Conservative Eulerian-Lagrangian Method (LCELM) that was used to discretize the systems (7) and (8) and the effective solute transport equation (13). LCELM is a numerical technique that has been developed for convection-dominated diffusive systems and is based on the operator splitting technique. Originally, LCELM was introduced to achieve the local conservation of mass for the problem of two-phase, immiscible, incompressible flow in porous media [2], and the convergence of a version of LCELM as applied to a semilinear parabolic problem in one and two space variables has been proved [3, 4].

#### 3.1 Locally Conservative Eulerian-Lagrangian Method

Consider the following initial value problem for an advection-diffusion equation:

\[
\nabla_{x, t} \cdot \left( \frac{\phi s(x, t)}{u(x, t)} \right) - \nabla \cdot (D \nabla s) + g(s) = 0, \quad x \in \Omega, \quad 0 \leq t \leq T.
\]

We want to compute an approximate solution \( S \) to \( s \) at each discrete time step. Let \( \{M_{ij}\} \) be the rectangular partition of uniform size \( h_x \times h_y \) of \( \Omega \). In order to define a predecessor set for \( M_{ij} \), let \( y(t; x) \) be the solution of the final value problem given by

\[
y' = u/\phi \quad \text{and} \quad y(t^n, x) = x.
\]
Then, let
\[ \partial M^n_{ij} = \{ y(t^{n-1}; x) : x \in \partial M_{ij} \}, \]  
and define the interior of \( \partial M^n_{ij} \) to be the predecessor set \( \tilde{M}_{ij} \) at time \( t^{n-1} \) corresponding to \( M_{ij} \) at time \( t^n \). Define the tube \( E^n_{ij} \) to be the set interior to \( M_{ij} \), \( \tilde{M}^n_{ij} \) and the lateral boundary \( F^n_{ij} \) defined by the integral curve \( y(t; x), t^{n-1} < t < t^n, x \in \partial M_{ij} \). Then, the solution of (14) satisfies the relation
\[ \int_{M_{ij}} \phi S^n d\mathbf{x} - \int_{\tilde{M}_{ij}} \phi S^{n-1} d\mathbf{x} - \int_{D_{ij}} \nabla \cdot (D \nabla s) d\mathbf{x} dt + \int_{D_{ij}} g(s) d\mathbf{x} dt = 0. \]  

In order to approximate the transport part, the sets \( \tilde{M}^n_{ij} \) and \( E^n_{ij} \) must be approximated. Define an approximate predecessor \( \hat{Q}^n_{ij} \) as the quadrilateral having vertices \( \hat{x}^n_{ij,k} = x_{ij,k} - \frac{u(x_{ij,k}, t^n)}{\phi} \Delta t \), where \( x_{ij,k}, k = 1, \ldots, 4 \), are the vertices of \( M_{ij} \).

Let \( \hat{E}^n_{ij} \) be the tube formed with top \( M_{ij} \) and bottom \( \hat{Q}^n_{ij} \). Then the approximate solution \( \bar{S} \) to the transport part of (14) can be computed by
\[ \int_{M_{ij}} \bar{S}^n d\mathbf{x} = \int_{\hat{Q}^n_{ij}} S^{n-1} d\mathbf{x}. \]  

Next, we approximate the solution of the diffusive part by a cell-centered finite difference method as follows:
\[ h_x^2 h_y^2 \phi(\bar{S}^n_{ij} - \bar{S}^{n-1}_{ij}) - (\Delta t) h_y^2 D_{11}(S^n_{(i+1)j} + S^n_{(i-1)j} - 2S^n_{ij}) 
- (\Delta t) h_x^2 D_{22}(S^n_{ij+1} + S^n_{ij-1} - 2S^n_{ij}) + (\Delta t) h_x^2 h_y^2 g(S^n_{ij}) = 0. \]  

When we apply LCEL to the upscaled transport equation (13), all the convolution terms are treated in \( g(c^*) \).

### 3.2 Approximation of the convolution terms

We will approximate the convolution terms using the method developed by Peszyńska [5]. Consider a convolution term of the form
\[ u_{t} \ast \tau(t) = \int_{0}^{t} u_{t}(x, s) \tau(t - s) \, ds, \ x \in \Omega, t \in I = (0, T). \]  

The convolution kernel \( \tau(\cdot) \) is related to the microscopic properties of the domain of the flow. Define the partition of \( I \) as follows: let \( N \geq 0 \) be integer, \( \Delta t = \frac{T}{N} \) be the time step, let \( t^k = k \Delta t, k = 0, \ldots, N, \) and \( I = \bigcup_{k=1}^{N} I^k \), \( I^k = (t^{k-1}, t^k] \). Denote the characteristic function of the subinterval \( I_k \) by \( \theta^k \), and define a family of functions \( \{ \xi^k \}_{k=1}^{N} \) by
\[ \xi^k(t) = \int_{0}^{t} \tau(t - s) \theta^k(s) \, ds, \]  

5
and define also the averages
\[ \eta^{i,k} = \frac{1}{\Delta t} \int_{t_{i-1}}^{t_{i}} \xi^{k}(t) \, dt, \quad 1 \leq i, k \leq N. \] (22)

Then we approximate \( u_{t} \ast \tau(t) \) at time \( t^{i} \) as follows:
\[ (u_{t} \ast \tau)(t^{i}) = \sum_{k=1}^{i} \eta^{i,k} u^{k} - u^{k-1} \Delta t. \] (23)

4 NUMERICAL RESULTS

In this section, we present our computational results for the upscaled coupled equations (6) and (13). Our domain \( \Omega \) is a rectangle of size \( 80 \times 20 \, \text{cm}^{2} \). Let the generic cell \( \Omega_{0} \) be a square of size \( l \times l \), and \( \Omega_{0s} \), centered inside \( \Omega_{0} \), be a square of size \( (l - \delta) \times (l - \delta) \). Therefore, the fast flow part \( \Omega_{0f} \) has uniform thickness around \( \Omega_{0s} \).

The porosity of \( \Omega_{f} \) is \( \phi_{f} = 0.45 \) and the porosity of \( \Omega_{s} \) is \( \phi_{s} = 0.4 \). We consider three different regimes of flow and transport depending on the ratio \( K_{\text{ratio}} = K_{f}/K_{s} \). These are \( K_{\text{ratio}} = 6, 300, 1800 \) and are called the low, intermediate, and high contrast cases, respectively. We assume that the permeability \( K_{f} \) is isotropic and \( K_{f} = 5.78822 \times 10^{3} \, \text{cm/h} \). We also assume that the medium is initially fully concentrated with the solute, i.e. \( c^{*} = 1, \ t = 0, \ x \in \partial \Omega \) and clear fluid is pumped into the medium at the left boundary, that is \( c^{*} = 0, \ t > 0, \ x \in \partial \Omega_{\text{left}} \). We impose no-flow conditions on \( v_{f} \cdot n \) along the top and bottom of the porous medium and \( v_{f} \cdot n = v_{l} = 15 \, \text{cm/h} \) along the left boundary and \( v_{f} \cdot n = v_{r} = 15 \, \text{cm/h} \) along the right boundary of the medium. In our simulation, we approximate the effective permeability with \( K^{*} = \frac{1}{l^{2}} (\delta^{2} + (l - \delta) \delta) \cdot K_{f} = \frac{\delta}{l} \cdot K_{f} \). The effective diffusion/dispersion tensor is computed in the same way, i.e. \( D^{*} = \frac{\delta}{l} D_{f} \). Then we can compute \( v^{*} = (v_{l} K^{*} / (K^{*} + \theta_{s} K_{s}), 0) \), and \( v^{*} = (v_{l} K_{s} / (K^{*} + \theta_{s} K_{s}), 0) \) follows.

We summarize our effective parameters for each flow regime in the Table 2. We shall present the breakthrough curves of the solute at the right side of the medium in three different contrast cases at the final time \( T = 10 \). Figure 2 shows the breakthrough curves using four different models; the obstacle problem, the traditional double porosity model, the model which includes the secondary diffusion term and the full model which includes all memory terms. We observe different tailing effects due to different memory terms. In high and intermediate contrast cases, the secondary diffusion and the secondary advection
terms do not seem to play an important role and, therefore, the traditional double-porosity model yields fairly good results. However, in the low contrast case, each memory term gives rise to a noticeable difference in the breakthrough curve. Moreover, breakthrough curves from different permeability heterogeneity display different tailing behaviors which are even clearer on the log-log scale in Figure 3. No significant tailing occurs in the low contrast case. In the high contrast case the tailing is long-term and diffusion driven, while the intermediate contrast case shows a flatter early part of tails which are primarily advective. These phenomena coincide with the observation made in lab experiments [6]. We will discuss some properties of the memory kernels and the analysis of the numerical methods used in this work in a forthcoming paper.

![Figure 2: Breakthrough curves using various models in high, intermediate, and low contrast cases from left to right.](image)
Figure 3: Breakthrough curves using various models on a log-log scale in high, intermediate, and low contrast cases from left to right.

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REFERENCES


