Two-scale computational modelling of water flow in unsaturated soils containing irregular-shaped inclusions

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SUMMARY

The focus of this paper is two-dimensional computational modelling of water flow in unsaturated soils consisting of weakly-conductive disconnected inclusions embedded in a highly-conductive connected matrix. When the inclusions are small, a two-scale Richards’ equation-based model has been proposed in the literature taking the form of an equation with effective parameters governing the macroscopic flow coupled with a microscopic equation, defined at each point in the macroscopic domain, governing the flow in the inclusions. This paper is devoted to a number of advances in the numerical implementation of this model. Namely, by treating the micro-scale as a two-dimensional problem our solution approach based on a control volume finite element method can be applied to irregular inclusion geometries, and, if necessary, modified to account for additional phenomena (e.g., imposing the macroscopic gradient on the micro-scale via a linear approximation of the macroscopic variable along the microscopic boundary). This is achieved with the help of an exponential integrator for advancing the solution in time. This time integration method completely avoids generation of the Jacobian matrix of the system and hence eases the computation when solving the two-scale model in a completely coupled manner. Numerical simulations are presented for a two-dimensional infiltration problem. Copyright © 2013 John Wiley & Sons, Ltd.

KEY WORDS: Two-scale; Multi-scale; Unsaturated flow; Control Volume Finite Element Method; Exponential integrators.

1. INTRODUCTION

A double porosity soil is a heterogeneous medium consisting of two soils (soil \(a\) and soil \(b\)) each with their own set of hydraulic properties (e.g. porosity, hydraulic conductivity, etc.). In this work, we consider the weakly conductive inclusions embedded in a highly conductive matrix problem of Szymkiewicz and Lewandowska [1]: soil \(a\) forms the connected matrix, soil \(b\) forms disconnected/isolated inclusions, and the hydraulic conductivity of soil \(a\) is orders of magnitude larger than that of soil \(b\) (see Figure 1). As the length scale of the soil heterogeneities becomes small, the computational cost of numerical simulations of the full two-scale model (i.e. Richards’ equation in the full heterogeneous geometry) quickly becomes prohibitive [2, 3, 4]. The numerical issues are further compounded by the presence of two time scales in the problem: a short time scale associated with the flow in the fast soil (soil \(a\)) and a long time scale associated with the flow in the slow soil (soil \(b\)).

A classic approach for the above problem is to replace the heterogeneous medium with a fictitious homogeneous medium and model the average flow behaviour at the macroscopic scale (i.e., at a...
scale much larger than the scale of the heterogeneities) [5]. Assuming a periodic geometry and using homogenization theory, a macroscopic equation can be derived taking the form of Richards’ equation with effective parameters [6]: the effective conductivity is defined in terms of the solution of an elliptic equation on the period (or unit cell) and accounts for the isotropic, orthotropic or anisotropic structure of the heterogeneous medium. This macroscopic approach works well provided the hydraulic conductivities of the soils are of the same order of magnitude [6, 1]. If, however, the conductivity of soil \( a \) is much larger than soil \( b \) (as is the focus of this paper), a typical two-scale phenomenon occurs: the flow in soil \( a \) is rapid and quickly surrounds the disconnected soil \( b \) inclusions before slowly infiltrating them. In this case, the macroscopic approach fails to account for the delay that is inherent in the flux entering the inclusions.

The reasons mentioned above have motivated the introduction of the class of two-scale models of double porosity [7, 8] or distributed microstructure [9, 10, 11, 12] type considered in this paper. In addition to an effective macroscopic equation, these models include, at each point in the macroscopic domain, an additional equation at the scale of the heterogeneities (microscopic scale). Coupling between scales is achieved by imposing the macroscopic value via a Dirichlet boundary condition on the interface between the two soils (boundary of the micro-scale domain) and by including the average flux across the interface as a source term at the macroscopic level to account for the delay effect. Such a two-scale model was derived for a Richards’ equation description of the flow by Lewandowska et al. [13] and since then has been further developed by other authors [13, 1, 14, 15]. In these papers, numerical results for macroscopically one- and two-dimensional problems have been given for simple geometries, including circular [1], rectangular [16, 14], spherical [15] and staggered rectangular shaped inclusions [14]. For circles and spheres, the microscopic equation reduces to a one dimensional problem. For other simple inclusion geometries (e.g. rectangular inclusions), where the problem is microscopically two-dimensional, the authors in these papers have employed a one dimensional numerical approximation to the microscopic equation (using a method proposed by Pruess and Narasimhan [17]), which, while reducing simulation times, sacrifices the true two-dimensional flow of water at the microscopic scale and overestimates the water infiltration into the inclusions by as much as 5% over a 25 hour simulation [14].

In this paper, we apply the ‘unified’ two-scale model of Szymkiewicz and Lewandowska [1] to a two-dimensional water infiltration problem and offer a number of advances in its numerical implementation. In particular, we outline a two-dimensional unstructured control volume finite element method that can be applied to irregular inclusion geometries, and, if desired, refined to account for additional phenomena, including gravitational effects at the microscopic scale, and a linear approximation of the macroscopic variable over the microscopic boundary (such a micro-scale boundary condition has been studied previously by Showalter [9, 10, 18]). Treating the micro-scale equation as a full two-dimensional problem is achieved with the help of an exponential integrator for advancing the numerical solution in time, which eases the two-scale computations since it totally avoids generating the Jacobian matrix.
The remaining sections of the paper are organised as follows. In the following section, we outline the two-scale model of Szymkiewicz and Lewandowska [1]. Section 3 presents our numerical implementation of the two-scale model based on an unstructured control volume finite element method at both scales and an exponential time stepping strategy, which allows the model to be applied to irregular inclusion geometries and solved simultaneously in a completely coupled manner. The section then concludes with a brief sketch of a MATLAB code for performing image-based meshing of irregular-shaped inclusion geometries (§3.3). Numerical simulation results for both inclusions geometries are presented in Section 4. A summary and conclusions of the work are given in Section 5.

2. TWO-SCALE MODEL

The microscopic scale is introduced into the formulation by assuming that at each point \( x = (x_1, x_2) \in \Omega \), there exists a micro-cell \( \Omega_x \) whose geometry is representative of the soil heterogeneity at that point (see Figure 2). The basic assumption in the derivation of the model is that the ratio of the characteristic length of \( \Omega_x \), denoted by \( l \), to the characteristic length of \( \Omega \), denoted by \( L \), is small, that is \( \varepsilon = l/L \ll 1 \). This assumption, which is known as separation of scales [19, 16], is necessary when deriving the model via homogenization since asymptotic expansions in the variable \( \varepsilon \) are assumed. Note that if the ratio is close to one (i.e., the scale of the soil heterogeneities are not small) then one would instead apply the full fine-scale model.

Before we proceed, some further notation and assumptions are required. We will assume that each cell \( \Omega_x = [0, a_1] \times [0, a_2] \) is an open rectangle in \( \mathbb{R}^2 \) with boundary \( \partial \Omega_x \) and further assume, for simplicity, that \( a_1 \) and \( a_2 \) are independent of \( x \). The sub-domains of \( \Omega_x \) occupied by soil \( a \) and soil \( b \) are denoted by \( \Omega_{x,a} \) and \( \Omega_{x,b} \), respectively. Furthermore, we let \( \Gamma_x \) denote the interface between the two soils within \( \Omega_x \). The coordinate variable \( y = (y_1, y_2) \in \Omega_x \) is defined on each cell \( \Omega_x \), under the assumption that the axial directions \( y_1 \) and \( y_2 \) align with \( x_1 \) and \( x_2 \) respectively.

The two-scale model of Szymkiewicz and Lewandowska [1] consists of a macroscopic equation:

\[
\frac{\partial}{\partial t} \left[ \theta_{\text{eff}}(h_a, x) \right] + \nabla_x \cdot \left[ -K_{\text{eff}}(h_a, x) \nabla_x (h_a + x_2) \right] = Q(x), \quad x \in \Omega, \tag{1a}
\]

where \( \theta_{\text{eff}}(h_a, x) = |\Omega_{x,a}| \theta_a(h_a)/(|\Omega_x|) \) (\(| \cdot | \) denotes area), coupled with a microscopic equation, defined at each point \( x \in \Omega \), governing the flow in the inclusions:

\[
\frac{\partial}{\partial t} \left[ \theta_b(h_b) \right] + \nabla_y \cdot \left[ -K_b(h_b) \nabla_y h_b \right] = 0, \quad y \in \Omega_{x,b}. \tag{1b}
\]

In the above equations, \( h_a [L] \) is the macroscopic primary variable (pressure head in soil \( a \)), \( h_b [L] \) is the microscopic primary variable (pressure head in soil \( b \)), and \( \theta_i [-] \) and \( K_i [L T^{-1}] \) are the
volumetric moisture content and hydraulic conductivity for soil $i$, respectively. At the macroscopic scale, gravity is assumed to act in the negative $x_2$ direction. Equality of the macroscopic and microscopic pressure head values is imposed at the soil interface

$$h_b = h_a, \quad y \in \Gamma_x, \quad x \in \Omega.$$  \hfill (1c)

The source term $Q$ quantifies the change in moisture content in $\Omega_{x,b}$ or, equivalently, the amount of fluid flux across the interface (from $\Omega_{x,b}$ to $\Omega_{x,a}$), both scaled by the area of $\Omega_x$

$$Q(x) = -\frac{1}{|\Omega_x|} \frac{\partial}{\partial t} \int_{\Omega_{x,b}} \theta_b(h_b) \, dy, \quad \text{or,}$$  \hfill (1d)

$$Q(x) = \frac{1}{|\Omega_x|} \int_{\Gamma_x} -K_b(h_b) \nabla y h_b \cdot n_{x,b} \, ds,$$  \hfill (1e)

where $n_{x,b}$ is the unit vector normal to $\Gamma_x$ directed outward from $\Omega_{x,b}$.

Note that the two-scale model is fully coupled with coupling occurring in both directions: the macroscopic equation (1a) features the source term $Q$ calculated from the microscopic variable $h_b$ (equations 1d and 1e) and the microscopic equation (1b) is paired with the boundary condition (1c) in which the macroscopic variable $h_a$ appears. Only soil $a$ participates in the macroscopic flow because only it is macroscopically connected. This model represents a significant increase in complexity compared with a classical macroscopic model: for every $x \in \Omega$ the solution of a separate partial differential equation is required. Note that if desired one may include gravitational effects at the microscopic scale by replacing $h_b$ by $(h_b + y_2)$ in equation (1b).

The effective hydraulic conductivity $K_{\text{eff}} \in \mathbb{R}^{2 \times 2}$ is a matrix with $j$th column equal to

$$[K_{\text{eff}}(h, x)]_{\ast j} = \frac{1}{|\Omega_x|} \int_{\Omega_a} K(h, y) \nabla y (u_j + y_j) \, dy,$$  \hfill (2)

where

$$K(h, y) = \begin{cases} K_a(h) & \text{if } y \in \Omega_{x,a} \\ K_b(h) & \text{if } y \in \Omega_{x,b} \end{cases},$$  \hfill (3)

and $u_j$ is the solution of the periodic cell problem:

$$\nabla y \cdot (K(h, y) \nabla y (u_j + y_j)) = 0, \quad y \in \Omega_x, \quad u_j \text{ is } \Omega_x-\text{periodic},$$  \hfill (4a)

$$\frac{1}{|\Omega_x|} \int_{\Omega_a} u_j \, dy = 0.$$  \hfill (4c)

The system (1)–(4) is the unified model for bimodal porous media given by Szymkiewicz and Lewandowska [1] and comprises a model of distributed microstructure [9, 10, 11, 12] or double porosity [7, 8] type.

Remark 1

(i) When the conductivity of soil $a$ is much larger than that of soil $b$, the effective conductivity can be defined over $\Omega_{x,a}$ only (see [1, eqs 16–18]). The definition (2)–(4), however, is applicable regardless of the conductivity ratio [16, 20].

(ii) The solution of the problem described by equations (4a) and (4b) is unique only up to an additive constant [19]; however, any of these solutions will do as only the gradient of $u_j$ is required in the definition of the effective conductivity (2). Nevertheless, to obtain a unique solution we follow the usual approach [1] of pairing the equations with the zero mean constraint (4c).
We will complement the two-scale model with the following initial and boundary conditions:

\[ h_a - h_0(x) = 0, \quad x \in \Omega, \quad t = 0, \quad (5a) \]
\[ K_{\text{eff}}(h_a, x) \nabla_x (h_a + x_2) \cdot n_\Omega - \gamma(x) = 0, \quad x \in \partial \Omega, \quad t > 0, \quad (5b) \]
\[ h_b - h_0(x) = 0, \quad y \in \Omega_{x,b}, \quad t = 0, \quad (5c) \]

where \( n_\Omega \) is the unit vector normal to \( \partial \Omega \) directed outward from \( \Omega \) and \( \gamma : x \in \partial \Omega \rightarrow \mathbb{R} \) controls the influx of water at the boundary. Also, as an alternative to the microscopic boundary condition at the soil interface (1c), we also allow for the microscopic value to vary linearly according to the macroscopic gradient:

\[ h_b = h_a + (\nabla_x h_a) \cdot (y - y_e), \quad y \in \Gamma_x, \quad x \in \Omega, \quad (6) \]

where \( y_e = \frac{1}{2}(a_1, a_2) \) is the centre of the micro-cell \( \Omega_x \). Because the inclusions are macroscopically disconnected we do not, however, include the divergence of the microscopic flux in the source term \( Q \) that accounts for the “secondary flux” flowing through the cell structure (see [9, 10, 12] for details).

To close the model we use the popular van Genuchten [21] relations:

\[ \theta_i(h) = \theta_{\text{res},i} + (\theta_{\text{sat},i} - \theta_{\text{res},i}) S_c(h), \quad (7a) \]
\[ K_i(h) = K_{\text{sat},i} S_c(h)^{1/2} \left[ 1 - (1 - S_c(h)^{1/m_i})^{m_i} \right]^2, \quad (7b) \]

where \( S_c \) is the effective saturation defined as

\[ S_c(h) = (1 + (-\alpha_i h)^{n_i})^{-m_i}, \quad (7c) \]

\( m_i = 1 - 1/n_i \) (Mualem’s hypothesis [22]) and the constants \( \theta_{\text{res},i}, \theta_{\text{sat},i}, \alpha_i, n_i \) and \( K_{\text{sat},i} \) characterise the hydraulic properties of soil \( i \): \( \theta_{\text{res},i} \) and \( \theta_{\text{sat},i} \) are the residual and saturated values of the moisture content (minimum and maximum values, respectively), \( \alpha_i \) is related to the pore density maximum, \( n_i \) is related to the pore size distribution and \( K_{\text{sat},i} \) is the saturated hydraulic conductivity (\( K_i(h) = K_{\text{sat},i} \) when \( S_c = 1 \)) [23]. These parameters are identified for a given soil by fitting the curves (7) to measured data in a least squares sense [23].

3. NUMERICAL IMPLEMENTATION

In this section, we present a numerical solution strategy for the two-scale model using an unstructured vertex-centered control volume finite element method. The three underlying principles of the method are that the discrete unknowns are positioned at the vertices in the mesh, control volumes are formed around each node by connecting the centroid of each element to the midpoint of its edges and finite element shape functions are used for flux approximation at control volume edges. We treat the microscopic equation as a full two-dimensional problem and use triangular elements to allow the method to be applied to irregular-shaped inclusions. Separate formulations for the two definitions of the source term, given in equations (1d) and (1e), are presented.

3.1. Discretisation in space

We consider a triangulation of the macroscopic domain \( \Omega \) consisting of \( N_{\text{macro}} \) nodes located at the coordinates \( x_i \) \((i = 1, \ldots, N_{\text{macro}})\) and assign to each of these nodes a micro-cell \( \Omega_{x_i} \), (see Figure 3). The corresponding microscopic domains \( \Omega_{x_i,b} \) (soil \( b \) component of micro-cell \( \Omega_{x_i} \)) are also meshed using triangular elements each consisting of \( N_{\text{micro},i} \) nodes located at the coordinates \( y_{i,1}, \ldots, y_{i,N_{\text{micro},i}} \). Note that it is impossible for triangle edges to perfectly align with curved boundaries and interfaces: the interface \( \Gamma_{x_i} \) in the microscopic mesh and the boundary \( \partial \Omega \) in the macroscopic mesh are approximated by polygonal curves consisting of a number of line segments.
These curves are denoted by $\tilde{\Gamma}_x$ and $\partial \tilde{\Omega}$, respectively, and the regions bounded by these curves as $\tilde{\Omega}_{x_i,b}$ and $\tilde{\Omega}$, respectively. In the working that follows, we adopt the following notation. The (two-dimensional) control volume for an arbitrary macroscopic node $i$ is denoted by $V_i$ and the (two-dimensional) control volume for an arbitrary microscopic node $j$ (associated with macroscopic node $i$) is denoted by $V_{i,j}$. The symbol $\sigma$ will be used to denote an arbitrary edge at both scales (see Figure 3). The macroscopic and microscopic discrete unknowns at the nodes are labelled $h_{a,i}$ and $h_{b,i,j}$, respectively. Following the usual control volume theory, the macroscopic equation (1a) is integrated over $V_i$ to give

$$\frac{d}{dt} \int_{V_i} \theta_{\text{eff}}(h_{a,x}) \, dx = \sum_{\sigma \in E_i} \int_{\sigma} K_{\text{eff}}(h_{a,x}) \nabla_x (h_{a,x} + x_2) \cdot n_{i,\sigma} \, ds + \int_{V_i} Q(x) \, dx,$$

(8)

where $E_i$ is the set of edges that make up the boundary of $V_i$ and $n_{i,\sigma}$ is the unit vector normal to edge $\sigma$ directed outward from macroscopic node $i$ (see Figure 3). We approximate the first integral on the right-hand side of equation (8) by the following quantity:

$$F_{i,\sigma} = \begin{cases} |\sigma| \left( \sum_{k=1}^{N_{\text{macro}}} K_{\text{eff}}(h_{a,k,x_k}) \psi_k(x_\sigma) \right) \left( \sum_{k=1}^{N_{\text{macro}}} h_{a,k} (\nabla_x \psi_k)(x_\sigma) + e_2 \right) \cdot n_{i,\sigma} & \text{if } \sigma \subset \tilde{\Omega} \\
-|\sigma| \gamma(x_\sigma) & \text{if } \sigma \subset \partial \tilde{\Omega},
\end{cases}$$

where $x_\sigma$ is the midpoint of edge $\sigma$. Calculation of the nodal values of the effective conductivity $K_{\text{eff}}(h_{a,k}, x_k)$ is presented later in §4.2. For each macroscopic node $i$, the function $\psi_i(x)$ is defined as the unique piecewise linear function (piecewise on the triangular elements) that takes the value one at node $i$ ($x = x_i$) and zero elsewhere, that is,

$$\psi_i(x_j) = \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\
0 & \text{if } i \neq j.
\end{cases}$$

(9)

Note that $\psi_i(x)$ vanishes over all elements that do not contain $i$ as a vertex and that the gradient $(\nabla_x \psi_i)(x)$ is piecewise constant and not defined at the vertices or edges of the triangles. The
functions (9) provide a convenient way to write down a global representation of the numerical flux at edges. For each edge \( \sigma \), the form of the approximation is equivalent to one obtained using linear finite element shape functions for triangular elements (see, e.g., [24, Example 1.11]).

The microscopic equation (1b) is integrated over the control volume \( V_{i,j} \) to give

\[
\frac{d}{dt} \int_{V_{i,j}} \theta_i(h_b) \, dy = \sum_{\sigma \in E_{i,j}} \int K_h(h_b) \nabla y h_b \cdot n_{i,j,\sigma} \, ds ,
\]  

(10)

where \( E_{i,j} \) is the set of edges that make up the boundary of \( V_{i,j} \) and \( n_{i,j,\sigma} \) is the unit vector normal to edge \( \sigma \) directed outward from microscopic node \( i,j \) (see Figure 3). We approximate the integrals on the left and right hand sides of equation (10) by the following quantities, respectively:

\[
\Psi_{i,j} = |V_{i,j}| \theta_b(h_{b,i,j}) ,
\]

\[
F_{i,j,\sigma} = |\sigma| \left( \sum_{k=1}^{N_{\text{micro},i}} K_h(h_{b,i,k}) \psi_i(y_{\sigma}) \right) \left( \sum_{k=1}^{N_{\text{micro},i}} h_{b,i,k}(\nabla h_{\psi_i}(y_{\sigma})) \cdot n_{i,j,\sigma} ,
\]

where \( y_{\sigma} \) denotes the coordinates of the midpoint of edge \( \sigma \). We have obtained \( \Psi_{i,j} \) by employing the usual quadrature approximation: evaluate the integrand at the node and multiply by the area of the control volume. The function \( \psi_i(y) \) is defined as the unique piecewise linear function (piecewise on the triangular elements) satisfying \( \psi_i(y_{t,i}) = \delta_{jk} \).

The discrete values of \( h_b \) located on the interface \( \Gamma_{\sigma} \), do not enter our solution procedure as unknowns since their values at each point in time are known from the Dirichlet boundary conditions (1c) or (6). For each microscopic domain, \( \Omega_{\text{micro},i} \), we assume that there are \( B_i \) boundary nodes and \( N_{\text{micro},i} \), interior nodes and label them \( b_1, \ldots, b_{B_i} \) and \( d_1, \ldots, d_{N_{\text{micro},i}} \), respectively. Equation (8) is therefore written down only for \( j = d_1, \ldots, d_{N_{\text{micro},i}} \). For each macroscopic node \( i \), the microscopic discrete values of \( h_b \) along the interface are computed using equation (1c):

\[
h_{b,i,j} = h_{a,i} ,
\]  

(11)

for all \( j = b_1, \ldots, b_{B_i} \), or the following discretisation of equation (6):

\[
h_{b,i,j} = h_{a,i} + \left( \frac{1}{|V_i|} \sum_{\sigma \in E_i} \left( \sum_{k=1}^{N_{\text{macro}}} h_{a,k} \psi_k(x_{\sigma}) \right) n_{i,\sigma} \right) (y_{i,j} - y_e) ,
\]  

(12)

for all \( j = b_1, \ldots, b_{B_i} \). Since the gradient of \( \psi_i(x) \) isn’t defined at \( x_i \), we have used the following approximation:

\[
(\nabla h_{a})(x_i) \approx \frac{1}{|V_i|} \sum_{\sigma \in E_i} \left( \sum_{k=1}^{N_{\text{macro}}} h_{a,k} \psi_k(x_{\sigma}) \right) n_{i,\sigma} ,
\]  

(13)

in equation (12), which arises from the result that

\[
\int_{V_i} \nabla h_{a} \, dx = \sum_{\sigma \in E_i} \int_{\sigma} h_{a} n_{i,\sigma} \, ds .
\]  

(14)

For the macroscopic equation, the discretisation of the second term on the right hand side of equation (8) depends on which definition of the source term is used (equation 1d or 1e). We present two separate formulations for each definition below.

**Formulation 1: Source term defined according to definition (1d).** In this case, the second term on the right hand side of equations (8) contains a time derivative, which we combine with the time derivative on the left-hand side as follows:

\[
\frac{d}{dt} \int_{V_i} \left[ \theta_c h_{a} + \frac{1}{|\Omega_{\text{micro},i}|} \int_{\Omega_{\text{micro},i}} \theta_b(h_b) \, dy \right] dx = \sum_{\sigma \in E_i} \int_{\sigma} K_{\text{eff}}(h_a, x) \nabla x (h_a + x_2) \cdot n_{i,\sigma} \, ds .
\]
The integral over \( V_i \) on the left-hand side of the above equation is approximated by evaluating the integrand at node \( i \) and multiplying by the area of \( V_i \) and then approximating the integral over \( \Omega_{x_i,b} \) using a sum over the control volumes:

\[
\int_{V_i} \left[ \theta_{\text{eff}}(h_a, x) + \frac{1}{|\Omega_{x_i}|} \int_{\Omega_{x_i,b}} \theta_b(h_b) \, dy \right] \, dx \approx |V_i| \left( \theta_{\text{eff}}(h_a,i, x_i) + \frac{1}{|\Omega_{x_i}|} \int_{\Omega_{x_i,b}} \theta_b(h_b) \, dy \right),
\]

\[\approx \frac{|V_i|}{|\Omega_{x_i}|} \left( |\Omega_{x_i,a}| \theta_a(h_{a,i}) + \sum_{j=1}^{\text{N\text{micro},i}} \theta_b(h_{b,i,j}) |V_{i,j}| \right) = \Psi_i. \tag{15}\]

In summary, we have derived the following coupled system of ordinary differential equations:

\[
\frac{d\Psi_{i,d}}{dt} = G_{i,j}, \quad j = d_1, \ldots, d_{\text{N\text{micro},i}}, \tag{17a}\]

\[
\frac{d\Psi_i}{dt} = G_i, \tag{17b}\]

for each macroscopic node \( i \), where

\[
G_i = \sum_{\sigma \in E_i} F_{i,\sigma}, \quad \text{and} \quad G_{i,j} = \sum_{\sigma \in E_{i,j}} F_{i,j,\sigma}.
\]

Numerous time integration methods exist that can be applied to the system (17) in its current form (e.g., the backward Euler method or methods based on the backward differentiation formula). Exponential integrators, however, require the system to be expressed in autonomous form:

\[
\frac{du}{dt} = g(u), \tag{18}\]

where \( u \in \mathbb{R}^N \) is the vector of discrete unknowns. To do this, we apply a chain rule to the left-hand side of the system (17) and then express it as follows:

\[
\frac{d}{dt} \begin{bmatrix}
    h_{b,i,d_1} \\
    \vdots \\
    h_{b,i,d_{\text{N\text{micro},i}}} \\
    h_{a,i} \\
\end{bmatrix} = \begin{bmatrix}
    R_{i,d_1} \\
    \vdots \\
    R_{i,d_{\text{N\text{micro},i}}} \\
    R_i \\
\end{bmatrix}, \tag{19}\]

where we define

\[
\begin{bmatrix}
    G_{i,d_1} \\
    \vdots \\
    G_{i,d_{\text{N\text{micro},i}}} \\
    G_i \\
\end{bmatrix} = \begin{bmatrix}
    \frac{\partial \Psi_{i,d_1}}{\partial h_{b,i,d_1}} & \cdots & \frac{\partial \Psi_{i,d_1}}{\partial h_{b,i,d_{\text{N\text{micro},i}}} & \frac{\partial \Psi_{i,d_1}}{\partial h_{a,i}} \\
    \vdots & \ddots & \vdots & \vdots \\
    \frac{\partial \Psi_{i,d_{\text{N\text{micro},i}}}}{\partial h_{b,i,d_1}} & \cdots & \frac{\partial \Psi_{i,d_{\text{N\text{micro},i}}}}{\partial h_{b,i,d_{\text{N\text{micro},i}}} & \frac{\partial \Psi_{i,d_{\text{N\text{micro},i}}}}{\partial h_{a,i}} \\
    \frac{\partial \Psi_{i}}{\partial h_{b,i,d_1}} & \cdots & \frac{\partial \Psi_{i}}{\partial h_{b,i,d_{\text{N\text{micro},i}}} & \frac{\partial \Psi_{i}}{\partial h_{a,i}} \\
\end{bmatrix}^{-1} \begin{bmatrix}
    R_{i,d_1} \\
    \vdots \\
    R_{i,d_{\text{N\text{micro},i}}} \\
    R_i \\
\end{bmatrix}. \tag{20}\]

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The derivatives in the above equation are computed analytically using the definition of $\theta_a(h)$ and $\theta_b(h)$ in equation (7a). Since $\Psi_{i,j}$ is a function of $h_{b,i,j}$ only, we have the following results

\[
\frac{\partial \Psi_{i,k}}{\partial h_{b,i,j}} = 0 \quad \text{if } j \neq k, \quad (21a)
\]

\[
\frac{\partial \Psi_{i,k}}{\partial h_{a,i}} = 0 \quad \text{for all } k = d_1, \ldots, d_{N_{\text{micro},i}}. \quad (21b)
\]

It follows that the matrix being inverted in equation (20) is lower diagonal with each entry below the main diagonal equal to zero apart from the last row, which contains all non-zero entries. Thus, the product in equation (20) can be computed efficiently using forward substitution as follows:

\[
R_{i,d_j} = \left( \frac{\partial \Psi_{i,d_j}}{\partial h_{b,i,d_j}} \right)^{-1} G_{i,d_j}, \quad j = 1, \ldots, \tilde{N}_{\text{micro},i},
\]

\[
R_i = \left( \frac{\partial \Psi_{i}}{\partial h_{a,i}} \right)^{-1} \left( G_i - \sum_{k=1}^{\tilde{N}_{\text{micro},i}} \frac{\partial \psi_{i}}{\partial h_{b,i,d_k}} R_{i,d_k} \right).
\]

Note that the above formulation is not valid when the discrete values of $h_b$ along the interface are computed using equation (12). The presence of the macroscopic gradient creates additional coupling between macroscopic and microscopic nodes. Since the sum in equation (16) is taken over all microscopic nodes (both boundary and interior nodes) associated with macroscopic node $i$, $\Psi_i$ is a function of not only the macroscopic unknown $h_{a,i}$ and the microscopic unknowns $h_{b,i,j}$ ($j = d_1, \ldots, d_{\tilde{N}_{\text{micro},i}}$) but also the macroscopic unknowns at neighbouring macroscopic nodes to node $i$. As result, the above formulation cannot be applied when the boundary condition (12) is employed.

**Formulation 2. Source term defined according to definition (1e).** In this case, equation (8) is rewritten as follows:

\[
\frac{d}{dt} \int_{V_i} \theta_{\text{eff}}(h_a, \mathbf{x}) \, d\mathbf{x} = \sum_{\sigma \in E_i} \int_{\sigma} K_{\text{eff}}(h_a, \mathbf{x}) \nabla_x (h_a + x_2) \cdot \mathbf{n}_{i,\sigma} \, ds \quad + \int_{V_i} \left[ \frac{1}{|\Omega_x|} \int_{\Gamma_x} -K_b(h_b) \nabla_y h_b \cdot \mathbf{n}_{x,b} \, ds \right] d\mathbf{x}, \quad (22)
\]

We approximate the first integral on the left-hand side and second term on the right-hand side of equation (22) by the quantities:

\[
\Psi_i = |V_i| \theta_{\text{eff}}(h_{a,i}, \mathbf{x}_i) = \frac{|V_i|}{|\Omega_x|} |\Omega_{x,a}| \theta_a(h_{a,i}),
\]

\[
S_i = -|V_i| |\Omega_x| \sum_{\sigma \in B_i} |\sigma| \left( \sum_{k=1}^{N_{\text{micro},i}} K_b(h_{b,i,k}) \psi_{i,k}(y_\sigma) \right) \left( \sum_{k=1}^{N_{\text{micro},i}} h_{b,i,k}(\nabla_y \psi_{i,k})(y_{\sigma,c}) \cdot \mathbf{n}_{i,j} \right),
\]

where $B_i$ is the set of edges the comprise the interface $\Gamma_{x_i}$. Note that $\nabla_y \psi_{i,j}$ is not defined at the edges of the triangles, so the gradient approximation cannot be evaluated at $y_\sigma$ when calculating the flux across the interface $\Gamma_x$. The edge $\sigma$, however, forms the edge of an element and it is the centroid of this element (denoted $y_{\sigma,c}$) at which the approximation is performed. In summary, for each macroscopic node $i$, we have derived a system in the form of (17) where

\[
G_i = S_i + \sum_{\sigma \in E_i} F_{i,\sigma}, \quad \text{and} \quad G_{i,j} = \sum_{\sigma \in E_{i,j}} F_{i,j,\sigma}.
\]

Note that in the formulation above the additional coupling between macroscopic and microscopic nodes created from the macroscopic gradient in the boundary condition (12) presents itself in the
term $S_i$ defined above, which appears on the right-hand side of equation (17). We conclude that this approach (Formulation 2) is applicable for both equations (11) and (12). Since $\Psi_i$ is a function of $h_{a,i}$ only and $\Psi_{i,j}$ is a function of $h_{b,i,j}$ only we have

$$\frac{\partial \Psi_i}{\partial h_{b,i,j}} = 0 \quad \text{for all } j = 1, \ldots, N_{\text{micro},i},$$

in addition to the results (21). It follows that the matrix being inverted in the product (20) is diagonal, so it is simple to form.

Regardless of which formulation above is employed, we have derived an initial value problem involving a system of ordinary differential equations in autonomous form (18) with the following properties:

(i) The $(j + \sum_{k=1}^{i-1} (\tilde{N}_{\text{micro},k} + 1))$th entries of $u$ and $g(u)$ are equal to $h_{b,i,d_j}$ and $R_{i,d_j}$, respectively, for all $j = 1, \ldots, \tilde{N}_{\text{micro},i}$ and $i = 1, \ldots, N_{\text{macro}}$.

(ii) The $(\sum_{k=1}^{i} (\tilde{N}_{\text{micro},k} + 1))$th entries of $u$ and $g(u)$ are equal to $h_{a,i}$ and $R_i$, respectively, for all $i = 1, \ldots, N_{\text{macro}}$.

(iii) The number of equations/unknowns is $N = N_{\text{macro}} + \sum_{k=1}^{N_{\text{macro}}} \tilde{N}_{\text{micro},k}$.

(iv) The initial values are $h_{b,i,d_j} = h_{a,i} = h_0(x_i)$ for all $j = 1, \ldots, \tilde{N}_{\text{micro},i}$ and $i = 1, \ldots, N_{\text{macro}}$.

Remark 2
Consider the special case when each microscopic mesh has the same number of nodes and the same number of interior nodes (i.e., $N_{\text{micro},i} = \tilde{N}_{\text{micro}}$ and $\tilde{N}_{\text{micro},i} = \tilde{N}_{\text{micro}}$ for all $i = 1, \ldots, N_{\text{macro}}$). This would be true, for example, in the case when the micro-cell geometry does not vary in space (provided the same mesh is used for each micro-cell). In this simple case, the $(j + (i-1)(\tilde{N}_{\text{micro}} + 1))$th entries of $u$ and $g(u)$ are equal to $h_{b,i,d_j}$ and $R_{i,d_j}$, respectively, the $i(\tilde{N}_{\text{micro}} + 1)$th entries of $u$ and $g(u)$ are equal to $h_{a,i}$ and $R_i$, respectively, and the number of equations/unknowns is $N = (N_{\text{macro}} + 1)\tilde{N}_{\text{micro}}$.

3.2. Discretisation in time

Existing time integration methods used for the two-scale model of Szymkiewicz and Lewandowska [1] have employed a backward Euler time discretisation [15, 16, 1, 14] and a Newton method to solve the resulting system of nonlinear equations [16]. To avoid a large coefficient matrix in Newton’s method, the macroscopic and microscopic equations are decoupled [15], which sacrifices the true two-way coupling embedded within the model. As previously mentioned, a novel contribution of this paper is the use of an exponential integrator to perform the time discretisation. The main attraction of exponential integrators over standard implicit integrators (e.g., the backward Euler method) is that Krylov subspace methods for approximating matrix-function vector products involving the exponential function converge rapidly. This means that the integrators can be implemented efficiently without the computational overhead associated with preconditioning, which in many cases requires generation and factorisation of all or part of the large sparse Jacobian matrix.

We employ the exponential Rosenbrock-Euler method [25] with the step-size control strategy proposed by Carr, Moroney and Turner [26] to solve the system of ordinary differential equations (18) numerically. This method has performed well in previous problems involving wood drying [27, 28] and unsaturated water flow [26]. The method relates the solutions at $t = t_n$ (denoted by
$u_n$) and $t = t_{n+1}$ (denoted by $u_{n+1}$) via the relation:

$$u_{n+1} = u_n + \tau_n \varphi(\tau_n J(u_n)) g(u_n),$$

(23)

where $\tau_n = t_{n+1} - t_n$ is the step size, $J$ is the Jacobian matrix of $g(u)$ and $\varphi(z) = (e^z - 1)/z$.

The formula is derived by approximating $g(u)$ by the first two terms of its Taylor polynomial and then solving the resulting linear system of differential equations exactly [26]. An important observation is that the scheme (23) is explicit, that is, $u_{n+1}$ is defined explicitly in terms of $u_n$, so there is no nonlinear or linear system of equations to solve. Instead the matrix-function vector product $\varphi(\tau_n J(u_n)) g(u_n)$ needs to be computed at each step, which we do using Krylov subspaces as described in previous work [26, 28]. Our method requires only matrix-vector products with $J$, which are computed using in the standard way by using a finite difference approximation involving evaluations of $g(u)$ [29, §3.2.1].

3.3. Mesh generation of micro-cell geometries

For irregular geometries, we use imaged-based meshing techniques and the finite element mesh generator GMSH [30] to generate the microscopic meshes from a bitmap image of the micro-cell. Our code, which we have implemented in MATLAB, is summarised graphically in Figure 4 and in the following steps:

(i) Read bitmap image of the micro-cell into MATLAB from the graphics file and convert to a binary image.

(ii) Use the MATLAB function `bwboundaries` to identify the coordinates of the boundary pixels of the inclusions.

(iii) Scale coordinates of the boundary pixels to the appropriate size of the micro-cell.

Figure 4. Mesh generation procedure using MATLAB. Legend: Interface nodes (●), sub-domain corresponding to soil a (■), sub-domain corresponding to soil b (□).

(i) Read bitmap image of the micro-cell into MATLAB from the graphics file and convert to a binary image.

(ii) Use the MATLAB function `bwboundaries` to identify the coordinates of the boundary pixels of the inclusions.

(iii) Scale coordinates of the boundary pixels to the appropriate size of the micro-cell.
(iv) Create a GMSH .geo file in MATLAB that defines the geometry of the domain. Boundary points of the inclusions are defined as points in GMSH (using the Point command) and BSplines curves are created that trace the inclusion boundaries (using the BSpline command).

(v) Run GMSH in ‘batch-mode’ from within MATLAB to mesh the geometry.

(vi) Read .msh file into MATLAB and build element and node arrays.

The code accommodates the microscopic domain for the two-scale model $\Omega_{x,b}$ (Figure 4f) and the domain for the periodic cell problem $\Omega_a$ (Figure 4d) but will not work if $\Omega_{x,b}$ overlaps the boundary of the micro-cell $\Omega_x$, that is, the inclusions must be interior to the cell.

4. RESULTS

Numerical simulation results for the two-scale model are presented in this section for a two-dimensional problem involving infiltration into a dry region. All simulations are performed using the second formulation developed in §3.1 (Formulation 2) because it can be applied to both microscopic boundary conditions (1c) and (6). For each simulation, we assume that the micro-cell does not vary in space: the geometry of micro-cell ($\Omega_x$) is independent of the macroscopic coordinate variable ($x$). This is the special case given in the remark in §3.1.

4.1. Test Problem

We consider infiltration into a two-dimensional square domain of width and height 50 cm (macroscopic domain $\Omega = [0, 50] \times [0, 50]$) (see Figure 5). All boundaries are impermeable apart from a 20 cm section located on the left hand side of the upper boundary ($0 \leq x_1 \leq 20$ cm), where a constant infiltration rate of $0.3 \text{ cm h}^{-1}$ is imposed, and the lower boundary ($x_2 = 0$) where free drainage ($\partial h/\partial x_2 = 0$) is applied. Initially, the capillary pressure head is uniformly equal to $-2000 \text{ cm}$ (at both scales). This problem has been previously been presented by Szymkiewicz and Lewandowska [14], however, we will use the micro-cell geometry shown in Figure 5 that contains irregular-shaped inclusions.

For all simulations, we assume the two soils differ only in the saturated hydraulic conductivity $K_{sat}$. Note that this means that the conductivity ratio $K_b(h)/K_a(h)$ is constant for all values of the pressure head $h$. We use the following parameters values that correspond to a typical sandy loam [14]: $\theta_{res} = 0.058$ (residual moisture content), $\theta_{sat} = 0.41$ (saturated moisture content), $\alpha = 0.073 \text{ cm}^{-1}$ (parameter related to pore density maximum) and $n = 1.89$ (parameter related to the pore size distribution). The saturated hydraulic conductivity of soil $a$ (macroscopically connected soil) is set equal to 4.4 cm h$^{-1}$. Different parameter values of the saturated hydraulic conductivity of the inclusions (soil $b$) are then investigated corresponding to the conductivity ratios $K_b/K_a = 10^{-2}$ and $10^{-6}$.

4.2. Computing the effective hydraulic conductivity

Under the assumption that the micro-cell geometry does not vary in space we will have a single global effective conductivity $K_{eff}$ defined for the entire macroscopic domain $\Omega$. Recall, that the effective conductivity $K_{eff}$ is defined in terms of the solution of the periodic cell problem (4), which continuously relates the pressure head $h$ to the value of $K_{eff}$. Rather than solve this problem throughout the simulation, standard practice is to compute $K_{eff}$ for a pre-determined sequence of discrete values of $h$ and then interpolate to evaluate $K_{eff}$ at any $h$ [14]. The sequence of discrete values must span the entire range of $h$ that are possible throughout the simulation. In order to capture the highly nonlinear behaviour of the hydraulic conductivity curve as $h \rightarrow 0$ we choose a geometric sequence of 100 pressure head values: $h_n = h_1 r^{n-1}$ for $n = 1, \ldots, 100$, where $h_1 = -2000 \text{ cm}$ and $r$ is computed to satisfy $h_{100} = -1 \text{ cm}$. Such a choice for the range is based on the initial condition, a simulation time of 40 hours and the values of the hydraulic properties used. We note that for a
A numerical solution of the periodic cell problem (4) is found for each combination of \( j = 1, 2 \) and discrete value of \( h \) (200 problems in total). Each problem is solved numerically using a control volume finite element method with an unstructured mesh consisting of 1266 triangular elements and 674 nodes (this mesh is shown in Figure 4d). The resulting spatially-discrete system is linear and solved using MATLAB’s backslash operator and represents a total pre-processing contribution to the simulation time of order one minute. Note that, for the soil parameter values given in the previous section it turns out that periodic cell problems (4) need only be solved once for each value of \( j = 1, 2 \). This can be seen by scaling equation (4a) by \( K_a(h) \): since \( K_b/K_a \) is fixed, the solution is equal for all \( h \). However, our goal is to produce a general code suitable for any values of the hydraulic parameters, so we do not take advantage of this in our implementation. We found that the larger conductivity of soil \( a \) dominates over the smaller conductivity of soil \( b \) producing negligible differences in the effective conductivity between the two conductivity ratios. The discrete entries \([K_{\text{eff}}(h_n)]_{ij}\) for \( K_b/K_a = 10^{-2} \) are plotted against the discrete values \( h_n, n = 1, \ldots, 100 \), in Figure 6 using a log (base 10) scale along the \( h \) axis. Due to the anisotropic nature of the micro-cell, the effective conductivity has non-zero off-diagonal entries and non-equal diagonal entries.

Piecewise linear interpolation of the entries of \( K_{\text{eff}} \) corresponding to the discrete values of \( h \) are used to evaluate the effective conductivity for any value of the pressure head. The relationship between \( K_{\text{eff}} \) and \( h \) is highly nonlinear, however, Figure 6 indicates that a piecewise linear function relating the entries of \( K_{\text{eff}} \) to \( \log_{10}(-h) \) is reasonable. For \( h_n < h < h_{n+1} \), we obtain the following estimate:

\[
[K_{\text{eff}}(h)]_{ij} := [K_{\text{eff}}(h_n)]_{ij} + \left( [K_{\text{eff}}(h_{n+1})]_{ij} - [K_{\text{eff}}(h_n)]_{ij} \right) \frac{\log_{10}(-h) - \log_{10}(-h_n)}{\log_{10}(-h_{n+1}) - \log_{10}(-h_n)}.
\]

Note that the interpolant requires only one evaluation of the \( \log_{10} \) function. The remaining terms are computed once prior to the simulation and stored thereafter.

4.3. Two-scale simulations

Numerical solutions are obtained using a structured macroscopic mesh consisting of 1681 nodes (40 × 40 grid with uniform node spacing of 1.25 cm) and an unstructured microscopic mesh consisting of 532 triangular elements and 316 nodes (this mesh is shown in Figure 4f) giving a total number of unknowns equal to 374,863. Due to the geometry of the macro-scale domain we have used a rectangular grid: the equations given in §3.1 still apply, however, the definition of \( \psi_i(x) \) changes from piecewise linear to piecewise bilinear. The level of refinement used on the micro-scale is equivalent to the level used when solving the periodic cell problem for the effective conductivity in the previous section. We have implemented the code in a hybrid Matlab/C framework: the vector-valued function \( g(u) \) in equation (18) is implemented as a MEX-file (MATLAB Executable) written in C. The computation time for each simulation is roughly 2 hours on a MacBook Pro with a 2.7 GHz Intel Core i7 processor and 4 GB of RAM running MAC OS X and MATLAB R2011a.

Simulation results are shown in Figures 10–12 using microscopic boundary condition (1c). Recall that the numerical solution of the two-scale model provides both the macroscopic pressure head field (\( x \in \Omega \)) and the microscopic pressure head field (\( y \in \Omega_{x,b} \)) at each macroscopic node. In each figure, we display the microscopic field at two selected points: (10, 40) and (30, 30). After 40 hours of infiltration, one point is located in the wetting front (30, 30) and the other in the wet zone behind the front (10, 40). To highlight the simulated physical configuration, the pressure head at the micro-scale in soil \( a (y \in \Omega_{x,a}) \) is visualised as uniformly equal to the macroscopic value. Note that the contour plots are not linear in the pressure head: the contours are chosen to correspond to increments of 0.1 in the effective saturation (e.g., \( h = -6 \, \text{cm} \) and \( h = -10 \, \text{cm} \) are approximately equivalent to \( S_e = 0.9 \) and \( S_e = 0.8 \), respectively).

The effect of the conductivity ratio on the microscopic solution is clearly evident from the microscopic fields at (10, 40). For the largest conductivity ratio \( K_b/K_a = 10^{-2} \), after 40 hours of infiltration, the inclusions (soil \( b \)) have been completely infiltrated with the pressure head matching the macroscopic value. This is in contrast to the smallest conductivity ratio where the pressure head is almost unchanged from its initial state since water has effectively bypassed the inclusions because...
of their low conductivity. Another important observation is that the wetting front propagates faster as the conductivity ratio \( K_b/K_a \) is reduced. This behaviour cannot be attributed to the effective conductivity (since negligible differences in \( K_{eff} \) were observed across the three conductivity ratios). Rather, it is a direct result of the source term \( Q \) coupling the macroscopic and microscopic fields. Since the test problem involves infiltration, the source term \( Q \) is always negative (sink)
because the moisture content is always increasing (see equation 1d). Therefore, the smaller the conductivity ratio, the slower the moisture content is increasing in the inclusions, which produces a larger value for $Q$ and an increase across the pressure head field.

Simulation results are shown in Figure 13 using microscopic boundary condition (6), where the microscopic value varies linearly according to the macroscopic gradient. When implementing this
boundary condition we found that one has to be careful that the perturbation \( \nabla_x h_a \cdot (y - y_c) \) is not too large to overshoot the unsaturated condition \( h < 0 \). To avoid this issue we have used a micro-cell of width and height equal to 0.5 cm and we note that the use of this boundary condition should be restricted to real-world applications where the macroscopic element size far exceeds that of the micro-cell. Imposing the macroscopic gradient on the microscopic scale produces more realistic solutions at the microscopic scale with the macroscopic wetting front clearly visible at the microscopic scale.

5. CONCLUSIONS

We have provided a number of advances in numerically solving the two-scale model of Szymkiewicz and Lewandowska [1] for simulating unsaturated flow in double porosity soils. In particular, our numerical approach allows the model to be applied to irregular inclusion geometries and solved simultaneously in a completely coupled manner thanks to the use of a two-dimensional unstructured control volume finite element method at the microscopic scale and an exponential Rosenbrock time integration method, respectively. This represents a significant contribution to the literature as previous papers [14, 15, 1] have employed a one-dimensional method at the micro-scale, which is only applicable to simple geometries, and have decoupled the macroscopic and microscopic equations in the solution procedure. Treating the micro-scale equation as a full two-dimensional problem also allows the model to be refined to account for additional phenomena if desired, for example, a non-uniform microscopic boundary condition using a linear approximation of the macroscopic value along the microscopic boundary. Altogether, two separate formulations for the spatial discretisation of the model were developed: one for each of the two definitions of the source term. We recommend the second formulation, where the source term is defined as the average flux across the micro-scale boundary, as it is better equipped to treat the additional coupling that arises when the macroscopic gradient is imposed on the microscopic scale.

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