



HAL
open science

Moving away from macroscopic modelling of of transport processes in porous media: two-scale approaches and their applications

Elliot Carr, Patrick Perré, I. I. Turner

► To cite this version:

Elliot Carr, Patrick Perré, I. I. Turner. Moving away from macroscopic modelling of of transport processes in porous media: two-scale approaches and their applications. 19th International Drying Symposium IDS'2014, Aug 2014, Lyon, France. hal-01794730

HAL Id: hal-01794730

<https://hal.science/hal-01794730>

Submitted on 17 May 2018

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

MOVING AWAY FROM MACROSCOPIC MODELLING OF TRANSPORT PROCESSES IN POROUS MEDIA: TWO-SCALE APPROACHES AND THEIR APPLICATIONS

E. Carr^{1*}, P. Perré¹, I. Turner²

¹*École Centrale Paris, Laboratory of Chemical Engineering and Materials (LGPM)
Grande Voie des Vignes, Châtenay-Malabry, 92290, France*

²*Mathematical Sciences School, Queensland University of Technology,
2 George Street, Brisbane, QLD 4000, Australia*

*Corresponding author: Tel.: +33 6 82 54 17 15, E-mail: elliott.carr@ecp.fr

Abstract: A classic approach for modeling transport phenomena in heterogeneous media is to adopt a larger macroscopic scale of description, where the transport is assumed to be smooth in space and time. However, because non-equilibrium effects at the scale of the heterogeneities (micro-scale) are not accounted for, the macroscopic approach fails in some configurations where both scales have to be considered simultaneously. This paper outlines two popular two-scale approaches for such configurations. For each approach, numerical simulations highlighting the capabilities of the model are presented for an example problem, including low temperature drying of softwood and water flow in heterogeneous materials.

Keywords: multi-scale modeling, two-scale modeling, heterogeneous media, wood drying

INTRODUCTION

Macroscopic approaches for modeling transport processes in a heterogeneous medium, for example a composite material or a porous medium, are well established. In porous media, to overcome the impossible task of solving the microscopic transport equations on the highly complex porous geometry, the macroscopic approach adopts a larger scale of description. At this length scale, the fluid phases are viewed as fictitious continua and volume averaging is used to derive balance equations from the standard conservation laws. The resulting macroscopic equations resemble those of a continuum with the exception that volume-averaged quantities and effective parameters now appear in the equations^[1]. Such an approach has been widely used to simulate transport processes in porous media, however, it fails in some documented cases. For example, the macroscopic formulation of coupled heat and mass transfer known as TransPore^[2-4], which has been extensively applied over the past twenty years to model and simulate the drying process, fails when applied to hardwood^[5].

Another problem where the macroscopic approach is often used is modeling fluid flow in a composite material that exhibits small-scale heterogeneity in physical properties such as permeability or porosity.

In this case, numerical solution of the governing partial differential equations is intractable due to the massive number of elements and vertices required to mesh the full heterogeneous geometry and capture the small material interfaces. To overcome these impracticalities, the macroscopic approach again consists of adopting a larger scale of description, where the heterogeneous medium can be viewed as a fictitious homogeneous medium, and a macroscopic equation with effective parameters can be derived. While the macroscopic model works well provided the assumption of local equilibrium holds (which is only true if the properties of the different materials are of the same order of magnitude), it fails if the assumption is violated. A common example is fluid flow in a two material medium where one material is connected and has high conductivity/permeability and the other material forms disconnected inclusions and has low conductivity/permeability. In this case, the flow in the connected material is rapid and a macroscopic model cannot account for the delay that occurs in the flux entering the inclusions. A classic example of such a configuration is fluid flow in fractured rocks^[6].

The aforementioned limitations of macroscopic approaches have motivated the introduction of methods that attempt to describe the transport processes on two scales, macroscopic and microscopic. For porous media, the microscopic

scale refers to the pore-scale where as for a composite material it refers to the scale of the heterogeneities. In this paper, we consider perhaps the two most prominent two-scale approaches: the heterogeneous multi-scale methods and the distributed microstructure models. The central idea of both approaches is the same, namely, that solving the microscopic transport equations on a number of small domains (micro-cells) sparsely distributed throughout the full heterogeneous medium is much less expensive than solving the full microscopic problem. In the next sections, we present the general framework of both approaches, briefly discuss their numerical implementation and demonstrate their application to an example problem.

HETEROGENEOUS MULTI-SCALE METHODS

Heterogeneous multi-scale methods^[7,8] are among those multi-scale approaches that assume local equilibrium at the micro-scale. In these methods, the form of the macroscopic flux is not proposed prior to the simulation but instead it is estimated throughout the simulation by solving the microscopic equation on micro-cells that have been strategically positioned at points where macroscopic flux estimation is required. The microscopic equation is solved under steady state conditions^[9] or evolved to a quasi-steady state^[7,8], at which point the macroscopic flux is estimated and the macroscopic solution then evolved. The objective of this approach is purely to describe the macroscopic behavior of the flow: the microscopic solution does not represent the solution to the full microscopic model at that point in space. For this reason the method is restricted to problems where the macroscopic scale is the only scale of interest.

Example: Low temperature convective drying of wood in the hygroscopic range

Heterogeneous multi-scale methods have been applied to simulate water flow in heterogeneous soils governed by the Richards' equation^[7,8]. Recently, a similar idea was used to simulate low temperature convective drying of softwood in the hygroscopic range^[9]. Under low temperature drying conditions, the assumption of a fixed gaseous pressure is valid, which means that only balance equations for the conservation of water and energy are required, giving the following pair of coupled macroscopic equations:

Macroscopic conservation of water and energy

$$\frac{\partial \psi_M^{(w)}}{\partial t} + \nabla \cdot q_M^{(w)} = 0 \quad (1)$$

$$\frac{\partial \psi_M^{(e)}}{\partial t} + \nabla \cdot q_M^{(e)} = 0 \quad (2)$$

where the conserved quantities are defined in terms of the primary variables: moisture content (X_M) and temperature (T_M). The subscript M is used to denote a macroscopic quantity and the subscript m a microscopic quantity. Each time the macroscopic fluxes need to be estimated, one solves the following pair of coupled steady state equations on the underlying pore structure specified by the geometry of the micro-cell at the given point:

Micro-cell steady state problem

$$\nabla \cdot q_m^{(w)} = 0 \quad (3)$$

$$\nabla \cdot q_m^{(e)} = 0 \quad (4)$$

Once a solution to the steady state problem has been obtained, the macroscopic moisture and thermal fluxes are computed by averaging the microscopic fluxes over the micro-cell:

$$q_M^{(w)} = \frac{1}{|Y|} \int_Y q_m^{(w)} dy \quad (5)$$

$$q_M^{(e)} = \frac{1}{|Y|} \int_Y q_m^{(e)} dy \quad (6)$$

where the micro-cell domain is denoted by Y and $|Y|$ is the area of the cell.

In the hygroscopic range, liquid water is absent from the pores so the void space in the porous medium is composed of air and water vapor only. Thus, the liquid mass flux at the microscopic consists of two contributions: bound water diffusion in the solid phase and water vapor diffusion in the gaseous phase. The transport of energy is governed by heat conduction (Fourier's Law) and the diffusive energy fluxes associated with bound water and vapor. For the full form of the microscopic fluxes the reader is referred to the literature^[9].

Additional coupling between the macroscopic and microscopic variable fields is described below:

- (i) Calibration of the macroscopic and microscopic conserved quantities is enforced

$$\psi_M^{(w)} = \frac{1}{|Y|} \int_Y \psi_m^{(w)} dy \quad (7)$$

$$\psi_M^{(e)} = \frac{1}{|Y|} \int_Y \psi_m^{(e)} dy \quad (8)$$

where the microscopic conserved quantities are defined in terms of the microscopic primary variables: moisture content (X_m) and temperature (T_m).

- (i) The macroscopic gradients of moisture content and temperature are imposed on the microscopic boundary via the following quasi-periodic boundary conditions:

$$X_m(a, y_2) = X_m(0, y_2) + a \frac{\partial X_M}{\partial x_1} \quad (9)$$

$$X_m(y_1, b) = X_m(y_1, 0) + b \frac{\partial X_M}{\partial x_2} \quad (10)$$

$$T_m(a, y_2) = T_m(0, y_2) + a \frac{\partial T_M}{\partial x_1} \quad (11)$$

$$T_m(y_1, b) = T_m(y_1, 0) + b \frac{\partial T_M}{\partial x_2} \quad (12)$$

where a and b are the width and height of the micro-cell Y , respectively.

Clearly, the two-scale model described above requires a significant increase in computational resources (e.g., memory and computation time) compared with a standard macroscopic approach. The extreme size of the numerical problem becomes apparent when applying a control volume finite element (CVFE) method to the macroscopic equations. In this case, macroscopic flux estimation is required at the midpoint of each control volume edge in the mesh throughout the entire simulation. Each time the flux is estimated one must solve the steady state problem numerically on the micro-cell (Eqs. 3 and 4) using an appropriate numerical strategy (e.g. a CVFE method together with a Newton iteration). In this work, the discrete macroscopic solution is advanced in time using an exponential Rosenbrock method^[9].

To highlight the capabilities of the model we present simulation results for low temperature convective drying of a small cross-section of softwood of size 5cm x 2.5cm. The micro-cell geometry is assumed to be fixed in space and time with size $50\mu\text{m} \times 40.963\mu\text{m}$. Two different micro-cell configurations are tested representing a cell in wood with and without pits (see Figs. 1 and 2). Initially, the moisture content and temperature are uniformly equal to 0.275kgkg^{-1} and 50°C , respectively. For the specific drying boundary conditions and parameters used the reader is referred to the literature^[9]. All simulations were performed with a macroscopic mesh containing 928 triangular elements and 552 nodes in total, however, due to the symmetry of the problem only one quarter of these are computed on. The simulation time was approximately 5 hours when implemented in a hybrid MATLAB/C code 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 using a microscopic mesh comprising 576 nodes.

The significant effect of the micro-cell configuration on the macroscopic moisture content fields is demonstrated in Figs. 2-7. The inclusion of pits eases the moisture transfer along the width of the cross-section (parallel to the direction of the pits) leading to a significantly faster drying rate and a quasi-flat moisture field after 18 hours of drying (Fig. 8). This phenomenon is explained by the fact that gaseous phase is connected in the direction of the width of the board (see Fig. 1). Since the mass flux is more conductive in the gaseous phase than in the solid phase, the connectivity of the gaseous phase increases the magnitude of the mass flux.

It is worth noting that one could also exhibit the microscopic distributions of moisture content (X_m) and temperature (T_m). However, these solutions are not representative of the actual distribution at the pore-scale. It is for this reason that we believe that this two-scale model closely aligns with a macroscopic approach, where the effective parameters are supplied using homogenization theory^[5].

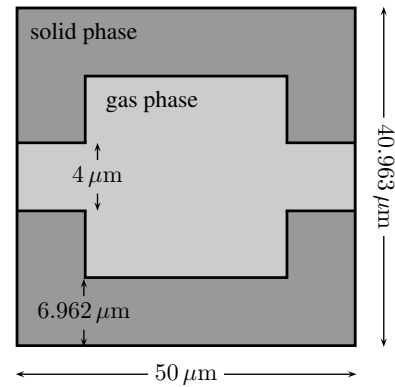


Fig. 1. Micro-cell configuration (pits)

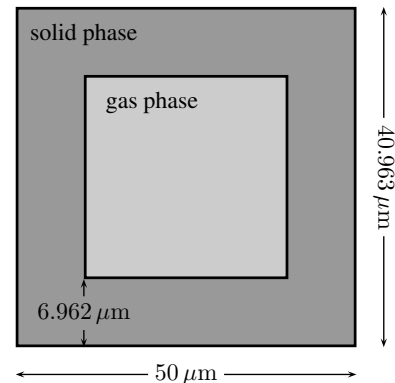


Fig. 2. Micro-cell configuration (no pits)

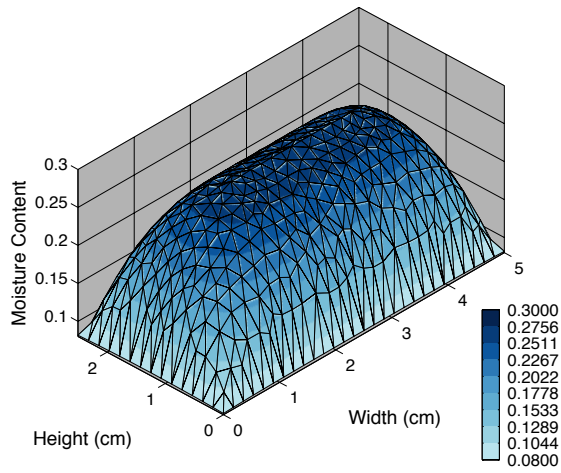


Fig. 3. Macroscopic moisture content field after 6 hours (no pits)

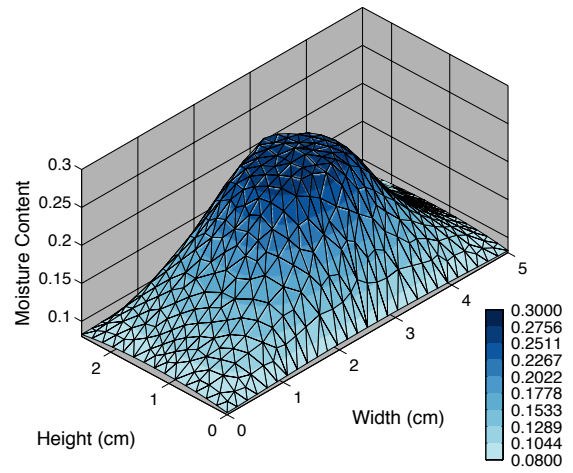


Fig. 6. Macroscopic moisture content field after 6 hours (pits)

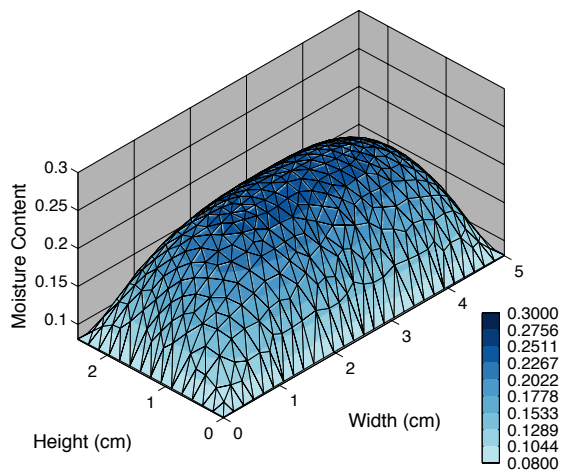


Fig. 4. Macroscopic moisture content field after 12 hours (no pits)

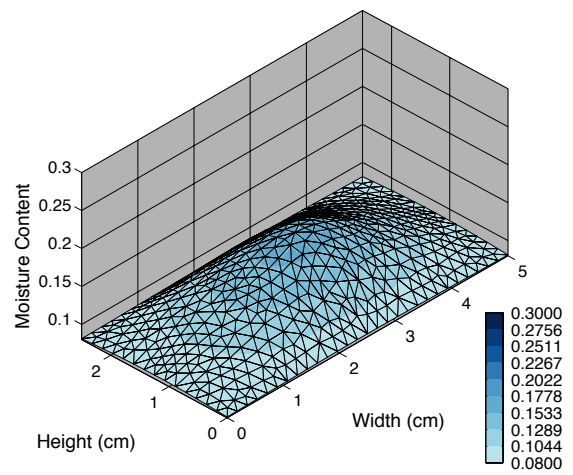


Fig. 7. Macroscopic moisture content field after 12 hours (pits)

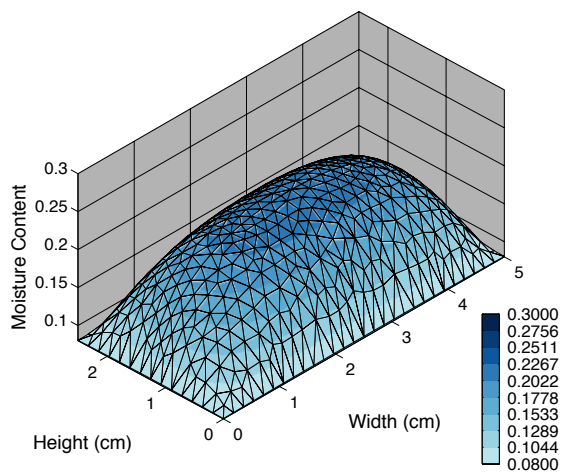


Fig. 5. Macroscopic moisture content field after 18 hours (no pits)

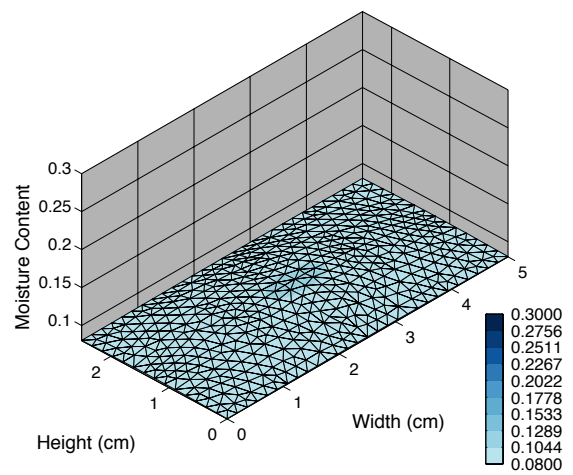


Fig. 8. Macroscopic moisture content field after 18 hours (pits)

DISTRIBUTED MICROSTRUCTURE MODELS

Unlike the heterogeneous multi-scale methods, distributed microstructure models do not assume local equilibrium at the microscopic scale. These models are designed specifically for a heterogeneous medium composed of two materials, where one material has high conductivity/permeability and is macroscopically connected (known as the matrix or the conductive phase) while the other has low conductivity/permeability and forms disconnected inclusions (also known as the storage phase). The underlying idea is that a macroscopic equation describes the global flow in the macroscopically connected material and a family of microscopic equations describes the local flow in the isolated inclusions. Coupling between scales occurs on the material interface within each micro-cell via a Dirichlet condition matching the microscopic and macroscopic variables and a source term at the macroscopic level representing the flux passing from the inclusions to the connected material. Recent work^[10] has permitted such models to 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).

Example: Water flow in heterogeneous soils

We consider a two-scale distributed microstructure model that uses a Richards' equation description of the flow. Richards' equation is commonly used to describe unsaturated flow of water in heterogeneous soils and represents a simplified form of the full two-phase (air and water) flow model under the assumption that the air phase is held at constant (atmospheric) pressure. The two-scale model consists of the following coupled macroscopic and microscopic equation:

Macroscopic conservation of water

$$\frac{\partial}{\partial t}(\varepsilon_M \theta_M) + \nabla \cdot (-K_{eff}(h_M) \nabla (h_M + x_2)) = Q \quad (13)$$

Microscopic conservation of water

$$\frac{\partial \theta_m}{\partial t} + \nabla \cdot (-K_m(h_m) \nabla h_m) = 0 \quad \text{on } Y_m \quad (14)$$

where $\varepsilon_M = |Y_M|/|Y|$, h_M is the macroscopic primary variable (pressure head in the matrix), h_m is the microscopic primary variable (pressure head in the inclusions), K_{eff} is the effective conductivity given according to homogenization theory^[10,11] and Y_m is the sub-domain of the micro-cell occupied by the weakly conductive inclusion (see Fig. 9). As previously mentioned, coupling between scales occurs in two ways:

- (i) Equality of the macroscopic and microscopic variables is imposed on the material interface, which forms the boundary condition for the microscopic problem:

$$h_m = h_M \quad \text{on } \Gamma \quad (15)$$

- (ii) The source term Q quantifies the amount of fluid flux that passes through the material interface (from the inclusions to the connected material) scaled by the area of the micro-cell:

$$Q = \frac{1}{|Y|} \int_{\Gamma} -K_m(h_m) \nabla h_m \cdot n_{\Gamma} dy \quad (16)$$

where n_{Γ} is the unit vector normal to the interface directed outward from the inclusion.

This model represents a significant increase in complexity compared with a classical macroscopic approach: at each macroscopic node the solution of separate partial differential equation is required (Eq. 14). The difference with the heterogeneous multi-scale method, however, is that both the macroscopic and microscopic equations are completely coupled and evolved using the same time step.

To close the model the van Genuchten relationships are used that express the moisture content and hydraulic conductivity in terms of the pressure head:

$$\theta(h) = \theta_{res} + (\theta_{sat} - \theta_{res}) S_e(h) \quad (17)$$

$$K(h) = K_{sat} S_e(h)^{1/2} [1 - (1 - S_e(h)^{1/m})^m]^2 \quad (18)$$

where $m = 1 - 1/n$ and the effective saturation

$$S_e(h) = [1 + (-\alpha h)^n]^{-m} \quad (19)$$

The various parameters included in the relations describe the hydraulic properties of the material^[10].

To highlight the capabilities of the model, we present numerical simulation results for a water infiltration problem into a square domain of size 30cm by 30cm consisting of weakly conductive inclusions embedded in a highly conductive material. All boundaries are no flux apart from a 10cm section at the center of the top boundary, where a constant infiltration rate of 0.3cmh^{-1} is applied. Initially, the domain is very dry with the pressure head set equal to -20cm everywhere at both scales. The hydraulic properties of both materials are the same apart from the saturated hydraulic conductivity, which is 1000 times smaller in the inclusions (see Table 1).

Table 1. Hydraulic properties

	K_{sat}	θ_{res}	θ_{sat}	α	n
Matrix	4.4	0.058	0.41	0.073	1.89
Inclusions	0.0044	0.058	0.41	0.073	1.89

The two-scale model is solved using a CVFE method applied to a macroscopic mesh consisting of 961 nodes (30 by 30 grid with 1cm spacing between grid points). At each macroscopic node, the microscopic equation (3) is solved on the micro-cell depicted in Fig. 9 using an unstructured mesh consisting of 186 nodes. The resulting discrete differential system has dimension $N = 961 + 961 \times 186 = 179,707$, which is solved numerically using an exponential Rosenbrock-Euler method^[10]. For a simulation of 20 hours, the computation time was approximately 40 minutes when implemented in a hybrid MATLAB/C code 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.

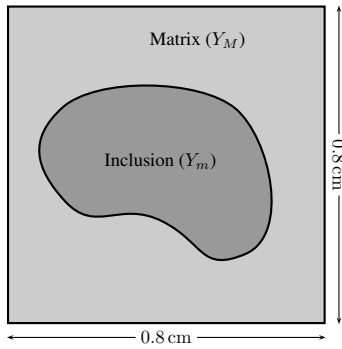


Fig. 9. Micro-cell configuration.

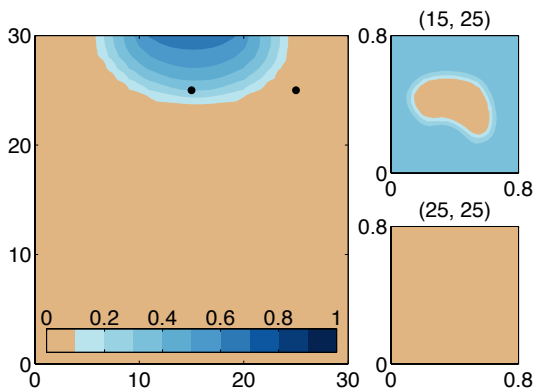


Fig. 10. Saturation contours after 5 hours.

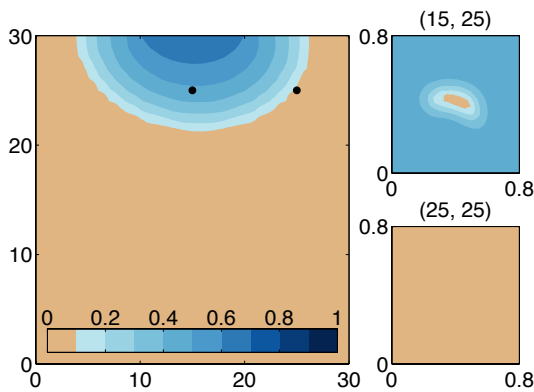


Fig. 11. Saturation contours after 8 hours.

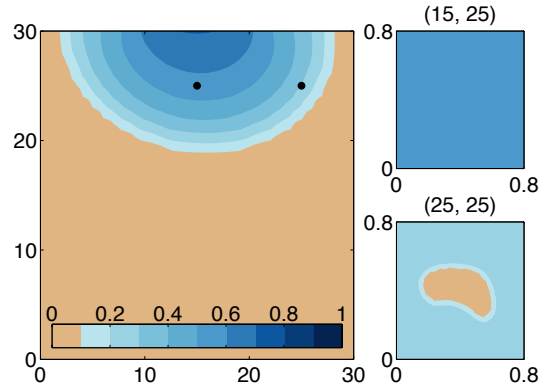


Fig. 12. Saturation contours after 12 hours.

As evident in Figs. 10-12, the distributed microstructure model is quite powerful, providing local descriptions of the flow behavior at the microscopic scale of the inclusions in addition to a global description of the flow in the full macroscopic domain. The microscopic solution is shown at two chosen points, however, in reality it is stored at every macroscopic node. After 5 hours of infiltration the saturation in the inclusion located at the macroscopic point (15,25) is unchanged from its initial state due to the low inclusion conductivity. As the simulation progresses, the inclusion is slowly infiltrated (Fig. 11) and eventually reaches an equilibrium state with the surrounding matrix after 12 hours (Fig. 12). This behavior is even clearer in Fig. 13, where the evolution of the saturation in the matrix and the center of the inclusion are profiled versus time. Initially, the saturation increase in the matrix (high conductivity material) is rapid and delayed in the inclusion (low conductivity material) before eventually reaching the matrix value after approximately 13 hours. It is worth noting that such non-equilibrium behavior at the microscopic scale cannot be captured by a classical macroscopic model.

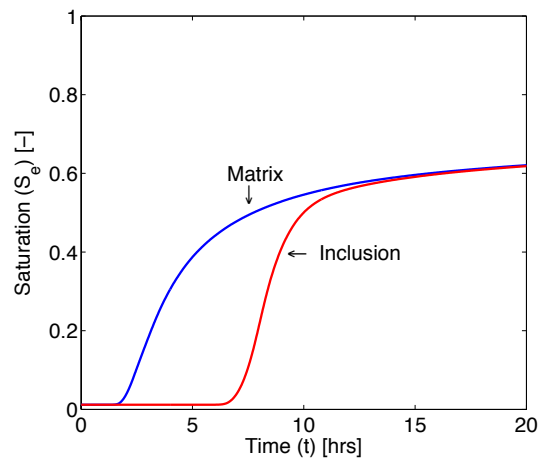


Fig. 13. Comparison of the evolution of the saturation in the matrix and inclusion located at (15,25).

CONCLUSIONS

This paper gave an overview of two current two-scale modeling approaches for simulating transport in porous media and demonstrated their application to two important problems: low temperature drying of wood in the hygroscopic range and unsaturated water flow in soils exhibiting small-scale heterogeneities. A clear limitation of the heterogeneous multi-scale methods is the assumption of local equilibrium at the microscopic scale, which means that the method is restricted to problems where this assumption holds true. On the other hand, while the distributed microstructure models allow for non-equilibrium behavior at the microscopic scale, they are limited to the specific problem of a heterogeneous medium comprising weakly conductive inclusions embedded in a highly conductive matrix. In conclusion, the need for a more general two-scale formulation for heterogeneous media is evident.

NOMENCLATURE

Y	micro-cell domain	–
X	moisture content	kgkg ⁻¹
T	temperature	°C
q	flux vector	–
K	hydraulic conductivity	cmh ⁻¹
K_{eff}	effective hydraulic conductivity	cmh ⁻¹
t	time	h
h	pressure head	cm
n	curve-fitted soil parameter	–
m	curve-fitted soil parameter	–
\underline{Q}	source term	h ⁻¹
\bar{S}_e	effective saturation	–

Greek letters

α	curve-fitted soil parameter	cm ⁻¹
θ	volumetric moisture content	–
θ_{res}	residual moisture content	–
θ_{sat}	saturated moisture content	–
ψ	conserved quantity	–
Γ	material interface	–

Subscripts

M	macroscopic scale
m	microscopic scale

ACKNOWLEDGEMENTS

The first author would like to thank the Laboratory of Chemical Engineering & Materials (LGPM) and its Centre of Excellence for White Biotechnology (CEBB) at École Centrale Paris for postdoctoral funding.

REFERENCES

- Whitaker, S. Coupled transport in multiphase systems: a theory of drying. *Advances in Heat Transfer* **1998**, 31, 1–104.
- Perré, P.; Turner, I.W. TransPore: a generic heat and mass transfer computational model for understanding and visualising the drying of porous media. *Drying Technology* **1999**, 17 (7), 1273–1289.
- Perré, P.; Turner, I.W. A heterogeneous wood drying computational model that accounts for material property variation across growth rings. *Chemical Engineering Journal* **2002**, 86, 117–131.
- Perré, P.; Turner, I.W. A mesoscopic drying model applied to the growth rings of softwood: mesh generation and simulation results. *Maderas. Ciencia y tecnología* **2008**, 10 (3), 251–274.
- Perré, P. Multiscale aspects of heat and mass transfer during drying. *Transport in Porous Media* **2007**, 33 (11), 2463–2478.
- Douglas, Jr, J.; Pesynska M.; Showalter R.E., Single phase flow in partially fissured media. *Transport Porous Media* **1997**, 28 (3), 285–306.
- Chen, F.; Ren, L. Application of the finite difference heterogeneous multiscale method to the Richards' equation. *Water Resources Research* **2007**, 44, W07413.
- Abdulle, A.; E, W. Finite difference heterogeneous multi-scale method for homogenization problems. *Journal of Computational Physics* **2003**, 191, 18–39.
- Carr, E.J.; Turner, I.W.; Perré, P. A dual-scale modeling approach for drying hygroscopic porous media. *Multiscale Modeling and Simulation* **2013**, 11 (1), 362–384.
- Carr, E.J.; Turner, I.W. Two-scale computational modelling of water flow in unsaturated soils containing irregular-shaped inclusions. *International Journal for Numerical Methods in Engineering* **2014**, 98 (3), 157–173.
- Szymkiewicz, A.; Lewandowska, J. Unified macroscopic model for unsaturated water flow in soils of bimodal porosity. *Hydrological Sciences Journal* **2006**, 51 (6), 1106–1124.