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Uncertainty analysis and validation of the estimation of effective hydraulic properties at the Darcy scale

A. Mesgouez *, S. Buis, S. Ruy, G. Lefeuve-Mesgouez

Université d'Avignon et des Pays de Vaucluse, UMR1114 EMMAH, Faculté des Sciences, F-84000 Avignon, France
INRA, UMR1114 EMMAH, F-84914 Avignon, France

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SUMMARY

The determination of the hydraulic properties of heterogeneous soils or porous media remains challenging. In the present study, we focus on determining the effective properties of heterogeneous porous media at the Darcy scale with an analysis of their uncertainties.

Preliminary, experimental measurements of the hydraulic properties of each component of the heterogeneous medium are obtained. The properties of the effective medium, representing an equivalent homogeneous material, are determined numerically by simulating a water flow in a three-dimensional representation of the heterogeneous medium, under steady-state scenarios and using its component properties. One of the major aspects of this study is to take into account the uncertainties of these properties in the computation and evaluation of the effective properties. This is done using a bootstrap method.

Numerical evaporation experiments are conducted both on the heterogeneous and on the effective homogeneous materials to evaluate the effectiveness of the proposed approach. First, the impact of the uncertainties of the component properties on the simulated water matric potential is found to be high for the heterogeneous material configuration. Second, it is shown that the strategy developed herein leads to a reduction of this impact. Finally, the adequacy between the mean of the simulations for the two configurations confirms the suitability of the homogenization approach, even in the case of dynamic scenarios.

Although it is applied to green roof substrates, a two-component media composed of bark compost and pozzolan used in the construction of buildings, the methodology proposed in this study is generic.

1. Introduction

At the Darcy scale, heterogeneous media can be represented in different ways. Basically, a heterogeneous medium can be modeled either using a spatial distribution of properties inside a single unit (Khaleel et al., 2002; Mantaglou and Gelhar, 1987; Russo, 1992; Vogel et al., 2010; Yeah et al., 1985 among others), or using a patchwork of homogeneous sub-units (Bechtold et al., 2012; Samouëlian et al., 2011; Wildenschild and Jensen, 1999a). A combination of both approaches (Javaux and Vanclooster, 2006a; Zhang et al., 2010) can also be used. A detailed description of the various representations can be found in the reviews of Renard and de Marsily (1997) or Vereecken et al. (2007). In our study, we refer to the second way of representation, based on a patchwork of homogeneous sub-units.

The determination of these sub-units is a difficult task and can be performed in different ways. Invasive methods for delineating three-dimensional natural soil units include pedological or geological observations (Bierkens and van der Gaast, 1998; Javaux and Vanclooster, 2006b; Ma et al., 2010; Samouëlian et al., 2011) and dye tracing experiments (Javaux and Vanclooster, 2006a). Non-invasive methods such as two-dimensional electrical resistivity tomography (Besson et al., 2004; Tabbagh et al., 2000) or three-dimensional X-ray computed assist tomography (Duliu, 1999) can also be used. The alternative approach is to work on remolded porous media, such as calibrated sands, to precisely control the heterogeneity pattern and the distribution of hydraulic properties (Bechtold et al., 2012; Danquigny and Ackerer, 2005; Wildenschild and Jensen, 1999b). In our study, we refer to this last way of representation.

* Corresponding author at: Université d'Avignon et des Pays de Vaucluse, UMR1114 EMMAH, Faculté des Sciences, F-84000 Avignon, France. Tel.: +33 490144463; fax: +33 490144409.

E-mail addresses: arnaud.mesgouez@univ-avignon.fr (A. Mesgouez), sbuis@avignon.inra.fr (S. Buis), ruy@avignon.inra.fr (S. Ruy), gaelle.mesgouez@univ-avignon.fr (G. Lefeuve-Mesgouez).

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When working on a patch of homogeneous sub-units, each component of the heterogeneous medium is considered as a single-phase continuum described by macroscopic laws (the Darcy law and the Richards equation). Water flow simulation or water balance computation can then be performed on the elementary volume by using a numerical solver of the Richards equation accounting for the spatial heterogeneity of the hydraulic properties. The spatial structure must be known to distribute the hydraulic properties of each material on the volume of interest. Moreover, solving the Richards equation can be tedious, in particular for three-dimensional flow in complex heterogeneous geometry (Herbst et al., 2008). A simpler approach consists in replacing the explicit three-dimensional structure of the heterogeneous volume by a homogeneous medium, wherein the properties of the homogenized medium take into account the hydraulic properties of each material, in such a way that simulations conducted on both domains yield similar water fluxes under identical boundary conditions (Samouëlian et al., 2011). Such medium properties are then called effective properties. The effective medium is still obtained at the Darcy scale. The homogenization approach can then be considered as an upscaling technique from a continuum scale to a larger continuum one.

Due to the recent advances in computing capabilities, numerical approaches are now widely used for the determination of effective properties (Samouëlian et al., 2007; Vogel et al., 2010). The objective of this study is to contribute to the evaluation of this approach. Several authors noted that simulations conducted using effective parameters may differ from simulations conducted with spatially distributed parameters (Vogel et al., 2008, 2010) or from experimental data measured on heterogeneous media (Wildenschild and Jensen, 1999b). In addition, though several authors estimated the effective hydraulic properties of various natural soils (Javaux and Vanclooster, 2006a; Samouëlian et al., 2011; Vogel and Roth, 1998), no study, to our knowledge, integrates a complete uncertainty evaluation of this procedure. The process of estimating the hydraulic properties of a given material includes however various sources of uncertainties (Mohrath et al., 1997; Peters and Durner, 2008; see also Section 2.2 of this article). These uncertainties significantly affect the results of numerical simulations (Christiaens and Feyen, 2001; Coppola et al., 2009; Pan et al., 2009) and thus the estimation of effective properties or their evaluation using dynamic scenarios. In this study, we propose to estimate the uncertainties on the effective hydraulic properties of a real heterogeneous material, and to evaluate these properties and the impact of their uncertainties by comparing simulations of a dynamic process using either the heterogeneous medium or the effective homogeneous material.

The methodology proposed in this article is generic. It is applied here to green roof substrates, hereafter called substrate or complex substrate. It is a composite of compressible materials, namely organic matter (bark compost) used as fertilizer, and of aggregates of volcanic rock (pozzolan) used as rigid skeleton. This two-component material is considered to serve a number of beneficial purposes that can help in the management of various environmental problems, such as the reduction of air pollution or of the carbon footprints of cities (Yang et al., 2008), the improvement of storm water management (Carter and Jackson, 2007) and the improvement of energy efficiency in buildings (Ouldboukhitine et al., 2012).

2. Materials and methods

The methodology followed in this study is sketched up in Fig. 1. The heterogeneous material under study is composed of a combination of bark compost and pozzolan. In the first step, water retention and hydraulic conductivity are measured for both materials using ad hoc experimental procedures for different water matric potential and on different samples. The hydraulic properties are then estimated by fitting parametric models to the experimental data. The uncertainties on these properties are estimated using a bootstrap method.

In the second step, effective hydraulic parameters are determined by simulating numerically the water flow in a three-dimensional representation of the heterogeneous material taking into account the uncertainties on the hydraulic properties of each constitutive materials and on the spatial distribution of the materials using Monte Carlo random sampling. The effective hydraulic properties and associated uncertainties are then estimated in the same way as for single material properties but using the simulated water retention and conductivity values.

Finally, in the third step, the reliability of the computed effective hydraulic properties is evaluated. Simulations of the evolution of water matric potential versus time are performed under dynamic scenarios with the effective medium and the heterogeneous material taking into account the uncertainties on their hydraulic properties and the spatial distribution of the materials. Their mean behaviors are cross-checked and the impact of the uncertainties is compared.

The following subsections give details on the models used for fitting hydraulic properties, the methodology followed for estimating their uncertainties, the numerical configuration of the water flow simulations, the method used for computing the effective properties and the evaluation of the homogenization approach. The experimental procedures used for measuring water retention and hydraulic conductivity for bark compost and pozzolan and the specific C++ parallelized code used for solving the Richards equation are described in Appendices A and B respectively.

2.1. Models of hydraulic properties

The van Genuchten model (van Genuchten, 1980) is fitted to the experimental data to obtain the hydraulic properties, from which we deduce the water retention curve, i.e. the relation between $\theta(h,\mathbf{x},t)$ $[L^3L^{-3}]$, the volumetric water content, and $h(\mathbf{x},t)$ $[L]$, the water matric potential, as follows

$$\theta(h,\mathbf{x},t) = \theta_r(\mathbf{x}) + (\theta_s(\mathbf{x}) - \theta_r(\mathbf{x})) \times \left[1 + \left(\frac{h(\mathbf{x},t)}{h_e(\mathbf{x})}\right)^n\right]^{-m} \quad (1)$$

where $\mathbf{x}$ $[L]$ are the spatial coordinates, t $[T]$ is the time, θ_r $[L^3L^{-3}]$ is the residual volumetric water content, θ_s $[L^3L^{-3}]$ is the water content at saturation, $h_e[L]$ is a scale parameter, n $[-]$ and m $[-]$ are shape parameters with $m = 1 - 1/n$.

The Mualem-van Genuchten model (van Genuchten, 1980) is fitted to the experimental data to obtain the hydraulic properties, from which we deduce the hydraulic conductivity curve, i.e. the relation between $K(h,\mathbf{x},t)$ $[LT^{-1}]$, the hydraulic conductivity, and $h(\mathbf{x},t)$, the matric water potential, as follows

$$K(h,\mathbf{x},t) = K_{Sat}(\mathbf{x}).\frac{\left[1-(h(\mathbf{x},t)/h_e(\mathbf{x}))^{n-1}\times\left(1+(h(\mathbf{x},t)/h_e(\mathbf{x}))^n\right)^{-m}\right]^2}{\left[1+(h(\mathbf{x},t)/h_e(\mathbf{x}))^n\right]^{m/2}} \quad (2)$$

The values of the parameters of the hydraulic models are estimated by fitting these models on all the available observations. These fits are performed using non-linear least squares regression with a trust-region-reflective minimizer (Coleman and Li, 1996). The method of estimating the uncertainties for these properties is detailed in the following subsection.

2.2. Uncertainty evaluation methodology

As already mentioned, various approximations and errors can be sources of uncertainty when estimating the hydraulic properties of a material. The following typology is proposed to classify these sources of uncertainty: