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How efficient are one-dimensional models to reproduce the hydrodynamic behavior of structured soils subjected to multi-step outflow experiments?

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SUMMARY

In this paper we investigate numerically the three following questions: (1) Do MSO data show the impact of soil structure on water flow? (2) If so, to what extent are the common one-dimensional hydraulic models able to apprehend any preferential flow features? and (3) What are the predictive capabilities of these models parameterized with MSO data? A Bayesian framework was used to infer the hydraulic models under virtual MSO conditions, for soil samples with different levels of heterogeneity. This, by coupling the HYDRUS-1D model with the DiffeRential Evolution Adaptive Metropolis algorithm (DREAM). Regarding questions 1 and 2, our findings indicate that (i) large outflow observed during the first steps of MSO may express the behavior of a real macropore, or of structural heterogeneity inside the soil core; (ii) this behavior cannot be characterized with the MV (Mualem, 1976; van Genuchten, 1980) and DR (Durner, 1994) models whereas mobile–immobile (Philip, 1968; van Genuchten and Wierenga, 1976, MIM) and dual-permeability (Gerke and van Genuchten, 1993a,b, DUAL) preferential flow models can provide excellent fits depending on the soil architecture type; (iii) in the presence of macropores, the DUAL model performed excellently despite frequent convergence problems of the HYDRUS-1D code. Furthermore, neglecting the first MSO steps can result in a perfect match of the soil matrix behavior by the MV model. Regarding question 3, a virtual infiltration front experiment reveals that predictive capabilities of the MIM model parameterized with MSO are not satisfactorily. This indicates that the MIM model underlying concept induce excellent MSO fits for wrong reasons. Similar findings hold for the DUAL model and soil architectures other than macroporous. For a macroporous soil, i.e., the conceptual structure for which the DUAL model was designed, the latter model parameterized with MSO data can provide consistent results under infiltration conditions. This, however, should be verified with real soils. Lastly, neglecting the first MSO steps to calibrate the MV model may induce, in the presence of macropores, significant errors when predicting the matrix behavior under infiltration. This because of the macropore-matrix water transfer.

Introduction

Many soils exhibit preferential flow due to macropores and structural heterogeneity. This has large implications in increasing drainage and accelerating the movement of contaminants through the soil profile (see, e.g., Javaux and Vanclooster, 2004; Javaux et al., 2006a). In order to protect aquifers and soils from contaminants, characterizing and modeling the hydrodynamic behavior of such soils is an important and challenging issue. Several conditions have to be met in order to predict preferential flow in soils. First, experimental protocols are needed to characterize the soil hydraulic behavior. Second, hydraulic models need to be able to generate, amongst others, large velocities close to saturation with an abrupt decrease for smaller matrix potentials. Third, these models should have parameters that are easy to identify and should present predictive power over a broad hydraulic range.

Previous studies have shown that soil structure can be considered as an heterogeneous ensemble of form-elements that are comparable in size with the scale of observation whereas soil texture is composed by much smaller elements, independently of the scale considered (Vogel and Roth, 2003). It has been suggested that structured porous media cannot be characterized in an effective way, i.e., by solving Richards equation with a deterministic parameter set (Vogel and Roth, 2003). Instead, the structure should be explicitly accounted for, whereas the textural heterogeneity could be statistically characterized.

In soil hydrology, several standard methods exist to characterize the soil hydraulic curves at the core scale, a volume generally comprised between 100 and 1000 cm^3. Among them, the multi-step outflow (MSO) technique is a widely used method to characterize the hydraulic properties of undisturbed soil cores (see, e.g., van Dam et al., 1994; Hollenbeke and Jensen, 1998; Zurmühl and

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Durner, 1998; Tuli et al., 2001; Javaux and Vanclooster, 2006b; Vogel et al., 2008, and many others). This approach is based on transient experiments where a porous medium sample is saturated with water and then drained by decreasing the boundary pressure stepwise, e.g., matric potential at the lower boundary. The hydraulic model parameters of the Mualem–van Genuchten (MV) model (Mualem, 1976; van Genuchten, 1980) are then obtained from the inverse solution of the one-dimensional Richards' equation, based on cumulative outflow and/or water potential at a certain depth measurements. However, poor matches between the observations and the inverted model outputs are sometimes observed. In those cases, large outflow during the first step(s), that is classically attributed to macropores, is often observed. Hence, given the soil structure definition of Vogel and Roth (2003), it is questionable to what extent the MSO method can be used to characterize the behavior of an heterogeneous soil in an effective way, and if so, which one-dimensional modeling approach, that cannot reproduce explicitly the soil structure, could be able to simulate the MSO data time series generated by soil architecture. To the best of our knowledge, only one study has partly addressed this issue, by investigating the effect of microscale heterogeneity on MSO outputs for a sandy material (Vogel et al., 2008).

Numerous one-dimensional models have been built to reproduce the hydraulic behavior of structured and/or heterogeneous soils. Among the most widely used are the following. The multimodal porosity model of Durner (1994, DR), the mobile–immobile dual porosity model (Philip, 1968; van Genuchten and Wierenga, 1976, MIM) and the dual-permeability model of Gerke and van Genuchten (1993a,b, DUAL). At present, only few studies have compared these models in their ability to simulate the impact of soil architecture on water flow. Moreover, the parameter identifiability of these models by calibration techniques is currently still open to question. To quote Šimůnek et al. (2003): "very little is currently known about the possibilities and potential problems of applying the inverse modeling techniques to preferential flow models".

In this work we investigate the ability of four one-dimensional hydraulic models (MV, DR, MIM and DUAL models) coupled with the Richards' equation, to reproduce the hydraulic behavior of structured soil cores during a MSO experiment. The three main questions that we address are: (1) Can MSO data show the impact of soil structure on water flow? (2) If so, to what extent can conceptual one-dimensional hydraulic models reproduce the hydraulic behavior of heterogeneous soils under MSO conditions? and (3) What are the predictive capabilities of such simplified models parameterized with MSO data?

We used three-dimensional numerical simulations to study the impact of structural and textural heterogeneity on water flow at the soil core scale. Virtual structured soil cores with micro- and macro-structures were generated and subjected to MSO experiments. Output data were then used to invert the one-dimensional hydraulic models. The parametrized models were in turn subjected to a virtual infiltration front experiment, and results were compared to the three-dimensional ground "truth".

To assess parameter uncertainty resulting from the calibration process, the inversions were carried out within a formal Bayesian framework using the DiffeRential Evolution Adaptive Metropolis (DREAM) Markov Chain Monte Carlo (MCMC) algorithm (Vrugt et al., 2008).

Description of the tested hydraulic models

The four analyzed hydraulic models use the 1-D Richards' equation:

$$\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z}+1\right)\right] \quad (1)$$

where z is the vertical coordinate (positive upwards) (L), t is time (T), h is the pressure head (L), θ is the volumetric water content (–) and K is the unsaturated hydraulic conductivity function (LT^{-1}).

The first model is the classical Mualem–van Genuchten (MV) unimodal model (Mualem, 1976; van Genuchten, 1980) that requires six parameters:

$$S_e(h)=\frac{\theta(h)-\theta_r}{\theta_s-\theta_r}=\frac{1}{(1+|\alpha h|^n)^m} \quad (2)$$

$$K(S_e)=K_S S_e^{\tau}\left[1-\left(1-S_e^{1/m}\right)^m\right]^2 \quad (3)$$

where S_e is the saturation ratio, θ_r and θ_s denote the residual and saturated volumetric water contents, K_S is the saturated hydraulic conductivity (LT^{-1}), α(L^{-1}), n (–), m (–) and τ (–) are empirical fitting parameters. In this work, we assume that $m = 1 - 1/n$ and consider θ_s to be easily measurable. This reduces the parameter estimation problem to the identification of θ_r, α, n, K_S, and τ.

Durner (1994) proposed water retention and hydraulic conductivity functions (DR) for multi-modal pore size distributions exhibiting k inflection points.

$$S_e(h)=\frac{\theta(h)-\theta_r}{\theta_s-\theta_r}=\sum_{i=1}^{k}w_i\frac{1}{(1+|\alpha_i h|^{n_i})^{m_i}} \quad (4)$$

$$K(S_e)=K_S\left(\sum_{i=1}^{k}w_iS_{e_i}\right)^{\tau}\frac{\left(\sum_{i=1}^{2}w_i\alpha_i\left[1-\left(1-S_e^{1/m_i}\right)^{m}_i\right]\right)^2}{\left(\sum_{i=1}^{2}w_i\alpha_i\right)^2} \quad (5)$$

The w_i denote weighting factors for the various modes, which sum up to one. In this work, we consider a bimodal pore size distribution, hence $k = 2$ in Eqs. (4) and (5). Assuming that θ_s may be easily measured, the number of parameters to be optimized is eight: $\theta_r,\ \alpha_1,\ n_1,\ K_S,\ \tau, w_2,\ \alpha_2,\ n_2$.

The two models considered so far assume the soil to consist of a one single domain and one mobile phase. In contrast, the mobile–immobile dual porosity model (MIM, Philip, 1968; van Genuchten and Wierenga, 1976) assumes two domains for water flow. The water flow process occurs within two distinct regions: a high velocity region (constituted by fractures, inter-agreggates or macropores; subscript f) where the water movement is convective, and a low permeability region (made of aggregates or rock matrix; subscript m) where water equilibrates with the mobile region only. This model is particularly justified in fractured or very aggregated porous media (Vanclooster et al., 1992; Vanderborght et al., 1996; Wallach and Parlange, 1998). The total water content over both domains, θ, is given by:

$$\theta=\theta_f+\theta_m \quad (6)$$

where θ_f is the mobile water content, i.e., water content of the fractures, and θ_m is the immobile water content, i.e., water content of the matrix. The dual-porosity formulation for the MIM model is given by (Šimůnek et al., 2003):

$$\frac{\partial\theta_f}{\partial t}=\frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z}+1\right)\right]-S_f-\Gamma_w \quad (7)$$

$$\frac{\partial\theta_m}{\partial t}=-S_m+\Gamma_w \quad (8)$$

where S_f and S_m (T^{-1}) are sink terms for both regions and Γ_w (T^{-1}) is the mass transfer rate for water from the inter- to the intra-aggregate pores. According to Philip (1968) and Šimůnek et al. (2003), Γ_w can be assumed to be proportional to the difference in saturation ratio of the two regions using: