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Non-equilibrium in soil hydraulic modelling

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SUMMARY

A notorious problem in modelling water dynamics within the unsaturated zone is preferential flow and temporal non-equilibrium between water content and water potential. These phenomena originate from the ubiquitous spatial heterogeneity of soil hydraulic properties and substantially hampers the prediction of solute transport from the soil surface towards groundwater. The characteristic scale of these processes is the soil profile or 'pedon scale' where modelling of water dynamics is typically based on the well established Richards equation which has been augmented by various conceptual approaches to represent preferential flow phenomena. In this paper we investigate through numerical case studies hydraulic non-equilibrium during infiltration of water into relatively dry, heterogeneous soil profiles, which is the most prominent scenario where non-equilibrium conditions affect the overall dynamics of water and solutes. We start from well-defined local heterogeneities in a two-dimensional domain and we analyze the dynamics of water content and water potential at the models full spatial resolution. Based on our numerical results we approach the problem of how to represent the heterogeneous setting by an effective one-dimensional description. For practical purposes of large scale applications, such one-dimensional schemes are highly required. As a prerequisite, soil types need to be represented by a reduced set of effective hydraulic properties. The main challenge is to preserve preferential flow phenomena in such simplified one-dimensional models. We demonstrate that classical approaches of volume averaging do not reflect non-equilibrium effects. From the different concepts for representing hydraulic non-equilibrium we focus on an approach proposed by (Ross, P., Smettem, K.R.J., 2000. A simple treatment of physical non-equilibrium water flow in soil. Soil Sci. Soc. Am. J. 64, 1926–1930.) to decouple water content and water potential. This concept is corroborated by our numerical results and we discuss the possibility to link non-equilibrium dynamics and the related model parameters to observable structural properties of the material.

Introduction

Water dynamics within the unsaturated zone has a multitude of different but characteristic spatial scales. Clearly, they are associated with the structural properties of terrestrial systems: the pore scale where fluid flow actually happens, soil aggregates with an internal and an external porous network each having a characteristic scale and pore size distribution, the scale of soil horizons and the heterogeneous spatial distribution of soil types and related properties in the field.

A general question is how to transfer information from smaller to larger scales to correctly represent the emergent properties and phenomena at the larger scale without carrying along all the small scale details. This refers to the issue of 'upscaling' which is actually a hot topic in vadose zone hydrology. For a recent review see Vereecken et al. (2007). It is mainly motivated by the fact that more often than not there is a discrepancy between the measurement scale of soil hydraulic properties and the scale of interest or the scale of modelling (Corwin et al., 2006).

At the pore scale fluid dynamics is described by Navier–Stokes equation and the geometry of the pore space is taken explicitly into account. The only parameters are the properties of the fluid (i.e. density and viscosity). At the larger scale of soil horizons and soil profiles, Richards equation is widely used and accepted to model water dynamics in soil based on water content θ and water matric potential ψ_m as continuous state variables. The detailed porous structure of the material is considered through the effective properties, the water retention curve $\theta(\psi_m)$ and the hydraulic conductivity function $K(\theta)$. These hydraulic properties can be defined for control volumes considerably larger than the size of single pores.

With increasing the spatial scale of modelling water flow in soil, the required averaging over larger control volumes becomes more and more afflicted by rigorous physical constraints since the local conductivity and the local phase saturation are not necessarily lying on the well-defined curves when averaged over these

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volumes. The state variables θ and ψ_m may deviate from the static water retention curve violating a fundamental assumption of the model. During infiltration and drainage processes it has been found theoretically (Roth, 2008) but also observed experimentally (Topp et al., 1967; Vachaud et al., 1972; Wildenschild et al., 2001) that water content is considerably lagging behind the water potential given by the equilibrium water retention curve. This phenomenon is referred to as 'hydraulic non-equilibrium' in this paper. Recently, Vogel and Ippisch (2008) presented an approach to estimate the critical averaging volume for Richards equation above which hydraulic non-equilibrium can be expected. This critical size came out to be pretty small, in the range of centimeters.

In this paper we explore the transition from local equilibrium conditions towards hydraulic non-equilibrium. This is based on numerical case studies where the small scale heterogeneity is resolved explicitly and the detailed numerical results can be compared to effective one-dimensional models. Such effective models are highly required while the challenge is to preserve non-equilibrium dynamics including preferential flow phenomena. Another formidable challenge is that the related parameters should be obtainable from soil properties which are more easily available or at least can be measured independently and the effective model should be applicable at arbitrary flow rates and not just to those for which the model was calibrated.

Theoretical considerations

Modelling water dynamics at the scale of soil profiles and beyond is typically based on Richards equation

$$\partial_t\theta - \nabla\cdot[K(\psi_m)[\nabla\psi_m - \rho g]] = 0. \tag{1}$$

with ρ and g the density of water and the acceleration due to gravity, ψ_m the soil water potential, θ the volumetric water content, and $K(\psi_m)$ the hydraulic conductivity function. Since θ and ψ_m are coupled through the water retention characteristics $\theta(\psi_m)$ Richards equation can be solved numerically. This requires discretization in time and space. While the discrete time steps are usually adapted according to the requirements of the problem and its admissible solution, the discretization in space is typically fixed on a regular grid having a fixed grid constant h $[L]$ so that the space is partitioned into nodes with volumes h^3 in case of three-dimensional water dynamics. Thus, Richards equation implies that within these control volumes the hydraulic state variables θ and ψ_m are in equilibrium with respect to the local water retention curve $\theta(\psi_m)$. Another requirement is that meaningful values for θ and ψ_m within the control volumes can be given. This means that the control volume need to be considerably larger than single pores which marks the limit of Richards equation towards the smaller pore scale. Towards larger scales the control volumes need to be increased due to computational demands. Particularly for transient conditions with moving wetting and drying fronts as typical for top soils the requirement of hydraulic equilibrium is challenged (Roth, 2008).

For infiltration processes, it has been recently shown by Vogel and Ippisch (2008) that the critical length h_{crit} of a control volume for sand is in the range of only a few centimeters while for loamy soil it is somewhat larger. It has been obtained as the length scale where the characteristic time for gravity driven convective flow (proportional to h) is shorter than the characteristic time for diffusive equilibration through capillary forces (proportional to h^2). Such a critical length scale marks the transition towards hydraulic non-equilibrium where water content and water potential are not directly coupled anymore by a static water retention characteristic. At this point the application of Richards equation in its classical form starts to be doubtable.

The decoupling of θ and ψ_m has also been observed experimentally. Wildenschild et al. (2001) analyzed water content and water potential during transient drainage experiments. They found that for a sandy material the water content was considerably lagging behind the water potential while for a loamy soil this effect was not apparent. Hydraulic non-equilibrium is an important aspect also for preferential flow phenomena especially during infiltration (Jarvis, 2007). In case of a large variance in local hydraulic properties the infiltration front moves preferentially through highly conductive regions at high water potentials while the surrounding low conductive matrix remains dry at a much lower water potential. This is the typical case for macropores within a dense soil matrix at high precipitation rates and relatively dry initial conditions.

It should be noted that the hydraulic non-equilibrium considered here is different from the physical non-equilibrium with respect to solute transport which is also relevant in terms of preferential flow. The latter describes non-equilibrated solute concentrations within a heterogeneous velocity field. This may as well occur within stationary flow fields while hydraulic non-equilibrium is explicitly linked to transient conditions.

The problem of hydraulic non-equilibrium can be solved by computing power when all relevant heterogeneities are represented explicitly at the 'equilibrium scale', meaning that the control volumes are small enough such that θ and ψ_m can be assumed to be always in equilibrium. One approach in this direction was made by Vogel et al. (2006) who modelled solute transport in a 3D soil block of about one cubic meter using a numerical grid at the centimetric scale to explicitly represent soil horizons including subscale heterogeneity and macroporous regions. In such a set up, non-equilibrium effects at the larger scale including preferential flow are emergent properties depending on the small scale heterogeneity and the external forcing. However, although computing power is steadily increasing, the required information on the subscale structure and the related hydraulic properties is typically not available.

As an alternative, effective one-dimensional models are used to represent the non-equilibrium effects. Most of them are based on the separation of the flow domain in two different regions following the concept of multi-domains (Gerke and van Genuchten, 1993). Recent reviews have been provided by Gerke (2006) and Simunek et al. (2003). A general difficulty related to multi-domain models is how to get the parameters of the different domains, especially the required exchange term between them. Typically, these parameters need to be fitted to some experimental observations because the separation into different domains is in the first place a conceptual approach and the different domains are not obvious from the structure of the material. This might be possible in some cases where the structural properties are clearly separated as, e.g. macropores within a compact soil matrix. However, even then the obtained parameters are often not stationary and depend highly on the flow rate.

Another approach has been presented by Ross and Smettem (2000) who suggested to decouple water content and water potential to represent non-equilibrium conditions within a control volume. They combine the classical Richards equation (1) with a kinetic description of the water dynamics towards equilibrium by adding an additional differential equation

$$\partial_t\theta = (\theta_e - \theta)/\tau, \tag{2}$$

where θ is the actual water content which might be different from the equilibrium water content θ_e. The dynamics towards the equilibrium water content is described by a simple linear kinetics so that only one additional relaxation parameter τ $[1/T]$ is required. Using this model, Ross and Smettem (2000) successfully described infiltration into undisturbed soil samples exhibiting preferential flow phenomena.