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Modeling Non-equilibrium Water Flow in Multistep Outflow and Multistep Flux Experiments

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Abstract

During the last 50 years, experimental observations have shown that the soil hydraulic properties estimated under static and dynamic flow conditions can substantially differ. These observations are often described by the terms “dynamic non-equilibrium” or “dynamic effects.” The way in which hydraulic non-equilibrium is expressed in experimental data depends on experimental boundary conditions. During experiments with controlled pressure head boundary conditions, non-equilibrium effects appear as a relaxation in the cumulative outflow / system-averaged water content data, while the pressure head in the soil column indicates hydrostatic equilibrium. For experiments with flux boundary conditions, non-equilibrium effects appear as a relaxation of the pressure head while the flux density and macroscopic water content distribution appear static. These phenomena are often attributed to processes such as air-water-interface reconfiguration, pore-water blockage, air entrapment, dynamic contact angles, among others. We have developed a model to quantitatively describe hydraulic non-equilibrium during variably saturated flow. The model considers two continua at the macroscopic scale: one continuum is described by the Richards equation and the second, associated with non-equilibrium water flow, by an extended Richards equation using the non-equilibrium approach of Ross and Smettem. The new model called DNE was implemented by extending the Hydrus-1D code. Numerical simulations with the DNE model demonstrate its ability to describe the dynamic effects occurring in transient flow experiments very well.

1. Introduction

The Richards equation is the most widely used model for describing water flow in the unsaturated zone. It has a clear physical basis and its applicability has been proved in various experimental studies in the laboratory and the field. The use of the Richards equation for the purpose of prediction requires knowledge of the soil-water characteristics, i.e. the water retention and the hydraulic conductivity curve. The water retention curve relates the water content \(\theta\) with the pressure head \(h\) and is parameterized by a monotonous function \(\theta(h)\), which is easily used in numerical simulations. Traditional theory assumes that the water retention curve is independent of the soil water flow regime. However, observations reveal that water retention curves determined under static equilibrium and dynamic conditions can differ. For this reason, the Richards equation often cannot describe observations of soil water dynamics in laboratory experiments. These observations are often described as dynamic non-equilibrium (NE) effects and are known since the work of Topp et al. (1967).

Diamantopoulos and Durner (2012) presented a comprehensive review on this phenomenon that focused on dynamic NE observations, hypothesized causes and modeling approaches. In this contribution, we review only the key studies concerning NE. Topp et al. (1967) performed laboratory experiments in sandy soils and measured the water retention curves (drainage) for
three different flow cases: static, steady-state and dynamic. They drained their sample by controlling the pressure in the gas phase. They found that although the retention curves were almost the same for static equilibrium and steady state flow experiments, the dynamic retention curves significantly differed. Specifically, for the same pressure head value, the water content was higher in the case of transient experiments compared with the other two cases. Similar water dynamics are also observed in multistep outflow experiments (MSO). Figure 1 shows experimental results for an MSO experiment presented by Diamantopoulos et al. (2012). After an applied pressure step at the lower boundary, the pressure head in the soil quickly reaches the equilibrium state. However, the time series of cumulative outflow shows two stages. During the first stage, immediately after the change in the applied pressure head, a large volume of water quickly flows out from the soil column. This is followed by a second stage with a much slower flow in the column toward hydraulic equilibrium. The crucial point is that these data cannot be described by the Richards equation because it cannot predict different equilibration times for \( \theta \) and \( h \) due to the tight coupling by the retention curve.

![Figure 1](image.png)

Figure 1. Non-equilibrium water flow during an MSO experiment. After a pressure head change at the boundary, the pressure head in the soil quickly equilibrates whereas outflow of water continues.

Poulovassilis (1974) investigated the effect of water flow on the water retention curve by conducting constant flux infiltration experiments in a soil column equipped with five tensiometers. After achieving uniform steady-state flow and uniform water content and pressure head throughout the soil column, he sealed both ends of the soil column and placed it horizontally. He observed that all tensiometers recorded a pressure head increase (suction decrease) while the water content inside the column remained constant. Recently, Weller et al. (2011) presented an automated method for direct measurements of hydraulic conductivity by a succession of unit-gradient experiments. They applied constant fluxes at the upper boundary of the soil column and set the pressure head at the lower boundary equal to the pressure head of water near the surface. Under these conditions, the hydraulic conductivity equals the applied flux density. Their experiments started with a saturated soil column and the applied fluxes were
decreased in steps. As was expected, pressure head measured in the soil dropped immediately after each applied step, but rose to higher levels afterwards, even though the column-averaged water content remained constant. Weller et al. (2011) also observed this phenomenon for increasing fluxes, but in this case the pressure head decreased during the relaxation period. Similar to what has been stated earlier, the observations of Poulouvasillis (1974) and Weller et al. (2011) cannot be described by the Richards equation because of its inherent assumption of a flux-invariant $\theta$-$h$-$K$ relationship.

The above studies reveal that for a given pressure head boundary condition, dynamic NE effects appear as a relaxation in the cumulative outflow data (or water content), whereas for a given flux boundary condition, they appear as a relaxation of the pressure head. Diamantopoulos et al. (2012) proposed a model for describing dynamic NE water flow in the case of MSO experiments. The model assumes two continua at the macroscopic scale. In the first continuum, water flow is described by the Richards equation, whereas in the second continuum, water flow is described by the Ross and Smettem (2000) model. In this article, we investigate the possibility of describing the two major dynamic NE observations outlined above with this model.

2. Model

2.1. Richards Equation

Variably saturated water flow in homogeneous porous media is generally described by the Richards equation:

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

(1)

where $\theta$ [L$^3$ L$^{-1}$] is the water content, $t$ [T] is time, $z$ [L] is the vertical coordinate, positive downwards, $h$ [L] is the pressure head and $K$ [L T$^{-1}$] is the unsaturated hydraulic conductivity.

2.2. Dual–Fraction Non–Equilibrium Model (DNE)

The DNE model assumes two fractions of water in the same porous system, one fraction $f_{eq}$ in instantaneous equilibrium with the local pressure head, and the second fraction $f_{ne}$ for which the equilibration of water content is time dependent. By assuming that the pressure heads in the two regions quickly equilibrate relative to the movement of water in the main flow direction, the main equation describing water flow becomes (Diamantopoulos et al., 2012):

$$(1 - f_{ne}) \frac{\partial \theta_{eq}}{\partial t} + f_{ne} \frac{\partial \theta_{ne}}{\partial t} = \frac{\partial}{\partial z} \left[ K(\theta) \left( \frac{\partial h}{\partial z} - 1 \right) \right]$$

(2)

with

$$\frac{\partial \theta_{ne}}{\partial t} = \frac{\left( \theta_{eq} - \theta_{ne} \right)}{\tau}$$

(3)
where $\tau$ describes the equilibration of water content in the non-equilibrium region [T], and $K$ is a function of the water content $\theta$. For more information about the model, the reader is referred to Diamantopoulos et al. (2012).

2.3. Parameterization of Hydraulic Properties

The unsaturated soil hydraulic properties are parameterized with the van Genuchten–Mualem (VGM) model (van Genuchten, 1980). The retention function and the hydraulic conductivity function (as a function of water content $\theta$) are given by:

$$
\theta(h) = \begin{cases} 
\theta_s + (\theta_r - \theta_s) \cdot (1 + |\alpha h|^n)^{-n}, & h < 0 \\
\theta_s, & h \geq 0
\end{cases}
$$

(4)

$$
S_s = \frac{\theta - \theta_r}{\theta_s - \theta_r}
$$

(5)

$$
K(S_s) = K_s \cdot S_s^m \left[ 1 - (1 - S_s^{1/m})^m \right]
$$

(6)

where, $\theta_s$ and $\theta_r$ [L$^3$ L$^{-3}$] are saturated and residual water contents, respectively, $\alpha$ [L$^{-1}$], $n$ [-], $m$ [-] and $l$ [-] are shape parameters and $m = 1 - \frac{1}{n}$, $n > 1$.

2.4. Inverse Modeling

The laboratory experiments were evaluated by inverse modeling. The objective function used for determining the unknown parameters $p$ from measurements of cumulative outflow and pressure head data in the case of the MSO experiment and pressure head data in the case of the multistep flux experiment is given by:

$$
O(p) = \sum_{j=1}^{M} w_j \sum_{i=1}^{N_j} r_{ij}(p)^2
$$

(7)

where $M$ is the number of the data groups used in the objective function ($M = 2$ for MSO and $M = 1$ for multistep flux experiments), $N_j$ is the number of data for each group and $r_{ij}$ are the residuals, i.e. the differences between observed and model–predicted data. The estimation of the model parameters is done by minimizing Eq. (7) with respect to the parameter vector $p$. This was achieved by the globally convergent evolutionary scheme SCE-UA (Duan et al., 1992). Numerical simulations with both the Richards equation and the DNE model were done with a modified version of Hydrus-1D (Šimůnek et al., 2008).
3. Material and Methods

3.1. Multistep Outflow (MSO) Experiment

The DNE model was tested against experimental results from an MSO experiment presented by Diamantopoulos et al. (2012). In that experiment, an undisturbed soil column 7.2 cm in height was collected from the subsoil horizon (35–45 cm) of a Luvisol (Schelle et al., 2011). The column was placed on a 0.7 cm thick porous plate that was covered by a fine-pored diaphragm. A tensiometer (T5, UMS Munich) was installed at a 1.8 cm depth measured from the top to record pressure head. The sample was slowly saturated from the bottom. The initial water content was calculated from the water content at the end of the experiment, and the cumulative water loss throughout the experiment. The bulk density, porosity and initial water content were 1.67 g cm$^{-3}$, 0.371 cm$^{-3}$ cm$^{-3}$ and 0.334 cm$^{-3}$ cm$^{-3}$, respectively. The saturated hydraulic conductivity of the plate ($K_p$) and soil ($K_s$) were 1.0 cm h$^{-1}$ and 2.7 cm h$^{-1}$, respectively. In the inverse simulations with the Richards equation and the DNE model, both saturated conductivities were fixed to these measured values.

3.2. Multistep Flux (MSF) Experiment

We tested the DNE model against experimental data from MSF experiments presented by Weller et al. (2011). They obtained direct measurements of unsaturated hydraulic conductivity by imposing gravity flow to one sandy undisturbed soil column as was described in the introduction. For more information about the material type or the experimental procedure, the reader is referred to Weller et al. (2011).

4. Results

4.1. MSO

Figure 2 illustrates results of a sensitivity analysis in which the effect of the non-equilibrium parameters $\tau$ and $f_{ne}$ for a multistep outflow and inflow experiment were analyzed for a sandy material. The first case (blue line) represents equilibrium flow described by the Richards equation. Figure 2a shows the prediction of the DNE model for a drainage–imbibition experiment and for increasing values of parameter $\tau$ (2, 4 and 8 h) when all the water is assumed to be in non-equilibrium ($f_{ne} = 1$). This corresponds to the Ross and Smettem (2000) NE model, which obviously is able to predict the basic observation that after an abrupt change in the applied pressure head at the lower boundary, the pressure head in the soil equilibrates faster than the cumulative outflow data. However, the equilibration dynamics always follow an exponential form, which is in contrast to the observations. As described previously, outflow data often show an equilibration in two stages. After each applied step, there is a quick outflow followed by a period with slower outflow. As shown in Figure 2b, this can be simulated by the DNE model. Figure 2b shows that the greater the value of $f_{ne}$, the smaller the amount of water that leaves the soil column after each applied pressure head.
Figure 2. Sensitivity analysis of DNE model for MSO experimental type. (a): the effect of $r$ parameter; (b): the effect of $f_{ne}$ parameter

Figure 3 shows measured and fitted outflow and pressure head data for a MSO experiment for a loamy sand soil. The experimental data show that after each pressure change at the lower boundary, the equilibration of the pressure head data in the column is quicker than that of the cumulative outflow data. The blue line illustrates that this cannot be described by the Richards equation since it assumes simultaneous equilibration between pressure head and water content (or cumulative outflow). Accordingly, any attempt to describe the data leads to misfits. On the contrary, the DNE model describes both the pressure head and outflow data very well. Any remaining discrepancies between measured and simulated outflow data, especially in the second and third step, can be attributed to the limited flexibility of the van Genuchten-Mualem model of the soil hydraulic properties. The fitted parameter $r$ and $f_{ne}$ were 3.2 h and 0.76, respectively.

Figure 3. Observed and simulated cumulative outflow and pressure head data for an undisturbed loamy sand. The fitted data are calculated using the Richards equation and the dual-fraction non-equilibrium (DNE) model.
4.2. MSF

Figures 4a and b show results of a sensitivity analyses for both non-equilibrium parameters of the DNE model for an MSF experiment. At the beginning, we assume a series of steady fluxes decreasing stepwise corresponding to a drainage experiment; after 150 hours, we assume increasing fluxes corresponding to an imbibition experiment. The Richards equation predicts that after an applied flux at the upper boundary, water content and pressure head in the soil immediately change and assume the relationship defined by the soil water retention curve. Figure 4a shows that the DNE model can predict the capillary overshoot presented by Weller et al. (2011) in both the drainage and imbibition sequence of the MSF experiment. At a constant value of the $f_{ne}$ parameter, increasing $r$ values result in slower equilibration of the pressure head after each applied flux. Additionally, the magnitude of the pressure head drop after each flux change is controlled by parameter $f_{ne}$ (Figure 4b).

![Figure 4. Sensitivity analysis of DNE model for MSF experimental type. (a): the effect of $r$ parameter; (b): the effect of $f_{ne}$ parameter](image)

Figure 5 shows the experimental and simulated data from the study of Weller et al. (2011). The experimental data were digitized from figure 4 in Weller et al. (2011). Figure 5 shows that after a stepwise change of the applied flux at the upper boundary, the pressure head drops as expected (drainage), but then it rises again to a higher value. The Richards equation predicts that after the establishment of steady state flux with constant water content in the soil, the pressure head remains constant as well and corresponds to the pressure head value obtained from the retention curve. This contradicts the experimental findings. In contrast, the DNE model predicts the observed slow equilibration of the pressure head data even if the water content remains constant and the agreement between fitted model predictions and experimental data is excellent. The fitted parameter $r$ and $f_{ne}$ were 19 h and 0.37, respectively.
Figure 5. Observed and simulated pressure head data for an undisturbed sand (Weller et al., 2011). The fitted data are calculated using the Richards equation and the dual-fraction non-equilibrium (DNE) model. The experimental data were digitized from Figure 4 in Weller et al. (2011).

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