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Single-porosity and dual-porosity modeling of water flow and solute transport in subsurface-drained fields using effective field-scale parameters

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Abstract

Water and solute flux from the subsurface drains of macroporous agricultural fields are simulated using two-dimensional single-porosity and dual-porosity models. Field-averaged (i.e. effective) parameters are calibrated from drainage outflow and validated for water flow and the transport of non-reactive solutes applied at discrete locations on the field. Both the single-porosity and the dual-porosity simulations capture the observed trends in the drainage hydrographs, with the dual-porosity model performing slightly better than the single-porosity model. The values of the effective hydrologic parameters, however, were not fully characteristic of macroporous soils. The physical meaning of the effective parameters was further questioned as neither the single-porosity nor the dual-porosity models could simulate the rapid transport of solutes to the subsurface drain. The discrepancies between the simulated and observed solute flux indicate that the actual spatial area contributing to drainage outflow in the field experiment was much greater than the integrated area of the simulated domain over which the effective parameters were calibrated. Supplementary simulations using parameters calibrated from solute flux data (outflow solute concentration multiplied by the outflow water flux) also fail to match both water and solute fluxes. The failure of the simulations is attributable to factors such as non-unique parameters and problems with representing a three-dimensional heterogeneous domain as a two-dimensional homogeneous system, including a misrepresentation of macropore flow paths. This study shows the fallacy of interpreting a hydrograph fit as evidence of the physical meaning of model parameters.

Keywords: Dual-porosity; HYDRUS-2D; Effective parameters; Subsurface-drains; Model calibration

1. Introduction

Agricultural landscapes consist of multi-scale heterogeneities that influence the movement of water and chemicals. Usually, a detailed quantification of spatial variability is either impractical or

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impossible. Consequently, models for predicting flow and transport through the vadose zone must somehow simplify the representation of the transport domain, yet still effectively reproduce the flow and transport response at a control plane or outlet point. In a deterministic model, this is often accomplished by assuming a representative elementary volume (REV), which proposes that a medium can be represented by homogenized (i.e. effective) parameters provided there is a separation of scales such that the characteristic volume of spatial heterogeneities is much smaller than macroscopic size of the transport domain (Royer et al., 2002).

The REV assumption is commonly invoked to calibrate effective model parameters from catchment outflow hydrographs for rainfall-runoff models. Often the legitimacy of these models is validated solely on the basis of hydrograph prediction (Beven, 1993; Beran, 1999). Using the outflow response as an exclusive measure of performance, however, is being increasingly questioned as these models fail to represent the actual drainage pathways and the physical processes occurring within the flow domain (Binley et al., 1991; Jain et al., 1992; Blazkova et al., 2002). Consequently, models become more sophisticated to better account for the internal system structure. The increased sophistication results in increased parameterization requirements. Because it is typically infeasible to make detailed distributed measurements, the added parameters must be estimated based on the same hydrograph information, which leads to a higher likelihood of non-unique parameter sets and an ill-posed inverse calibration problem—even for simple, small-scale systems (Hopmans and Šimůnek, 1997; Durner et al., 1997; Madsen et al., 2002; Doherty and Johnston, 2003).

While the REV approach to finding effective parameters is simple in concept, verifying its existence can be complicated. (Baveye and Sposito, 1984; Berkowitz et al., 1988; Neuman and Orr, 1993; Lugo et al., 1998; Tartakovsky and Neuman, 1998a,b,c; Indelman, 2002; Fernandez-Garcia et al., 2002; Royer et al., 2002). Neuman and Orr (1993) demonstrated mathematically that while effective values may be found for infinite subsurface domains, the flux for bounded systems becomes non-local, and thus, an average flow model generally does not exist. For radially converging flow systems, however, they showed that effective parameters could be found depending on the correlation structure and physical dimensions of the domain.

Temporal variability also creates difficulties in finding effective parameters. Tartakovsky and Neuman (1998b) reported that for porous media, an effective hydraulic conductivity will exist in the 'strict sense' only when the mean head and the residual flux are constant in space and time. Though this is not possible under transient flow—except if the storativity is zero or time approaches infinity—there are a number of cases, where effective hydraulic conductivities can be approximated in real, Laplace and/or Fourier spaces (Tartakovsky and Neuman, 1998b,c).

Some of the more complex flow and transport domains are subsurface-drained agricultural fields of the US Midwest region. Analogous to catchment hydrographs, the subsurface drain response is an aggregation of the spatial and temporal variability across that part of the field that contributes to drainage outflow. Consequently, the drainage hydrograph may be useful for estimating effective parameters if the transport domain can be approximated as a radially converging flow system, spatial correlation lengths of variability in the soil properties are small compared to the field dimensions, and rainfall events are limited to a realistic range of magnitudes such that the field volume contributing to the outflow does not appreciably change between events. Still, even when these conditions are met, the non-linear processes in the vadose zone, coupled with flow and transport through macropore networks that are abundant in these soils, may violate the ergodic hypothesis (Yeh, 1997) and the representations of the driving processes.

As in catchment modeling, using the outlet response to derive effective hydraulic properties for subsurface-drained fields is not new (Hoffman and Schwab, 1964; Skaggs, 1976), and automated inverse procedures have been developed and tested for a variety of systems of different scales and for a number of boundary conditions (Durner et al., 1997; Hopmans and Šimůnek, 1997; Jacques et al., 1997; Šimůnek et al., 1998). De Vos et al. (1997) used the inverse procedure in the HYDRUS-2D flow and transport model to estimate effective field-scale parameters from measurements of drainage outflow and groundwater level fluctuations. The effective parameter model could satisfactorily reproduce the overall