Journal of Hydrology 521 (2015) 261–273

Contents lists available at ScienceDirect

Journal of Hydrology

journal homepage: www.elsevier.com/locate/jhydrol

Temporal moment analysis for stochastic-advective vertical solute transport in heterogeneous unsaturated soils

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ARTICLE INFO

Article history:
Received 26 February 2014
Received in revised form 27 October 2014
Accepted 30 November 2014
Available online 5 December 2014
This manuscript was handled by Peter K. Kitanidis, Editor-in-Chief, with the assistance of Roseanna M. Neupauer, Associate Editor

Keywords:
Temporal moments
Infiltration
Solute transport
Sharp-front models
Upscaling

SUMMARY

Temporal moment analysis of solute transport in unsaturated soils subjected to rainfall events is typically achieved by the numerical solution of the flow field from the Richards equation followed by a numerical solution of the advection–dispersion equation before computing moments. These numerical solutions are computationally very intensive, and may not provide the insights that are possible from simpler analytical representations. In this study, temporal moments of solute transport for unsteady unsaturated flows under rainfall conditions at the soil surface are presented for the first time. A local-scale model for water movement is derived from a sharp front approximation and is combined with a model for transport of solute particles along the main characteristics of the flow field. Expressions for travel times from the local-scale model are first presented for pre- and post-ponding conditions. These local solutions are upscaled to field-scale solute transport by adopting a log-normally distributed spatial hydraulic conductivity field. Semi-analytical expressions are developed for temporal moments of travel times. These expressions are compared to 1-D Monte Carlo simulation results, and to 3-D numerical results for model corroboration. The model is used to investigate the behavior of macroscopic Eulerian effective velocities and dispersion at the field-scale. Expressions for asymptotic effective properties show that effective velocity achieves a constant value while effective dispersion increases linearly with depth. The roles of pre-ponding and post-ponding conditions in determining field-scale dispersion are described.

1. Introduction

An understanding of field-scale solute transport in soils is essential for quantifying the fate and movement of surface applied chemicals, and for evaluating the fluxes of contaminants past control planes that are needed to devise suitable abatement strategies. However, field-scale flow and solute transport through the unsaturated zone are highly complex because of the nonlinear nature of the governing equations and the natural variability exhibited by field soils.

Dagan and Bresler (1979) were among the first to model field-scale flow and solute transport in the unsaturated zone for vertical steady flow conditions using a stochastic theory. The flow domain was represented as an ensemble of statistically independent homogeneous soil columns (i.e., no vertical heterogeneity). Jury (1982), Jury et al. (1986), and Jury and Scotter (1994) developed transfer function models based on a systems approach to predict mean solute concentration past a control plane at a field-scale. Simmons (1982) considered stochastic–convective transport with nonuniform flow, and related the average concentration to travel times that were assumed to follow either a normal or a lognormal distribution. Yeh et al. (1982, 1985a–c) used a numerical three-dimensional stochastic approach and a linearized perturbation method to examine the effects of spatial variability in hydraulic conductivity on steady unsaturated flow. Russo (1998) combined the analyses of Yeh et al. (1985a,b) with a stochastic-Lagrangian approach proposed by Dagan (1984, 1989) and derived velocity covariance and macrodispersion tensors for unsaturated flow conditions.

For simplification, many studies have focused on steady state, gravity-dominated unsaturated flow to describe field-scale solute behavior. The velocity flow field under these conditions is stationary and hence formulation of analytical or semi-analytical expressions is possible (Vanderborght et al., 2006). However, steady state and gravity dominated flow conditions are more appropriate at only large times, for small values of seepage velocities, and for moisture contents close to saturation (Elrick et al., 1979). The studies performed by Yeh et al. (1985a,b) and Russo (1998, 2003) do consider the three-dimensional anisotropic structure of the soil,

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http://dx.doi.org/10.1016/j.jhydrol.2014.11.076
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but were conducted with several underlying assumptions. The spectral perturbation approach adopted in these studies was combined with the assumption of first order approximation of velocity covariance and displacement covariance tensors and thus, the results are limited to formations with log unsaturated conductivity variance less than unity (Russo, 1998). Furthermore, the results are restricted to conditions of constant mean-head gradient when describing the flow field.

While assumptions of steady and gravity-dominated flows (Bresler and Dagan, 1983) have led to useful results, transient conditions are arguably just as prevalent, if not more so. The flow and transport in the unsaturated zone near the soil surface are generally a result of transient climatic or human induced boundary conditions (rainfall, or irrigation) (Butters, 1987; Russo et al., 1989; Vanderborght et al., 2006). As a result, the velocity fields near the soil surface are non-stationary both in time and space. Obtaining analytical solutions for the nonlinear Richards equation and the contaminant transport equations under transient flow conditions and in bounded domains is far more complex (Vanderborght et al., 2006).

Stochastic theories have often been used for describing transient flow and transport problems at the field-scale. Mantoglou and Gelhar (1987a–c) described large scale transient unsaturated flow in spatially variable soils by extending the spectral perturbation approach of Yeh et al. (1985a,b). This was accomplished by introducing assumptions such as spatial and temporal stationarity of local hydraulic soil properties, stratified soil formation, and infinite flow domain. Unlü et al. (1990) studied one-dimensional unsaturated flow for transient redistribution through Monte-Carlo simulations and observed good agreement with the spectral perturbation approach except near the soil surface. Mantoglou (1992) utilized the distributed parameter estimation theory of McLaughlin and Wood (1988a,b) to describe transient unsaturated flow conditions under a more general stochastic framework. Liedl (1994) proposed a different perturbation model for transient unsaturated flow that resulted in a set of partial differential equations governing the statistical moments of saturation. Zhang (1999), unlike Liedl (1994) and Mantoglou (1992), derived linear equations for the second moment that were decoupled from the nonlinear first moment (mean) equation for pressure head, Darcy flux and seepage velocity. In all these studies, the linearized moment equations were solved numerically to obtain effective hydraulic parameters and two-point (cross) covariances of dependent variables (Mantoglou, 1992; Zhang, 1999).

Three-dimensional stochastic theories and models have provided fundamental insights into the role of spatial variability of soil properties on hydraulic parameters (Vereecken et al., 2007). However, there are several constraints that limit the applicability of these models. The perturbation approach is only valid for mild variations in soil water contents and is not applicable to highly heterogeneous soils. The equations arising from the stochastic theory are very complex to solve (even numerically) because of intercoupling, nonlinearity and high dimensionality (Loll and Moldrup, 1998). The computational demand to solve the moment equations for three-dimensional transient flow in unsaturated zone is so high that researchers often find it more efficient to implement Monte Carlo simulations (Vereecken et al., 2007). Another major constraint is the accurate estimation of necessary statistics from measured field-data, namely, correlation lengths and covariance functions between parameters that require a very detailed and expensive field campaign (Mantoglou, 1992). Measurement errors in key soil properties can significantly impact the predictions by stochastic models and, as a consequence, the decisions based on these predictions (Holt et al., 2003). The details of the strong connectivity structure between soil hydraulic parameters that is required for accurate modeling is however difficult to recover from local-scale sampling techniques (Neuweiler and Cirpka, 2005; Neuweiler and Vogel, 2007). Algorithms for generation of random fields typically assume second-order stationarity. Lack of rapid and novel assessment techniques of spatial variability in unsaturated zone properties and proper field validation is a major impediment to accurate implementation of stochastic theories. Furthermore, these models assume equivalence of spatial means and ensemble averages. This may constitute a serious limitation when correlation length scales of hydraulic properties are not orders of magnitude smaller than field dimensions.

Other than stochastic models, numerous studies have adopted deterministic modeling with statistical sampling to describe flow and transport in the unsaturated zone. These studies were often based on coupling of numerical or analytical solutions of the governing partial differential equations of unsaturated water flow and advection–dispersion equations subject to appropriate initial and boundary conditions (e.g., Dagan and Bresler, 1983; Bresler and Dagan, 1983; Jensen and Refsgaard, 1991; Rubin and Or, 1993; Chen et al., 1994a, 1994b; Smith and Diekkrtiger, 1992; Russo et al., 2006). Spatial variability is typically described by theoretical distributions fitted to measured values of the spatially variable parameters. Further, the spatially averaged flow properties are obtained either in a Monte-Carlo framework using sampling of the input distributions, or using a numerical approach that combines a statistical generation method to produce realizations of the heterogeneous formation properties that preserve correlation of soil properties, with an efficient numerical method to solve the PDEs that govern flow and transport in the heterogeneous unsaturated zone of the soil (Russo et al., 2006). Although, these studies were useful, for many practical applications these numerical solutions are too complex, time consuming, prone to numerical error, not amenable to developing closed form analytical solutions, and do not provide direct insights into how output variables are controlled by the spatial variability of soil parameters.

Recognizing that limitations exist with stochastic three dimensional models and Monte-Carlo based numerical solutions of the non-linear PDEs, it is desirable to develop analytical solutions for field-scale flow and solute transport in the unsaturated zone of soils based on physical models under transient flow conditions. Several studies have advocated the use of simplified local models, with the expectation that large-scale variability in soil parameters will minimize or eliminate the impact of errors in the simplified models (Dagan and Bresler, 1983; Bresler and Dagan, 1983; Govindaraju et al., 1992; Chen et al., 1994a,b). Specifically, Chen et al. (1994a,b) in their study related to prediction of field-scale moisture content, compared numerical solutions of the three-dimensional Richards equation with a stochastic model based on perturbation theory and an analytical solution derived using the Green-Ampt model. Their results based on the Green-Ampt model matched very well with the Richards equation solutions, and in case of high field-scale variability, performed better than the stochastic model solutions.

Numerous studies have used temporal moment analyses for obtaining simple representations of aggregated transport properties (Valocchi, 1985; Fernàndez-Garcia et al., 2005; Govindaraju and Das, 2007). For instance, the first temporal moment is a measure of the average travel time of solute molecules in the system from their entry point to the control plane (Skopp, 1985). The second moment reflects the effect of solute spreading mechanisms such as diffusion, hydrodynamic dispersion, kinetic sorption (Valocchi, 1989), and macro-dispersion resulting from heterogeneity in soil properties (Gelhar and Axness, 1983; Dagan, 1986). Along similar lines, in this study, expressions for first two temporal moments and field-scale effective velocity and dispersion are derived utilizing a sharp front approximation for water movement. First, local-scale models of flow and transport of a conservative