

Vadose Zone Modeling: Introduction and Importance

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MANY MODELS of varying degree of complexity and dimensionality have been developed during the past several decades to quantify the basic physical and chemical processes affecting water flow and pollutant transport in the unsaturated zone. These models are now being used increasingly for a wide range of applications in research and management of natural subsurface systems. Modeling approaches range from relatively simple analytical and semianalytical models to more complex numerical codes that permit consideration of a large number of simultaneous nonlinear processes. While analytical and semianalytical solutions are still used for relatively simple applications, the ever-increasing power of personal computers, as well as supercomputers, and the development of more accurate, numerically stable, and often parallelized (Hardelauf et al., 2007) solution techniques have given rise to the much wider use of numerical models in recent decades (Šimůnek, 2005).

This special section of the *Vadose Zone Journal* documents the tremendous progress in vadose zone modeling over the last three decades. The section is divided into two parts. Part 1 includes six papers that describe the latest developments or specific applications of some of the most widely used models for simulating various processes in the vadose zone. These papers cover the following models (in the alphabetical order): HYDRUS (Šimůnek et al., 2008), MODFLOW-SURFACT (Panday and Huyakorn, 2008), STOMP (White et al., 2008), SWAP (van Dam et al., 2008), TOUGH2 (Finsterle et al., 2008), and VS2DI (Healy, 2008). The authors of HYDRUS review their efforts over some 30 yr in developing their various analytical and numerical tools (Šimůnek et al., 2008), while the authors of TOUGH2 describe recent developments and new processes that have been considered in their model (Finsterle et al., 2008). Authors of MODFLOW-SURFACT (Panday and Huyakorn, 2008), VS2DI (Healy, 2008), and SWAP (van Dam et al., 2008) provide basic descriptions of their models and their general capabilities. Finally, authors of STOMP (White et al., 2008) present a sophisticated application of their model.

The second part of this special section includes 15 papers that describe modeling of specific vadose zone processes or associated applications. Contributions include two papers that review colloid and colloid-facilitated contaminant transport in the vadose zone (Bradford and Torkzaban, 2008; Flury and Qiu, 2008, respectively), two papers that address reactive biogeochemical transport under transient flow conditions (Jacques et al., 2008; Szegedi et al., 2008), two papers related to multiphase flow and remediation (Class et al., 2008; Hodges and Falta, 2008), and one paper that reviews (Furman, 2008) and two papers that develop new tools for modeling surface–subsurface interactions (Twarakavi et al., 2008; van Walsum and Groenendijk, 2008). The topics of preferential and nonequilibrium flow and transport in the vadose zone are covered by Šimůnek and van Genuchten (2008) and Kodešová et al. (2008). Individual papers deal with salt leaching under subsurface drip irrigation and saline, shallow groundwater conditions (Hanson et al., 2008), spatially distributed water fluxes in soil under banana plants (Sansoulet et al., 2008), modeling of processes in subsurface flow constructed wetlands (Langergraber, 2008), and inverse modeling of subsurface flow and transport properties using recent advances in global optimization, parallel computing and sequential data assimilation (Vrugt et al., 2008). There are, however, some obvious gaps and uncovered processes, such as coupled water, vapor and heat transport, and large-scale model applications, not addressed in this special issue. Readers interested in these topics are referred, for example, to recent papers by Cahill and Parlange (1998), Saito et al. (2006), or Twarakavi et al. (2008).

Part 1: Vadose Zone Models

This special section opens with two papers dedicated to the HYDRUS (Šimůnek et al., 2008) and TOUGH2 (Finsterle et al., 2008) models. These models are commonly used by contributors to the *Vadose Zone Journal*. While one of the HYDRUS models was used in more than 60 published manuscripts during the first six years of the journal,

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an entire special issue was recently dedicated to applications of TOUGH2 [Vadose Zone Journal 6(1), 2008].

Šimůnek et al. (2008) review the history of development, the main processes involved, and selected applications of a large number of popularly used computer tools for studying vadose zone flow and transport processes developed collaboratively between the U.S. Salinity Laboratory, the University of California, Riverside, and PC-Progress over the past 20 yr. These tools include numerical models for one- or multidimensional variably saturated flow and transport [e.g., HYDRUS-1D, HYDRUS-2D, and HYDRUS (2D/3D)], analytical models for solute transport in soils and groundwater (e.g., CXTFIT and STANMOD), and tools or databases for analyzing or predicting the unsaturated soil hydraulic properties (e.g., RETC, Rosetta, and UNSODA). These modeling tools cover a large number of processes, from relatively simple one-dimensional solute transport problems to multidimensional flow and transport applications to relatively complex problems involving a range of biogeochemical reactions. An example of the latter is the HP1 (Jacques et al., 2008) program, which couples the HYDRUS-1D software package with the PHREEQC geochemical code (Parkhurst and Appelo, 1999).

Finsterle et al. (2008) discuss fundamental and computational challenges in simulating vadose zone processes and present examples of recent developments of the TOUGH suite of codes aimed at addressing some of these issues. The TOUGH suite of simulators includes several related codes simulating, for example, nonisothermal multiphase flow (e.g., TOUGH2, T2VOC), reactive biogeochemical transport (TOUGHREACT) and rock mechanical processes (TOUGH-FLAC). Finsterle et al. (2008) either list or discuss several recent applications of TOUGH. These applications involve, for example, simulation of CO₂ sequestration in brine-saturated formations while considering hysteresis and gas entrapment, evaluation of the presence of water and ice on Mars while considering processes of freezing and thawing, and reactive biogeochemical transport. Key references to described simulators and their recent advanced applications are also provided.

Panday and Huyakorn (2008) describe the MODFLOW SURFACT model, the name of which indicates that this model include modules developed for MODFLOW (Harbaugh et al., 2000), probably the most widely used groundwater flow model, to extend its capabilities to simulate unsaturated flow, recharge, fracture flow, and contaminant transport. It is interesting to note that the wide variety of MODFLOW SURFACT capabilities is achieved by solving only one flow equation and one transport equation. The Richards flow equation can be solved with standard retention functions, with bimodal or multimodal relative permeability curves, or with pseudo-soil retention functions. The equation can also be recast in terms of air phase flow to analyze subsurface air flow behavior. The transport equation can include an immobile multicomponent nonaqueous phase liquid (NAPL) phase with equilibrium partitioning and mass transfer between phases, as well as dual-porosity capabilities to analyze transport in fractured media. Finally, two example problems are presented that demonstrate the use of MODFLOW SURFACT to evaluate alternative designs for dense nonaqueous phase liquid remediation and to simulate the movement of a contaminant in a fractured system.

Healy (2008) presents first a brief overview of approaches for simulating water, solute, and heat transport through variably saturated porous media, including a brief description of the most widely used numerical models. He then discusses assumptions involved in the development of the VS2DI package and presents examples of its uses for a variety of applications. These examples include an evaluation of the influence of the unsaturated zone on piezometer responses in unconfined aquifers during aquifer tests, an estimation of ground–surface water exchange, and an analysis of water movement in soils in response to evapotranspiration. Finally, he analyzes advantages and limitations of the VS2DI package for different applications.

In their paper, van Dam et al. (2008) review both the main and special features of the one-dimensional SWAP model. While the main features—water flow, and solutes and heat transport in the vadose zone—are similar as in the above models, SWAP has several unique features. These include generic crop growth, swelling and shrinking processes, versatile top boundary conditions, macroporous flow, and relatively complex interactions, although handled in a simplified manner, of soil water with groundwater and surface water. van Dam et al. (2008) also review several case studies of SWAP applications that appeared in recent literature. These applications involve an evaluation of agricultural water productivity, regional nutrient management, and groundwater conservation by surface water management. To conclude their paper, van Dam et al. (2008) provide their vision of the future SWAP developments for the coming 5 to 10 yr.

Finally, authors of STOMP (White et al., 2008) present a sophisticated application of their model to investigate the distribution and remediation (soil vapor extraction) of carbon tetrachloride in the deep vadose zone at the Hanford site, near Richland, WA. High-resolution simulations were executed in three dimensions using layered and heterogeneous distributions of soil properties. The use of only a single processor to solve this problem with STOMP was not practical because of the complexity of the problem and the long simulation times. To overcome these limitations, White et al. (2008) present the developed and application of a scalable version of STOMP for faster execution on parallel computers.

Part 2: Modeling of Vadose Zone Processes

While the first part of this special section is devoted to numerical models simulating water flow, heat transport, and contaminant transport in the vadose zone, the second part presents reviews of important vadose zone processes and applications of models simulating these processes.

Colloid and Colloid-Facilitated Contaminant Transport

The first two papers in this part review processes involved in colloid and colloid-facilitated contaminant transport in the vadose zone. Pore-scale processes and models relevant for colloid transport and retention in unsaturated porous media are thoroughly reviewed by Bradford and Torkzaban (2008). While the majority of literature devoted to colloid transport studies these processes at the laboratory column scale, this review discusses our current knowledge of physical and chemical mechanisms, factors, and models of colloid transport and retention at the smaller scales: interface, collector, and pore. Bradford and Torkzaban (2008) first study the interaction energy and adhesive, hydrodynamic, and

non-Derjaguin–Landau–Verwey–Overbeek forces and/or torques that act on colloids near the solid–water and air–water interfaces. They discuss the hydrodynamic mechanisms, such as lifting, sliding, and rolling, that can cause colloid removal from an interface. Then they numerically solve the Navier–Stokes equation at the collector scale, that is, around a single solid grain or an air bubble, and evaluate the potential for colloid attachment in the presence of hydrodynamic forces from a balance of applied and adhesive torques. Here, they discuss processes such as diffusion, interception, and sedimentation that affect colloid attachment. Finally, they carry out similar analysis at the pore scale that differs from the collector scale by the presence of small pore spaces associated with multiple interfaces and zones of relative flow stagnation and where new processes such as straining, wedging, retention at the triple point, bridging, or mechanical filtration can take place.

Flury and Qiu (2008) review the current knowledge and modeling of colloid-facilitated contaminant transport in the vadose zone. Their review indicates that colloid-facilitated transport models consider mechanisms that control both colloid and solute (contaminant) transport, their mutual interactions, and mass transfer to and from the solid and air phases. The presence of an air phase in the vadose zone is reported to affect colloid-facilitated contaminant transport in several ways; for example, colloids can be trapped in immobile water, strained in thin water films and in the smallest regions of the pore space, or attached to the air–water interface itself. Flury and Qiu (2008) indicate that modeling of colloid-facilitated contaminant transport in the vadose zone has mostly been theoretical, tested only with column experiments; field applications are still lacking.

Biogeochemical Transport

Two articles demonstrate the use of biogeochemical transport and reactions models that simultaneously consider water flow, solute transport and complex chemical reactions. Both models are based on the geochemical speciation model PHREEQC (Parkhurst and Appelo, 1999).

Jacques et al. (2008) first review interactions between physical and biogeochemical processes in the vadose zone and their mutual feedbacks. They then present a hypothetical example involving the migration of several chemical species over a 200-yr time period. In this application, they use the multicomponent transport model HP1 (Jacques and Šimůnek, 2005) that resulted from coupling of the HYDRUS-1D water flow and solute transport model (Šimůnek et al., 2008) with PHREEQC to evaluate the potential environmental impact of long-term applications of mineral fertilizers containing small amounts of uranium to agricultural soils. They account for interactions between uranium and organic matter, phosphate, and carbonate, consider surface complexation as the major solid-phase interaction, and couple all geochemical processes with transient soil water flow. Jacques et al. (2008) demonstrate how transient water contents and fluxes affect soil pH and hence, the retention, bioavailability, and fluxes of various solute components. Leaching of uranium from the soil profile occurred faster in the transient flow simulation than in the steady-state simulation, as a result of the interplay between changing hydrological and geochemical soil conditions.

Szegedi et al. (2008) present the RhizoMath model for simulating coupled solute transport and speciation in the rhizosphere. RhizoMath resulted from coupling routines developed in the

mathematical package MATLAB, simulating either one-dimensional or radial solute transport with PHREEQC. Their paper presents both the model development and its verification. In its most complex application presented here, RhizoMath is able to describe the observed effects of citrate exudates on the simultaneous transport of arsenate and phosphate that compete for surface binding sites with each other and with other oxyanions such as citrate.

Multiphase Flow and Remediation

Contamination of the vadose zone with NAPLs poses a risk to soil and water quality at many hazardous waste sites. Two papers related to multiphase flow and remediation of NAPLs in the vadose zone are included here.

Class et al. (2008) demonstrate how dominant multiphase flow and transport processes at a NAPL-contaminated site can change over distinct timescales. For example, multiphase flow is the dominant mechanism at early times following the release of a NAPL into the subsurface, whereas compositional and/or nonisothermal effects become more important at longer time scales and/or during active remediation. The authors propose and illustrate how models of varying complexity can be sequentially coupled to simulate such problems. Adjusting the model complexity to the dominant processes results in significant savings of computation time and thus enables the user to make predictions for complex flow and transport scenarios over longer time spans.

Hodges and Falta (2008) numerically investigate the ability of cold air injection to control the vertical movement of the steam during steam flooding in the shallow vadose zone. Cold air injection is found to provide good control of the vertical steam movement when using approximately equal air and steam volumetric flow rates, but it may also result in the need to treat a larger volume of contaminated air. These authors report that the most effective design for steam flooding appears to be a low-permeability surface cap in conjunction with air injection above the steam injector.

Surface–Subsurface Processes

The cycling of water in the environment involves water in the atmosphere, surface waters, and water in the subsurface. While water fluxes between these three domains are continuous and directly affect each other, water movement and storage in individual domains are usually described by specialized models that consider only one domain, while the other two domains are represented simply as boundary conditions, and thus, interactions between individual domains are greatly simplified. The same is also true for the subsurface, where specialized models exist for the vadose zone and the groundwater. To describe mutual interactions between the three domains, the specialized models need to be coupled. In his review, Furman (2008) focuses on different ways of coupling hydrological models for surface and subsurface domains. He first reviews the governing equations for surface and subsurface flow, and the coupling physics and mathematics. He starts with relatively complex systems and shows how these systems are frequently simplified. He then discusses the physical alternatives for internal (between surface and subsurface) boundary conditions and numerical alternatives for coupling the systems. He identifies four different coupling schemes: uncoupled,

degenerated uncoupled, iteratively coupled, and fully coupled. Finally, he discusses how various, widely used models, deal with coupling of processes in different zones.

Although water flow through the variably saturated (vadose) zone is an important part of the hydrologic cycle because it influences partitioning of water among various flow components—runoff, infiltration, evapotranspiration, groundwater recharge, and vadose zone storage—vadose zone flow processes have rarely been properly represented in large-scale hydrological models. While Furman (2008) deals mainly with the problem of coupling surface and subsurface models, Twarakavi et al. (2008) review various approaches that can be used to account for processes in the vadose zone when simulating groundwater flow with MODFLOW (Harbaugh et al., 2000). In particular, Twarakavi et al. (2008) evaluate the newly developed HYDRUS package for MODFLOW and compare it with other available approaches. Because the HYDRUS package solves the Richards equation for water movement in the vadose zone, it can thus consider processes, such as precipitation, infiltration, evaporation, redistribution, capillary rise, plant water uptake, water accumulation at the ground surface, surface runoff, and soil moisture storage and therefore can evaluate the effects of these processes on groundwater flow and storage. The authors present several test examples of increasing complexity to document the functionality of the HYDRUS package in the MODFLOW environment.

An alternative approach to account for vadose zone fluxes in groundwater modeling is presented by van Walsum and Groenendijk (2008). They describe an approach in which a sequence of steady-state water content profiles (for the vadose zone) is used to perform dynamic simulations. The appropriate profiles are selected on the basis of water balances at the aggregate scale of control volumes. The performance of the simplified approach is evaluated by comparing results to those of a model that solves the Richards equation.

Nonequilibrium and Preferential Flow

Preferential and nonequilibrium flow and transport are often considered to hamper accurate predictions of contaminant transport in soils and fractured rocks (Šimůnek et al., 2003). Since several reviews of nonequilibrium flow have recently appeared, or will soon appear, in the literature (Šimůnek et al., 2003; Gerke, 2006; Köhne et al., personal communication, 2008), we do not include an additional review here. Instead, this special section includes one paper (Šimůnek and van Genuchten, 2008) that reviews the wide range of approaches for simulating preferential flow and transport in the HYDRUS-1D model, and another (Kodešová et al., 2008) that discusses the impact of soil micromorphological features on nonequilibrium water flow and herbicide transport in soils.

The large number of physical and chemical nonequilibrium approaches available in the latest version of HYDRUS-1D are described by Šimůnek and van Genuchten (2008). Since nonequilibrium models for water flow have been reviewed relatively recently (Šimůnek et al., 2003), this paper focuses mainly on solute transport. The various models are divided into three groups: physical nonequilibrium transport models, chemical nonequilibrium transport models, and physical and chemical nonequilibrium transport models. These models range from classical models simulating uniform flow and transport to traditional

dual-porosity physical and two-site chemical nonequilibrium models to complex dual-permeability models that consider both physical and chemical nonequilibrium. The presented models form a hierarchical system from which different formulations can be selected for different applications, depending on available information and data. Šimůnek and van Genuchten (2008) present several examples calculated with the different nonequilibrium approaches to show the effect of various transport and reaction parameters and to demonstrate the consequences of increased complexity in the models. They also discuss implications for the formulation of the inverse problem.

The impact of soil micromorphological features on water flow and herbicide transport in three different soil types is discussed by Kodešová et al. (2008). Micromorphological properties characterizing the soil pore structure were studied on images of thin soil sections taken with a camera. The soil micromorphological images were used to analyze soil porous systems, to count pores of different diameters, to distinguish the possible characters of water flow, and to select appropriate numerical models for three different soil types. Soil hydraulic properties for selected models were then estimated using a multistep outflow and ponded infiltration experiments, and numerical inversion. Finally, field observations of water flow and herbicide transport were successfully simulated using single-porosity and either dual-porosity or dual-permeability flow and transport models in HYDRUS-1D.

Agricultural Applications

Most early models for studying variably saturated water flow in the vadose zone were initially used in agricultural research to optimize moisture conditions for crop production. This focus has increasingly shifted to environmental research, with the primary concern now being the subsurface fate and transport of a wide range of contaminants, such as pesticides, nutrients, pathogens, pharmaceuticals, viruses, bacteria, colloids, toxic trace elements, radionuclides, and/or fumigants, but also the evaluation of water recharge through the vadose zone. In the category of agricultural applications, there are two papers, the first one dealing with salt leaching under subsurface drip irrigation (Hanson et al., 2008) and the second evaluating spatially distributed water fluxes under banana plants (Sansoulet et al., 2008).

Hanson et al. (2008) use the HYDRUS-2D software package to evaluate salt leaching under conditions found in many commercial fields in the San Joaquin Valley, California. Here drip irrigation is often used in fields that have saline, shallow ground water. HYDRUS-2D was used in this study to estimate actual leaching fractions, including localized leaching below the drip emitter. Simulations were conducted for different amounts of applied water, water table depths, and irrigation water salinity. The spatially varying soil wetting patterns that occur under drip irrigation caused the localized leaching. Results show that some localized leaching occur even for water applications of 60% of the potential evapotranspiration, typically considered to be severe deficit irrigation. The authors conclude that the commonly used fieldwide water balance approach is inappropriate for estimating actual leaching fractions under drip irrigation.

Sansoulet et al. (2008) used suction lysimeters to collect spatially distributed water fluxes in an Andisol under banana plants. The main cause for the spatial heterogeneity of recharge fluxes at the 1-m depth was not the spatial variability of the

subsurface environment but rather, uneven infiltration of water due to aboveground interception and redistribution of rainfall by the plant canopy that caused significant stemflow. Drainage volumes under the banana stem were up to six times higher than elsewhere, as these other areas were sheltered from direct rainfall by the banana leaves and received only throughfall. Collected experimental data and spatially distributed drainage fluxes are well reproduced by the HYDRUS software package, simulating three-dimensional variably saturated water flow for boundary conditions reflecting spatially varying infiltration fluxes. Sansoulet et al. (2008) question the common practice of applying fertilizers and pesticides at the foot of the plant, as the abundant stemflow may leach soluble nutrients or pesticides from the root zone into deeper horizons and eventually into the groundwater.

Constructed Wetlands

Langergraber (2008) provides a thorough review of numerical tools available for modeling various biogeochemical processes in subsurface constructed wetlands, that is, engineered systems that provide a natural way for simple, inexpensive, and robust wastewater treatment. Understanding the constructed wetland function is difficult since a large number of coupled physical, chemical, and biological processes occur simultaneously. Numerical models are thus indispensable for understanding these complex systems. Langergraber (2008) reviews five models of different complexity that consider variably saturated flow and transport, as well as typical wetland reactions. Several example applications of the multicomponent reactive transport module CW2D of HYDRUS (Langergraber and Šimůnek, 2006) are given.

Inverse Problem

In the first part of their article, Vrugt et al. (2008) review the current state-of-the-art of inverse modeling for estimating unsaturated flow and transport processes. They provide the historical background and summarize various solution algorithms used to solve the parameter estimation problem. In the second part, they discuss their recent work on improved optimization and data assimilation methods for inverse estimation of distributed flow and transport model parameters using parallel computing capabilities. Finally, in the third part, they demonstrate these new methods with three case studies involving the calibration of a fully coupled three-dimensional vapor extraction model, the multiobjective inverse estimation of soil hydraulic properties of a one-dimension flow model, and the simultaneous estimation of parameters and states in a groundwater solute mixture model.

Future Outlook

Historically, vadose zone models were used essentially only in national laboratories or by premium research institutes and universities. Today, sophisticated numerical models are available to every college student or consulting practitioner. Although more and more complex numerical models are being developed, some of these tools can only be accessed by a few highly specialized individuals or teams. There is therefore an increasing need to make these tools available and accessible to the public by the development of graphics-based user interfaces that can tremendously simplify the use of these tools. Similarly, while many of the advanced numerical models have been parallelized to run on supercomputers or computer clusters running either Unix or

Linux operating systems, there is also a need to develop parallelized versions of these models that can run on regular PCs with multicore processors.

Future advances in vadose zone modeling will also be limited by our basic understanding of the fundamental physics, chemistry, and biology that occurs in the subsurface environments. As our knowledge increases and this information is incorporated into models, more physically meaningful tools can be generated to help study and manage the vadose zone.

While not covered in this special section, research on new numerical techniques, linear and nonlinear solvers, grid generation, parallel computing techniques, visualization, optimization techniques, and other areas (USDOE, 2001) is taking place that will have an important impact on future developments in vadose zone modeling. Additionally, there is a need to develop and implement spatial and temporal error estimators and adaptive local grid and time-step refinement algorithms into vadose zone models to automatically minimize these errors. To facilitate the use of numerical models by regulators and consulting practitioners, it would be extremely helpful to develop algorithms that would automatically alert users about a model's possible limitations or that could even automatically select more accurate alternative approaches.

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