Advanced Vadose Zone Simulations Using TOUGH

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ABSTRACT

The vadose zone can be characterized as a complex subsurface system in which intricate physical and biogeochemical processes occur in response to a variety of natural forcings and human activities. This makes it difficult to describe, understand, and predict the behavior of this specific subsurface system. The TOUGH nonisothermal multiphase flow simulators are well-suited to perform advanced vadose zone studies. The conceptual models underlying the TOUGH simulators are capable of representing features specific to the vadose zone, and of addressing a variety of coupled phenomena. Moreover, the simulators are integrated into software tools that enable advanced data analysis, optimization, and system-level modeling. We discuss fundamental and computational challenges in simulating vadose zone processes, review recent advances in modeling such systems, and demonstrate some capabilities of the TOUGH suite of codes using illustrative examples.

INTRODUCTION

Water flow through variably saturated porous media is commonly described by the Richards equation (Richards, 1931). The Richards equation exhibits strong nonlinearities, which calls for numerical solution methods whenever the model is applied to realistic systems. The TOUGH suite of numerical simulators for nonisothermal flows of multiphase, multicomponent fluids in permeable (fractured and porous) media (Pruess et al., 1999; Pruess, 2004a) is based on conceptualizations and methodologies that are well suited for the solution of vadose zone flow and transport problems. Moreover, the emphasis of TOUGH on an accurate description of hydrogeological features, physical processes, and thermodynamic properties makes it a useful tool for studying and predicting more complex phenomena occurring near the land surface or in deeper unsaturated zones, either using the classical Richards equation or employing more complex, nonisothermal multiphase flow and reactive transport processes. Table 1 shows a summary of the main TOUGH codes.

In this review article, we discuss some of the modeling issues specific to the simulation of vadose zone processes, and present examples of recent developments of the TOUGH suite of codes aimed at addressing some of these issues. Table 2 summarizes the simulation capabilities and applications presented in this paper along with key references.

VADOSE ZONE MODELING CHALLENGES

Traditionally, soil physicists and agronomists perform vadose zone modeling studies that focus on the prediction of moisture, soil-gas, and heat flow as well as nutrient and pesticide transport in the shallow, variably saturated crop root zone. In addition to these traditional applications, the scope of numerical simulations in the unsaturated zone has been considerably broadened both in terms of systems and processes considered. The depth and horizontal scale of vadose zone systems studied by numerical models has been greatly expanded, and may include deep unsaturated zones that are affected by contamination, considered for storage of carbon dioxide and nuclear waste, or used for the extraction of geothermal energy, natural gas, or methane from hydrate accumulations. Soil moisture balances and the interaction between the subsurface, surface waters, and the atmosphere are studied on the hillslope, watershed, and global scales. On the other end of the spectrum, effects such as preferential flow, biogeochemical reactions, and certain geomechanical behavior occur on much smaller scales that are below the size of a commonly used computational element or even smaller than the representative elementary volume as defined in groundwater hydrology.

In addition to considering unsaturated flow of water and transport of tracers or non-reactive components, vadose zone hydrology has evolved to study complex processes of nonisothermal, multiphase, multicomponent fluid flow coupled to biogeochemical reactions. The multiscale, multiphysics nature of vadose zone processes poses significant conceptual and numerical challenges. In addition, advanced measurement techniques and analysis methods are needed to obtain the characterization data for site-specific models. Finally, the vadose zone has to be integrated into a larger system, which may include not only other natural subsystems, but also engineering components as well as economic and regulatory aspects.

The modeling challenges mentioned above can be grouped into three categories: (1) challenges resulting from the heterogeneity and complexity of the physical and biogeochemical processes occurring in the vadose zone; (2) challenges resulting from the position of the vadose zone at the interface between different spheres (atmosphere, biosphere, hydrosphere); and (3) computational challenges resulting from the coupling of subsystems and processes involving many spatial and temporal scales.

The first group of challenges includes the characterization and incorporation of heterogeneity, which affects flow behavior (fingering, flow focusing, lateral diversion, preferential and fast flow, water perching) and transport behavior (channelization, plume spreading). Moreover, biogeochemical reactions not only depend on heterogeneity in chemical and mineralogical composition, but they are also affected by details of the flow patterns and transport processes to which they are strongly coupled. Also note that under unsaturated or multiphase flow conditions, the impact of heterogeneity on these processes may be self-enhancing or self-controlling, which affects the conceptualization of such processes in a numerical model.

The characterization of heterogeneity is further complicated because the soil structure may exhibit both systematic and random features on multiple scales. Additionally, sensors used for monitoring the vadose zone and for measuring its properties have different support scales, and averaging these properties often leads to effective parameters that are process-specific, scale-dependent, and anisotropic.

The TOUGH simulators have been used extensively to analyze the impact of heterogeneity on vadose zone processes (Pruess, 1998, 1999, 2004b; Pruess et al., 2002). Such studies include the use of high-resolution simulations with a massively parallelized version of the code (Wu et al., 2002; Zhang et al., 2003) and the development of a joint hydrological-geophysical inversion approach to characterize heterogeneity and to reduce systematic modeling errors (Kowalsky et al., 2005; Finsterle and Kowalsky, 2007; Lehikoinen et al., 2007).

The classic approach for describing unsaturated flow based on the Richards equation has been successful but limited. One limitation stems from the difficulty in obtaining characterization data for specifying the relative permeability and capillary pressure curves. In addition, the functional form of these curves is difficult to assess and may greatly impact modeling results. For example, if a standard hysteretic capillary pressure model is used, key phenomena (such as hysteresis in the relative permeabilities and history-dependent gas entrapment) may be neglected. The hysteresis model implemented in TOUGH is presented in Doughty (2007) and will be summarized below. Similarly, fast-flow through macropores or fractures may be described by an effective continuum model with multimodal characteristic curves. However, as demonstrated by Doughty (1999), the applicability of an effective continuum model is limited to cases where the assumption of thermodynamic equilibrium between the continua is valid. In addition to the active fracture model by Liu et al. (1998), the TOUGH simulators include dual- and triple-continuum (Wu et al., 2004) formulations with multiple interacting continua to accurately capture exchanges of fluids and heat between regions of the porous medium of vastly different flow and transport characteristics.

The vadose zone, being bounded by the land surface and the groundwater table, is in direct contact with the biosphere and strongly affected by human activities. Interaction among these various interfaces leads to a second group of modeling challenges. The processes at the vadose zone boundaries are often highly dynamic (infiltration events, evapotranspiration, heat transfer, water table fluctuations); more importantly, they may need to be fully coupled to account for feedback mechanisms (e.g., evaporation, root water uptake). The TOUGH codes accurately account for phase transitions (evaporation and condensation, including the related latent heat effects) as well as multiphase diffusion (e.g., of water vapor), allowing the simulation of evaporation and dry-out processes. Simplified approaches to simulate evaporation using the Richards equation have been recently implemented (Ghezzehei et al., 2004). TOUGH has also been coupled to the National Center for Atmospheric Research (NCAR) Community Land Model CLM3 (http://www.cgd.ucar.edu/tss/clm/index.html) for the simulation of energy and moisture dynamics between the atmosphere and the subsurface (Pan et al., 2007). Finally, integration of TOUGH2 and iTOUGH2 into the GoldSim model (GoldSim Technology Group, 2006) provides the means to study the interaction between the subsurface environment and related natural and engineered components on a system level (Zhang et al., 2007).

The third group of challenges is related to the computational difficulties in dealing with highly nonlinear, coupled processes that occur on multiple scales and with potentially different characteristic time constants. Spatial discretization in the TOUGH codes is based on the integral finite difference approach (Narasimhan and Witherspoon, 1976), in which the basic mass conservation equations are directly discretized in their integral form (Pruess et al., 1999; Pruess, 2004a). This scheme provides great flexibility in handling complex geometries, multiregion approaches, and a variety of boundary conditions. Higher-order schemes have also been implemented (Pruess, 1991b; Oldenburg and Pruess, 2000). Nonlinearities are treated using Newton-Raphson iterations with a residual-based convergence criterion. Parallelization of the forward (Wu et al.,

2002) and inverse (Finsterle, 1998) runs help make tractable the solution of larger simulation and optimization problems. Nevertheless, phase changes, strong nonlinearities in characteristic curves near residual saturations, sharp saturation and reaction fronts, and the coupling of counteracting processes on disparate scales are among the features causing numerical difficulties that require careful attention by the code developer and sometimes case-by-case intervention by the user.

The remainder of this review article discusses a few select capabilities recently implemented in various TOUGH modules. These examples address diverse issues from all three groups of challenges related to vadose zone modeling mentioned above.

SELECT CAPABILITIES AND APPLICATIONS

Hysteresis with Gas Entrapment

Numerical modeling has been used extensively in the past few years to study geologic storage of CO_2 in brine-saturated formations. At depths commonly considered for CO_2 storage (>800 m), CO_2 primarily exists as a gas-like supercritical phase, which is the non-wetting phase, while some CO_2 dissolves in the brine, which is the wetting phase. Interactions between the two fluid phases are represented at the grid-block scale by capillary pressure and relative permeability functions. The amount of CO_2 potentially trapped in the subsurface depends on hysteresis effects. Given the underlying trapping mechanism, it is necessary to develop a hysteresis model that is capable of simulating history-dependent gas entrapment.

During periods of CO_2 injection into brine-saturated formations, the resulting CO_2 plume grows continuously, that is, all locations follow the primary drainage branch of the capillary pressure curve at all times, and this branch can be replicated using a non-hysteretic formulation. However, for post-injection periods, when the CO_2 plume moves upward and updip due to buoyancy forces, different locations experience drainage and imbibition at different times, necessitating the use of a hysteretic formulation.

In a hysteretic model, some parameters depend only on the process (drainage or imbibition) that is occurring, so it is convenient to subdivide the characteristic curves into drainage branches and imbibition branches (see Figure 2 below). The parameters describing gas entrapment, however, depend on the value of the saturation when the grid block makes a transition from drainage to imbibition or vice versa, the so-called turning-point saturations. Because turning-point saturations are different in each grid block, these parameters are spatially variable and history-dependent. The most critical parameter is the residual gas saturation, denoted S_{gr}^{Δ}, which is the saturation below which gas is immobile (i.e., the saturation below which immiscible CO_2 is trapped). For the primary drainage curve, S_{gr}^{Δ} = 0, but for imbibition, S_{gr}^{Δ} increases as the liquid saturation at the drainage-to-imbibition turning point, denoted S_{l}^{Δ}, decreases. Thus, grid blocks that once contained the most CO_2 are those which trap the most CO_2. The maximum possible value of S_{gr}^{Δ} is $S_{gr\max}$, which is obtained for the minimum possible value of S_{l}^{Δ}; this minimum turning-point saturation is generally equal to the irreducible liquid saturation S_{lr}. The value of S_{gr}^{Δ} determines the history- and location dependent amount of CO_2 that can be trapped. Note that gas entrapment cannot be adequately simulated using a model that is solely based on the Richards equation, in which gas is considered a passive bystander; a two-phase formulation is needed (Faybishenko, 1995).

We consider an application in which CO_2 is injected into a porous formation 100 m thick located at a depth of 1,000 m. This system is represented by an axisymmetric model with the injection well in the center. The porosity of the formation is 25%, horizontal permeability is 2×10^{-13} m^2, and vertical permeability is 1×10^{-13} m^2. The overburden above the storage formation extends to the surface and is assumed to have the same properties as the storage formation itself; thus, there is no low-permeability caprock. Initially, the brine saturation is 100% everywhere in the model, pore pressure is hydrostatic with a pressure of 1 bar at the surface, and temperature follows the geothermal gradient of 30 ^oC/km, with the temperature at the surface and base of the model held constant at 15 ^oC and 45 ^oC, respectively. The salinity of the pore water is assumed to be 100,000 ppm. Fluid and heat flow are fully coupled in the simulations.

The numerical simulations begin with injection of 900,000 tons of CO_2 into the porous formation at a constant rate of 30,000 tons per day for one month. (This rate of CO_2 corresponds roughly to emissions of a 1,000 MW coal-fired power plant.) After injection stops, the only driving force in the model tending to cause movement of the CO_2 is buoyancy. Simulations continue for 1,000 years.

Figure 1 shows the CO_2 plume at a series of times. During the one-month injection period, the CO_2 plume is expanding in all directions, and the hysteretic-model results do not differ from what would be obtained with a non-hysteretic model. Thereafter, the leading edge of the plume, where drainage occurs and S_{gr} is zero, continues to advance (reaching the surface at about 700 years), while the trailing edge of the plume, where imbibition occurs and S_{gr} is large, remains largely trapped. This combination of processes cannot be replicated with a non-hysteretic model or a hysteretic model that does not include phase trapping. If a non-hysteretic model with a small value of S_{gr} is used, most of the plume escapes through the ground surface within 10 years; whereas a non-hysteretic model with a large value of S_{gr} produces a plume that never reaches the surface and remains entirely trapped indefinitely.

Figure 2 shows the capillary pressure and relative permeability paths followed for several locations in the CO_2 plume. All paths begin at $S_l = 1$ along the primary drainage curve; the transition to an imbibition scanning curve occurs at S_l^{Δ} (shown by arrows); as $|P_c| \rightarrow 0$ and $k_{rg} \rightarrow 0$ on the imbibition curves, $S_l \rightarrow (1 - S_{gr}^{\Delta})$ (shown by black-outlined dots). Thus grid blocks near the plume center, which get much drier during the injection period and therefore have a small S_l^{Δ}, have a much larger S_{gr}^{Δ}, and consequently trap more CO_2 than do grid blocks barely reached by the plume. More details about this modeling capability and the related application can be found in Doughty (2007).

Hydrological Processes in Permafrost

Subsurface flow is governed by the characteristics of the porous medium, the fluid properties, and constitutive relations describing the interaction between the porous medium and the fluids. The equation-of-state modules of the TOUGH codes provide an accurate description of the thermophysical properties of the considered fluid mixtures. Specifically, the properties of water are calculated within experimental accuracy from steam table equations as given by the International Formulation Committee (IFC, 1967).

As part of the ongoing re-engineering of TOUGH, the temperature and pressure range available for the calculation of water properties has been expanded to include the phase transition from liquid or gas to ice and vice versa. The enthalpy, sublimation pressure, as well as fusion and melting pressures of ice (on the ice-vapor and ice-liquid equilibrium lines of the water phase diagram) are computed using regression equations from data obtained by the National Institute for Science and Technology. Within the ice phase (to $T = 50$ K and $P \approx 200$ MPa), ice densities are determined using the ice compressibility model of Marion and Jakubowski (2004) and the thermal expansivity data from Tanaka (1999). The ice enthalpy is computed using the heat capacity polynomial equation with the coefficients reported in Yaws (1999). Changes in fluid capillary pressure and relative permeability relations as a function of ice saturation are also accounted for.

Simulating freezing and melting processes is essential to improve our understanding of permafrost regions (e.g., to study the hydrological response to climate change). These processes also occur during the formation and dissociation of gas hydrates deposited in permafrost and sub-oceanic formations (Moridis, 2003; Moridis et al., 2005). The extended equation-of-state for water is implemented in the re-engineered version of TOUGH2, named TOUGH+. To demonstrate the capability of the TOUGH+GasH2O code to handle melting ice and steam fronts in a single model, we simulated the extreme thermal conditions encountered when a heat-generating power-source (e.g., from a landing vehicle) is buried into permafrost on Mars. A heat source of 250 W is assumed to be embedded in the shallow Martian subsurface. Below a depth of 0.2 m, the pore space contains 50% ice and 50% carbon dioxide at an atmospheric pressure of only 713 Pa and a temperature of -80 °C; above the permafrost is a layer of completely dry sediment.

Figure 3 shows the distribution of temperature, water and ice saturations after 10 sols ("Martian days;" 1 sol = 88,620 sec). In the immediate vicinity of the heat source the ice has been melted and the water vaporized. Liquid water only exists in a relatively thin region with temperatures between about 0 and 60 °C. At the outer edge of this region, the water freezes, creating an ice barrier that effectively prevents convective heat transport in radial direction. Water vapor (and associated thermal energy) is redirected upwards where it escapes to the Martian atmosphere. The simulations predict that the zone disturbed by a buried heat source is very limited. Specifically, liquid water is confined to a narrow region, reducing the risk that terrestrial microorganisms that may have been carried by the landing vehicle could survive and proliferate. More details about this simulation study can be found in Moridis and Pruess (2006).

Biogeochemical Reactions

Understanding and predicting the fate of nutrients and contaminants in the vadose zone requires simulation of biogeochemical reactions. Accounting for biogeochemical reactions is also important because most redox reactions occurring in the shallow subsurface are catalyzed by bacteria. Geochemical and microbiological reactions are strongly coupled to flow and transport processes, and—depending on the scale at which they are studied—may not reach local equilibrium and thus require kinetic rate laws. A multi-regional formulation for intra-aqueous kinetic reactions and biodegradation has been incorporated into TOUGHREACT (Xu and Pruess, 2001; Xu et al., 2006), which considers a variety of subsurface thermo-physical-chemical processes for a wide range of hydrological and chemical conditions. Interactions between mineral assemblages and fluids can be modeled assuming local equilibrium or kinetics. The gas phase may be chemically active, and precipitation and dissolution reactions may change formation porosity and permeability. Reactions among primary species (including intra-aqueous and sorption reaction kinetics and biodegradation) are described using a general rate law that accounts for multiple mechanisms and multiple products, concentration-dependent (Monod) rate expressions, and inhibition terms.

Since most bacteria grow within a relatively immobile biofilm on solid surfaces, a three-region model is proposed that consists of (1) a mobile region, (2) an immobile region, which includes stagnant water and biomass, and (3) a solid particle region where mineral dissolution or precipitation and surface reactions may occur (Figure 4). Instead of explicitly considering every pore and particle, the three regions are lumped into three overlapping continua, which are discretized separately and connected to each other. If necessary, each region can be further discretized to better resolve steep gradients and sharp reaction fronts. This concept is similar to the MINC model (multiple interacting continua; Pruess and Narasimhan (1985)) and the triple-continuum approach of Wu et al. (2004), both implemented in the TOUGH simulators. These models resolve global fluid and heat flow through a fractured (or macropore) system, while accounting for the local exchange between the fractures and the matrix. The extension of the MINC method to reactive geochemical transport is described in Xu and Pruess (2001).

Reactive transport of denitrification was simulated using both a single-continuum and a multi-region model, and the results are compared to data from the column experiments of von Gunten and Zobrist (1993). While the single-continuum model fails to reproduce the nitrate concentration profiles, the multi-region model (see Figure 5) captures the system behavior reasonably well, even though the volume of the immobile region needed to be increased (potentially reflecting bacterial growth) at later times.

The biogeochemical transport simulation capabilities of TOUGHREACT will be useful for many subsurface problems, including acid mine drainage remediation, organic matter decomposition, oil and gas maturation, sulfite reduction in oil fields, and effective environmental remediation of groundwater contamination. More details about TOUGHREACT and its applications can be found in Xu and Pruess (2001), Xu et al. (2001), and Xu (2007).

Parameter Estimation and Model Structure Identification

An accurate description of physical processes, biogeochemical reactions, and fluid properties is a prerequisite for a reliable prediction of vadose zone systems. However, a major source of prediction uncertainty lies in our incomplete knowledge of the subsurface structure and the related soil properties. The complexity of soil formation as well as depositional and erosional processes result in an equally complex, usually highly heterogeneous, but not entirely random subsurface structure. While several stochastic methods exist to describe and simulate subsurface structures (using, for example, geostatistics (Deutsch and Journel, 1992) or lithofacies modeling (Carle and Fogg, 1996)), the determination of the actual structure at a given site remains challenging. In addition to identifying the geometry of the stratal soil architecture, hydrogeologic and geochemical parameters need to be assigned. These parameters are often scale-dependent, specific to the process being simulated, and related to other aspects of the conceptual model. Finally, initial and boundary conditions are either unknown or uncertain, so they need to be parameterized and estimated along with the structure and soil properties. Inverse modeling is a means to obtain parameters that in some sense can be considered optimal for a given model. However, it is important to realize that an error in the conceptual model can yield parameter estimates that are biased or even meaningless; it is therefore essential to address the impact of systematic errors (in the data and the conceptual model) when calibrating a vadose zone model.

The iTOUGH2 code (Finsterle, 2004; http://www-esd.lbl.gov/iTOUGH2) provides inverse modeling capabilities for most modules of the TOUGH suite of simulators. iTOUGH2 solves a nonlinear optimization problem to determine TOUGH input parameters based on measured data for which corresponding TOUGH output is calculated. This means that any aspect of the model that can be parameterized—including boundary conditions and the soil structure—can be subjected to estimation by inverse modeling. Moreover, standard TOUGH output variables can be used to calculate new quantities that can then define the objective for optimization—including geophysical data or also costs.

This flexibility has been exploited to develop a joint inversion approach, in which hydrological and geophysical data are inverted to estimate hydrogeological, geostatistical, and petrophysical parameters (Kowalsky et al., 2004; 2005; Finsterle and Kowalsky, 2007). In this approach, the potential estimation bias introduced by a systematic error in the conceptual model (specifically in the representation of subsurface heterogeneity) is reduced by adjusting the model structure itself during the optimization process. The increased need for data that contain information about the subsurface structure is met by adding geophysical data. The inclusion of hydrogeological data in the joint inversion approach ensures that a relation can be established between the geophysical signals and soil properties that determine fluid flow (note that this may require the estimation of additional parameters, such as those of a petrophysical relationship). An example is shown in Figure 6, where a highly heterogeneous, anisotropic soil structure and its related properties are determined by the joint inversion of hydrological data (infiltration rates and neutron probe measurements) and geophysical data (arrival times from a cross-hole ground penetrating radar survey). Details about this specific application can be found in Finsterle and Kowalsky (2007).

Since inverse modeling usually deals with the difference between the measured and calculated system response, systematic errors may stem from errors in both the data and the model, and it is often difficult (and sometimes irrelevant) to distinguish between the two sources. For example, data from laboratory experiments may show a systematic deviation (trend) from the expected behavior. If the trend is a result of a leak in the testing apparatus, it can be considered a data error, or an error in the model, as the model does not properly represent the experimental conditions. Depending on the statistical properties of the residuals, the problem can be resolved using robust estimators (Finsterle and Najita, 1997), through explicit simulation of the processes expected to have influenced the data and associated parameter estimation (Finsterle and Persoff, 1997), through the estimation of a correction parameter (Kowalsky et al., 2005), or through the development of a statistical approximation error model (Lehikoinen et al., 2007). All these approaches are being examined in the context of vadose zone characterization using the TOUGH suite of forward and inverse models.

Coupling with Other Models

Since the vadose zone is in direct contact with the land surface, it is essential to consider hydrologic and chemical interactions between the atmosphere, land surface, and subsurface. In addition, anthropogenic activities (such as land cultivation, irrigation, hydraulic engineering projects, waste disposal) may profoundly affect the vadose zone and other related natural systems. These coupled impacts on the water and chemical cycles also influence (and are influenced by) the economic and regulatory environment.

Considering the vadose zone as a disconnected subsystem raises difficult questions regarding the boundary conditions to be employed at the land surface. While net infiltration can be estimated using experimentally based parameterization models (for a review, see Faybishenko (2007)), evapotranspiration (a potentially significant contributor to the moisture balance at the surface, specifically in arid regions) is a coupled process that requires a physical description of both surface and subsurface conditions. Conversely, land hydrologic responses to meteorological forcing involve complicated exchanges of moisture and energy between soil, vegetation, snowpack, groundwater, and the overlying atmospheric boundary layer. The NCAR Community Land Model CLM3 is a model primarily developed to meet the needs of regional climate modeling. In CLM3, radiation, sensible and latent heat transfer, zonal and meridional surface stresses, and ecological and hydrological processes are simulated as interrelated subprocesses. However, the subsurface moisture flow in CLM3 is only considered in a simplified manner. CLM3 has been coupled to TOUGH2 through an internal interface that includes flux and state variables shared by the two submodels. Specifically, TOUGH2 uses infiltration, evaporation, and root-uptake rates, calculated by CLM3, as sink or source terms, while CLM3 uses saturation and capillary pressure profiles, calculated by TOUGH2, as state variables.

Simulation results show (see Figure 7) that the coupled model greatly improves the prediction of water table elevation, evapotranspiration, surface temperature, and soil moisture, as evaluated using 18 years of data observed at a real site (Pan et al., 2007). The new model can be extended to include an atmospheric simulation model to simulate hydraulic processes from the top of the atmosphere to deep in the ground.

In addition to coupling atmospheric, land surface, and subsurface processes, the vadose zone is linked to many other environmental and engineered systems. The interaction among these subsystems can be better understood, analyzed, and optimized using a system-level modeling tool such as GoldSim (GoldSim Technology Group, 2006; http://www.goldsim.com). For example, decisions regarding the use of biofuels as an alternative energy source need to be based on an analysis of the interactions between regional hydrological cycles, water and energy needs for biofuel production, impacts on the vadose zone and groundwater resources, as well as economic and regulatory parameters. Uncertainties and risks associated with each submodel and its parameters also need to be evaluated. To support system-level studies involving subsurface flow and transport processes, both TOUGH2 and iTOUGH2 have been linked to GoldSim. This coupling provides the capability to simulate the interaction between the vadose zone and various engineered components, to analyze the economic impact of environmental management decisions, to perform risk analysis studies, and to optimize testing and monitoring designs. Moreover, GoldSim provides a convenient graphical interface to control TOUGH simulations and to visualize modeling results. Figure 8 shows an example of a TOUGH-GoldSim application that focuses on evaluating the feasibility of carbon sequestration with enhanced gas recovery, where the economic benefits of enhanced methane production is directly weighed against the costs and benefits of CO_2 capture and injection. In this example, the reservoir simulations are performed using a module for multicomponent gas mixtures of methane and CO_2 (Oldenburg et al., 2004). More details about this application can be found in Zhang et al. (2007).

Finally, the integration of a subsurface process simulator into a system-level modeling tool that also includes an economic model provides an opportunity to evaluate and optimize water management decisions. Optimization routines provided by GoldSim or iTOUGH2 can also be used to determine operational parameters of a remediation project (an example is discussed in Finsterle (2005)).

CONCLUDING REMARKS

To understand and predict the response of the vadose zone to naturally occurring hydrological events or anthropogenic interference requires the use of sophisticated numerical modeling capabilities. The TOUGH suite of simulators is well suited to address the conceptual and computational challenges that are specific to unsaturated subsurface systems. The accurate process description implemented in TOUGH provides the basis for the analysis of the vadose zone and its interactions with other subsystems. However, we believe that an integrated approach to site characterization and predictive modeling is needed to reduce the impact of systematic modeling errors on our forecast of vadose zone system behavior.

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Table 1. The TOUGH suite of simulators: Main codes

Simulator	Comment	Reference
TOUGH2	General-purpose simulator for nonisothermal two-phase systems	Pruess, 1991a
T2VOC	Nonisothermal three-phase simulator for environmental applications	Falta et al., 1995
iTOUGH2	Inverse modeling, sensitivity analysis, and uncertainty propagation analysis for TOUGH2 and T2VOC	Finsterle, 1999a, b, c
TOUGH2 V2.0	Updated version of TOUGH2, with added process descriptions and fluid properties modules	Pruess et al., 1999
TMVOC	Nonisothermal three-phase simulator for multicomponent hydrocarbon mixtures	Pruess and Battistelli, 2002
TOUGH-FLAC	Simulator for coupled nonisothermal multiphase flow and rockmechanical processes	Rutqvist et al., 2002
TOUGHREACT	Simulator for nonisothermal multiphase flow and reactive biogeochemical transport	Xu et al., 2004
TOUGH+	Re-engineered version of TOUGH2 V2.0 with enhanced process descriptions and added fluid property modules	(research code)

Table 2. TOUGH simulation capabilities and applications

Simulation capability	Application	Reference
Hysteresis with gas entrapment	CO_2 sequestration	Doughty (2007)
Freezing and melting	Ice on Mars	Moridis et al. (2006)
Reactive biogeochemical transport	Denitrification	Xu (2007)
Joint hydrological-geophysical inversion	Vadose zone characterization	Finsterle and Kowalsky (2007); Kowalsky et al. (2004, 2005)
Coupling to land surface model	Watershed moisture prediction	Pan et al. (2007)
Integration into system-level model	Enhanced gas production and CO_2 sequestration	Zhang et al. (2007)

FIGURE CAPTIONS

Figure 1. CO_2 plume evolution (from Doughty, 2007). The single black contour line shows $S_g = 0$. The colored points identify the locations for which characteristic curves are shown in Figure 2.

Figure 2. Hysteretic capillary pressure (top) and relative permeability (bottom) paths for several grid blocks within the CO_2 plume (from Doughty, 2007). Grid-block locations are shown in Figure 1. All paths start at $S_l = 1$ on the primary drainage curve.

Figure 3. Simulation of heat source buried in Martian permafrost (from Moridis and Pruess, 2006). (a) temperature, (b) water saturation, and (c) ice saturation after 10 sols.

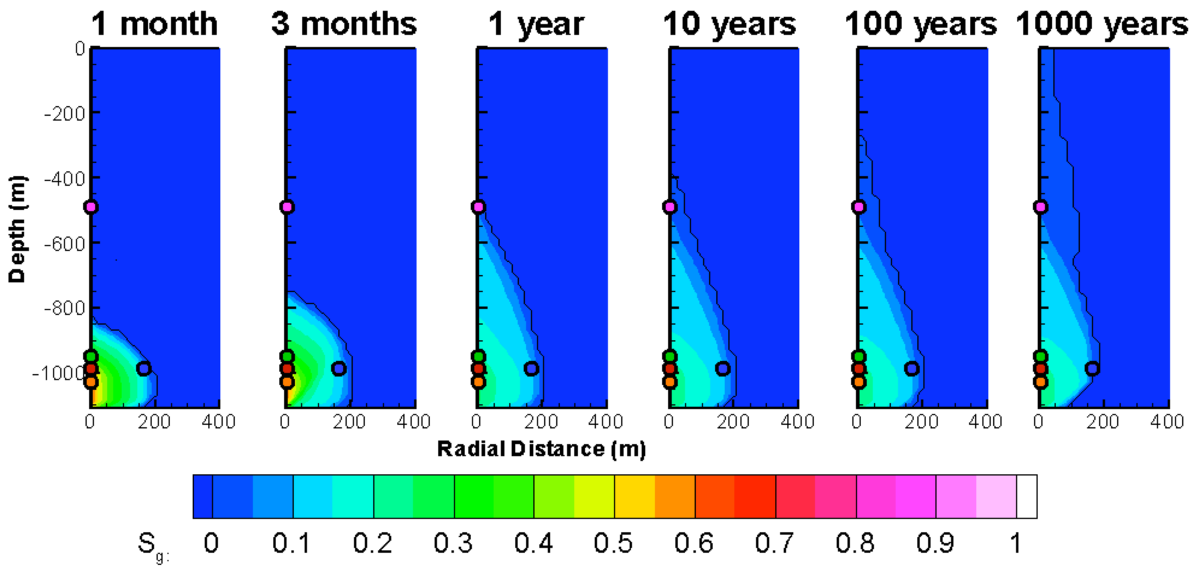
Figure 4. Schematic representation of a multi-region model for resolving local diffusive transport (from Xu, 2007).

Figure 5. Nitrate concentrations obtained with the multi-region model after 7 and 14 days (from Xu, 2007); measured data are from von Gunten and Zobrist (1993).

Figure 6. Demonstration of joint hydrological-geophysical inversion approach for soil structure identification (from Finsterle and Kowalsky, 2007). (a) Liquid saturation distribution after one day of water release, locations of neutron probes in boreholes (squares), and GPR straight-ray paths used for inversion; (b) site-specific permeability field obtained by the joint estimation of geostatistical, hydrogeological, and petrophysical parameters.

Figure 7. Comparison between observed and simulated daily water tables using CLM3 and the coupled CLM3-TOUGH2 simulators (from Pan et al., 2007).

Figure 8. System-level model for the evaluation of carbon sequestration with enhanced gas recovery (from Zhang et al., 2007). Carbon dioxide injection and methane production are simulated using TOUGH2; the link to the engineering components and an economic analysis is provided by GoldSim.



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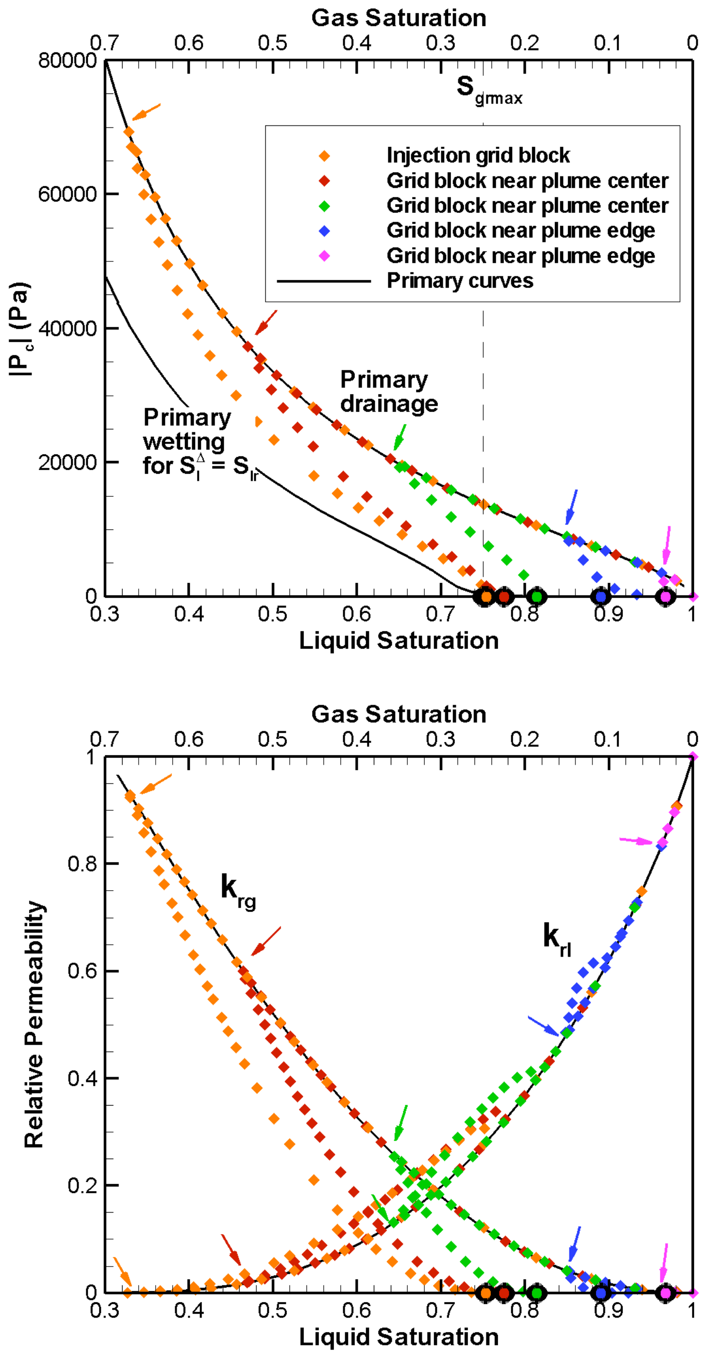

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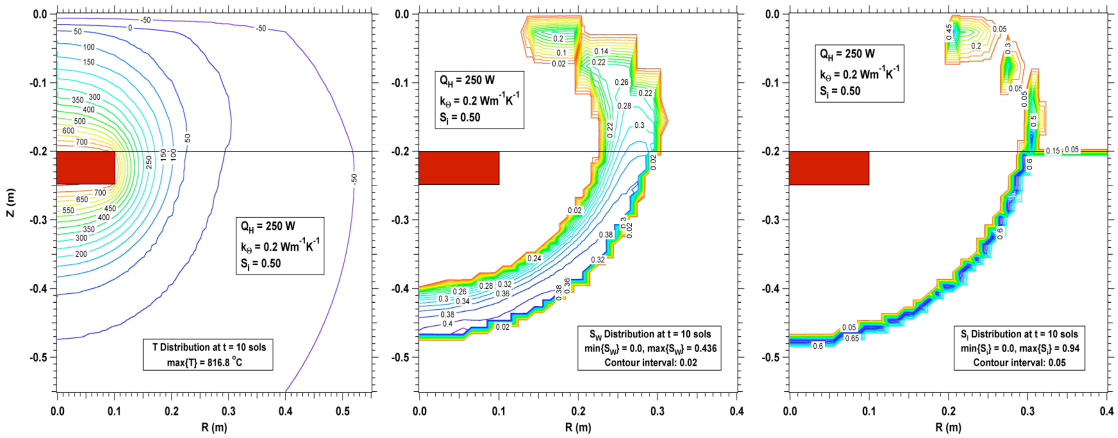

(a) (b) (c)

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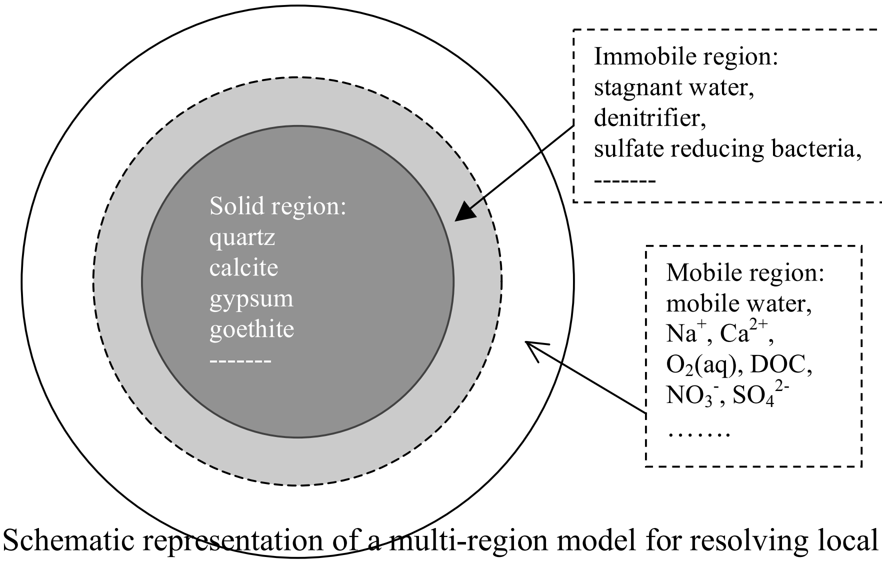

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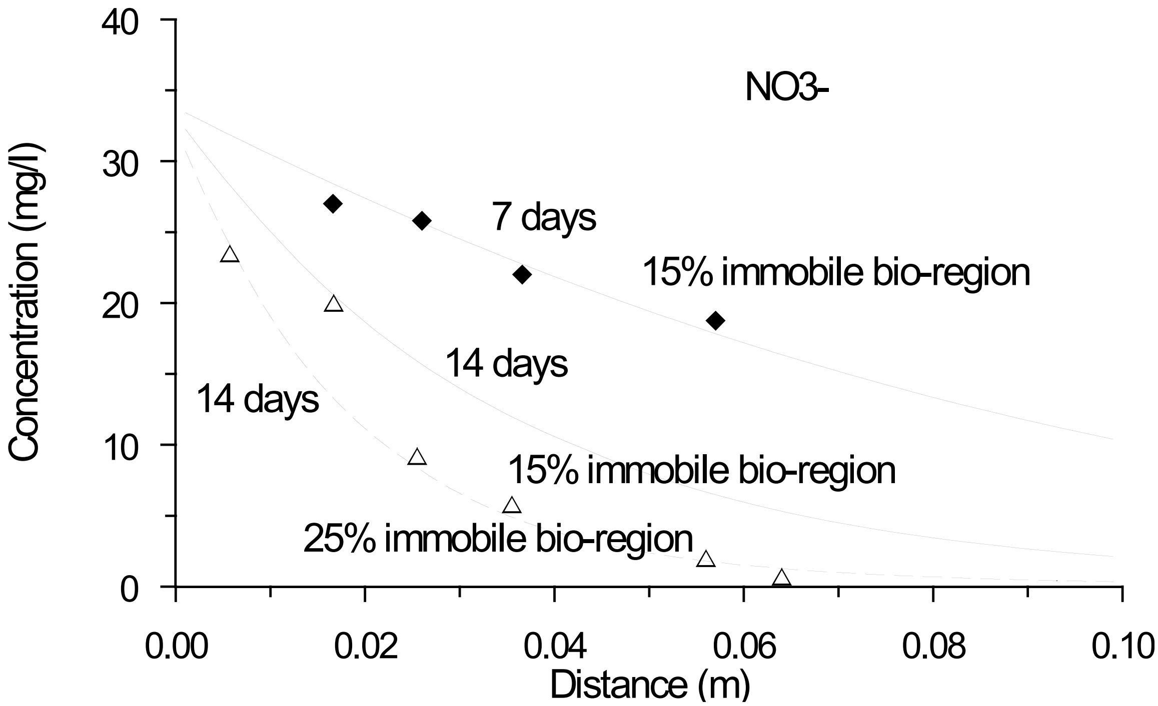

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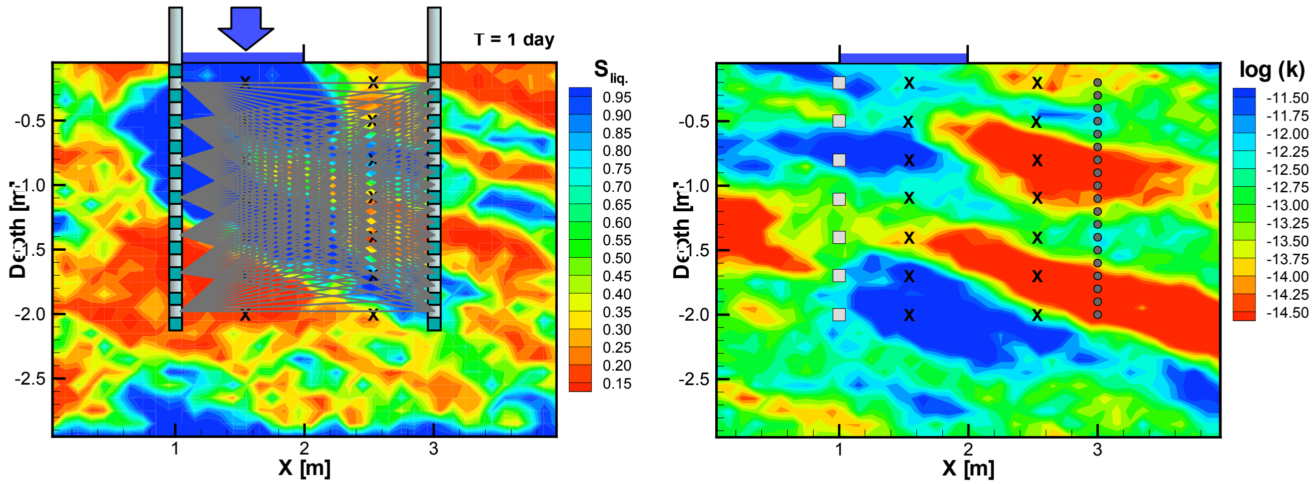

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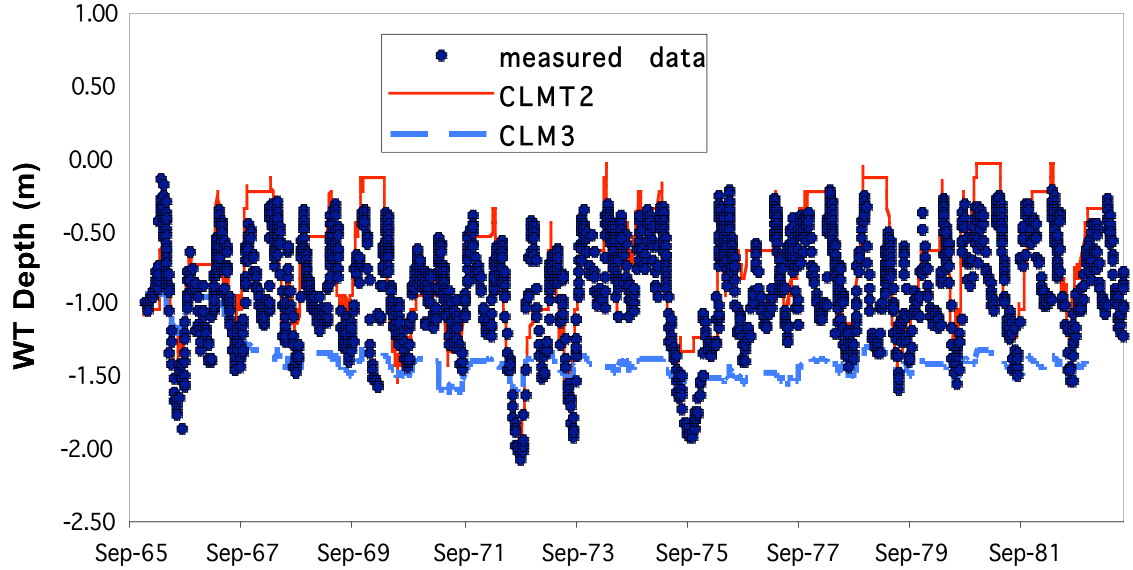

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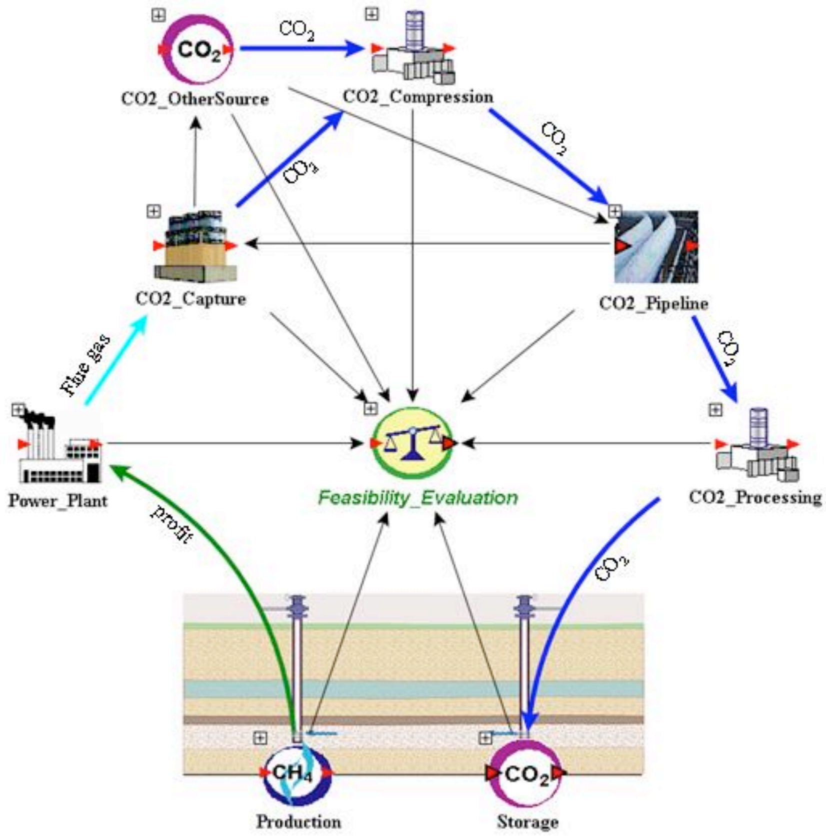

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