Preface: Recent Advances in Modeling Multiphase Flow and Transport with the TOUGH Family of Codes

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ABSTRACT

A symposium on research carried out using the TOUGH family of numerical codes was held from May 15 to 17, 2006, at the Lawrence Berkeley National Laboratory. This special issue of the *Vadose Zone Journal* contains revised and expanded versions of a selected set of papers presented at this symposium (TOUGH Symposium 2006; http://esd.lbl.gov/TOUGHsymposium), all of which focus on multiphase flow, including flow in the vadose zone.

Situations involving flow of multiple fluids in the subsurface, including the case of flow in the vadose zone, are commonly encountered in many environmental and water resources problems. These problems are associated with water resources management, irrigation, remediation of aquifers contaminated with waste products and non-aqueous phase liquids (NAPLs), and disposal of nuclear wastes in fractured-rock sites, among others. The complexities of multiphase flow and transport processes in the subsurface are attributed to a number of factors, including: (1) The effect of subsurface heterogeneity and difficulties in characterizing the heterogeneity at different scales of interest, (2) the coupling that occur between physical, chemical, biological and ecological processes, and (3) strong nonlinearities involved in the flow and transport that (combined with heterogeneity) may give rise to episodic or intermittent flow behavior. With all the advances that have been made in improving our understanding of these processes through laboratory and field studies, numerical modeling of these complex processes in naturally heterogeneous subsurface formations still remains a major challenge.

The papers in this special issue of the *Vadose Zone Journal* present recent modeling advances that have been made to address some aspects of this challenge. The focus is on the TOUGH family of codes, a suite of general-purpose numerical simulators for multidimensional fluid and heat flows in porous and fractured media (Pruess et al., 1999; Pruess, 2004; Finsterle, 2004; http://esd.lbl.gov/TOUGH2). The articles that are selected for this issue are a subset of presentations given at the TOUGH Symposium 2006, which brought together developers and users of the TOUGH family of codes at the Lawrence Berkeley National Laboratory (LBNL) in Berkeley, California, for three days in May 2006 (http://esd.lbl.gov/TOUGHsymposium). The papers presented at this symposium covered a wide range of topics, including those associated with vadose zone hydrology, environmental engineering, hydrocarbon and gas hydrate recovery, carbon sequestration, nuclear waste isolation, mining engineering, and geothermal reservoir engineering. The papers reflected the continuing trend toward increased sophistication of the capabilities and applications of TOUGH family of codes. This special issue contains revised and expanded versions of eight selected papers from the TOUGH Symposium 2006, focusing on issues related to multiphase (including unsaturated) flow and transport in the subsurface.

Reliable prediction of subsurface flow and contaminant transport depends to a large degree on the accuracy with which the spatial distribution of process-relevant model parameters can be identified and quantified. Finsterle and Kowalsky (2007, this issue) present a stochastic approach where the high-resolution imaging capabilities of geophysical methods are combined with flow-process-specific information obtained from the inversion of hydrological data. The approach has been implemented into the iTOUGH2 inversion code and is demonstrated for the joint use of synthetic time-lapse ground-penetrating radar travel times and hydrological data collected during a simulated ponded infiltration experiment at a highly heterogeneous site.

Air sparging is a remediation technology developed to remove volatile organic contaminants from entrapment zones below the water table, using air injection. Most multiphase flow models ignore heterogeneity effects at a sub-gridblock scale on local mass transfer and assume local equilibrium between liquid and gas phases. VanAntwerp et al. (2007, this issue) use data from a two-dimensional laboratory-scale experiment and a field-scale air-sparging test to evaluate a newly developed dual-domain approach (used to handle effects of sub-grid heterogeneity). They find that the approach provides an improved fit of the model to the test data that was used.

The need to consider aqueous and sorption reaction kinetics and microbiological processes arises in many subsurface contamination problems. By incorporating these processes to the TOUGH family of codes, more complex problems involving multiphase fluid and heat flow, as well as geochemical interaction, can be addressed. Xu (2007, this issue) presents a formulation for incorporating kinetic rates among primary species into mass-balance equations, and proposes a general multi-region model for hydrological transport, coupled with microbiological and geochemical processes, to handle the effects of heterogeneity. This author shows that the relevant simulation results are consistent with data from a published column experiment of denitrification and sulfate reduction.

Spills of organic waste products and chemicals frequently occur at coastal sites where industrial plants are located. The migration of organic compounds spilled in the subsurface of coastal sites is influenced by sea water intrusion into aquifers discharging to the sea. Battistelli (2007, this issue) presents an improved version of TMVOC (which belongs to the TOUGH2 family of codes) to model the migration of multi-component organic mixtures under multiphase flow conditions. His TMVOC simulations demonstrate the effects of sea water intrusion on the distribution of contaminants within a coastal aquifer.

An understanding of the hydrologic interactions among atmosphere, land surface, and subsurface is key to understanding the water cycle that supports our life system on Earth. Pan et al. (2007, this issue) present a model that simulates the land-surface and subsurface hydrologic response to meteorological forcing by combining TOUGH2 and a state-of-the-art land-surface model to simulate such interactions. Preliminary simulation results show that the coupled model greatly improves the predictions of the water table elevation, evapotranspiration, surface temperature, and moisture at a real watershed.

Episodic or intermittent water flow has been observed under a number of scenarios in unsaturated flow systems. These non-uniform processes are significant, because relatively large volumes of water can move rapidly through the unsaturated system, carrying water and possibly contaminants to greater depths. Podgorney and Fairly (2007, this issue) examine the modeled behavior of water flow through a simplified system of a sand column underlain by a vertical capillary tube and compare the results with observed episodic-flow data from the literature. They find that simulation results using TOUGH2, based on a newly proposed constitutive relationship, can capture the observed flow behavior for the flow system under consideration.

Numerical dispersion is a common problem that is encountered when modeling contaminant transport in multiphase systems using coarse, multidimensional regular or irregular grids. Wu and Forsyth (2007, this issue) investigate several total-variation-diminishing schemes by testing them with T2R3D, one of the TOUGH family of codes. They present an application to demonstrate that these schemes are able to effectively reduce numerical dispersion.

Recharge into granitic bedrock under a melting snowpack is investigated as part of a study designed to understand hydrologic processes involving snow at Yosemite National Park in the Sierra Nevada Mountain of California. Field tests have been performed in the park, and a variety of data sets have been gathered. Flint et al. (2007, this issue) discuss the field tests and use TOUGH2 to interpret the field data and evaluate the potential for vertical flow into the fractured rock (which contributes to the groundwater recharge) and lateral flow at the bedrock/soil interface.

Numerical simulators are playing an increasingly important role in advancing our understanding of flow and transport processes in the subsurface. For many application problems, it is desirable to employ a single family of codes (such as the TOUGH family of codes) with capabilities to handle a range of physical, biochemical, and ecological processes and their interactions. It is our hope that this collection of articles will help the modeling community in exploring a variety of possible subsurface applications of the TOUGH family of codes. Finally, although it may be considered common sense, we would like to emphasize that simulation results from any numerical model (or simulator) are useful only when the model is carefully validated with data collected at appropriate scales, and only when the model is able to capture the key physical mechanisms for the flow and transport processes under consideration.

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We would like to dedicate this special issue of the *Vadose Zone Journal* to Dr. Gudmundur S. Bodvarsson (Bo), the Director of the Earth Sciences Division at LBNL. On November 29, 2006, Bo passed away unexpectedly at the age of 54. Bo had been a user and developer of the TOUGH family of codes and their precursors since his student days in the late 1970s. His strong support and involvement in research and development activities related to the TOUGH family of codes will be sorely missed.

References

Battistelli, A. 2007. Modeling multiphase organic spills in coastal sites with TMVOC V.2.0. Vadose Zone J. (this issue).

Finsterle, S. 2004. Multiphase inverse modeling: Review and iTOUGH2 applications. Vadose Zone J. 3:747–762.

Finsterle, S., and M. B. Kowalsky. 2007. Joint hydrological-geophysical inversion for soil structure identification. Vadose Zone J. (this issue).

Flint, A.L., L. E. Flint, and M. D. Dettinger. 2007. Modeling soil moisture processes and recharge under a melting snowpack. Vadose Zone J. (this issue).

Pruess, K., C. Oldenburg, and G. Moridis. 1999. TOUGH2 user's guide, Version 2.0. Rep. LBNL-43134, Lawrence Berkeley Natl. Lab., Berkeley, California.

Pruess, K. 2004. The TOUGH codes—a family of simulation tools for multiphase flow and transport processes in permeable media. Vadose Zone J. 3:738–746.

Pan, L., J. Jin, N. Miller, Y.S. Wu, and G. S. Bodvarsson. 2007. Modeling hydraulic responses to meteorological forcing: From canopy to aquifer. Vadose Zone J. (this issue).

Podgorney, R. K., and J. P. Fairley. 2007. Investigation of episodic flow from unsaturated porous media into a macropore. Vadose Zone J. (this issue).

VanAntwerp, D.J., R. W. Falta, and J. S. Gierke. 2007. Numerical simulation of field scale contaminant mass transfer during air sparging. Vadose Zone J. (this issue).

Wu, Y. S., and P. A. Forsyth. 2007. Efficient schemes for reducing numerical dispersion in modeling multiphase transport through heterogeneous geological media. Vadose Zone J. (this issue).

Xu, T. 2007. Incorporation of aqueous reaction kinetics and biodegradation into TOUGHREACT: Application of a multi-region model to hydrobiogeochemical transport of denitrification and sulfate reduction. Vadose Zone J. (this issue).