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**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.

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

92 The papers in this special issue of the *Vadose Zone Journal* present recent modeling
93 advances that have been made to address some aspects of this challenge. The focus is on
94 the TOUGH family of codes, a suite of general-purpose numerical simulators for
95 multidimensional fluid and heat flows in porous and fractured media (Pruess et al., 1999;
96 Pruess, 2004; Finsterle, 2004; <http://esd.lbl.gov/TOUGH2>). The articles that are selected
97 for this issue are a subset of presentations given at the TOUGH Symposium 2006, which
98 brought together developers and users of the TOUGH family of codes at the Lawrence
99 Berkeley National Laboratory (LBNL) in Berkeley, California, for three days in May
100 2006 (<http://esd.lbl.gov/TOUGHsymposium>). The papers presented at this symposium
101 covered a wide range of topics, including those associated with vadose zone hydrology,
102 environmental engineering, hydrocarbon and gas hydrate recovery, carbon sequestration,
103 nuclear waste isolation, mining engineering, and geothermal reservoir engineering. The
104 papers reflected the continuing trend toward increased sophistication of the capabilities
105 and applications of TOUGH family of codes. This special issue contains revised and
106 expanded versions of eight selected papers from the TOUGH Symposium 2006, focusing
107 on issues related to multiphase (including unsaturated) flow and transport in the
108 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.

201   ACKNOWLEDGEMENTS AND DEDICATION

202   We thank the authors for their interesting contributions, and the reviewers for their
203 thoughtful and constructive review comments.

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

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