Vadose Zone Journal
Special Section

Preface

# Research Advances in Vadose Zone Hydrology Through Simulations with the TOUGH Codes

Numerical simulators are playing an increasingly important role in advancing our fundamental understanding of hydrological systems. They are indispensable tools for managing groundwater resources, analyzing proposed and actual remediation activities at contaminated sites, optimizing recovery of oil, gas, and geothermal energy, evaluating subsurface structures and mining activities, designing monitoring systems, assessing the long-term impacts of chemical and nuclear waste disposal, and devising improved irrigation and drainage practices in agricultural areas, among many other applications. The complexity of subsurface hydrology in the vadose zone calls for sophisticated modeling codes capable of handling the strong nonlinearities involved, the interactions of coupled physical, chemical and biological processes, and the multiscale heterogeneities inherent in such systems.

The papers in this special section of *Vadose Zone Journal* are illustrative of the enormous potential of such numerical simulators as applied to the vadose zone. The papers describe recent developments and applications of one particular set of codes, the TOUGH family of codes, as applied to nonisothermal flow and transport in heterogeneous porous and fractured media (http://www-esd.lbl.gov/TOUGH2). The contributions were selected from presentations given at the TOUGH Symposium 2003, which brought together developers and users of the TOUGH codes at the Lawrence Berkeley National Laboratory (LBNL) in Berkeley, California, for three days of information exchange in May 2003 (http://www-esd.lbl.gov/TOUGHsymposium). The papers presented at the symposium covered a wide range of topics, including geothermal reservoir engineering, fracture flow and vadose zone hydrology, nuclear waste disposal, mining engineering, reactive chemical transport, environmental remediation, and gas transport. This Special Section of *Vadose Zone Journal* contains revised and expanded versions of selected papers from the symposium, with special attention to issues related to the vadose zone and unsaturated flow systems.

The first paper, written by the original developer of TOUGH, Karsten Pruess, provides an overview of the history of the TOUGH codes, the main physical processes considered, their mathematical and numerical implementation, and case studies. That paper is followed by a review article summarizing inverse modeling applications performed by iTOUGH2. A subsequent group of papers deals with diverse unsaturated zone systems, highlighting the versatility of the code to handle a variety of processes in different geologic settings. Simulation capabilities of the TOUGH codes are increasingly used for geologic carbon sequestration studies as testified by the next group of papers. The final series of papers demonstrates the use of the TOUGH codes in support of remediation and engineering applications. These studies discuss biological and reactive

chemical transport simulations, the design of clean-up operations and landfill management, and the analysis of engineered soil stabilization.

As guest editors, we thank the authors for their interesting contributions, and the many reviewers for their careful and constructive review comments. Finally, on behalf of all of the authors and ourselves, we express our sincerest appreciation to Rien van Genuchten for providing the opportunity to publish these papers together in a Special Section of *Vadose Zone Journal*.

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