CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

TRIP REPORT

SUBJECT: The TOUGH2 Symposium and Workshop

DATE/PLACE: May 12–17, 2003

AUTHOR: Lauren Browning and Randall Fedors

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Berkeley, CA

PERSONS PRESENT: L. Browning (CNWRA), Randall Fedors (CNWRA), and about 90 people at the Symposium and 20 at the Workshop.

BACKGROUND AND PURPOSE OF TRIP:

TOUGH is a family of thermal-hydrological-geochemical codes that the U.S. Department of Energy (DOE) plans to use in support a potential license application for a nuclear waste repository at Yucca Mountain, Nevada. TOUGH2 is the second, and most recent, version of the TOUGH family of codes. The TOUGH2 family of codes is currently being used by about 300 organizations in 33 countries to evaluate a wide range of natural resource and environmental problems.

TOUGH2 permits numerical analysis of nonisothermal flow of multicomponent, multiphase fluids in porous, fractured materials in up to three dimensions. Specific modeling applications are accommodated by selection and implementation of one or more modules within the TOUGH family of codes. The TOUGHREACT module, for example, works in concert with the TOUGH2 simulator to permit analysis of chemical reactions between solid phases, water and gases along flow pathways.TOUGH2 and the associated modules are written in standard FORTRAN77, and can be run on any platform.

The main goal of attending the TOUGH2 Symposium and Workshop was to learn more about the strengths and limitations of the TOUGH2 family of codes to facilitate more rigorous review of DOE flow and transport and reactive transport models that may be used in a potential license application for a nuclear waste repository at Yucca Mountain, Nevada. Sessions on Fracture Flow and Vadose Zone Hydrology, Nuclear Waste Isolation, Nuclear Waste, and Reactive Transport were highly relevant to NRC's evaluation of the proposed repository at Yucca Mountain, Nevada. L. Browning attended the Symposium and Workshop as a Professional Development activity, and R. Fedors attended in support of the Thermal Effects on Flow and Unsaturated and Saturated Flow Under Isothermal Conditions Key Technical Issues.

This report describes the fourth TOUGH Symposium and Workshop conducted at Lawrence Berkeley National Laboratory. Earlier TOUGH Symposia were conducted in 1990, 1995, and 1998. The TOUGH2 Symposium consisted of oral and poster presentations intended to encourage discussions on applications and recent code enhancements of the TOUGH codes. Following the TOUGH2 Symposium, a three day training course was conducted to provide hands-on experience using the TOUGH2 codes to address common hydrogeochemical problems. Additional information about the TOUGH2 codes and the associated Symposium and Workshop can be found at: http://esd.lbl.gov/TOUGHsymposium.

MEETING SUMMARY:

The TOUGH2 Symposium consisted of 10 oral sessions and a set of evening poster sessions. Most presentations highlighted successful TOUGH2 applications for diverse science and engineering problems. However, the Symposium also included a session on "Tricks of the Trade" that was designed to encourage discussion of problems encountered during model development and to offer some simple solutions to some recurrent problems. In addition, two poster session introduced new modules and code developments, including pre- and post-processing capabilities.

Two papers in the session on Fracture Flow and Vadose Hydrology dealt with fingering and rivulet flow in fractures. R. Podgorney (Idaho National Engineering and Environmental Laboratory) described a laboratory experiment where blocks of limestone were mounted in a sealed frame and a constant flux was applied at the top boundary. Three regimes were identified (i) fracture dominated flow, in which flow occurred as a continuous phase in the fracture; (ii) transitional flow, in which flow occurred in discrete, disconnected drops in the fracture; and (iii) matrix dominated flow. The transitional regime spanned several orders of magnitude of specific flux. It was noted that convergent pathways for rivulets or pulses occurred, but divergent pathways did not occur. The fracture dominated flow regime was successfully modeled using a discrete feature model (separate elements representing the fracture) and the matrix dominated flow regime was successfully modeled using an equivalent continuum approach. The transitional regime was not adequately described by either modeling approach, primarily because the dynamics of flow were not adequately represented by the Richards Equation for unsaturated flow. It was also suggested that fast pathways could develop at lower flux rates than previously believed.

In the same session, H.H. Liu (Lawrence Berkeley National Laboratory) proposed that subgrid representation of fracture flow has fractal properties. The distribution of secondary mineralization on fracture surfaces at Yucca Mountain was used to support the fractal behavior of flow patterns. The active-fracture model is currently used to simulate unsaturated flow at Yucca Mountain. The number of actively flowing fractures calculated using the active-fracture model matched the percentage of fractures with coatings. A closed-form relation was presented between fractal flow behavior and the active-fracture model in TOUGH2. Liu concluded that the connection between fractal behavior and the results from the active-fracture model provided support for the validity of the active-fracture model.

Two papers in the Nuclear Waste Isolation session discussed the effect of evaporation on matrix diversion around drifts and on water movement at a seepage face in drifts. Evaporation associated with ventilation during in situ liquid injection tests at Yucca Mountain was interpreted by NRC to have affected DOE estimates of seepage, particularly the seepage threshold (i.e., the concept that no seepage into drifts will occur for low percolation rates). R. Ahlers (formerly of Lawrence Berkeley National Laboratory) presented a method for simulating evaporation from a seepage face using the computationally efficient Richards Equation module in TOUGH2. An expression for effective permeability was modified to account for the diffusive flux of evaporation from specified grid cells at drift walls. The alternative, computationally expensive approach would be to explicitly simulate liquid, gas, and heat flow. T. Ghezzehei (Lawrence Berkeley National Laboratory) evaluated the effectiveness of lateral diversion around the drifts when evaporation is occurring at the drift wall face using the updated TOUGH module described by R. Ahlers (see above). Ghezzehei presented data obtained from the tunnels at Yucca Mountain on the evaporative boundary layer thickness (of the air adjacent to the tunnel wall) for ventilated (5-7 mm) and unventilated (20 mm) conditions assuming isothermal vapor diffusion. It was shown that seepage fluctuations in liquid injection tests were captured better when using the Richards Equation module of TOUGH that contained the evaporation model than with the previous analytical approaches applied directly to the seepage data. Utilization of the evaporation module in TOUGH also allows for heterogeneity to be incorporated into the modeling of the liquid injection tests.

In the Nuclear Waste session, Y. Tsang (for G. Bodvarsson, Lawrence Berkeley National Laboratory) presented a summary of numerical modeling successes and limitations for the Yucca Mountain Project. Her presentation covered ambient, thermohydrological, thermal-hydrological-chemical, and thermal-hydrological-mechanical models. During the discussion period following her presentation, the topic of grid resolution for simulating flow in fractured rocks was brought up by K. Pruess (Lawrence Berkeley National Laboratory) as a possible limitation of the models. For example, Pruess' work suggests that isothermal and nonisothermal seepage rates are underestimated by the grid resolution used in the Yucca Mountain Project.

In discussions with A. Flint (U.S. Geological Survey), it was determined that documentation of three large-scale field tests at Yucca Mountain is in preparation. The three are the Alcove 1 test, the Pagany Wash test during the El Nino winter of 1998, and the Ghost Dance Fault test. The authors were not aware of the last test, which assessed infiltration over faulted and nonfaulted areas. Documentation of the first two tests was requested in Agreement TSPAI.3.02, but was not fully satisfied by in the DOE report.

Several new modules and developments were presented at the Symposium. For example, J. Kim (Argonne National Laboratory) and S. Finsterle (Lawrence Berkeley National Laboratory) improved the efficiency of the ECO2 module of the TOUGH2 code by applying the automatic differentiation method. The method decreased calculation times for the Jacobian matrix, which is required to handle nonlinearities arising at each iteration. The ECO2 module is designed to accurately simulate CO_2 sequestration in aquifers. K. Pruess introduced a new module called TMVOC, which permits simulation of multiple volatile organic chemicals. Another module, EOSN, was designed by C. Shar (Lawrence Berkeley National Laboratory) and K. Pruess to simulate transport of noble gases in the subsurface. L. Pan (Lawrence Berkeley National Laboratory) developed an interactive grid generator for TOUGH2, and K. Ito (Lawrence Berkeley National Laboratory) and Yongkoo Seol (Lawrence Berkeley National Laboratory) developed a 3-dimensional discrete fracture network generator to examine fracture-matrix interaction using TOUGH2 models.

V. Javeri, of GRS in Germany, led an oral session devoted to gas transport. Several presentations focused on CO_2 sequestration in aquifers. K. Pruess (Lawrence Berkeley National Laboratory) presented numerical simulation of leakage from a geologic disposal reservoir for CO_2, with transitions between super- and sub-critical conditions. C. Doughty discussed simulations of supercritical CO_2 injection into heterogeneous porous media that she performed with K. Pruess. C. Oldenburg presented an analysis of innovative methods to enhance both gas recovery and natural gas storage.

Other recent applications of TOUGH2 family of codes that were highlighted in the Symposium sessions included: geothermal reservoir engineering, geothermal engineering, gas transport and vadose zone hydrology, environmental engineering, reactive transport, mining engineering, and environmental remediation.

A 3-day TOUGH2 training course was conducted immediately after the TOUGH2 Symposium. Although the underlying physics, numerical approach and mathematical implementations in

TOUGH2 were summarized, the course work focused mainly on learning to apply the TOUGH2 code and some of its most commonly used modules to solve science and engineering problems. The majority of the short course was spent analyzing and preparing input data files for the EOS1, EOS3, and T2VOC modules. Study problems included 2 component flow and transport in a 2 phase nonisothermal system.

CONCLUSIONS: The TOUGH2 Symposium and Workshop provided a very effective and time-efficient introduction to the TOUGH2 family of codes. Increased familiarity with the code is expected to improve the ability of CNWRA staff to provide rigorous technical analyses of DOE simulations used in support of a potential license application for Yucca Mountain, Nevada.

PROBLEMS ENCOUNTERED: None.

PENDING ACTIONS: None.

RECOMMENDATIONS: The TOUGH2 Symposium and Workshop is highly recommended to technical staff who regularly develop flow and transport/reactive transport simulations, or who will be reviewing DOE flow and transport/reactive transport simulations involving the geologic disposal of nuclear waste.

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