

# **CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES**

## **TRIP REPORT**

**SUBJECT:** Subsurface Multi-Phase Fluid Flow and Remediation Modeling  
(20.06002.01.011)

**DATE/PLACE:** September 19–21, 2003  
International Groundwater Modeling Center  
Colorado School of Mines  
Golden, Colorado

**AUTHORS:** Chandrika Manepally

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### **PERSONS PRESENT:**

Seven professional hydrogeologic modelers participated in this course, including staff from S.S. Papadopoulos and Associates, Intera Inc., and the Geological Survey of Finland. The instructor was Dr. John McCray, an Assistant Professor at the University of Texas at Austin and formerly a faculty member at the Colorado School of Mines. He has been practicing and teaching applied modeling in the academic and geohydrologic-consulting arena for 10 years.

### **BACKGROUND AND PURPOSE OF TRIP:**

TOUGH2 is a numerical simulator for nonisothermal flow of multi-component, multi-phase fluids in one-, two-, and three-dimensional porous and fractured media. The main objective of attending this course was to improve understanding of the TOUGH2/T2VOC code to strengthen reviews of DOE flow and transport models that may be used in a potential license application for a nuclear waste repository at Yucca Mountain, Nevada. TOUGH2 is used extensively in many DOE modeling activities related to the potential Yucca Mountain license application. This course was offered as one of the numerous short courses at the *MODFLOW and More 2003: Understanding through Modeling* conference.

### **SUMMARY OF PERTINENT POINTS:**

This course covered subsurface multi-phase fluid flow modeling concepts and techniques using TOUGH2/T2VOC. The principles and numerical analyses of multi-phase flow and transport processes, and the application of state-of-the-art numerical codes to site-specific subsurface flow and transport problems were presented.

### **SUMMARY OF ACTIVITIES:**

The course began with a detailed conceptual and mathematical description of multi-phase fluid flow and inter-phase partitioning of organic chemicals between phases. The capabilities and areas of application of TOUGH2/T2VOC were presented. The second session involved details regarding the preparation of the TOUGH2/T2VOC input files and understanding the output files. The input data is organized in blocks which are defined by keywords. The formatting details are provided in the user's manual. Hands-on computer sessions provided an opportunity to become familiar with the TOUGH2/T2VOC software packages. Input files were reviewed to learn the

various keywords and options available. The use of T2VOC capabilities to model a contaminant transport problem and issues like using appropriate boundary conditions, laboratory and field hydrologic data were also discussed. A new window-based GUI, PetraSim™, was used for data input and output visualization. PetraSim is a fully integrated interface with an interactive preprocessor and postprocessor. Users can construct and run a TOUGH2/T2VOC simulation and view the results entirely within PetraSim. Further information regarding this software can be obtained at this website: <http://www.thunderheadeng.com/petrasim/>

#### **CONCLUSIONS:**

This course provided an overview of the code structure and capabilities of the TOUGH2/T2VOC code. The DOE models using this code include the multi-scale thermohydrological model, the site-scale unsaturated zone ambient flow model, and the Drift-Scale Heater Test coupled thermohydrological-chemical model. These models, and others, are expected to be major components of the potential license application. Participation in this course enhanced staff's abilities to thoroughly review DOE approach and model results regarding flow in the unsaturated zone.

#### **PROBLEMS ENCOUNTERED:**

Participants encountered some problems as schedule change information was not provided in a timely manner.


#### **PENDING ACTIONS:**

Future plans include requesting an executable version of TOUGH2 and developing alternate conceptual models at CNWRA.

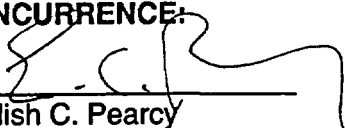
#### **RECOMMENDATIONS:**

Recommend attendance by CNWRA staff at future MODFLOW conference and short courses.


#### **SIGNATURES:**

  
Chandrika Manepally  
Geohydrology and Geochemistry

10/20/03  
Date

**CONCURRENCE:**  
  
English C. Percy  
Manager, Geohydrology and Geochemistry

10/22/03  
Date

  
Patrick C. Mackin  
Director of Administration

10/22/2003  
Date