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Authors
Finsterle, Stefan
Oldenburg, Curtis M.

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Technical Program and Abstracts of the
Second International

TOUGH SYMPOSIUM

May 15–17, 2006

Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, California, U.S.A.

EDITED BY
STEFAN FINSTERLE AND CURTIS M. OLDENBURG
Foreword

Welcome to the TOUGH Symposium 2006. Within this bound volume are the Symposium Program and Abstracts for approximately sixty papers to be presented in both oral and poster formats. The full papers are available as PDF files linked from the Symposium Program posted on the TOUGH Symposium 2006 website

http://esd.lbl.gov/TOUGHsymposium/program.html

Additional updated information including any changes to the Program will also be available at the website.

The papers cover a wide range of application areas and reflect the continuing trend toward increased sophistication of the TOUGH codes. A CD containing the proceedings papers will be published immediately following the Symposium and sent to all participants. As in the prior Symposium, selected papers will be invited for submission to a number of journals for inclusion in Special Issues focused on applications and developments of the TOUGH codes. These journals include, Geothermics, Energy Conversion and Management, Journal of Nuclear Science and Technology, and the Vadose Zone Journal.

The Organizing Committee wishes to thank in advance the session chairs, presenters, panel speakers, and participants for their ongoing interest in the TOUGH codes. The support from various agencies and offices in the U.S. and around the world for the development and application of the TOUGH codes is greatly appreciated. We also are grateful to Thunderhead Engineering, INTERA, and Industrial Research Limited for financial support of the Poster Session and Symposium Banquet.

Stefan Finsterle
Curtis M. Oldenburg

Berkeley, May 5, 2006
TOUGH SYMPOSIUM 2006

Technical Program
Lawrence Berkeley National Laboratory
Berkeley, California
Building 50 Auditorium
May 15–17, 2006

Agenda Outline

MONDAY, MAY 15, 2006

7:30 am  Registration
8:30 am  Oral Session: Environmental Engineering
10:15 am  Coffee Break
10:45 am  Oral Session: Environmental Engineering (cont.)
12:00 noon  Lunch
1:30 pm  Oral Session: Geothermal Reservoir Engineering
3:10 pm  Oral Session: Geotechnical Engineering
5:30 pm  Poster Session and Reception, LBNL Cafeteria

TUESDAY, MAY 16, 2006

8:30 am  Oral Session: Carbon Dioxide Storage
9:45 am  Coffee Break
10:15 am  Oral Session: Carbon Dioxide Storage (cont.)
11:30 am  Lunch
1:00 pm  Oral Session: Vadose Zone Hydrology
2:40 pm  Coffee Break
3:10 pm  Oral Session: Reactive Geochemistry
6:30 pm  Banquet, International House

WEDNESDAY, MAY 17, 2006

8:30 am  Oral Session: Nuclear Waste
10:10 am  Coffee Break
10:40 am  Oral Session: Gas Hydrates
11:30 am  Lunch
1:00 pm  Tricks-of-the-Trade
2:30 pm  Coffee Break
3:00 pm  Panel Discussion
4:30 pm  Adjourn
**Monday, May 15, 2006, Morning Sessions**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Speaker/Institution</th>
</tr>
</thead>
<tbody>
<tr>
<td>7:30</td>
<td>Registration, Building 50 Auditorium Foyer</td>
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<tr>
<td>8:30 am</td>
<td>Welcome</td>
<td>Bo Bodvarsson, Director, Earth Sciences Division, LBNL</td>
</tr>
<tr>
<td>8:35 am</td>
<td>Opening Remarks</td>
<td>Karsten Pruess</td>
</tr>
<tr>
<td>8:45 am</td>
<td>Announcements</td>
<td>Organizing Committee</td>
</tr>
<tr>
<td>9:00 am</td>
<td><strong>Modeling Organic Spills in Coastal Sites with TMVOC V.2.0</strong></td>
<td>Alfredo Battistelli (Snamprogetti SpA, Fano, Italy)</td>
</tr>
<tr>
<td>9:25 am</td>
<td><strong>Multiphase Modeling and Inversion Methods for Controlling Landfill Bioreactor</strong></td>
<td>Terhi Kling, Juhani Korkealaakso (Technical Research Centre of Finland, VTT, Finland)</td>
</tr>
<tr>
<td>9:50 am</td>
<td><strong>Radionuclide Transport through a Low-Permeability Natural Gas Reservoir</strong></td>
<td>Clay Cooper, Ming Ye, Jenny Chapman (Desert Research Institute)</td>
</tr>
<tr>
<td>10:15 am</td>
<td><em>Coffee Break</em></td>
<td></td>
</tr>
<tr>
<td>10:45 am</td>
<td><strong>Modeling Kinetic Interphase Mass Transfer During Field Scale Air Sparging Operations with a Dual Domain Approach</strong></td>
<td>Darby VanAntwerp, Ron Falta (Clemson University, Clemson, SC)</td>
</tr>
<tr>
<td>11:10 am</td>
<td><strong>Modeling NAPL Source Zone Formation in Stochastically Heterogeneous Layered Media - a Comparison with Experimental Results</strong></td>
<td>Fritjof Fagerlund, Auli Niemi (Uppsala University, Sweden), Tissa Illangasekare (Colorado School of Mines, Golden, CO)</td>
</tr>
<tr>
<td>11:35 am</td>
<td><strong>TOUGH+GasH2O Study of the Effects of a Heat Source Buried in the Martian Permafrost</strong></td>
<td>George Moridis, Karsten Pruess (LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>12:00 noon</td>
<td><em>Lunch, LBNL Cafeteria</em></td>
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</tbody>
</table>
## Monday, May 15, 2006, Afternoon Sessions

### Geothermal Reservoir Engineering

**Session Chair: Mario César Suárez Arriaga**

<table>
<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Presenters</th>
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</thead>
<tbody>
<tr>
<td>1:30 pm</td>
<td>Reservoir Model of the Hengill Volcano, Iceland, Becomes Central Issue in Environmental Impact Studies and Licensing</td>
<td>Grimur Björnsson, Einar Gunnlaugsson (Reykjavik Energy, Iceland), Arnar Hjartarson (Iceland Geosurvey, Iceland)</td>
</tr>
<tr>
<td>1:55 pm</td>
<td>Evaluation of C-14 as a Natural Tracer for Injected Fluids at the Aidlin Sector of the Geysers Geothermal System through Modeling of Mineral-Water-Gas Reactions</td>
<td>Patrick Dobson, Eric Sonnenthal, Jennifer Lewicki, Mack Kennedy (LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>2:20 pm</td>
<td>Shear Slip Analysis in Multi-Phase Fluid Flow Reservoir Engineering Applications Using TOUGH-FLAC</td>
<td>Jonny Rutqvist (LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>2:45 pm</td>
<td>Modeling of Gas Composition and Gravity Signals at the Phlegrean Fields Caldera</td>
<td>Micol Todesco, Giovanni Chiodini, Giovanna Berrino (Istituto Nazionale di Geofisica e Vulcanologia, Italy)</td>
</tr>
<tr>
<td>3:10 pm</td>
<td>Coffee Break</td>
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</table>

### Geotechnical Engineering

**Session Chair: Julio Garcia**

<table>
<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Presenters</th>
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</thead>
<tbody>
<tr>
<td>3:40 pm</td>
<td>Flooding of an Abandoned Salt Mine – Modeling Two-Phase Flow in Complex Mine Structures</td>
<td>Joachim Poppei, Gerhard Mayer, Nicolas Hubscherlen, Georg Resele (Colenco Power Engineering Ltd., Baden, Switzerland)</td>
</tr>
<tr>
<td>4:05 pm</td>
<td>ASCATA - A TOUGH2 Based Program for Automated Simulation of Compressed Air Tunnel Advance</td>
<td>Gerhard Steger, Stephan Semprich (TU Graz, Austria)</td>
</tr>
<tr>
<td>4:30 pm</td>
<td>Enhanced Seepage and its Effect on Slope Stability under Torrential Precipitate during Flood Discharge Event on a Large Hydroelectric Station</td>
<td>Mo Xu¹, Guoping Lu², Ying Ma¹, Xiaobing Kank (¹ Chengdu University, Chengdu, China; ² LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>4:55 pm</td>
<td>The Lihir Open Pit Gold Mine Revisited</td>
<td>Stephen White, John Burnell (Industrial Research Ltd, Lower Hutt, New Zealand), Markos Melaku, Roy Johnstone (Lihir Management Company Ltd, Port Moresby, Papua New Guinea)</td>
</tr>
</tbody>
</table>
### Carbon Dioxide Storage and Gas Hydrates

<table>
<thead>
<tr>
<th>Session</th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>P1</td>
<td>System-Level Modeling for Geological CO₂ Storage</td>
<td>Yingqi Zhang, Curt Oldenburg, Stefan Finsterle, Bo Bodvarsson (LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>P2</td>
<td>Sequestration of CO₂ in the Altmark Natural Gas Field, Germany: Mobility Control to Extend Enhanced Gas Recovery</td>
<td>Dorothee Rebscher¹, F. May², Curtis Oldenburg¹ (¹ LBNL, Berkeley, CA; ² Bundesanstalt für Geowissenschaften und Rohstoffe (BGR), Hannover, Germany)</td>
</tr>
<tr>
<td>P3</td>
<td>Comparison of Kinetic and Equilibrium Reaction Models in Simulating the Behavior of Gas Hydrates in Porous Media</td>
<td>Michael Kowalsky, George Moridis (LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>P4</td>
<td>Depressurization-Induced Gas Production from Class 1 and 2 Hydrate Deposits</td>
<td>George Moridis, Michael Kowalsky (LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>P5</td>
<td>Relative Permeability Estimates for Methane Hydrate-Bearing Sand</td>
<td>Yongkoo Seol, Timothy Kneafsey, Liviu Tomutsa, George Moridis (LBNL, Berkeley, CA)</td>
</tr>
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</table>

### Computation Methods, Pre- and Post-Processing

<table>
<thead>
<tr>
<th>Session</th>
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<th>Authors</th>
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</thead>
<tbody>
<tr>
<td>P6</td>
<td>Efficient Scheme for Reducing Numerical Dispersion in Modeling Multiphase Chemical Transport in Porous and Fractured Media</td>
<td>Yu-Shu Wu (LBNL, Berkeley, CA), Peter Forsyth (University of Waterloo, Ontario, Canada)</td>
</tr>
<tr>
<td>P7</td>
<td>Enhancing Scalability and Efficiency of TOUGH_MP for Linux Clusters</td>
<td>Keni Zhang, Yu-Shu Wu (LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>P8</td>
<td>Using PetraSim to Create, Execute, and Post-Process TOUGH2 Models</td>
<td>Alison Alcott (RockWare Inc., Golden CO), Daniel Swenson, Brian Hardeman (Thunderhead Engineering, Manhattan, KS)</td>
</tr>
<tr>
<td>P9</td>
<td>Some Topological Aspects of (Un)Structured Generation of Meshes: A Possible Enhancement of Meshmaker in TOUGH</td>
<td>Juan Carlos Díaz Patiño, Ricardo Pacheco, Mario César Suárez Arriaga (Michoacán University, México)</td>
</tr>
<tr>
<td>P11</td>
<td>IGGI, A Computing Framework for Large Scale Parametric Simulations: Application to Uncertainty Analysis with TOUGHREACT</td>
<td>Fabrice Dupros, F. Boulahy, J. Vairon (BRGM, Orléans, France), P. Lombard (ICATIS, Meylan, France), N. Capit, J-F. Méhaut (Laboratoire ID-IMAG, Montbonnot Saint Martin, France)</td>
</tr>
<tr>
<td>P12</td>
<td>GeoCad2—A Pre- and Post-Processor for TOUGH2</td>
<td>Stephen White (IRL, New Zealand)</td>
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### Reactive Geochemistry and Environmental Engineering

<table>
<thead>
<tr>
<th>Session</th>
<th>Title</th>
<th>Authors</th>
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</thead>
<tbody>
<tr>
<td>P13</td>
<td>Simulation of Salt Water Intrusion</td>
<td>Kenzi Karasaki (LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>P14</td>
<td>The Relative Importance of Variable Water Infiltration Rate and Geological Heterogeneity for Three-Phase TCE Transport in a Porous Medium</td>
<td>Hanna Zandin, Auli Niemi (Uppsala University, Uppsala, Sweden)</td>
</tr>
<tr>
<td>P15</td>
<td>Implementation of the Pitzer Activity Model into TOUGHREACT for Modeling Concentrated Solutions</td>
<td>Guoxiang Zhang, Nic Spycher, Eric Sonnenthal, Carl Steefel (LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>P16</td>
<td>Modeling of the Laboratory Experiments Interaction of the Hot NaNO₃-NaOH Brine with Sandstone Rocks from Deep Radionuclide Repository Site, Using TOUGHREACT</td>
<td>Alexey Kiryukhin (Institute of Volcanology and Seismology, Kamchatksky, Russia), E. P. Kaymin, E. V. Zakharova (Institute of Physical Chemistry, Moscow, Russia), A. A. Graphchikov (Institute of Mieralogy, Chernogolovka, Russia), A. A. Zubkov (Siberia Chemical Plant, Severesk, Russia)</td>
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<tr>
<td>Paper</td>
<td>Title</td>
<td>Authors</td>
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<tr>
<td>P17</td>
<td>Simulation of the Effects of Hydrophilic Polymer Adsorption on Two-Phase Flow of Oil-Water Mixtures</td>
<td>Michele Carpita, Marica Marcolini, Alfredo Battistelli (Snamprogetti SpA, Fano, Italy)</td>
</tr>
<tr>
<td>P18</td>
<td>Modeling the Pauzhetsky Geothermal Field, Kamchatka, Russia, Using iTOUGH2</td>
<td>A. V. Kiryukhin¹, N. P. Asaulova², S. Finsterle³, T. V. Rychkova¹, N. Obora¹ (¹ Institute of Volcanology and Seismology, Kamchatksy, Russia; ² Kamchatskburgoteomgia Enterprise, Kamchatka, Russia; ³ LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>P19</td>
<td>TOUGH and the Boundary Element Method in the Estimation of the Natural State of Geothermal Submarine Systems</td>
<td>Mario César Suárez Arriaga (Michoacán University, México), Fernando Samaniego (National University of México, México)</td>
</tr>
<tr>
<td>P20</td>
<td>Modeling of Helium and Heat Transport in an Extensional Basin Using the Noble Gas Module EOSN in TOUGH2</td>
<td>Judy Andrews, Martin Saar (University of Minnesota–Twin Cities, Minneapolis, MN)</td>
</tr>
<tr>
<td>P21</td>
<td>Three Dimensional Analyses of Coupled Gas, Heat and Nuclide Transport in a Repository Including Rock Salt Convergence</td>
<td>Vijen Javeri (Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, Köln, Germany)</td>
</tr>
<tr>
<td>P22</td>
<td>Design and Analysis of a Gas Threshold Pressure Test in a Low-Permeability Clay at ANDRA’s Underground Research Laboratory, Bure (France)</td>
<td>Rainer Senger (INTERA Inc., Austin, TX), Cristian Enachescu (Golder Associates GmbH, Celle, Germany), Thomas Doe (Golder Associates Inc., Redmond, WA), Marc Distinguin, Jacques Delay (Andra, France)</td>
</tr>
<tr>
<td>P23</td>
<td>A Coupled Model for Natural Convection in Heated Subsurface Enclosures Embedded in Fractured Rock: TOUGH2 Enhancements and Simulation Examples</td>
<td>Nicholaus Halecky¹,², Jens Birkholzer¹, Steve Webb³, P. F. Peterson¹, Bo Bodvarsson¹ (¹ LBNL, Berkeley, CA; ² Sandia National Laboratories, Albuquerque, NM; ³ University of California, Berkeley, CA)</td>
</tr>
<tr>
<td>P24</td>
<td>Modifying TOUGH2 to Support Modeling of Gas Transport through Saturated Compacted Bentonite as Part of the Large-Scale Gas Injection Test (LASGIT) in Sweden</td>
<td>Nicola Calder, John Avis, Rainer Senger (INTERA Engineering Ltd., Ottawa, Canada), Helen Leung (Ontario Power Generation, Toronto, Canada)</td>
</tr>
<tr>
<td>P25</td>
<td>Coupling TOUGH2 with CLM3: Developing a Coupled Land Surface and Subsurface Model</td>
<td>Lehua Pan, Jiming Jin, Norm Miller, Yu-Shu Wu, Bo Bodvarsson (LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>P26</td>
<td>Validation of the Active Fracture Model for Unsaturated Flow in Heterogeneous Fractured Rock Using Numerical Experiments</td>
<td>Quanlin Zhou (ETIC Engineering Inc., Oakland, CA)</td>
</tr>
<tr>
<td>P27</td>
<td>Numerical Simulation and Parameter Estimation Using Borehole Flowmeter Logging in Low Permeability Rocks</td>
<td>Kazumasa Ito, Naoto Takeno, Yoji Seki, Kazuki Naito, and Yoshio Watanabe (AIST, Japan)</td>
</tr>
<tr>
<td>P28</td>
<td>Modeling of Physical Observations of Water Diversion in a Capillary Barrier Using a Centrifuge</td>
<td>Hideo Nakajima (Research Center for Deep Geological Environments, Tsukuba, Japan), Julio Garcia (ETIC Engineering, Oakland Inc., CA), Robert Podgornoy (INL, Idaho Falls, ID)</td>
</tr>
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</table>
**Tuesday, May 16, 2006, Morning Sessions**  

**Carbon Dioxide Storage**

*Session Chair: Stephen White*

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Presenter(s)</th>
</tr>
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<tbody>
<tr>
<td>8:30 am</td>
<td>ECO2N - A New TOUGH2 Fluid Property Module for Studies of CO₂ Storage in Saline Aquifers</td>
<td>Karsten Pruess, Nicolas Spycher (LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>8:55 am</td>
<td>Numerical Modeling of CO₂ Injection Test at Nagaoka Test Site in Nigata, Japan</td>
<td>Tatsuya Sato (GERD, Japan), Young Hong, Stephen White (IRL, New Zealand), Ziqiu Xue (RITE)</td>
</tr>
<tr>
<td>9:20 am</td>
<td>Joule-Thomson Cooling Due to Injection of CO₂ into Depleted Gas Reservoirs</td>
<td>Curtis Oldenburg (LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>9:45 am</td>
<td>Coffee Break</td>
<td></td>
</tr>
<tr>
<td>10:15 am</td>
<td>Modeling Geologic Storage of Carbon Dioxide: Comparison of Non-Hysteretic and Hysteretic Characteristic Curves</td>
<td>Christine Doughty (LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>10:40 am</td>
<td>Modeling CO₂ Injection with Halite Precipitation Using an Extended Verma &amp; Pruess Porosity-Permeability Model</td>
<td>Michele Carpita, Thomas Gioris, Alfredo Battistelli (Snamprogetti SpA, Italy)</td>
</tr>
<tr>
<td>11:05 am</td>
<td>A Long-Term 2D Vertical Modeling of the CO₂ Storage at Sleipner (North Sea) Using TOUGHREACT</td>
<td>Pascal Audigane, I. Gaus (BRGM, Orléans, France), Karsten Pruess, Tianfu Xu, (LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>11:30 am</td>
<td>Lunch, LBNL Cafeteria</td>
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</table>
**Tuesday, May 16, 2006, Afternoon Sessions**

### Vadose Zone Hydrology

*Session Chair: Lorraine Flint*

<table>
<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Presenters</th>
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</thead>
<tbody>
<tr>
<td>1:00 pm</td>
<td>Investigation of Episodic Flow Events between Unsaturated Porous Media and Macropore Domains Using TOUGH2</td>
<td>Robert Podgornay (INL, Idaho Falls, ID), Jerry Fairley (University of Idaho, Moscow, ID)</td>
</tr>
<tr>
<td>1:25 pm</td>
<td>Investigating Nonlinear Rainfall-Runoff Response from a Trenched Hillslope Using TOUGH2 3-D Simulations</td>
<td>April James, Jeffrey McDonnell (Oregon State University, Corvallis, OR)</td>
</tr>
<tr>
<td>1:50 pm</td>
<td>Modeling Soil Moisture Processes and Recharge under a Melting Snowpack</td>
<td>Alan Flint, Lorraine Flint (USGS, Sacramento, CA)</td>
</tr>
<tr>
<td>2:15 pm</td>
<td>Joint Hydrological-Geophysical Inversion for Soil Structure Identification</td>
<td>Stefan Finsterle, Michael Kowalsky (LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>2:40 pm</td>
<td><strong>Coffee Break</strong></td>
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### Reactive Geochemistry

*Session Chair: Nicolas Spycher*

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<tr>
<th>Time</th>
<th>Title</th>
<th>Presenters</th>
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</thead>
<tbody>
<tr>
<td>3:10 pm</td>
<td>Incorporation of Aqueous Reaction and Sorption Kinetics and Biodegradation into TOUGHREACT</td>
<td>Tianfu Xu (LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>3:35 pm</td>
<td>TOUGHREACT/ECO2 on Reactive Transport Modeling of CO₂ in a Geological Repository</td>
<td>Hakan Alkan, W. Müller, G. Bracke (Institute of Safety Technology, Germany)</td>
</tr>
<tr>
<td>4:00 pm</td>
<td>Solubility Enhanced Retardation of Neptunium in the Unsaturated Zone at Yucca Mountain, Nevada</td>
<td>Guoping Lu, Tianfu Xu (LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>4:25 pm</td>
<td>Uncertainty in the Reactive Transport Model Response to an Alkaline Perturbation in a Clay Formation</td>
<td>André Burnol¹, P. Blanc¹, Tianfu Xu², Nicolas Spycher², E. C. Gaucher¹ (¹ BRGM, Orléans, France; ² LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>6:30 pm</td>
<td><strong>Banquet, International House</strong></td>
<td></td>
</tr>
<tr>
<td>7:30 pm</td>
<td>Why do Volcanoes (Only Sometimes) Erupt Explosively?</td>
<td>Michael Manga (University of California, Berkeley, CA)</td>
</tr>
<tr>
<td>8:30 pm</td>
<td>Bus leaving for Hotels Durant and Shattuck</td>
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## Wednesday, May 17, 2006, Morning Sessions

### Nuclear Waste

*Session Chair: Bo Bodvarsson*

<table>
<thead>
<tr>
<th>Time</th>
<th>Topic</th>
<th>Speakers</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:30 am</td>
<td>TOUGH2/iTOUGH2 Analysis of the Gas Migration Test (GMT) at the Grimsel Test Site (Switzerland)</td>
<td>Rainer Senger, (INTERA Inc., Austin, TX), Bill Lanyon Fracture Systems Ltd, Cornwall, UK, Paul Marschall, Stratis Vomvoris (NAGRA, Wettingen, Switzerland), Ai Fujiwara (RWMC, Tokyo, Japan)</td>
</tr>
<tr>
<td>8:55 am</td>
<td>Simulations of the Hydrogen Migration out of Intermediate Level Radioactive Waste Emplacement Drifts Using TOUGH2</td>
<td>Jean Talandier (Andra, Châtenay-Malabry, France), Gerhard Mayer, Jean Croisé (Colenco Power Engineering AG, Baden, Switzerland)</td>
</tr>
<tr>
<td>9:20 am</td>
<td>Three Dimensional Analyses of Combined Gas and Nuclide Transport in a Repository Considering Coupled Hydro-Geomechanical Processes</td>
<td>Vjen Javeri (Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, Köln, Germany)</td>
</tr>
<tr>
<td>9:45 am</td>
<td>Joint Inversion of Ground-Penetrating Radar and Thermal-Hydrological Data Collected During a Large-Scale Heater Test</td>
<td>Michael Kowalsky, Jens Birkholzer, Stefan Finsterle, John Peterson, Sumit Mukhopadhyay, Yvonne Tsang (LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>10:10 am</td>
<td><strong>Coffee Break</strong></td>
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</table>

### Gas Hydrates

*Session Chair: George Moridis*

<table>
<thead>
<tr>
<th>Time</th>
<th>Topic</th>
<th>Speakers</th>
</tr>
</thead>
<tbody>
<tr>
<td>10:40 am</td>
<td>Numerical Simulation of Gas Hydrate Dissociation in a Large Heterogeneous Porous Sample</td>
<td>Arvind Gupta¹, Timothy Kneafsey², George Moridis⁵, Yongkoo Seol⁷, Michael Kowalsky⁷, E. D. Sloan¹ ('Colorado School of Mines, Golden, CO'; ² LBNL, Berkeley, CA)</td>
</tr>
<tr>
<td>11:05 am</td>
<td>Gas Production by Depressurization from Hypothetical Class 1G and Class 1W Hydrate Reservoirs</td>
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ENVIRONMENTAL ENGINEERING
MODELLING ORGANIC SPILLS IN COASTAL SITES WITH TMVOC V.2.0

Alfredo Battistelli

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ABSTRACT
Contaminant spills are frequently encountered in coastal sites where many industrial plants are located. Among them, refineries are and petrochemical plants are often built close to the sea for easy transport of crude oil and final by-products. The migration of organic compounds spilled in the subsurface of coastal sites can be influenced by the effects of sea water intrusion in the aquifers discharging to the sea.

An improved version of TMVOC numerical simulator can model the migration of multi-component organic mixtures under multiphase conditions accounting for the effects of sodium chloride dissolved in the aqueous phase on thermophysical properties of groundwater, following the basic approach used for saline brines in the EWASG module. An overview of the thermodynamic formulation is presented, together with main hypotheses and assumptions.

Then, simulations of a multi-component organic spill using a 2D vertical numerical model are presented to show main code capabilities and to highlight the effects of sea water intrusion on the distribution of contaminants within the aquifer. The effects of the construction of an impervious wall on the NAPL plume migration is also investigated.
MULTIPHASE MODELING AND INVERSION METHODS
FOR CONTROLLING A LANDFILL BIOREACTOR

Terhi Kling and Juhani Korkealaakso

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ABSTRACT
In this study multiphase modeling and inversion methods implemented with the TOUGH2 and iTOUGH2
models are applied for controlling a landfill bioreactor. During a two year (2003-2004) leachate
recirculation experiment at Ämmässuo, Finland, data were collected and a modeling approach developed
for predicting the effects of leachate recirculation. During the construction of the full-scale bioreactor,
modeling will support the planning of the monitoring system. An initial simulation model has been
created for the whole landfill area. The model will be updated with all the new data from the area, and the
approach will be further developed in order to be able to control the final bioreactor after the closing of
the landfill in 2007.
TRITIUM TRANSPORT THROUGH A LOW-PERMEABILITY NATURAL GAS RESERVOIR

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ABSTRACT

The U.S. Department of Energy and its predecessor agencies conducted a program in the 1960s and 1970s to evaluate technology for the nuclear stimulation of low-permeability gas reservoirs. Two of the sites were located in the Piceance Basin of Colorado, and the devices were detonated in low-permeability Cretaceous sandstones and shales. At each of the sites, transport of long-lived gas-phase radionuclides is of greatest concern—these are primarily $^3$H, $^{14}$C, and $^{85}$Kr. Using TOUGH2 and EOS7r, we conducted simulations to explore the controls and evaluate the length and time scales of $^3$H transport toward a nearby hypothetical producing gas well. The simulations were conducted such that diffusive transport occurred for a 35-year period starting from the nuclear detonation and prior to the start of production. The permeability in the vicinity of the hypothetical production well was then changed to account for hydraulic (production) fractures, and the simulator was restarted to evaluate 30 years of gas production from the well. Depending upon the location and magnitude of production, tritium transport could be controlled by both diffusion and advection caused by gas production. After gas production ceased, the remnant pressure field controlled gas migration for a time equal to the amount of time that gas production occurred (i.e., an additional 30 yr). We found that in locations where diffusion was dominant, the mass fraction field of tritium was highly dependent upon the chosen tortuosity model.
MODELING KINETIC INTERPHASE MASS TRANSFER DURING FIELD SCALE AIR SPARGING OPERATIONS WITH A DUAL DOMAIN APPROACH

Darby VanAntwerp and Ronald W. Falta

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ABSTRACT

Previous numerical simulations of air sparging using T2VOC and similar codes have demonstrated that the basic injected gas flow patterns that occur below the water table during air sparging can be simulated. These earlier simulations, however did not attempt to model rates of contaminant removal during air sparging. Various laboratory and field test data suggest that air sparging contaminant removal tends to be a non-equilibrium process at local scales. This means that the local equilibrium assumption used in each normal gridblock of a T2VOC or TMVOC simulation will result in an overprediction of the rate of contaminant removal. A simple way to include this local kinetic mass transfer is to use a dual domain formulation, where the bulk characteristics of the porous media are preserved, but where gas is allowed to flow preferentially through part of the domain. In this type of model, the local mass transfer rate is determined by the rate of diffusion from higher water content locations into the locations with flowing gas. Simulations of an air sparging field experiment using TMVOC show that the apparent mass transfer coefficient is scale-dependent, decreasing with increasing scale. In particular, sparging mass transfer coefficients measured at the laboratory scale are about 100 times larger than those calibrated to the field data.
MODELLING NAPL SOURCE ZONE FORMATION IN STOCHASTICALLY HETEROGENEOUS LAYERED MEDIA— A COMPARISON WITH EXPERIMENTAL RESULTS

Fritjof Fagerlund 1,2, Auli Niemi 1, Tissa Illangasekare 2

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ABSTRACT
Understanding and characterisation of subsurface occurrences of DNAPLs are important for the assessment of mass transfer from entrapped sources. Subsurface NAPL migration and the formation of immobile source zones of groundwater contamination were studied using soil flume experiments. The saturated medium is a two-layered mildly dipping system with known, stochastically generated, heterogeneity. Spatial NAPL distributions were monitored continuously using multiple energy x-ray attenuation techniques, which allows precise measurements of fluid saturations. Digital images were also taken.

Experimental results are compared to preliminary modelling results using two constitutive models: BCB by Brooks and Corey (1964) and Burdine (1953) and VGM by van Genuchten (1980) and Mualem (1976), both including a simple model of NAPL entrapment. Results indicate that the final immobile NAPL distribution is largely governed by capillary barriers during, infiltration, displacement and immobilisation of the NAPL. The description capillary pressure – fluid saturation relations is therefore a key factor in the modelling of NAPL source zone formation.

Both constitutive models reproduced the main features of the NAPL migration but overestimated immobile NAPL saturations in coarse sands enclosed by capillary barriers as well as the speed of migration. A hysteretic constitutive model is deemed likely to improve model results.
TOUGH+GASH₂O STUDY OF THE EFFECTS OF A HEAT SOURCE BURIED IN THE MARTIAN PERMAFROST

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Earth Sciences Division
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ABSTRACT
We use TOUGH+AirH₂O to study the effects of a heat source buried in the Martian permafrost to evaluate the possibility of establishing a wet zone of liquid water, in which terrestrial microorganisms could survive and multiply. Analysis of the problem indicates that (1) only a limited permafrost volume (not exceeding 0.35 m in radius) is affected, (2) a “wet” zone with limited amounts of liquid water develops (not exceeding 8 and 0.7 kg for a 250 W and a 62.5 W source, respectively), (3) the wet zone persists for a long time, becomes practically stationary after \( t = 20 \) sols because of venting into the Martian atmosphere, and its thickness is limited and decreases slowly over time, (4) a “dry” zone (where \( S_g > 90\% \)) evolves, continues to expand (albeit slowly) with time, but its extent remains limited, and (5) the ice front surrounding the wet zone is self-sharpening. For a range of initial conditions investigated, evolution of the liquid water mass occurs at approximately the same rate, reaches roughly the same maximum, and occurs at about the same time (10 to 20 sols; 1 sol = 24.39 hours).
Session 2
GEOTHERMAL RESERVOIR ENGINEERING
APPLYING RESERVOIR MODEL OF THE HENGILL VOLCANO IN POWER PLANT DECISION MAKING AND ENVIRONMENTAL IMPACT STUDIES

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ABSTRACT

Environmental impact studies are currently an integral part for development and harnessing of high-temperature geothermal resources in Iceland. State and municipal licensing authorities are increasingly concerned with subjects like sustainable development and renewable production. Consequently they find numerical reservoir models, which forecast only 20 to 30 years of generation, insufficient for the environmental licensing process. An existing, large-scale 3-D reservoir model of the Hengill volcano has therefore been applied to address these critical issues.

In the model study we consider 360 MWe and 700 MWt generations in two sub-areas of Hengill. Due to limited production history, reservoir performance under full load is predicted for maximum 30 years. At that future point in time, all generation is stopped and recovery histories of fluid and heat reserves computed. We observe that model pressures recover back to natural state levels in similar time as generation has been ongoing, 30-60 years. This behavior is related to open boundaries of the reservoir model, confirmed by 20 years of generation in Nesjavellir. The heat reserve, on the other hand, requires up to 1000 years for recovery. We conclude that large geothermal power plants in Hengill produce at rates exceeding natural recharge. In order to make the generation renewable, either resting periods are required or that production is later reduced to boundary recharge rates. These power plants should, nevertheless, qualify as sustainable development due to technical and scientific advancements that accompany intense field activities. To achieve this goal of sustainable development we find critical that all relevant field data and scientific publications, gathered during project life, are documented and made open to the public.
EVALUATION OF C-14 AS A NATURAL TRACER FOR INJECTED FLUIDS AT THE AIDLIN SECTOR OF THE GEYSERS GEOTHERMAL SYSTEM THROUGH MODELING OF MINERAL-WATER-GAS REACTIONS

Patrick Dobson, Eric Sonnenthal, Jennifer Lewicki, and Mack Kennedy

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ABSTRACT

The use of reactive isotopic tracers coupled to the reactions between water, gases, and minerals within a full thermal-hydrological reservoir simulation allows for an improved method of investigating flow and heat transfer in geothermal systems. A combined field and modeling study has been initiated to evaluate the effects of fluid injection on in-situ and produced gas compositions and isotopic ratios as they are related to heat and mass transfer between fluids in fractures and the rock matrix, and mineral-water-gas reactions. Field sampling of produced fluids from the Aidlin steam field was conducted prior to the initiation of reclaimed water injection to establish a baseline for the geothermal reservoir fluid chemistry. Subsequent sampling will evaluate changes that result from injection of larger volumes of water that are distinctly different in chemical composition from reservoir fluids and previously injected condensate.

A reactive-transport model for 14C was developed and applied to the Aidlin geothermal system. A 1-D grid was developed to evaluate the effects of water injection and subsequent water-rock-gas interaction on the compositions of the produced fluids using TOUGHREACT. This model uses a dual-permeability model of the fracture-matrix system, and contains the principal minerals (K-feldspar, plagioclase, calcite, silica polymorphs) that occur in the metagraywackes that comprise the geothermal reservoir. Initial simulation results predict that the gas phase CO2 in the reservoir will become more enriched in 14C as air-equilibrated injectate water (with a modern carbon signature) is incorporated into the system, and that these changes will precede accompanying decreases in reservoir temperature. The effects of injection on 14C in the rock matrix will be lessened somewhat due to the dissolution of matrix calcite with “dead” carbon. Changes in the abundance of 14C and the composition of isotopic tracers such as 3C/12C, 18O/16O, and D/H measured periodically in production well fluids during injection of wastewater in the Aidlin field will be used to test the ability of the TOUGHREACT simulator to predict how interactions between injectate water and the mineral, gas, and steam phases present in the geothermal reservoir will affect the composition and enthalpy of produced fluids over time.
SHEAR SLIP ANALYSIS IN MULTI-PHASE FLUID FLOW RESERVOIR ENGINEERING APPLICATIONS USING TOUGH-FLAC

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ABSTRACT
This paper describes and demonstrates the use of the coupled TOUGH-FLAC simulator for geomechanical shear-slip (failure) analysis in multiphase fluid-flow reservoir-engineering applications. Two approaches for analyzing shear-slip are described, one using continuum stress-strain analysis and another using discrete fault analysis. The use of shear-slip analysis in TOUGH-FLAC is demonstrated on application examples related to CO₂ sequestration and geothermal energy extraction. In the case of CO₂ sequestration, the shear-slip analysis is used to evaluate maximum sustainable CO₂-injection pressure under increasing reservoir pressure, whereas in the case of geothermal energy extraction, the shear-slip analysis is used to study induced seismicity during steam production under decreasing reservoir pressure and temperature.
MODELING OF GAS COMPOSITION AND GRAVITY SIGNALS
AT THE PHLEGREAN FIELDS CALDERA

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ABSTRACT

Hydrothermal systems are known to play an important role in the evolution of active calderas: these volcanic systems periodically undergo dramatic unrest crises, commonly involving ground deformation, seismic activity and important changes in several geophysical and geochemical parameters monitored at the surface. These unrest crises may, or may not, culminate with a renewal of the eruptive activity, but in any case they bear important consequences in densely populated regions. Early warning and a prompt evaluation of the state of evolution of the volcanic system are therefore essential to ensure proper mitigation measures. A proper interpretation of monitoring data, however, is only achieved within the framework of a robust conceptual model of the system. Recent research work carried out at the Phlegrean Fields shows that the recent evolution of the caldera is consistent with the presence of a pulsating magmatic source, periodically discharging CO₂-enriched fluids into a shallow hydrothermal system. Such pulsating degassing affects the amount of heat and fluids entering the hydrothermal system, the distribution of fluid phases throughout the system, and their composition. As a consequence, degassing controls not only the composition of fluids discharged at the surface, but also ground displacement and gravity residuals. In this work, the TOUGH2 code has been applied to study how different degassing scenarios could affect the composition of discharged fluids and the gravity signals recorded at the surface.
Session 3
GEOTECHNICAL ENGINEERING
FLOODING OF AN ABANDONED SALT MINE—
MODELING TWO-PHASE FLOW IN COMPLEX MINE STRUCTURES

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ABSTRACT
The TOUGH module EOS7 has been used to model the conditions in a former salt mine during and after flooding. Of particular interest are the conditions in a small part of the mine where radioactive wastes are stored under an extremely low permeability backfill. The salt rock between the waste emplacement cavern and the cavern underneath is disturbed and, therefore, has significant permeability. The structure of the relevant parts of the complex underground mine was simplified and then discretized with our own pre-processing software MAGICS to generate a 3D mesh consisting of about 18,000 hexahedrons.

The two-phase flow occurring when a highly viscous and very dense flooding fluid is introduced into the mine was modeled successfully with the TOUGH module EOS7. Sensitivity analyses were performed to evaluate the influence of uncertain parameters.

Post-processing and the 3D visualization of the results with TECPILOT have greatly enhanced the understanding of how the flooding fluid advances through the complex underground mine and how air may be trapped in the process.

The modeling study has shown that the air trapped below the low permeability backfill will most probably prevent the flooding fluid from getting into contact with the wastes. However, a contact cannot be completely ruled out because of capillary effects.
ASCATA—A TOUGH2 BASED PROGRAM FOR AUTOMATED SIMULATION OF COMPRESSED AIR TUNNEL ADVANCE

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ABSTRACT

In compressed air tunneling an excess air pressure is applied inside the tunnel to prevent groundwater-inflow. Due to the excess pressure compressed air partly penetrates into the surrounding ground. The costs for the continuous generation of the compressed air may reach a significant share of the total tunnel construction costs. Especially contractors are therefore interested in predictions of the expected air losses to determine the capacity of the air supply equipment on site and to estimate the energy costs for the generation of the compressed air. Consulting engineers want to know how the escaping air influences surface settlements and tunnel face stability.

ASCATA—a TOUGH2 based program, was developed in order to compute the transient air flow rates during the tunnel advance and to simulate the effects of the escaping compressed air to the ground. TOUGH2 was chosen as core of the new program because of the available flow module EOS3 (active air and water flow) and the open source code which, among other things, allowed for the implementation of an automatic advance sequence.

Initially, an introduction of tunneling under compressed air is given in the paper. In the following, the main features of the developed program are described. Special attention is given to the algorithms which are used for the automatic advance simulation. The functionality of the program is demonstrated by two case studies.
ENHANCED SEEPAGE AND ITS EFFECT ON SLOPE STABILITY
UNDER TORRENTIAL PRECIPITATE DURING FLOOD DISCHARGE EVENT
ON A LARGE HYDROELECTRIC STATION

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ABSTRACT

During flood season, it is a common practice for a hydropower reservoir to discharge its excessive
flooding water when necessary. The discharging water generates rain and fog localized over the area
surrounding the flood-discharge structure plunge pool. The precipitate could be as intensified as a
torrential storm. For example, in Nuozadu Hydroelectric Station on Lancang River in Yunnan, China, the
localized rain can be as heavy as up to 200 to 300 mm/hr and last for 5 days. The rainy area could extend
about 500 m along the river, about 300 m wide across, and about 200 m high. The heavy rain results in
alteration of flow condition of the slope in the energy dissipation area of the discharging floodwater,
which, in turn, adversely affects the stability and safety of the engineering slope. Conventional practice
treats the subsurface as saturated, neglecting the suction of the rock matrix associated with unsaturated
condition. This leads to an overestimation of pore water pressure and thus a severe underestimation of
the effective stress. An underestimated effective stress incurs engineering costs much higher than
otherwise in protection of the slope, as it calls for more-conservative engineering measures. In this paper,
we focused on the response of seepage during discharging events at Nuozadu Hydroelectric Station. Both
subsurface flow simulation and laboratory experiment were performed to evaluate the seepage alteration
and its impact on slope stability. The seepage model was developed and calibrated with field- and
laboratory-measured rock properties and saturation data. The relation of seepage to slope stability is
established through correlating saturation with measured rock mechanical data. Results show that the
effective stress could be much better represented with the proposed unsaturated flow approach. This
study represents one of the first few similar field study cases on this active research area, concerning
slope stability issues on intensified infiltration during flood discharge events at large hydroelectric
stations. Its methodology and general conclusions are applicable to general slope sites on hydropower
structures.
THE LIHIR OPEN PIT GOLD MINE REVISITED

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ABSTRACT

In the last TOUGH2 workshop (White et al. 2003) we described initial modelling of the geothermal system and groundwater in the vicinity of the open pit Lihir gold mine. This mine pit is planned ultimately to reach more than 200 meters below sea level and is being dug into an active geothermal system with some of the area to be mined at boiling-point for depth conditions. Cooling and depressurisation of the geothermal resource associated with the gold mineralisation is an essential part of the mining operation. Previous modelling was based on data from eight deep, deviated geothermal wells completed during 1999 and information from the shallower mineral exploration wells drilled and tested in the 1980's.

Currently the mine is over 150 meters below sea level and more than 30 geothermal wells plus a number of steam relief and new pumped dewatering wells have been drilled. Two power stations have been built to provide a total of 36 MW of electricity for use in the gold refining process. The new geothermal drilling has shown that the productive reservoir beneath the mine pit to be fracture dominated with a low effective porosity, partially isolated from the shallow reservoir.

This system provides a number of challenges to the modeller with coupling between the groundwater, the sea and the geothermal system all being important and the need to take account of the changing surface topography as the mine pit is deepened.

Use was made of iTOUGH2 running on a cluster of LINUX workstations to aid the fitting of some model parameters. Using this program in a parallel computational environment (Finsterle 1998) was essential to complete the parameter fitting in an acceptable time.

Recently we have also made use of a new version of Multi-TOUGH2 (Zhang et al. 2001), also on a LINUX cluster and this has significantly reduced the processing time required to calculate initial states for some of the large models developed.
Session 4
CARBON DIOXIDE STORAGE AND GAS HYDRATES
(Posters)
SYSTEM-LEVEL MODELING FOR GEOLOGICAL STORAGE OF CO₂

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ABSTRACT
One way to reduce the effects of anthropogenic greenhouse gases on climate is to inject carbon dioxide (CO₂) from industrial sources into deep geological formations such as brine formations or depleted oil or gas reservoirs. Research has and is being conducted to improve understanding of factors affecting particular aspects of geological CO₂ storage, such as performance, capacity, and health, safety and environmental (HSE) issues, as well as to lower the cost of CO₂ capture and related processes. However, there has been less emphasis to date on system-level analyses of geological CO₂ storage that consider geological, economic, and environmental issues by linking detailed representations of engineering components and associated economic models. The objective of this study is to develop a system-level model for geological CO₂ storage, including CO₂ capture and separation, compression, pipeline transportation to the storage site, and CO₂ injection. Within our system model we are incorporating detailed reservoir simulations of CO₂ injection and potential leakage with associated HSE effects. The platform of the system-level modeling is GoldSim. The application of the system model is focused on evaluating the feasibility of carbon sequestration with enhanced gas recovery (CSEGR) in the Rio Vista region of California. The reservoir simulations are performed using a special module of the TOUGH2 simulator, EOS7C, for multicomponent gas mixtures of methane and CO₂ or methane and nitrogen. Using this approach, the economic benefits of enhanced gas recovery can be directly weighed against the costs, risks, and benefits of CO₂ injection.
SEQUESTRATION OF CO₂ IN THE ALTMARK NATURAL GAS FIELD, GERMANY: MOBILITY CONTROL TO EXTEND ENHANCED GAS RECOVERY

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ABSTRACT
We are investigating the technical feasibility of injecting CO₂ for carbon sequestration with enhanced gas recovery (CSEGR) in the depleted Altmark natural gas reservoir of the North German Basin. Our approach is numerical simulation using TOUGH2/EOS7C with modifications to include a gelling fluid for mobility control to retard CO₂ breakthrough. The Altmark reservoir is a faulted and compartmented anticlinal structure covered by a massive salt cap rock. The reservoir itself is composed of alternating sandstone, claystone, and siltstone at a depth of approximately 3000 m. The reservoir pressure is approximately 20 MPa, the temperature is about 120 °C. The average usable storage porosity in sand layers is estimated to be 8 %. The permeabilities vary from 0.5 mD to 1000 mD, representing hydrostratigraphic units with higher amounts of clay and silt, and higher amounts of sand, respectively. The natural gas is rich in nitrogen, ranging from 40-90 %, with an average methane content of 32 %. The model includes vertical zoning representing the Salzwedel-Peckensen part of the Altmark reservoir, discretized as nine layers with six different rock types spanning 226 m of total thickness. The geometry modeled is a quarter of a five-spot pattern with a well spacing of 2.1 km. Various injection and production strategies were investigated. In general, the high-permeability layers allow breakthrough of CO₂ at the production well after only 3–10 years. In order to extend the enhanced gas recovery period, different mobility-reducing strategies were tested, i.e., water and gel injection into the high-permeability layers to control CO₂ mobility. The simulations suggest that pre-CSEGR injection can be used to delay CO₂ breakthrough. In general, CSEGR appears to be promising for increasing gas production in the Altmark gas fields while simultaneously sequestering CO₂.
ABSTRACT

In this study we compare the use of kinetic and equilibrium reaction models in the simulation of gas (methane) hydrates in porous media. Our objective is to evaluate through numerical simulation the importance of employing kinetic versus equilibrium reaction models for predicting the response of hydrate-bearing systems to external stimuli, such as changes in pressure and temperature. Specifically, we (1) analyze and compare the responses simulated using both reaction models for production scenarios in various geological settings and for the case of depressurization in a core during extraction; and (2) examine the sensitivity to factors such as initial hydrate saturation, hydrate reaction surface area, and numerical discretization. We find that for systems undergoing thermal stimulation and depressurization, the calculated responses for both reaction models are remarkably similar, though some differences are observed at early times. Given these observations, and since the computational demands for the kinetic reaction model far exceed those for the equilibrium reaction model, the use of the equilibrium reaction model often appears to be justified and preferred for simulating the behavior of gas hydrates. This work was supported in part by the U.S. Dept. of Energy under Contract No. DE-AC03-76SF00098.
DEPRESSURIZATION-INDUCED GAS PRODUCTION FROM CLASS 1 AND CLASS 2 HYDRATE DEPOSITS

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ABSTRACT
Class 1 hydrate deposits are characterized by a Hydrate-Bearing Layer (HBL) underlain by a two-phase zone involving mobile gas. In Class 2 deposits, a mobile water zone underlies the hydrate zone. Using TOUGH+HYDRATE to study the depressurization-induced gas production from such deposits, we determine that large volumes of gas can be readily produced at high rates for long times using conventional technology. To avoid blockage caused by hydrate formation in the vicinity of the well, wellbore heating is a necessity during production.

Dissociation in Class 1W deposits (involving water and hydrate in the HBL) proceeds in distinct stages, while it is continuous in Class 1G deposits (defined by water and gas in the HBL). These hydrates are shown to contribute significantly to the production rate (up to 65% and 75% for Class 1W and 1G, respectively) and to the cumulative volume of produced gas (up to 45% and 54% for Class 1W and 1G, respectively). Large gas volumes can be produced from Class 2 hydrates, but the continuously increasing gas production attains a substantial rate after a long lead time. Additionally, the permeability of the confining boundaries plays a significant role in Class 2 deposits.

Production from Class 1 (and, to a lesser extent, from Class 2) deposits leads to the emergence of a second dissociation front (in addition to the original ascending hydrate interface) that forms at the top of the hydrate interval and advances downward. Capillary pressure effects lead to hydrate lensing, i.e., the emergence of distinct banded structures of alternating high-low hydrate saturation, which form channels and shells and have a significant effect on production.
ABSTRACT
The relative permeability to fluids in hydrate-bearing sediments is an important parameter for predicting natural gas production from gas hydrate reservoirs. We estimated the relative permeability parameters (van Genuchten $\alpha$ and $m$) in a hydrate-bearing sand by means of inverse modeling, which involved matching water saturation predictions with observations from a controlled waterflood experiment. We used x-ray computed tomography (CT) scanning to determine both the porosity and the hydrate and aqueous phase saturation distributions in the samples. X-ray CT images showed that hydrate and aqueous phase saturations are non-uniform, and that water flow focuses in regions of lower hydrate saturation. The relative permeability parameters were estimated at two locations in each sample. Differences between the estimated parameter sets at the two locations were attributed to heterogeneity in the hydrate saturation. Better estimates of the relative permeability parameters require further refinement of the experimental design, and better description of heterogeneity in the numerical inversions.
Session 5
COMPUTATION METHODS, PRE- AND POST-PROCESSING
(Posters)
EFFICIENT SCHEMES FOR REDUCING NUMERICAL DISPERSION IN MODELING MULTIPHASE TRANSPORT THROUGH POROUS AND FRACTURED MEDIA

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ABSTRACT

Numerical issues with modeling transport of chemicals or solute in realistic large-scale subsurface systems have been a serious concern, even with the continual progress made in both simulation algorithms and computer hardware in the past few decades. The problem remains and becomes even more difficult when dealing with chemical transport in a multiphase flow system using coarse, multidimensional regular or irregular grids, because of the known effects of numerical dispersion associated with moving plume fronts. We have investigated several total-variation-diminishing (TVD) or flux-limiter schemes by implementing and testing them in the T2R3D code, one of the TOUGH2 family of codes. The objectives of this paper are (1) to investigate the possibility of applying these TVD schemes, using multi-dimensional irregular unstructured grids, and (2) to help select more accurate spatial averaging methods for simulating chemical transport given a numerical grid or spatial discretization. We present an application example to show that such TVD schemes are able to effectively reduce numerical dispersion.
ENHANCING SCALABILITY AND EFFICIENCY OF TOUGH2_MP FOR LINUX CLUSTERS

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ABSTRACT
TOUGH2_MP, the parallel version TOUGH2 code, has been enhanced by implementing more efficient communication schemes. This enhancement is achieved through reducing the amount of small-size messages and the volume of large messages. The message exchange speed is further improved by using non-blocking communications for both linear and nonlinear iterations. In addition, we have modified the AZTEC parallel linear-equation solver to nonblocking communication. Through the improvement of code structuring and bug fixing, the new version code is now more stable, while demonstrating similar or even better nonlinear iteration converging speed than the original TOUGH2 code. As a result, the new version of TOUGH2_MP is improved significantly in its efficiency. In this paper, the scalability and efficiency of the parallel code are demonstrated by solving two large-scale problems. The testing results indicate that speedup of the code may depend on both problem size and complexity. In general, the code has excellent scalability in memory requirement as well as computing time.
USING PETRASIM TO CREATE, EXECUTE, AND POST-PROCESS TOUGH2 MODELS

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ABSTRACT

Although powerful, the TOUGH2 codes were initially developed as research tools, using a text-based input file. This presents significant hurdles to a new user, who must create an input file that describes a valid mesh and specifies the appropriate solution controls. Possible simulator options are often activated by flags that are confusing and may appear in unrelated locations in the input file. It is hard enough to solve non-isothermal, multi-component, multi-phase problems without the additional difficulty of preparing complex and lengthy input files. In addition, the user must develop their own toolkit to display results. Even experienced users may need additional help to exploit models with tens of thousands of cells or to enable rapid remeshing for convergence studies.

PetraSim – an integrated program for TOUGH2 model creation, analysis, and results display – has undergone continual development since its first release in August, 2002. The latest version includes support for TOUGHREACT and TOUGH-Fx/HYDRATE. New features to be demonstrated in version 3.0 include: support for “extra cells” that are not part of the physical mesh (used for special boundary conditions, etc.), display of a 2D image (such as a map) in the 3D views, improved support for wells, improved 2D editor performance including cell search features, and several other interface enhancements.

Use of PetraSim and the TOUGH2 programs will be demonstrated in the poster session.
SOME TOPOLOGICAL ASPECTS OF THE (UN) STRUCTURED GENERATION OF MESHES: A POSSIBLE ENHANCEMENT OF MESHMAKER IN TOUGH2

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ABSTRACT

The non-linear partial differential equations solved in TOUGH by the Integral Finite Difference Technique, need the construction of meshes with diverse degrees of sophistication to model the geometry of physical systems in 2D or 3D domains with boundaries that can be of complex shapes. The main mathematical tools required to create efficient grids are differential geometry, tensor analysis and topology. We present several results from topology and geometry applied to practical grid generation.

Structured mesh generation is the first step in the solution of problems with boundary conforming meshes. Structured meshes deal with the construction of coordinate curves in 2D and of coordinate surfaces in 3D. The intersection of these curves and surfaces produces mesh points and cells inside the solution domain. The grid cells are generally four sided geometric objects in 2D and finite volumes with six curved faces in 3D. The connectivity of points is the manner in which grid points are connected to each other in the solution domain. This connectivity depends on the overall generation scheme used. The Cartesian coordinates of every point can be stored in specific matrices with geometric and topological information. A variational approach is used for grid properties (orthogonality, longitude, area and smoothness) that can be controlled by the minimization of a functional. In unstructured meshes the connectivity between grid points can vary from point to point and it has to be described explicitly by an appropriate and particular data structure. This characteristic makes the unstructured solution algorithms more expensive in computational cost but more flexible and useful when employed in adaptive solutions of transient flows and moving boundary problems. This scheme is widely used in many applications of the Finite Element Method and in the Galerkin Discontinuous approach. We introduce a unstructured mesh generation using the Delaunay triangulation in 2D. The Delaunay tetrahedrization holds in 3D. In the first part we work in two dimensions using classic constructions from Euclidean geometry. In the second part we introduce topological concepts to generate meshes in three dimensions. We developed Fortran and Visual C codes to show some results in 2D. The practical aspects of this work could be useful as enhanced options for the TOUGH2 Meshmaker module.
TOUGH+: THE NEW GENERATION OF OBJECT-ORIENTED FAMILY OF CODES FOR THE SOLUTION OF PROBLEMS OF FLOW AND TRANSPORT IN THE SUBSURFACE

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ABSTRACT

TOUGH+ is the successor to the TOUGH2 family of codes for multi-component, multiphase fluid and heat flow developed at the Lawrence Berkeley National Laboratory. It is written in standard FORTRAN 95/2000/2003 to take advantage of all the object-oriented capabilities and the enhanced computational features of that language. While TOUGH+ has a very different syntax and architecture than TOUGH2, it maintains full backward compatibility with existing TOUGH2 input data files.

The new code employs dynamic memory allocation, thus minimizing storage requirements. It follows the tenets of Object-Oriented Programming (OOP), and involves data encapsulation, polymorphism, derived types and classes (defining the various objects), pointers, constructors and destructors, dynamic linkage, inheritance, operator overloading, and complete interoperability with C/C++ subroutines. The TOUGH+ code is based on a modular structure that is designed for maximum traceability and ease of expansion, and enhanced interoperability of FORTRAN95/2000/2003. Additionally, the TOUGH+ codes include enhanced capabilities, allowing (a) complex domain geometries with both expanded and new domain discretization capabilities, (b) extended phase changes (covering the entire gas-to-liquid-to-solid range), (c) equations of state describing the behavior of real gas mixtures of interest to subsurface science, (d) expanded initialization capabilities, and (e) time-variable boundary conditions.
IGGI, A COMPUTING FRAMEWORK FOR LARGE SCALE PARAMETRIC SIMULATIONS: APPLICATION TO UNCERTAINTY ANALYSIS WITH TOUGHREACT

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ABSTRACT

IGGI stands for infrastructure for grids, cluster and intranet. This research project partially funded by the French government is aiming at developing technologies allowing the access and the gathering of the whole computing resources spread over the intranet of a company. This could include dedicated computing power or personal computers. The project is collaboration between BRGM, INRIA and Mandriva.

Scientific computing has evolved for last few years and commodity-based components can run a wide range of applications. In this study, our focus will be on the software environment required to carry out large scale parametric simulations, but we will also report on experience of the deployment of such an infrastructure in the day to day life of an intranet.

The IGGI software suite is mainly based on two components: ComputeMode\textsuperscript{TM} which smoothly aggregates idle user machine to a virtual computing cluster. This is done through a transparent switch of the PC to a secondary, protected mode from which it boots from the ComputeMode server taking advantage of the PXE protocol. The second IGGI component is CIGRI which scheduled and executed computing tasks on the idle nodes of clusters.

Special attention has been paid on the end-users ability to perform easily parametric simulations. Transparent access to the batch-scheduler, checkpoint and migration of the application will be exposed for the test-case of the analysis of uncertainty with TOUGHREACT: “Uncertainty in predictions of transfer model response to a thermal and alkaline perturbation in clay”.

The calculations reported were carried out using idle computing capacity on personal computers inside the BRGM. This new architecture is particularly well suited to explore the wide range of perturbations in highly coupled problems.
Session 6
REACTIVE GEOCHEMISTRY AND ENVIRONMENTAL ENGINEERING (Posters)
SIMULATION OF SALT WATER INTRUSION

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ABSTRACT

We have modeled laboratory experiments of saltwater intrusion using TOUGH2/EOS7. Matching laboratory and simulation results turned out to be quite challenging partly because of numerical dispersion and partly because the experiments were not very well controlled. In order to understand better the effects of numerical dispersion, we simulated the so-called Henry problem, in which a large dispersion coefficient is assumed resulting in a wide transition zone between freshwater and saltwater. Henry attributed the large dispersion to the effect of tidally induced motion. We imposed a sinusoidal boundary condition to see if a large transition zone can be created without explicitly modeling dispersion. However, for the parameters used we were not able to do so. It is still plausible that a wide transition zone is caused by formation heterogeneity. Nonetheless, we question the validity of the use of a large dispersion coefficient where the velocity is very low, or where the flow is in the opposite direction of the concentration gradient.
A MODELING CASE STUDY OF NAPL TRANSPORT IN POROUS MEDIUM UNDER THE INFLUENCE OF VARIABLE WATER INFILTRATION AND GEOLOGICAL HETEROGENEITY

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ABSTRACT

The subsurface migration of non-aqueous phase liquids (NAPLs) is influenced by, among other factors, geological heterogeneity and water infiltration rates. In order to determine the simultaneous influence of these two factors, T2VOC is used to model NAPL release scenarios. The scenarios are hypothetical but selected to represent typical Scandinavian climatic and geological conditions.

The conceptual model consists of a two-dimensional vertical cross-section representing part of the unsaturated zone of a porous medium. A DNAPL – trichloroethylene (TCE) – is injected as a 2 m wide source either at the ground surface or at different depths. Varying water infiltration rates are introduced at the upper boundary representing seasonal and short-term changes in groundwater recharge.

Results show that the combined effect on NAPL migration from heterogeneity and variable water infiltration is highly dependent on the magnitude and time-scale of variation in water infiltration. For natural water infiltration rates changing monthly around an annual mean, the effect of heterogeneity is superior to that of water infiltration. Even for more short-term variations in water infiltration, the heterogeneity is clearly more significant. For natural infiltration variability characteristics of Scandinavian conditions as tested here, heterogeneity can therefore be concluded to be more important to consider than variations in water infiltration rates.

When short-term water infiltration rate is increased drastically, a notable effect can be seen on NAPL migration. When the water pulse arrives to a given depth, a small increase in NAPL saturation can first be observed, followed by a more pronounced decrease. The observed decrease can be concluded to be a result of an increased dissolution due to the higher aqueous phase flow. For the heterogeneous case, this effect is more apparent than for the corresponding homogeneous case. Furthermore, the effect is more pronounced the sooner the water pulse occurs after the NAPL release. Hence, a high NAPL saturation at the time when the water pulse arrives tends to increase its effects.
IMPLEMENTATION OF A PITZER ACTIVITY MODEL INTO TOUGHREACT FOR MODELING CONCENTRATED SOLUTIONS

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ABSTRACT
TOUGHREACT is a general-purpose reactive geochemical transport numerical simulator. It deals with multiphase flow, solute transport and geochemical reactions including aqueous complexation, mineral dissolution/ precipitation and cation exchange. Making use of an extended Debye-Hückel ion activity model, this simulator can handle solutions concentrated to slightly above ~1 molal with caution, and only for NaCl-dominant waters at ionic strengths up to ~4 molal. However, brines produced under natural and artificial conditions are often more concentrated. To handle such brines, a Pitzer activity model was implemented in TOUGHREACT, based on the standard Harvie-Moller-Weare (HMW) formulation that accounts for all binary and ternary combinations of interaction terms. The vapor-pressure-lowering effect caused by the low water activity in brines was also accounted for by this code. The extended version was verified and tested using published results from laboratory experiments and benchmarked against other computer codes. This new version of TOUGHREACT is being applied to the investigation of boiling and evaporation within and around the proposed high-level nuclear waste emplacement tunnels at Yucca Mountain, Nevada. An example application is presented. Processes considered in the example include evaporation of porewater to near dryness, formation of highly concentrated brines, precipitation of deliquescent salts, and generation of acid gases.
MODELING OF THE LABORATORY TESTS OF INTERACTION OF THE NaNO₃-NaOH FLUIDS WITH SANDSTONE ROCKS FROM DEEP RADIONUCLIDE REPOSITORY SITE, USING TOUGHREACT

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ABSTRACT

TOUGHREACT modeling was used to reproduce laboratory tests with sandstones samples collected from deep radionuclide repository site in Siberia Chemical Plant. Laboratory test include injection of alkaline fluids into sandstones samples at 70°C. Some minerals were restrained in the model to precipitate or dissolve according to laboratory test results. Modeling results were compared with observed test data (mineral phases change, transient concentrations data at the outlet of sample column). Model and test convergence in mineral phases (Na-smectite and kaolinite precipitation in the model, quartz, microcline, chlorite and biotite dissolution in the model) were obtained due to restrain orders for some minerals to precipitate/dissolve. Nevertheless it was not found possible to generate sodium in the model (while sodium clearly observed in the test). Transient chemical concentrations data at the outlet of sample column match Na only. Possible improvements of the TOUGHREACT based model to better match observed data are concluded.
SIMULATION OF THE EFFECTS OF HYDROPHILIC POLYMER ADSORPTION ON TWO-PHASE FLOW OF OIL-WATER MIXTURES

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ABSTRACT

Injection of water-soluble polymers in oil or gas producing wells can be an effective way to control water production where other technologies (gels, cements) cannot be applied. These treatments are relatively simple and inexpensive and the risk of impairing the permeability of the hydrocarbon producing layer is small. Numerical simulation techniques can be useful to design and interpret laboratory tests and predict the performances of polymeric solution treatments in actual field conditions.

We first developed a simplified model of pore networks to evaluate changes in the effective permeability of the aqueous phase due to polymer adsorption, and then we implemented the obtained relationships between adsorbed thickness and water relative permeability into the TMVOC reservoir simulator. The pore network is described according to an extension of V&P tube in series model, suitable also for fractured rocks. The adsorbed polymer reduces the pore volume available for flow, thus reducing the effective permeability of the wetting phase compared to the original pore network. It is assumed that water and oil/gas relative permeability curves are conveniently described by a Corey’s type function, with or without adsorbed polymer. The model estimates the reduction of water relative permeability and evaluates the new parameters of Corey’s curve as a function of adsorbed polymer thickness. These parameters are regressed using polynomial correlations which are then supplied through the input file to a modified version of TMVOC simulator.

The adsorption isotherm parameters, as well as those necessary to evaluate the relationship between adsorbed mass and adsorbed layer thickness, can be evaluated by inverse simulation of core flood experiments, which is performed by running TMVOC under the PEST code.
Session 7
GEOTHERMAL RESERVOIR ENGINEERING
(Posters)
MODELING THE PAUZHETSKY GEOTHERMAL FIELD, KAMCHATKA, RUSSIA, USING iTOUGH2

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ABSTRACT

The forward TOUGH2 modeling study of the Pauzhetsky geothermal field was followed by an iTOUGH2 analysis to obtain more reliable reservoir parameter estimations. The model was automatically calibrated against (1) natural state and (2) production data. For the natural state modeling, calibration data include 68 points (2 natural discharge rates, 14 reservoir pressures at -250 m.a.s.l., and 52 reservoir vertically averaged temperatures). The different quality of the calibration points was expressed by specifying appropriate standard deviations. Preliminary estimates of the principal parameters are: (1) permeability $k = 87$ mD, and (2) an upflow rate $Q_b = 40.5$ kg/s.

For the modeling of the exploitation phase, calibration data include 60 datasets: enthalpies of the exploitation wells (10 data sets), pressures in monitoring wells (24 data sets), and temperatures in monitoring wells (26 data sets), with a total of 15,030 calibration points. The following parameters are estimated: (1) reservoir compressibility, (2) reservoir fracture porosity, and (3) infiltration “window” permeabilities. Model calibration will be followed by an analysis of the sustainable capacity of the Pauzhetsky field.
TOUGH AND THE BOUNDARY ELEMENT METHOD IN THE ESTIMATION OF THE NATURAL STATE OF GEOTHERMAL SUBMARINE SYSTEMS

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ABSTRACT
In this work we present a general updated description of geothermal submarine reservoirs and an evaluation of the amount of energy contained in these important natural systems. To estimate the natural state of these reservoirs we use the classical Boundary Element Method (BEM) and suggest a simple way to couple this technique to TOUGH2 through the INPUT file. Submarine geothermal reservoirs contain essentially an infinite amount of energy. The deep submarine heat is related to the existence of hydrothermal vents emerging in many places along the oceanic spreading centers between tectonic plates. These systems have a total length of about 65,000 km in the Earth’s oceanic crust. The deep resources are located at certain places along the rifts between tectonic plates of the oceanic crust at more than 2000 m below sea level. Shallow resources are found near to continental platforms between 1 m and 50 m depth and are related to faults and fractures close to the coasts. Both types of resources exist in the Gulf of California, Mexico. To model these systems the initial mathematical problem is expressed in terms of boundary integral equations, fundamental solutions and boundary conditions of mixed type. The field main functions are pressure and temperature. The versatility and power of the BEM allows the efficient treatment of very complex or unknown reservoir’s geometry, without requiring discretization of the whole domain occupied by the system. This capability permits to test quickly different boundary conditions to estimate several thermodynamic initial states at any desired interior point of the domain occupied by the reservoir under specific conditions. Unfortunately, the classical BEM is limited to single phase flow in homogeneous media and cannot be fully applied to flow problems in heterogeneous systems. In this last case there is no fundamental solution. To overcome this difficulty, after an initial state is estimated, TOUGH2 can be used to improve the initial simulation. The few available data on hydrothermal vents are very useful to estimate the amount of energy out flowing from the ocean floor. In this way, it is possible to estimate initial conditions knowing only heat fluxes and temperatures at fissures and chimneys using this hybrid technique.
COUPLING AND DECOUPLING OF HEAT AND HELIUM TRANSPORT IN A GEOTHERMAL RESERVOIR

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ABSTRACT

We present two- and three-dimensional simulations of heat and helium transport for a generalized graben system to systematically investigate how various interacting parameters influence coupling and decoupling of heat and helium signals. We confirm findings of previous studies by other authors including the occurrence of spatial decoupling of heat and helium due to variations in their respective diffusivities, entrapment of helium by low permeability layers, and the preference of helium for fracture flow. We continue by assessing the impact of radiogenic heat and helium production and buoyancy-driven convection within a fracture system and within a crystalline basement layer on the distribution of temperature, helium, and isotopic ratios of helium. We find that processes deep within the subsurface can have a large effect on near-surface mantle/magmatic heat and helium signatures. Additionally, we show the significance of distinguishing between the decoupling of heat and helium due to transport phenomena and the decoupling of heat and helium signals due to other subsurface processes. The results of our investigation have applications to geothermal reservoir analyses, mantle heat versus mantle helium estimations, and studies using heat and/or helium as natural tracers of groundwater flow.
Session 8
NUCLEAR WASTE
(Posters)
THREE DIMENSIONAL ANALYSES OF COUPLED GAS, HEAT AND NUCLIDE TRANSPORT IN A REPOSITORY INCLUDING ROCK SALT CONVERGENCE

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ABSTRACT
For a repository system for spent fuel elements in rock salt, coupled three dimensional transport of gas, heat and nuclide is studied with a modified version of computer code TOUGH2/EOS7R. Variable hydrodynamic properties of compactible filling material like crushed salt are determined considering convergence of rock salt depending on fluid pressure and temperature. Among other observations, the analyses show that a two dimensional analysis can be sufficient and reasonable, if the gas transport in an isothermal configuration is a major issue. However, if the heat and/or nuclide transport are to be investigated additionally, a three dimensional approach can be necessary to adequately quantify the consequences of the combined transport processes.
DESIGN AND ANALYSIS OF A GAS THRESHOLD PRESSURE TEST IN A LOW-PERMEABILITY CLAY FORMATION AT ANDRA’S UNDERGROUND RESEARCH LABORATORY, BURE (FRANCE)

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ABSTRACT

A gas threshold pressure test (GTPT) in a deep borehole at Andra’s Underground Research Laboratory near Bure, France was conducted to better understand gas transport processes in the low-permeability clay formation under constant rate gas injection conditions. A hydrotest preceding the gas test was performed to estimate the interval transmissivity, static formation pressure, and the flow model in the vicinity of the test section. This information served as the basis for the design and analysis of the gas test to determine the gas threshold pressure of the formation. The gas threshold pressure is typically identified from the pressure buildup curve indicating a deviation from linear increase when the gas starts to migrate into the formation.

The GTPT at Bure showed a sudden pressure decline after continuous gas injection which suggested fracturing of the formation. A second gas injection phase was performed and verified the fracture development and the pressure recoveries following both gas injection phases indicated the same equilibration pressure, which corresponds to the gas threshold pressure of the undisturbed formation.

The GTPT response was analyzed using the two-phase simulator TOUGH2. Even though the standard version of TOUGH2 does not consider coupled mechanical processes associated with the observed fracturing, we used an analytical fracture mechanics analysis to estimate the fracture volume, aperture, and extent. The fracture analysis indicated a horizontal fracture with relatively small lateral extent of a few meters and a maximum aperture of less than 1 mm. The simulation of the initial fracture response used a restart option to incorporate the inferred fracture characteristics in the numerical model. The closure and re-opening of the fracture during the subsequent recovery and second gas injection phase was implemented by calibrating a pressure-dependent permeability relationship for the fracture elements. The analysis further showed that by the end of the first and second recovery phase the fracture did not completely close, characterized by significantly higher permeability (i.e., more than one order of magnitude) than that of the undisturbed rock. The simulations indicated non-linear behavior in terms of fracture closure during the first recovery phase and re-opening during the second gas injection phase. In addition to the fracture behavior that could be quantified, the initial objective of the GTPT was also accomplished. The pressure recoveries following the fracturing could be used in a Horner extrapolation to estimate the gas threshold pressure of the undisturbed formation.
A COUPLED MODEL FOR NATURAL CONVECTION AND CONDENSATION IN HEATED SUBSURFACE ENCLOSURES EMBEDDED IN FRACTURED ROCK

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ABSTRACT
In heated tunnels such as those designated for emplacement of radioactive waste at Yucca Mountain, axial temperature gradients may cause natural convection processes that can significantly influence the moisture conditions in the tunnels and in the surrounding fractured rock. Large-scale convection cells would provide an effective mechanism for axial vapor transport, driving moisture out of the formation away from the heated tunnel section into cool end sections (where no waste is emplaced). To study such processes, we have developed and applied an enhanced version of TOUGH2, adding a new module that solves for natural convection in open cavities. The new TOUGH2 simulator simultaneously handles (1) the flow and energy transport processes in the fractured rock; (2) the flow and energy transport processes in the cavity; and (3) the heat and mass exchange at the rock-cavity interface. The new module is applied to simulate the future thermal-hydrological (TH) conditions within and near a representative waste emplacement tunnel at Yucca Mountain. Particular focus is on the potential for condensation along the emplacement section, a possible result of heat output differences between individual waste packages.
MODIFYING TOUGH2 TO SUPPORT MODELING OF GAS-TRANSPORT THROUGH SATURATED COMPACTED BENTONITE AS PART OF THE LARGE-SCALE GAS INJECTION TEST (LASGIT) IN SWEDEN

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ABSTRACT

The LASGIT (Large Scale Gas Injection Test) project is a full-scale test of gas transport in bentonite at the Aspö Hard Rock Laboratory in Sweden. Simulating conditions in a deep geologic repository for spent fuel, an empty copper container surrounded by compacted bentonite blocks is placed within a large-diameter borehole in the host rock of the Hard Rock Laboratory. Once the buffer is completely saturated with groundwater, He gas is injected from ports on the container and monitored as it migrates from the container through the bentonite buffer to the host rock. The intent of the LASGIT experiment is to improve the understanding of gas migration through the engineered barrier of a deep geologic repository for spent fuel and to validate different modeling approaches which may be used in future safety assessments.

A preliminary gas-transport model of the LASGIT experiment was developed with a modified version of TOUGH2. This paper will describe the modifications to the TOUGH2 code, present the implementation of the LASGIT experiment in a numerical model and discuss preliminary model results.

Development of the gas-transport model required modifications to TOUGH2 to simulate expected gas transport mechanisms. While the mechanism for gas transport within bentonite is not well known, three potential mechanisms have been proposed (Hoch et al., 2004):

- conventional two-phase flow through a porous medium
- stress- or pressure-induced microscopic fracturing of the bentonite to provide pathways for gas flow
- stress- or pressure-induced macroscopic fracturing of the bentonite to provide pathways for gas flow

Each of these mechanisms may work individually or simultaneously. TOUGH2 was modified to include a pressure-dependent permeability function to simulate micro- or macro- fracturing and a permeability-dependent capillary pressure function to simulate fracture dilation. Additional modifications to TOUGH2 were implemented to simulate He gas.

A 3-D radial mesh was generated representing the copper container and the surrounding bentonite. The mesh is refined surrounding injection ports in the copper container used to inject gas at localized breach points. The 3D mesh was generated and the pressure and saturation model results were visualized with mView, a numeric model pre- and post- processor.

At present, the LASGIT experiment has been installed and the water saturation phase has begun. The preliminary model will be used to evaluate gas-injection test design, and will be further developed for detailed test analysis.
Session 9
VADOSE ZONE AND FRACTURE HYDROLOGY
(Posters)
COUPLING TOUGH2 WITH CLM3: DEVELOPING A COUPLED LAND SURFACE AND SUBSURFACE MODEL

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ABSTRACT
An understanding of the hydrologic interactions among atmosphere, land surface, and subsurface is one of the keys to understanding the water cycling system that supports our life system on earth. The inherent coupled processes and complex feedback structures among subsystems make such interactions difficult to simulate. In this paper, we present a model that simulates the land surface and subsurface hydrologic response to meteorological forcing. This model combines a state of the art land surface model, the NCAR Community Land Model version 3 (CLM3), with a variably saturated groundwater model, the TOUGH2, through an internal interface that includes flux and state variables shared by the two submodels. Specifically, TOUGH2 uses infiltration, evaporation, and root-uptake rates, calculated by CLM3, as source/sink terms in its simulation; CLM3 uses saturation and capillary pressure profiles, calculated by TOUGH2, as state variables in its simulation. This new model, CLMT2, preserves the best aspects of both submodels: the state of the art modeling capability of surface energy and hydrologic processes (including snow, runoff, freezing/melting, evapotranspiration, radiation, and biophysiological processes) from CLM3 and the more realistic physical process based modeling capability of subsurface hydrologic processes (including heterogeneity, three dimensional flow, seamless combining of unsaturated and saturated zone, and groundwater table) from TOUGH2. The preliminary simulation results show that the coupled model greatly improved the predictions of the groundwater table, evapotranspiration, and surface temperature at a real watershed, as evaluated using 18 years of observed data. The new model is also ready to be coupled with an atmospheric simulation model, representing one of the first top of the atmosphere to deep ground atmosphere land surface subsurface models.
VALIDATION OF THE ACTIVE FRACTURE MODEL FOR UNSATURATED FRACTURE FLOW USING NUMERICAL EXPERIMENTS

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ABSTRACT
The active fracture model has been successfully applied to modeling unsaturated flow and transport in fractured rock at Yucca Mountain, Nevada. It accounts for complex flow features (e.g., preferential flow) observed in the field in a relatively large scale model. In this model, the effects of active, water-conducting fractures on effective liquid saturation \( S_e \), capillary pressure \( P_c \), relative permeability \( k_r \), and fracture-matrix interface area are taken into account in the framework of the van Genuchten constitutive equations, with an additional parameter \( \gamma \) introduced to represent fraction of active fractures. This parameter is often obtained through model calibration. However, a direct relationship between the magnitude of \( \gamma \) and the fractured-rock characteristics has not been achieved so far. Our paper aims at demonstrating (1) whether the effective \( k_r - P_c - S_e \) relationships in the active fracture model can be reproduced using numerical experiments, and (2) whether the \( \gamma \) parameter can be linked to the spatial variabilities of fracture geometric and hydraulic properties. The numerical experiments were conducted in four steps: (1) generating random fields of log fracture permeability, with varying correlation lengths and standard deviations; (2) simulating steady-state unsaturated flow in fractured rock using TOUGH2; (3) upscaling effective, flux-weighted \( S_e \), \( P_c \), \( k_r \) values for the entire flow system; and (4) deriving the effective \( k_r - P_c - S_e \) constitutive relationships with the \( S_e \) values varying with specified top boundary conditions. Our results indicate that (1) the effective \( k_r - P_c - S_e \) relationships are different from the local-scale, homogeneous \( k_r - P_c - S_e \) ones, indicating the effects of active fractures with high flow rates, (2) such difference increases with increasing degree of heterogeneity, and (3) the \( \gamma \) parameter increases with increasing degree of fracture-permeability heterogeneity, and (4) it changes with \( S_e \), which is different from the constant-value assumption usually established in the active fracture model.
NUMERICAL SIMULATION AND PARAMETER ESTIMATION USING BOREHOLE FLOWMETER LOGGING IN LOW PERMEABILITY ROCKS

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ABSTRACT

Hydraulic properties of low permeability rocks are indispensable to construct a three dimensional rock property model for the performance assessment or safety estimation of the underground nuclear waste disposal. However, the efficient and accurate estimation of hydraulic properties of low permeability rocks is difficult with the in-situ borehole hydraulic tests, such as injection test or slug test.

The borehole flowmeter logging is a useful method to estimate a magnitude of seepage or inflow between borehole and surrounding rocks. However, because of the low sensitivity of conventional flowmeter logging and the lack of the numerical analyses to estimate hydraulic properties, the observation results were usually used for a qualitative estimation of the relative magnitude of the permeability of fractures across the borehole.

The authors improved the heat-pulse type borehole flowmeter up to 0.03cm/s in detection limit, and applied it to an actual field investigation. The site scale numerical model was constructed from the geologic survey, and basic hydraulic properties were estimated from the hydraulic test and matching of piezometric pressure in boreholes.

In order to simulate the vertical flow velocity along an open borehole in the natural site scale groundwater flow system, the authors developed hybrid RZ2D and rectangular mesh construction program for TOUGH2, and applied it to the site scale model. In this paper, the results of the numerical simulations are compared to the measured velocity profile for the more detailed estimation of hydraulic properties along a borehole.
MODELING OF PHYSICAL OBSERVATIONS OF WATER DIVERSION IN A
CAPILLARY BARRIER USING A CENTRIFUGE

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ABSTRACT
Water flow behavior in capillary barriers has been primarily investigated using mathematical models, with few physical experiments conducted in comparison. The centrifuge modeling technique for studies of unsaturated flow is receiving attention as a rapid physical observation method. This method was used to conduct a number of capillary barrier experiments in this study to examine the relationship between the infiltration intensity and the diversion length.

The objectives of this study are to demonstrate centrifuge experiments of water movement in a fine-over-coarse layer system in order to gain basic knowledge of capillary barriers and to cross-evaluate the centrifuge technique with TOUGH2 simulations of capillary barriers. Particular interests of this study were the water diversion length variability associated with the rainfall intensity, and their representation within the TOUGH2 code.
Session 10
CARBON DIOXIDE STORAGE
ECO2N - A NEW TOUGH2 FLUID PROPERTY MODULE FOR STUDIES OF CO2 STORAGE IN SALINE AQUIFERS

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ABSTRACT
ECO2N is a fluid property module for the TOUGH2 simulator (Version 2.0) that was designed for applications to geologic storage of CO2 in saline aquifers. It includes a comprehensive description of the thermodynamics and thermophysical properties of H2O - NaCl - CO2 mixtures, that reproduces fluid properties largely within experimental error for the temperature, pressure and salinity conditions of interest (10 °C ≤ T ≤ 110 °C; P ≤ 600 bar; salinity up to full halite saturation). Flow processes can be modeled isothermally or non-isothermally, and phase conditions represented may include a single (aqueous or CO2-rich) phase, as well as two-phase mixtures. Fluid phases may appear or disappear in the course of a simulation, and solid salt may precipitate or dissolve. ECO2N can model super- as well as sub-critical conditions, but it does not make a distinction between liquid and gaseous CO2. This paper highlights significant features of ECO2N, and presents illustrative applications.
NUMERICAL MODELING OF CO₂ INJECTION TEST AT NAGAOKA TEST SITE IN NIGATA, JAPAN

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ABSTRACT

The Research Institute of Innovative Technology for the Earth (RITE) is responsible for the five-year project, “Research and Development of Geological Sequestration Technology for Carbon Dioxide”. The project aims to establish a technology that provides stable, safe and long-term geological sequestration of carbon dioxide emitted from large-scale sources in Japan.

In this project a CO₂ injection test was carried out at Nagaoka in the Niigata prefecture. An injection well and three monitoring wells were drilled at test site and super-critical CO₂ injected into a saline sandstone aquifer at a depth of approximately 1100 meters and a rate of approximately 20 - 40 tones/day. The injection test started in July 2003 and continued until November 2004. Monitoring was begun before injection using the monitor wells and is still continuing.

The main purposes of the Nagaoka experiment are to:
• study the actual behavior of CO₂ in an aquifer,
• test simulation methods by comparing model results with measured data and
• gain a general understanding of the behavior of sub-surface CO₂.

The work described in this paper addresses the progress of the second part of these namely, “test simulation methods by comparing model results with measured data”. To this end, we have developed one and three-dimensional models of the reservoir and carried out a number of simulations. We have used iTOUGH2 and ECO2 to determine a number of key reservoir parameters, in particular permeability and residual gas saturation, and ChemTOUGH2 to investigate likely long-term chemical changes in the reservoir.

As part of the experiment several cross-hole tomography runs were performed. These provide the location of the gas bubble on a plane between two monitor wells. This was found to be in good agreement with the results of the three dimensional simulation of the experiment.

Interestingly, the iTOUGH2 calculation of residual gas saturation found the optimum value was zero although some authors have suggested that a value as high as 0.3 is appropriate. This is an important parameter in determining the long-term fate of sequestered CO2 and we believe this is an important finding.
JOULE-THOMSON COOLING DUE TO CO₂ INJECTION INTO NATURAL GAS RESERVOIRS

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ABSTRACT
Depleted natural gas reservoirs are a promising target for Carbon Sequestration with Enhanced Gas Recovery (CSEGR). The focus of this study is on evaluating the importance of Joule-Thomson cooling during CO₂ injection into depleted natural gas reservoirs. Joule-Thomson cooling is the adiabatic cooling or heating that accompanies the expansion of a real gas. If Joule-Thomson cooling were extreme, injectivity and formation permeability could be altered by the freezing of residual water, formation of hydrates, and fracturing due to thermal stresses. The TOUGH2/EOS7C module for CO₂-CH₄-H₂O mixtures is used as the simulation analysis tool. For verification of EOS7C, the classic Joule-Thomson expansion experiment is modeled for pure CO₂ resulting in Joule-Thomson coefficients in agreement with standard references to within 5-7%. For demonstration purposes, a case with a large pressure drop (~50 bars) is presented in order to show that temperature can drop by more than 20 °C by this effect. Two more realistic constant-rate injection cases show that for typical systems in the Sacramento Valley, California, the Joule-Thomson cooling effect is minimal. This simulation study shows that for constant-rate injections into high-permeability reservoirs, the Joule-Thomson cooling effect is not expected to create significant problems for CSEGR.
MODELING GEOLOGIC STORAGE OF CARBON DIOXIDE: COMPARISON OF NON-HYSTERETIC AND HYSTERETIC CHARACTERISTIC CURVES

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ABSTRACT
TOUGH2 models of geologic storage of carbon dioxide (CO₂) in brine-bearing formations use characteristic curves to represent the interactions of non-wetting-phase CO₂ and wetting-phase brine. When a problem includes both injection of CO₂ (a drainage process) and its subsequent post-injection evolution (a combination of drainage and wetting), hysteretic characteristic curves are required to correctly capture the behavior of the CO₂ plume. In the hysteretic formulation, capillary pressure and relative permeability depend not only on the current grid-block saturation, but also on the history of the saturation in the grid block. For a problem that involves only drainage or only wetting, a non-hysteretic formulation, in which capillary pressure and relative permeability depend only on the current value of the grid-block saturation, is adequate. For the hysteretic formulation to be robust computationally, care must be taken to ensure the differentiability of the characteristic curves both within and beyond the turning-point saturations where transitions between branches of the curves occur. Two example problems involving geologic CO₂ storage are simulated using non-hysteretic and hysteretic models, to illustrate the applicability and limitations of non-hysteretic methods: the first considers leakage of CO₂ from the storage formation to the ground surface, while the second examines the role of heterogeneity within the storage formation.
MODELING CO₂ INJECTION WITH HALITE PRECIPITATION USING AN EXTENDED VERMA & PRUESS POROSITY-PERMEABILITY MODEL

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ABSTRACT
The precipitation of halite around a CO₂ injection well has been studied to investigate the possible effects on well injectivity decline for a pilot test concerning the CO₂ injection in a depleted gas reservoir. The numerical simulations performed with TMGAS, a version of the TMVOC simulator with 1D and 2D radial systems, show that the injection of dry supercritical CO₂ vaporizes the formation brine promoting the NaCl concentration and the precipitation of halite. Different behaviors are observed depending on the initial liquid saturation: when the brine has a low mobility, the evaporation front advances with limited halite precipitation and only minor effects on well injectivity. On the other hand, when the brine has enough mobility, the precipitation front is recharged by the brine flowing towards the wellbore, due to the strong capillary pressure gradient driven by the evaporation. In this case the concentrated precipitation can strongly reduce the formation permeability. These effects depend on formation properties and on the porosity-permeability relationship which describes the effects of halite precipitation. Effects, an extension of the so-called tube in series model of Verma and Pruess was developed, with pore size distribution evaluated from the measured grain size distribution of the sandy formation considered for execution of the pilot CO₂ sequestration test.
A LONG TERM 2D VERTICAL MODELLING STUDY OF CO₂ STORAGE AT SLEIPNER (NORTH SEA) USING TOUGHREACT

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ABSTRACT
This paper presents a numerical modeling study of the long term storage of CO₂ in a saline aquifer at Sleipner in the North Sea. The simulation aims at predicting how CO₂ will be transformed because of geochemical reactions with minerals present in the host rock and with species present in the brine.

TOUGHREACT allows simulating hydrodynamics, thermodynamics and geochemical processes involved in CO₂ storage in saline aquifers. A 2D vertical radial geometry model was used with a layered system containing a porous sand formation with four semi-permeable layers. A different mineralogy is applied for the “sand” system and for the “shale” system. Long term simulations have been performed over a time period of 10 000 years. A balance evolution of the amount of CO₂ stored (i) as supercritical phase, (ii) as dissolved in the brines and (iii) as a mineral phase due to carbonate precipitation is presented to conclude the study.
Session 11
VADOSE ZONE HYDROLOGY
INVESTIGATION OF EPISODIC FLOW EVENTS FROM UNSATURATED SAND MEDIA INTO MACROPORES

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ABSTRACT
Episodic or intermittent flow has been observed under a number of scenarios in unsaturated flow systems under constant influx boundary conditions. Flow systems characterized by a sand media underlain by a macropore, as well as discrete fracture networks, have been cited in recent literature as examples of systems that can exhibit episodic outflow behavior. Episodic outflow events are significant because relatively large volumes of water can move rapidly through an unsaturated system, carrying water and possibly contaminants to depth greatly ahead of a diffusive wetting front. In this study, we examine the modeled behavior of water flow through a sand column underlain by a vertical capillary tube in order to assess the potential for rapid vertical water movement, and compare the results to conventional modeling approaches and with experimental data from the literature. Capillary pressure relationships were developed for the macropore domain that capture the complex interrelationships between the sand materials above and control the flow out of the system. Modeling results using the new relative permeability and capillary pressure functions capture the behavior observed in laboratory experiments remarkably well, while simulations using conventional relative permeability and capillary pressure functions fail to capture some of the observed flow dynamics.
INVESTIGATING NONLINEAR RAINFALL-RUNOFF RESPONSE FROM A TRENCHED HILLSLOPE USING TOUGH2 3-D SIMULATIONS

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ABSTRACT

In this short paper we describe the Panola Mountain Experimental Watershed trenched hillslope field site, the existing experimental dataset and a preliminary simulation of the hillslope rainfall-runoff response using the Panola hillslope 3-D TOUGH2 model. Extensive previous field studies on this experimental hillslope have developed a valuable reference dataset to which simulation of the development of subsurface lateral flow during storm events can be compared. The most recent studies of Tromp-van Meerveld and McDonnell (2006a,b,c) observed a threshold ‘fill and spill’ response during storms events resulting from the irregular bedrock topography of depression storage of transient groundwater pockets that eventually spilled over a small bedrock ridge to form connected subsurface stormflow. Here we describe preliminary simulations with the Panola hillslope 3-D TOUGH2 model and present a test simulation of a 63 mm storm event compared to experimental data. This storm is above the 55 mm size at which ‘fill and spill’ behavior has been observed. Further application of the Panola hillslope model will extend to an investigation of hillslope classification.
MODELING SOIL MOISTURE PROCESSES AND RECHARGE UNDER A MELTING SNOWPACK

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ABSTRACT

Recharge into bedrock under a melting snowpack is being investigated as part of a study designed to understand hydrologic processes involving snow at Yosemite National Park in the Sierra Nevada Mountains of California. Snowpack measurements, accompanied by water content and matric potential measurements of the soil under the snowpack, allowed for estimates of infiltration into the soil during snowmelt, and percolation into the bedrock. Infiltration rates into the soil exceeded the permeability of the bedrock and caused ponding to be sustained at the soil-bedrock interface during the snow melt period. During a 7-day period with no measured snowmelt, drainage of the ponded water into the underlying fractured granitic bedrock was estimated to be 16 mm/day. The numerical simulator, TOUGH2, was used to reproduce the field data and evaluate the potential for vertical flow into the fractured bedrock or lateral flow at the bedrock/soil interface. The field data and model results support the notion that although most snowmelt on shallow soils overlying relatively impermeable upland bedrock tends to run off and contribute directly to streamflow, at least some of the snowmelt can infiltrate and potentially provide recharge to local or regional aquifers.
JOINT HYDROLOGICAL-GEOPHYSICAL INVERSION FOR SOIL STRUCTURE IDENTIFICATION

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ABSTRACT
Reliable prediction of subsurface flow and contaminant transport depends on the accuracy with which the values and spatial distribution of process-relevant model parameters can be identified. Successful characterization methods for complex soil systems are based on (1) an adequate parameterization of the subsurface, capable of capturing both random and structured aspects of the heterogeneous system, and (2) site-specific data that are sufficiently sensitive to the processes of interest. We present a stochastic approach where the high-resolution imaging capability of geophysical methods is combined with the process-specific information obtained from the inversion of hydrological data. Geostatistical concepts are employed as a flexible means to describe and characterize subsurface structures. The key features of the proposed approach are (1) the joint inversion of geophysical and hydrological raw data, avoiding the intermediate step of creating a (non-unique and potentially biased) tomogram of geophysical properties, (2) the concurrent estimation of hydrological and petrophysical parameters in addition to (3) the determination of geostatistical parameters from the joint inversion of hydrological and geophysical data; this approach is fundamentally different from inference of geostatistical parameters from an analysis of spatially distributed property 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 (GPR) travel times and hydrological data collected during a simulated ponded infiltration experiment at a highly heterogeneous site.
Session 12
REACTIVE GEOCHEMISTRY
INCORPORATION OF AQUEOUS REACTION AND SORPTION KINETICS AND BIODEGRADATION INTO TOUGHREACT

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ABSTRACT
The needs for considering aqueous and sorption kinetics and microbiological processes arises in many subsurface problems, such as environmental and acid mine remediation. A general rate expression has been implemented into TOUGHREACT, which considers multiple mechanisms (pathways) and includes multiple product, Monod, and inhibition terms. In this paper, the formulation for incorporating kinetic rates among primary species into the mass balance equations is presented. A batch sulfide oxidation problem is simulated. The resulting concentrations are consistent with simple hand calculations. A 1-D reactive transport problem with kinetic biodegradation and sorption was investigated, which models the processes when a pulse of water containing NTA (nitrylotriacetate) and cobalt is injected into a column. The problem has several interacting chemical processes that are common to many environmental problems: biologically-mediated degradation of an organic substrate, bacterial cell growth and decay, metal sorption and aqueous speciation including metal-ligand complexation. The TOUGHREACT simulation results agree very well with those obtained with other simulators.
ABSTRACT
This study reports a numerical investigation of the transport/retention mechanisms and rates of generated CO₂ in a radioactive waste repository in rock salt using TOUGHREACT. The ECO2 module is applied for equation of state. A 2-dimensional grid model is created with refinements in the regions of interests (waste and backfill). All cavities in the modelled repository area are backfilled with a Mg(OH)₂ based material. The pore volume is saturated with MgCl₂ rich brine. Hydrostatic and local geothermal gradients determine the initial conditions for the simulated area. The gas generation rates are derived from realistic scenarios reported earlier.

The ability of TOUGHREACT for more detailed applications of reactive transport under given repository conditions is investigated. The compositions of mineral phases and of the aqueous phase require an adaptation of the thermodynamic database.

The geochemical stability of a backfill based on Mg(OH)₂ under repository conditions is re-evaluated in further runs using TOUGHREACT. The impact of transport and retention of CO₂ dissolved in brine as well as the precipitation of carbonates as magnetite and calcite mainly on long term safety are analysed successfully using TOUGHREACT.
SOLUBILITY ENHANCED RETARDATION OF NEPTUNIUM IN THE UNSATURATED ZONE AT YUCCA MOUNTAIN, NEVADA

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ABSTRACT
(This abstract is in review by the Yucca Mountain Project.)
UNCERTAINTY IN THE REACTIVE TRANSPORT MODEL RESPONSE TO AN ALKALINE PERTURBATION IN A CLAY FORMATION

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ABSTRACT

The mineral alteration in the concrete barrier and in the clay formation around long-lived intermediate-level radioactive waste in the French deep geological disposal concept is evaluated using numerical modeling. There are concerns that the mineralogical composition of the surrounded clay will not be stable under the high alkaline pore fluid conditions caused by concrete (pH~12). Conversely, the infiltration of CO₂-rich groundwater from the clay formation into initially unsaturated concrete, at the high temperature (T~70°C) produced from the decay of radionuclides, could cause carbonation, thereby potentially affecting critical performance functions of this barrier. This could also lead to significant changes in porosity, which would affect aqueous diffusive transport of long-lived radionuclides. All these processes are therefore intimately coupled and advanced reactive transport models are required for long-term performance assessment. The uncertainty in predictions of these models is one major question that must be answered. A mass-transfer model response to an alkaline perturbation in clay with standard model values is first simulated using the two-phase non-isothermal reactive transport code TOUGHREACT. The selection of input parameters is thereafter designed to sample uncertainties in a wide range of physico-chemical processes without making a priori assumptions about the relative importance of different feedbacks. This “base-case” simulation is perturbed by setting a parameter to a minimum, intermediate or maximum value or by switching on/off a process. This sensitivity analysis is conducted using grid computing facilities of BRGM (http://iggi.imag.fr).

Our evaluation of the preliminary results suggests that the resaturation and the heating of the near-field will be of long enough duration to cause a limited carbonation through all the width of the concrete barrier. Another prediction is the possibility of self-sealing at the concrete/clay interface. Further research is however required to discuss the effect of such evolution on the desirable performance function of both barriers.
Session 13
NUCLEAR WASTE
TOUGH2/ITOUGH2 ANALYSIS OF THE GAS MIGRATION TEST (GMT) AT THE GRIMSEL TEST SITE (SWITZERLAND)

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ABSTRACT

The Gas Migration Test (GMT) at the Grimsel Test Site (GTS) underground laboratory in central Switzerland was designed to investigate gas migration through an engineered barrier system (EBS). The EBS consists of a concrete silo embedded in a sand/bentonite buffer emplaced in a silo cavern that intersects a shear zone in the surrounding granite host rock. The experiment was performed in a series of stages: (1) excavation of the access drift and silo cavern, (2) construction and instrumentation, (3) saturation of the EBS, (4) water tests, (5) long-term gas injection at different rates, (6) post-gas water testing, (7) gas injection with a “cocktail” of gas tracers, and (8) depressurization and dismantling.

A numerical model of the GMT was implemented with the two-phase flow code TOUGH2, representing the GMT silo with a multi-layered radially-symmetric mesh and the surrounding water-conducting granite shear zone with a 2D vertical feature. The different stages of the experiment were simulated in sequence using the results of the previous stage as initial conditions for the subsequent stage. Two-phase flow parameters for the EBS were derived from laboratory experiments on core samples of the different materials that comprise the EBS, while hydraulic properties of the sand/bentonite and of relevant interface zones were calibrated to the pressure responses in the silo and selected piezometers in the sand/bentonite. The results of the numerical modeling of the GMT experiment show that the main features and processes of the different stages of the experiment could be reasonably well reproduced. In addition to standard two-phase flow processes, inferred coupled hydromechanical phenomena were implemented using pressure-dependent permeability relationships on interfaces at the top of the silo and between the sand/bentonite and the granite host rock. Changes in the hydraulic properties of the sand/bentonite that occurred during the different test stages were incorporated by updating material properties for the simulation of the test stages. Time-dependent permeability relationships were calibrated for the tunnel seal to account for the gradual decrease in water inflow from the upper cavern into the access tunnel and the drift.
SIMULATIONS OF THE HYDROGEN MIGRATION OUT OF INTERMEDIATE-LEVEL RADIOACTIVE WASTE DISPOSAL DRIFTS USING TOUGH2

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ABSTRACT
Corrosion and radiolysis processes cause hydrogen to be generated in a repository for intermediate-level radioactive waste (ILW) for at least 10,000 years after the closure of the facility. Two model configurations have been used for the TOUGH2 simulations to investigate the impact of the hydrogen in terms of the pressure build-up and the gas saturation level in the disposal drift and in the surrounding argillaceous rock formation.

1. Cross-section (2D) through the disposal drift, perpendicular to its axis: The overpressure caused by the hydrogen has been found to be less than the expected frac pressure, for the production rate and scheme considered.

2. Longitudinal vertical section (3D) through the disposal, access and main drifts: The flow of gas/water from the disposal drift through/around the sealing plug in the access drift has been found to have limited impact on the overpressure inside the disposal drift.
THREE DIMENSIONAL ANALYSES OF COMBINED GAS AND NUCLIDE TRANSPORT IN A REPOSITORY CONSIDERING COUPLED HYDRO-GEOMECHANICAL PROCESSES

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ABSTRACT
To study the coupled hydrologic-geomechanical processes and their influence on gas and nuclide transport in a two phase flow configuration in a porous medium, a linear coupling of the hydrodynamic code TOUGH2 and the mechanic code FLAC3D is described and applied to analyze three dimensional isothermal gas and nuclide transport in a repository for nuclear waste in a deep geological rock formation like clay rock or rock salt. According to stress dependent hydrological properties such as porosity, permeability and capillary pressure, the influence of coupled processes on a two phase flow can be relevant. The coupled analyses can be applied to quantify the safety margin related to hydro-fracturing due to fluid pressure build-up.
JOINT INVERSION OF GROUND-PENETRATING RADAR
AND THERMAL-HYDROLOGICAL DATA
COLLECTED DURING A LARGE-SCALE HEATER TEST

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Sumit Mukhopadhyay, and Yvonne Tsang

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ABSTRACT
(This abstract is in review by the Yucca Mountain Project.)
Session 14
GAS HYDRATES
ESTIMATION OF COMPOSITE THERMAL CONDUCTIVITY OF A HETEROGENEOUS METHANE HYDRATE SAMPLE USING ITOUGH2

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ABSTRACT
We determined the composite thermal conductivity ($k_\theta$) of a porous methane hydrate sample (composed of hydrate, water, and methane gas) as a function of density using iTOUGH2. X-ray computed tomography (CT) was used to visualize and quantify the density changes that occurred during hydrate formation from granular ice. The composite thermal conductivity was estimated and validated by minimizing the differences between the observed and the predicted thermal response using history matching. The estimated density-dependent composite thermal conductivity ranged between 0.25 and 0.58 W/m/K.
GAS PRODUCTION BY DEPRESSURIZATION FROM HYPOTHETICAL CLASS 1G AND CLASS 1W HYDRATE RESERVOIRS

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ABSTRACT

A study on recovery of gas from a Class 1G hydrate deposit (mobile gas in the hydrate zone) and a Class 1W hydrate deposit (mobile water in the hydrate zone) is presented in this text. During the production from these reservoirs, a second dissociation front appears at the top of the hydrate interval. This front develops and advances downward in addition to the original hydrate interface. Two production schemes; with and without well-bore heating (case A and case B), show the same replenishment rate of produced hydrate under the conditions studied. For the case with well-bore heating and 20 years production life, hydrate dissociation contributes up to 50% of the production rate and up to 38% of the cumulative volume of produced gas. High-low alternating hydrate saturation layers (hydrate lens) are observed in both types of reservoirs for both cases of well-bore heating.
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