Modeling Coupled Geomechanical and Flow Processes Associated with Nuclear Waste Disposal: Some Recent Studies at LBNL

Presented by Jens Birkholzer* and Jonny Rutqvist
Lawrence Berkeley National Laboratory

*UFD Technical Lead for International Activities

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Outline

- **Part 1: Current US and LBNL Disposal R&D**
  - Status of the United States Repository Program
  - DOE Used Fuel Disposition Campaign (UFD)
  - Brief Overview of LBNL’s Current and Planned Clay Disposal R&D Activities within UFD

- **Part 2: Coupled THM Modeling At LBNL**
  - THM Modeling of the Yucca Mountain Drift Scale Test
  - TOUGH-FLAC Simulator
  - Extensions to TOUGH-FLAC for Clay and Bentonite Modeling
  - Preliminary Clay and Bentonite Applications
Nuclear Waste Program Status in the United States

- In 2010, the Obama administration officially withdrew its pending license application for Yucca Mountain.
- A Blue Ribbon Commission was established to review for nuclear waste storage, processing and disposal, and just released a final report providing recommendations for a safe long-term waste solution.
- DOE’s Office of Nuclear Energy (DOE-NE) is now responsible for nuclear waste disposal activities, replacing the Office of Civilian Radioactive Waste Management (OCRWM).
- NE nuclear waste activities reside within the Used Fuel Disposition (UFD) Campaign which was established in 2009.
- UFD’s mission is to identify alternatives to Yucca Mountain and conduct research and technology development to enable long-term storage and disposal of used nuclear fuel and wastes.
- No regulatory framework exists for sites other than Yucca Mountain, and only generic (site-independent) disposal R&D can be conducted.
Several lawsuits are still pending charging that DOE had no right to withdraw license application for Yucca Mountain.

NRC has continued its evaluation of the license application, and has recently been forced by congress to release its Safety Evaluation Report (heavily redacted).

State of Nevada recently forced NRC to restart legal process of license hearings and invitations were sent out before process was stopped.

Political pressure is mounting in congress about the sudden end of the Yucca Mountain license application.

House Committee on Energy and Commerce recently recommended to place $25 M to “continue the Yucca Mountain license application activity.”
The BRC strongly supports mined geologic repositories as the preferred path forward. It also recommends R&D on deep borehole disposal, but its support for this concept appears to be more lukewarm.

The BRC supports the generic work being done by the Used Fuel Disposition campaign, including research on different geological media and design of better engineered barriers.

The BRC supports the “safety case” concept as consisting of much more than a narrow reliance on quantitative PA analyses.

The BRC suggests that a new approach is needed to site and develop nuclear waste management and disposal facilities in the United States in the future, which would need to be 1) consent-based, (2) transparent, (3) phased, (4) adaptive, (5) standards- and science-based.
Used Fuel Disposition Campaign
Structure

- **DOE Nuclear Energy**
- **Oversees UFD Activities**

- Used Fuel Disposition Campaign

- UFD management coordinates R&D activities of individual national laboratories
- National laboratories are sub-contractors to DOE to conduct specific R&D projects
UFD Work Activities

- Two main areas: **Storage & Transportation Research** and **Disposal Research**
- Disposal Research is not site specific
- R&D Gap Evaluation, Lessons Learned Activities, Inventory Assessments, and FEPs Analysis support R&D planning
- International collaboration is viewed as a central part of future R&D
UFD Disposal Research Activities

Engineered Barrier Systems (EBS)  
Natural Systems Evaluations

NEAR FIELD

EBS BUFFER  
Backfill, Liner, Seals  
[BENTONITE BUFFER]  
[CLAY, SALT BACKFILL]  
[DEEP BOREHOLE SEAL]

GEOSPHERE

Host Rock and Other Geologic Units  
[GRANITIC ROCKS]  
[CLAY/SHALE]  
[SALT]

BIOSPHERE

Surface

Thermal Load Management & (Repository) Design Concepts

Disposal System Environment Modeling

SUPPORT, ANALYSIS & EXPERIMENTAL ACTIVITIES

- Engineered Materials Performance  
- Features, Events & Processes  
- Low Level Waste Disposition Issues  
- Inventory Projections  
- (corrosion, degradation studies)  
- (how R&D is organized and prioritized)  
- (part of total nuclear waste consideration)  
- (LLW/HLW, used fuel, open → closed fuel cycles)
Disposal R&D Planning and Objectives

Objectives:
- Develop science and engineering tools
- Confirm advanced modeling approaches
- Provide sound technical basis for disposal system evaluations
Relevant R&D Issues in Clay/Shale Host Rock

**Disturbed Zone (DZ) Evolution:**
- evolution of stress-changes due to excavation
- fracturing due to ventilation and thermal stresses
- self-sealing processes
- modeling excavation and emplacement

**Transport Processes:**
- multi-species diffusion through compacted clays
- advective transport in near-field disturbed zone (e.g., continuity of fracture pathways)
- impact of bedding planes on fracture transport

**Geological Conditions and Processes:**
- regional assessment of clay/shales in US
- fracture/fault reactivation
- intrusion and collapse structures
- heterogeneity and in-situ stress conditions

**Coupled Processes:**
- long-term property changes (creep, subcritical crack growth)
- gas generation and pressure buildup
- constitutive relationships for deformation and hydraulic properties
- salinity and other geochemical effects on swelling
- hyperalkaline solutions
- waste heat effects on chemistry/mineralogy
- interaction between host rock and EBS components
International Activities in Disposal R&D

- Yucca Mountain was so unique with respect to design and geologic environment that overlap with international R&D was quite limited.
- With UFD addressing alternative disposal designs and geologic environments, DOE views international collaboration as a very beneficial strategy of advancing R&D.
- Next step is engagement of UFD researchers in ongoing or upcoming underground in situ experiments (and related lab/modeling work).
- DOE is in the process of establishing formal collaborative R&D arrangements with three ongoing international initiatives.

Mont Terri: International underground research laboratory (URL) in clay in Switzerland

Colloid Formation and Migration Project at Grimsel: URL in granite in Switzerland

DECOVALEX (Development of Coupled Models and their Validation against Experiments): Model comparison against experiments.
Brief Overview of Current or Planned Clay/Shale Research Activities at LBNL
Regional Assessment of US Clay/Shale Formations

- Assessment of geologic/hydrologic criteria for clay/shale host rocks
- Combined with other criteria (societal, land use, population density) in a GIS system
Clay and Bentonite Diffusion

Diffusive Double Layer

Molecular Dynamics

Reactive Transport Modeling

Diffusion Experiments
- Diffusion cell experiments to characterize the effects of chemical speciation (anion, cation, neutral) on apparent diffusion rates
- Employ synchrotron X-ray spectroscopic and electron-based imaging techniques to evaluate diffusion on scales of microns up to one mm
Disturbed-zone behavior strongly affected by THMC processes related to excavation, ventilation, emplacement of EBS materials, and heat. DZ flow paths depend on fracture generation and healing, as well as longitudinal interconnectedness.

Develop a predictive modeling capability that allows simulating the evolution of small-scale to large-scale disturbed zone flow paths as a function of time and relevant THMC conditions.
Disturbed Zone Coupled Processes Modeling

**TOUGH-FLAC: Coupled THM**

- Fluid and heat transport
- Coupling module
- Stress and strain analysis

**TOUGHREACT: Coupled THC**

**TOUGHREACT-FLAC: Coupled THMC**

- New constitutive relationships for clay/shale/bentonite behavior
Discrete Fracture-Matrix Models for DZ

- Develop discrete modeling capability for flow and transport in DZ
- Evaluate continuity of fracture flow and transport paths
- Include impact of fracturing, self-sealing, and other coupled processes
- Coupling of fracture generation propagation code with flow and transport simulator

Morphology-Based Discrete Damage Models with Rigid-Body Spring Network (Asahina, 2011)

Drying Shrinkage Patterns (Asahina, 2011)
Planned Experiments

Bentonite Temperature Constraints
• Bentonite testing at high T and P, variable S
• Mechanical and chemical analysis

Fracture Growth and Sealing
• Image rock properties and fracture growth/sealing during chemical/thermal/stress alteration
• Model THMC processes with TOUGHREACT-FLAC3D and fracture damage codes

Triaxial Loading and Fluid Flow

ALS Synchrotron Micro-CT Imaging

- Grain
- Calcite

200 microns
Coupled THM Modeling at LBNL
In the early and mid-1980s Coupled processes associated with nuclear waste repositories were discussed for the first time in a series of workshops and international symposiums at Berkeley Lab (Tsang, 1987).


**TOUGH-FLAC** code for coupled THM analysis under multi-phase flow conditions (Rutqvist et al. 2002, Rutqvist and Tsang 2003)
Since the early 1990s, LBNL has participated in an international cooperative project **DECOVALEX** (DEvelopment of COupled MOdels and their VALidation against EXperiments). DECOVALEX is sponsored by nuclear waste agencies in 10 countries involving some 20 research organizations.

- LBNL Research Team for SKI (Sweden), DOE (US), NDA (UK).
- 4 journal special issues, 3 books, and special conferences.
- An excellent venue for international collaboration!
A large number of Bench Mark Tests (BMTs) focusing on long-term coupled THM processes, both in the near field and EBS, and surrounding rocks (crystalline rock):

- The US unsaturated zone repository
- The Japanese H12 repository design with vertical deposition holes.
- The KBS-3 for the Swedish proposed site.
- The Canadian conceptual design for a repository in granite with horizontal deposition tunnels.
- The Spanish EBS system emplaced in granite with horizontal deposition tunnels.
Coupled THM Modeling at LBNL 1980-2009 (4)

1) The Kamaishi Mine heater test, Japan.
2) The FEBEX in situ experiment at the Grimsel Test Site, Switzerland.
3) The Drift Scale Test at Yucca Mountain, Nevada.
4) The Tunnel Sealing Experiment (TSX) at URL Canada.
5) The French Tournemire site in indurate clay.

Yucca Mountain Drift Scale Test
Nevada (1997-2007)

FEBEX In Situ Heating Test
Switzerland (1997-??)
Yucca Mountain Drift Scale Test (1997-2007)

Conceptual Model for Stress versus Permeability Coupling

\[ b = b_r + b_{max} \cdot \exp(d \cdot \sigma_n) \]

Fracture Aperture, \( b \)

Normal Stress, \( \sigma_n \)

Two-Dimensional Model

Dual-Permeability Medium: Matrix & Fracture

Heated Drift
• Thermally induced stresses near the heated drift tightens fractures to a smaller aperture
• At about 15 to 25 m above the heater drift there is a reduction in horizontal stress that results in opening of vertical fractures
• TH processes (including evaporation, vapor flow, condensation) causes drying and wetting of fractures
Permeability Correction Factor $F_k = \frac{k}{k_i}$

Test interval 76:4 located close to the heat source:

- **Increased Compressive Stress**
- **Increased Liquid Saturation**
- **Decreased Permeability**

Wet conditions:
- **Low Stress**: Reduced $k$
- **High Stress**: Reduced $k$

Dry conditions:
- **Low Stress**: Increased $k$
- **High Stress**: Increased $k$

**Reduced $k$**

**Increased $k$**

**Decreased Permeability Correction Factor $F_k$**

**Heating**

**Reduction caused by thermal stress normal to vertical fractures**

**Additional reduction due to wetting in fractures**

- **Measured**
- **Calculated TM**
- **Calculated TM+TH**

**76:4**

- $k_i = 8.62 \times 10^{-14}$ m$^2$
- $L = 10.0$ m
Developed as a pragmatic approach for modeling coupled multiphase flow, heat transport and geomechanics, by linking the two established codes TOUGH2 and FLAC3D.

A great advantage with the adopted approach is that both codes are continuously developed (by others) and widely used in both academia and industry.
TOUGH2 part: Fluid and heat transport

- Research code that is widely used in the fields of geothermal energy, environmental hydrology, reservoir engineering, CO$_2$ sequestration and methane-hydrates
- Calculates coupled fluid flow and heat transport
- Multiphase fluid flow (i.e. gas and liquid)
- Multi-component (i.e. CO$_2$, water, salt)
- Many specially developed fluid property Equation of State (EOS) modules (e.g. brine-CO$_2$ mixture under supercritical conditions, and methane-hydrates)
A commercial code for rock and soil mechanics, which has been applied for soil and rock slope stability, mining, tunneling, oil and gas reservoir engineering.

- Calculates coupled hydrological-mechanical and thermo-mechanical analysis of geological media in 3D.
- Elasto-plastic, visco-elastic, poroelastic.
- Various constitutive models for mechanical behavior of soil, rock and faults.

**FLAC3D part:** Stress and strain analysis.
Two codes are coupled through a coupled Thermal-Hydrological-Mechanical (THM) model of hydrate-bearing sediments:

**Direct couplings:** Pore volume change, effective stress, thermal strain, and swelling

**Indirect couplings:** Changes in mechanical and hydraulic properties
Nuclear Waste Disposal: Geomechanics

Geomechanics

- Fracture flow paths exist ubiquitously in host rock
- Question about geomechanical changes is not whether new fractures are being created in the perturbed state
- Rather the question is how permeabilities of existing fractures may be affected over time

Unsaturated Fractured Tuff

Yucca Mountain Site

Clay/Shale Repository (e.g., Switzerland)

Saturated Low-Permeability Host Rock

Geomechanics

- Undisturbed host rock is virtually impermeable
- Question about geomechanical changes is whether connected fracture pathways may be generated in the disturbed zone and how they evolve over time
- Perturbation stems from excavation, ventilation, backfilling, and heating
THE BBM MODEL AND TOUGH-FLAC

Implemented the Barcelona Basic Model (BBM) into the TOUGH-FLAC simulator for rigorous modeling of thermo-elasto-plastic behavior of unsaturated soils (Gens. 1995)
### Testing and Documentation of BBM in Tough-FLAC

Tests against literature data

<table>
<thead>
<tr>
<th>Test</th>
<th>Processes</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>AGJ1</td>
<td>Volumetric deformation induced by wetting at increasing confining stress</td>
<td>Alonso et al. (1990)</td>
</tr>
<tr>
<td>AGJ2</td>
<td>Effect of alternate application of load and suction.</td>
<td>Alonso et al. (1990)</td>
</tr>
<tr>
<td>AGJ4</td>
<td>Shear tests for different suction.</td>
<td>Alonso et al. (1990)</td>
</tr>
<tr>
<td>AGJ6</td>
<td>Shear tests on partially saturated Kaoline</td>
<td>Alonso et al. (1990)</td>
</tr>
<tr>
<td>K&amp;A1</td>
<td>Compression test of MX80 bentonite with constant suction</td>
<td>Kristensson and Åkesson (2008)</td>
</tr>
<tr>
<td>K&amp;A2</td>
<td>Elastoplastic behavior of during a swelling test of MX-80 bentonite</td>
<td>Kristensson and Åkesson (2008)</td>
</tr>
<tr>
<td>K&amp;A3</td>
<td>Triaxial compression of MX-80 bentonite</td>
<td>Kristensson and Åkesson (2008)</td>
</tr>
<tr>
<td>GTS1</td>
<td>Odometer and direct shear test on bentonite-sand mixture</td>
<td>Romero et al (2002)</td>
</tr>
</tbody>
</table>

Example: K&A3 Triaxial Compression test of MX80 bentonite

![Graph showing TESTING AND DOCUMENTATION OF BBM IN TOUGH-FLAC](image)

Good agreement with independent model results and experimental data.
Study of a bentonite back-filled repository in clay host rock

- Use of Opalinus clay stone properties of host rock
- Bentonite properties from FEBEX in situ test in Grimsel, Switzerland.
- Waste emplacement in bentonite-backfilled horizontal tunnels
- GDSE heat load
- Adjust tunnel and canister spacing to limit max temperature to less than 100°C

Modeling sequence: 1) Pre-excavation, 2) Excavation, 3) Waste and buffer emplacement, 4) Post-closure coupled processes modeling
THM driven buffer/rock interactions: 1) Delayed buffer resaturation due to low rock permeability, 2) thermal-pressurization in rock affects pressure and stress evolution in buffer
Complex THM evolution of buffer: buffer modulus changes orders of magnitude as a result of stressing and saturation changes and the final porosity distribution becomes slightly uneven in this case.
Buffer swelling important for rock stress evolution at the rock wall (provides confining stress)
New Constitutive Relationships

**BBM Model**

The Barcelona Basic Model (BBM) describes a large number of typical features of the mechanical behavior of unsaturated clay/bentonite (Alonso and Gens, 1992; Gens et al. 2006)

>> Mechanical behavior as a function of saturation

**Dual-Structure Model**

Dual-structure models allow to establish a relation between swelling pressure and chemical variables. Microstructure describes diffuse double layer for interactions at particle level.

>> Mechanical behavior as a function of chemistry

**Modified Hooke’s Law**

The modified Hooke’s law considers rock mass as a combination of hard and soft parts and derived results are consistent with a large number of experimental observations.

>> Improved relationship between stress, fracture aperture, and permeability
Current Status of LBNL Clay Modeling

- We are expanding our coupled processes modeling capabilities from crystalline fractured rocks to clay host rock environments.
- Extension of TOUGH-FLAC-BBM to Barcelona Expansive Model (BExM) that considers micro and macro structural interactions (ongoing)
- This approach and model development will serve as a framework for further extension to coupled THMC behavior (i.e. adding coupling to chemistry)
- Test the models against published laboratory data (including irreversible behavior upon cyclic wetting-drying, and swelling under different water salinity)
- Apply TOUGH-FLAC and BExM within the international DECOVALEX project and Mont Terri field experiments
UFD Storage & Transportation Activities

- UFD Storage & Transportation objectives roll up to three points:
  - Develop the technical basis for extended storage of used nuclear fuel
  - Develop the technical basis for fuel retrievability and transportation after extended storage
  - Develop the technical basis for transportation of high burnup used nuclear fuel
LBNL Focus: Clay Repositories

- Review of Science Gaps
- Prioritization of R&D Opportunities
- Capability Development of Tools, Methods, Models
- Improved Process Understanding of Generic Systems
- Validation with Data from Generic URLs

A Review of Key Processes and Outstanding Issues Related to Radioactive Waste Repositories in Clay Formations

Fuel Cycle Research & Development

Prepared for U.S. Department of Energy
Used Fuel Disposition Campaign

Chin-Fu Tsang, LBNL
Jens Birkholzer, LBNL
Hui-Hai Liu, LBNL
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Disturbed Zone Flow Paths

DZ flow paths depend on fracture generation and healing, as well as longitudinal interconnectedness.

Develop a predictive modeling capability that allows simulating the evolution of small-scale to large-scale disturbed zone flow paths as a function of time and relevant mechanical-thermal-chemical conditions.