Used Fuel Disposition Campaign

Process Modeling and Investigations For Clay/Shale Repositories: Natural Barrier System

Hui-Hai Liu, Jim Houseworth, Jonny Rutqvist, Fei Chen, Liange Zhang, Jens Birkholzer, Lianchong Li, Daisuke Asahina, Stefan Finsterle, Seiji Nakagawa, Tim Kneafsey, Jonathan Ajo-Franklin
Lawrence Berkeley National Laboratory

UFD NBS Telecom
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FY13 Work Activities

- **THMC Model Capabilities for Clay Repositories**
  - Coupled Thermal-Hydrological-Mechanical (THM) Discrete Fracture Model (DFM) for Argillaceous Rock, Including Fracture Propagation (Asahina/Houseworth/Birkholzer)
  - Constitutive relationships and HM Modeling of the Mine-by Test at Mont Terri (Liu/Li/Birkholzer)

- **Thermal Limit Testing**
  - High Temperature Laboratory Experiments (Nakagawa/Kneafsey/Ajo-Franklin/Birkholzer)
  - Detailed Mechanistic Modeling of THMC Alterations (Zheng/Finsterle/Birkholzer)
  - Impact of High-Temperature THMC Changes on Radionuclide Transport and Other PA drivers (Finsterle/Zheng/Birkholzer)

- **Radionuclide Interaction and Transport in Representative Geologic Environments**
  - Modeling Radionuclide Interaction and Transport in Clay Formations (Zheng)
FY13 Work Activities

- **Modeling hydrologic flows in representative geologic media**
  - *Investigation of Non-Darcy Flow Behavior in Clay* (Liu/Li/Birkholzer)

- **International Collaborations**
  - *THM Modeling of FE Heater test at Mont Terri URL* (Rutqvist/Chen/Birkholzer)
  - *Discrete Fracture Interpretation of the HG-A Test at Mont Terri* (Asahina/Houseworth/Birkholzer)

- **Deliverables**
  - Level 2 - *THMC modeling of the near field evolution of a generic clay repository: Model validation and demonstration* (08/15/2013)
  - Level 4 - *Report on THMC effects on radionuclide transport in a clay repository* (8/15/13)
  - Level 4 - *Report on hydrologic flows in low permeability media* (11/13/13)
  - Level 4 - *Report on international collaborations on FE heater and HG-A tests* (11/6/13)
The two-part Hooke’s model (TPHM) was implemented into the TOUGH-FLAC3D code and tested against data from the Mine-by Test at Mont Terri URL.

A new three-dimensional DFN modeling tool for coupled flow and geomechanical processes, capable of addressing fracture initiation and propagation, was developed.

Preliminary TH and THM model simulations of the FE test at the Mont Terri URL were performed for the purpose of validating modeling capabilities for THM processes.

The TOUGHREACT-FLAC3D (THMC) simulator was further enhanced and used for a preliminary evaluation of the THMC impact on radionuclide transport processes.
Argillaceous formations that may be available for nuclear waste disposal are typically saturated
- Suitability of argillaceous rock rests in large part on an effective and robust low-permeability attribute.

Fracturing is the most likely threat to the low-permeability attribute of an argillaceous rock:
- Repository-induced THMC disturbances cause fracturing along repository openings.
- Natural disturbances (e.g., abnormal pressure-induced hydrofractures) cause fracturing at the formation scale.

Fractures in argillaceous rock tend to be short-lived because of self-sealing behavior:
- Can lead to poorly-connected fractures during fracturing episode.
- Potential fracture-matrix cross-flow interaction.
- Coupled process DFMs more representative.

Modified from Bauer et al., 2003
Cosgrove, 2001

Mercia Mudstone, Bristol Channel Basin, UK: natural hydraulic fractures filled with sand and gypsum.

Cosgrove, 2001

Blümling et al., 2007
Coupled Thermal-Hydrological-Mechanical (THM) Discrete Fracture Model (DFM) for Argillaceous Rock

- **THM dynamic fracturing model based on coupling** TOUGH2 thermal-hydrological model with Rigid-Body-Spring Network (RBSN) geomechanical fracture-damage model
  - Both operate on same Voronoi grid; fractures are mapped onto edges of Voronoi cells
  - Flow /transport and coupled HM /TM processes have been analyzed and compared with analytical models or alternative numerical models
  - Fracture initiation and propagation coupled with hydrologic model has been analyzed for problem of desiccation-induced fracturing

- **FY13 work activities**
  - Validate desiccation-induced fracturing model against experimental data from literature
  - Implement coupling for
    - strain effects on porosity, permeability
    - fluid pressure-geomechanics for hydraulic fracturing
  - Evaluate repository-induced and natural fracturing, more complex fracture networks, and self-sealing
  - Conduct HG-A modeling (see international collaboration)
Objective

Constitutive relationships are key elements for modeling coupled processes. The major objective is to develop and validate the relationships for clay rock.

Approach

Based on two-part Hook’s model and TOUGH2-Flac3D.

FY13 Work

- FY12 work is a preliminary 2D study that cannot capture all the important features of the Mine-by test at Mont Terri. A 3D model will be developed in FY13 to incorporate all the events in the test.
- Modeling results will be compared with available data from the Mine-by test including displacement and pore pressure as a function of time.
Thermal Limit Testing: High Temperature Laboratory Experiments

Objective:
Investigate the impact of heat-induced chemical alterations (smectite-to-illite transformation) of buffer and backfill materials (bentonite) and clay host rock on their geomechanical and hydrological properties (mechanical strength, permeability, seismic velocity)

Approach
- Test bentonite clay with a range of (1) porosity (density), (2) water content (below saturation), (3) KCl concentration
- Multiple samples are heated (from 100°C to 300°C) in sealed, spring-loaded cylindrical titanium miniature pressure vessels
- Changes in volume, acoustic velocity, permeability, and mechanical strength are examined for different heating durations
- Chemical/mineral testing in collaboration with LANL
- Integration with modeling work (TOUGHREACT-FLAC3D)

FY2013 Work
- Fabrication of miniature pressure vessels
- Preparation of experimental system
- Acquisition and baseline characterization of clay samples
- Preliminary experiments for verifying system performance
Motivation

- Illitization, the transformation of smectite to illite, results in a loss of swelling capability of EBS and clay host rock.
- The rate of illitization increases as temperature increases, with about two orders of increase if temperature increase from 100 to 150 °C according to a theoretical model.
- However, many factors such as the availability of potassium, proton and water constrain the illitization. A model that could consider all the relevant factors is needed to evaluate the illitization in EBS and clay host rock.
- The mechanical and hydraulic consequences of illitization also need to be evaluated.
Objective:
Evaluating the degree of illitization in EBS and clay host rock under high temperature (100 to 200 °C) conditions and the subsequent effects on the mechanical and hydraulic properties of EBS and clay host rock

Approach
- Detailed mechanistic modeling with TOUGHREACT and TOUGHREACT-FLAC3D

FY2013 Work
- Establishing the geochemical conceptual model based on detailed understanding of the reaction network of illitization under typical clay repository environment.
- Developing a THC model to evaluate the degree of illitization in EBS and clay host rock for temperature from 100 to 200 °C under different geochemical and hydraulic conditions.
- Developing coupled THMC model to assess the swelling pressure and hydraulic conductivity changes as a consequence of illitization
Thermal Limit Testing:
Impact of High-Temperature THMC Changes on Radionuclide Transport and Other PA drivers

Objective:
Develop modeling methodology supporting PA of a high-temperature repository
Design and optimization of high-temperature repository

■ Approach
- Identify high-temperature scenarios and related effects (see previous task)
- Determine method to include THMC effects in system-level models
  ▪ Coupled process models
  ▪ Empirical correlations
  ▪ Reduced-order modeling
- Define performance measures to be used for analysis
- Develop simulation and uncertainty quantification methodology for evaluation of (potentially correlated) scenarios and parameter cases
- Determine scenarios and parameters with significant influence on high-temperature repository performance
- Outline future analysis and optimization studies
Objective:
Modeling radionuclide reactive transport in clay formation with a focus on using data from other labs for surface complexation model improvement and further enhancing the THMC modeling capability

■ Approach
  - Detailed mechanistic modeling with TOUGHREACT

■ FY2013 Work
  - Building surface complexation reaction network based on experimental data for U and Pu sorption on clays and iron hydroxidizes from UFD (e.g. U sorption study at LBNL or Pu sorption study at LLNL) and other sources. If possible, compile these reactions into a consistent database
  - Incorporating temperature effect into surface complexation reactions and testing them with available data
  - Developing a THC model to evaluate the migration of U and Pu in clay formation under different geochemical and hydraulic conditions
  - Implementing more constitutive mechanical-chemical coupling relations such as linking BExM (Barcelona Expansive Model) with chemical reactions to enhance our capability of simulating THMC processes
Excavation Damaged Zone (EDZ) is a critical feature impacting repository performance.

Desaturation and resaturation are important for EDZ evolution (shrinkage-induced fracture; fracture self-sealing).

Water flow from host rock to EBS is critical for buffer to function (swelling).
Approach and FY13 Work Scope

- Development of approach to incorporate temperature impact based on data from petroleum literature.
- Development of a modeling capability for non-Darcy flow by incorporating FY12 development into TOUGH2 code.
- Integration with LANL’s neutron-scattering test results.

Cui et al. (2008)

Miller and Low (1963)
Objective:
In situ investigations and model validation related to repository induced coupled thermo-hydro-mechanical (THM) processes and their effect on the host rock

Approach
- TOUGH-FLAC simulator using layered (anisotropic) rock mass THM model of Opalinus Clay and Barcelona Basic Model (BBM) for bentonite THM behavior.

FY2013 Work
- Develop a 3D TOUGH-FLAC model (grid) of the FE Heater test based on current preliminary 2D model.
- Conduct modeling of laboratory THM experiments for parameterization of BBM material parameters related to granular bentonite buffer materials.
- Modeling of FE tunnel excavation with comparison to measured rock mass responses when data available.
- 3D model predictions of THM evolution during heating test
The HG-A test is being conducted at the Mont Terri URL
- HG-A microtunnel is 13 m long, 1 m in diameter
- array of instrumented boreholes measuring stress, strain, fluid pressure, and water content during water and gas injection

The test is focused on:
- conceptual understanding of damage zones around cylindrical excavations
- hydraulic conductivity of the Opalinus Clay on the tunnel scale
- self-sealing processes along the damage zones around backfilled tunnels
- gas leakage rates from sealed tunnel sections

For FY13, the coupled THM-DFM will be used to examine test data and interpret EDZ
- disturbed zone fracturing
- hydraulic behavior
- fluid-displacement processes
- fracture self-sealing

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