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Fuel Cycle Technologies

R&D Activities Supporting Disposal in Clay/Shale Repositories

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DOE-NE Used Fuel Disposition Campaign

Presented to the

Nuclear Waste Technical Review Board

Fall 2011 Board Meeting

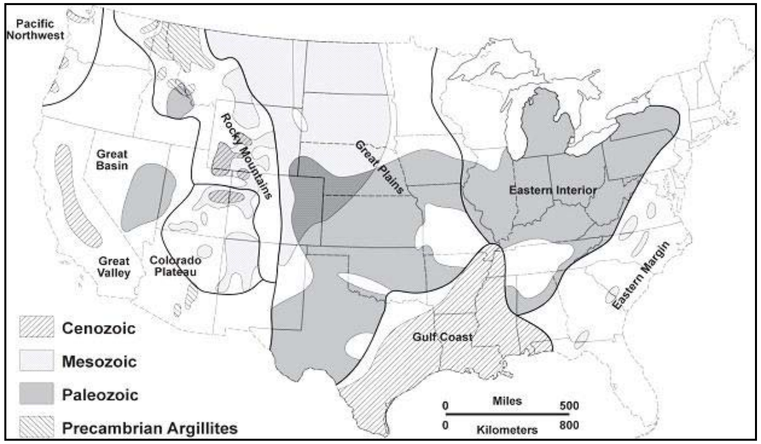
Salt Lake City, Utah, September 13, 2011

Outline

- **Background on Clay/Shale Repositories**
- **R&D Planning and Objectives**
- **Key Science Issues and Examples of Disposal R&D**
- **THMC Coupled Behavior in Disturbed Zone**
  - Capability Development
  - Improved Process Understanding
  - Field-Based Confirmation
- **Diffusion in Compacted Clay and Bentonite**
  - Capability Development
  - Improved Process Understanding
  - Field-Based Confirmation

Reasons for Interest in Clay/Shale Repository Environments

- Clay and shale formations have several features conducive to waste isolation
  - Stable
  - Low permeability
  - Diffusion dominated
  - Relatively homogeneous
  - Self sealing
  - Sorptive
  - Reducing

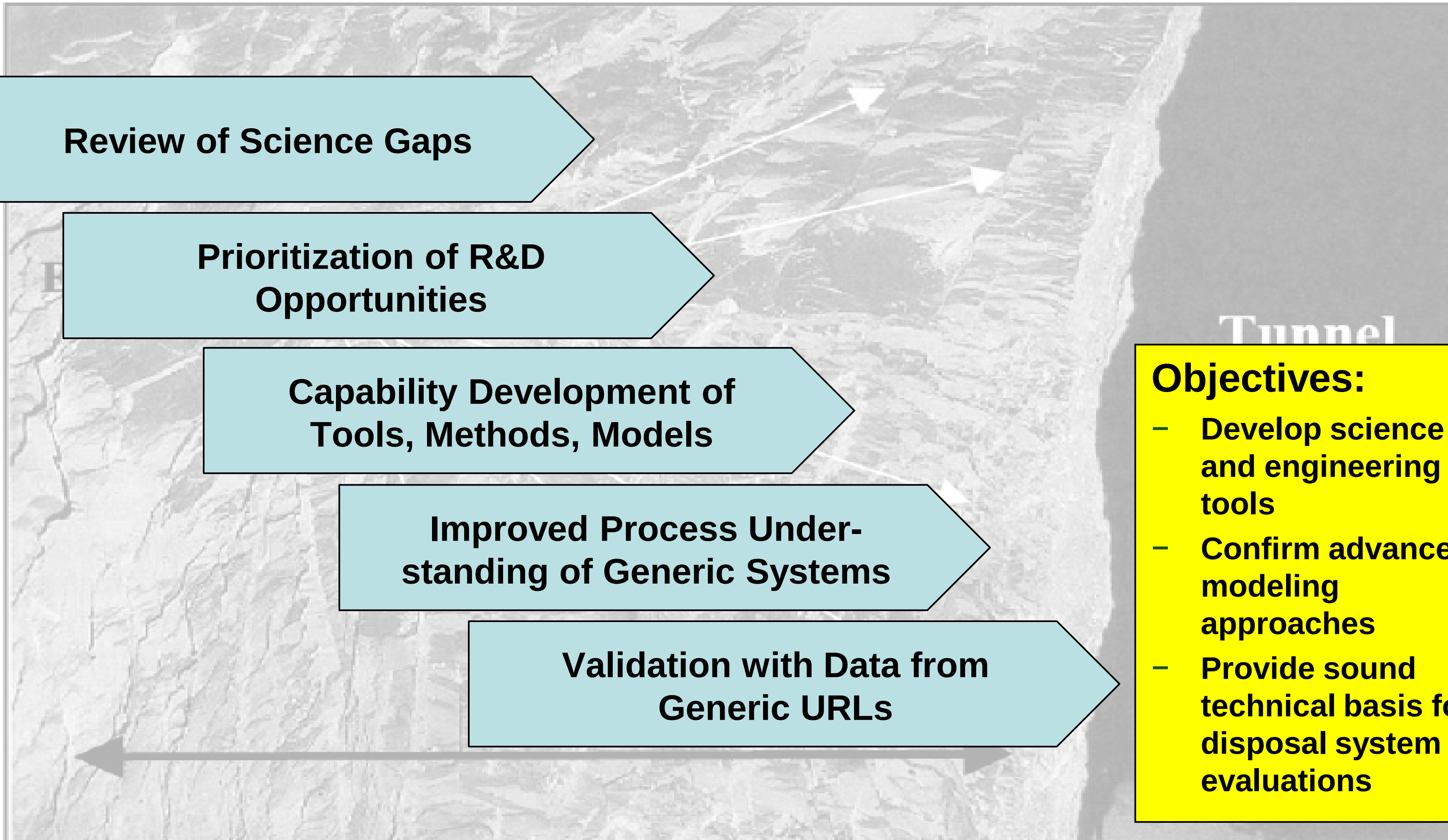


(Gonzales and Johnson, 1984)

- Clay is considered as a host geologic environment in Belgium (Boom Clay), France (Callovo-Oxfordian Clay) and Switzerland (Opalinus Clay)
- Clay buffers (bentonite) are included as engineered barriers in several disposal system concepts with granite and/or clay host rocks

➢ Main performance drivers related to clay/shale host rock and bentonite backfill:
  - Advective transport paths, either natural or induced via degradation/damage
  - Diffusive and sorptive behavior

R&D Planning, Steps and Objectives



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

Objectives:

- Develop science and engineering tools
- Confirm advanced modeling approaches
- Provide sound technical basis for disposal system evaluations

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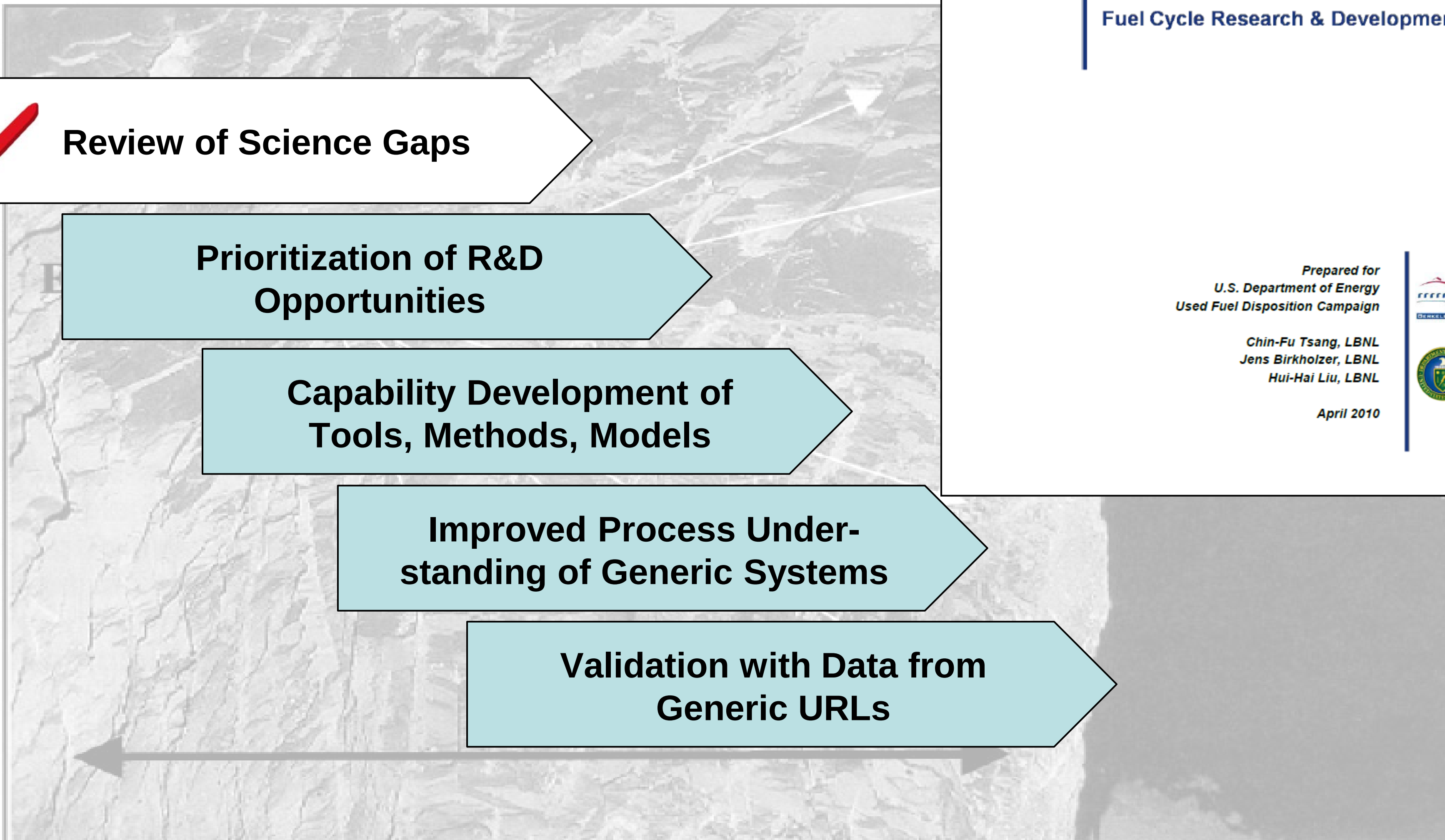
R&D Planning ... Obje...



- ✔ **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

April 2010

R&D Planni
Obje

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


Used Fuel Disposition Campaign Disposal Research and Development Roadmap

Fuel Cycle Research & Development

Prepared for
U.S. Department of Energy
Used Fuel Disposition Campaign
March 2011
FCR&D-USED-2011-000065 REV 0

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R&D Planni… Obje…

Review of Science Gaps

Review of International Activities and Active Collaboration with International Partners

Validation with Data from Generic URLs

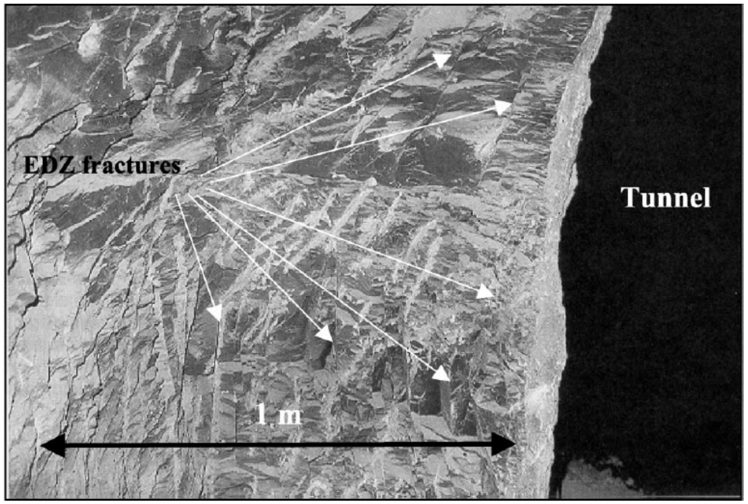
Disposal R&D in the Used Fuel Disposition Campaign: A Discussion of Opportunities for Active International Collaboration

Fuel Cycle Research & Development

Prepared for
U.S. Department of Energy
Used Fuel Disposition
Jens Birkholzer
Lawrence Berkeley National Laboratory
June 2011
FCRD-USED-2011-000225

Relevant R&D Issues in Clay/Shale Host Rock

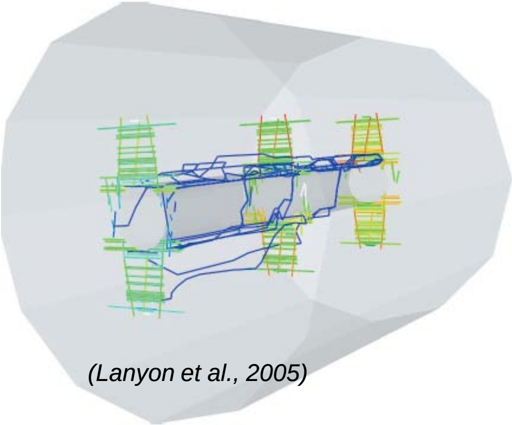
Disturbed Zone (DZ) Evolution:
- evolution of stress-changes due to excavation
- fracturing due to ventilation and thermal stresses
- self-sealing processes
- modeling excavation and emplacement



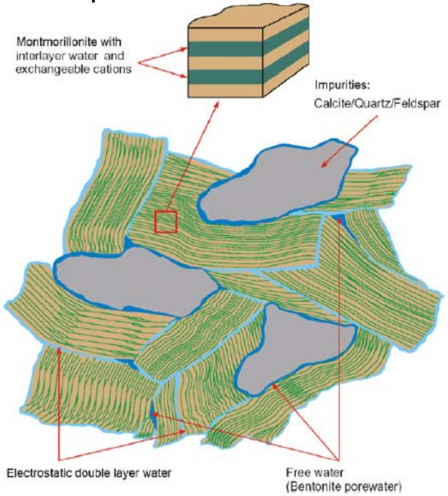
(Bossart et al., 2002)

Geological Conditions and Processes:
- fracture/fault reactivation
- intrusion and collapse structures
- heterogeneity and in-situ stress conditions

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



(Lanyon et al., 2005)

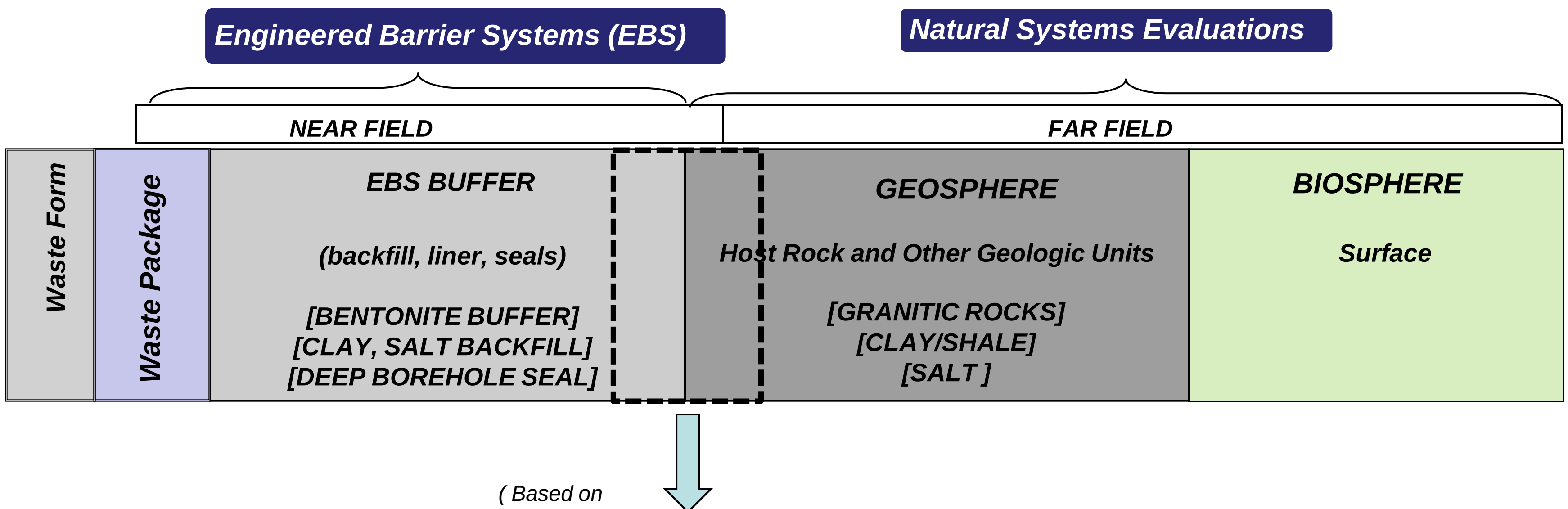


(Tournassat & Appelo, 2011)

Coupled THM+C 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

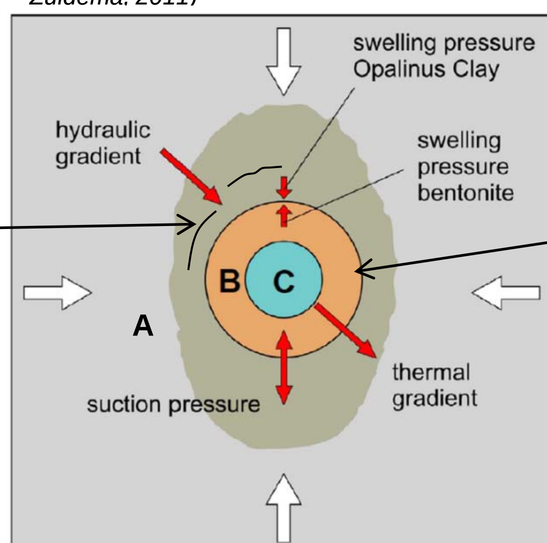
Examples of Specific Disposal R&D Activities

Examples of Disposal R&D Activities



(Based on Zuidema, 2011)

THMC Behavior in Disturbed Zone and Impact on Flow Properties



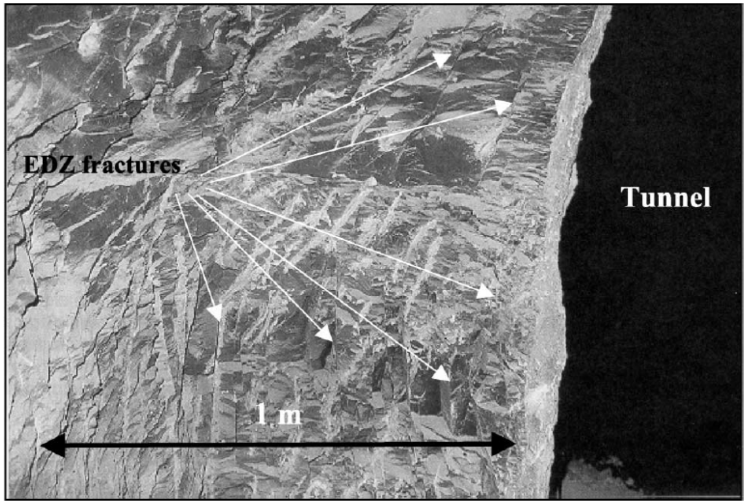
Diffusion in Compacted Clay and Bentonite

A: Host rock

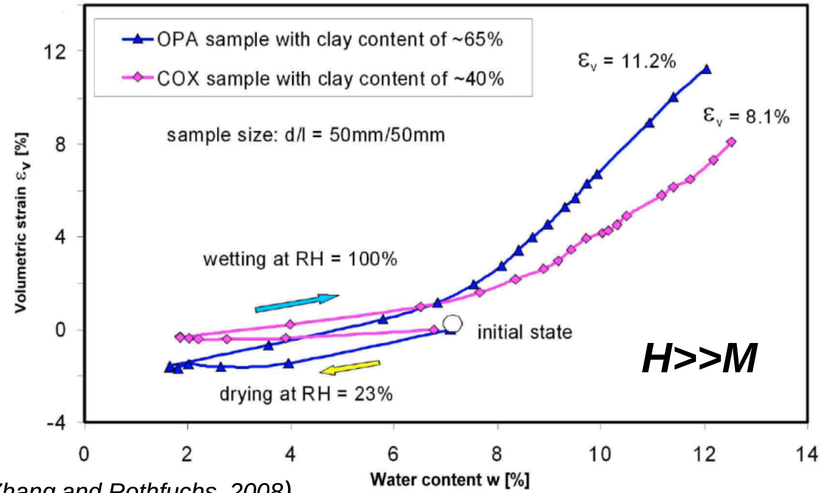
B: Clay-based backfill

C: Waste package

THMC Disturbed Zone: Relevant Coupling

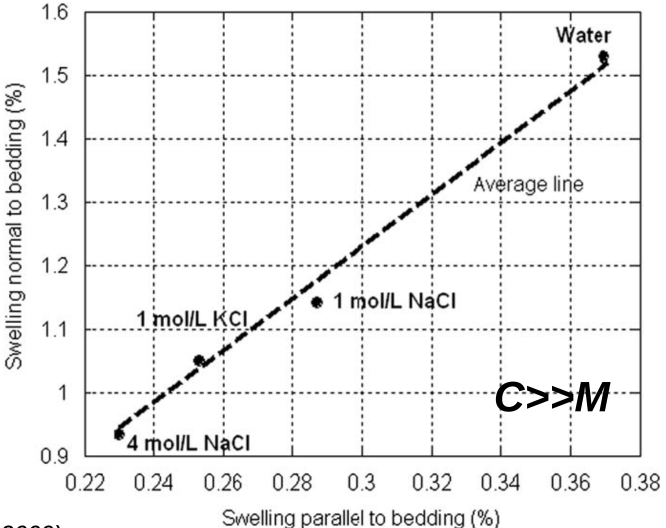


(Bossart et al., 2002)



(Zhang and Rothfuchs, 2008)

Disturbed-zone behavior strongly affected by coupled THMC processes related to excavation, ventilation, emplacement of EBS materials, and heat



(Wakin et al., 2009)

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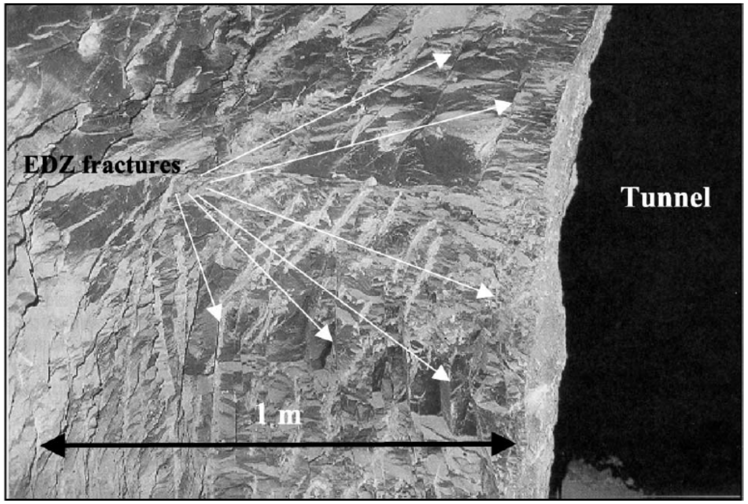
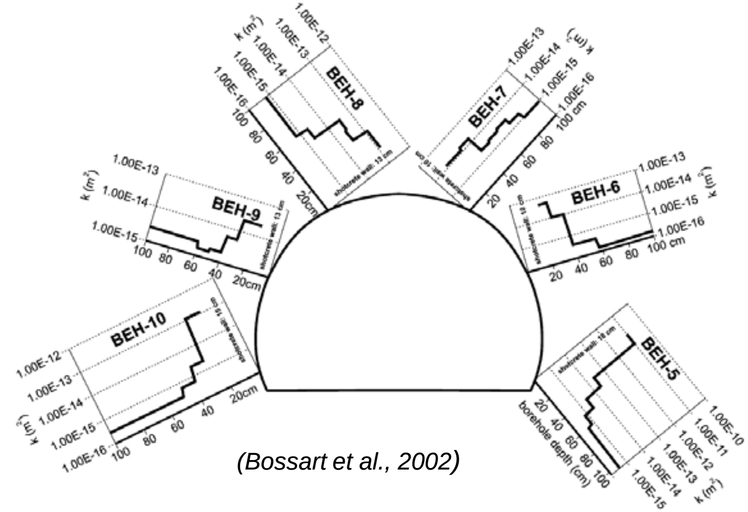
THMC Disturbed Zone: Disturbed Zone Flow Paths

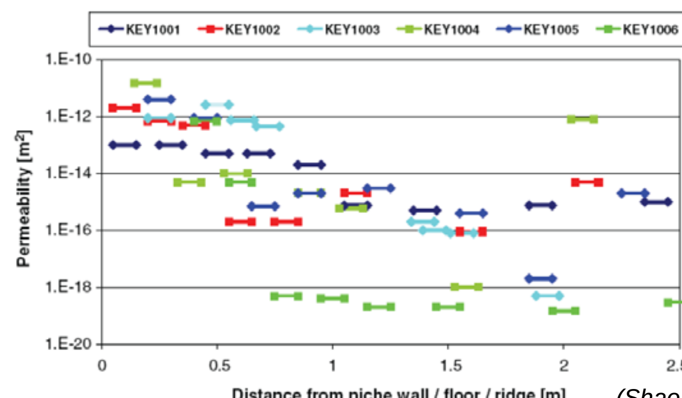


(Bossart et al., 2002)



(Bossart et al., 2002)

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

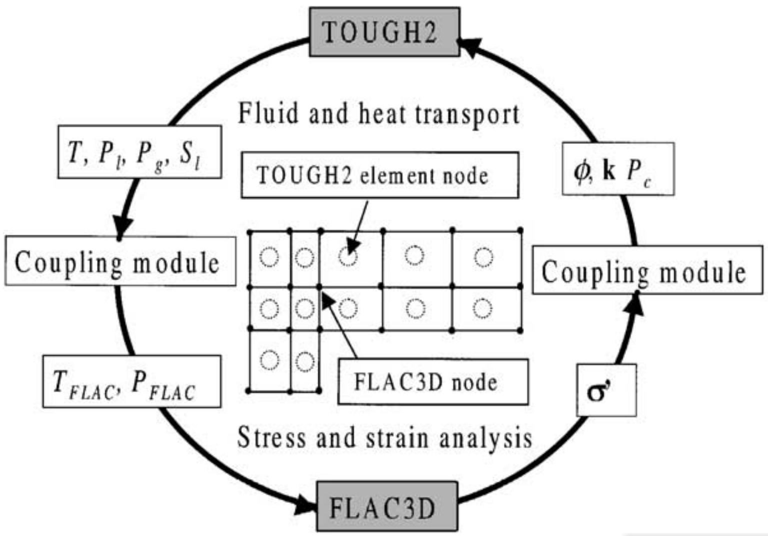


(Shao et al., 2008)

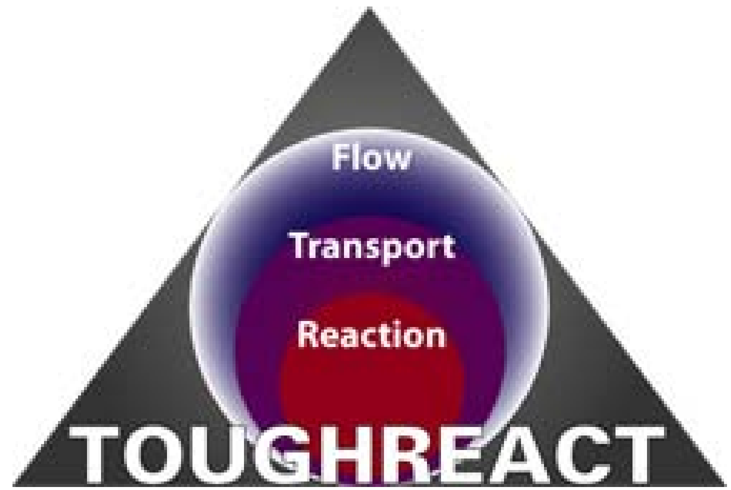
Develop a predictive modeling capability that allows simulating the evolution of small-scale to large-scale disturbed zone flow paths as a function of time and relevant mechanical-thermal-chemical conditions

THMC Disturbed Zone: Fully Coupled THMC Simulator

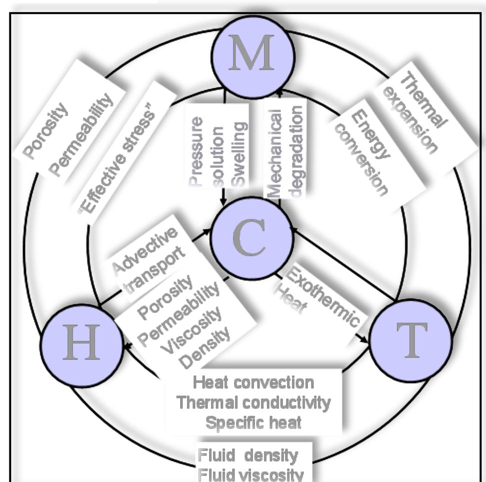
TOUGH2-FLAC3D: Coupled THM



TOUGHREACT: Coupled THC



TOUGHREACT-FLAC3D: Coupled THMC



New constitutive relationships for clay/shale/bentonite behavior

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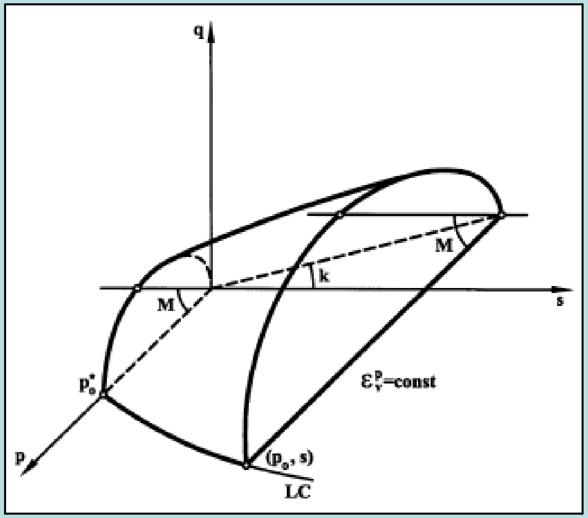
THMC Disturbed Zone: Constitutive Relationships

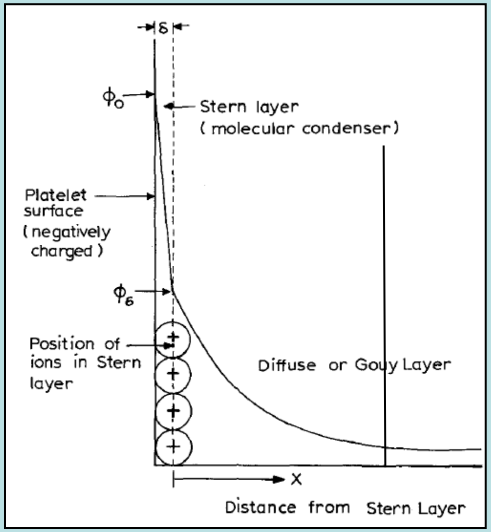
BBM Model



The Barcelona Basic Model (BBM) describes a large number of typical features of the mechanical behavior of unsaturated clay/bentonite and is one of the most advanced and accepted models.

>> Mechanical behavior as a function of saturation

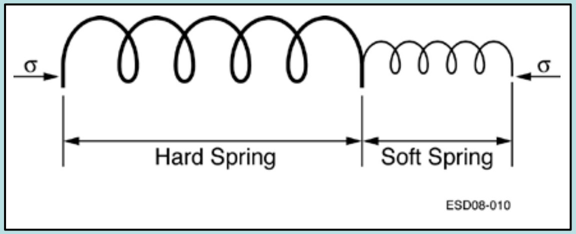
Dual-Structure Model

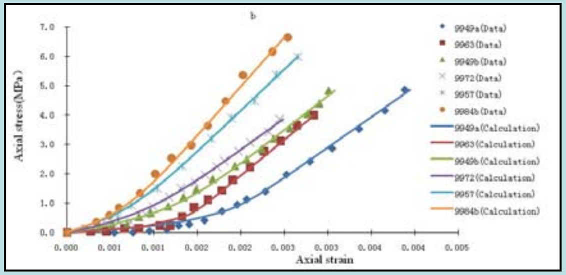


Dual-structure models allow to establish a relation between swelling pressure and chemical variables. Microstructure describes diffuse double layer for interactions at particle level.

>> 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

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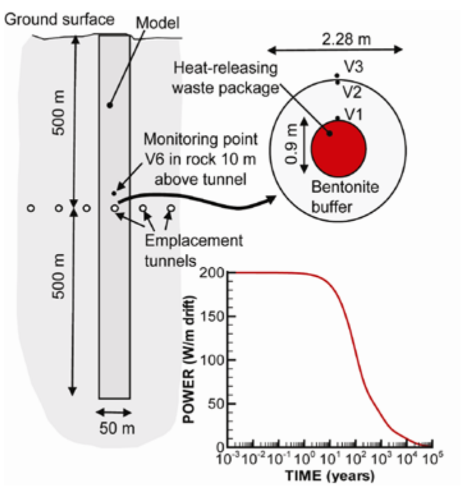
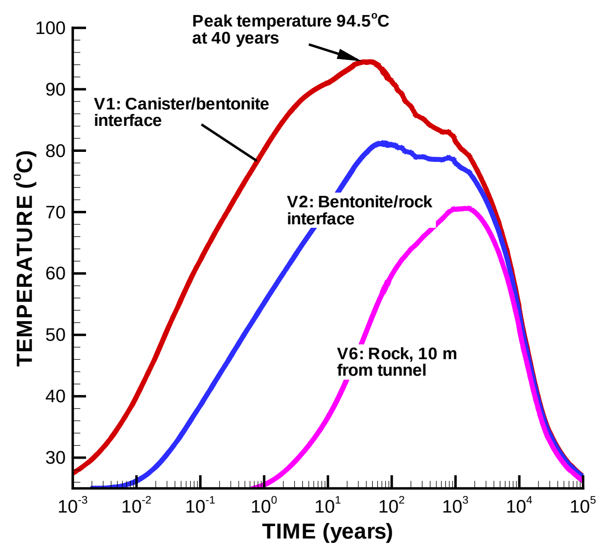
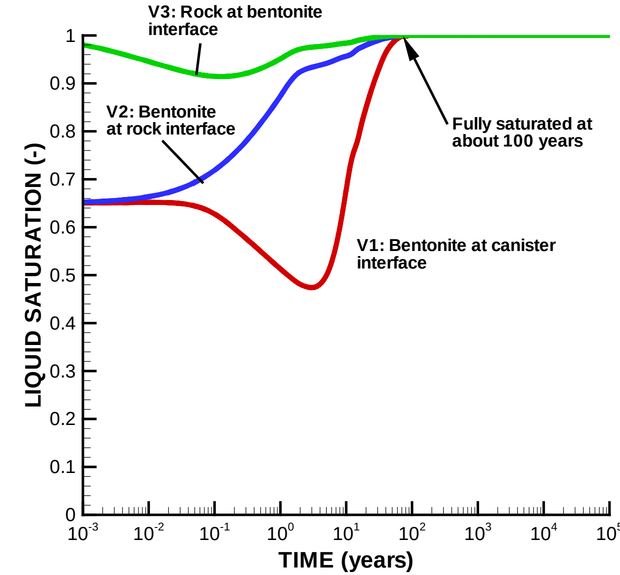
Thermo-Elasto-Plastic Behavior: Generic Modeling Results

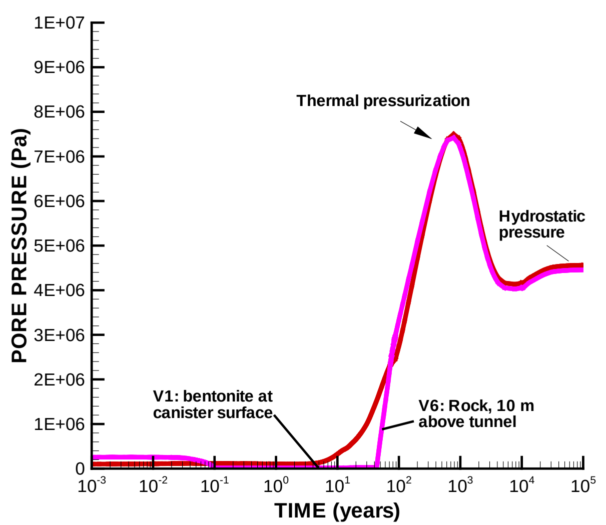


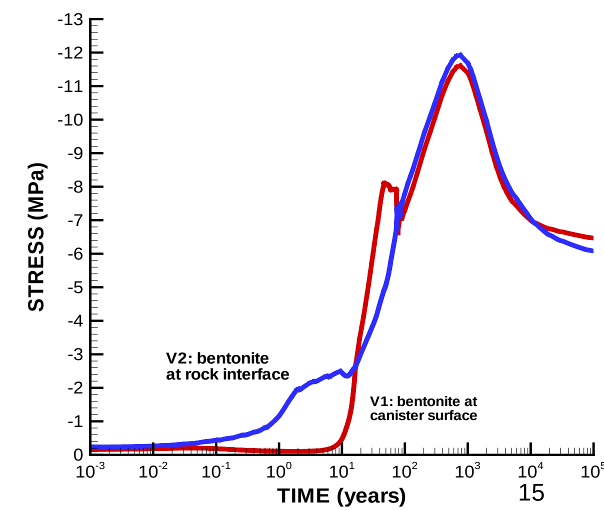




THM driven buffer/rock interactions:

1) Delayed buffer resaturation due to low rock permeability
2) Thermal-pressurization in rock affects pressure and stress evolution in buffer





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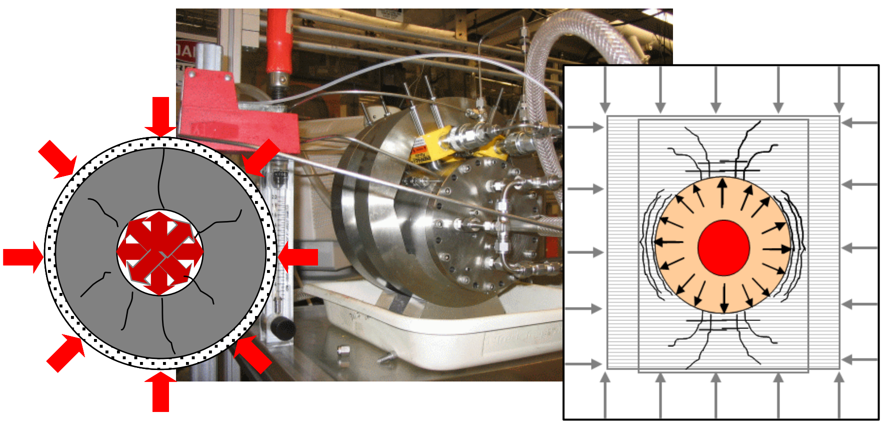
Future Work: Improved Process Understanding

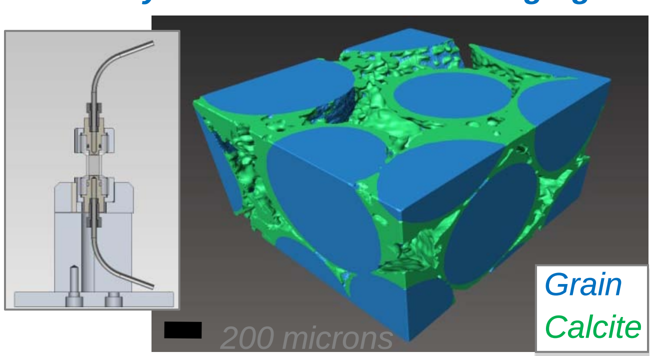
Fracture Growth and Sealing

- 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

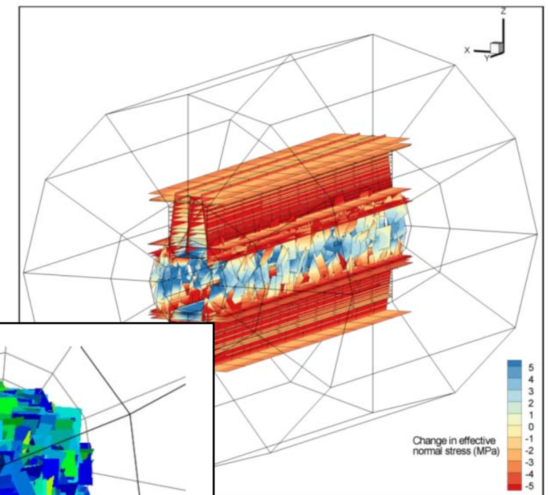


ALS Synchrotron Micro-CT Imaging



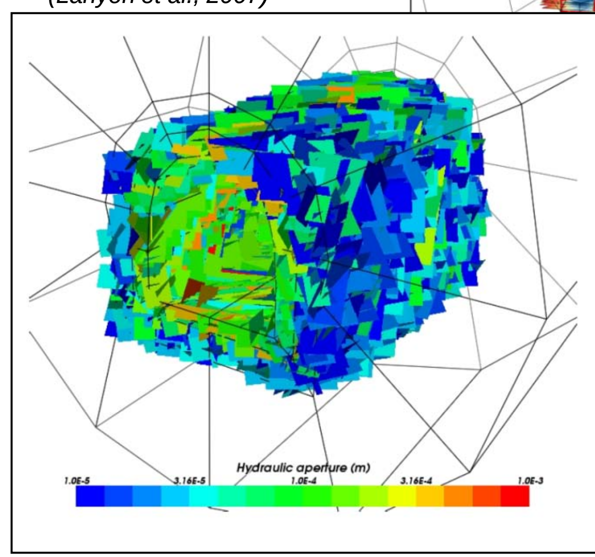
Discrete Fracture-Matrix Models for DZ

- Develop discrete modeling capability for flow and transport in DZ (see also Painter presentation)
- Evaluate continuity of fracture flow and transport paths
- Include impact of fracturing, self-sealing, and other coupled processes



(Lanyon et al., 2007)

(Lanyon et al., 2007)



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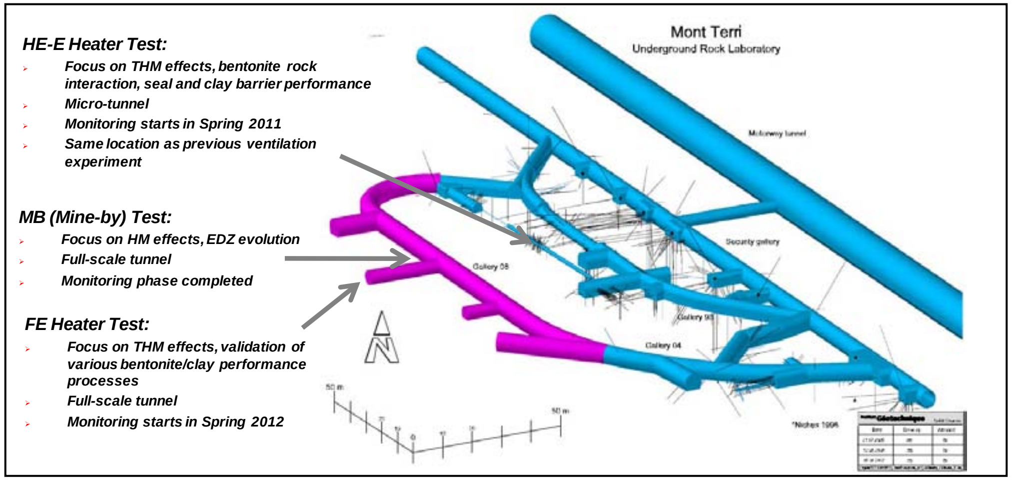
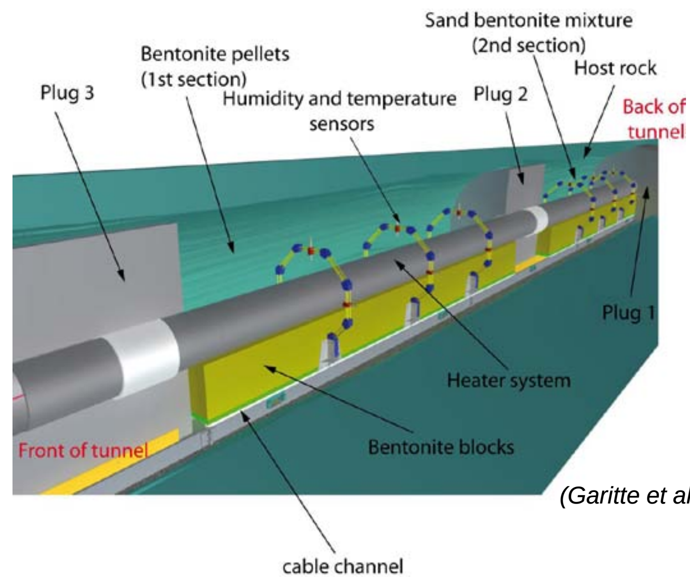
Future Work: Validation with Field Data from International URLs

Generic URL at Mont Terri in Switzerland



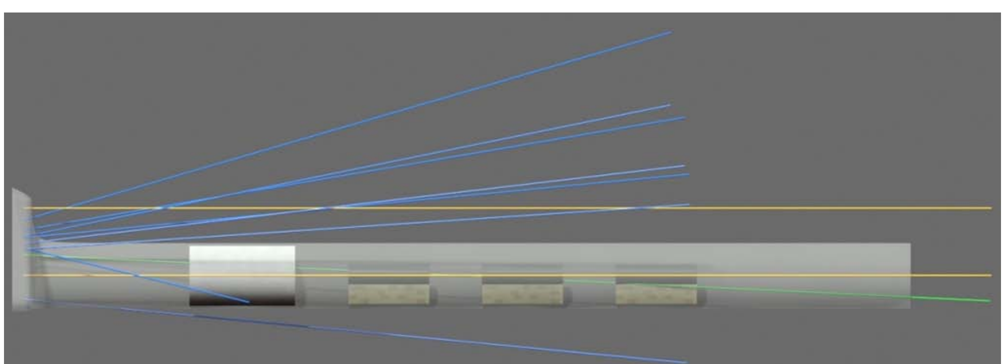
(Based on Garitte et al., 2010)

HE-E Heater Test



(Garitte et al., 2011)

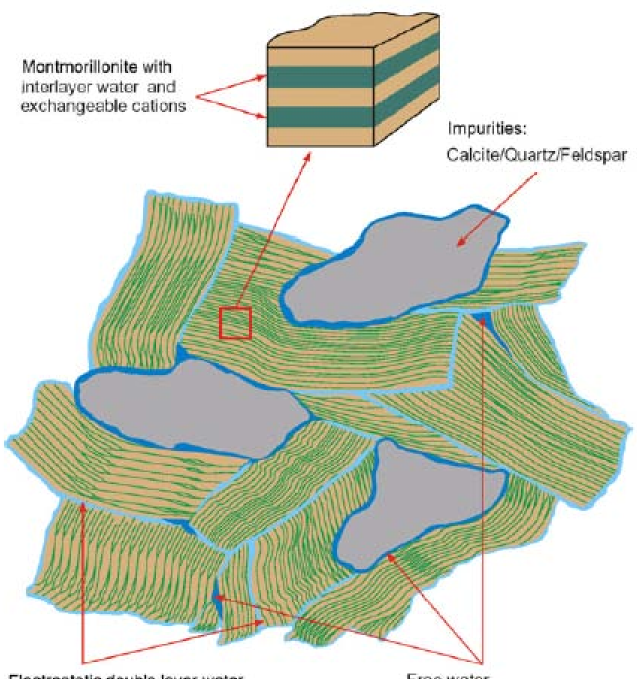
FE Heater Test



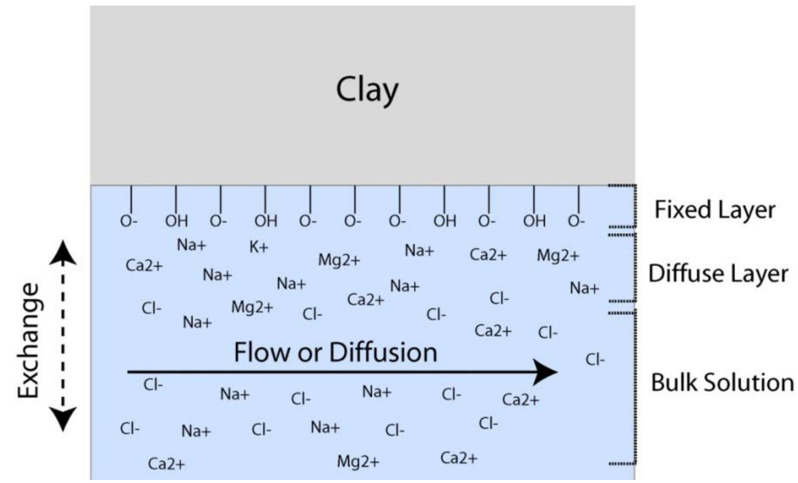
(Vietor, 2011)

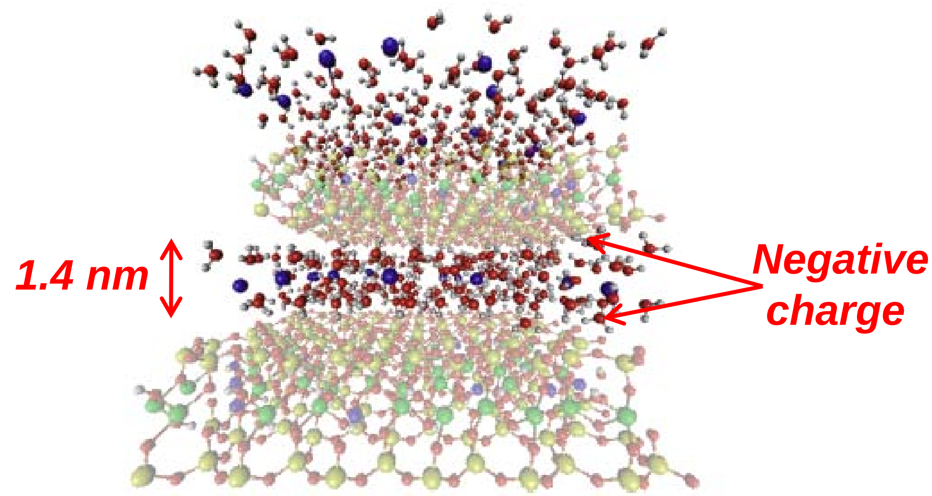
Clay and Bentonite Diffusion: Capability Development

- Nanometer size of pores in compacted clays and bentonite means that free water in bulk solution may not be connected
- Observations suggest that anions are excluded from double layer or interlayers, while cations and neutral species may diffuse in double or interlayers, subject to sorption
- Apparent diffusion rates are affected by chemical speciation, electrical double-layer structure at clay-water interface, and amount of interlayer water



(Tournassat & Appelo, 2011)



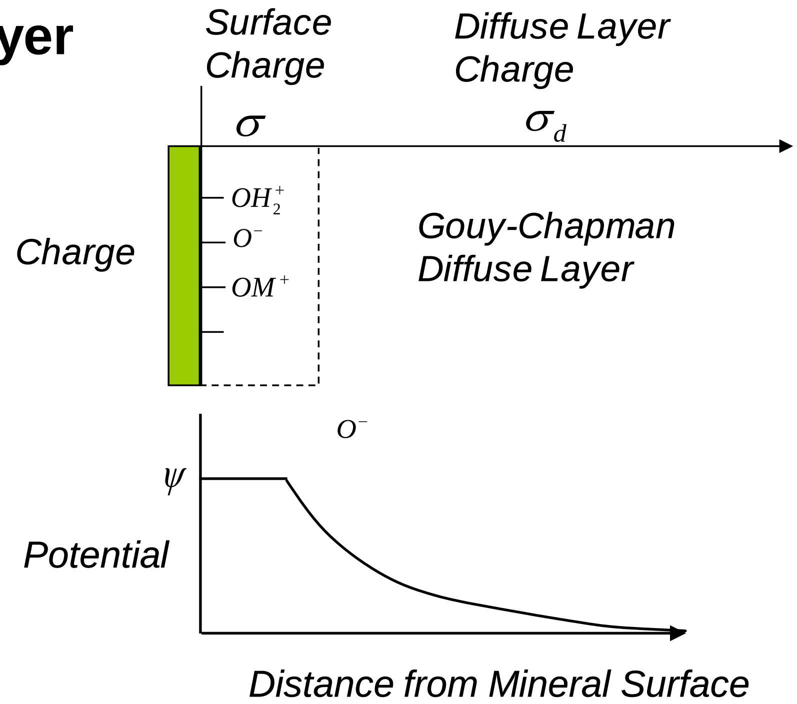


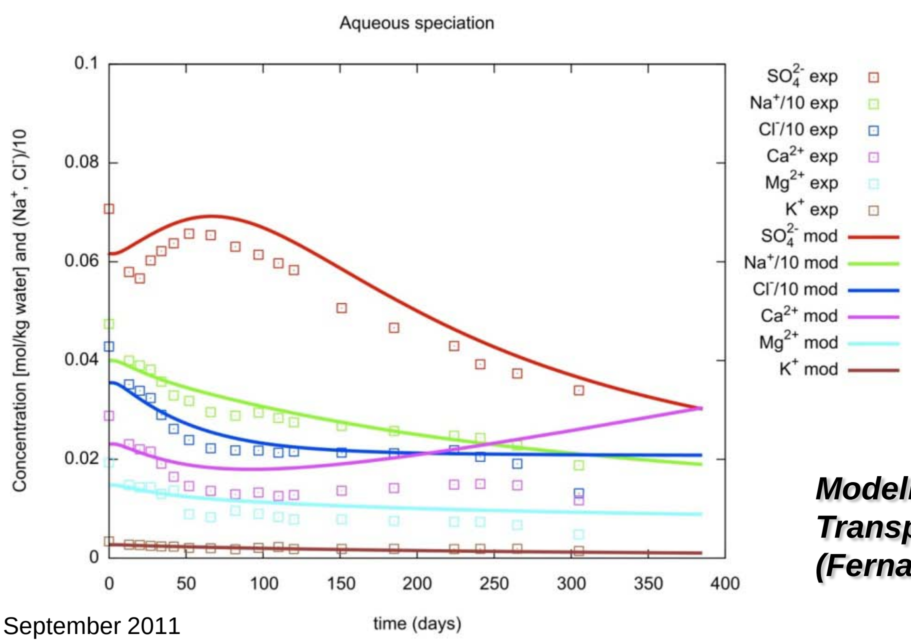
Two-layer hydrate of Na-montmorillonite, the predominant mineral phase in compacted bentonite, with Na (blue), water O (red), and water H (white) atoms in the interlayer and Si (yellow), Al (green), Mg (blue), O (red), and H (white) atoms (Bourg and Sposito, 2010).

Clay and Bentonite Diffusion: Coupled Model Approach

Model Formulation for Diffuse Double Layer

- Solve for charge of mineral surface using surface complexation approach
- Calculate diffuse layer thickness (and volume) as a function of ionic strength
- Solve for a) potential of surface and b) mean potential of diffuse layer using Donnan equilibrium model
- Diffuse solutes separately in macro- and micropores





Modeling of Multicomponent Transport Experiment (Fernandez et al., 2011)

Clay and Bentonite Diffusion: Improved Process Understanding

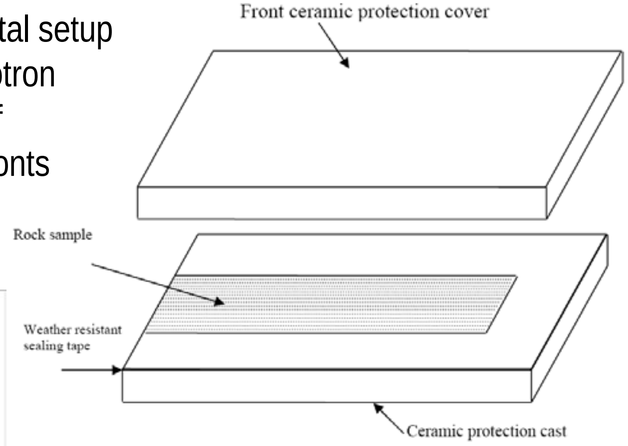
Diffusion Experiments

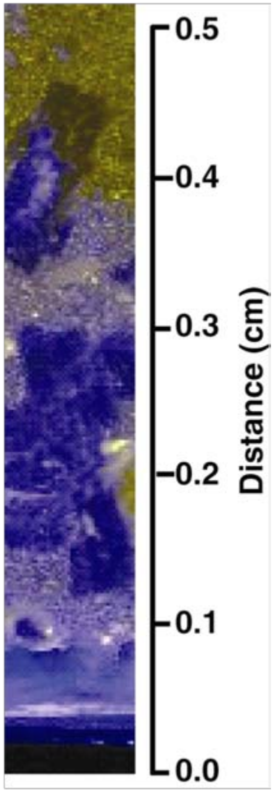
- Conducted under a variety of chemical solution conditions and degrees of compaction, to characterize the effects of chemical speciation (anion, cation, neutral) on apparent diffusion rates and its dependence on compaction

- With varied experimental temperatures and total concentrations, with a goal to determine activation energies and to distinguish between various (diffusion) processes consistent with a model-based data interpretation

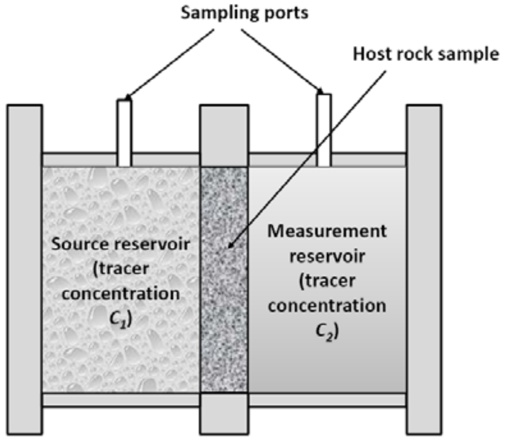
- Employ synchrotron X-ray spectroscopic and electron-based imaging techniques to evaluate diffusion on scales of microns up to one mm

Experimental setup for synchrotron mapping of diffusion fronts





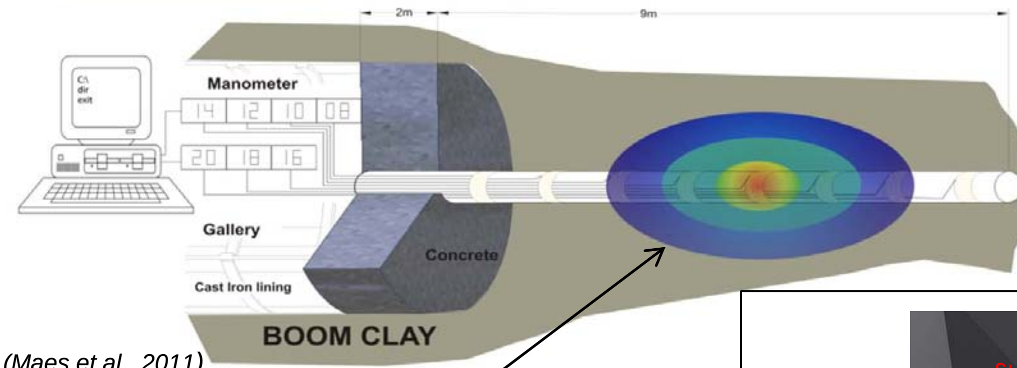
mXRF result using bromide tracer



Experimental setup for diffusion cell

Options for Validation with Field Data from International URLs

RN Migration Experiment at HADES URL in Belgium

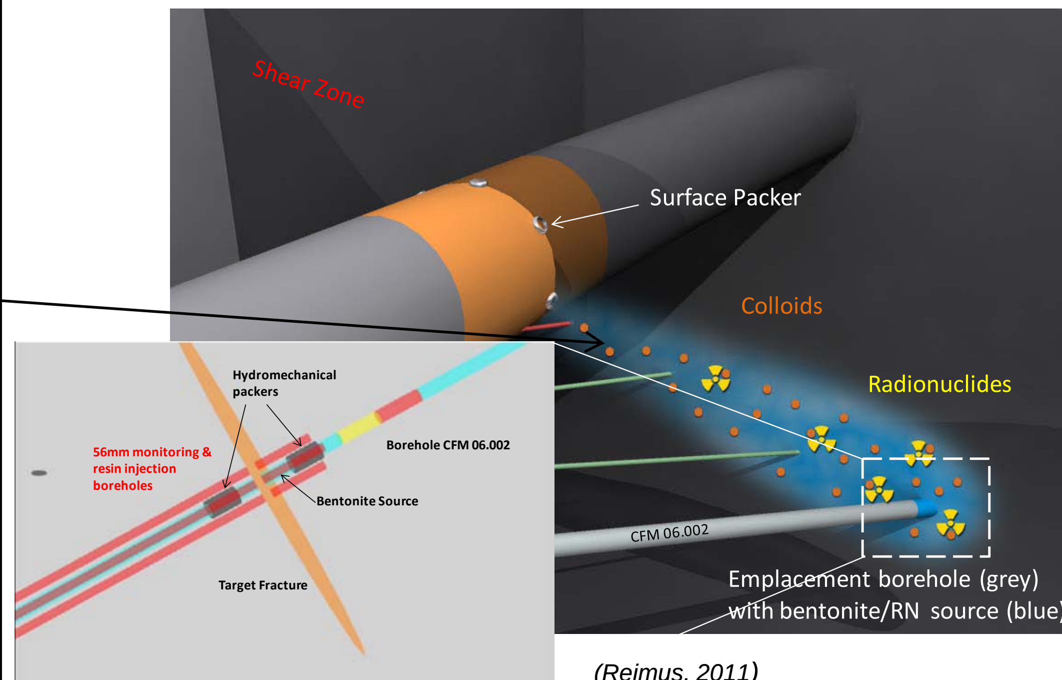


(Maes et al., 2011)

Diffusive transport

Advective transport in shear zone

RN Tracer Test at Grimsel Test Site in Switzerland



(Reimus, 2011)

Questions?