The mission of ESD’s Nuclear Energy and Waste (NEW) Program is to perform earth-sciences related research concerning the safe and secure use of nuclear energy and the safe long-term storage and disposal of used nuclear fuel and waste.
• Nuclear Energy Trends in the US

– The Obama administration supports building the “the next-generation nuclear reactors that are smaller and safer and cleaner and cheaper.” Ohio State University-March 22, 2012

– The administration also points out that “with rising oil prices and a warming climate, nuclear energy will only become more important.” Seoul, Korea - March 26, 2012

– In part triggered by financial incentives and loan guarantees, several new reactors are currently planned, approved, and constructed in the US, the first time in decades

– Following the accident at Fukushima Daiichi, the DOE, the NRC and the nuclear industry initiated a review of all operating and planned reactors in the US
• Used Nuclear Fuel in the US: Today and Tomorrow

- Nuclear waste disposition remains one of the most critical issues for expansion of nuclear energy
- Even without any new reactors, the amount of discharged spent fuel will double till 2060
• Status of Nuclear Waste Disposal in the US

  – In 2010, the Obama administration officially withdrew its pending license application for Yucca Mountain. However, lawsuits are pending and political pressure is mounting in Congress about the sudden end of the license application.

  – Nuclear waste activities reside within DOE’s 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, transportation, and disposal of used nuclear fuel and wastes.

  – To date, no regulatory framework exists for sites other than Yucca Mountain, and only generic (site-independent) disposal R&D can be conducted within UFD.

  – UFD disposal objectives are therefore to provide the technical basis for viable disposal options and to develop science and engineering tools for implementation (“repository ready”)

  – Blue Ribbon Commission generally supportive of UFD focus and objectives. The commission also suggests using nuclear utility contributions to provide stable funding for management and disposition of waste
• R&D Staff in FY2012 (~50)
• **Understanding Disposal System Performance**
  - Characterize geologic and hydrogeologic conditions
  - Evaluate barrier integrity over time
  - Predict radionuclide transport

![](image)

• **LBNL’s Core Expertise**
  - Characterize repository sites with novel instrumentation and interpretation methods
  - Monitor flow and transport processes in complex lab and field experiments
  - Evaluate and predict the system behavior with multi-physics computer models
  - Mechanistic understanding of coupled THMC processes and their relevance
Main Disposal Research Themes for DOE-UFD

- Prediction of Borosilicate Glass Corrosion Over Geologic Times
- Integrated Studies of Diffusion in Tight Clay-Based Materials
- THMC Behavior in Disturbed Zone (DZ) and Backfill and Impact on Transport Properties
- Clay Behavior at Very High Temperatures
- Regional Assessments and Characterization of Clay Formations Using GIS
• Predicting Extent and Evolution of Disturbed Zone

Coupled fracture-damage modeling
• To simulate evolving fracture network and hydrologic processes in disturbed zone
• Simulates fracture initiation and propagation using Rigid-Body-Spring Network (RBSN) method and coupled to TOUGH for TH processes

TOUGH-FLAC framework for THM continuum models
• New constitutive relationships for clay/shale/bentonite (e.g., BBM model, two-part Hooke’s model)
• New relationship for non-Darcian flow in clays
• Coupling with reactive transport for MC coupling (e.g., swelling effects from pore-water variation, mineralogy)
• Large-strain mode with deformable grids (i.e., for salt)

Field Applications in Underground Research Labs

HE-E Heater Test at Mont Terri
Coupled THM Fracture-Damage Model
Daisuke Asahina, Jim Houseworth, Jens Birkholzer

• Problem: modeling evolving fracture network and hydrologic processes in damage zone around drifts in clay rock for nuclear waste disposal

• Geomechanics, including fracture initiation and propagation, using Rigid-Body-Spring Network (RBSN) model

• RBSN is coupled with TOUGH2 for thermal-hydrological processes in evolving discrete fractures and permeable rock matrix

Motivation: Engineered Barrier System (EBS) is typically composed of bentonite; Clay rock is one important type of hosting formation; THMC processes are closely coupled in bentonite and clay formation. THMC modeling with MC coupling through diffuse double-layer theory (Zheng et al., 2013 IHLRWM).

The geochemical induced swelling/shrinkage of host clay rock involves the combined effect of variation in pore-water ion concentration, exchangeable cations, and the amount of smectite, it occurs exclusively in the near field and is affected by many hydrogeology and geochemical parameters.
Non-Darcian Flow in Clay

H.H. Liu and Jens Birkholzer

Problem Addressed:
The commonly used Darcy Law cannot accurately capture water flow process (in clay) that is important for performance of a clay repository.

Approach and Results:
• Test data sets show the existence of non-Darcian flow behavior for both saturated and unsaturated clay media.
• The behavior may be a result of strong water-solid interaction (Low, 1961; Chen et al., 2008).
• A new relationship between water flux and hydraulic gradient is developed (Liu et al. 2011; Liu and Birkholzer, 2012).
• An empirical relationship between permeability and threshold hydraulic gradient (a measure of non-Darcian behavior) is obtained (Liu and Birkholzer 2012).


• Clay and Bentonite Diffusion

Improved Methods for Ion Transport Through Compacted Clay

- Clay and bentonite diffusion
- Bentonite pore water
- Quartz/feldspar grains
- Interlayer water

Molecular Dynamics for Nanopore Diffusion

- Diffusion cell experiments to characterize apparent diffusion rates under variable chemical (and temperature) conditions
- Employ synchrotron X-ray spectroscopic and electron-based imaging techniques

Microcontinuum Modeling

- Mean electrostatic (or Donnan) potential approach with dynamic changes in double layer thickness
- Improved description of transport and electrical double layer by solving the full Poisson-Boltzmann equation between charged clay surfaces
- Application to DR-A Test at Mont Terri

Diffusion and Sorption Laboratory Experiments

- Diffusion cell experiments to characterize apparent diffusion rates under variable chemical (and temperature) conditions
- Employ synchrotron X-ray spectroscopic and electron-based imaging techniques
Modeling diffusion in clay nanopores
Michael Holmboe, Ian Bourg

- Our MD simulations predict that the activation energy of diffusion of Na\(^+\) \((E_a)\) increases substantially with compaction \((E_a\) values in the 2- and 1-layer hydrates of Na-montmorillonite are 2.3 and 5.4 kJ mol\(^{-1}\) higher than in bulk liquid water).

- In laboratory diffusion experiments, our collaborators at Hokkaido U. measured a 2 to 5 kJ mol\(^{-1}\) increase in \(E_a\) in conditions where the 2-layer hydrate is observed.

- Our results provide clear evidence that Na\(^+\) diffusion in compacted smectite occurs primarily through the clay interlayer nanopores.
Uranium(VI) Diffusion in Bentonite under Variable Chemical Conditions

Ruth M. Tinnacher and James A. Davis

Current diffusion model paradigm: \[ \text{Flux} = D_a \left( \delta^2 C / \delta x^2 \right); \] \( C \) is radionuclide concentration

\( D_a \) is apparent diffusion coefficient = \( D_e / (\omega + \rho K_d) \)

\( D_e \) is “effective” diffusion coefficient, \( \omega \) = porosity, \( \rho \) = bentonite density, \( K_d \) = sorption coefficient.

Problem: Uranium \( K_d \) values are highly variable with chemical conditions

Objective: Surface complexation model to replace \( K_d \) values in diffusion model

Mean Electrostatic Potential and Poisson-Boltzmann Approach to Ion Transport in Compacted Clay
Carl Steefel, et al.

Higher ionic strength front diffuses through clay, reducing EDL porosity, increasing bulk porosity

\[ \frac{\partial^2 \phi}{\partial x^2} = \frac{-e}{\varepsilon} \sum_i z_i C_i \exp \left( \frac{-z_i e \varphi(x)}{k_B T} \right) \]

Dynamic model for electrical double layer thickness as a function of ionic strength with Mean Electrostatic Potential approach

\[ \frac{\partial}{\partial t} \left[ \phi^B C_i^B + \phi^{EDL} C_i^{EDL} \right] = \frac{\partial}{\partial t} \left[ \phi^B C_i^B + \left( A_{clay} \lambda_{DL} \beta_{DL} / \sqrt{T} \right) C_i^{EDL} \right] \]

Two-dimensional cation transport between charged clay surfaces simulated with Poisson-Boltzmann equation

Steefel et al, 2013
Modeling Anion Diffusion in Opalinus Clay at the Mont Terri Site, Switzerland

Carl Steefel, et al.

Simulation of tracer and anion transport from borehole to Opalinus Clay using Mean Electrostatic Potential approach
Microcontinuum Modeling of Borosilicate Glass Corrosion over Geologic Time Scales
Steefel, et al.

Ripening and densification of silica-rich corrosion layer leads to a reduction in diffusion rates and slowing of corrosion

Modeling of Poiseuille flow and reaction in microfluidic experiments quantifies corrosion rates
Assessment of Alternative Host-Rock Distribution in the U.S. Using GIS

Patrick Dobson (LBNL), Frank Perry (LANL), Rick Kelley (LANL)

- Develop GIS data base for mapping distribution, depth, and thickness of alternative repository host rocks (shale, salt, granite)
- Other screening factors can be incorporated into system
- Work will be presented at 2013 IHLRWMC (Perry et al.)
Petroleum Analogues for Natural Disturbances of Argillaceous Rock

- Problem: identify varieties of natural disturbances observed in argillaceous rock that could affect nuclear waste disposal
- Argillaceous rock also serves as caprocks for many petroleum accumulations worldwide
- Investigations of caprock leakage reveal numerous types of disturbances
  - mainly piercement structures associated with fluid overpressure
  - observations of disturbances have been found in a variety of geologic settings, active and passive continental margins, intracratonic basins, etc.

• International Projects in Waste Disposal

**Funded by DOE UFD**
- DOE views international collaboration as a very beneficial strategy of advancing R&D
- Focus is on collaborative R&D with access to tests in underground research labs
- DOE has formal collaborative R&D with ongoing programs in Europe and Asia
- Current LBNL work involves modeling support of in situ heater tests, mine-by and EDZ tests, and diffusion experiments

**Funded by international programs**
- Fault zone characterization (NUMO-Japan)
- Flowing Fluid Electric Conductivity Logging (JAEA-Japan)
- Modeling support with TOUGH family of codes (Various)
Fault Zone Characterization

Kenzi Karasaki, Christine Doughty, Mark Conrad, Erika Gasperikova, and Paul Cook

• Developed dedicated fault zone testing site
• Conducted multi-disciplinary field characterization
  – Geologic, geophysical, geochemical and hydraulic tools
• Inferred permeability structure of fault zone
• Constructed geohydrological model
Flowing Fluid Electric Conductivity Logging

Christine Doughty and Chin-Fu Tsang

- Wellbore logging method to characterize permeable zones of fractured rock
- **Basic Concept**
  - Fill well with low-FEC (DI) water
  - Pump at a low rate
  - Native water with bigger FEC pulled into well from fractures
  - Shows as peaks in FEC log
  - Analyzing transient development of peaks to determine depth, flow rate, and salinity of fractures
- **Recent Enhancements**
  - Repeat FFEC logging using different pumping rates to determine transmissivity $T/T_{tot}$ and hydraulic head $I\Delta p_i$ of fractures
  - Apply to artesian wells
  - Identify regional groundwater flow through fractured rock (e.g., $z=450-500$, equal and opposite head)
- **Applications**
  - Characterize fractured rock for nuclear waste storage
  - Assess fracture flow before and after fracking operations for geothermal energy or petroleum extraction

• International Collaboration – On the Web

Go To: http://esd.lbl.gov/research/programs/new/research_areas/international/
• **Seismic Safety of Power Plants**

Develop and utilize new integrated modeling approaches for improved seismic and structural design analysis

– Develop models for seismic wave propagation and ground motion
– Improve time-domain analysis for soil-structure interaction
– Evaluate technical benefits and limitations of base-isolation technologies
– Improve models for non-linear structural system response

Current projects:

• NRC: New framework for seismic regulation of nuclear power plants, with emphasis on new soil-structure interaction analysis and base-isolation technology
• DOE-NEAMS: Advanced seismic analysis and design of nuclear power plants (with other national labs)

Based on McCallen, 2010
NRC-Supported Projects on Nuclear Power Reactor Safety

Emphasizing Seismic Safety Issues
Robert J. Budnitz (P.I.)

• Starting in 2008, NRC has supported 5 interlocking and interacting research projects in the area of the seismic safety of nuclear power plants (NPPs).

• The most important technical advances have been
  – in improving time-domain analysis of soil-structure interaction phenomena;
  – in understanding the technical benefits and limitations of seismic-base-isolation technologies for potential use beneath NPPs;
  – in proposing and analyzing potential improvements in the framework for seismic design and regulation of NPPs, leading to advances toward more performance-based and risk-informed design and regulation;
  – in improving our understanding of how much correlation exists in the failure mechanisms when identical co-located NPP components respond in very large earthquakes.

• Another major accomplishment is that LBNL is now “on the map” in terms of credibility with the NRC after decades with almost no reactor programs to point to.

• Collaborators: B. Jeremic (UC-Davis), A. Whittaker (SUNY-Buffalo), B. Stojadinovic (ETH-Zurich), all of whom are LBNL affiliates.
• **Safety of Critical Infrastructure in Seismic Events**
  – Network of seismic stations at LBNL
  – Data can be used for verification and demonstration of integrated approach