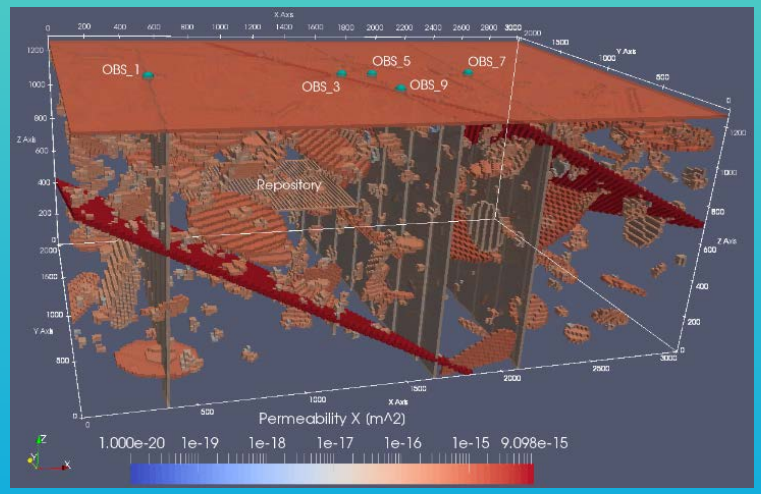

Overview of DOE R&D Efforts Related to a Clay-Based Repository and Clay-Based Engineered Barriers

U.S. Nuclear Waste Technical Review Board
Summer 2022 Board Meeting
September 13 - 14, 2022
Arlington, Virginia

SAND2022-10271 PE

Chris Camphouse
Sandia National Laboratories

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Outline

- Argillite and Engineered Barrier System R&D Control Accounts
- International Collaborations, 5-Year Plan
- Argillite Disposal R&D Activities, 5-Year Plan
- EBS R&D Crosscut Activities, 5-Year Plan
- Conclusions

Argillite and Engineered Barrier System R&D Control Accounts

Why Argillite?

Argillite (hardened mudstone) geologic formations are being considered worldwide for geologic disposal of high-level radioactive waste. Why?

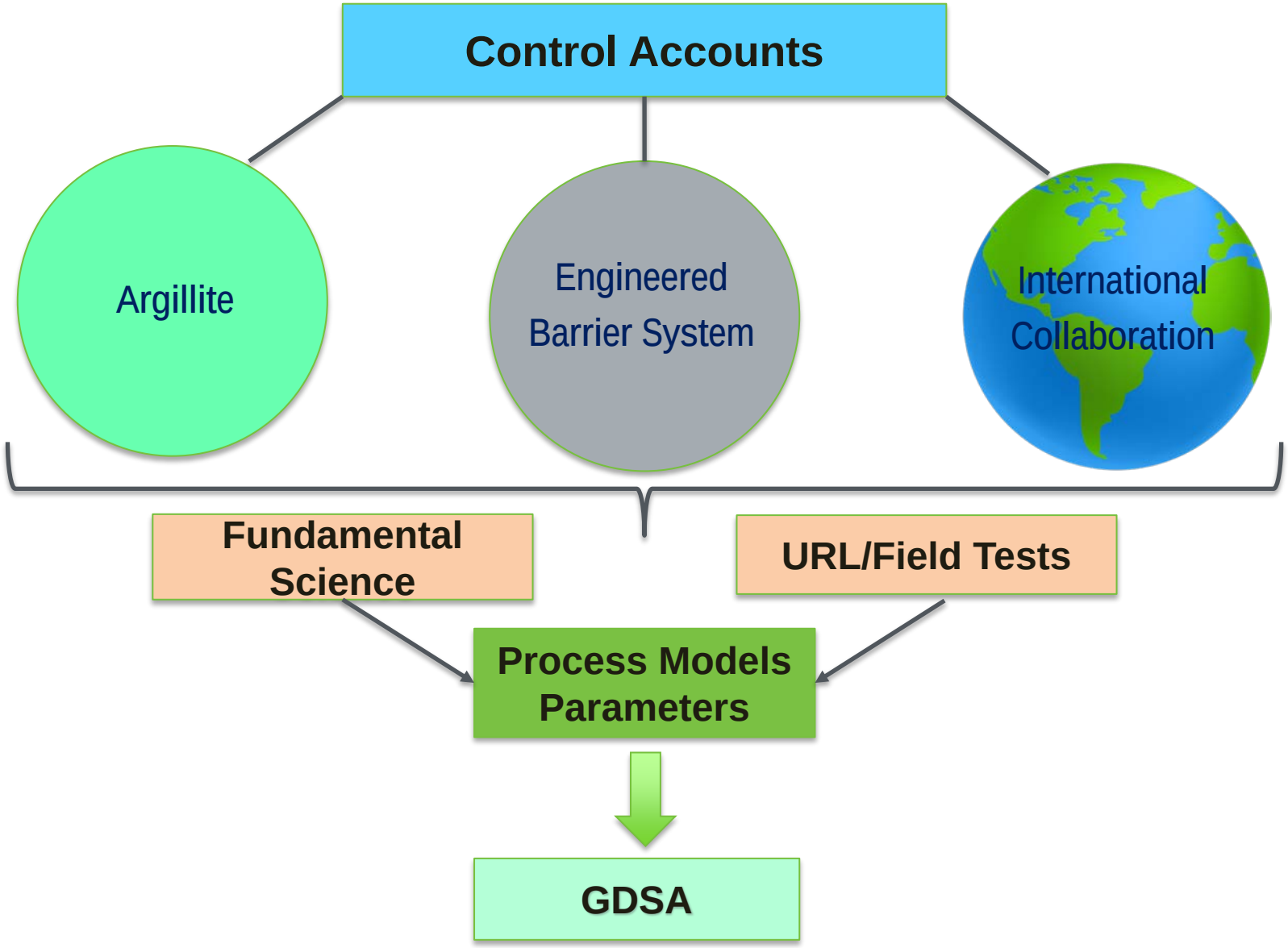
Argillite host rocks typically exhibit:

- Low permeability
- Low diffusion coefficient
- High retention capacity for radionuclides
- In general, can be self-sealing

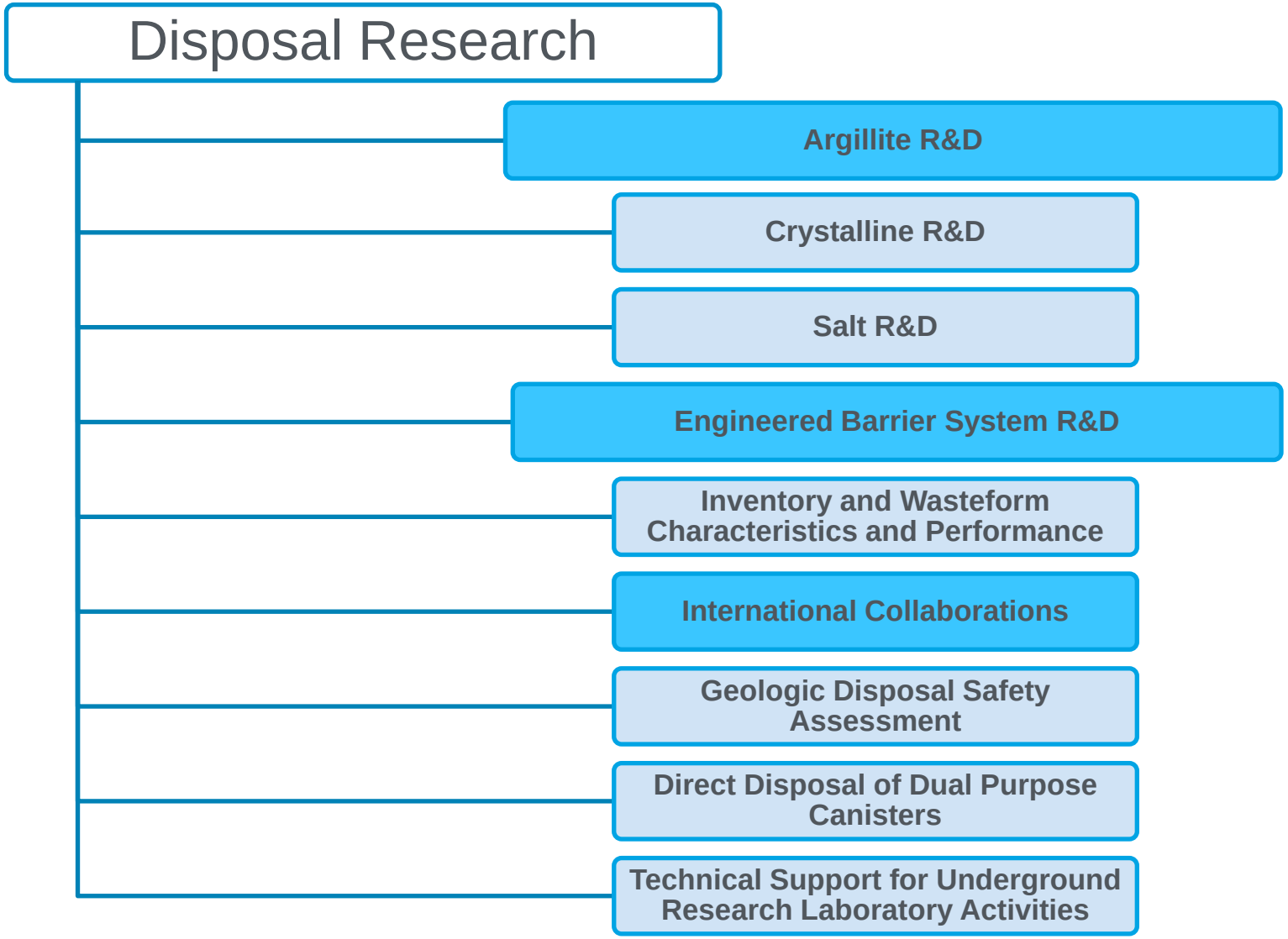
These properties comprise an attractive natural barrier in terms of geologic disposal.

Mont Terri Underground Research Laboratory, Switzerland

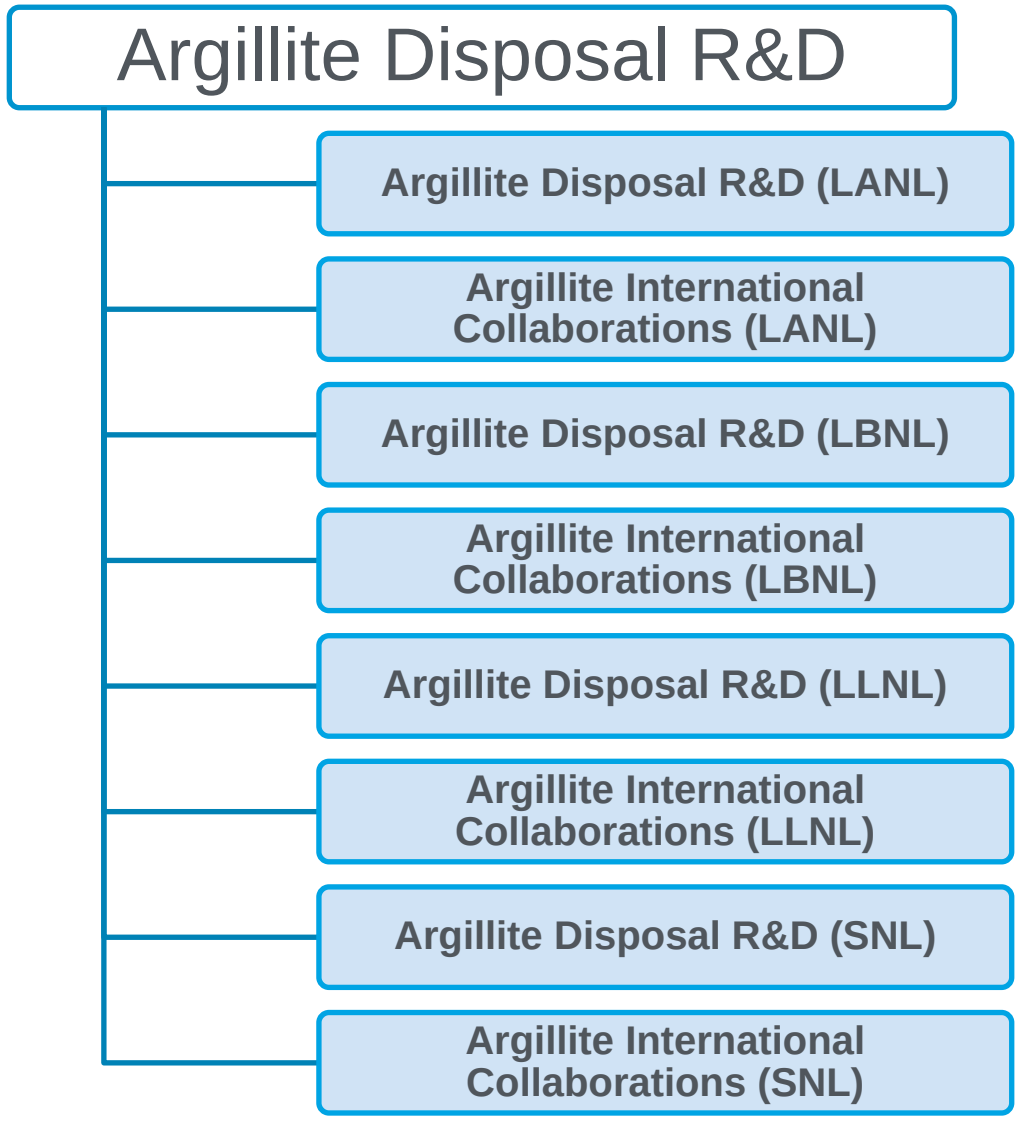
Argillite Host Rock and Engineered Barrier R&D

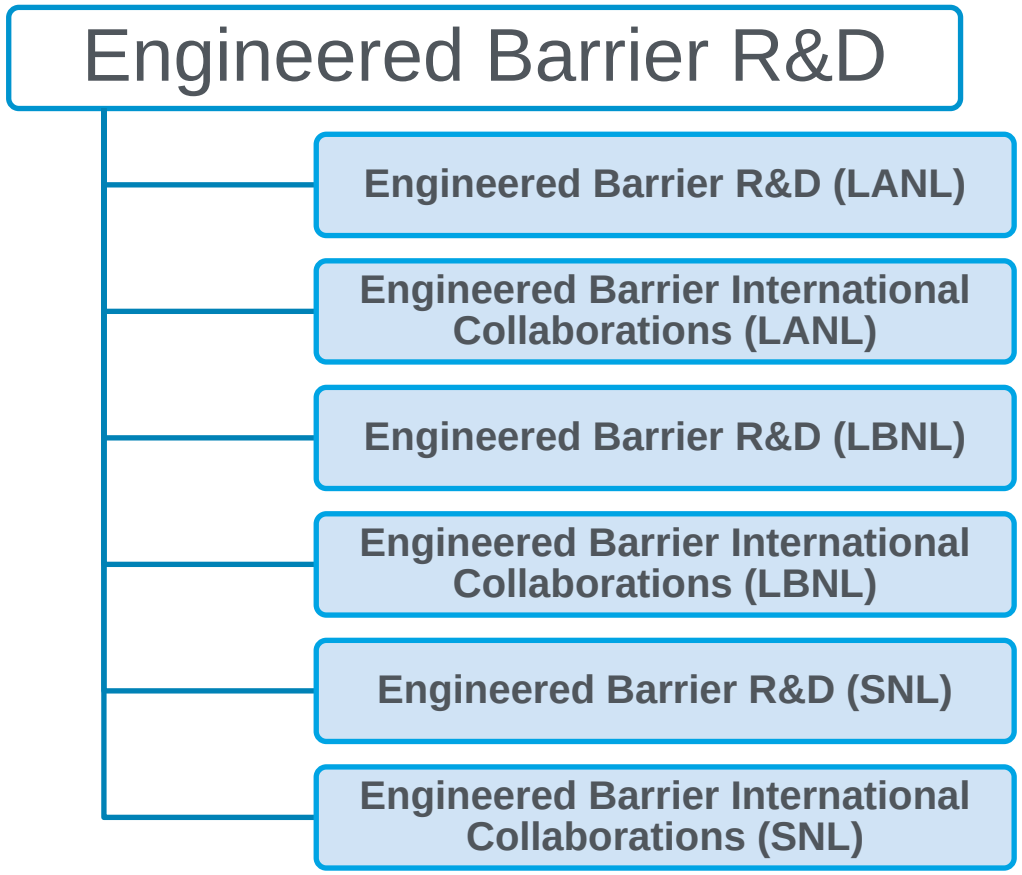


Spent Fuel and Waste Science and Technology Disposal Research Control Accounts



Control Account Drill Downs





International collaboration is a significant component, with funding commensurate to R&D work packages.

International Collaborations, 5-Year Plan

Benefits of International Collaboration

Scientific and Technical Benefits

- Tap into global knowledge, stay abreast of science advances, and gain access to international datasets and experiments
- Test and validate advanced process-modeling and experimental tools
- Understand research needs arising from critical (and sometimes surprising) issues related to “real” rocks and sites
- Leverage resources and share cost of science campaigns, in particular large experimental projects

Other Benefits

- Build valuable relationships and re-establish the U.S. disposal research program as a committed international partner
- Work towards a common set of disposal best practices and lessons learned (e.g., risk communication and site selection)
- Attract and build a new generation of “waste disposal” scientists

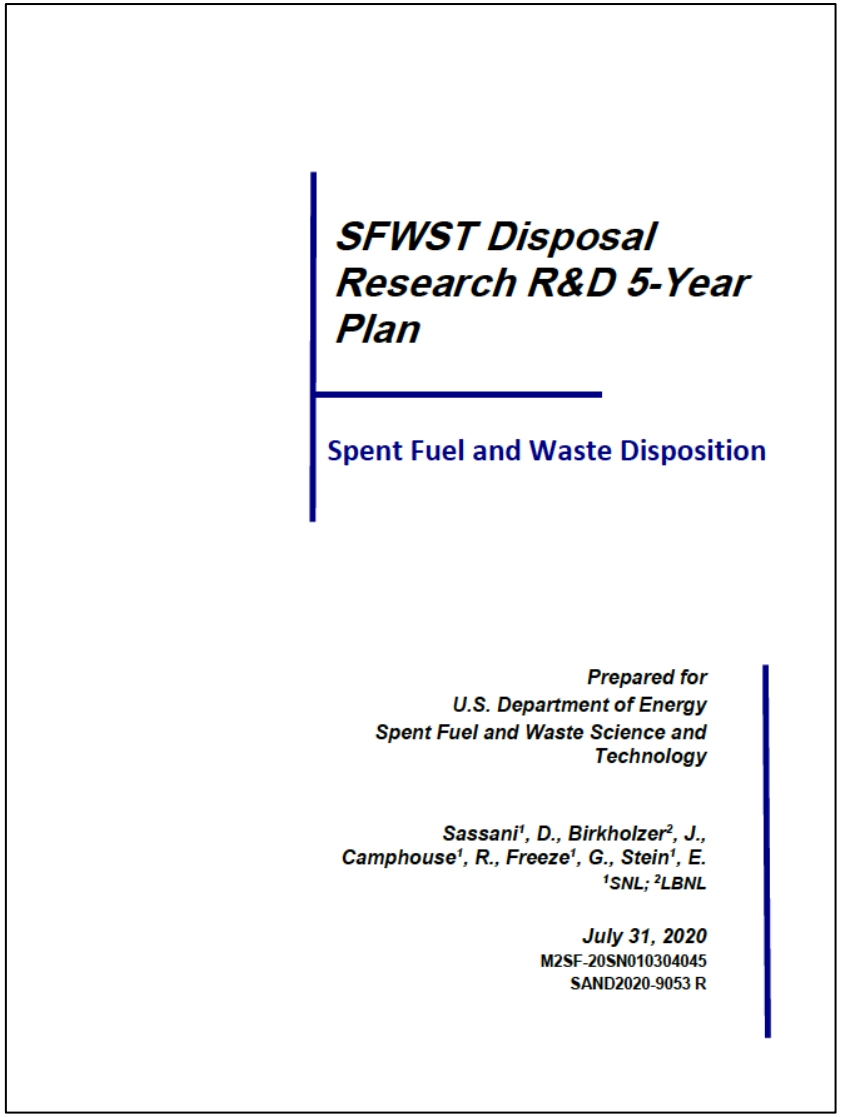
Prioritization Principles

- Prioritize international R&D activities based on key issues, technical merit, relevance to safety, and cost/benefit
- Emphasize active R&D participation and access to experiments in underground research laboratories (URLs)
- Balance portfolio across host rocks, repository designs, and key R&D areas

Disposal Research Five-Year Plan (International Collaboration)

International Collaboration Thrust Topics

- Near-Term Thrust Topics
  - ✓ **Continue participation within international R&D** in URLs for a range of geologic systems
  - ✓ Pursue a **more active role in conducting experimental work** in international URLs
  - ✓ Contribute to **integration and confidence building** for Generic Disposal System Analysis
  - ✓ Continued assessment of **new international opportunities:** Gas Transport, Diffusion Behavior, Sealing Elements, In Situ Corrosion
- Longer-Term Thrust Topics (ongoing or planned)
  - ✓ Utilize international activities for **workforce development in disposal science**
  - Develop best practices and technologies for **site selection and characterization**



SFWST Disposal Research R&D 5-Year Plan

Spent Fuel and Waste Disposition

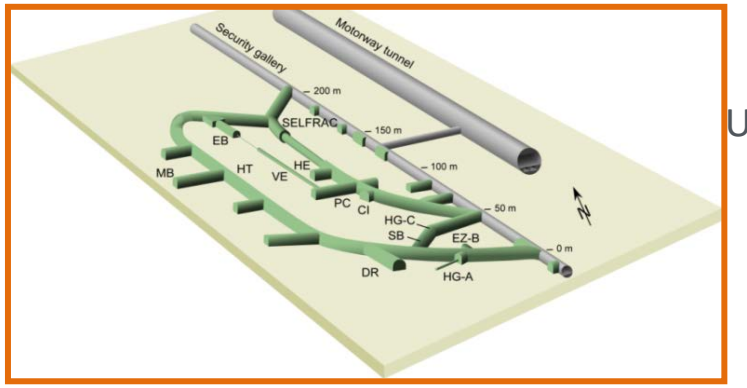
Prepared for
U.S. Department of Energy
Spent Fuel and Waste Science and Technology

Sassani[1], D., Birkholzer[2], J., Camphouse[1], R., Freeze[1], G., Stein[1], E.
[1]SNL; [2]LBNL

July 31, 2020
M2SF-20SN010304045
SAND2020-9053 R

DECOVALEX Project: Model Comparison Against Experiments

- Comparative analyses of multiple approaches, conceptual models, and simplifications applied to the same problem
- Broad portfolio of challenges, designs, host rocks, processes
- Tasks closely reflecting interests of international waste disposal funding organizations
- In-depth and regular discussions among national agencies and research teams with different views
- Excellent publication records, training standard of PhD students, and international visibility and reputation
- A successful long-term platform of information and knowledge exchange



Leverage International Underground Research Labs (e.g. Mont Terri, Switzerland)

Advanced experiments

In-depth comparison and discussion

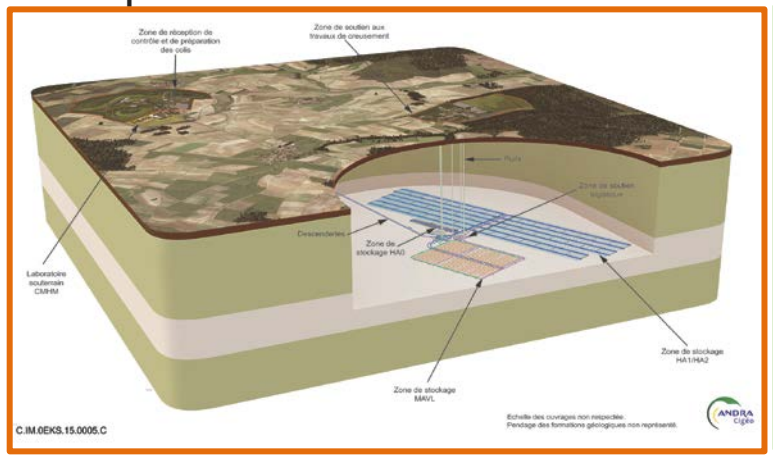
Multiple research teams

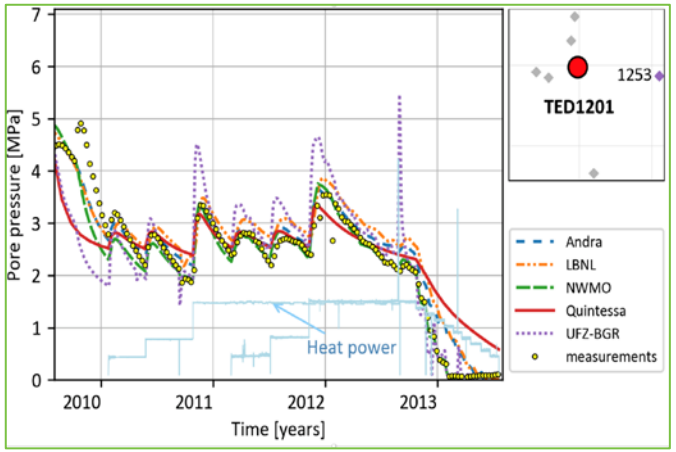
Team	Person	F.O.	Country	Code
BGR	Wang Xuerui	BGR	Germany	OpenGeoSys
CAS	Pengzhi Pan	CAS	China	EPCA3D
LBNL	Jonny Rutqvist	DOE	USA	TOUGH-FLAC
ENSI	Bastian Graupner	ENSI	Switzerland	OpenGeoSys
CNSC	Son T. Nguyen	IRSN	Canada/France	COMSOL
JAEA	Keisuke Maekawa	JAEA	Japan	THAMES
KAERI	Changsoo Lee	KAERI	South Korea	FLAC
CNWRA	Chandrika Manepally	NRC	USA	FLAC-xFlo

DECOVALEX for THM

From DECOVALEX 2019

- Evaluate upscaling methods for THM processes in clay host rock at Bure URL in France
- Scale up from Argillite small-scale boreholes heater tests to a micro-tunnel heater test and then to an entire waste repository (French design)
- Task led by Andra involved five modeling teams, from five different countries (including the U.S.)
- Comparison between these modeling teams provided confidence that upscaling methods for THM repository predictions are tractable and robust

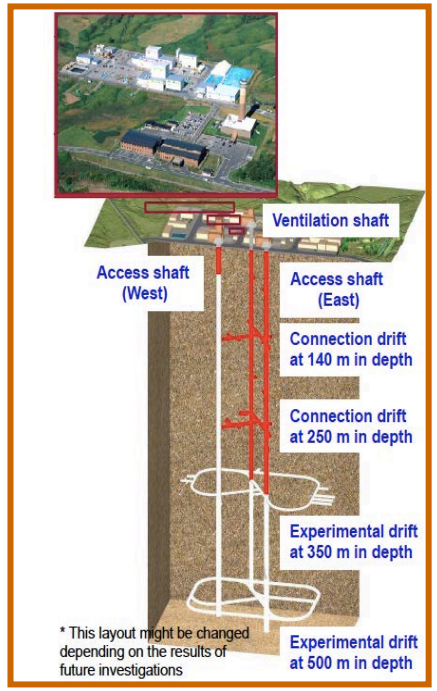




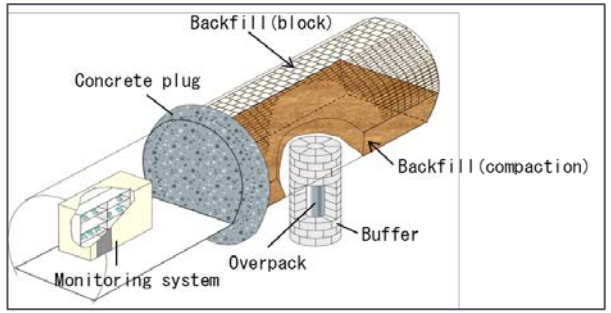
Extensions to DECOVALEX 2023

Full-Scale THM Demonstration Experiments

- THM Modeling of the Full Scale emplacement Experiment in Opalinus Clay at Mont Terri
- Full-scale Engineered Barrier System Experiment at Horonobe URL



Horonobe URL, Japan



Argillite Disposal R&D Activities, 5-Year Plan

Argillite 5-Year R&D Plan

- Priority is given to
  - Engagements in international activities (DECOVALEX-2023, HotBENT, and others),
  - Integration of experimental and modeling activities of barrier material (engineered/natural) interactions at elevated temperatures for generic disposal concepts in argillite.
  - Use of novel approaches to evaluate barrier material dynamic behavior and stability under repository conditions.

Near-Term Thrust Topics (Next 1- to 2-year period)

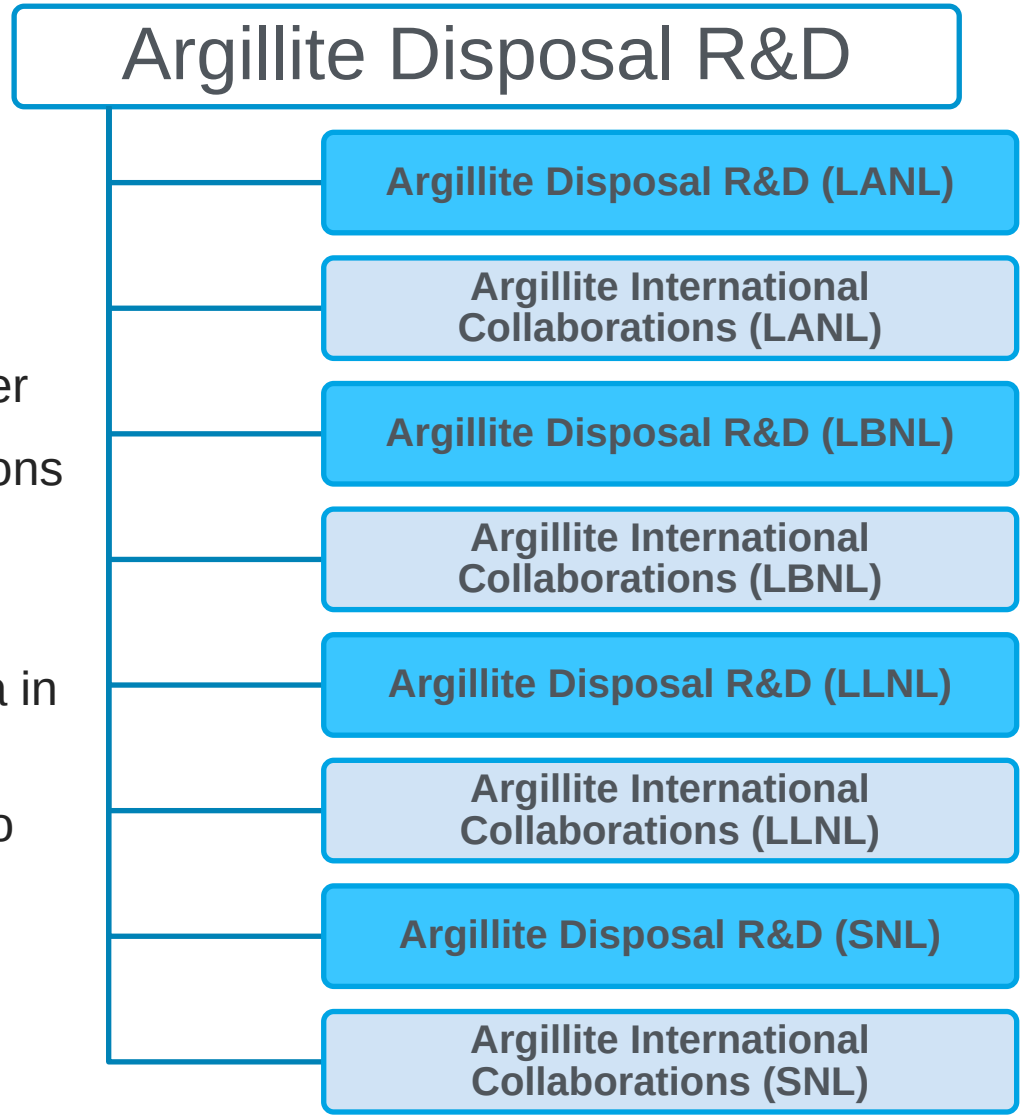
a) *Elucidation of the coupled thermal, hydrologic, mechanical, and chemical (THMC) processes affecting repository performance and*
b) *Development of multi-fidelity approaches for integration of process models into the GDSA Framework*

Longer-Term Thrust Topics (Next 3- to 5-year period)

a) *Simplifying the representations of THMC processes occurring from within the EBS*
b) *International collaborations with inputs on field testing and process understanding*

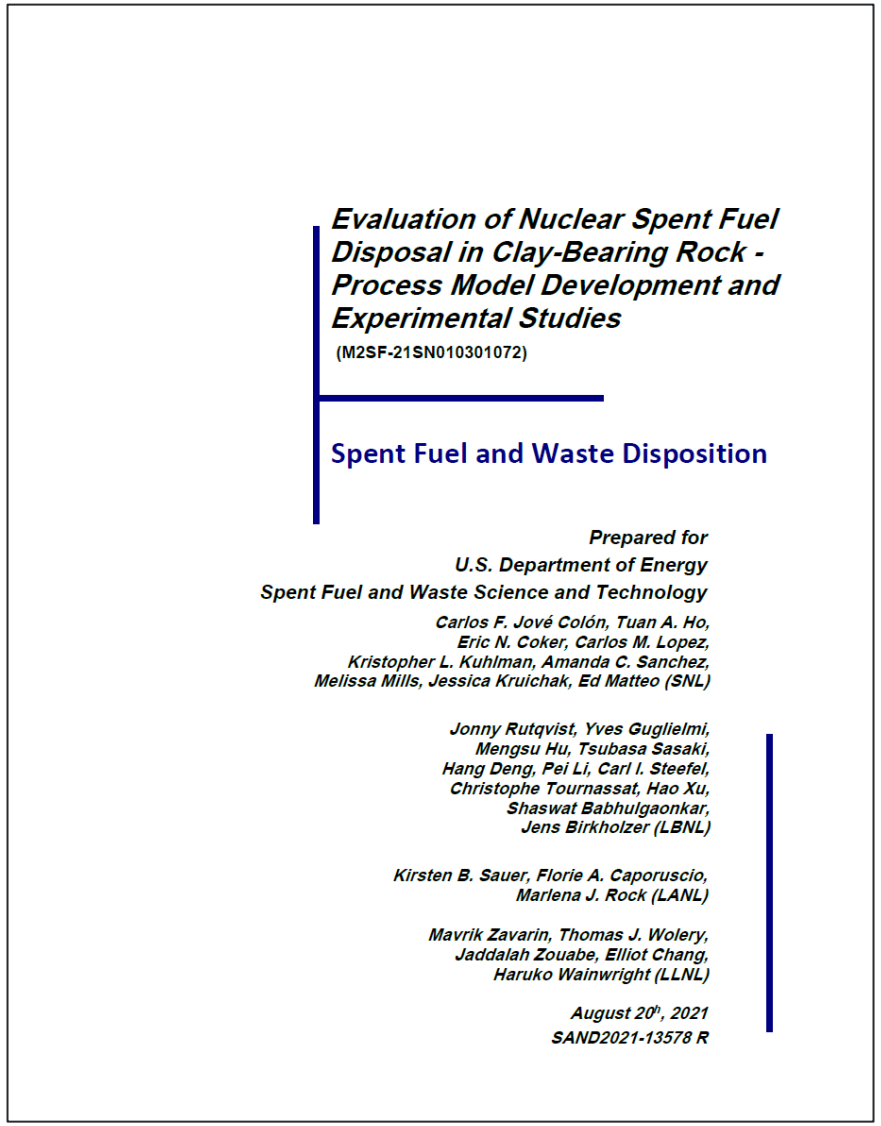
Highlights of Argillite Disposal R&D Activities

- Experimental Activities: Barrier Material Interactions at High Temperatures
- PFLOTRAN THC Modeling
- Modeling of the Long-Term Integrity of the Argillite Host Rock Barrier
- Machine-Learning (ML) approach for radionuclide-mineral interactions & surface complexation database development
- Updates to thermodynamic database development
- Molecular dynamics (MD) simulation of water transport phenomena in smectite
- Integrating Coupled THC Processes for Radionuclide Transport into GDSA
- HotBENT Heated/Unheated Column Experiments



Highlights of Argillite R&D Accomplishments

- Development of a comprehensive suite of experiments focused on hydrothermal interactions of bentonite clay, steel materials, and argillaceous wall rock.
- Integration of characterization studies with thermodynamic modeling, including engineered barrier solids and host rock material.
- Simulations of bentonite swelling and model development to simulate permeability and damage behavior in the EDZ.
- THC modeling of bentonite barrier – fluid interactions via PFLOTRAN.
- Thermodynamic database development for thermodynamic properties of aqueous, solids, and gas species.



Evaluation of Nuclear Spent Fuel Disposal in Clay-Bearing Rock - Process Model Development and Experimental Studies

(M2SF-21SN010301072)

Spent Fuel and Waste Disposition

Prepared for
U.S. Department of Energy
Spent Fuel and Waste Science and Technology

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Jonny Rutqvist, Yves Guglielmi, Mengsu Hu, Tsubasa Sasaki, Hang Deng, Pei Li, Carl I. Steefel, Christophe Tournassat, Hao Xu, Shaswat Babhulgaonkar, Jens Birkholzer (LBNL)

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August 20th, 2021
SAND2021-13578 R

EBS R&D Crosscut Activities, 5-Year Plan

Engineered Barrier 5-Year R&D Plan

- Priority is given to
  - HotBENT Field Test and supporting complementary activities,
  - DECOVALEX 2023 THM modeling and validation activities, using data from Mont Terri FE experiment,
  - Integration between hydrothermal experimental methods and cement-host media studies.

Near-Term Thrust Topics (Next 1- to 2-year period)

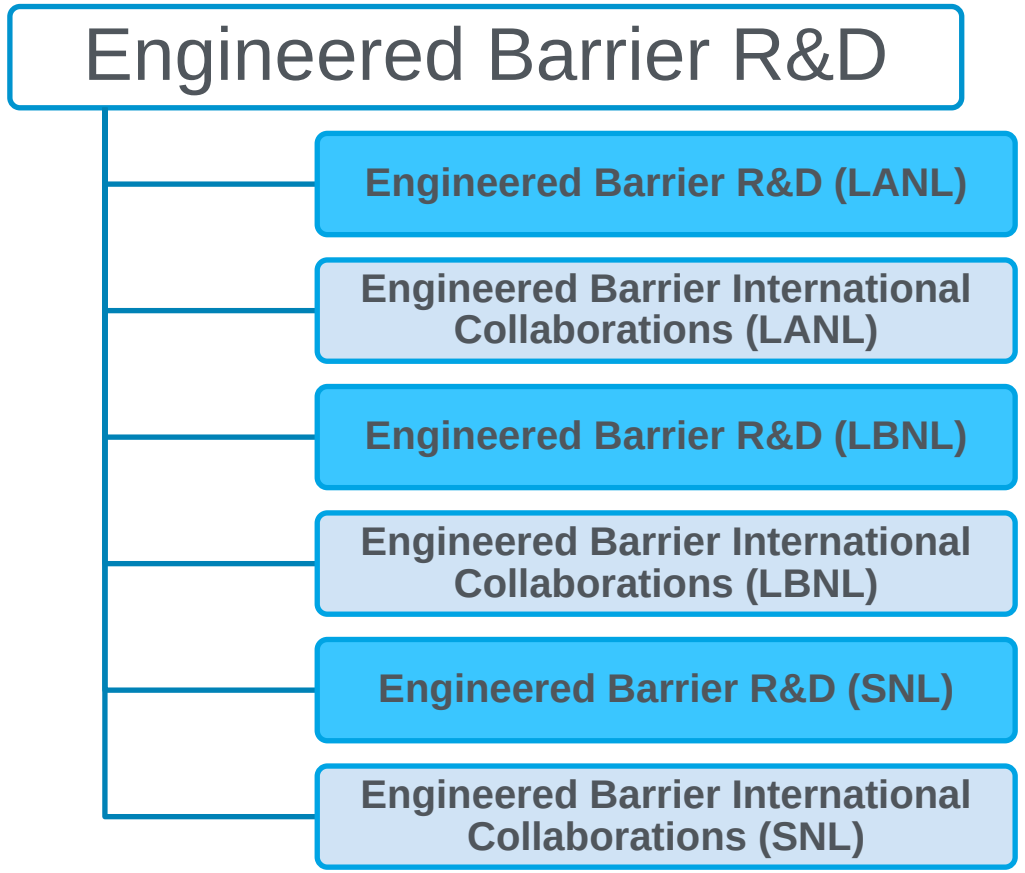
a) *Analysis of thermal, mechanical, and chemical processes that will influence performance of EBS designs for each host media*
b) *Understanding of bentonite buffer drying and re-saturation processes (i.e., thermal-hydrologic behavior)*

Longer-Term Thrust Topics (Next 3- to 5-year period)

a) *International collaboration and URL studies for EBS performance and design materials (e.g., cement)*

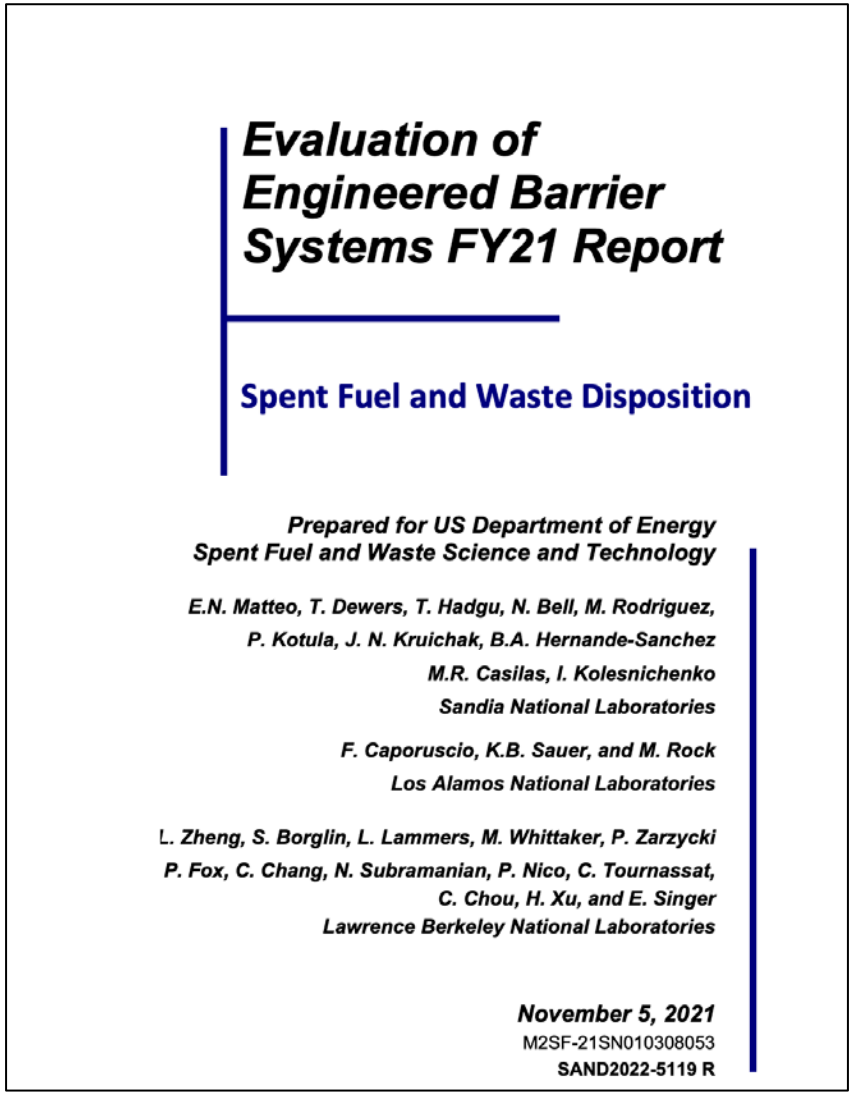
EBS R&D Activity Crosscuts with Argillite

- Fundamental Process Understanding
  - Integrity of Repository Seals
    - Drift and shaft seals
    - Degradation evolution, esp. permeability evolution
  - Processes at material interfaces
    - Engineered materials and Disturbed Rock Zone (DRZ)
    - Waste Package materials and backfill/buffer
  - Representing and understanding complex processes
    - Coupled processes
      - Chemo-mechanics
      - Thermal-Hydrologic-Mechanical-Chemical
    - Multi-phase flow
    - Multi-scale phenomenon
      - Linking microstructural scale to continuum scale



Highlights of EBS R&D Accomplishments (w.r.t. Argillite/Clay)

- THM model development of the Full-scale Emplacement (FE) heater test at the Mont Terri URL, Switzerland.
- Extension of clay swelling thermodynamic modeling to higher electrolyte concentrations.
- Reactive molecular simulations for modeling of bentonite radionuclide retention.
- Sorption and diffusion experiments on bentonite.
- THMC evolution of bentonite via analysis of large-scale field experiments.



Evaluation of Engineered Barrier Systems FY21 Report

Spent Fuel and Waste Disposition

Prepared for US Department of Energy
Spent Fuel and Waste Science and Technology

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Los Alamos National Laboratories

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P. Fox, C. Chang, N. Subramanian, P. Nico, C. Tournassat,
C. Chou, H. Xu, and E. Singer
Lawrence Berkeley National Laboratories

November 5, 2021
M2SF-21SN010308053
SAND2022-5119 R

Nuclear Energy University Program (NEUP)

U.S. University Nuclear Energy R&D for DOE Waste Disposal Needs

Since 2020, there have been 14 NEUP awards to teams investigating disposal R&D aspects significant to argillite host rock and engineered barriers.

Some Highlights

- Backfill Material Advancements
- High Temperature Effects
- Adsorption and Reduction Studies
- THMC Processes for Bentonite
- Database Development
- Engineered Barrier Material

Conclusions

- Argillite R&D activities are extensive in scale, from bench lab work to URL field testing.
- Collaborations are extensive, from university to international partners.
- Engineered barrier R&D is complementary, develops technical understanding of the barrier/argillite host rock system.
- Argillite and EBS R&D activities provide technical underpinnings for GDSA models and representations.
- Annual milestone reports contain detailed summaries of R&D activities and results.

References

- Birkholzer, J., *Introduction and Overview of International Disposal Research*. Presented at the SFWST Annual Work Group Virtual Meeting. 10 – 12 May 2022.
- Birkholzer, J. and A. Bond., "Clay Research in the International DECOVALEX Model Comparison Project: An Overview of Past and Current Modeling Tasks". *8th International Conference on Clays in Natural and Engineered Waste Barriers for Radioactive Waste Confinement.* 13 – 16 June 2022. Nancy, France.
- Birkholzer, J. et al., *International Collaboration Activities in Geologic Disposal Research: FY21 Progress.* FY21 International Collaboration Report for SFWST. 30 September 2021. LBNL-2001433.
- Jove-Colon, C. et al., *Evaluation of Nuclear Spent Fuel Disposal in Clay-Bearing Rock – Process Model Development and Experimental Studies.* FY21 Argillite Disposal Report for SFWST. 20 August 2021. SAND2021-13578 R.
- Matteo, E. et al., *Evaluation of Engineered Barrier Systems FY21 Report*. FY21 Engineered Barrier System Report for SFWST. 5 November 2021. SAND2022-5119 R.
- Sassani, D., Birkholzer, J., Camphouse, R., Freeze, G., and E. Stein. *SFWST Disposal Research R&D 5-Year Plan – FY2021 Update*. 12 August 2021. SAND2021-12491 R.

Thank you for your kind attention.