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ARGILLITE AND CRYSTALLINE DISPOSAL RESEARCH: ACCOMPLISHMENTS AND PATH-FORWARD

Fuel Cycle Research & Development

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

Carlos Jove-Colon, Kevin McMahon, Yifeng Wang, Sandia National Laboratories

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Acronym List

DECOVALEX	DEvelopment of COupled models and their VALidation against EXperiments
DOE	Department of Energy
DOE-NE	DOE Office of Nuclear Energy
DR	Disposal Research
EBS	Engineered Barrier System
FCRD	Fuel Cycle Research and Development
FCT	Fuel Cycle Technologies
FEBEX	Full-scale Engineering Barrier EXperiments
FEPs	Features, Events and Processes
GDSA	Generic Disposal Systems Analysis
HLW	High Level Waste
KAERI	Korean Atomic Energy Research Institute
KURT	KAERI Underground Research Tunnel
NFSTPP	Nuclear Fuel Storage and Transportation Program Plan
NRC	Nuclear Regulatory Commission
NTD	National Technical Director
PA	Performance Assessment
QA	Quality Assurance
R&D	Research & Development
UFD	Used Fuel Disposition
UFDC	Used Fuel Disposition Campaign
UNF	Used Nuclear Fuel
URL	Underground Research Laboratory

I. Introduction

The intention of this document is to provide a path-forward for research and development (R&D) for two host rock media-specific (argillite and crystalline) disposal research work packages within the Used Fuel Disposition Campaign (UFDC). The two work packages, Argillite Disposal R&D and Crystalline Disposal R&D, support the achievement of the overarching mission and objectives of the Department of Energy Office of Nuclear Energy Fuel Cycle Technologies Program. These two work packages cover many of the fundamental technical issues that will have multiple implications to other disposal research work packages by bridging knowledge gaps to support the development of the safety case.

The path-forward begins with the assumption of target dates that are set out in the January 2013 *DOE Strategy for the Management and Disposal of Used Nuclear Fuel and High-Level Radioactive Waste* (http://energy.gov/downloads/strategy-management-and-disposal-used-nuclear-fuel-and-high-level-radioactive-waste).

The path-forward will be maintained as a living document and will be updated as needed in response to available funding and the progress of multiple R&D tasks in the Used Fuel Disposition Campaign and the Fuel Cycle Technologies Program. This path forward is developed based on the report of "Used Fuel Disposition Campaign Disposal Research and Development Roadmap (FCR&D-USED-2011-000065 REV0)" (DOE, 2011). This document delineates the goals and objectives of the UFDC R&D program, needs for generic disposal concept design, and summarizes the prioritization of R&D issues.

II. Fuel Cycle Technologies Program Mission and Objectives

Nuclear energy is a prominent part of a reliable, sustainable energy mix and has demonstrated remarkable performance over decades of use. Despite this key role, nuclear energy use presents challenges including mounting stockpiles of used nuclear fuel (UNF) and high-level radioactive waste (HLW) and a potential for nuclear proliferation. The United States must address these challenges in order to meet our goals for energy, environmental and economic security. In response, the U.S. Department of Energy Office of Nuclear Energy (DOE-NE) established the Fuel Cycle Technologies (FCT) program (http://energy.gov/ne/fuel-cycle-technologies). Within the FCT program, the UFDC goal is to develop a comprehensive R&D program to evaluate the waste isolation performance of a subsurface geologic repository in various types of host rock media.

Long-term resolution of the aforementioned challenges entails development of sustainable systems that reduce waste while improving resource utilization and safety. To identify potential solutions, the FCT program adopted a results-oriented, science-based approach towards R&D that takes advantage of advances in high-performance computing (HPC) to evaluate and integrate theory and experimental data with advanced modeling and simulation.

The *FCT program mission* is multi-faceted, tackling current issues with the nation's UNF inventory and maximizing performance and safety of the existing nuclear fleet. Concurrently, it is also developing advanced systems for the future that will ensure nuclear energy's continued role as a clean, safe, and sustainable energy source. FCT programs goals that are directly addressed by the UFDC are in boldface type.

FCT Near-Term Goals

- **Strengthen the technical and scientific basis for extended storage of UNF and HLW, and work with industry to develop and demonstrate solutions.**
- Identify and test options to enhance accident tolerance of the current reactor fleet.
- Identify and select preferred fuel cycle options that address key challenges, including deployment of advanced uranium enrichment technologies to enhance national energy security.

FCT Medium-Term Goals

- **Deploy the selected extended storage solution while developing the scientific basis for permanent disposal options in a geologic repository.**
- Demonstrate and deploy the selected enhancements for accident tolerance.
- Conduct science-based, engineering-driven research to fully evaluate and characterize the selected sustainable fuel cycle options.[a]

FCT Long-Term Goals

- **Implement safe strategies for management of UNF and HLW, including both storage and permanent disposal solutions.**
- Deploy advanced nuclear systems for safe, affordable, and secure nuclear-generated electricity while continuing to test enabling technologies for future deployment.

III. UFDC Mission, Objectives and Challenges

UFDC Mission

The mission of the UFDC is to identify alternatives and to conduct scientific research and technology development to enable storage, transportation and disposal of used nuclear fuel and wastes generated by existing and future nuclear fuel cycles.

Recognizing that the current system for managing UNF and HLW is viable for several decades, the UFDC has established *near-term* (5-yr) and *medium-term* (10-yr) *objectives* to meet the overarching goals for used fuel and high-level waste management, building on research completed in these areas since 2009. Objectives shown below include only those applicable to disposal research.

[a] A sustainable fuel cycle is one that: improves uranium utilization, maximizes energy generation, minimizes waste generation, improves safety, and limits proliferation risk.

Disposal Research Objectives

UFDC Challenge

Provide a sound technical basis for supporting the DOE strategy for managing the back end of the nuclear fuel cycle, including the identification and evaluation of safe and secure options for storage, transportation, and permanent disposal of radioactive wastes resulting from existing and future fuel cycles.

Near-Term Disposal Research Objectives (2016–2020)

- Field a deep borehole test, with drilling beginning in 2016 and testing complete in 2019.
- Complete evaluation of the direct disposal of dual-purpose canisters.
- Develop the experimental and modeling basis for understanding long-term performance of disposal systems in clay/shale and crystalline rock.
- The aforementioned development will be integrated with the Generic Disposal System Analysis (GDSA) model activities to identify gaps, develop process models, provide parameter feeds and support requirements providing the capability for a robust repository performance assessment (PA) model by 2020.

Long-Term Disposal Research Objectives (2020–2025)

- Develop the technical basis of the Deep Borehole Disposal concept with Deep Borehole Field Test data.
- Support implementation of integrated storage, transportation and disposal concepts.
- Support integration of disposal research activities with GDSA-PA modeling for the evaluation of repository performance.

IV. Disposal Research and Development (R&D)

Safe disposal of radioactive waste is accomplished by isolating the waste from the human environment for sufficiently long time periods, as required by regulatory standards. Isolation is achieved through a combination of engineered and natural barriers (e.g., robust waste packages, and very slow radionuclide transport through the surrounding engineered barrier and rock), essentially resulting in no radiological risk to the biosphere for many thousands of years when these barriers perform as expected. Over the very long time periods necessary to isolate the wastes, the engineered barriers may degrade, allowing radionuclides still present in the waste to be released at a low rate into the natural system. The natural system will act to reduce and delay the subsequent migration of radionuclides to the accessible environment to levels stipulated by regulatory standards, typically well below naturally-occurring background radiation levels. Understanding when radionuclides may begin to be released from the disposal system, the rate at which they may be released, and how they might migrate through the natural system are primary factors in demonstrating the safety performance of a disposal system concept.

Geologic disposal concepts are typically complex systems with physical and chemical couplings between the disposed waste, engineered barrier materials, and the natural system. The long-term radionuclide isolation capabilities and characteristics of a waste disposal environment are dependent on the details of the site, and the form and composition of the wastes to be disposed. Disposal systems can be geographically large and the distance over which materials could potentially migrate can be long. In addition, because of the long time frames involved, precise predictions of repository performance are not possible, and uncertainty must be acknowledged in the decision-making process. Quantifying, propagating, and reducing this uncertainty through safety assessments have been and continue to be challenges in demonstrating the viability and safety of geologic disposal. Disposal R&D focuses on gathering sufficient data (laboratory and field) and developing high-fidelity computational models for evaluating and demonstrating long-term disposal system performance and safety.

Evaluations indicate that, based on existing information, reasonable designs, and generic safety assessment models, it is likely that mined geologic repositories (i.e. in salt, argillaceous, or crystalline rocks) or deep borehole disposal facilities that are capable of safely isolating used nuclear fuel and high-level radioactive waste from the public and the environment can be developed in the U.S.

Given the generic nature of this work, the R&D activities formulated in this path-forward document will focus on general capability development, generic data collection, and enhanced understanding of geologic media and processes involved in waste disposal through integrated modeling, laboratory and field work. Models and methods for improved understanding can be developed without site-specific data from an actual site considered for disposal in the U.S. Data from representative geologic environments obtained through international scientific collaborations and literature studies can potentially be used for the generic R&D, to ensure that the envisioned models and methods work for the intended purpose.

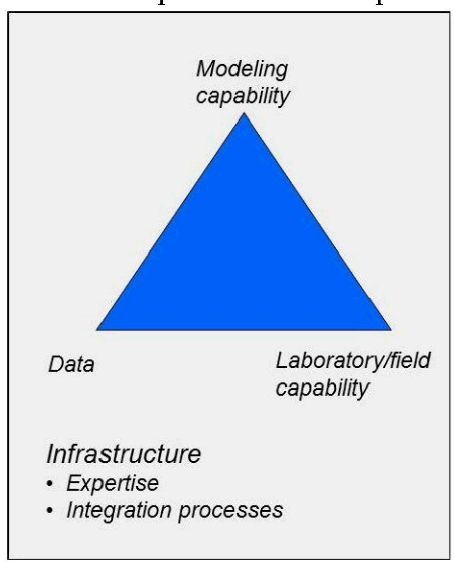

FIGURE 1: Key components of UFDC capability development

The capabilities to be developed in this path-forward include (1) numerical models and modeling tools, (2) experimental techniques and field testing capabilities that can be used for validating and/or verifying the models, and (3) technical data that are needed to support computational simulations. In a more general sense, this effort will also include the development of necessary infrastructure (e.g. maintaining appropriate technical expertise and developing appropriate system integration processes among different UFDC work packages) to support actual site screening, site selection, site characterization, and eventually the repository license application (Figure 1). For model development, it should be noted that multiple-fidelity models will be needed for different applications, ranging from support of simple FEP screening assessments to ultimately a comprehensive license application. The modeling tools to be developed should be able to accommodate this and other needs.

V. Disposal Research Necessary to Meet DOE Strategy Goals

In order to meet the goals set out in the *DOE Strategy* for the disposal of UNF and HLW it is necessary to recognize that specific research and development tasks must be completed within a defined timeline. This section identifies an approximate timeline and tasks required to meet the stated goals. Some items listed below are not specifically research and development tasks but must be completed in order to achieve the stated goal.

❖ R&D task.

2026 Permanent repository sited

Requirements:

❖ Completed GIS database [by 2018]
❖ Defined site characterization process [by 2018]
  o Site screening and characterization process defined and implemented
  o Features, events and processes (FEPs) defined for each site
- Defined inventory of what will go into the repository
  o Include detailed attributes of waste forms as intended for disposal
- Defined list of candidate sites [2022]
- Defined down-selection process from volunteer sites [2026]
❖ Predictive modeling tools validated [by 2022]
  o Data collected for specific candidate sites
  o Preliminary conceptual repository design to perform analysis
❖ Metrics for a suitable site evaluation defined [by 2020]
  o Performance measures that will be calculated by the model
  o Metrics may be a reiteration of NRC-defined regulations for a repository
  o Considerations: dose, thermal load, cost, time, etc.
- Cost analyses
- QA program in place
- EIS started

2038 Repository site license application submitted

2042 Repository designed and licensed

Requirements:

❖ Site characterization complete [by 2034]
  o Iterative process with system performance analysis
  **Typically plan for ~15 yrs, but this does not fit within the current estimated timeline.
- Underground Research Laboratory testing
❖ Understanding of data and processes is sufficient to support licenses [complete by 2034 to support license application; work will continue through licensing approval]
- Repository design and plans for operation sufficient for licensing
  ❖ Iterative process with system analysis [2026 – 2034]
  o Freeze design in 2034
❖ Pre- and post-closure safety analyses

    - Model must be available prior to this step [model evolves 2026-2034]
    - Post-closure analysis as a component of preparing the license application [2034-2038]
- ❖ Performance confirmation program in place [defined by 2038; implemented through closure and post-closure monitoring]
    - Includes instrumentation and monitoring plan in place
    - Assess what instrumentation is available at present and when would need to be available
- License in-hand
    - Milestones for licensing:
        - Submit license [4-yrs to license; submit by 2038]
        - Complete characterization [4-yrs to prepare license application; complete characterization by 2034]
        - Site characterization [2026 – 2034, defined by established timeline rather than by duration desired by technical staff]
- Detailed design in-hand
- Surface facilities designed
- FEIS completed

2048 Repository constructed and operations commenced

Requirements:

- Construction and startup schedule must be maintained
- Note: Yucca Mountain assumed that the first waste shipment would be received 9 yrs after license was in hand.

VI. Current Specific Disposal Research Activities Applicable to Argillite and Crystalline

DR – Specific Host Rock R&D

The objectives of the Host Rock R&D activities are to develop experimental and computational capabilities and to perform modeling analyses to support the development of disposal concepts in various geologic media in the near- and far-field environment of disposal. Understanding interactions occurring between fuel waste and various natural and engineered barriers within various design concepts is important for determining design flexibility and optimization, establishing requirements for waste form performance, and providing a scientific basis underlying the safety cases for optional disposal systems.

Host Rock Research: Argillite *(clay-bearing host rock)*

The argillite work package is focused on the evaluation of important processes in the analysis of disposal design concepts and related materials for nuclear fuel disposal in this type of clay-bearing repository media.

Current activities include:

- Model development
  - Develop constitutive relationships for coupled processes.
  - Evaluate relevant physico-chemical processes for clay/shale disposal.
  - Develop thermodynamic databases and modeling approaches for chemical equilibria and sorption with insights from experimentally-based studies.
  - Develop process models to quantify the effects of chemical, electrochemical, and radiolysis reactions; physical mass transport processes; and environmental conditions on fuel matrix degradation, radionuclide release rates, and canister/overpack performance.
- Conduct clay damage and discrete fracture studies.
- Establish a scientifically sound thermal limit on argillite host rock via high temperature laboratory tests.
- International collaborations:
  - Collaborate on testing at the Mont Terri Underground Research Laboratory (URL) in argillite in Switzerland.
  - Collaborate through DEvelopment of COupled models and their VALidation against EXperiments (DECOVALEX), an international cooperative research project on mathematical models of coupled thermal-hydrological-mechanical processing for safety analysis of radioactive waste repositories.
  - Collaborations with the FEBEX-DP activity on the dismantling of the FEBEX heater test experiment at the Grimsel URL site, Switzerland.

Host Rock Research: Crystalline

The crystalline work packages are aimed at advancing our understanding of long-term disposal of used fuel in crystalline rocks and to develop necessary experimental and computational capabilities to evaluate various disposal concepts in such media.

Current activities include:

- Support to develop of a total system performance assessment model for crystalline media. This activity helps develop the first version of the PA model for crystalline rocks by providing conceptual and mathematical models as well as model input parameters.
- Continuing the development of the fuel degradation model and initiating the waste package degradation model.
- Synthesis of colloid formation and transport-related work and formulating a colloid-facilitated transport model for total system performance assessments.
- Modeling of fluid flow and transport in fractured crystalline rocks: task will continue to demonstrate the potential application of the discrete fracture network model and the fracture continuum model to actual field testing data obtained from international collaborations. Develop a strategy to integrate these types of process models into a total system performance assessment model.
- Experimental investigation of radionuclide interactions with natural and engineered materials: Continue the work on actinide sorption and diffusion in clays and in granitic materials, with an aim to

develop a comprehensive process model for total system performance assessment and to maintain certain levels of experimental activities.

- Investigation of thermal limits of clay materials: Start systematical measurements swelling and cation exchange capacities for clays subjected to various thermal treatments.

International collaborations: International collaborations are crucial for the activities proposed for this work package. These collaborations will include: KURT tests, SKB-BRIE tests, DECOVALEX, Mont Terri and FEBX-DP tests.

DR – Generic Disposal Systems Analysis (GDSA)

The objective of the Generic Disposal System Analysis (GDSA) activity is to develop the necessary system model architecture to support the evaluation of post-closure risk. Modeling will be at sufficient rigor to support the intended use and maintain the flexibility in the system model architecture to meet the evolving needs of the DOE NE and UFD missions. Models will have the capability to produce risk information throughout the potential future phases of the mission, including prioritization of R&D needs, down selection of geologic disposal options, and site selection and screening. The generic disposal system modeling and analysis capability, including uncertainty, will cover a range of disposal options (e.g., salt, argillite, crystalline, deep borehole).

Additionally, the UFD Disposal Research R&D Roadmap is an evolving document that will ensure that the technical information needed to implement new national policy for managing the back end of the nuclear fuel cycle is available when decisions are made to move forward. It is focused on generic research and development work undertaken today that will support future site-specific work. As DR continues to evolve, it is necessary to update the R&D Roadmap to provide both tactical and strategic guidance for the direction of DR. The DR R&D Roadmap will be updated and managed under the Generic Disposal Systems Analysis activity.

Current activities include:

- Develop a source term conceptual model applicable to all generic disposal options.
- Integrate updated conceptual models of subsystem processes and couplings developed under other work packages; leverage existing computational capabilities.
- Develop and simulate reference cases for generic salt, argillite, and crystalline (granitic) disposal systems.
- Review and update of the DR R&D Roadmap.

DR – Deep Borehole Disposal

The objective of the Deep Borehole Disposal activity is to advance the deep borehole disposal technical basis needed to demonstrate the viability of this disposal concept and make progress towards implementing a full-scale demonstration.

Current activities include:

- Utilize the regional geology database to support site selection for the deep borehole field test.
- Evaluate sub-regional geology and other information for a drilling demonstration project.
- Develop reference designs for disposal of alternative waste forms.
- Evaluate borehole seals for chemical, mineralogical and physical stability in the deep borehole environment.

Planned activities include initiation of a field demonstration test to evaluate the feasibility of the deep borehole disposal concept, conditional on programmatic approval. Specific activities associated with the first year of a deep borehole field demonstration test using surrogate waste will include:

- Establishment of a project management structure.
- Preliminary characterization and evaluation of one or more candidate sites for a field test.
- Selection of a site for a field test, including land acquisition.
- Development of a conceptual design and requirements for borehole construction.
- Development of a conceptual design and requirements for disposal canisters and waste handling.
- Evaluation of regulatory and legal requirements, including obtaining necessary permits.
- Modeling to support site evaluation and test design.

DR – International Disposal R&D

The International Disposal control account is established to ensure the integration and coordination of UFD-supported activities among participating national laboratories and comparable programs outside the US. UFD management will be advised of international opportunities that complement ongoing campaign R&D and of activities that have the greatest potential for substantive technical advances. International collaboration is a beneficial and cost-effective strategy for advancing disposal science with regards to multiple disposal options and different geologic environments.

DR – DOE Managed HLW and SNF Research and Analysis

This disposal research activity is intended to establish a path for the permanent disposal of high-level radioactive waste and SNF derived from national defense nuclear activities and R&D activities of the Department of Energy (DOE). In FY-16, specific attention will be given to the activities needed to implement a plan for disposal of the subject wastes within the DOE's existing authority under the Atomic Energy Act of 1954, and fully consistent with the requirements of the Nuclear Waste Policy Act of 1982, as amended.

VII. Summary of Progress and Path-Forward of Disposal Research Activities Applicable to Argillite and Crystalline

Host Rock Research: Argillite

The shale/argillite disposal R&D activity is focused on the evaluation of important processes in the analysis of disposal design concepts and related materials for nuclear fuel disposal in clay-bearing repository media. Various key characteristic of engineered barrier design concept evaluation, research tools and, methodologies applied to the evaluation of performance requirements for disposal in argillite/shale media. This include multi-barrier concepts that will be considered to assess adequacy of disposal concepts for clay rock. A multi-faceted integration of knowledge and evidence gathering is required to demonstrate the appropriate confidence level of repository performance at a geological disposal site. This level of integration between various work packages, particularly performance assessment, is also necessary to build the safety case along with the necessary system requirements (safety and performance) in the decision-making process.

Current progress on R&D activities applicable to clay/shale/argillite media are summarized as follows:

Evaluation of Used Fuel Disposition in Clay-Bearing Rock: Reactive-Transport Modeling of the Near Field Environment

- Non-isothermal 1D reactive-transport modeling of the EBS using the PFLOTRAN simulation code.
    - Thermally-driven phase transformation reactions of hydration/dehydration reactions (e.g., gypsum → anhydrite) can generate volume differences of ~60% leading to porosity increases in the EBS bulk regions and at interfaces.
    - Dissolution/precipitation reactions leading also to porosity enhancement and/or reduction.
    - Changes in pore solution chemistry and temperature are key factors in determining the alteration mineral assemblage.

International collaborations: Simulation of Heater Test Experiments at URls and EBS Material Characterization Studies

- Standard X-ray Micro-(CT) and synchrotron X-ray microCT (SXR-μCT) imaging reveals the wide occurrence of microcracks in FEBEX-DP project (Grimsel URL, Switzerland) bentonite samples as a result of dehydration and shrinkage. Microcracks can influence moisture transport and clay swelling in clay barrier material.
- The application of scanning characterization techniques (e.g., micro-XRF and SEM/EDS/BSEI) are useful in the compositional characterization of EBS barrier materials and their alteration modes.
- Thermal-Hydrological-Mechanical (THM) and Heater Test Modeling implementation of the Barcelona Expansive Model (BExM in TOUGH-FLAC computer codes). Successful completion of DECOVALEX-2015 modeling associated with the Mont Terri HE-E experiment and Horonobe

EBS experiment. Currently analyzing field data from the largest ongoing underground heater test in the world: Mont Terri FE experiment.

- Thermal-Hydrological-Mechanical-Chemical (THMC) model implementation of the BExM to link mechanical process with chemistry to simultaneously incorporate the effects of exchangeable cations, ionic strength of pore water and abundance of swelling clay on the swelling stress of bentonite.

Discrete Fracture Network (DFN) Approach for THM Damage Modeling in Argillaceous Rock:

- An effective coupling between the TOUGH2 (Thermal-Hydrological simulation code) and the Rigid Body Spring Network (RBSN) approach has been implemented and applied to hydraulic fracturing and damage deformation simulations.

Experimental studies of EBS Materials

- Experimental work focus: Opalinus wall rock interactions with EBS clay backfill, copper alteration and corrosion rates, steel/bentonite interface phase reactions at elevated temperatures.
- Alteration mineralogy in Opalinus Clay upon heating develops wairakite along cracks and edges. Mine run bentonite contains clinoptilolite, and transforms to analcime at high temperatures, releasing both SiO_2 and water.
- Pit corrosion is the driving force in copper degradation at high temperatures. Copper reacts with H_2S (aq, g) to produce chalcocite and covellite.
- The interface between bentonite and steel develops a well characterized Fe-saponite phyllosilicate (particularly at 300°C), that grows perpendicular to the steel surface. Pit corrosion of low carbon steel was common and resulted in a corrosion rate of 1083 µm/yr.

Thermodynamic Database Development and Sorption Database Integration

- Evaluation of a thermodynamic data using concept of “links” to the chemical elements in their reference forms.
- Coupling of the PHREEQC computer code with the parameter estimation / optimization software PEST was tested to fit U(VI)-quartz sorption dataset.
- Ongoing NEA TDB project activities include upcoming releases and/or ongoing review activities of chemical thermodynamic data.

Fuel Matrix Degradation Model (FMDM): Canister Corrosion and the Effect of Hydrogen on Used Fuel Degradation Rates

- Integration of the Fuel Matrix Degradation Model (FMDM) with the GDSA-PA model
- Electrochemical steel corrosion model implementation that couples in-package steel corrosion with fuel degradation. This includes mechanistic modeling of H_2 effects and its impact on source term calculations for in-package steel corrosion and used nuclear fuel.

Radiolysis Model Formulation for Integration with the FMDM

- Radiolysis model for calculating radiolytic generation of H_2O_2 in the presence of aqueous species like Br^- accounting for dependencies on H_2.

A summary of R&D path-forward objectives for disposal in argillite are:

- To evaluate physico-chemical processes for backfilled engineered barriers systems (EBS) and materials relevant to spent nuclear fuel disposal in clay/shale host-rock media. These evaluations will encompass multi-laboratory efforts for the development of EBS design concepts and application of Thermal-Mechanical-Chemical (TMC) experimental work to assess barrier material interactions with subsurface fluids and other barrier materials, their stability at high temperatures, and the implications of these processes to the evaluation of thermal limits.
- Coordinate the scope and integration of results produced by various R&D activities in other national laboratories for use across SFWST-related repository science work packages.
- Integrate and implement models for spent fuel degradation and radionuclide mobilization to evaluate the source term consistent with argillite or granite repository environments. Also, create synthesis reports documenting the work produced by various laboratory groups.
- Engage with the generic disposal system analysis performance assessment (GDSA-PA) activity to develop process models supporting the GDSA-PA model and to provide the parameter feeds to the model.
- Develop thermodynamic databases (e.g., cement and clay) along with modeling approaches for chemical equilibria and sorption, with insights from experimentally-based studies. Thermodynamic databases and associated models are key to the evaluation of multiphase multicomponent interactions between fluids, and barrier materials and spent fuel. Further, seek engagements with international partners and other multi-institutional collaborative efforts to enhance and bridge advancements in the analysis, expansion, and implementation of thermodynamic databases and modeling in nuclear waste repository science.
- To expand existing R&D partnerships with international programs in nuclear waste disposal underground research laboratory (URL) activities to create a bridge with other groups conducting nuclear waste disposal research. This activity will involve model calibration of clay properties based on FE heater test (Mt. Terri) and comparison of results with other teams. Participate in programs such as FEBEX-DP (dismantling phase) to interrogate material properties through sample characterization and controlled disassembling of the engineered barrier. Participation in the current phase of the DECOVALEX international collaboration program.

Host Rock Research: Crystalline

The objective of the Crystalline Disposal R&D activity is to advance our understanding of long-term disposal of used fuel in crystalline rocks and to develop necessary experimental and computational capabilities to evaluate various disposal concepts in such media. Major accomplishments are summarized as follows:

Development of Fuel Matrix Degradation Model (FMDM)

- Similar to the Argillite Disposal R&D activity, the Crystalline Disposal R&D work also supports development of the FMDM electrochemical steel corrosion model coupling in-package steel corrosion with used fuel degradation. The emphasis on integration with the GDSA-PA model is also supported by this activity.

Uranium Interaction with Engineered Materials

- A new surface complexation model (SCM) for U(VI) adsorption onto Na-montmorillonite has been developed to cover a wide range of chemical solution conditions. This model specifically accounts for the 'spillover' of the electrostatic surface potential of basal cation exchange sites on the surface potential of neighboring edge sites.

Colloid-Facilitated Radionuclide Transport

- A comprehensive literature review and data synthesis has been conducted on colloid-facilitated radionuclide transport (CFRT), and a scheme for the implementation of the CFRT model in performance assessment has been proposed.
- A comprehensive model interpretation has been performed for the Grimsel Test Site (GTS) CFRT tests, yielding valuable insights for modeling of radionuclide transport, and particularly of CFRT, in saturated fractured crystalline rocks.
- It is shown that the actinides Th, Pu and Am, and the fission product ^{137}Cs, are the most likely radionuclides to experience colloid-facilitated transport over long time and distance scales (at least for bentonite colloids in a fractured crystalline setting). However, the time and distance scales of the GTS tests were very short relative to time and distance scales of relevance for nuclear waste repository performance assessments.
- The GTS results collectively suggest that CFRT is likely to be more efficient at lower radionuclide concentrations than at higher concentrations because a greater fraction of the radionuclide mass will then tend to become associated with strong, low abundance adsorption sites on the colloids.

D*evelopment and demonstration of Discrete Fracture Network (DFN) model*

- Evaluated the correlation between fracture size and fracture transmissivity. Characterized how different fracture size-transmissivity relationships influence flow and transport simulations through sparse three- dimensional discrete fracture networks, based on Forsmark fracture characteristics provided by the SKB site characterization study.

- Adopting a correlation between a fracture size and its transmissivity leads to earlier breakthrough times and higher effective permeability when compared to networks where no correlation is used.
- Developed an analysis and visualization tool for the characterization of flow in constrained networks using the concept of a flow topology graph (FTG).

Comparison of Fracture Continuum Model (FCM) with DFN model

- Both the DFN and FCM fracture models can be used to characterize fractures in crystalline rock.
- DFN is based on flow and transport in fractures only. FCM is based on both matrix and fracture flow and transport. Comparison of the two models required significant upgrades to the FCM codes.
- Results of the two fracture models are similar when modified FCM methods are used. Results are largely different when the original FCM method is used with matrix diffusion included. Therefore, the rock matrix can play a role in advective as well as in diffusive transport.
- It is anticipated that a relatively large number of realizations of these methods might be required for a performance assessment of a crystalline rock geologic repository.

Based on the work accomplished in FY16 and prior years in the Crystalline Disposal R&D activity, a summary of path-forward objectives is recommended:

- Continue to focus on two key topics related to deep geologic disposal of spent fuel in crystalline rocks:
    - Better characterization and understanding of fractured media and fluid flow and transport in such media, and designing effective engineered barrier systems (EBS) for waste isolation.
    - Specific attention will be given to the development of next-generation buffer materials for waste isolation and to a mechanistic understanding of alteration products (e.g. iron oxides) of EBS components as secondary waste forms for radionuclide retention.
- Help the generic disposal system analysis (GDSA) team to develop a total system performance assessment (TSPA) model and provide the parameter feeds to the model. One goal of this effort is to have a PA model matured enough over next two years to be able to simulate a typical thermal-hydrologic-chemical (THC) evolution history of a repository in a crystalline medium.
- Continue to synthesize technical results in a few selected areas to demonstrate tangible progress in the research. The focus areas will include thermal limits of bentonite and smectite illitization and modeling approaches of fluid flow and transport in fractured geologic media.
- The modeling work will move towards model demonstrations and applications using actual field data. For the process model development, an emphasis will be placed on the integration with total system model development.
- Fully leverage international collaborations, especially with Sweden SKB URL and DECOVALEX.
- Closely collaborate and integrate with other work packages, especially those on disposal in argillite, deep borehole disposal, and DOE-managed high-level waste (HLW) and spent nuclear fuel (SNF) Research.

VIII. References

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