SFWST Disposal Research R&D 5-Year Plan – FY2023 Update

Spent Fuel and Waste Disposition

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

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August 14, 2023

M2SF-23SN010304083
SAND2024-01688R

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APPENDIX E

NFCSC DOCUMENT COVER SHEET[1]

Name/Title of Deliverable/Milestone/Revision No. SFWST Disposal Research R&D 5-Year Plan – FY2023 Update
Work Package Title and Number: SF-23SN01030408 GDSA - Framework Development - SNL
Work Package WBS Number: 1.08.01.03.04
Responsible Work Package Manager: Paul Mariner (Name/Signature)
Date Submitted: 8/14/23

Quality Rigor Level for Deliverable/Milestone[2]	☐ QRL-1 ☐ Nuclear Data	☐ QRL-2	☒ QRL-3	☐ QRL-4 Lab QA Program[3]

This deliverable was prepared in accordance with Sandia National Laboratories *(Participant/National Laboratory Name)*

QA program which meets the requirements of

☒ DOE Order 414.1 ☐ NQA-1 ☐ Other

This Deliverable was subjected to:

☒ Technical Review

Technical Review (TR)

Review Documentation Provided

☐ Signed TR Report or,
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☐ Peer Review

Peer Review (PR)

Review Documentation Provided

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Name and Signature of Reviewers

Stephanie Booth

NOTE 1: *Appendix E should be filled out and submitted with the deliverable. Or, if the PICS:NE system permits, completely enter all applicable information in the PICS:NE Deliverable Form. The requirement is to ensure that all applicable information is entered either in the PICS:NE system or by using the NFCSC Document Cover Sheet.*

- *In some cases there may be a milestone where an item is being fabricated, maintenance is being performed on a facility, or a document is being issued through a formal document control process where it specifically calls out a formal review of the document. In these cases, documentation (e.g., inspection report, maintenance request, work planning package documentation or the documented review of the issued document through the document control process) of the completion of the activity, along with the Document Cover Sheet, is sufficient to demonstrate achieving the milestone.*

NOTE 2: *If QRL 1, 2, or 3 is not assigned, then the QRL 4 box must be checked, and the work is understood to be performed using laboratory QA requirements. This includes any deliverable developed in conformance with the respective National Laboratory / Participant, DOE or NNSA-approved QA Program.*

NOTE 3: *If the lab has an NQA-1 program and the work to be conducted requires an NQA-1 program, then the QRL-1 box must be checked in the work Package and on the Appendix E cover sheet and the work must be performed in accordance with the Lab's NQA-1 program. The QRL-4 box should not be checked.*

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SUMMARY

This FY2023 report is the second update to the Disposal Research (DR) Research and Development (R&D) 5-year plan for the Spent Fuel and Waste Science and Technology (SFWST) Campaign DR R&D activities. In the planning for FY2020 in the U.S. Department of Energy (DOE) NE-81 SFWST Campaign, the DOE requested development of a high-level summary plan for activities in the DR R&D program for the next five (5)-year period, with periodic updates to this summary plan. The DR R&D 5-year plan was provided to the DOE based initially on the FY2020 priorities and program structure (initial 2020 version of this 5-year plan) and provides a strategic summary guide to the work within the DR R&D technical areas (Control Accounts, CA), focusing on the highest priority technical thrusts. This 5-year plan is a living document (planned to be updated periodically) that provides review of SFWST R&D accomplishments (as seen on the 2021 revision of this 5-year plan), describes changes to technical R&D prioritization based on (a) progress in each technical area (including external technical understanding) with specific accomplishments and (b) any changes in SFWST Campaign objectives and/or funding levels (i.e., Program Direction). Updates to this 5-year plan include the DR R&D adjustments to high-priority knowledge gaps to be investigated in the near-term, as well as the updated longer-term DR R&D directions for the program activities. This plan fulfills the Milestone M2SF-23SN010304083 in DR Work Package (WP) SF-23SN01030408 (GDSA - Framework Development – SNL).

This document is structured with three main sections. Section 1 contains background on the detailed evaluation and prioritization of the SFWST DR R&D technical work with a review of both the original Roadmap Report (DOE, 2012) and the Reassessment of the Roadmap (Sevougian et al., 2019)[a]. Those two large-scale strategic planning activities provide the detailed technical bases for overarching prioritization of the DR R&D Program activities (full reassessment occurs about once every seven years), whereas this plan is an overview of the DR Program as it exists looking forward based on technical progress and more focused changes in program emphasis in each technical area.

In Section 2, the summary plan for R&D technical activities is provided for each of the SFWST DR R&D technical areas (note these correspond generally to the work breakdown structure (WBS), Control Accounts for the DR R&D program for DOE NE-81). For each DR R&D technical area, the plan provides a summary of accomplishments since the previous DR plan update, a brief review of the changes in priority, and the planned major technical thrust topics slated for the next five years.

Recent accomplishments include:

- Leadership in both geologic disposal safety assessment (GDSA) and salt repository systems within the international DECOVALEX initiative, which brings more than 100 international researchers together to pursue a common set of research challenges associated with model validation
- Investigation of the effects expected from heat-generating waste, through both brine availability test in salt (BATS) Phase 1 (2020-2021) and BATS Phase 2 (2022-2023), measuring the effects of coupled physical and chemical processes associated with heating a packer-isolated central borehole in salt at the waste isolation pilot plant (WIPP)

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[a] The Disposal Research Program has just initiated the next stage of Detailed Program Planning (i.e., the Roadmap Reimagination) that is planned to be completed by the end of FY2026.

- Implementation of Next Generation Workflow (NGW) within the GDSA Framework, an easy-to-use graphical interface that allows the user to dictate workflow and provides reproducibility and traceability of the files and scripts used for a particular study (Mariner et al., 2020)
- Development and implementation of preliminary generic system models for two types of potential criticality events, a transient event and a steady-state event, in both an unsaturated repository in alluvium and in a saturated repository in shale (Price et al., 2022). These models have been implemented in the GDSA Framework
- Implementation of a Workforce Development pilot program, launched in 2022, to attract and train a diverse early-career workforce of nuclear waste disposal scientists
- Development and implementation of the first version of a nuclear waste management (NWM) taxonomy within the knowledge management activities with a formal governance plan for its ongoing maintenance

Also in Section 2, the detailed thrust topics are presented with discussions of the current/planned activities supporting those thrust topics. Those 5-year plans discuss the general schedules for the thrust topics of each DR R&D technical area (TA) and provide the expected technical emphasis in two parts: the near term (i.e., the more certain 1- to 2-year timeframe) and the longer term (i.e., the less certain 3- to 5-year timeframe). The near-term emphasis can be viewed as a representation of the present DR R&D portfolio with modest modifications that reflect emerging priorities and funding levels. In contrast, the 3- to 5-year period represents a longer-term vision of where the SFWST Campaign DR R&D is heading provided there is no major change to the Program Direction.

Section 3 provides an overview of high-level technical focus areas to cover the planned overarching priorities of the SFWST DR R&D work at a more strategic level for the next five (5) years. Some of those focus areas continue from prior R&D, whereas others have just started, and others have subparts that are yet to be initiated.

The previous Used Fuel Disposition (UFD; from FY2011-FY2017) Campaign and the current SFWST Campaign disposal R&D programs have focused on the evaluation of the viability of mined repositories in three primary generic geologic media (salt, clay/argillite, and crystalline rock; e.g., Sevougian et al., 2019). The host lithologies were selected because they have been considered and analyzed as potential repository host rocks both in the U.S. and internationally for several decades (e.g., Faybishenko et al., 2016). The generic host rock types were identified at a broad level: salt includes both bedded and domal salt; clay was defined to include a broad range of fine-grained sedimentary rock types including shales, argillites, claystones, as well as soft clays; and crystalline rock may include a range of lithologies such as metamorphic gneisses, granite, and other igneous rock types. Each of these primary generic host rock systems have their own TA investigating the detailed technical bases for that generic system. Additionally, supplementary evaluations (within either the TAs of direct disposal of dual-purpose canisters (DPC) and/or the GDSA) are conducted on generic unsaturated mined repository concepts regarding their capabilities to effectively release heat via ventilation to open emplacement tunnels and potential for criticality and consequences in such systems. Lastly, in FY2023, the SFWST program initiated the reinstatement of the deep borehole disposal concept for consideration of disposal of specialized waste forms and this is being implemented in the GDSA TA.

The above range of generic disposal systems evaluated thus far is not intended to represent a complete/comprehensive list of possible alternatives, and other options may also have the potential to provide safe long-term isolation. However, DOE and UFD/SFWST managers believe that R&D related to the evaluation of the selected generic media will be applicable to nearly any future program that relies on deep geologic disposal. The fundamental disposal R&D on these primary generic geologic host rock systems will continue to be the cornerstone of the SFWST Disposal R&D program to support geologic repository disposal solutions in the U.S.

The detailed portion of this 5-year plan is given in Section 2 and provides an assessment for each of the DR R&D TA below. The eleven TAs covered are:

- Argillite Disposal R&D
- Crystalline Disposal R&D
- Salt Disposal R&D
- Engineered Barrier System (EBS) R&D
- Inventory and Waste Form Characteristics and Performance
- Geologic Disposal Safety Assessment (GDSA)
- International Collaborations Disposal Research
- Direct Disposal of Dual-Purpose Canisters
- Technical Support for Underground Research Laboratory Activities
- Knowledge Management (Under Campaign Leadership)
- Advanced Fuels and Advanced Reactor Waste Streams Strategies (Under Campaign Leadership)

In this assessment, each DR R&D TA section includes an overview of the TA purpose and scope, accomplishments since the previous plan version, associated changes to priorities for the plan, and the 5-year plan for that TA. Each DR R&D TA 5-year plan includes sections that:

- Identify the primary thrust topics (these are the major technical priorities in each TA
  - for the near term (next 1- to 2-year period (i.e., our current DR R&D program))
  - for the longer term (3- to 5-year period (i.e., where the DR R&D may go in the future if Program Direction remains the same))
- Describe the activities in the TA that are addressing each of the thrust topics listed both for the program currently (i.e., near term), and how that may change going forward to the longer term. There is generally more detail available for the near-term thrust topics, with the longer-term thrust topics being discussed in comparison/contrast to the near-term thrusts.

This year (FY2023) we have initiated a couple of activities to get an early start on the next reevaluation of the SFWST Roadmap (referred to as the Roadmap Reimagination), which is the full reevaluation of the detailed SFWST Program Technical Priorities for R&D (see DOE, 2012 and Sevougian et al., 2019). Given the expanding progress on details of the technical bases for generic disposal systems, growing technical capabilities in repository science, cutting edge development of system assessment tools, and the abundance of accumulated SFWST data and reports, the Roadmap Reimagination will include a shift back to more explicit mapping/prioritization/status using the features, events, and processes (FEP) for each of the generic repository concepts being considered. Using FEP to assess the SFWST Program R&D portfolio within the various generic disposal systems will elucidate aspects that are progressing well and technical topics that require further attention to poise the program to move into the next stage as efficiently as possible. This will also permit active development of the FEP exclusion/inclusion evaluations for each generic disposal concept to prepare for future site evaluations more fully after that next stage transition.

As shown in this plan for the next five years, the DR R&D will continue to focus on process model development within the generic geologic concepts, EBS, and waste forms/source terms, with the goal of prioritizing model implementation in GDSA Framework for different generic reference cases. At the end of the five years, it is anticipated that GDSA Framework and the reference cases will contain even more detailed representations of relevant improved process models and/or surrogate models. Such progress will facilitate more diverse demonstrations of safety assessments, sensitivity analyses, and more robust programmatic prioritization of targeted DR R&D activities.

Beyond the core efforts to evaluate generic geologic systems for disposal behavior and constrain their key generic natural barrier capabilities with systematic integration of process-level understanding with system evolution of natural and engineered barriers. Additionally, the SFWST Campaign DR R&D activities will maintain a specific focus in the next five years on the following four areas: GDSA Capabilities Development and Demonstration; International Collaboration and Underground Research Laboratories; EBS Representations; and Evaluation of Potential Direct Disposal of DPCs. Another focus area is the work on advanced reactors spent fuel and other waste streams, which is expected to continue at an extent based on Program Direction in this area (i.e., DOE direction, appropriations, etc.).

ACKNOWLEDGEMENTS

This work was supported by the U.S. Department of Energy Office of Nuclear Energy, through the Office of Spent Fuel and Waste Science and Technology (SFWST) Research and Development Campaign (DOE NE-81) within the Office of Spent Fuel and Waste Disposition.

The authors acknowledge the contributions to this activity of the following Sandia National Laboratories (SNL) team members: Carlos Jove-Colon, Kris Kuhlman, Tara LaForce, Paul Mariner, Ed Matteo, Paul Meacham, Melissa Mills, Michael Nole, Sylvia Saltzstein, Laura Swiler, Yifeng Wang, and Phil Weck, for discussions and input on technical aspects and integration of this work.

In addition, the authors thank the staff from U.S. Department of Energy Office of Nuclear Energy (DOE-NE) SFWST Staff—Daniel Fagnant (DOE NE-81), Prasad Nair (DOE NE-81), Tim Gunter (Disposal Research Technical Lead, DOE NE-81) and William Boyle (Director, DOE NE-81)—for their discussions, oversight and guidance on the R&D outlined in this report.

This report was improved by a technical review from Stephanie Booth (SNL).

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ACRONYMS

AR	advanced reactor
ARWS	advanced reactor waste streams
ATF	accident tolerant fuel
BATS	Brine Availability Test in Salt
BEMAR	Back-End Management of Advanced Reactors
BENFC	back-end of the nuclear fuel cycle
CA	control accounts
CI-D	Cement-Clay Interaction Test
COSC	Collisional Orogeny in the Scandinavian Caledonides
DECOVALEX	DEvelopment of COupled models and their VALidation against EXperiments
DFN	discrete fracture network
DHLW	DOE-managed High-Level Waste
DOE	Department of Energy
DOE EM	(DOE) Environmental Management
DOE NE	(DOE) Nuclear Energy
DPC	Dual Purpose Canister
DR	Disposal Research
DR-C	Diffusion in a Thermal Gradient Experiment
DSNF	DOE-managed Spent Nuclear Fuel
EBS	Engineered Barrier System
EBS-TF	Engineered Barrier System – Task Force
EDZ	Excavation Disturbed Zone
EM	(DOE) Environmental Management
FE	Full-scale Emplacement Experiment
FEBEX-DP	Full-scale Engineered Barrier EXperiment – Dismantling Project
FEP	Features, Events, or Processes
FY	Fiscal Year
GDSA	Geologic Disposal Safety Assessment
GRS	Gesellschaft fuer Reaktorsicherheit
GT	Gas Transport Experiment
HLW	High-Level Waste
HOTBENT	High Temperature Effects (HOT) on BENTonite Buffers
HPC	High-Performance Computing
IAEC	Israel Atomic Energy Commission
IPT	Integrated project team
ISC	Important to the Safety Case
IWM	Integrated Waste Management
KM	Knowledge Management
LANL	Los Alamos National Laboratories

LBNL	Lawrence Berkeley National Laboratories
LDT	Long-Term Diffusion Test
L-SCIE	LLNL Surface Complexation/Ion Exchange
MD	molecular dynamic
ML	machine learning
NE	(DOE) Nuclear Energy
NEA	Nuclear Energy Agency
NEFC	Nuclear Energy Fuel Cycle
NGW	Next Generation Workflow
N-TH	Neutronic-Thermal Hydraulic
NWM	nuclear waste management
NWTRB	Nuclear Waste Technical Review Board
OECD-NEA	Organisation for Economic Co-operation and Development - Nuclear Energy Agency
OUO	Official use only
OWL	Online Waste Laboratory
PA	Performance Assessment
PFLOTRAN	Parallel FLOw and TRANsport
PWR	Pressurized Water Reactor
R&D	Research and Development
S&T	storage and transportation
SA	sensitivity analysis
SAL	State-of-the-art Level
SCM	Surface complexation models
SET	Bore Sealing Test
SFD	Spent Fuel Database
SFWST	Spent Fuel and Waste Science and Technology
SKB	Swedish Nuclear Fuel and Waste Management Co
SNF	spent nuclear fuel
SNL	Sandia National Laboratories
SSRS	SQL Server Reporting Services
SW-A	Large-scale Sandwich Experiment
TA	Technical Area
TDB	Thermodynamic Database
THM	thermal-hydrologic-mechanical
THMC	thermal, hydrologic, mechanical, and chemical
TPOC	technical points of contact
UFD	Used Fuel Disposition
UFDC	Used Fuel Disposition Campaign
UK	United Kingdom
URL	Underground Research Laboratory(ies)

U.S.	United States
UQ	Uncertainty Quantification
WIPP	Waste Isolation Pilot Plant
WP	Work Package

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SPENT FUEL AND WASTE DISPOSITION/SPENT FUEL AND WASTE SCIENCE AND TECHNOLOGY

1 INTRODUCTION

This five (5)-year plan for the Spent Fuel and Waste Science and Technology (SFWST) Campaign Disposal Research (DR) Research and Development (R&D) activities provides a strategic summary guide to the work within the DR R&D technical areas (TAs), focusing on the highest priority technical thrusts. This FY2023 report is the second update to the DR R&D 5-year plan for the SFWST Campaign DR R&D activities to provide review of SFWST R&D accomplishments and discuss technical R&D prioritization changes based on progress in areas including SFWST mission, external technical understanding, and changes in SFWST Campaign objectives and/or funding levels (i.e., Program Direction). Updates to this 5-year plan address the DR R&D that has been completed (accomplishments) and the additional high priority knowledge gaps to be investigated, as well as providing the updated DR R&D priorities for the next stages of activities. This plan fulfills the M2SF-23SN010304083 in DR Work Package (WP) SF-23SN01030408 (GDSA - Framework Development – SNL).

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Section 3 provides an overview of high-level technical focus areas to cover the planned overarching priorities of the SFWST DR R&D work at a more strategic level for the next five years. Some of those focus areas continue from prior R&D, whereas others have just started, and others have subparts that are yet to be initiated.

[b] The Disposal Research Program has just initiated the next stage of Detailed Program Planning (i.e., the Roadmap Reimagination) that is planned to be completed by the end of calendar year 2024.

1.1 Background and Initial Strategic Planning Roadmap

The SFWST Campaign of the U.S. DOE Office of Nuclear Energy (NE), Office of Spent Fuel and Waste Disposition (SFWD) is conducting R&D on deep geologic disposal of spent nuclear fuel (SNF) and high-level nuclear waste (HLW). The R&D addressing the disposal of SNF/HLW in the U.S. is currently generic (i.e., "non-site-specific") in scope, following the suspension of the Yucca Mountain Repository Project in 2010. However, to prepare for the eventuality of a repository siting process, the former Used Fuel Disposition Campaign (UFDC) of DOE-NE (which has been succeeded by the current SFWST Campaign) formulated an R&D Roadmap from 2010 to 2012 (DOE, 2012). That Roadmap defined generic R&D activities and developed their priorities appropriate for establishing sound technical bases for multiple deep geologic disposal options in the U.S., increasing confidence in the robustness of generic disposal concepts, and developing the tools needed to support disposal concept implementation. Note that those priorities were established, in part, by how important R&D would be for a potential (i.e., future) repository disposal program leading to a license application/safety case developed for a future site (see Decision Points in Figure 1-1). The DOE (2012) UFDC Roadmap also identified the importance of re-evaluating priorities in future years as knowledge is gained from the DOE's ongoing R&D activities.

Since 2012, significant knowledge has been gained from the UFDC/SFWST R&D activities in the U.S. program and via international collaborations, especially with countries that operate underground research laboratories (URL). From 2017 to 2019 an SFWST R&D Roadmap Update (Sevougian et al., 2019) was conducted to summarize the progress of ongoing generic disposal R&D activities relative to the 2012 Roadmap priorities, to identify gaps in the SFWST Campaign R&D, and to re-assesses SFWST R&D priorities and identify new activities of high priority, such as R&D on disposal of dual purpose canisters (DPC), which now contain a significant fraction of the Nation's commercial SNF inventory.

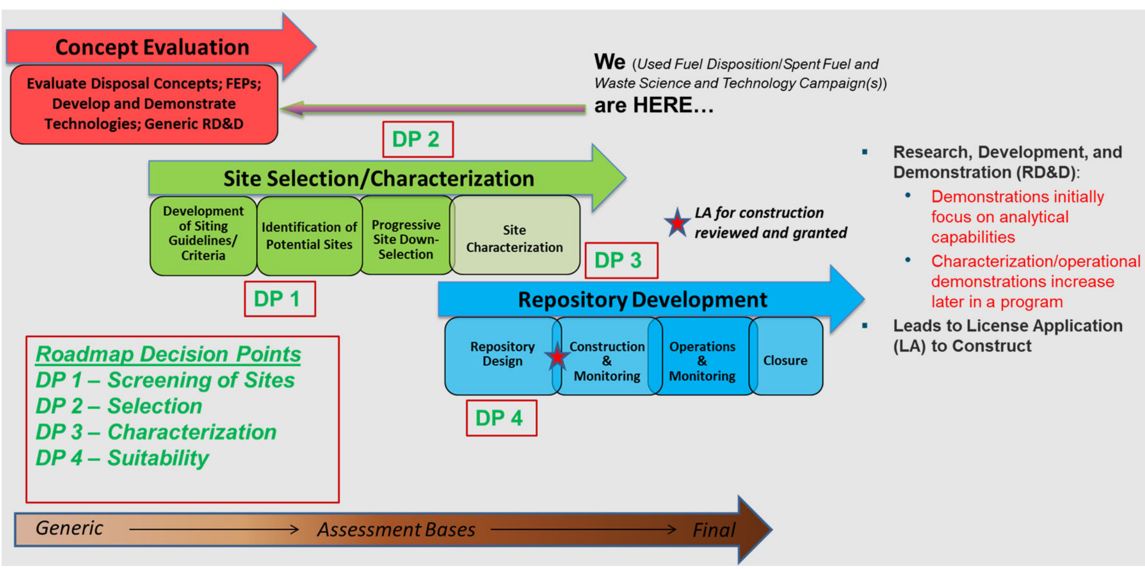

Figure 1-1 The technical lifecycle of a disposal program. Stages include concept evaluation of generic disposal concepts (current U.S. Program), site selection/characterization in which potential sites are considered and down selected for site characterization, and repository development that includes design, licensing for construction, licensing for operation, and licensing for closure. The decision points (DP 1 – 4) are those considered in the 2012 UFDC Roadmap, with the earlier decision points having the greatest weight.

As described in the 2012 UFDC Roadmap (DOE. 2012), the UFDC defined and utilized a systematic, decision-analysis-based approach to develop and prioritize the R&D portfolio. The approach involved several steps, including the identification of potential R&D issues like information needs and knowledge gaps, and the prioritization of these R&D issues based on metrics related to (1) their importance to constructing a future safety analysis at the decision points shown in Figure 1-1, and (2) the state of knowledge regarding the issue.

Each identified R&D issue in the 2012 Roadmap was derived from and/or equated to a FEP (Feature, Event, or Process) from the generic list of 208 FEP considered as important to repository performance. A suite of 354 such R&D issues was identified, which is greater than the original list of 208 FEP, because each FEP may have a different importance to a potential safety analysis, and/or a different state-of-the-art knowledge level, depending on which of the three generic host-rock concepts (argillite, crystalline, or salt) was being evaluated. Evaluation of the subsequent prioritization rankings of the 354 R&D issues pinpointed an important set of broader cross-cutting R&D categories, as well as a series of groupings of natural barrier system issues and EBS issues, that were helpful for defining the future R&D program at that time.

In the process of evaluating the R&D issues summarized in Appendix A of DOE (2012), UFDC scientists and engineers also identified several cross-cutting issues and R&D opportunities that do not correspond directly to individual issues in the UFDC Disposal R&D Roadmap Prioritization Information Matrix. However, they either cut across or integrate with, several of the specific R&D issues and have therefore been defined as, and been considered part of, the UFDC R&D portfolio. These prioritized cross-cutting issues defined in the UFD Campaign Roadmap (DOE, 2012) were used as the framework to develop the set of R&D activities within the UFD Campaign. The cross-cutting issues and their 2012 UFD Campaign Roadmap priorities are:

- HIGH: Design Concept Development
- HIGH: Disposal System Modeling
- LOW: Operations-Related Research and Technology Development
- MEDIUM: Knowledge Management
- MEDIUM: Site Screening and Selection Tools
- MEDIUM: Experimental and Analytical Techniques for Site Characterization
- MEDIUM: Underground Research Laboratories
- MEDIUM: R&D Capabilities Evaluation

The original 2012 UFDC Roadmap promised a re-evaluation of priorities in future years as knowledge was gained from ongoing activities in the U.S. and abroad (DOE, 2012, Sec. 2.4).

1.2 Roadmap Reassessment Purpose and Results

A full reassessment of R&D priorities was initiated during fiscal year 2018 (last quarter of 2017). At the SFWST Annual Meeting, Sassani (2018) provided a high-level assessment of how well the R&D Campaign had addressed the cross-cutting issues and priorities that the 2012 Roadmap summarized to drive the planning of the UFD/SFWST Campaign R&D activities. The full re-assessment culminated in a workshop of Campaign experts in early 2019, held at the University of Nevada in Las Vegas from January 15 to 17 to assess the priorities of existing R&D activities, as well as to identify and prioritize gaps in the R&D portfolio. In addition, a new document archive was developed to organize and store the various reports generated by the disposal R&D work packages over the course of the UFD and SFWST Campaigns (Sevougian et al., 2019).

Though Sassani (2018) indicated the UFD/SFWST Campaign had made appropriate (relative to the priority assigned) progress in a number of the cross-cutting issues such as the high priority issues of *Design Concept Development* and *Disposal System Modeling*, it was also noted that the Campaign R&D progress seemed to fall short in the medium priority issues of *Knowledge Management* and *Experimental and Analytical Techniques for Site Characterization*. Additionally, further gaps were identified in the high priority FEP for waste package degradation and engineered barriers chemistry coupled processes, as well as for some additional medium priority FEP such as cladding degradation (Sassani, 2018; see highlights in backup materials in the referenced work). Because a number of these last topical areas generally rely on more site-specific environmental conditions, it was not very surprising to see developmental lag in the generic R&D program for those.

The full re-assessment workshop results and analyses in Sevougian et al. (2019) provide both a more extensive evaluation of the full range of R&D activities within the SFWST Campaign and a robust basis for planning the direction of the future Campaign work. The Roadmap reassessment captured the gaps noted here, as well as other gaps, many of which are related to the recently started evaluation of direct disposal of spent fuel stored in DPC related to the specific thermal and inventory characteristics of those DPC. The Roadmap Reassessment is summarized below with an overview of the results.

The objectives of the 2019 R&D Roadmap Reassessment (Sevougian et al., 2019) included the following:

(1). Recap the original 2012 Roadmap results and conclusions.

(2). Document the 2019 Roadmap Update Workshop approach, process, and evaluations.

(3). Summarize the status, progress, and priority of 2019 SFWST R&D Activities and their relation to the FEP important to various host rocks and repository designs.

(4). Identify the generic R&D still needed to advance the state-of-the-art for important R&D Activities and associated FEP.

(5). Identify important FEP that have not been addressed adequately by Campaign R&D Activities (i.e., identify gaps).

(6). Present a new document archive for UFD and SFWST milestone reports.

Objectives 3 and 4 are primarily addressed in a series of appendices in Sevougian et al., (2019) that capture the wealth of consensus information compiled by SFWST Campaign experts during the three-day Roadmap Update Workshop. Regarding objective 5, the update exercise identified a number of gap activities that represent future R&D necessary to adequately advance the state of the art of several high- and medium-priority FEP. These gaps tended to be focused in the areas related to the engineered barriers, for example cladding and waste package degradation, as these investigations are more challenging for generic system studies due to higher reliance on the details of chemical conditions in the system. Note that the details of the 2019 Roadmap systematic reevaluation process, summarized in Appendix A, were similar in many ways to that used in the 2012 Roadmap (DOE, 2012), but with differences related to the progress that has been made within the campaign.

In Sassani (2018), it was found that two high-priority areas that were not covered well included waste package degradation and cladding degradation investigations. It was also found in the full set of gap activities identified in the full reassessment workshop that more work on these two specific R&D topics was a priority for crystalline, DPC activities, and EBS activities. The Roadmap reassessment identified other gaps in other areas (see summary in Appendix A; and Sevougian et al., 2019 Appendix I) covering flow and transport in natural systems, thermally coupled processes in the EBS, re-wetting/re-saturation processes, DPC system modeling and criticality processes, coupled chemical systems and waste form degradation, and gas migration. Additionally, the need was identified for more active integration within the DR R&D areas, especially among the host-rock based process models and the Geologic Disposal Safety Assessment (GDSA) models (for the generic geologic repository Reference Cases) with emphasis on the method for models being integrated into the GDSA Framework. Other integration needs to include developing more connections with the SFWST Campaign Storage and Transportation (S&T) R&D, and the need for further integration with other DOE-NE campaigns that provide data/models for waste form degradation. These considerations helped to define overarching areas of R&D focus found in Section 3.

Similar to the cross-cutting issues defined in the UFDC Roadmap (DOE, 2012), the current SFWST Campaign DR R&D program will move forward with its own areas of focused R&D for the next 5-year planning period. Some of these focus areas are the same as defined as in the UFDC Roadmap (DOE 2012), for example the GDSA capabilities development and demonstration, which underpins quantitative analysis of the post-closure safety of generic repository systems. Other focus areas are based on new program direction for specific R&D (e.g., evaluation of direct disposal of DPC). These areas of R&D focus are strategic points for integration/synthesis of the R&D being executed across the DR R&D program. For example, the generic geologic systems being studied remain a core effort, though it is expected that the specific R&D thrust topics (discussed in Section 2 below) in each generic geologic system would likely evolve over time.

1.3 Next Roadmap Reevaluation Initiation

In FY2023 we have initiated a couple of activities to obtain an early start on the next reevaluation of the SFWST Roadmap. This third cycle of strategic planning (over a year ahead of the seven-year strategic planning cycle) is referred to as the *Roadmap Reimagination*. Given the expanding progress on details of the technical bases for generic disposal systems, growing technical capabilities in repository science, cutting edge development of system assessment tools, and the abundance of accumulated SFWST data and process understanding, the Roadmap Reimagination is shifting back to more explicit prioritization/status of the FEP for each of the generic repository concepts being considered as the basis for strategic planning. The first activity entails developing a real-time, online accessible FEP list capability for all SFWST investigators (work package managers and their key technical investigators) to use to map their SFWST program activities to the specific sub-FEP aspects (the bulleted listing for the generic FEP list at their most detailed level) that are being addressed. This should both (a) enhance integration because all users will be able to see all activities/investigators evaluating specific FEP aspects and (b) provide ready assessment of "how complete" work is on any FEP, and make it straightforward to identify where gaps exist in the program R&D. We began development of prototype of this FEP tool in FY2023, completed high-level review of that tool, and it is being modified for use by a wider group of managers and technical staff in this next fiscal year. A second additional activity we initiated is to establish a Library of GDSA Reference Cases for all the generic repository concepts. The Reference Case Library will include the model definitions, files, documentation, and results of those demonstration cases for each of the generic repository concepts. This Library will contain the details of these safety analyses/demonstrations with the GDSA capabilities, as well as providing a readily accessible communication context for these capabilities.

Once the online FEP tool is ready, it will undergo a trial usage by a subset of the work package managers/control account managers (targeting mid-FY24), revised as needed, then implemented for each generic repository concept, and put into full usage (starting roughly end of FY24 to mid-FY25). The online FEP tool will allow real-time input/usage and output of sub-FEP listings of activities such that the DR technical staff/managers will be able to more readily assess how to better integrate their work, assess changes in priorities, determine when their work will be complete enough for the sub-FEP and generic concept GDSA as needed, and identify gaps in R&D. Once fully populated, the online FEP tool would be used by the program staff to reevaluate the SFWST Roadmap and poise the U.S. for moving efficiently into the next stage of an active repository program (Figure 1-2).

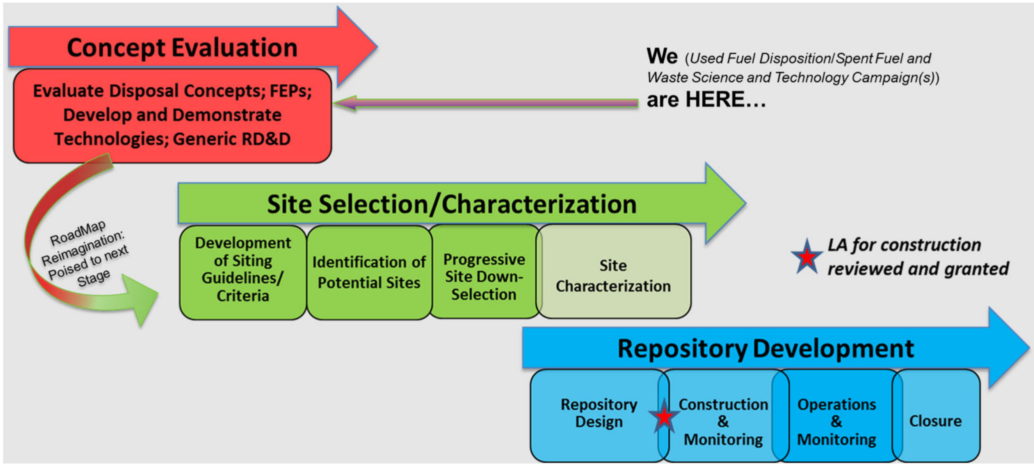

Figure 1-2. In the Roadmap Reimagination, the focus will be to ensure the SFWST Program is poised to leap into the next stage of a Repository Program Lifecycle. The starting point for such a next stage would depend explicitly on changes in Program Direction.

The primary linkage between the technical bases for any repository concept and the safety analysis for that concept is the set of FEP include/exclude assessments. Those FEP analyses provide the essential detailed discussion of the technical bases of each FEP to conclude which FEP to incorporate/include directly into (or exclude from) the GDSA. The FEP analyses are a primary part of system Performance Assessment (PA) that provide some indication of how much more work there is remaining on the technical bases and constructing the (generic) GDSA Reference Case for any (generic) disposal system. In conjunction with this active FEP progress tracking capability, a library of GDSA Reference Cases would be developed to include: (1) summary descriptions for each generic disposal concept, the bases, and documentation/reports developed for each Reference Case, (2) the models files, and (3) the results output of the Reference Case. This library will be developed for internal purposes of tracking progress but will also include a publicly accessible site for communication of the safety assessment capabilities and disposal concepts being evaluated. Eventually, the online FEP Lists will be a substantial part of the documentation/technical bases of why FEP were excluded from/included into the most current GDSA generic disposal concepts reference cases. The SFWST goal is to have these tools finalized and fully populated with existing information by the end of FY2026, The SFWST generic disposal program would them be poised as much as possible to leap readily into any program (beyond the current one for generic disposal concepts) that Congress/the government would direct at some point in the future.

In conjunction with this early start to our Roadmap Reimagination, the SFWST program is working to have a more explicit/coherent mapping of our technical points of contact to the European R&D program EURAD-2. EURAD-2 is a ~5-year European Commission collaborative program (https://www.ejp-eurad.eu/news/eurad-2-core-group-communication-may-2023) set to execute a set of repository R&D work that will largely be selected for funding in the Fall of 2023 and intended to commence Autumn 2024. EURAD-2 requested the SFWST campaign to map technical points of contact to the eventual funded projects based on U.S. DOE interest in TAs for in-kind collaboration with the projects selected. Our DOE Technical Lead agreed to provide a set of technical points of contact (TPOC) to be the primary (with secondary/backup TPOC) to each funded project of U.S. DOE interest (see section below on International). SFWST collaboration in such International Programs provides an essential linkage to active site-specific investigations in multiple geologic systems around the world. This provides both active experience in URLs in field scale experimental/characterization investigations, as well as connection to disposal programs performing site-specific evaluations. These two aspects are essential expertise to maintain in the U.S. program and will be areas for growth moving into the next stage of a disposal program in the U.S. Such concerted collaborative aspects of International R&D on disposal programs will be a longer-term targeted thrust for each relevant TA.

Beyond the core efforts to evaluate generic geologic systems for disposal behavior and constrain their key generic natural barrier capabilities with systematic integration of process-level understanding with system evolution of natural and engineered barriers. Additionally, the SFWST Campaign DR R&D activities will maintain a specific focus in the next five years on the following four areas: GDSA Capabilities Development and Demonstration; International Collaboration and URLs; EBS Representations; and Evaluation of Potential Direct Disposal of DPCs. These areas of technical focus were defined based on both the Roadmap Reassessment results (Sevougian et al., 2019), discussions among the DR technical managers and the National Technical Director, and input from the DOE NE leads. These four areas are discussed further in Section 3. Another focus area is the work on advanced reactors spent fuel and other waste streams, which is expected to continue at an extent based on Program Direction in this area (i.e., DOE direction, appropriations, etc.).

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2 PLANS WITHIN THE SFWST CAMPAIGN DISPOSAL RESEARCH R&D TECHNICAL AREAS

The detailed portion of this 5-year plan is given below and provides an assessment for each of the DR R&D technical areas (TAs) below. Note that the DR R&D TAs covered here correspond to the Control Accounts within the work breakdown structure (WBS) in the DOE PICS:NE management system, which contains the details of the planned R&D activities, as well as the milestones/deliverables/reports generated from executing the work. The eleven TAs covered below are:

- Argillite Disposal R&D – developing the technical bases for the natural and engineered barriers in generic argillite (e.g., clay/shale) repository concepts, including international collaboration.
- Crystalline Disposal R&D – developing the technical bases for the natural and engineered barriers in generic crystalline (e.g., granite/gneiss) repository concepts, including international collaboration.
- Salt Disposal R&D – developing the technical bases for the natural and engineered barriers in generic salt (e.g., bedded/domal) repository concepts, including international collaboration.
- Engineered Barrier System (EBS) R&D – developing the technical bases for the generic integrated EBS across all generic repository concepts, including international collaboration.
- Inventory and Waste Form Characteristics and Performance – developing the technical bases for the inventory and characteristics of waste forms for generic repository concepts, including their performance over geologic time.
- Geologic Disposal Safety Assessment (GDSA) – developing the performance assessment scenarios, safety analyses capabilities, and safety constraints for all generic repository concepts being evaluated.
- International Collaborations Disposal Research – integrating the SFWST International collaborations within the program, growing the future DR workforce, and managing the interface to the international community.
- Direct Disposal of DPCs – assessing the feasibility of directly disposing of DPC, developing the technical bases for modifications to prevent the post-closure criticality, and assessing the safety impacts of any post-closure criticality.
- Technical Support for URL Activities – proposed field-based subsurface studies that could be applied in existing underground facilities to collect data applicable to generic repository concepts.
- Knowledge Management (Under Campaign Leadership) – capturing tacit knowledge throughout the back-end of the nuclear fuel cycle (BENFC) that will be lost and providing multiple pathways for staff to access/digest/utilize the information.
- Advanced Fuels and Advanced Reactor Waste Streams Strategies (Under Campaign Leadership) – evaluating the potential SNF (and other waste streams) from proposed advanced reactor concepts for potential R&D issues to be addressed with further R&D.

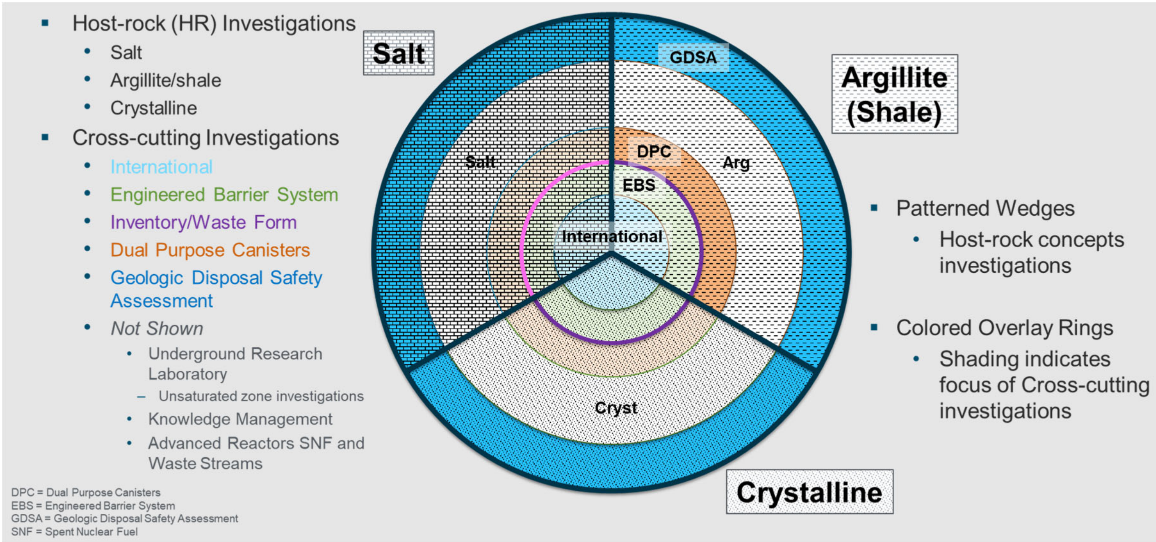


Figure 2-1. A pie diagram in which the host-rock technical areas investigations that focus on technical bases of the natural barriers of the generic geologic systems are shown as the patterned wedges of the pie. Technical areas investigations that are cross-cutting (to the generic host-rock concepts) are shown as concentric rings of various colors, the shading of which indicates more or less focus in the generic geologic systems. The three areas not shown are either not directly relevant to the three primary generic host rocks here (URL) or are more generally applicable to the entirety of the SFWST Program.

The eleven TAs (shown in Figure 2-1 relating the cross-cutting investigations TAs to the Host-rock investigation TAs) cover virtually all the technical work being done within the SFWST Campaign DR R&D program. The first nine of these describe the work explicitly in the nine control accounts defined and executed under the DR R&D program (WBS 1.08.01.03) of the SFWST program. However, some technical R&D work that applies to both the S&T R&D program (WBS 1.08.01.02) *and* the DR R&D program is being executed within the Campaign Leadership (CL) program (WBS 1.08.01.01) area, either as single events requested by Program Direction, or as multi-year projects that span the entire SFWST technical arena. One very good example of this is the development of the *Knowledge Management* (KM) repository (see Section 2.10) that started as a mechanism to capture tacit knowledge of senior experts (focusing initially within the program of Disposal Research), including those involved with licensing/certification processes from previous repository programs. This KM work is ongoing, has expanded to cover S&T R&D (as well as to the entire set of work in the DOE Office of SFWD), and is becoming more desired across the SFWST Campaign (as well as in other technical venues), and will likely grow further in the coming years with even more integration internationally. Another set of technical work that spans storage, transportation, and disposal R&D analyses is evaluating R&D issues with the BENFC for advanced reactors spent fuels and other waste streams. These two TAs are covered in their own subsections below the nine DR R&D TAs.

In this assessment each DR R&D TA section includes an overview of the TA purpose and scope, accomplishments since the previous plan version, associated changes to priorities for the plan, and the plan for that TA. Each DR R&D TA 5-year plan includes sections that:

- Identify the primary thrust topics (these are the major technical priorities in each TA)
    - for the near term (next 1- to 2-year period – i.e., our current DR R&D program)
    - for the longer term (3- to 5-year period - i.e., where the DR R&D may go in the future if Program Direction remains the same)

- Describe the activities in the TA that are addressing each of the thrust topics listed both for the program currently (i.e., near term), and how that may change going forward to the longer term. There is generally more detail available for the near-term thrust topics, with the longer-term thrust topics being discussed in comparison/contrast to the near-term thrusts.

In all the subsections below covering the TA, the level of detail relates to the breadth of scope in each TA. More detailed plans for some TAs reflect those TAs that contain more R&D activities to cover in that area (e.g., GDSA, DPC, International) and shorter plans (e.g., the *Knowledge Management*) reflect the more limited scope of that TA. The periodic update (about every two years) to this 5-year plan will address the DR R&D work that has been completed (major accomplishments), the additional knowledge gaps remaining, updates to the DR R&D priorities, and shifts in resources for the next stages of activities. For each of the DR R&D TAs, the review of accomplishments completed during the previous period will be used to inform the updated priorities, technical thrusts, and any major shifts in resource allocation for the updated 5-year plan discussions.

In the next five years, the DR R&D will continue to focus on process model development within the generic geologic concepts, EBS, and waste forms/source terms, with the goal of prioritizing model implementation in GDSA Framework for different generic reference cases. At the end of the five years, it is anticipated that GDSA Framework and the reference cases will contain even more detailed representations of relevant improved process models and/or surrogate models. Such progress will facilitate more diverse demonstrations of safety assessments, sensitivity analyses, and more robust programmatic prioritization of targeted DR R&D activities. As described briefly above, the next stage of re-evaluation of the DR Roadmap (the Roadmap Reimagination) is getting an early start with a goal of completion by the end of FY2026. Those changes to priorities would be incorporated into a future iteration of this 5-year plan after that more detailed SFWST Roadmap Reimagination is completed.

2.1 Argillite Disposal R&D

Integration across disposal R&D activities is important for the argillite media scope of work because all argillite research covers areas related to engineered/natural barrier system investigations, noting that data obtained from international URL activities are key to argillite R&D objectives. The various R&D efforts on disposal in argillaceous geologic media encompass development and application of coupled thermal, hydrologic, mechanical, and chemical (THMC) process models, international collaborations on repository science R&D (e.g., HotBENT, DECOVALEX-2023, SKB Task Force on EBS), experimental studies on engineered barrier material interactions plus host-rock (argillite) including solute transport, molecular dynamic (MD) simulations and thermal studies of water transport during clay hydration/dehydration (swelling/shrinkage), MD studies of hydrogen gas interactions in smectite interlayers, and advances in thermodynamic and surface complexation databases for geochemical modeling. The purpose of these R&D efforts is to inform the analysis of disposal concepts and provide data (field- and laboratory-scale) necessary to gauge barrier behaviors and process-model development for the representation of deep geological repository environments. Integration with GDSA activities includes linking THMC process in Performance Assessment (PA) and evaluating of groundwater chemistries in shale formations.

2.1.1 Accomplishments and Discussion

In the years since the previous version of this DR R&D Plan, the major accomplishments are:

- Use of MD simulations to elucidate swelling clay dehydration behavior as a two-stage process. This is supported by thermal analysis (TGA/DSC) and *in situ* XRD experiments. These thermal and structural analyses combined with molecular modeling are key to the mechanistic behavior of clay hydration/dehydration.
- Investigating the effect of shale-creep on the long-term performance of an argillite repository. This includes applications of the shale creep model for brittle and sealing shale plus its

implementation in a THM coupled process model platform to evaluate potential damage. Also, applications of machine learning (ML) to evaluate fault stability testing (Mont Terri URL).

- Reactive transport modeling of engineered barrier interactions from laboratory- and field-scale testing activities. This modeling effort permits the evaluation of chemical and transport parameters for interactions occurring at barrier material interfaces.
- Active involvement in DECOVALEX-2023 and other international collaboration activities (e.g., Mont Terri), many of which crosscut key aspects of process model development and validation. This also includes the HotBENT heater test and related column experiments at LBNL, and the SKB Task Force on EBS modeling of cement-bentonite interactions. Engagement with the Nuclear Energy Agency (NEA) on thermodynamic database development.
- Hydrothermal experiments of clay/metal/cement engineered barrier materials and host-rock (argillite) material interactions. The results of recent experiments revealed the occurrence and co-existence of zeolite and cement minerals during barrier material interactions at elevated temperatures.
- Applications of ML approaches to the evaluation of sorption databases. A data-driven approach is used to develop a chemistry-driven ML method to predict metal adsorption onto mineral surfaces.

These accomplishments in modeling and experimental approaches are key to the characterization of chemical and physical phenomena that could impact the long-term safety assessment of heat-generating nuclear waste disposition in deep clay/shale/argillaceous rock. This information is crucial to the characterization of thermal effects on bentonite clay barrier performance and constrains parameter inputs to process models in the evaluation of generic argillite repository disposal concepts.

2.1.2 Summary Discussion of Major Changes to Priorities

Given the accomplishments in this TA, as well as the changes/drivers on priorities (e.g., Program Direction; external data/understanding advancements, etc.,), the following major changes in priorities are:

- Increased priority is given to:
    - Engagements in international activities (DECOVALEX-2023, HotBENT, SKB Task Force for EBS, 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.
    - Application of reactive-transport modeling approaches to barrier / host-rock material interactions under (non)isothermal conditions.
    - Application of data-driven and ML approaches to evaluate sorption data and develop efficient predictive methods for metal sorption.
- Decreased priority is given to:
    - Past international activities that have been largely completed (e.g., FEBEX-DP). However, ongoing research may still be carried out for strategic approaches obtain knowledge from availability of barrier material.
    - Past activities supported by the disposal in argillite work package on waste form degradation modeling and experiments. Note that these activities have been transferred to another Control Account/Technical Area dedicated to waste form R&D work.

The Thrust Topics in the next Section are consistent with these updated priorities.

2.1.3 Planned Thrust Topics and Summaries

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

a) *Elucidation of the coupled THMC processes affecting repository performance*

b) *Development of multi-fidelity approaches for integration of process models into the GDSA Framework*

c) *Existing international collaborations such as DECOVALEX-2028, HotBENT, SKB Task Force for EBS*

These three near-term thrust topics are interrelated and though they are the current focus areas, it is expected they will also continue into the longer term as well. Continuing work includes expanding the applicability of coupled process models to elevated temperatures and integration of DPC-relevant information related to thermal management. These models include calculations of the permeability and porosity evolution of the EBS in clay formations using continuum approaches.

Simplifying the representations of THMC processes occurring from within the EBS out into the argillite host rock is also a longer-term thrust with the goal to get these representations to include only the most essential variables for ease of implementation in the GDSA models. In the shorter term, one option is to develop response surfaces for key parameters (e.g., for permeability, porosity, cation exchange capacity, swelling stress) as a function of other system variables such as temperature. Longer-term thrusts include the development of reduced order/simplified model representations for the complex argillite process models.

Partnerships with current international programs will be nurtured and expanded in the near-term to foster continued collaborations aimed at gaining advanced knowledge of nuclear waste disposal research from ongoing URL activities worldwide.

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

a) *Simplifying the representations of THMC processes occurring from within the EBS*

b) *A more coherent integration of large-scale international programs (e.g., EURAD-2 5-year program kicking off in 2024)*

These two longer-term thrust topics are complementary to the collaborative work as it provides constraints to evaluate, enhance, and validate our process-level understanding in this area. Expansion of in-kind collaboration with integrated international programs will be a focus of continued enhancement, for example, see discussion of EURAD-2 in Section 1.3. Emphasis will be given to THM and HM modeling activities for heater test experiments at international URL's and other relevant activities (e.g., DECOVALEX- DEvelopment of COupled models and their VALidation against EXperiments). Specific examples of these are the heater tests at the Horonobe URL site in Japan and HotBENT at the Grimsel test site in Switzerland. The Grimsel site has provided a large suite of barrier material samples (bentonite, cement, rock) for characterization and experimental studies of fluid-bentonite interactions. These activities will continue during the next five years. Additional international collaborations include continued modeling of heater test and CI-D experiments at Mont Terri. Also, participation in the SKB Task Force (TF) on EBS for the modeling of cement-bentonite interactions. Continue the engagement with the OECD-NEA thermodynamic database (TDB) project development and the review of the thermodynamic data volumes produced by this project. Taken collectively, these international collaborations are intended to provide access to the data needed to develop, test, calibrate, and validate coupled process models. Such data sets will allow for detailed assessment of process models to identify the key THMC variables that are the major ones versus those that may not need to be explicitly included in EBS THMC models for GDSA.

2.2 Crystalline Disposal R&D

The objective of the Crystalline Disposal R&D is to advance our understanding of long-term disposal of used fuel in generic crystalline rock (i.e., granite and other related lithologies) and to develop necessary experimental and computational capabilities to evaluate generic disposal concepts in such media. The R&D activities aim to:

- Assist the GDSA team to develop a robust generic crystalline repository PA model.
- Provide the GDSA with the essential minimal set of process models to support the GDSA goals.
- Evaluate the different approaches taken by international researchers to understand how robustly the models are constrained to determine their level of rigor and readiness levels for implementation.
- Fully leverage international collaborations for data collection, as well as model development and validation.
- Closely collaborate with other TAs, especially those on disposal in argillite and EBS design, to more fully develop generic repository disposal concepts and bases.

The crystalline R&D thrust area has a significant focus on opportunities to improve process understanding and process model representations of the processes most import to repository performance. Due to the fractured nature of the disposal media, the design concept in a crystalline host will place a higher reliance on the EBS performance than other generic host-rock types. Thus, the thrust area will focus on: (1) a better characterization and understanding of fractured media and fluid flow/transport therein; and (2) designing an effective EBS for waste isolation. The modeling activities will give more emphasis on model validation and demonstration using field and in-situ testing data obtained through international collaborations with an objective to reduce model uncertainties.

2.2.1 Accomplishments and Discussion

In the years since the previous version of this DR R&D Plan, significant progress has been made in both experimental and modeling arenas in evaluation of used fuel disposal in crystalline rocks, especially in model demonstration using field data.

- *Excavation disturbed zone (EDZ) characterization:* The laboratory experiments on intact rock core samples were completed to assess permeability evolution under triaxial loading and thermal changes. Results show almost one order of magnitude permeability reduction due to heating under 90 °C, which may indicate that pressure solution occurred on crack surfaces. Subsequent reduction in the confining stress did not result in permeability recovery, which could be attributed to mineral precipitation and crack filling on the free surface of larger cracks. Such thermally induced microcrack closure and irreversible permeability reduction would improve the hydrological barrier performance of the EDZ around a waste repository tunnel.
- *Discrete Fracture Network (DFN) Model Development:* Many model-based studies assume fractures to be smooth planes. However, real-world fractures are known to have rough surface asperities. An effort was made to account for fracture roughness by assuming textures with different connectivity structure and to understand how this impacts transport behavior. It was demonstrated that fracture roughness could control important features of flow and mass transport. The relative impact of advective transport compared to retention due to matrix diffusion has also been investigated. It was found that flow and solute transport through low-permeability fractured media could be generally determined at short time scales while at longer time scales matrix diffusion could also influence solute transport.

- *Understanding stress effects on DFN and transport:* The DFN modeling effort has focused on characterizing the combined effects of stress and variable network properties on flow and transport in three-dimensional fracture networks. There has been extensive research in recent years into the effects of external/applied stress on flow and transport in single fractures, but very little research at the network scale, which is highly relevant to the performance assessment of a repository in crystalline rocks, where stress conditions may change over the lifetime of disposal sites. The work explored how changing the length distribution and orientation of fracture families in different DFNs, subjected to anisotropic stress, might affect flow and transport observables. A total of nine different networks and 30 realizations of each were considered. Governing equations for geomechanics, flow, and transport were solved for each network, and a comparison was made between stressed networks to reference cases with no fracture response to stress. It was found that changing both the length distribution of fractures and orientation would affect how stress was accommodated by changing apertures in the networks, which in turn changed the degree of flow channeling in the network and breakthrough times of particles. It was also found that the presence of large fractures particularly could affect the breakthrough behavior, as well as fractures that might exert more shear failure and dilation, which could be linked back to their initial orientation in the networks.
- *In-situ evaluation of transmissive fractures:* In-situ transmissive fracture testing was performed in collaboration with the Collisional Orogeny in the Scandinavian Caledonides (COSC) scientific team. The research aims to provide insights on the problem of nuclear waste disposal in crystalline formations. The following field tests were carried out: pressure buildup tests, pressure falloff tests, and constant flow rate tests in the COSC-1 borehole. Two approaches were used to evaluate stress conditions: an inversion of the displacement data, and a fully coupled, forward numerical simulation of fracture stimulation and fluid flow using the distinct element code 3DEC. These analyses provided insights into the stress state for the borehole, as well as how the fractures responded to hydraulic stimulation.
- *Model validation for fluid flow and transport in fractured rocks:* Updated modeling analyses were conducted on DECOVALEX Task C inflow and recovery simulations. The inflow simulations included a study of boundary conditions related to domain size by comparing inflow results for the base case domain (200 m × 300 m × 200 m - site scale) with that of a much larger domain (1386 m × 1486 m × 806 m). The comparisons were done for ten fracture realizations. Pressure distribution simulation results for one of the realizations show that the site-scale domain exhibited boundary effects while the larger domain had no such effects. As a result, the inflow results for the ten realizations using the larger domain show significantly reduced values compared to the base case domain. Thus, the inflow is better predicted with the larger domain. Updated simulations were also conducted to model water-filling and pressure recovery of a plugged closure test drift at the Mizunami URL in Japan.
- *Study of thermal and chemical stability of bentonite:* Bentonite (mainly smectite) has been proposed as a buffer material in a nuclear waste repository, due to its low permeability, high swelling capability, and high ion exchange capacity. To evaluate the performance of the material, it is important to understand a possible hydrothermal alteration of smectite to illite. Experiments were conducted to investigate the hydrothermal alteration of smectite under various physical and chemical conditions to identify key controlling factors of the process. The experiments were performed on less than 2 µm fractions of Na-rich or K-exchanged smectite in DI water or 1M KCl solution at 200 °C for various liquid/solid ratios over a time period up to 112 days. Multiple analysis techniques were used to characterize the solid and liquid products to determine the extent of the conversion and the related mineral structural changes. Experimental results suggest that the conversion could be relatively fast at the optimal conditions, much faster than previously postulated. A high K^+ concentration in the solution is required to trigger the

structural transition of a low charge smectite layer to a high charge illite layer. This transition appears to be continuous, thus contradicting the dissolution-precipitation mechanism for smectite to illite transformation. Based on the solution chemistry measurements, the equilibrium constant for the transformation of K-exchanged SWy-2 smectite to illite is estimated. In addition, the overall conversion is limited, to a large extent, by the dissolved silica concentration in the solution. Given a generally low potassium content, an extremely low liquid:solid ratio, and an extremely slow diffusion in an actual EBS, the extent of smectite conversion to illite in a repository environment, if it happens, would be limited. The conversion can be further inhibited by introducing brucite and amorphous silica as chemical additives to the buffer material.

- *Understanding bentonite swelling behaviors and colloid stability:* An effort was made to evaluate uncertainties related to bentonite behavior under disturbances, such as high temperature or swelling induced by changes in groundwater ionic strength, to understand the implications for colloid-facilitated transport of radionuclides. Column experiments were designed to test the effects of temperature on bentonite mineralogy and electrochemical properties. The results suggest that, at elevated temperature, morphological and mineralogical changes to the bentonite occur that could potentially increase its sorption capacity. Elevated temperatures could also reduce the repulsive force between colloids, lowering their stability. A new method was also developed to quantify the anisotropy of bentonite swelling to inform bentonite swelling and erosion models.

- *Development of new generation buffer materials for high temperature and high pH environments:* Saponite, a tri-octahedral smectite with an ideal formula of $Mg_3(Si, Al)_4O_{10}(OH)_2 \bullet 4H_2O$ for an Mg-end member (saponite-15Å), has similar swelling properties as montmorillonite and therefore can be considered as a potential candidate buffer material for nuclear waste disposal. An experimental study was conducted to investigate the chemical stability of this material under alkaline conditions (pH ~12) at high temperatures (up to 150 °C) and saturated vapor pressures over the experimental durations of about three weeks. Alkaline conditions in a geologic repository can be induced by borosilicate waste forms or cementitious materials introduced as structural components such as seals, liners, and plugs. The experiment was conducted to simulate the interactions of saponite with portlandite [$Ca(OH)_2$]-saturated solutions at 60 °C and 150 °C. The results indicated that saponite is chemically more stable in these environments than montmorillonite and remained unchanged after the interactions. The stability is attributed to its low solubility, with dissolved-magnesium concentrations in the portlandite-saturated solutions estimated to be $< 4 \times 10^{-7}$ mol•kg^{-1} or 2×10^{-7} mol•kg^{-1} at 60 °C or 150 °C, respectively. For a comparison, the experiment was also conducted to investigate the interactions of montmorillonite (SWy-2) with a portlandite-saturated solution at 150 °C. The results indicate that montmorillonite is not stable, leading to the formation of zeolite (phillipsite) after nine days of reaction. This study thus demonstrates the possibility of using saponite as a promising candidate buffer material (alternative to the currently proposed montmorillonite) in an alkaline and elevated-temperature disposal environment.

- *Understanding radionuclide sequestration by corrosion products:* Surface complexation models (SCM), which aim to quantify sorption processes, play a key role in repository performance assessments. Although enormous efforts have been made to develop reliable SCMs, obtaining global consensus among reported SCMs is still challenging since each SCM had been constructed with different foundations. In light of the limitation, this effort aims to develop a more comprehensive SCM framework by compiling raw sorption data and the relevant surface complexation reactions reported from various literature sources. A data flow framework was established for SCM database development. The framework consists of sorption database (i.e., L-SCIE (LLNL Surface Complexation/Ion Exchange)), a surface titration model, and a SCM. L-SCIE database provides input data for surface titration/complexation models, and data processing and fitting routine have been done within each model. In addition, experiments were conducted to further investigate radionuclide sequestration through coprecipitation. The incorporation of radionuclides into corrosion phases may limit the rate of radionuclide release by sequestering a portion of the radionuclide source term. Therefore, there is a need to evaluate the incorporation of Pu and other radionuclides into various Fe-oxide phases, and to understand the behavior of coprecipitated phases during mineral recrystallization processes and during re-oxidation events. This effort focused on completing our analysis of radionuclide incorporation into Fe oxide phases and evaluation of partitioning coefficient λMe values across a range of radionuclides relevant to PA models. The processes of sorption and coprecipitation of a trace element within a mineral matrix can be parameterized using the Doerner-Hoskins relationship.

- *Waste package material development:* Corrosion-resistant waste packages are a key component of a multiple barrier system for waste isolation. A new concept has been evaluated; that lead/lead-alloy materials could be an excellent alternative material to copper for waste package outer layers, owing to their corrosion resistance (especially to hydrogen sulfide attack) and radiation-shielding capability. Long-term corrosion experiments show that lead is passivated by its corrosion products, such as cerussite ($PbCO_3$) and tarnowitzite $(Ca,Pb)CO_3$, in carbonate-bearing groundwaters. This is based primarily on the formation of a dense surface layer of corrosion products and the low solubility of the corrosion products. The low solubility of cerussite ($<10^{-6}$ mol kg^{-1}) reflects its greater thermodynamic stability (i.e., it is more favored to form) compared to galena (PbS) in a typical disposal environment; thus, the issue of sulfide-induced metal corrosion that applies to copper could be eliminated in the case of lead.
- *Enhancement of bentonite thermal conductivity:* The low thermal conductivity of bentonite (~0.5 W/m-K) combined with a thermally hot waste package may result in a high surface temperature on the package that may potentially affect the surrounding buffer material. The thermal conductivity of bentonite could be effectively enhanced by embedding copper mesh across the buffer layer. A simple calculation based on Rayleigh's model indicates that a thermal conductivity value of 5 W/m-K required for effective heat dissipation can be achieved simply by adding ~ 1 volume % of copper mesh into bentonite. As a result, the peak surface temperature on a large waste package such as a DPC can be reduced, perhaps significantly reducing surface storage time for waste cooling to facilitate direct disposal of DPC.

2.2.2 Summary Discussion of Major Changes to Priorities

Given the accomplishments in this TA, as well as the changes/drivers on Priorities (e.g., Program Direction; external data/understanding advancements, etc.,), the following major changes in priorities are:

- Increased priority is given to:
  - Improved representation of coupled THM processes affecting fracture transmissivity
  - Improved statistical sampling and representation of fracture networks
  - New generation of EBS materials including new buffer and waste package materials
- Decreased priority is given to:
  - Model development of DFNs

These prioritization changes are reflected by the progress made and new processes to be considered:

- A major part of the DFN model development has been completed. The focus will be shifted from model development to model validation and demonstration with field data.

- The potential impacts of glaciation/deglaciation on the properties of fracture networks need to be considered for long-term performance assessments, which requires a consideration of full coupling between mechanical and hydrological processes.

2.2.3 Planned Thrust Topics and Summaries

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

a) *Flow and transport in fractures, including matrix diffusion*

b) *Improved representation of coupled THM processes affecting fracture transmissivity*

c) *Existing international collaborations, particularly DECOVALEX-2028*

These three interrelated near-term thrusts for constraining processes for crystalline systems focus on the fracture network representation and the major THM processes that may modify the transmissivity of that network. A primary thrust is advanced capability development for generating DFNs in high-performance computing (HPC) systems for use in the GDSA Framework. In the near-term, model capability development will support assessment of coupled THM processes affecting fracture transmissivity and use multi-fidelity approaches to evaluate the uncertainty introduced by the stochastic nature of fracture networks. This area will continue to focus on model capability demonstrations using actual field data obtained from international collaborations. Systematic investigations of the potential effects of fracture geometry and distribution on fracture connectivity and field-scale permeability will continue. Such work may feed long-term studies delineating site characterization and siting characteristics.

Validation of models and parameters is an important component of the near-term focus. Significant international collaborations will be continued so that experimental data acquired in ongoing international URL programs can be leveraged to the crystalline R&D area.

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

a) *Performance of candidate buffer materials under a range of disposal conditions*

b) *Continued integration of large-scale international programs such as EURAD-2 and DECOVALEX-2028*

The interaction between the host rock and the EBS has been an important research thrust in the crystalline area and will continue to be because of fast transport in natural fracture systems. Engineered buffer materials in the EBS are an important component for waste isolation in a crystalline repository. This area is pursuing development of a new generation of buffer materials that can be tailored to disposal environments for effective waste isolation. This effort includes molecular modeling and experiments to constrain and parameterize radionuclide interactions with newly developed buffer materials or corrosion products of EBS components. The goal of this modeling effort is the development of a continuum model used to simulate fluid flow and transport in the EBS materials as they degrade. Such a model will be to evaluate the efficacy of new buffer materials and EBS design options. International collaborations have been, and will continue to be, a significant aspect of the crystalline research area. These activities include continued participation in DECOVALEX (for validation models), as well as collating and analyzing data from international URL and the EURAD-2 five-year program.

2.3 Salt Disposal R&D

Salt formations are an attractive host rock for deep geologic disposal of SNF and HLW because the high thermal conductivity of salt dissipates heat, while its low water content, porosity, and permeability inhibit radionuclide transport. In addition, salt experiences visco-plastic deformation and recrystallization: fractures will heal, disposal drifts will creep closed, and granular salt backfill in waste disposal drifts will consolidate until its properties are equivalent to those of intact salt.

The objective of the Salt TA is to develop conceptual and numerical models describing the response of natural and engineered features in a salt repository to excavation of the repository and emplacement of heat-generating waste. This understanding is important to both operational and long-term safety of a salt repository. Salt deformation affects drift stability; brine migration will impact corrosion of waste forms and waste packages, gas generation, and in-package criticality; and radionuclide transport may be affected by the evolution of the disturbed rock zone, granular salt backfill, and cement seals.

Salt disposal R&D supports multiple aspects of the safety assessment process, including:

(1). Development of generic disposal system concepts,

(2). identification of FEP, and development of generic evolutionary scenarios,

(3). development of the quantitative technical bases necessary for system simulation, including system conceptual models, characteristics, and process model development, and

(4). confidence building through collaboration with experts around the world to develop international consensus and best practices.

Primary R&D thrusts in the salt TA are (1) observing the effect of heat on brine availability and salt deformation in the EDZ (Brine Availability Test in Salt - BATS); (2) evolution of engineered barriers in salt (granular salt reconsolidation, compatibility, and evolution of cementitious seals); and (3) development of coupled process models and parameterization of requisite constitutive relationships. Activities are coordinated with the EBS, GDSA, and International TAs, and address high priority topical areas identified in the 2019 DR R&D Roadmap Reassessment, including high-temperature processes (e.g., temperature-dependent constitutive models), coupled process models in salt, and evolution of cement seals.

2.3.1 Accomplishments and Discussion

In the years since the previous version of this DR R&D Plan, the major accomplishments are:

- Effect of heat on salt
    - To investigate the effects expected from heat-generating waste, both BATS Phase 1 (2020-2021) and BATS Phase 2 (2022-2023) have measured the effects of coupled physical and chemical processes associated with heating a packer-isolated central borehole in salt at WIPP, the nation's only currently active URL for nuclear waste disposal. BATS comprises a series of observation/measurement boreholes (centered around the heated borehole) that contain equipment for water-vapor monitoring and brine sample collection. Surrounding these are smaller-diameter satellite boreholes instrumented to measure temperature, electrical resistivity, distributed strain and temperature, acoustic emissions, cement seal compatibility, and perform gas injection. An unheated control borehole array is located down the drift from the heated array. Currently, a second heated array (Phase 2) has been instrumented and additional series of heating and cooling tests gas tracers are underway. The data acquired to this point have shed light on several aspects of brine availability and elucidated test design revisions that will likely improve data collection to further refine our understanding of thermal effects (Kuhlman et al., 2022).
- Model development
    - Progress on model development benefits from the unique and extensive dataset collected at BATS, which enhances the U.S.' leadership in salt repository science. The Salt Team has led a four-year international collaborative task as part of DECOVALEX 2023 (2020 to 2023) and is proposing a follow-on task as part of DECOVALEX 2027. Participants are developing models of the coupled thermal-hydro-mechanical (THM) processes associated with brine production and damage evolution associated with emplacement of heat-

generating waste in salt. Modeling teams from four countries (U.S., Germany, UK, and Netherlands) have completed a series of increasingly complex model benchmarks and data from the BATS experiment for comparison across programs.

- Several salt-specific features have been implemented in PFLOTRAN, to support DECOVALEX and RANGERS modeling efforts (e.g., changing porosity due to soluble matrix and implementation of brine equations of state), through collaboration with GDSA model developers.
- The U.S. benefits from several ongoing collaborative projects that are part of a long-standing bilateral agreement with Germany. In the last year, a comprehensive report laying the groundwork for validation of temperature- and moisture-dependent constitutive models for reconsolidation of granular salt backfill was published (Kuhlman et al., 2021; Czaikowski et al., 2020).

The BATS is providing a wealth of data for process understanding, is re-developing U.S. expertise on URL test development, and facilitating model benchmark comparisons and model validation activities in the international disposal research community.

2.3.2 Summary Discussion of Major Changes to Priorities

Because salt disposal R&D activities are ongoing (activity plans extend through several consecutive phases), there are no major changes in priorities. Rather, the specific focus of activities in the next one to two years will build on the previous year's accomplishments. The thrust topics in the next section are consistent with these priorities.

2.3.3 Planned Thrust Topics and Summaries

Primary R&D thrusts in the Salt TA are (1) measuring the effect of heat on brine availability and salt deformation in the EDZ (BATS –Figure 2-2); (2) evolution of engineered barriers in salt (granular salt reconsolidation, compatibility, and evolution of cementitious seals); and (3) development of coupled process models and parameterization of requisite constitutive relationships. Activities are coordinated with the EBS, GDSA, and International Technical Areas, and address high priority topical areas identified in the 2019 DR R&D Roadmap Reassessment, including high-temperature processes (e.g., temperature-dependent constitutive models), coupled process models in salt, and evolution of cement seals.

Figure 2-2. BATS Phase 2; photo of BATS 2 array (left), and layout of in-drift equipment (right).

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

a) *Effects of different power levels on salt*

- Phase 2 of BATS, ongoing since 2022, will continue performing heated testing at different power levels in the new array of boreholes, utilizing a refined experimental design. We are collecting data that are beginning to show a connection between the mechanical (i.e., damage), hydrological, and chemical aspects of the test at different temperature levels. We continue to monitor the evolution of damage and gas permeability in the salt, in response to heating the salt to different temperatures. Additional heating schedules (i.e., slower radioactive decay and periodic heating) will be investigated to better discriminate the nature of damage and healing in the damaged zone surrounding a drift in salt.

b) *Confidence and international relationship building*

- The DR R&D Salt team has a leadership role in the NEA's Salt Club, as Kris Kuhlman has been the NEA Salt Club chair since January 2021. Melissa Mills and Kris Kuhlman are co-organizers of the U.S./German Workshop on Salt Repository Research, Design & Operation (with 2024 being its 14^{th} meeting). The Salt DR team members are leading international efforts focused on scenario development and human intrusion for generic salt disposal concepts, with participation on other modeling and laboratory efforts on engineered barriers and granular salt reconsolidation.

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

Many of the activities in the Salt TA have multi-year plans. At BATS, a long-term heater test (months to years), including a sealed heater test (i.e., no gas circulation) are proposed as part of a BATS follow-on phase. A long-term heater test would help constrain the stability of brine production over time and may allow observation of heat-accelerated salt creep. A sealed heater test would evaluate the impacts of the applied boundary condition at the borehole (constant relative humidity or no-flow). Additionally, facility improvements for BATS at WIPP are proposed to allow additional investigations such as gas permeability testing, large-scale strain monitoring, (Kuhlman et al., 2022). Follow-on BATS tests at WIPP (i.e., BATS3) are proposed to have a more decentralized approach (i.e., smaller, independent tests in adjacent smaller borehole arrays), rather than being coordinated and focused on a single central heater. Ongoing international collaborations, such as DECOVALEX-2028 and the U.S./German workshop will also be longer-term thrusts.

2.4 Engineered Barrier System (EBS) R&D

EBS R&D activities support all three of the generic host-rock types (argillite, crystalline, salt) with the specific EBS characteristic differing depending on the host-rock system. Because of this, EBS research activities address a wide range of topics on design materials and barrier performance. In addition, consideration of direct disposal of DPC expands the consideration of higher temperature conditions and chemical effects from potential additional DPC filler materials within the EBS environment. Because of all these aspects, EBS research thrusts are aimed at assessing the feasibility, applicability, evolution, and performance of EBS concepts in a given generic geologic medium and given a particular waste inventory.

The R&D activities focus on understanding EBS components evolutions and interactions within the EBS, as well as interactions between the host media and the EBS. A primary goal is to advance the development of process models that can be implemented directly within the GDSA platform or that can contribute to the safety case such as building confidence, providing further insight into the processes being modeled, and/or establishing better constraints on barrier performance, etc.

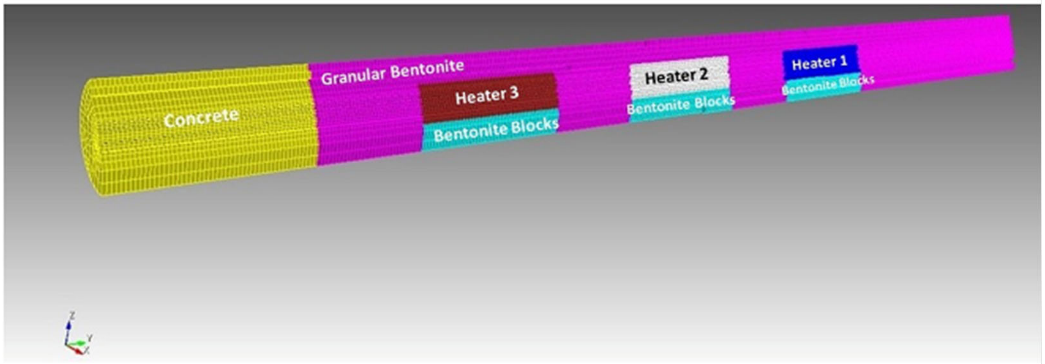


Figure 2-3. Model representation of the full-scale emplacement (FE) heater test experimental tunnel, used as part of DECOVALEX Task C activities.

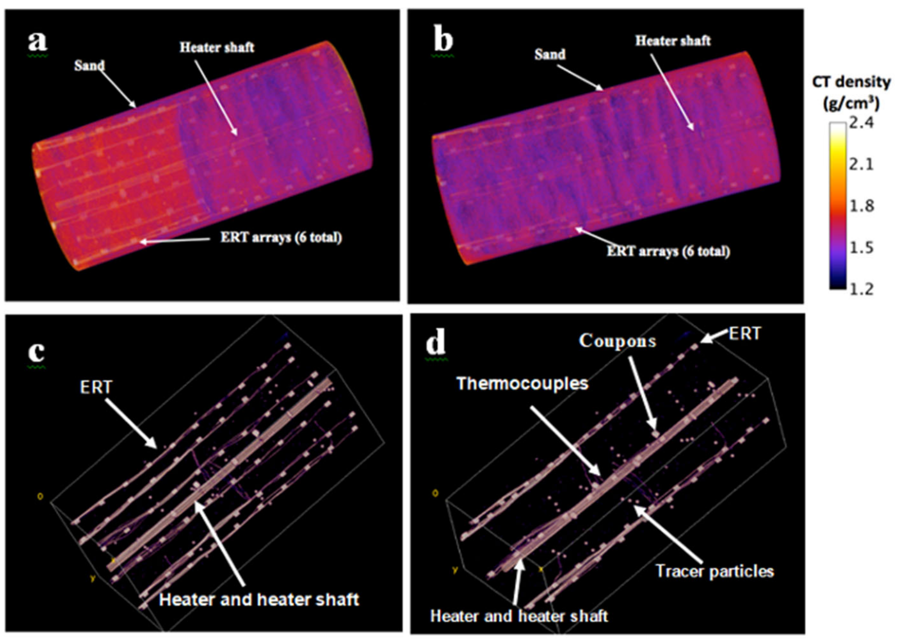


Figure 2-4. Benchscale Column Test to support HotBENT 3-D -- CT images from the showing the initial density distribution in the (a) non-heated and (b)heated columns. (c) and (d) present key instrumentations—heater and heater shaft, thermocouples, tracer particles, metal coupons, ERT and sensor wires.

2.4.1 Accomplishments and Discussion

In the years since the previous version of this DR R&D Plan, the major accomplishments are:

- Continued support of and participation in the HotBENT Field Test, including preliminary modelling of the field test and a bench-scale bentonite column test to better understand saturation behavior of the bentonite at higher thermal loads. A major and notable accomplishment for the HotBENT heater field test was the start of the experimental phase, marked by the heater start up that occurred in 2023.
- Hydrothermal bench-scale tests to study interactions of EBS materials, including bentonite, host rock, waste package materials, and cement liners, under repository conditions. Particular emphasis will be on understanding the effect of higher temperature, as would be expected for DPC direct disposal.

- Combined experimental and modelling study focused on understanding evolution of cement-host media interfaces. This includes novel methods for characterizing cement-host rock interfaces, as well as code comparison of state of the art 1-D leaching code (LeachXS) with PFLOTRAN.
- Development and evaluation of next-generation buffer materials. This includes lab testing, characterization, and molecular-scale modeling to better understand potential anionic sorbent materials.

Overall, the EBS activities are working to create and implement process models to understand fundamental processes. These activities in the EBS work-scope can be described in broad terms via three categories:

(1). Evaluating the integrity of repository plugs and seals, including shaft and drift seals; the main thrust is to understand how these closures evolve with time. Of particular interest is permeability evolution, as this is typically an important parameter in performance assessment. Sorption processes/interaction of radionuclides with EBS materials make up another important parameter space for investigation.

(2). Understanding of seals evolution is facilitated by understanding processes at material interfaces. This includes engineered or geotechnical materials and disturbed rock zone interfaces, as well as the interface of waste package materials and buffer/backfill.

(3). Many of the processes at material interface are complex and can include coupled processes, multi-phase flow, and multi-scale phenomenon.

2.4.2 Summary Discussion of Major Changes to Priorities

Given the accomplishments in this TA, as well as the changes/drivers on Priorities (e.g., Program Direction; external data/understanding advancements, etc.,), the following major changes in priorities are:

- Increased priority is given to:
  - HotBENT Field Test and supporting complementary activities,
  - Sorption and transport of radionuclides in bentonites, and
  - Integration between hydrothermal experimental methods and cement-host media studies.
  - Next-generation buffer materials (crosscut with Crystalline WP)
  - EURAD-2, in particular the bentonite focused ANCHORS project will provide a new opportunity for international collaboration.
- Decreased priority is given to:
  - DECOVALEX 2023, Task C (which is winding down in FY24).

The Thrust Topics in the next section are consistent with these updated priorities.

2.4.3 Planned Thrust Topics and Summaries

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)*

c) *Existing international collaborations such as DECOVALEX-2028, HotBENT, EBS Task Force*

The three near-term thrust topics are examples of a general approach for EBS investigations that are somewhat tailored to each generic disposal concept and a specific focus on bentonite backfill thermal-hydrologic processes that may be similar/common for a number of generic concepts. Advancing models of multiphase transport and its effects on buffer/backfill and response to varying thermal and mechanical conditions in the repository drift is being used to evaluate radionuclide transport in the EBS. Modeling and experimental activities are underway to assess performance of EBS components in the disposal environment, including buffer/backfill, waste package materials, waste forms (including SNF), and shaft and drift seal materials longevity and chemical effects.

Improved understanding of the effects of this dry-out on the resultant clay pore matrices, and on fluid permeability, is being pursued. Restoration or healing of pore matrices upon re-saturation (when the repository has cooled down) is also a target of improved understanding. Experiments and modeling will be conducted to elucidate these phenomena in such a way that the results can help to improve confidence in predictions of buffer permeability evolution under more realistic repository conditions. Many current international partnerships will continue to be developed and enhanced for both barrier performance understanding and constraints on materials evolution and chemical effects in the EBS. These partnerships are both near-term and longer-term thrusts.

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)

International activities include participation in the Engineered Barriers System Task Force (EBS-TF – an international consortium that works collaboratively to study issues most critical to EBS Design and Performance). Participation in the EBS-TF, HotBENT, and DECOVALEX has continually provided an opportunity to stay up to date on the latest international advances in EBS design and performance, but more importantly gives access to test data and samples from underground field tests of EBS performance. These current activities will continue to remain an important to EBS involvement in international collaborations and URL studies. The EURAD-2 projects are an emerging opportunity for EBS to participate in bentonite-based research in collaboration with international experts. The EURAD-2 ANCHORS project will begin in FY25 and figure to be an important aspect of EBS International collaboration over the next several years.

2.5 Inventory and Waste Form Characteristics and Performance

At the beginning of fiscal year 2021, a number of waste form relevant activities were moved into the *Inventory and Waste Form Characteristics and Performance* TA to integrate the ongoing activities in this area. These activities fall into four areas covering (1) the Online Waste Library (OWL) inventory database for DOE-managed high-level waste (DHLW) and DOE-managed spent nuclear fuel (DSNF), (2) cladding degradation conceptual model development, (3) advance isotopic measurements on high-burn-up SNF, and (4) waste form testing, modeling, and performance. This last area encompasses the integration of models for both commercial spent nuclear fuel (CSNF) and high-level waste (HLW) glass degradation for use in GDSA, as well as the current suite of testing activities investigating SNF behavior within the DR program and the integrated planning for further testing of CSNF degradation behavior. This TA integrates this work with the intent to dispose of these waste forms in a deep geologic repository. It is recognized that the DHLW includes wastes that may be dispositioned in the future with a different waste classification that would perhaps entail a different disposal pathway. In this work, the theoretical geologic repository for wastes, including DSNF and DHLW, is assumed to be a deep mined generic geologic repository.

The purpose of the work directly on the OWL is to provide the inventory data on DSNF and DHLW for safety assessment analyses of generic repositories for these wastes and their waste forms. Additional work on specific waste form characteristics includes assessing the inventory data and ensuring information exists for disposal of relevant radionuclides, as well as evaluating the waste form degradation behavior of waste forms for implementation of waste form degradation models in the GDSA Framework. To this end, there are related activities in the waste form testing, modeling, and performance investigating the modeling assessments of Stage III (accelerated, "resumptive") rates for HLW glass degradation, first principles calculations of clarkeite ($Na_2U_2O_7$) structures, and electrochemical model development for SNF (UO_2) degradation.

2.5.1 Accomplishments and Discussion

In the years since the previous version of this DR R&D Plan, the major accomplishments are:

- OWL database activities focused on completing the release of OWL Version 3.0 (SAND2021-14487W) on November 18, 2021, and OWL version 4.0 (SAND2022-12754W) on September 26, 2022. In OWL Version 3.0, the most significant change was the addition of sodium-bonded fuel produced from DOE's experimental fast-neutron breeder reactor program. OWL version 4.0 included 17 new radionuclides, added to make more complete decay chain information available for future PFLOTRAN analyses. Other changes involved error corrections and enhancements.
- Short-term activities for OWL also included the continued updating of the listing and inventory data for DOE-managed HLW and SNF radioactive wastes that are potential candidates for deep geologic disposal. These data include those assessed in the previous disposal options evaluation work, and any newly identified additional wastes and/or waste forms. OWL supporting documents were also updated to maintain traceability of OWL inventory data.
- Advances on several ongoing, multiyear, expansion projects were also made in OWL, regarding: (1) the development of a GDSA interface for OWL; (2) the expansion of OWL for vessel information; and (3) leveraging selected information from INL's Spent Fuel Database (SFD). For the first expansion project focusing on developing a GDSA interface for OWL, the goal is to build the capability within OWL to generate input parameter files for use in PFLOTRAN. The information required in radionuclide inventory input files for PFLOTRAN depends on whether the input file is for waste packages containing SNF or for waste packages containing HLW glass. The focus for the first area of integration was on developing an input file for HLW glass because OWL currently contains more information about HLW glass than SNF. Regular discussions between the OWL and PFLOTRAN teams during this past year have resulted in the selection of specific inventory and waste information for glass waste along with efforts to implement the selection. For the second expansion project which involves adding vessel information to OWL, the OWL team is creating a new subsite with information on vessels (e.g., containers, canisters, casks, waste packages) designed for storage, transportation, and/or disposal of nuclear waste. The types of information being compiled include dimensional characteristics, weights, regulatory certification for usage, waste types and waste forms that could potentially utilize these vessels, material properties of the vessels, etc. Due to the complexity of this expansion, new database infrastructure was developed to help facilitate and manage workflow. Its implementation is ongoing. Another area of progress is the vessel information modeling, which has resulted in the creation of tables that are currently being reviewed and readied for testing. For the third expansion project, which involves leveraging selected information from INL's SFD for use in OWL, the OWL team selected a subset of information with a focus on future needs for PFLOTRAN modeling and sent a data request to INL. INL responded with the requested information in spreadsheet format from the current SFD version (version 8.1.8) and marked the information as official use only (OUO). Planning is currently underway regarding how best to incorporate some of the content requested into OWL. This cooperative effort allows the two databases to complement each other. Access to the SFD is limited by necessity because it is a Nuclear Quality Assurance-1 (NQA-1) database, which

contains classified information. Even with OUO (or controlled unclassified information (CUI), as appropriate) restrictions, the information, once included in OWL, will be more accessible to a wider group of users. Also, as part of OWL, this information can be analyzed within the context of DOE-managed wastes beyond just DSNF.

- As part of the waste form testing, modeling, and performance activities, density functional theory investigation of all known crystalline clarkeite polymorphs and their temperature-driven phase transitions were carried out to evaluate their relative stability as a function of temperature (Weck et al., 2023).
- Evaluated thermodynamic data updates for zeolites (Zeo19) and clays to conduct EQ3/6 reaction path calculations of HLW glass (Jové Colón et al., 2022). The Zeo19 and ALTGLASS^{TM} databases for HLW glass degradation data were used to constrain rate parameters in reaction path simulations.
- Development of a thermodynamically based electrochemical model for SNF degradation using SNL Zuzax code suite (Jove Colon et al., 2023). The objective of this model is to capture electrochemical reaction feedbacks due to changes in solution chemistry using species standard thermodynamic properties, macroscopic balances for energy and transport, and reactions kinetics.
- Generated a conceptual model for cladding degradation that is to be utilized in both safety assessments and in criticality evaluations for DPC direct disposal (Brady et al., 2022).
- Initiated an integrated planning activity to evaluate knowledge gaps and prioritize new testing on SNF within the DR Program (Meszaros et al., 2022). The draft plan is being augmented through multi-National Laboratory workshops (including each of the participating labs in this TA); it is expected that the plan will be finalized in FY23 with the intent to start additional testing work with the highest priority thereafter.

It is expected that these modeling activities relevant to waste form degradation will be integrated with multi-laboratory experimental/testing efforts to accurately represent the evolution of in-package chemistry under repository conditions and key source term processes in GDSA-PA.

2.5.2 Summary Discussion of Major Changes to Priorities

Priorities in this area are unchanged, except that the expanded activities have been added to both the near-term and longer-term thrust topics. Most efforts focused on OWL remain at the same priority as before, although OWL will need to migrate from its current SharePoint site on the SNL External Collaboration Network (ECN) to the Cloud by ca. 2025. Other activities are still evolving or were initiated recently.

2.5.3 Planned Thrust Topics and Summaries

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

a) *Migrating OWL from SharePoint on the SNL ECN to the cloud*
b) *Development of basic interface GDSA scripts to access and read OWL data*
c) *Develop Glass Waste Degradation Expertise*
d) *Finalize SNF testing gap analyses and prioritization*

The primary thrusts for the OWL inventory work in the short-term are: (a) the migration of OWL from its current SharePoint site on the SNL ECN to the Cloud and (b) the development of basic GDSA interface scripts to access and read OWL data to allow a more automated approach to generating inventory input for the GDSA Framework.

Regarding item (a) above, by ca. 2025, SNL SharePoint database will have to migrate to the Cloud. The current implementation of OWL SharePoint site on the SNL ECN relies on the use of SQL Server Reporting Services (SSRS), which will no longer be available in the cloud (i.e., there is currently no Software-as-a-Service (SaaS) for SSRS on Microsoft Azure cloud computing platform). As part of OWL migration to the cloud, significant effort and resources might be required to convert current SSRS reports to paginated reports in Microsoft Power Business Intelligence (BI) on Azure cloud computing platform.

With respect to item (b), once developed, these scripts will enable GDSA models using PFLOTRAN to perform standard database queries of the OWL. Short-term activities will also include the continued updating of the listing and inventory data for DOE-managed HLW and SNF radioactive wastes that are potential candidates for deep geologic disposal. These data include those assessed in the previous disposal options evaluation work, and any newly identified additional wastes and/or waste forms.

HLW glass degradation rate is described to occur in three major stages (I, II, III). The Stage III behavior is characterized by a resurgence in HLW glass dissolution rate associated with the precipitation of a secondary phases (Vienna et al., 2018; Neeway et al., 2020). As part of cross-campaign integration, the existing data and conceptual models for Stage III (accelerated, also referred to as “resumptive”) degradation rates for HLW glass were assessed. This effort still provides the groundwork and develops expertise for evaluating any future enhanced models (as developed/delivered from another NE Campaign). Such expertise will facilitate implementing any process model of HLW glass degradation that includes Stage III effects for use within the GDSA Framework.

The integrated planning activity to evaluate knowledge gaps and their prioritization along with new testing activities on SNF degradation was initiated in Meszaros et al. (2022). This work was followed up by Jové Colón et al. (2023) resulting in a revised gap list (10 gaps) and their prioritization. Further, the proposed waste form testing activities were also revised and expanded. The integrated planning for the proposed SNF testing activities analyses and their prioritization will focus on a testing strategy/plan in the upcoming fiscal year. As with the gap analysis effort, this work will utilize experts from each of the National Laboratories involved in the DR modeling and testing of SNF to develop a prioritization of testing activities based on the gap analysis to close those gaps. It is intended that the highest prioritized tests will be initiated in the next 1-to-2-year period.

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

a) *Maintain OWL Inventory Content and Interface OWL with Other Databases*

b) *Consider Additional OWL Interface Capabilities for the GDSA Framework*

c) *Execute prioritized SNF testing to collect data needed to address gaps*

d) *Coherent integration of large-scale international programs, particularly EURAD-2*

The longer-term thrusts in this TA are generally on-going efforts (i.e., maintaining the data sets within the OWL (inventory content) for any changes/updates, and adding additional inventory data sets, as needed for GDSA). In addition, OWL capability expansion activities are also possible over the next five years. Such activities could include interfacing OWL with other databases, such as the DOE SNF Database at INL on the numerous entries for DOE-managed SNF. This effort would involve defining data exchanges to facilitate future testing of integration protocols. Longer-term activities would include construction of the next stage development of the OWL to add capabilities for generating turn-key inventory output for safety assessment simulations. The OWL could also be augmented to include data sets for available radioactive waste “vessels”, for example cans/canisters/packages. Such additional data tables would include dimensional characteristics (inner and outer), masses, material properties, certification for usage, indication for which wastes/waste forms these are meant to enclose, as appropriate, etc. These data sets would be incorporated in much the same manner as the data for the wastes/waste forms. An initial vessel information model has been developed during FY23 and is currently being tested with a sample dataset. OWL capabilities could be developed to facilitate a more active integration with the GDSA Framework (e.g., generation of "as packaged inventory" from user-selected waste forms and vessels, and disposal date) for disposal analyses, and potentially with other codes for transportation/storage systems assessment. Once developed, such OWL capabilities could be used to simulate disposal of selected OWL inventories in mined geologic disposal concepts in a variety of generic geologic media (e.g., salt, clay/shale rocks, and crystalline host lithologies).

In addition to the above improvements in the inventory work, the third longer-term thrust is the execution of the prioritized SNF testing based on the completed strategy/plan. It would be intended to complete at least the first series of newly initiated SNF testing within this longer-term period, potentially with any needed update to the gap analysis and prioritization based on insights gained through the testing. Collaborations will be developed under EURAD-2 aimed at improved quantification and mechanistic understanding of the release of safety relevant radionuclides covering most representative types of SNF and of the fuel evolution both prior and posterior to contact with ground water to better predict the radionuclide source term for post-closure safety assessment.

2.6 Geologic Disposal Safety Assessment

The objective of the GDSA TA is to develop and continuously maintain a state-of-the-art software framework for probabilistic post-closure performance assessment analyses of facilities for deep geologic disposal of nuclear waste. This unified software framework provides the U.S. DOE with robust, sophisticated simulation and analysis tools that will support site selection, site characterization, and licensing for the nation's next deep geologic disposal facility. The GDSA TA is the nexus for integration of concepts, models, and understanding developed in other SFWST disposal research TAs. Leadership and participation in international collaborations promotes innovation, ensures a world-class standard of practice, and engages the next generation of scientists in this compelling problem of national interest.

GDSA Framework (https://pa.sandia.gov) is an open-source software framework developed to leverage the U.S. DOE's HPC resources. The availability of this unique computing capability enables appropriately detailed modeling of the coupled physical and chemical processes affecting repository evolution and radionuclide transport, implementation of model domains with geologic fidelity, forward simulation over the 10^4- to 10^6-year timescale typically required by regulation, and propagation of uncertainty over many realizations of the problem.

Open-source software development makes the simulation and analysis tools within GDSA Framework freely available to regulators, stakeholders, and the scientific community at large, thus promoting collaboration, driving development, and importantly, enabling transparent decision-making in a regulatory environment.

Primary R&D thrusts in the GDSA TA are (1) advanced simulation capability; (2) state-of-the-art uncertainty and sensitivity analysis methods; (3) traceable, user-friendly workflow; (4) repository systems analysis, including simulation of generic reference case repositories in argillite, crystalline, salt, and unsaturated host rocks; and (5) development of geologic models, including generic archetypes for different host rocks and an interactive web-based application for visualization of regional geology in the U.S.

2.6.1 Accomplishments and Discussion

In the years since the previous version of this DR R&D Plan, the major accomplishments are:

- *Advanced simulation capability*
  - GDSA Framework integrates coupled physical and chemical process models and material-specific constitutive models in PFLOTRAN (Lichtner et al., 2019), a multiphase flow and reactive transport simulator. The range of conditions over which multiphase flow and solute transport can be simulated was improved by completing the implementation of advanced linear and nonlinear solvers, adding options for characteristic curves, and

prototyping a solute transport mode that can handle complete dry-out in the model domain (Nole et al., 2022; 2023). Integration with other TAs drove development of simulation capability (Nole et al., 2022; 2023). For DPC criticality consequence analyses capabilities added include temperature-dependent material property changes associated with illitization of bentonite buffer and a degradation model for internal components of the canister. For simulations of salt repository concepts a flow mode with fully implicit coupling of salinity allows simulation of density-driven flow and a soluble rock matrix. For simulations of crystalline repository concepts, gas transport was added to the fracture-matrix diffusion model and a conceptual model for buffer erosion and canister corrosion was developed. GDSA-specific software quality assurance (QA) is also being developed through PFLOTRAN's generic QA test suite, which compares simulation results to analytical solution and a handful of other codes (e.g., TOUGH). Machine learning surrogate models for fuel matrix dissolution are under development that incorporate time-dependence (Mariner et al., 2023).

  - Implementation of the main functionality of the biosphere model was completed (Ghosh et al., 2022). The open-source biosphere model incorporates multiple exposure pathways consistent with the NEA FEP list and a flexible, modular architecture consistent with recommendations from the IAEA.
  - Since FY21, a PFLOTRAN beginner short course is being offered to collaborators internationally. In FY23, advanced short course material was developed focusing on the key components to building a fractured crystalline reference case model. Topics include multi-continuum vs ECPM formulations for fracture flow and transport, generating deterministic and stochastic fracture networks with dfnWorks, upscaling fracture properties to ECPM for use in PFLOTRAN, and performing sensitivity analysis on a miniature crystalline reference case using Dakota.

- *Uncertainty and sensitivity analysis*
  - Uncertainty quantification and sensitivity analysis (UQ/SA) methods in GDSA Framework are primarily available through Dakota (Adams et al., 2020), an open source HPC interface for coupling physics simulations to both tried-and-true and cutting-edge methods of UQ/SA, optimization, and parameter estimation. The GDSA team demonstrated the potential of multi-fidelity uncertainty and sensitivity methods to increase efficiency that advanced the crystalline reference case with improved representation of fracture networks (Swiler et al., 2021a; Swiler, 2022). Two focus areas in 2022 included analysis of the transmissivity relationship used in the DFN (correlated constant vs. correlated depth-dependent transmissivity) and model form uncertainty introduced by the FMD surrogate model in the crystalline case (Swiler, 2022). In 2023, we performed sensitivity analysis on a generic shale reference case (Swiler, 2023).
  - GDSA leads an international team in comparison of sensitivity analysis methods, a milestone in the ongoing process of developing an international consensus on best practices for sensitivity analyses for repository performance assessment (Swiler et al., 2021b). The past 18 months have focused on SA of three more complex repository cases with more advanced SA methods: Volume 2 of the comparison report is expected to be complete this coming year.

- *Workflow*
  - The GDSA team put the framework in GDSA Framework with the Next Generation Workflow (NGW; Orient et al., 2020), an easy-to-use graphical interface that allows the user to dictate workflow and that provides reproducibility and traceability of the files and scripts used for a particular study (Mariner et al., 2020). The workflow incorporates significant post-processing capabilities that automate sensitivity analysis and was

demonstrated on the crystalline reference case (Swiler et al., 2021a). A journal paper summarizing the NGW and the way it can be used to facilitate advanced studies such as nested samples has been submitted (Portone et al., 2023) and tutorial material for NGW has been prepared and delivered (Swiler et al., 2022).

- *Repository systems analysis*
    - Reference cases describing generic repositories in argillite, salt, crystalline, and unsaturated host rocks provide a platform for integrating concepts, demonstrating capability, and driving development of simulation software and analysis methods. Conceptual models and simulations that account for high temperature impacts associated with direct disposal of DPCs are a priority. The primary focus areas since 2020 have been international collaboration on PA studies through leadership of a DECOVALEX task, testing and extending capability of the workflow.
    - The GDSA Repository Systems Analysis and Framework teams are leading a 4-year task for DECOVALEX2023 in which PA simulation and analysis methods are applied to generic crystalline and salt reference cases. Since the task began in 2020, ten teams from seven countries have collaboratively developed reference case scenarios that are amenable to a wide variety of conceptual and simulation approaches and published them in a publicly available document (LaForce et al., 2023). The in-house simulation studies to date are in (LaForce et al., 2021, LaForce et al., 2022).
    - Framework testing and extensions have included studies utilizing a newly developed simulation capability for disturbed rock zone evolution that includes waste packages representative of DPCs in inventory, development and simulation of an unsaturated alluvium reference base case, and development and utilization of open-source meshing software VoroCrust (LaForce et al., 2021, LaForce et al., 2022)

The above accomplishments represent advances in modeling and simulation accounting for high-temperature impacts (such as those associated with direct disposal of DPCs); development of breadth and depth in reference case concepts; confidence building through international collaboration, information exchange, and benchmarking; and improvements to performance and workflow necessary to sustain a forward-looking, agile simulation and analysis framework.

2.6.2 Summary Discussion of Major Changes to Priorities

Because GDSA activities are ongoing (activity plans extend through several consecutive phases), there are no major changes in priorities. Rather, the specific focus of activities in the next one to two years will build on the previous year's accomplishments. The Thrust Topics in the next Section are consistent with these priorities.

2.6.3 Planned Thrust Topics and Summaries

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

a) *Advanced simulation capability*
    - Near term advancements in PFLOTRAN capability will continue to focus on high priority topical areas while building on previous accomplishments. These efforts will include continuing to advance high-temperature simulation capability; implementing material-specific waste package degradation models; addressing the coupled thermal-hydro-mechanical-chemical processes affecting buffer evolution, backfill consolidation, and drift convergence; and examining the coupled thermal-hydro-chemical processes affecting waste form degradation, radionuclide release, radionuclide transport, and transport in high ionic strength solutions. Multi-fidelity model implementation, including mechanistic models derived from detailed process understanding, reduced order models, and machine

learning emulators, enhances computational efficiency and dovetails with integration of advanced UQ/SA methods. Simulator verification will be also pursued through formal software QA. Simulator performance improvements will be pursued and include use of machine learning techniques (e.g., augment nonlinear solvers).

- Other software development tasks will include ongoing development of open-source biosphere simulation software; addition of capability to dfnWorks (Hyman et al., 2015), software for generating DFNs and simulating particle transport; and release of an open-source version of Vorocrust (Abdelkader et al., 2020), an automated meshing tool for generating conforming meshes of complex engineered and geologic features.
- Future assessment of the GDSA Framework capability will be facilitated by a tracking tool being developed by the GDSA team that will associate repository reference case FEP (and FEP parts) with GDSA Framework capability status, current and planned R&D activities across DR, Roadmap priorities, and 5-year plan thrusts. This tool will help track the completeness of GDSA Framework and will aid in prioritizing remaining DR R&D needed to fully develop GDSA Framework.

b) *Uncertainty and sensitivity analysis*

- Uncertainty quantification and sensitivity analysis (UQ/SA) methods in GDSA Framework will be advanced in two ways. First, the team will continue to identify and demonstrate methods consistent with the current standard of practice that add value to deep geologic repository performance assessment such as surrogate (meta) modeling, variance decomposition, multi-fidelity analysis, and evaluation of model form uncertainty. The team will continue to take a leadership role in international collaboration on these topics. Second, the team will begin to evaluate the reliability of methods dependent surrogate models through techniques such as cross-validation and development of quantitative metrics for assessing goodness of surrogates.

c) *Workflow*

- Transparent, traceable workflows increase stakeholder confidence and user-friendliness. In the next 1 to 2 years, GDSA automation will be further developed using NGW and two additional important workflows will be established: an open-source framework (scripted in Python) that automates software (PFLOTRAN) verification testing; and a workflow that streamlines data transfer from the geologic model to the meshing software and ultimately to the simulator. Two classes of workflows in NGW are being developed: one that performs a single loop sample study and one that supports nested sampling.
- Integration of GDSA Framework with the OWL will be initiated. This integration will provide quality-assured radionuclide inventories for simulations involving defense-related waste streams.

d) *Repository systems analysis*

- In the near term, a main priority will be simulation and analysis of the salt and crystalline reference cases developed for the DECOVALEX-2023 task. This task will drive development of models of bentonite backfill evolution and waste package degradation (crystalline) and of salt consolidation and creep; and advance understanding of uncertainties associated with simulation and analysis methods. GDSA will also continue to develop the shale reference case and continue to integrate with other TAs to advance analyses of direct disposal of DPCs, understanding of high-temperature FEP, and scenario development methodology. In addition, performance assessment techniques will be further developed and implemented in reference cases to quantify the relative contributions of specific features and processes to overall repository performance in reference case simulations.

e) *Geologic modeling*

- Geologic modeling involves two primary efforts: generation of representative 3-dimensional (3D) regional geology models that inform reference case concepts and simulations, and development of an interactive web-based application (https://gis1.inl.gov/regionalgeology/) for visualizing argillite, salt, and crystalline formations in the U.S. In the near term, geologic models of a generic unsaturated alluvial basin and of regional argillite stratigraphy will be linked into the meshing workflow described above; and 3D subsurface visualization tools will be developed within the web application.

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

In future years, capability development will continue to address high-priority topical areas and integrate new process understanding acquired in other SFWST TAs. Identification and prioritization of activities will be aided by a database that tracks progress and links activities to important FEP of the reference cases. Model development and implementation may include multi-fidelity approaches to simulation of coupled processes in salt, interior waste package chemistry, gas flow in the EBS, and physical and chemical evolution of cement seals. Reference case simulations will continue to evolve to incorporate new software (VoroCrust meshing and Dakota NGW), designs, concepts, and models as they are developed. The current DECOVALEX PA comparison will be finalized, and a new round focused on UQ/SA will be initiated, subject to continued sponsorship in DECOVALEX-2027.

In general, simulation capability will move toward a more sophisticated representation of a larger set of FEP affecting repository performance; software development will integrate with process modelers with emphasis on traceability, computational efficiency, and streamlining the process of adding new models to GDSA codes; UQ/SA will incorporate best practices consistent with up-to-date standards of practice; and the geologic modeling and meshing workflow will flexibly incorporate refined representations of engineered and geologic features as appropriate.

Depending on program direction, the tools and expertise that reside in the GDSA TA could be expanded for eventual use in site evaluation, selection, and eventual characterization. The DOE's HPC platform, PFLOTRAN's multi-physics simulation capability, and Dakota's cutting-edge analysis tools together enable sophisticated methods of inverse modeling and data assimilation that are well-suited to interpretation of large, complex datasets and development of material parameterizations that incorporate uncertainty and stochastic variability. Together, the GDSA, Argillite, Crystalline, Salt, and International Technical Areas can leverage international collaborations to access site characterization data, to develop expertise in site evaluation methodology, to compare uncertainty and sensitivity analysis methods, and to test technical approaches to data collection and interpretation.

2.7 International Collaborations Disposal Research

The SFWST Campaign has a balanced portfolio of international collaboration activities in disposal research, addressing relevant R&D challenges in fields like near-field perturbation, engineered barrier integrity, radionuclide transport, and integrated system analysis. These activities form a central element of SFWST's disposal research, and significant advances have been made across different host rock types and engineered barrier research challenges. International collaboration enables (1) leveraging a deep knowledge base regarding alternative repository environments developed across the world, (2) utilizing international research facilities (such as URL testing) not available in the U.S., and (3) sharing the cost of major research efforts such as full-scale in situ experiments or complex modeling efforts. SFWST currently has in place formal collaboration agreements with several international initiatives (DECOVALEX Project, Mont Terri Project, SKB Task Forces, HotBENT,) and multiple international partners. National lab scientists associated with the campaign are conducting a number of collaborative R&D activities that align with R&D priorities across most of the TAs discussed in this section. In these collaborations, SFWST scientists contribute world class analyses, models, and data for both process understanding and system risk modeling and assessment (Birkholzer et al., 2023.

A major focus of the International program are collaboration activities that provide access to and/or allow for participation in field experiments conducted in operating URLs in host rock environments not currently available in the U.S. Figure 2-5 gives a visual overview of activities conducted to date, experiments in bold denote currently active international collaborations. The figure graphically illustrates the breadth and focus of SFWST's international program. The research portfolio is equally distributed between engineered barrier, near-field and far-field focus, with an emphasis on argillite and crystalline host rock.

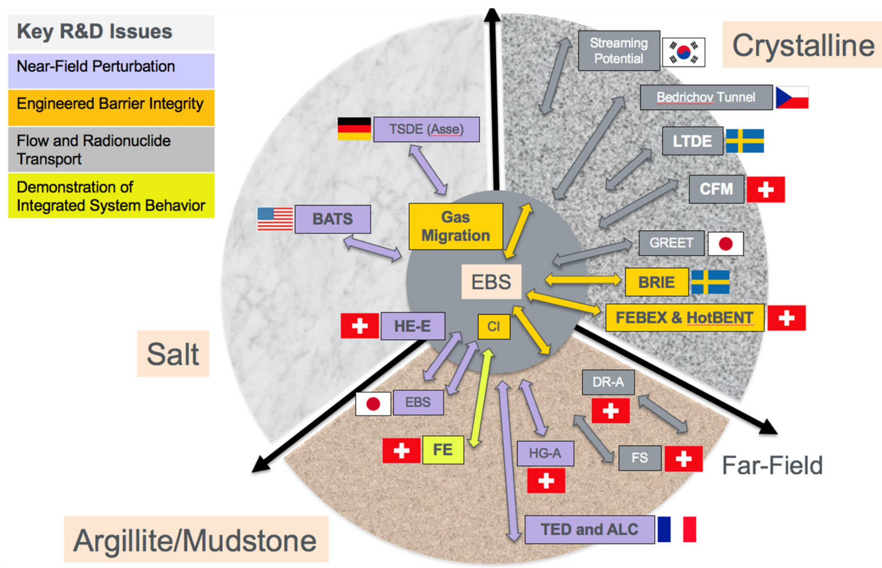


Figure 2-5. High-level overview of the major international experiments conducted in different countries that SFWD researchers have participated in since 2012. Experiments in bold denote currently active collaborations. See Table ES-1 in Birkholzer et al. (2023) for more information on each experiment.

Overall, the focus on international collaboration allows close integration with the international waste management R&D community in terms of best practices, new science advances, state of the art simulation tools, new monitoring and performance confirmation approaches, and lessons learned. The joint R&D with international researchers, the worldwide sharing of knowledge and experience, and the direct access to relevant data/experiments from a variety of URLs and host rocks provides an improved understanding of the current technical basis for disposal in a range of potential host rock environments. Comparison with experimental data allows for testing and validating predictive computational models for evaluation of disposal system performance in a variety of generic disposal system concepts. Comparison of model results with other international modeling groups, using their own simulation tools and conceptual understanding, enhances confidence in the robustness of predictive models used for performance assessment. The possibility of linking model differences to particular choices in conceptual model setup provides guidance into "best" modeling choices and understanding the effect of model uncertainty. These outcomes, including improved predictive models and a deep understanding of conceptual model uncertainties, can be directly incorporated into GDSA activities.

2.7.1 Accomplishments and Discussion

In the years since the previous version of this DR R&D Plan, the major accomplishments are:

- HotBENT: The objective of the international HotBENT project is to conduct a full-scale high-temperature heater experiment at the Grimsel Test Site in Switzerland. The construction and installation of HotBENT was finalized in 2021 and the full-scale *in-situ* experiment started officially on September 9, 2021, when heaters were turned on for the first time. After months of careful ramping up of heater power, all HotBENT heaters reached their final target temperatures of 175 °C or 200 °C in June 2022. SFWD has been very active since the beginning of HotBENT project and made significant contributions to the project: scoping calculation models were developed to facilitate the design, high temperature laboratory column tests and hydrothermal batch experiments were carried out to provide information that cannot be measured in the field test, predictive and interpretive models have been developed as part of the HotBENT Modeling Platform to deepen the understanding and improve modeling capabilities.

- DECOVALEX: The DECOVALEX Project (dEvelopment of cOupled Models and their VALidation Against eXperiments) is an international research collaboration and model comparison activity for coupled processes simulations in geologic repository systems (currently 17 project partners). SFWST scientists participated in a broad range of relevant modeling tasks associated with the current DECOVALEX Project phase referred to as DECOVALEX-2023, which was initiated in early 2020 and will run through December 2023. These tasks include *in-situ* tests on thermal and gas fracturing in argillite, gas migration in bentonite, a full-scale demonstration test in a clay host rock, a full-scale engineered barrier experiment, and a more fundamental task involving laboratory experiments fluid flow, shear, thermal and reaction processes. Furthermore, SFWD scientists are serving as task leads for two additional tasks, one focusing on brine migration in heated salt, and one on performance assessment. Planning for a new DECOVALEX Project phase is currently underway. This new phase, referred to as DECOVALEX-2027, will start in early 2024 and run for four years till the end of 2027.

- Active Role in Shaping International Efforts: One of the near-term thrust topics listed below calls for SFWST to consider moving from a mostly participatory role in ongoing *in-situ* experiments conducted by other nations to a more active role in conducting its own experimental program in international URLs. The advantage of active planning is obviously that the experimental focus and design can be better tailored to the SFWST campaign needs. In past years, SFWST's disposal program has started taking a much more active approach in shaping the future R&D portfolio of the international initiatives it has joined as a partner. For example, SFWST scientists play an important role in the international DECOVALEX Project serving, respectively as Chairman and Leads of two important modeling tasks. SFWST researchers are also leading a new modeling task in the SKB EBS Task Force, which at its center has a high-temperature column experiment conducted at LBNL. In addition, as pointed out above, DOE has co-developed with international partners the planning and design of the HotBENT Project, the full-scale high-temperature heater experiment planned at the Grimsel Test Site.

- Confidence Building in Performance Assessment Models: Another near-term thrust topic calls for international collaboration to contribute confidence building for GDSA. SFWST researchers have increased their international collaboration in this area: In Task F of the DECOVALEX-2023 project, confidence in performance assessment (PA) models and methods is enhanced by comparing PA modeling results from ten international disposal programs applied to the same reference cases, one involving a repository in a fractured crystalline host rock and another featuring a repository in a bedded salt formation.

- Next Generation Workforce Development: A longer-term goal described below is to utilize international collaboration activities as an opportunity to develop the next-generation workforce for disposal research in the U.S. To advance this cause, SFWST launched a new pilot program in 2022 to attract and train a diverse early-career workforce of nuclear waste disposal scientists. Initially designed as a pilot study involving a small number of national labs and partner universities, the effort considers three main areas, all of which are related to international research activities in SFWST.

- To stimulate student interest in nuclear waste research, the program worked towards developing free, virtual seminar series for interested undergraduate and graduate students, and young nuclear waste disposal researchers. In FY22 for example, SNL collaborated with Dr. Neven Ali, a lecturer at the University of New Mexico (UNM) Department of Nuclear Engineering, to develop a seminar series at UNM for the Fall 2021 and Fall 2022 semesters centered around current topics and challenges in radioactive waste management.
- To create a next-generation pipeline, both LBNL and SNL ran very successful summer internship programs in 2022: students with diversified background participated in a variety of research projects in LBNL and SNL associated with international disposal research, some of them were converted to long-term interns and may have the potential be hired as postdocs in the future. These programs have been expanded in 2023, adding LANL as another partner lab.
- To advance the pipeline, LBNL and SNL each hired a dedicated post-doc a three-year research project focused on international collaboration (e.g., the HotBENT or GDSA post-doc).

The above accomplishments provide a flavor of the benefits of international collaboration, which range from sharing of knowledge and best practices to active peer-to-peer research participation to jointly conducting complex *in-situ* experiments in international URLs not available in the U.S. and provide opportunities for workforce development. Integrating across several TAs including EBS R&D, Argillite Disposal R&D, Crystalline Disposal R&D, Salt Disposal R&D, and GDSA, the joint modeling and comparative analysis of complex *in-situ* experiments has led to better predictive models and directly contributes to confidence building of GDSA predictions.

2.7.2 Summary Discussion of Major Changes to Priorities

In this TA, there have been no major changes in priorities.

2.7.3 Planned Thrust Topics and Summaries

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

a) Continue participation within international R&D in URL for a range of geologic systems

The current international research portfolio, which spans across several TAs including Argillite Disposal R&D, Crystalline Disposal R&D, Salt Disposal R&D, EBS R&D, and GDSA, has been re-evaluated and re-prioritized in 2019 as part of a broad activity-based priority assessment across the campaign (Sevougian at el., 2019). We expect these priorities will remain largely intact over the next few years, while moderate revisions to the international portfolio will be made as new opportunities emerge and existing collaborations end (see below). Note that some key international activities involve long-term in situ experiments that will continue for years to come (e.g., the full-scale emplacement (FE) Heater Test at Mont Terri, HotBENT), while others such as DECOVALEX tasks have a limited timeline and will be replaced with new collaborative tasks.

b) Continue assessment of new international opportunities

Ongoing evaluation of existing and emerging opportunities for international collaboration is a key responsibility of the International Collaborations TA. We will continue to review, assess, and develop such opportunities in close integration with international partners, will evaluate technical merit and alignment with the current and planned work scope within SFWST work packages, and revise the portfolio of international R&D activities as appropriate. Examples of possible new collaboration activities might include:

- The new DECOVALEX-2027 phase, which will start in 2024, will likely comprise seven to eight tasks of high relevance to SFWST. We are currently working with DECOVALEX leadership to shape the task portfolio and participate in the next phase as makes sense.
- SKB has started dismantling of the inner Section of their Prototype Repository Heater Test at the Äspö Hard Rock Laboratory (HRL), Sweden. The full-scale test started in 2001 and is now the longest operation of a multi-barrier repository experiment in the world. SKB has incited the international community to participate in the dismantling project. Discussions with SFWST are underway.
- SFWST considers tunnel, shaft, and borehole sealing elements as a priority theme for engineered barriers research. Participation in international experiments is currently evaluated (e.g., the upcoming Large-scale Sandwich Experiment, SW-A, which tests a promising layered technology for shaft seals; or Andra's GES test which examines gas permeable seal).
- The SFWST program is currently evaluating technical alignment with the EURAD-2 European Commission collaborative program which will start a new round repository R&D work in the Fall of 2024. The goal is to encourage in-kind collaboration of SFWST scientists with projects funded under EURAD-2, for cross-benefit between these two large programs.

Assessment of new international opportunities will feed into the next stage of re-evaluation of the DR Roadmap (the Roadmap Reimagination).

c) *Pursue a more active role in conducting experimental work in international URLs*

The SFWST campaign will continue evaluating whether its international collaboration focus should move from a mostly participatory role in ongoing in situ experiments conducted by other nations to a more active role in conducting its own experimental program in international URLs. The advantage of active planning is that the experimental focus and design can be better tailored to the campaign needs. More such active collaborations will be considered in the future.

d) *Contribute to integration and confidence building for Geologic Disposal Safety Assessment*

The international research activities, with their focus on modeling and comparative analysis for complex in situ experiments, ultimately lead to better predictive models and thus directly contribute to confidence building for post-closure PA models. In the SFWST campaign, the work packages for international collaboration, for generic research on EBS and host-rock specific topics, and for GDSA need to be well integrated to make optimal use of improved process models leading to better safety assessments models. Confidence in PA models can also be enhanced by comparing PA methods to international standards, or by benchmarking PA studies against international data sets. Under leadership of SFWST scientists, the PA/UQ/SA benchmarking task in DECOVALEX 2023 has compared PA methodologies across multiple international disposal programs. Continuation of this PA/UQ/SA task is envisioned for the next DECOVALEX phase.

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

International collaboration will continue to be a central element of SFWST Campaign's disposal R&D over the next five years and beyond. As research priorities change and new opportunities for collaboration present themselves, the international research portfolio will be re-prioritized as appropriate. Many of the two-year themes discussed above will continue to drive the campaign planning. In addition, depending on the direction of the campaign and the progress made, international collaboration could be expanded to in several ways to serve other objectives. Below are two examples:

a) *Develop best practices and technologies for site selection and characterization*

The current campaign focus in disposal research is to (1) provide a sound technical basis for multiple disposal options in the U.S., (2) assess suitability and geographic distribution of host rock types,

(3) increase confidence in the robustness of generic disposal concepts, and (4) develop the science and engineering tools needed to support disposal concept implementation. As the campaign evolves, a suitable goal for international collaboration is to start learning more about siting and site characterization practices for geologic disposal, via engagement with countries that currently go through such efforts. At a minimum, such international collaboration would involve close observation and information exchanges, to gain a better understanding of best practices and lessons learned in disposal programs that are in different stages of siting. Or the campaign could be actively embedded in ongoing international site characterization efforts, for example, via joint development and testing of surface- and borehole-based characterization tools.

b) Utilize international activities for training/education of junior staff

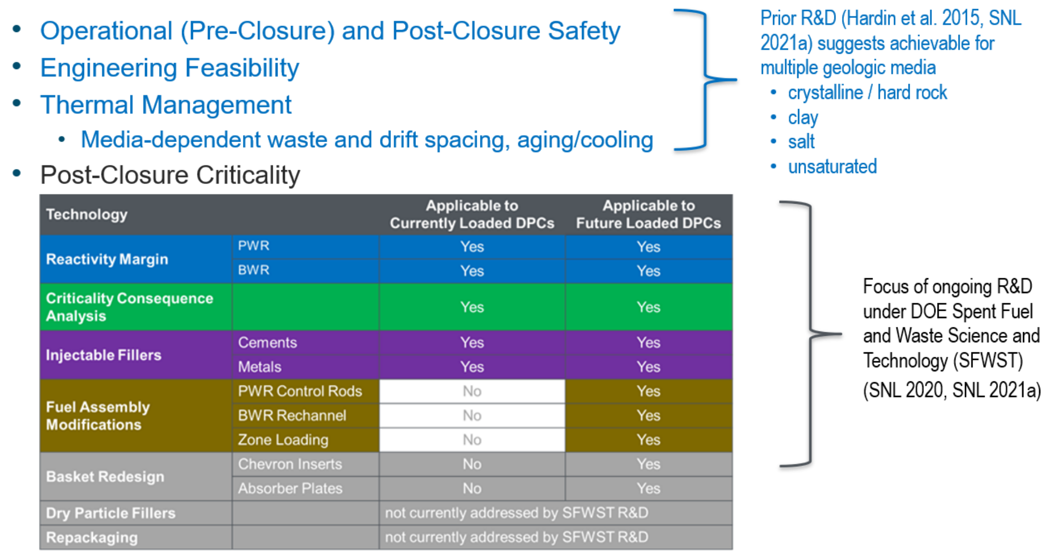
International collaboration has provided extremely valuable data sets from underground testing that are not only relevant to the SFWST's campaign R&D objectives but also provide for complex scientific challenges of high interest to young researchers. The campaign will continue to make a dedicated effort to use international collaboration activities as an opportunity to recruit and train early-career scientists to become the next-generation workforce for disposal research in the U.S.

2.8 Direct Disposal of Dual-Purpose Canisters

Commercial SNF is accumulating in dry storage at over 70 sites across the U.S. in DPCs, which are designed for S&T, but not disposal. DOE is investigating the technical feasibility of direct disposal of commercial SNF in DPCs, as an alternative to repackaging the commercial SNF into purpose-built disposal containers. Direct disposal of SNF in DPCs has the potential to simplify disposal operations, minimize the number of SNF shipments, reduce collective worker dose associated with repackaging, and significantly decrease the costs associated with geologic disposal.

The main technical challenges for disposal of SNF in DPCs are thermal management, handling and emplacement of large, heavy waste packages, and post-closure criticality (Hardin et al., 2015). In prior years, DOE has published reports addressing engineering challenges associated with the large size and weight of DPCs and thermal management of the large heat load. Potential higher peak temperature in generic repository systems is being addressed in thermally coupled processes in argillite, crystalline, salt, EBS, and GDSA TAs. Elevated pressures associated with thermal pressurization in argillite are being investigated in conjunction with GDSA. Current research also addresses post-closure criticality because modern DPCs depend on aluminum-based materials for neutron absorption during S&T, and those materials will degrade in a few decades when exposed to groundwater in a repository.

Specific research focus areas (see Figure 2-6) include: (1) direct disposal without modification (post-closure criticality consequence analysis, as-loaded reactivity margin analysis); (2) modification of already-loaded DPCs (with injectable filler materials for criticality control); and (3) modification of DPCs to be loaded in the future, or the fuel they contain (changing loading maps, adding disposal criticality control features, or basket redesign). Implementation of models for direct disposal of SNF in DPCs in generic repository systems remains a focus of this area to inform future policy decisions regarding storage and disposal of such SNF canisters.



Technology		Applicable to Currently Loaded DPCs	Applicable to Future Loaded DPCs
Reactivity Margin	PWR	Yes	Yes
	BWR	Yes	Yes
Criticality Consequence Analysis		Yes	Yes
Injectable Fillers	Cements	Yes	Yes
	Metals	Yes	Yes
Fuel Assembly Modifications	PWR Control Rods	No	Yes
	BWR Rechannel	No	Yes
	Zone Loading	No	Yes
Basket Redesign	Chevron Inserts	No	Yes
	Absorber Plates	No	Yes
Dry Particle Fillers		not currently addressed by SFWST R&D	
Repackaging		not currently addressed by SFWST R&D	

Figure 2-6. Overview of options to facilitate evaluation of feasibility of direct disposal of DPC.

2.8.1 Accomplishments and Discussion

In the years since the previous version of this DR R&D Plan, the major accomplishments are:

- *Probabilistic Post-Closure DPC Criticality Consequence Analyses* – Developed and implemented preliminary generic system models for two types of potential criticality events, a transient event, and a steady-state event, in both an unsaturated repository in alluvium and in a saturated repository in shale (Price et al., 2022). These models have been implemented in the GDSA Framework. Preliminary modeling has included joined thermal, hydrologic, and criticality processes in the repository and near-field to estimate the potential source term from a criticality event, investigate conditions that could lead to the permanent termination of a criticality event, and estimate consequences in terms of dose to a member of the public. Preliminary results indicate that the consequences of a steady-state criticality event in an unsaturated repository would be minimal because the lack of water limits the power and duration of such a criticality event, thereby limiting the temperature increase and inventory increase. Preliminary results also indicate that the occurrence of a steady-state criticality event in a saturated repository does not lead to an increase in dose to a member of the public. Work is ongoing regarding the consequences of transient criticality.
- *As-Loaded DPC Reactivity Margin Modeling* – Continued investigation of potential reactivity management strategies that can be used to reduce the number of canisters susceptible to criticality over the repository performance assessment period (Shaw et al., 2021). The investigations examined effects on reactivity of modifying baskets, modifying fuel assemblies, and optimizing the loading pattern. These approaches will allow criticality analysis to be incorporated in the decision-making process that will be used for canister loading.
- *DPC Injectable Filler Testing and Analysis* – Prepared and implemented a multi-year workplan for cement and metal filler development (SNL, 2021) that describes experimental work supported by simulation to advance the development and characterization of filler materials and filling methods. Ongoing experimental work focused on several different phosphate cements as promising filler materials; the calcium aluminate phosphate cements appear to show the most promise for advanced testing and scale-up. Metal filler work included simulation and experimental work related to evaluation of filler material compatibility with injection through a small diameter DPC drain port and final porosity of the metal casting.

- *Future DPC (Fuel/Basket) Modifications* – Focused on testing of advanced neutron absorber materials that could be used in future DPCs for long-term criticality control and DPC mechanical degradation modeling (Hardin & Jones, 2021).

The above accomplishments show progress in the near-term Thrust Topics. The criticality consequence analyses, and thermal scoping analysis provide promise that existing and future DPCs may be disposable without modification under certain conditions and/or geologies. R&D on injectable fillers and future DPC modifications may ultimately lead to techniques that reduce the probability of post-closure criticality for existing and future DPCs.

2.8.2 Summary Discussion of Major Changes to Priorities

There will be one major change in priority in the coming years: ending the work on testing of advanced neutron absorber materials that could be used in future DPCs for long-term criticality control. There are several reasons for this change: (1) modifying DPCs to include advanced neutron absorbers would require action on the part of the DPC manufacturers, not the DOE; and (2) it would take many years for these modified DPCs to be designed, licensed, and used by utilities; by then thousands more unmodified DPCs would be filled with SNF.

A new study has been started, investigating the possible extrusion of bentonite into a failed waste package. The purpose of this study is to characterize the movement of water and/or bentonite into a failed waste package under the conditions anticipated in a hypothetical saturated repository: high pressure gradient (~50 bar) across the waste package wall and approximately 50% void space inside a waste package.

2.8.3 Planned Thrust Topics and Summaries

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

a) *Probabilistic Post-Closure DPC Criticality Consequence Analyses*

The near-term focus of this thrust area is to continue to develop and implement a method for evaluating the consequences of potential criticality events on overall repository performance to determine if the consequences are acceptably low. Consequence screening is a new approach, not fully constrained in the U.S. or international repository R&D programs to the degree planned here. This approach includes developing a technical and regulatory strategy for low consequence analyses, developing a source term representing effects from criticality events, using coupled process modeling input, and identifying appropriate criticality FEP, key parameters, and metrics. Some of these efforts are continuing while others, such as identifying FEP that are affected by and/or can affect the occurrence of criticality, have been completed (Alsaed & Price, 2020).

Criticality scenario development with source term and near-field changes specific to different types of criticality events will continue to evaluate the consequences of post-closure criticality. Contributing activities will continue to couple nuclear dynamics (neutronics) and thermal hydraulics (N-TH coupling). Other activities will continue to include effects from mechanical/hydrologic/chemical/radiolytic changes in fuel/basket/canister performance into post-closure criticality consequence calculations.

This activity includes the following High Priority R&D Activities from the R&D Roadmap Reassessment (Sevougian et al., 2019, Table 3-5):

- Probabilistic post-closure DPC criticality consequence analyses
- Coupled multi-physics simulation of DPC post-closure (chemical, mechanical, thermal-hydraulic) including processes external to the waste package
- Source term development with and without criticality

b) As-Loaded DPC Reactivity Margin Modeling

Analyses of reactivity for several hundred as-loaded DPCs, for a stylized degradation case representing loss of all neutron absorbing materials (complete removal and replacement by water), will continue. These analyses include the compilation of fuel characteristics (type, burnup profiles, etc.) and canister data (basket design, fuel loading schema, etc.) for DPCs as that information becomes available and analysis (and re-analysis) of reactivity for stylized degradation cases, and for disposal environments (e.g., natural groundwaters, chloride brines). These analyses will also include optimizing fuel loading to reduce reactivity, with the goal of creating a methodology that utilities could implement while loading SNF that would meet loading requirements for heat and worker dose and reduce reactivity in the event of neutron absorber loss.

This activity includes the following High Priority R&D Activity from the R&D Roadmap Reassessment (Sevougian et al., 2019, Table 3-5):

- Maintain and populate DPC as loaded database

c) DPC Injectable Filler Testing and Analysis

The near-term focus of this thrust area is to develop and demonstrate fillers that could be injected as liquids into existing DPCs, where they solidify. One advantage of this activity would be demonstrating that fillers would be successful in displacing or excluding ground water from breached waste packages in a repository and preserving neutron absorbing materials to prevent criticality over the long-term. If successful, this approach could be used to treat both current and future DPCs as needed. The near-term investigations will continue to include mixing and handling of candidate filler materials, both cement and metal, and demonstration of filler injection into small-scale representations of DPC fuel/basket geometries. In addition, near-term investigations will include an evaluation and identification of the FEP that would be affected by the presence of fillers, The development of a concept of operations for a filler facility at a disposal site, as well as whether filling would occur via existing vent/drain ports or holes created for the purpose of injecting filler material.

This activity includes the following High Priority R&D Activity from the R&D Roadmap Reassessment (Sevougian et al., 2019, Table 3-5):

- DPC filler and neutron absorber degradation testing and analysis

d) Movement of Water and/or Backfill Material into a Failed Waste Package

The near-term focus of this new thrust area is to plan and conduct bench-scale experiments to study the movement of water and/or backfill material through a breach in a waste package and into that waste package under conditions expected in a saturated repository. The objective is to determine the conditions, if any, under which a swelling backfill material, such as clay, might intrude through a crack in a failed waste package into the void space of that waste package. Depending on the results of these experiments, it might be possible to leverage this process to reduce the reactivity of the fuel inside that waste package.

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

a) Probabilistic Post-Closure DPC Criticality Consequence Analyses

The longer-term focus of this thrust area is to develop a higher-fidelity, robust PA model that includes the integrated processes necessary to simulate the consequences of potential criticality events on overall repository performance. The integrated PA model would include a detailed source term representation (fuel, cladding, basket, and waste package physical and chemical evolution relevant to critical configurations), the effects of N-TH coupling, conditions external to waste packages (saturated and unsaturated repositories).

b) As-Loaded DPC Reactivity Margin Modeling

The longer-term focus of this thrust area is to continue to collect the data necessary to perform criticality analyses on as-loaded DPCs under the stylized degradation cases used in the past. This will provide the DOE with information regarding the number and percentage of DPCs that would remain subcritical during the post-closure period and will identify those DPCs that might need to be filled with filler material, should the DOE decide to purse that avenue rather than a low-consequence approach.

c) DPC Injectable Filler Testing and Analysis

The longer-term focus of this thrust area is the demonstration of the most promising filler materials and injection techniques at full- or near-full scale. This would also include large-scale representations of the geometries of the DPCs, baskets and other internals, and assemblies, and appropriate representation of the injection vent ports and filler tubes.

d) Movement of Water and/or Backfill Material into a Failed Waste Package

The longer-term focus of this thrust area is to continue to perform experiments, with the design, scope, and scale of later experiments being informed by the results of earlier experiments.

2.9 Technical Support for Underground Research Laboratory Activities

The DOE has an inactive URL in unsaturated tuff that will be leveraged to support R&D pertaining to generic disposal concepts, especially disposal concepts for unsaturated zone repositories. The URL has not been actively operated for an extended period of time (approximately 12 years) and all offsite electrical utility power has been disconnected remotely from the location. Power restoration is the first activity to utilize this URL for DR R&D on generic disposal concepts.

2.9.1 Accomplishments and Discussion

In the years since the previous version of this DR R&D Plan, restoration of power and lighting to the URL has continued to be delayed due to the impacts of the COVID-19 pandemic and performance of work contract issues. In this time, researchers working in this area have advanced the cosmic radiation test plan (Meszaros et al., 2021) and have purchased a single weather station and data acquisition system for the non-invasive monitoring of air/gas composition and movement in the tunnel that occurs both through the tunnel openings and through the unsaturated fractures of the host rocks. Additionally, a site survey was conducted to determine optimal locations for future installation of passive monitoring equipment (Figure 2-7).

Figure 2-7. Potential drift location for passive monitoring equipment.

2.9.2 Summary Discussion of Major Changes to Priorities

Given the accomplishments in this TA, there has been no change in priorities for these activities and the Thrust Topics in the next Section are consistent with this.

2.9.3 Planned Thrust Topics and Summaries

The URL TA has two operational objectives and two R&D thrusts at this stage of resuming operations. Operational objectives are to re-establish lighting and communications within the URL, and to develop planning and facility access protocols. The R&D thrusts are passive monitoring of atmospheric conditions in the underground, and measurement of cosmic ray background radiation (including muon detection). Both of these R&D activities serve as vehicles for achieving the second operational objective (develop planning and facility access protocols).

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

a) Operational

With the re-establishment of electric power and communications from the URL to outside locations, work can proceed by researchers in a safe and productive manner. In the next 1 to 2 years, operational activities will include installation and refurbishment of underground electrical, lighting, and communications equipment, and connection to surface power sources.

Underground activities will include cleaning of existing mine power centers; procurement and installation of approximately 6,500' of bare copper grounding/bonding conductor; refurbishment of approximately 100 subsurface light fixtures; procurement and installation of several hundred feet of low voltage and medium voltage portable power cables; and reconnection of 50 communication units.

Surface activities will include connecting two legacy diesel generators to the legacy underground power system through newly procured medium voltage unit substations. Two new earth ground points will be installed.

b) Passive monitoring

Passive monitoring instruments will be installed in the URL to quantify the impact of natural ventilation on in-drift conditions in an unsaturated zone URL. The test plan addresses planning and facility access protocols and proposes installing at least two instrument clusters to continuously measure barometric pressure, temperature, and air flow. In addition, one or more continuous gas stream analyzers will be installed to measure compositional components of the tunnel gases, for example the partial pressure of H_2O (humidity) and CO_2. Unmanned deployment of monitoring equipment to inaccessible areas is also desired, primarily for assessing radon and humidity levels in non-ventilated drifts.

c) Cosmic radiation

Muons, negatively charged particles with 200 times the mass of electrons, are created when cosmic rays hit particles in the Earth's atmosphere and can pass through hundreds of meters of solid material. The recent availability of portable detectors has enabled characterization of dense objects and subsurface features using muons. In the next 1 to 2 years, a muon detector as well as instruments for detection of other cosmic radiation (e.g., gammas, neutrons) will be installed in the URL for preliminary data collection. Long-term objectives are to develop non-destructive subsurface characterization methods using muon imaging, and to inform the design of sensitive physics experiments (e.g., rare-event searches) that require shielding from cosmic radiation. A test plan (Meszaros et al., 2021) describes the proposed detector.

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

Longer-term data collection is planned for both the passive monitoring and cosmic radiation detection activities. In both cases, outcomes may include characterization of subsurface heterogeneity, development of geologic or hydrogeologic models, and implementation of additional related experiments (e.g., non-invasive geophysical methods and seismic studies). Measurements of cosmic ray background as a function of depth in the URL could serve as an important input in designing future experiments to develop this technology for site characterization and safeguards and security applications.

When power, lighting, and communications are restored and planning and access protocols are in place, other opportunities to leverage the URL for generic R&D are expected to arise.

2.10 Knowledge Management

The primary goal of the Knowledge Management (KM) activity is to establish a KM program covering the entire Nuclear Energy Fuel Cycle (NEFC). The KM program began as a pilot program focused on knowledge relevant to the SFWST Campaign DR R&D program, but now has expanded to address knowledge of value to the entire back end of the fuel cycle. The loss of senior staff members, who are not only leaders and mentors but also seasoned subject matter experts in nuclear waste management (NWM), continues to call for an intentional approach to ensure an efficient and rigorous approach to capturing, cataloging, and archiving institutional NWM knowledge and enabling sharing of that knowledge to new staff. This KM activity has been collecting, organizing, and cataloging such knowledge while developing the tools to archive, transfer, and use this tacit knowledge from our colleagues nearing the end of their professional careers. Capturing and managing this knowledge avoids the costs and risks of recreating already known methodologies once again (or worse in multiple instances) and mitigates the potential complete loss of that tacit experience base.

The pilot effort that began in 2019 can now be considered complete. Numerous knowledge capture events have been conducted including KM workshops, focus groups, and deep dives, and an initial KM repository has been established and hundreds of documents collected there. Audience participation in the KM events has expanded to the entire DOE NE-8 and national laboratory community, as has the KM governance team.

There are still important objectives to pursue. For example,

- Supporting new staff in building expertise in NWM
- Increasing knowledge sharing and coordination across the DOE NWM community
- Ensuring better coordination and consistency in information management and knowledge repositories.
- Supporting consent-based siting programs by helping to ensure that accurate, current information is findable for all stakeholders.
- Capturing the knowledge, experience, and information gained from the Consortia Program and ensuring that it is maintained for future siting efforts.

2.10.1 Accomplishments and Discussion

In the years since the previous version of this DR R&D Plan, the KM program has matured significantly. In May 2023, a major update to the strategy document, *SFWD Knowledge Management Strategy Recommendations*, marked the conclusion of the pilot program for KM, capturing lessons learned and establishing a new set of KM program objectives. In addition to that milestone, the major accomplishments in KM activities include:

- Development and implementation of the first implementable version of a NWM taxonomy and a formal governance plan for its ongoing maintenance.
- Continuing the deep dive presentation series
- Incorporating the SFWD seminar series into the KM program
- Migrating the KM site to an externally accessible cloud SharePoint site.

The first implementable version of the NWM was completed in 2021. The taxonomy was developed with consultation from a KM contractor with taxonomy expertise. The fields and terms of the taxonomy reflect the practices of DOE OCRWM and were explicitly designed to be informed by and consistent with NRC terminology found in its storage, transportation, and disposal regulations and review plans. This taxonomy has now been implemented not only in the KM repository but also in the CURIE website. The *Taxonomy Governance Plan* (Meacham et al., 2022), which outlines a formalized process to updated and maintain the taxonomy over time and ensure its consistent use in multiple systems, was completed in September 2022.

The deep dives conducted since the last version of this plan include the following:

- June 7, 2022 — Yucca Mountain Total System Performance Assessment (TSPA-LA) Model (Day 1) — Speakers: David Sassani, Robert Howard, K. Pat Lee, Sunil Mehta
- June 14, 2022 — Yucca Mountain Total System Performance Assessment (TSPA-LA) Model (Day 2) — Speakers: Chris Camphouse, Cliff Hansen, Teklu Hadgu, and a two-hour SME panel discussion including Patrick Mattie, Sunil Mehta, K. Pat Lee, Cliff Hansen, Peter Swift, Robert MacKinnon and Mark Nutt, moderated by Laura Swiler and Chris Camphouse
- January 24, 2023 — knowledge transfer panel interview of William Boyle, NE-81
- January 25, 2023 — History of Public Interest in Siting Nuclear Waste Facilities — Andrew Newman, “Nevada, Nuclear Waste, and Assembly Joint Resolution 15 of 1975”; Thomas Cotton, “Setting the Stage: Nuclear Waste Management Policy up to 1982”; Tom Isaacs “Nuclear Waste Management 1983–1987: Siting and Survival”; Robert Mussler, “The Story of the Office of the Nuclear Waste Negotiator: A Volunteer Siting Effort Directed by Statute (1990-1995)”; Lake Barrett, “Lessons on Organization and Public Engagement: OCRWM 1988–2010.”

- May 23, 2023 — video capture of Yucca Mountain site tour with William Boyle.

Each of the above Deep Dives covered large amounts of materials and generated active discussion with questions being addressed by the participants to clarify materials and cover additional details. They were selected to capture critical knowledge at risk of being lost or to inform current program needs where knowledge gaps could be filled. For example, the TSPA Deep Dive was conducted because the TSPA model, which has been maintained live since 2010, was being shut down; the Deep Dive on the history of siting nuclear waste helped gather historical background, experiences, and lessons learned relevant to the current DOE consent-based siting effort; and the January interview and May site tour with William Boyle were designed in part as knowledge capture events. As with all prior Deep Dives, each event was recorded on video, transcribed, and collected on the Nuclear Waste Program Knowledge Management SharePoint site along with all their referenced source materials.

The SFWD Seminar Series that began as online brown bag events during the pandemic shutdown was restarted within the scope of KM to record and capture these presentations for future use. These are occasional online meeting presentations, conducted 1–3 times a month with presenters across the NE-8 organization sharing recent work.

The initial KM site was migrated to SNL external cloud SharePoint ensure accessibility to all NE-8 laboratory staff and federal staff.

2.10.2 Summary Discussion of Major Changes to Priorities

In the time since the prior version of this 5-year plan, priorities have shifted significantly. This shift in priorities comes from two main drivers:

(1). Direction from NE-8 for the KM program to serve both the NE-81 SFWST campaign and the NE-82 Integrated Waste Management (IWM) campaign.

(2). Restart of the consent-based siting program for a centralized interim storage facility.

These changes in priority accelerated previously planned thrusts for the long term to be immediate priorities. The two prior long-term thrust topics (to expand KM Repository to benefit larger portions of the NEFC community and to consider developing training courses) have already been initiated or largely accomplished. The accomplishments outlined above reflect those changes in priority.

2.10.3 Planned Thrust Topics and Summaries

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

a) Continued maintenance and development on KM repositories

b) Continued maintenance and development of the NWM taxonomy, especially with respect to development of terms relevant to social sciences and consent-based siting

c) Provide KM support to the consent-based siting program

d) Documentation of historical lessons learned

e) Developing training courses.

The key thrust for KM in the short-term is to maintain and develop the KM repositories (both the Nuclear Waste Program Knowledge Management SharePoint site as well as supporting content on the CURIE site); some of this is now a supporting, ongoing activity performed as new content is developed and added to these systems, but there is an ongoing effort to tag libraries containing the milestone reports from NE-81 and NE-82 with the NWM taxonomy to ensure that they are available across the program and can be readily found. The continued development of the NWM taxonomy, especially to include terms from social science and important to consent-based siting but also to further refine the taxonomy related to S&T will be a major focus. The KM team is supporting the consent-based siting program in a variety of ways, the most important being to capture, organized, and preserve information generated from the consortia program. Finally, a report summarizing lessons learned from the past repository site characterization program is planned for completion in FY24, and an effort to prepare a NWM primer training program for new staff has also be initiated.

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

a) *Expand KM Repository libraries to collect and organize a much larger volume of information.*

b) *Develop machine-learning techniques and tools to help automate tagging of information added to these libraries.*

Further development of KM Repository content and capabilities would continue in the long-term as more information is collected and linked. To support those goals and make the effort more efficient, the KM team is beginning to investigate use of ML tools that can help automate the application of document metadata. Document tagging is currently a time-consuming task requiring considerable training and expertise, but there is a path forward to developing and training large language models to analyze documents and apply the NWM taxonomy, which would allow the KM repository to rapidly expand its contents and still ensure that documents would be readily findable for system users. Such a tool would be able to be used in the future, wherever the NWM taxonomy might be implemented, including future document control or records systems.

2.11 Evaluating Disposal Pathways for Advanced Reactors SNF

The commercial nuclear reactor industry is developing advanced reactor (AR) fuel cycles and advanced fuel (e.g., accident tolerant fuel; ATF) for the existing fuel cycle. Waste streams from ARs span a variety of potential spent fuels (AR SNF) and other waste types. Some of the potential AR SNF are similar to existing DOE-managed spent nuclear fuels (DSNF) from previous reactors (e.g., TRISO particle fuels and metallic fuels within the DSNF inventory) and some of which may be different (e.g., molten salt reactor spent fuels—note that the molten salt reactor experiment—MSRE—at ORNL has not yet been "defueled"). The purpose of the SFWST work regarding potential AR SNF, and potential other waste streams, is to identify gaps and outline areas where further storage, transportation, and disposal R&D would contribute to their well-defined disposition pathways (Matteo et al., 2023). The analysis of disposition pathways is rooted in characterization of potential waste forms and the existing BENFC experience that can inform approaches to disposition of AR SNF and other waste streams (see SNL, 2014; Swift & Sassani, 2020, and Sassani et al., 2022 for examples).

The focus of this effort currently is on the disposition of potential AR SNF and other waste streams. Small modular reactors (SMRs) and microreactors are an emerging subset of AR concepts that are being developed, but in general these have spent fuel very similar to most current LWR fuels with some minor differences (e.g., shorter in length) that do not appear to introduce conceptual differences in storage, transportation, and disposal considerations. One primary difference of a subset of microreactors is the potential/desired transport of SNF within one such reactor after it is operated but has not been defueled from the reactor itself (i.e., wholesale microreactor transport after operation). For other SMR generating SNF similar to those produced in larger AR (e.g., molten salt reactors), those SMR SNF would be covered by evaluations of the comparable AR SNF. However, there is no current precedent for wholesale storage/transport/disposal of small-modular-/micro-reactors, and such a conceptual gap is outside the current scope included in this report as it involves substantial operational changes.

2.11.1 Accomplishments and Discussion

The work on potential AR SNF and waste streams was started about the time the last version of this plan was written. In the years since the previous version of this DR R&D Plan, the work on potential new fuel cycles based on potential AR has progressed through collection and synthesis of existing information to formulate a high-level strategy for both (a) developing assessments of R&D gaps (for storage and transportation) and (b) evaluating FEP to constrain any future disposal R&D (Matteo et al., 2023-draft M2 report). In that milestone, the major objectives include:

Develop a high-level strategy via three primary objectives:

(1). *Survey the range of AR SNF and associated waste streams in order to classify the AR SNF and other waste streams into groups to be evaluated.* To the extent possible, this includes understanding implementation of AR concepts such that additional waste streams associated with the AR fuel cycle can also be taken into consideration.

(2). *Collate and evaluate the previous experience on existing analogous SNF and waste streams* to build a knowledge base for evaluating storage, transportation, and disposal issues/technical gaps related to the AR SNF and other potential waste streams.

(3). *Identify technical gaps related to storage, transportation, and disposal of AR SNF and other waste streams.* Evaluate AR fuels and Advanced Reactor Waste Streams (ARWS) against precedent experience in the knowledge base to produce a detailed gaps analysis (for S&T R&D), and analyses of features, events, and processes (FEP, for disposal R&D). Such gap and FEP analyses can be used to identify additional R&D activities in order to close the gaps.

Based on those objectives, the strategy development completed the following:

- A subset of commercial advanced reactor concepts has been reviewed and summarized.
- The AR SNF and potential other waste streams (ARWS) from these reactor designs have been reviewed and summarized.
- Previous BENFC experience and existing pathways for disposition (storage, transportation, and disposal) of similar SNF and wastes have been reviewed and summarized.
- Preliminary technical gaps between previous BENFC experience/precedents and ARF and ARWS have been identified and summarized.
- The strategy and approaches to the detailed gap analyses and FEP analyses have been developed.

In addition to the strategy development and technical review of existing/publicly available information and data on advanced reactors, the DOE (within DOE NE-8) has initiated an Integrated Project Team (IPT) for the *Back-End Management of Advanced Reactors* (BEMAR). As with the technical evaluations, this group is focusing on the TRISO and metallic fueled AR designs, but including molten salt reactors and other reactor designs as needed. The same SFWST staff performing the technical evaluations for storage, transportation, and disposal are serving on and providing the technical input to the BEMAR. However, the BEMAR is an internal DOE CUI process as it deals directly with developers/vendors and their proprietary data sets in conjunction with the DOE General Counsel.

2.11.2 Summary Discussion of Major Changes to Priorities

This work was started in late FY21 (i.e., since the last version of this DR R&D 5-year plan) to cover the spent fuel and other waste streams potentially to be generated from advanced reactors in possible future nuclear fuel cycles. As such, there are no changes in priorities as those below are the first occurrence of prioritization in this plan.

2.11.3 Planned Thrust Topics and Summaries

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

a) Develop FEP analyses for DR for AR SNF and waste streams (in conjunction with developing detailed Gap analyses for Storage & Transportation R&D)

b) *Identify further R&D in disposal areas (and in storage & transportation R&D) for execution within SFWST on potential AR SNF and other waste streams*

c) *Continued Technical Support/Input to the DOE BEMAR IPT*

d) *Focus development of capabilities in Inventory and Waste Form Performance and in the GDSA areas to use for future R&D*

These thrust areas are essentially the triage R&D for addressing an AR design space that encompasses well over a hundred different designs, whereas any potential future fuel cycle will likely not utilize more than about three of them. For disposal purposes, assessing the various generic disposal concepts against an end-member repository inventory consisting of entirely one, two, or three types will entail a large degree of uncertainty in the results. Identifying the major potential performance issues with each AR SNF will be the first order of assessment with planning to close the gaps and identify barrier capabilities that would be needed to address additional performance needs in the generic system analyses. A number of the AR SNF are similar to DSNF and if generated in small quantities (~<3%) may be safely accommodated in an unsaturated-zone repository inventory (e.g., DOE, 2008), and potentially into other generic disposal concepts (SNL, 2014). However, for a future fuel cycle inventory in which an entire repository inventory is composed primarily (> ~50%) of one particular SNF type, two aspects of SNF performance in post-closure dominate the disposal considerations. For cost efficiency, SNF that is directly disposable is key because the cost of any treatment facility for the fuel cycle would be roughly the safe as the entire disposal cost. For post-closure safety, the SNF degradation rate will primarily determine the release rate for fission products that contribute to peak dose in most disposal environments (Swift & Sassani, 2020) and so waste form lifetimes should be substantial for the primary SNF inventory.

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

a) *Prioritize Disposal R&D for the three most likely AR designs identified for a potential fuel cycle*

b) *Provide R&D results that have more resolution on BENFC aspects of the three most likely future fuel cycle AR SNF and waste streams*

c) *Continued Technical Support/Input to the DOE BEMAR IPT*

In order to provide substantive assessment of the BENFC aspects for any specific AR fuel cycle, the definition of the likely AR to populate that fuel cycle is essential (see discussions in NAS, 2022). The initial assessments/analyses above will cover potential technical issues/gaps at a fairly coarse level of resolution because of both (a) needing to generalize across multiple somewhat different designs that may have some very specific difference in the SNF and waste streams that may be produced and (b) lumping the issues/gaps with three categories of effort expected to address that equate roughly to (a) easy-to-none, (b) moderate, and (c) challenging. Though the initial effort categorization may prove accurate enough for initial assessments, there will likely be areas where more effort could be applied to show that some potential issue for disposal may not holdup given some unknown specifics about the SNF and waste streams (all the developers information on these specifics tends to be proprietary information). Further degrees of effort to achieve higher resolution would likely only be rational to apply to the AR designs most likely to fill a potential future fuel cycle.

3 SUMMARY OF SFWST DR R&D HIGH-LEVEL TECHNICAL FOCUS AREAS FOR 5 -YEAR PLANNING

The previous Used Fuel Disposition (UFD; from FY2011-FY2017) Campaign and the current SFWST Campaign (FY2017 to present) Disposal R&D programs have focused on the evaluation of the viability of mined repositories in three generic geologic media (salt, clay/argillite, and crystalline rock; e.g., Sevougian et al., 2019), and, in addition to these mined repository disposal concepts, the evaluation of very deep boreholes in generic crystalline basement rock (Arnold et al., 2012; SNL, 2014; NWTRB, 2016; Freeze et al., 2019)[c]. The host lithologies were selected because they have been considered and analyzed as potential repository host rocks both in the U.S. and internationally for several decades (e.g., Faybishenko et al., 2016). The generic host rock types were identified at a broad level: salt includes both bedded and domal salt; clay was defined to include a broad range of fine-grained sedimentary rock types including shales, argillites, claystones, as well as soft clays; and crystalline rock may include a range of lithologies such as metamorphic gneisses, granite, and other igneous rock types. Recently, generic unsaturated system mined repository concepts are also being analyzed, especially regarding their capabilities to effectively release heat via ventilation in open emplacement tunnels. Lastly, in FY2023, the SFWST program initiated the reinstatement of the deep borehole disposal concept for consideration of disposal of specialized waste forms and this is being implemented in the GDSA TA.

The above range of generic disposal systems evaluated thus far is not intended to represent a complete and comprehensive list of possible alternatives, and other options may also have the potential to provide safe long-term isolation. However, DOE and UFD/SFWST managers believe that R&D related to the evaluation of the selected generic media would likely be applicable to nearly any future program that relied on deep geologic disposal. The fundamental disposal R&D on these various generic geologic host rock systems will continue to be the cornerstone of the SFWST Disposal R&D program to support geologic repository disposal solutions in the U.S.

As has been the case throughout the SFWST Campaign DR R&D program, there exists a continual need to have active integration among the process-level generic geologic systems studies and the performance assessment modeling (i.e., GDSA modeling). For example, studies of direct disposal of DPC actively integrate the existing stored spent fuel as packaged with disposal studies where models of the engineered barriers and natural system are actively being modified to address conditions based on the DPC characteristics. Within the SFWST Campaign there are programs of R&D addressing topics on S&T of SNF (e.g., Teague et al., 2019), in addition to DR. Further integration between DR R&D and relevant S&T R&D would provide better defined waste inventory characteristics/initial conditions for disposal. This would also enhance consistency of process interfaces such as SNF and cladding characteristics for disposal with direct ties to expected physical conditions after storage, and the degradation processes for post-closure behavior. The development of the conceptual model for cladding degradation is an example of direct involvement of the S&T R&D lead staff with post-closure geoscience staff. Another area for enhanced integration is the expected evolution of DPC (potentially the largest inventory for disposal) physical conditions in extended dry storage and their relevant life-cycle parameters (e.g., thermal, dose). This would facilitate preparing for eventual disposal and defining approaches for potential treatment/overpack needs for DPC direct disposal.

In addition to this internal SFWST Campaign integration, potential new technology (e.g., ATFs; probable advanced nuclear fuel cycle reactor fuels) may generate additional/new waste forms. Work on the high-

[c] DOE Campaign R&D for this concept was discontinued in 2017 and reinitiated in FY2023.

level strategy for assessing BENFC issues/gaps for new waste streams has just been initiated in the SFWST Campaign covering both DR and S&T approaches. Addressing potential new challenges in these areas would be facilitated by coordination with relevant efforts in other external waste management areas such as more active integration with the BENFC management processes within the IWM Campaign. Even beyond the direct NE-8 mission, potential changes to inventory and waste form processes within both DOE NE and DOE Environmental Management (EM) could further focus the growing need for robust R&D in the deep geologic disposal of radioactive wastes. Beyond the core efforts to evaluate generic geologic systems for disposal behavior and constrain their key generic natural barrier capabilities with systematic integration of process-level understanding with system evolution of natural and engineered barriers, the SFWST Campaign DR R&D activities will maintain a further focus in the next five years on the following four areas: GDSA Capabilities Development and Demonstration; International Collaboration and URLs; EBS Representations; and Evaluation of Potential Direct Disposal of DPCs.

A. GDSA Capabilities Development and Demonstration

This cross-cutting issue was covered well with the previous DR R&D that defined a number of reference cases for generic geologic disposal systems, and this overarching activity for developing and demonstrating safety assessments of such systems will remain central to repository science. The continued development and improvement of a world-class safety assessment capability relies on a seamless integration of complex process-level models for the generic geologic disposal systems and the EBS. Within this focus area, efforts include: (1) advanced simulation capability; (2) state-of-the-art uncertainty and sensitivity analysis methods; (3) traceable, user-friendly workflow; (4) repository systems analysis, including simulation of generic reference case repositories in argillite, crystalline, salt, and unsaturated host rocks; and (5) development of geologic models, including generic archetypes for different host rocks and an interactive web-based application for visualization of regional geology in the U.S.

B. International Collaboration and Underground Research Laboratories

The Campaign's continued participation within the international R&D community, especially with continued participation at a number of URLs in a range of geologic systems is an essential aspect of the core effort to evaluate multiple generic concepts for deep geologic disposal systems. This allows SFWST DR R&D investigators to not only contribute world-class analyses, models, and data for both process-level science and system risk modeling and performance assessment, but also provides collaborative access to world-leading URL investigations in the field and peer review by the international scientific community. Such direct studies provide enhanced leveraging of diverse knowledge, models, process understanding, and data sets and facilitate development of robust technical bases within the DR R&D program for multiple generic geologic disposal concepts. Goals in this focus area include providing more highly integrated capabilities for analyzing generic repository systems in argillite, crystalline, and salt host rocks, with integrated EBS treatments and GDSA demonstration capabilities.

C. Engineered Barrier System Representations

This focus area touches on each generic geologic system because there are a number of engineered barriers (e.g., the waste form including cladding, the waste package, canisters, and backfill) that are common to a number of disposal concepts. EBS research thrusts are aimed at assessing the feasibility, applicability, evolution, and performance of EBS concepts in a given generic geologic medium and given a particular waste inventory. R&D activities focus on understanding EBS components evolutions and interactions within the EBS, as well as interactions between the host media and the EBS. A primary goal is to advance the development of process models that can be implemented directly within the GDSA platform or that can contribute to the safety case such as building confidence, providing further insight into the processes being modeled, and/or establishing better constraints on barrier performance, etc.

D. Evaluation of Potential Direct Disposal of DPCs

This focus area is driven by the recent effort to evaluate the feasibility of directly disposing of the SNF in dry storage in DPC. Direct disposal of DPCs has the potential for significant cost savings and, lower worker health and safety doses as compared to repackaging the SNF for disposal. Current research addresses post-closure criticality control, because modern DPCs depend on aluminum-based materials for neutron absorption during S&T, and those materials will degrade in a few decades when exposed to groundwater in a repository. Specific research focus areas for post-closure criticality control include: (1) direct disposal without modification (as-loaded reactivity margin analysis, post-closure criticality consequence analysis); (2) modification of already-loaded DPCs (with injectable filler materials for criticality control); and (3) modification of DPCs to be loaded in the future, or the fuel they contain (adding disposal criticality control features, optimizing loading maps). Implementation of models for direct disposal of DPC in generic repository systems remains a focus of this area to inform future policy decisions regarding storage and disposal of such SNF canisters.

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4 SUMMARY AND CONCLUSIONS

In the planning for FY2020 in the U.S. DOE NE-81 SFWST Campaign, the DOE requested development of a plan for activities in the Disposal Research (DR) Research and Development (R&D) over a five (5)-year period, and DOE requested periodic updates to this plan. The DR R&D 5-year plan was provided to the DOE based on the FY2020 priorities and program structure (initial 2020 version of this 5-year plan) and represents a strategic guide to the work within the DR R&D TAs (i.e., the Control Accounts), focusing on the highest priority technical thrusts. This FY2023 report is the first update to the DR R&D 5-year plan for the SFWST Campaign DR R&D activities. This 5-year plan will be a living document and is planned to be updated periodically to provide review of accomplishments and for prioritization changes based on aspects including mission progress, external technical work, and changes in SFWST Campaign objectives and/or funding levels (i.e., Program Direction). The updates to this 5-year plan will address the DR R&D that has been completed (accomplishments) and the additional knowledge gaps to be investigated, with any updates to the DR R&D priorities for the next stages of activities.

This document is structured with three main sections. Section 1 contains the background on evaluation and prioritization of the SFWST DR R&D technical work with a review of both the original Roadmap Report (DOE, 2012) and the Reassessment of the Roadmap (Sevougian et al., 2019). In Section 2, the summary plan for R&D technical activities is provided for each of the SFWST DR R&D TAs (note these correspond to the work breakdown structure Control Accounts for the DR R&D program for DOE NE-81). For each DR R&D TA, the plan provides a summary of accomplishments since the previous plan update, a review of the changes in priority, and the planned major technical thrust topics slated for the next five years. The thrust topics are presented with discussions of the current/planned activities supporting those thrust topics. Those 5-year plans discuss the general schedules for the thrust topics of each DR R&D TA and provide the expected technical emphasis in two parts: the near term (i.e., the more certain 1- to 2-year timeframe) and the longer term (i.e., the less certain 3- to 5-year timeframe). The near-term emphasis can be viewed as a representation of the present DR R&D portfolio with modest modifications that reflect emerging priorities and funding levels. In contrast, the 3- to 5-year period represents a longer-term vision of where the SFWST Campaign DR R&D is heading provided there is no major change to the Program Direction. Section 3 provides an overview of high-level technical focus areas to cover the planned overarching priorities of the SFWST DR R&D work at a more strategic level for the next five years. Some of those focus areas continue from prior R&D, whereas others have just started, and others have subparts that are yet to be initiated. This plan fulfills the Milestone M2SF-21SN010304054 in DR Work Package (WP) SF-21SN01030405 (GDSA - Framework Development – SNL).

The previous UFD (from FY2011-FY2017) Campaign and the current SFWST Campaign (FY2017 to present) Disposal R&D programs have focused on the evaluation of the viability of mined repositories in three generic geologic media (salt, clay/argillite, and crystalline rock; e.g., Sevougian et al., 2019), and, in addition to these mined repository disposal concepts, the evaluation of very deep boreholes in generic crystalline basement rock (Arnold et al., 2012; SNL, 2014; NWTRB, 2016; Freeze et al., 2019)[d]. The host lithologies were selected because they have been considered and analyzed as potential repository host rocks both in the U.S. and internationally for several decades (e.g., Faybishenko et al., 2016). The generic host rock types were identified at a broad level: salt includes both bedded and domal salt; clay was defined to include a broad range of fine-grained sedimentary rock types including shales, argillites, claystones, as well as soft clays; and crystalline rock may include a range of lithologies such as

[d] DOE Campaign R&D for this concept was discontinued in 2017 and reinitiated in FY2023.

metamorphic gneisses, granite, and other igneous rock types. Recently, generic unsaturated system mined repository concepts are also being analyzed, especially regarding their capabilities to effectively release heat via ventilation in open emplacement tunnels. Lastly, in FY2023, the SFWST program initiated the reinstatement of the deep borehole disposal concept for consideration of disposal of specialized waste forms and this is being implemented in the GDSA Technical Area.

The above range of generic disposal systems evaluated thus far is not intended to represent a complete/comprehensive list of possible alternatives, and other options may also have the potential to provide safe long-term isolation. However, DOE and UFD/SFWST managers believe that R&D related to the evaluation of the selected generic media will be applicable to nearly any future program that relies on deep geologic disposal. The fundamental disposal R&D on these various generic geologic host rock systems will continue to be the cornerstone of the SFWST Disposal R&D program to support geologic repository disposal solutions in the U.S.

The detailed portion of this 5-year plan is given in Section 2 and provides an assessment for each of the DR R&D technical areas (TA) below. The eleven TA covered below are:

- Argillite Disposal R&D
- Crystalline Disposal R&D
- Salt Disposal R&D
- Engineered Barrier System (EBS) R&D
- Inventory and Waste Form Characteristics and Performance
- Geologic Disposal Safety Assessment
- International Collaboration Disposal Research
- Direct Disposal of Dual-Purpose Canisters
- Technical Support for Underground Research Laboratory Activities
- Knowledge Management
- Advanced Fuels and Advanced Reactor Waste Streams Strategies

In this assessment each DR R&D TA section includes an overview of the TA purpose and scope, accomplishments since the previous plan version, associated changes to priorities for the plan, and the 5-year plan for that TA. Each DR R&D TA 5-year plan includes sections that:

a. identify the primary thrust topics (these are the major technical priorities in each TA)
   i. for the near term (next 1- to 2-year period – i.e., our current DR R&D program)
   ii. for the longer term (3- to 5-year period – i.e., where the DR R&D may go in the future if Program Direction remains the same)
b. describe the activities in the TA that are addressing each of the thrust topics listed both for the program currently (i.e., near term), and how that may change going forward to the longer term. There is generally more detail available for the near-term thrust topics, with the longer-term thrust topics being discussed in comparison/contrast to the near-term thrusts.

In the next five years, the DR R&D will continue to focus on process model development within the generic geologic concepts, EBS, and waste forms/source terms, with the goal of prioritizing model implementation in GDSA Framework for different generic reference cases. At the end of the five years, it is anticipated that GDSA Framework and the reference cases will contain even more detailed representations of relevant improved process models and/or surrogate models. Such progress will facilitate more diverse demonstrations of safety assessments, sensitivity analyses, and more robust programmatic prioritization of targeted DR R&D activities.

This year (FY2023) we have initiated a couple of activities to get an early start on the next reevaluation of the SFWST Roadmap (referred to as the Roadmap Reimagination). Given the expanding progress on details of the technical bases for generic disposal systems, growing technical capabilities in repository science, cutting edge development of system assessment tools, and the abundance of accumulated SFWST data and process understanding, the Roadmap Reimagination will shift back to more explicit mapping/prioritization/status of the FEP for each of the generic repository concepts being considered. This entails developing a real-time, online accessible FEP list capability for all SFWST investigators (work package managers and their key technical investigators) to use to map their activities to the specific sub-FEP aspects (the bulleted listing for the generic FEP list at their most detailed level) that are being addressed. This should both (1) enhance integration because all users will be able to see all activities/investigators constraining specific FEP aspects and (2) provide ready assessment of "how complete" work is, and where gaps exist in the total program R&D. A prototype of this FEP tool began development this year, completed assessment, and is being modified for use. An additional focus moving forward will be to establish a Library of GDSA Reference Cases for the generic repository concepts including model definitions, documentation, and results of those demonstrations.

As an additional early start to our Roadmap Reimagination, our SFWST program is working to have a more explicit mapping of our technical points of contact to the EURAD-2 (a ~5-year European Commission collaborative program: https://www.ejp-eurad.eu/news/eurad-2-core-group-communication-may-2023) to execute a set of repository R&D work that will largely be selected for funding in the Fall of 2023 and intended to be started in Autumn 2024. Some of the organizers requested our SFWST campaign to map technical points of contact to the eventual funded projects based on our interest in the in-kind collaboration with the projects selected. Our DOE Technical Lead agreed that we would be interested in such organized collaboration and given our large international portfolio of work (see section below on International), we will provide a set of technical staff to be the primary U.S. contact to each funded project as there is interest in our collaboration. Our work in these International Programs provides an essential linkage to active site-specific investigations in multiple geologic systems around the world. This provides both active experience in URLs in field scale experimental/characterization investigations, as well as connection to disposal programs performing site-specific evaluations. These two aspects are essential expertise to maintain in the U.S. program and will be areas for growth moving into the next stage of a Disposal Program in the U.S.

Beyond the core efforts to evaluate generic geologic systems for disposal behavior and constrain their key generic natural barrier capabilities with systematic integration of process-level understanding with system evolution of natural and engineered barriers, the SFWST Campaign DR R&D activities will maintain a further focus in the next five years on the following four areas: GDSA Capabilities Development and Demonstration; International Collaboration and URLs; EBS Representations; and Evaluation of Potential Direct Disposal of DPCs. Additionally, the work on advanced reactors is expected to continue but the extent of it will be based on Program Direction in this area (i.e., DOE direction, budget appropriations, etc.).

As has been the case throughout the SFWST Campaign DR R&D program, there exists a continual need to have active integration among the process-level generic geologic systems studies and the performance assessment modeling (i.e., GDSA modeling). For example, studies of direct disposal of DPCs actively integrate the existing stored spent fuel as packaged with disposal studies where models of the engineered barriers and natural system are actively being modified to address conditions based on the DPCs characteristics. Within the SFWST Campaign there are programs of R&D addressing topics on S&T of SNF (e.g., Teague et al., 2019), in addition to DR. Further integration between DR R&D and relevant S&T R&D would provide better defined waste inventory characteristics/initial conditions for disposal. This would also enhance consistency of process interfaces such as SNF and cladding characteristics for disposal with direct ties to expected physical conditions after storage, and their degradation processes for post-closure behavior. The development of the conceptual model for cladding degradation is an example of direct involvement of the S&T R&D lead staff with post-closure DR geoscience staff. Another area for enhanced integration is the expected evolution of DPCs (potentially the largest inventory for disposal) physical conditions in extended dry storage and their relevant life-cycle parameters (e.g., thermal, dose). This would facilitate preparing for eventual disposal and defining approaches for potential treatment/overpack needs for DPC direct disposal.

In addition to this internal SFWST Campaign integration, potential new technology (e.g., ATFs; probable advanced nuclear fuel cycle reactor fuels) may generate additional/new waste forms. Work on the high-level strategy for assessing new waste streams has been initiated in the SFWST Campaign for both DR and S&T approaches. Addressing new challenges would be facilitated by coordination with relevant efforts in other external waste management areas such as more active integration with the BENFC management processes within the IWM Campaign. The IWM Campaign (DOE NE-82) provides a coherent interface with other DOE Offices (such as EM) that manage wastes that will ultimately be disposed in a deep geologic repository, and with external stakeholders including local government agencies and tribal nations. Even beyond the direct NE-8 mission, potential changes to inventory and waste form processes within both DOE NE and DOE EM could further focus the growing need for robust R&D in the deep geologic disposal of radioactive wastes. For example, within the DOE NE-4 R&D, development of new waste forms, ATFs, and advanced reactor fuel cycles with a variety of other fuel types and potentially treated waste streams (e.g., TRISO, metallic fueled reactors) also will become facets of future DR R&D.

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