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SFWST Disposal Research R&D 5-Year Plan – FY2021 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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APPENDIX E
NFCSC DOCUMENT COVER SHEET[1]

Name/Title of Deliverable/Milestone/Revision No.	SFWST Disposal Research R&D 5-Year Plan – FY2021 Update/M2SF-21SN010304054/ Draft-Internal Use Only
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This deliverable was prepared in accordance with Sandia National Laboratories
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QA program which meets the requirements of

☒ DOE Order 414.1 ☐ NQA-1 ☐ Other

This Deliverable was subjected to:

☒ Technical Review

☐ Peer Review

Technical Review (TR)
Review Documentation Provided

☐ Signed TR Report or,
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☐ Signature of TR Reviewer(s) below

Peer Review (PR)
Review Documentation Provided

☐ Signed PR Report or,
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Name and Signature of Reviewers
Patrick V. Brady (SNL) [as indicated in PICS:NE Deliverable Form]

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.*

SUMMARY

In the planning for FY2020 in the U.S. DOE NE-81 Spent Fuel and Waste Science and Technology (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 (Sassani et al., 2020) and represents a strategic guide to the work within the DR R&D technical areas (i.e., the Control Accounts), focusing on the highest priority technical thrusts. This FY2021 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 technical areas (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 technical area, 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 technical area 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. This plan fulfills the Milestone M2SF-21SN010304054 in DR Work Package (WP) SF-21SN01030405 (GDSA - Framework Development – SNL).

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 generic geologic media (salt, clay, 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. Recently, generic unsaturated system mined repository concepts are also being analyzed, especially regarding their capabilities to effectively release heat via ventilation to open emplacement tunnels.

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

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

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 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, 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 Underground Research Laboratories; Engineered Barrier System Representations; and Evaluation of Potential Direct Disposal of Dual Purpose Canisters.

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: David Sevougian (retired), Peter Swift (retired), Kevin McMahon (retired), Robert MacKinnon (retired), Sylvia Saltzstein, and Paul Mariner for discussions 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) —Prasad Nair (DOE NE-81), Tim Gunter (DOE NE-81) and William Boyle (DOE NE-8)—for their discussions, oversight and guidance on the R&D outlined in this report.

This report was improved by a technical review from Pat Brady (SNL).

CONTENTS

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ACRONYMS

BATS	Brine Availability Test in Salt
BWR	Boiling Water Reactor
CI-D	Cement-Clay Interaction Test
DECOVALEX	DEvelopment of COupled models and their VALidation against EXperiments
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
GAST	Gas Permeable Seal Test
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
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
NE	(DOE) Nuclear Energy
NGW	Next Generation Workflow
N-TH	Neutronic-Thermal Hydraulic
NWTRB	Nuclear Waste Technical Review Board
OECD-NEA	Organisation for Economic Co-operation and Development - Nuclear Energy Agency
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
SET	Bore Sealing Test
SFWST	Spent Fuel and Waste Science and Technology
SKB	Swedish Nuclear Fuel and Waste Management Co
SNF	Spent Nuclear Fuel
SNL	Sandia National Laboratories
SW-A	Large-scale Sandwich Experiment
TA	Technical Area
TCMH	Thermal-Chemical-Mechanical-Hydrologic
TDB	Thermodynamic Database
THM	Thermal-Hydrologic-Mechanical
THMC	Thermal-Chemical-Mechanical-Hydrologic
UFD	Used Fuel Disposition
UFDC	Used Fuel Disposition Campaign
UK	United Kingdom
URL	Underground Research Laboratory(ies)
US	United States
UQ	Uncertainty Quantification
WIPP	Waste Isolation Pilot Plant
WP	Work Package

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 guide to the work within the DR R&D technical areas, focusing on the highest priority technical thrusts. This FY2021 report is the first update to the DR R&D 5-year plan for the SFWST Campaign DR R&D activities to provide review of accomplishments and discuss 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.

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1.1 Background

The Spent Fuel and Waste Science and Technology (SFWST) Campaign of the U.S. Department of Energy (DOE) Office of Nuclear Energy (NE), Office of Spent Fuel and Waste Disposition (SFWD) is conducting research and development (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 was succeeded by the SFWST Campaign) formulated an R&D Roadmap (DOE 2012) outlining generic R&D activities and their priorities appropriate for developing a sound technical basis 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 the R&D would be for a potential (i.e., future) safety case developed for a future site. That 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 these activities through R&D in the U.S. and via international collaborations, especially with countries that operate underground research laboratories (URLs). In 2019 an R&D Roadmap Update (Sevougian et al., 2019) was conducted to summarize the progress of ongoing generic disposal R&D activities relative to the Roadmap priorities, to identify gaps in the Campaign R&D, and to re-assesses R&D priorities and identify new activities of high priority, such as R&D on disposal of DPC (dual purpose canisters), which now contain a significant fraction of the Nation's commercial SNF activity.

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" (information needs and knowledge gaps) and the prioritization of these R&D issues based on evaluation metrics (primarily their importance to a future post-closure safety case and the state of knowledge regarding the issue). Each identified R&D issue was derived from (actually, equated to) a FEP (Feature, Event, or Process) from the generic list of 208 FEPs 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 FEPs, because each FEP may have a different importance to a potential safety case 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 and a series of groupings of natural barrier system issues and engineered barrier system issues that were helpful for defining the future R&D program.

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 with the 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). A full re-assessment of R&D priorities was initiated during fiscal year 2018. Sassani (2018) provided a high-level assessment of how well the R&D Campaign had addressed the cross-cutting issues priorities that the Roadmap summarized to drive the planning of the UFD/SFWST Campaign R&D activities at the SFWD Annual Meeting. 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. 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). Those topical areas generally rely on more specific environmental conditions, so it was not surprising to see developmental lag in the generic R&D program for those.

1.2 Roadmap Reassessment Purpose and Results

The full re-assessment workshop results and analyses in Sevougian et al. (2019; Roadmap Reassessment) 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 dual-purpose canisters 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 FEPs 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 FEPs
5) Identify important FEPs 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 FEPs. 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 systems 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 engineered barrier system, rewetting/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 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 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 (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 five-year planning period. Some of these focus areas are the same as defined as in the UFDC Roadmap (DOE 2012), for example the geologic disposal system assessment (GDSA) capabilities development and demonstration, which underpins quantitative analysis of the post-closure safety of generic repository systems. Other focus areas are derived 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.

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 Underground Research Laboratories; Engineered Barrier System Representations; and Evaluation of Potential Direct Disposal of Dual Purpose Canisters. 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.

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

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

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

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:

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.

The ten technical areas addressed below cover virtually all the technical work being done within the SFWST Campaign DR R&D program. However, in a few cases, some technical R&D work has been executed within the management and integration area for the SFWST Campaign, either as single events requested by Program Direction, or as multi-year projects that span the entire technical arena. One very good example of this latter type is the development of the *Knowledge Management* repository (see Section 2.10) that started as a mechanism to capture tacit knowledge of senior experts within the program of Disposal Research, including those involved with licensing/certification processes from previous repository programs. This work is ongoing, is becoming more desired across the SFWST Campaign (as well as in other technical venues), and will likely grow further in the coming years, especially to expand to the S&T R&D program. In the sections below for the DR R&D TA, more detailed plans for some TA reflect those TA 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 to this 5-year plan will address the DR R&D work that has been completed (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 technical areas, a review of the 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 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. (Note that the DR R&D TA covered here correspond to the Control Accounts within the work breakdown structure in the DOE PICS:NE management system, which contains details of the planned R&D activities.)

2.1 Argillite Disposal R&D

Integration across disposal R&D activities is important for 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 THMC process models, international collaborations relevant to repository science R&D (e.g., HotBENT, DECOVALEX-2023), experimental interaction studies on engineered barrier materials plus host-rock (argillite) including solute transport, molecular dynamic (MD) simulations and thermal studies of water transport during (swelling) clay dehydration, 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 PA and evaluating of groundwater chemistries in shale formations.

2.1.1 Accomplishments and Discussion

In the ~one year 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.
- Initiated work related to investigating the effect of shale-creep on the long-term performance of an argillite repository. This includes identification of an appropriate shale creep model with available data plus its implementation in a THM coupled process model platform and applications of machine learning (ML) on meshing optimization of fracture media.
- Reactive transport modeling of barrier material leaching data using PFLOTRAN. This modeling effort permits the evaluation of chemical and transport parameters for interaction occurring at material interfaces.
- Active involvement in DECOVALEX-2023 and other international collaboration activities, many of which crosscut key aspects of process model development and validation. This also includes initiating analyses of material resulting from the HotBENT column experiment at LBNL.
- 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.

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

These two near-term thrust topics are interrelated and though they are the current focus areas, it is expected that 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. Other work includes support of in-package chemistry model development that incorporates first principles atomic (density functional theory – DFT) simulation work on U-bearing solids for retrieval of thermodynamic data at elevated temperatures.

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 outputs for the complex argillite process models.

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

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

These two longer-term thrust topics are complimentary as the collaborative work provides constraints to evaluate, enhance, and validate our process-level understanding in this area. Partnerships with current international programs will be nurtured and expanded in the coming years to create a collaboration bridge gaining advanced knowledge of nuclear waste disposal research from URL activities worldwide. 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 experiments at Mont Terri. Participation in the OECD-NEA thermodynamic database (TDB) project, particularly in the review of the ancillary thermodynamic data volume, is planned to take place as soon as within the next two years. 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 geologic disposal safety assessment (GDSA) team to develop a robust generic crystalline repository performance assessment model.
- Provide the GDSA with the essential "minimal" set of process models and model inputs to support the GDSA goals.
- Evaluating 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 Technical Areas, especially those on disposal in argillite and engineered barrier system 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 of most import to repository performance. Buffer erosion is a good example of an instance in which a new mechanistic representation can be developed, building on work that has already been done in Europe. Hydrologic properties of the EDZ represent another opportunity for improved representation. Overall, due to the fractured nature of the disposal media, modeling a repository in crystalline rocks may involve more issues with high reliance on the engineered barrier system performance than other generic host-rock types. Thus, the thrust area will focus on: (1) better characterization and understanding of fractured media and fluid flow/transport therein; and (2) designing effective engineered barrier systems (EBS) for waste isolation.

2.2.1 Accomplishments and Discussion

Since the implementation of this 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.

- *Discrete Fracture Network 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 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.
- *Rock testing capability development:* A high pressure (up to 10,000 psi), high temperature (up to 200˚C) triaxial loading system has been developed to enable long-term (days to months) laboratory experiments of flow simultaneously on multiple core samples under thermal, mechanical, and chemically controlled conditions. The system has been tested for the permeability measurements of granite samples obtained from the Grimsel Underground Research Laboratory.
- *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 x 300 m x 200 m- site scale) with that of a much larger domain (1386 m x 1486 m x 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 10 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 Underground Research Laboratory in Japan.
- *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 completely eliminated in the case of lead.

- *Enhancement of bentonite thermal conductivity:* The low thermal conductivity of bentonite (~ 0.5 W/mK) 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 to form fully connected high heat conduction pathways. 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 dual-purpose canister (DPC) can be reduced, perhaps significantly reducing the 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 Technical Area, 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
- Decreased priority is given to
  - Flow and transport in fractures, including matrix diffusion

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

- Major part of the discrete fracture network 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*

The two 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 discrete fracture networks in high performance-computing 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.

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

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

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.

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 technical area 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 may affect waste package corrosion; 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 features, events, and processes, 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 technical area are 1) measuring the effect of heat-generating waste on brine availability and salt deformation (Brine Availability Test in Salt); 2) evolution of engineered barriers in salt; and 3) development of coupled process models and constitutive relationships. Activities are coordinated with the EBS, GDSA, and International technical areas, and address high priority topical areas identified in the 2019 Disposal Research R&D Roadmap Reassessment, including high-temperature processes (i.e., temperature-dependent constitutive models), coupled process models in salt, and evolution of cement seals.

2.3.1 Accomplishments and Discussion

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

- *Effect of heat-generating waste*
  - To investigate the effects of heat-generating waste, the Brine Availability Test in Salt (BATS) measures the effects of coupled physical and chemical processes associated with emplacement of a heated borehole in a salt host rock in WIPP, the nation's only currently active underground research laboratory (URL) associated with nuclear waste disposal. BATS comprises a series of observation/measurement boreholes (centered around the heated borehole) that contain equipment for water-vapor sample collection and brine sample collection. Surrounding these are smaller-diameter satellite boreholes instrumented to measure temperature, electrical resistivity, distributed strain, and acoustic emissions. An identical control borehole array that is not heated is adjacent to the heated array. The first phase of BATS heating occurred during January to March 2020 with continuous data collection. Currently, additional series of heating and cooling with the addition of gas and liquid tracers are underway. The data acquired to this point has 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. 2021a).
- *Model development*
  - Progress on model development benefits from the unique and extensive dataset collected at BATS, which enhances the US' leadership in salt repository science. The Salt team is leading a four-year international collaborative task for DECOVALEX2023, in which participants are developing models of the coupled thermal-hydro-mechanical (THM) processes associated with emplacement of heat-generating waste in salt. In the first year of the task, modeling teams from four countries (US, Germany, UK & Netherlands) have completed a series of increasingly complex model benchmarks for comparison across programs. In the recently started next stage, the teams will validate their models against data collected at the BATS.
  - The US 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. 2021b; Czaikowski et al. 2020).

The BATS is providing both a wealth of data for process understanding, as well as 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 technical area are 1) measuring the effect of heat-generating waste on brine availability and salt deformation (Brine Availability Test in Salt); 2) evolution of engineered barriers in salt; and 3) development of coupled process models and constitutive relationships. Activities are coordinated with the EBS, GDSA, and International technical areas, and address high priority topical areas identified in the 2019 Disposal Research R&D Roadmap Reassessment, including high-temperature processes (i.e., temperature-dependent constitutive models), coupled process models in salt, and evolution of cement seals.

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

a) *Effect of heat-generating waste*

- Phase 1 of BATS will wrap-up with a sequence of heating and cooling cycles to investigate possible hysteretic (or irreversible) effects of heating on the response of the salt. Destructive post-test sampling will allow characterization of the heated salt and provide data pertaining to salt/brine/cement interactions (see below).
- Phase 2 of BATS, scheduled to begin in Fall 2021, will comprise a newly drilled array of boreholes and an improved experimental design. Phase 2 will investigate brine availability in an argillaceous unit at an elevation just below that of the clean halite in which the BATS Phase 1 heated array is located. The argillaceous unit is expected to provide a larger source of brine due to the presence of hydrated clay minerals.

b) *Evolution of engineered barriers in salt*

- Studies of the evolution of engineered barriers in salt repositories include two primary areas of investigation: cement seals and granular salt backfill (see Model Development). Both are the focus of international collaborations, and cement seal evolution is a component of BATS.
- Data pertaining to mechanical and chemical salt/brine/cement interactions will be collected at the end of BATS Phase 1 via overcoring of the test boreholes. A larger-diameter borehole adjacent to the heated borehole array includes a Sorel and salt cement plugging/sealing test. Strain gauges, thermistors, and relative humidity gauges are being used to monitor the cement seals during heating. A German collaborator (GRS) is conducting complementary poromechanical tests on similar cement, brine, and WIPP salt cores.

c) *Model development*

- In the second year of the four-year task for DECOVALEX2023, participants will develop models of the coupled thermal-hydro-mechanical processes associated with emplacement of heat-generating waste in salt and validate their models against data collected in Phase 1 of BATS.
- US-Germany joint projects will continue to work toward: 1) improving thermal-hydro-mechanical models for granular salt consolidation through model validation, consolidation experiments, and analysis of microstructural features; 2) improving constitutive models for salt deformation, including creep behavior at low stress, dependence of healing on temperature, and influence of inhomogeneities such as clay seams; and 3) designing geotechnical seals for drifts and shafts in a salt repository (Kuhlman et al. 2021b).

d) *Confidence Building*

- The DR R&D Salt team has a leadership role in the Nuclear Energy Agency's Salt Club. Following the publication of a comprehensive FEPs catalogue in collaboration with Germany (see GDSA Section), Salt team members are leading a Salt Club effort focused on scenario development for generic salt disposal concepts.

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

Many of the activities in the Salt technical area have multi-year plans. At BATS, a long-term heater test (months to years) is proposed to begin after completion of BATS Phase 2. A long-term test would determine the stability of brine production over time and may allow observation of heat-accelerated salt creep. Additionally, facility improvements at BATS are proposed to facilitate additional investigations such as gas permeability testing, large-scale strain monitoring, or experiments to understand waste package buoyancy effects (Kuhlman et al. 2021a). BATS data interpretation and model development and validation will continue through 2023 under the DECOVALEX project. In the next 3 to 5 years, process models and constitutive relationships developed in this project and in the US/German joint projects will be integrated into GDSA Framework for use in demonstrations of generic safety assessments and other repository systems analyses. The Salt Club scenario development effort is likely to provide evolutionary scenarios that drive generic reference case development and development of simulation capability for generic safety assessments.

2.4 Geologic Disposal Safety Assessment

The objective of the Geologic Disposal Safety Assessment (GDSA) technical area 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 US 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 technical area is the nexus for integration of concepts, models, and understanding developed in other SFWST disposal research technical areas. 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 US DOE's high-performance computing (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 technical area 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 US.

2.4.1 Accomplishments and Discussion

In the ~one year 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. Implementation of advanced linear and nonlinear solvers and options for smoothing capillary pressure variations at very low saturation improved PFLOTRAN's performance on simulations of temperature-driven desaturation and resaturation (Nole et al. 2021). Integration with the DPC, salt disposal, and international technical areas drove development of simulation capability, including a waste package criticality model, temperature-dependent thermal conductivity, bentonite and DRZ evolution models, and fracture-matrix diffusion (Nole et al. 2021). Recently developed neural network surrogate models for fuel matrix dissolution may reduce conservatism compared to a simple fractional rate law model while reducing computation time by a factor of 1000 compared to the mechanistic model used to train the surrogate (Mariner et al., 2020a).
    - Software requirements for a biosphere model were developed (Condon et al. 2020). The open-source biosphere model, which is in early stages of development, will incorporate multiple exposure pathways consistent with the NEA FEPs list and a flexible, modular architecture consistent with recommendations from the IAEA.
- *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 multifidelity uncertainty and sensitivity methods to increase efficiency that advanced the crystalline reference case with improved representation of fracture networks (Swiler et al. 2021a). GDSA led an international team in documenting a 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).
- *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. 2020b). The workflow incorporates significant post-processing capabilities that automate sensitivity analysis and was demonstrated on the crystalline reference case (Swiler et al. 2021a).

- *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 GDSA team published a review of disposal concepts for a high-temperature repository in shale (Stein et al. 2020); improved simulation capability for high-temperature unsaturated systems (Nole et al. 2021); and supported the DPC technical area by simulating the consequences of criticality in repository performance analyses (Price, 2021).
    - International collaborations focus on crystalline and salt generic repository concepts, including engineered barriers. The GDSA team is leading a 4-year task for DECOVALEX2023 in which performance assessment (PA) simulation and analysis methods applied to generic crystalline and salt reference cases will be compared (LaForce et al. 2020). Ten teams from 7 countries are collaboratively developing appropriate reference case scenarios and participating in benchmarking exercises. A US/German joint project finalized a report that documents FEPs in salt repositories (Freeze et al. 2020); and a broader coalition of countries initiated a collaborative effort to establish best practices for development of scenarios for evolution of salt repositories.

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.

2.4.2 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.

2.4.3 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 identified in the 2019 Disposal Research R&D Roadmap Reassessment while building on previous accomplishments. These efforts will include continuing to advance high-temperature simulation capability, implementing material-specific waste package degradation models, and addressing the coupled thermo-hydro-mechanical (THM) processes affecting buffer evolution, and the coupled thermo-hydro-chemical (THC) processes affecting radionuclide transport. 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.
- 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 discrete fracture networks 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.

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, multifidelity 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 on 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.
- Integration of GDSA Framework with the Online Waste Library will be initiated. This integration will provide quality-assured radionuclide inventories for simulations involving defense-related waste streams.

d) *Repository systems analysis*

- In the next 1 to 2 years, a main priority will be simulation and analysis of the salt and crystalline reference cases developed for the DECOVALEX2023 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 continue to integrate with other technical areas to advance analyses of direct disposal of DPCs, understanding of high-temperature FEPs, and scenario development methodology.

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 US. In the next 1 to 2 years, 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)

The research thrusts in the GDSA technical area are generally on-going efforts. In future years, capability development will continue to address high-priority topical areas and integrate new process understanding acquired in other SFWST technical areas. Model development and implementation may include multi-fidelity approaches to simulation of coupled processes in salt, in-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 designs, concepts, and models developed in other technical areas. The DECOVALEX PA comparison will progress from reference case development and simulation to uncertainty propagation and sensitivity analysis. In general, simulation capability will move toward a more sophisticated representation of a larger set of features, events, and processes affecting repository performance; 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 technical area 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, and to test technical approaches to data collection and interpretation.

2.5 Direct Disposal of Dual-Purpose Canisters

Commercial SNF is accumulating in dry storage at over 70 sites across the US in dual-purpose canisters (DPCs), which are designed for storage and transportation, 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 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 control (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-couple processes in argillite, crystalline, salt, EBS, and GDSA technical areas. Current research addresses post-closure criticality control, because modern DPCs depend on aluminum-based materials for neutron absorption during storage and transportation, and those materials will degrade in a few decades when exposed to groundwater in a repository.

Specific research focus areas (see Figure 1) 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 DPC in generic repository systems remains a focus of this area to inform future policy decisions regarding storage and disposal of such SNF canisters.

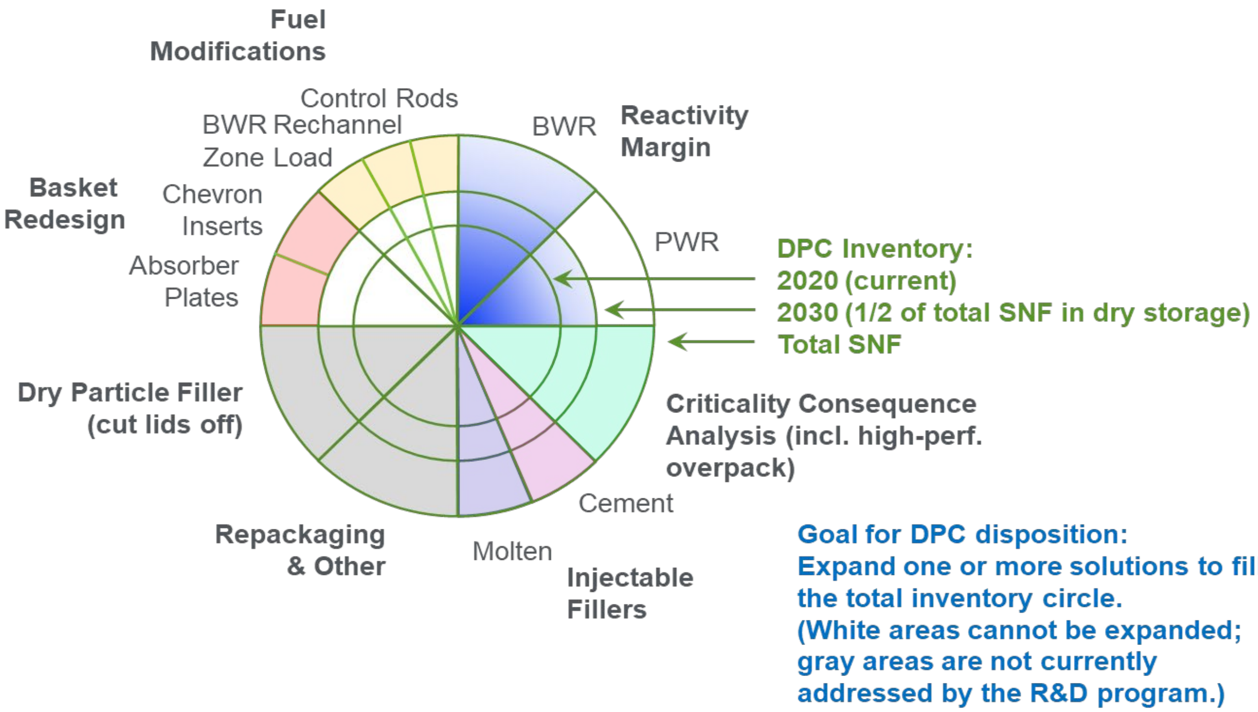

Figure 1. Overview of options to facilitate evaluation of feasibility of direct disposal of DPC. The pie slices represent research sub-topics within the four larger target quadrants of (clockwise from top left) changes to basket design, constraining reactivity margin, use of injectable fillers, and use of other methods involving opening the top of the DPC. The circumferential (i.e., circular) zones represent the DPC inventory that may be affected by the different methods. For example, the innermost ring reflects the current (2020) DPC inventory that cannot have their baskets redesigned (the upper left quadrant regions of this zone are shown as white).

2.5.1 Accomplishments and Discussion

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

- *Probabilistic Post-Closure DPC Criticality Consequence Analyses* – Developed preliminary generic system models for potential criticality events in an unsaturated repository in alluvium and in a saturated repository in shale (Price, 2021). These models have been implemented in the GDSA Framework. Preliminary modeling has included coupled thermal, hydrologic, and criticality processes in the repository and near-field to estimate the potential source term from a criticality event and investigate conditions that could lead to the permanent termination of a criticality event.
- *DPC Disposal Thermal Scoping Analysis* – Developed thermal modeling approaches to refine prior calculations of the near-field temperatures at or near DPC-based waste packages in a range of geologic media (Jones et al. 2021). The principal finding from this study is that the near-field temperatures at or near as-loaded DPC-based waste packages are much lower than previous conservative studies have suggested. This is because the present study exclusively uses thermal output projections for as-loaded DPCs, whereas previous studies have used bounding assumptions such that all waste packages contain high-burnup fuel.
- *DPC Injectable Filler Testing and Analysis* – Prepared a multi-year workplan for 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 phosphate cements as a promising filler material.

- *As-Loaded DPC Reactivity Margin Modeling* – Completed a preliminary 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 (Clarity et al. 2021). The investigations examined reloading the assemblies in the canisters at the Zion site using the individual assembly reactivity and an initial development of an artificial neural network (ANN) based approach for rapid estimation of canister reactivity that can be used for optimum loadings search. These approaches will allow criticality analysis to be incorporated in the decision-making process that will be used for canister loading.
- *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 and Jones 2021).

The above Accomplishments show progress in the near-term Thrust Topics. The criticality consequence analyses and thermal scoping analysis provide promise that some existing 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 safe long-term disposal of existing and future DPCs.

2.5.2 Summary Discussion of Major Changes to Priorities

Given the accomplishments in this Technical Area, there are no major changes in priorities. Progress was made towards some near-term Thrust Topics but outstanding R&D remains in all areas. The one accomplishment that may impact future thrusts is the DPC disposal thermal scoping analysis that showed lower near-field temperatures from existing as-loaded DPCs. This finding has the potential to reduce cooling/aging times for some DPCs and/or reduce the likelihood of degradation of certain near-field materials (e.g., bentonite backfill).

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

2.5.3 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 evaluate the consequences of potential criticality events on overall repository performance to determine if the consequences are acceptably low, which assumes a viable method for determining consequences. Consequence screening is a new approach, not fully constrained in an US or international repository R&D program 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.

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

Generic models to represent repository performance with criticality events have been developed for an unsaturated repository in alluvium and in a saturated repository in shale. A preliminary implementation of these models in a performance assessment (PA) model in the GDSA Framework has been initiated for high-level thermal, hydrologic, and criticality processes. Additional processes to be implemented include fuel, basket and waste package degradation (e.g., cladding unzipping, UO_2 alteration/dissolution, basket corrosion and collapse, and canister/overpack breach evolution), interaction (heat, mass) with the near-field, and N-TH coupling.

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

(D-01) Probabilistic post-closure DPC criticality consequence analyses

(D-04) Coupled multi-physics simulation of DPC post-closure (chemical, mechanical, thermal-hydraulic) including processes external to the waste package

(D-05) Source term development with and without criticality

b) As-Loaded DPC Reactivity Margin Modeling

Recent 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) have shown that some of these DPCs have sufficiently low k_{eff} for direct disposal even in degraded condition, because of the basket design and the as-loaded fuel characteristics. The focus of this thrust area is to continue these types of as-loaded analyses to identify existing DPCs that are amenable to direct disposal (i.e., have zero/low probability of criticality in any disposal environment). This includes compilation of fuel characteristics (type, burnup profiles, etc.) and canister data (basket design, fuel loading schema, etc.) for all DPCs and analysis (and re-analysis) of reactivity for stylized degradation cases, and for disposal environments (e.g., natural groundwaters, chloride brines).

Canisters loaded today (and in the future) have less reactivity margin, caused by larger capacity and more compact basket design, with more advanced burnup credit analysis. Therefore, these analyses will focus on older DPCs, particularly ones loaded more than 10 years ago as they are more likely to have zero/low probability of criticality in any disposal environment. A preliminary 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 was completed for the Zion site. Additional investigations at other sites with older DPCs will add to the knowledge base.

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, and displace or exclude ground water from breached waste packages in a repository, and preserve neutron absorbing materials to prevent criticality over the long-term. Fillers must have desirable behavior in injectability, radiolysis, material interactions, leachability, and have long-term durability in the disposal environment. If successful, this approach could be used to treat all DPCs including those loaded without modifications. Several potentially effective filler materials are being considered including aqueous cement slurries, and molten metals, alloys, and low-temperature glasses.

The near-term investigations include initial mixing and handling of candidate filler materials, and demonstration of filler injection into small-scale representations of DPC fuel/basket geometries. Experimental work identified phosphate cements as a promising filler material.

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

(D-03) DPC filler and neutron absorber degradation testing and analysis *d) Future DPC (Fuel/Basket) Modifications*

The near-term focus of this thrust area is to identify potential modifications to future DPCs so they will remain subcritical in any repository setting. These include: a) loading schema with the possibility to blend fuel assemblies from fuel pools based on reactivity (PWR and BWR fuel); b) disposal control rods (PWR fuel); c) disposal control rods or rechanneling (BWR fuel); and d) replacement absorber plates (some, but not all BWR fuel baskets). DPC modification could be combined with other options, to treat different sets of DPCs and limit the overall probability of a criticality event.

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) 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.

c) Future DPC (Fuel/Basket) Modifications

The longer-term focus of this thrust area is to further develop the most promising potential DPC fuel/basket modifications. This could include fabrications and/or demonstrations. An important consideration at this stage is the potential for DPC modifications to actually be implemented by vendors and/or utilities.

2.6 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 in regards to alternative repository environments developed across the world, (2) utilizing international research facilities (such as underground research laboratory 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, FEBEX-DP) 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 technical areas 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 and Faybishenko, 2020).

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 underground research laboratories in host rock environments not currently available in the U.S. Figure 2 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.

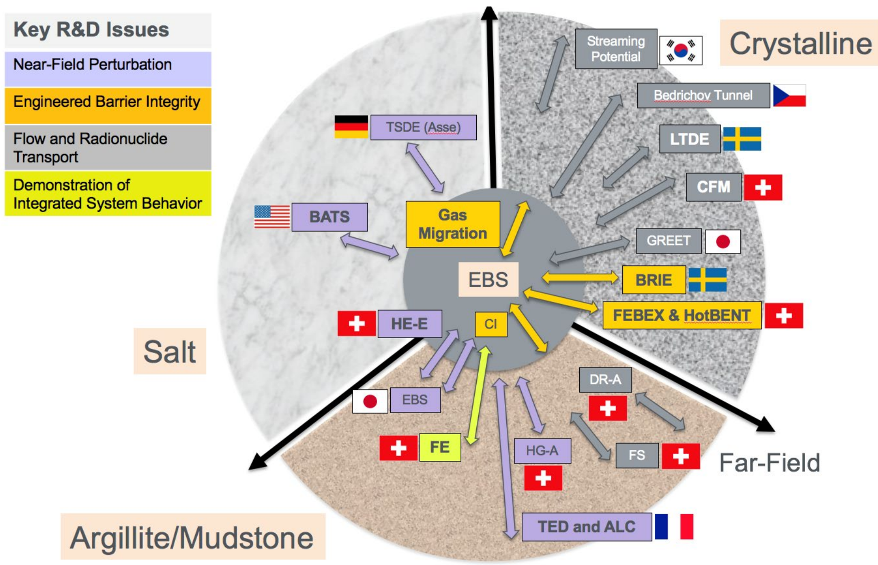

Figure 2. High-level overview of the major international experiments conducted in different countries that SFWD researchers have participated in since 2012. Experiments in bold denote currently active collaborations. See Table ES-1 in Birkholzer and Faybishenko (2020) for more information on each experiment.

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, lessons learned, etc. 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 underground research laboratories 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.

2.6.1 Accomplishments and Discussion

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

- HotBENT: Several international organizations (including SFWST) have in 2018 initiated a new collaboration project referred to as HotBENT to study the effects of high temperature on clay buffers and the near-field host rock. Because the impact of such processes on the performance of a repository are a challenge to be realistically modeled and not clearly assessed representatively at the smaller laboratory scale, the objective of HotBENT is to conduct a large *in-situ* heater test in an underground research laboratory in Switzerland. Significant progress has been made in the last year to construct and instrument the testbed in a fashion to support field-scale date collection; the collaborative experiment is now ready for operation and the heaters will be turned on in 2021.

- 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). A new DECOVALEX Project phase started in April 2020, with DOE participation in multiple new tasks. SFWST DR scientists are also serving as task leads for two of these tasks, one focusing on coupled processes and brine migration in heated salt, and another one on GDSA model comparisons. The new phase, referred to as DECOVALEX-2023, will run through December 2023. Much progress has been made in all seven of the current project tasks.
- 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 underground research laboratories (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.
- Training/Education of Junior Staff: 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 has recently developed a concept paper proposing a dedicated effort at National Labs 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 would consider three main areas: (1) Stimulating Student Interest in Nuclear Waste Research, (2) Creating the Pipeline with Undergraduate and Graduate Internship Programs, and (3) Advancing the Pipeline with Post-Doctoral Research Opportunities, all of which related to international research activities in SFWST.

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 technical areas including Engineered Barrier System R&D, Argillite Disposal R&D, Crystalline Disposal R&D, Salt Disposal R&D, and Geologic Disposal Safety Assessment, 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.

2.6.2 Summary Discussion of Major Changes to Priorities

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

2.6.3 Planned Thrust Topics and Summaries

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

a) *Continue participation within international R&D in underground research laboratories for a range of geologic systems*

The current international research portfolio, which spans across several technical areas including Engineered Barrier System R&D, Argillite Disposal R&D, Crystalline Disposal R&D, Salt Disposal R&D, and Geologic Disposal Safety Assessment, 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 that this revised portfolio will remain largely intact over the next two years. The current key activities either involve long-term in situ experiments that will continue for years to come (e.g., the full-scale FE Heater Test at Mont Terri, the recent fracture network modeling task related to the SKB Task Forces), or they are multi-year collaborations that have just been initiated based on the 2019 Roadmap Reassessment (e.g., the HotBENT experiment at Grimsel Test Site, or the new collaborative tasks defined in the DECOVALEX 2023 Project).

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 technical area. 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 make revisions to the portfolio of international R&D activities as appropriate. Examples of possible new activities might include:

- Additional joint field experiments addressing gas transport in engineered and natural barriers (e.g., participation in the Gas Transport, GT experiment at Mont Terri to better understand gas transport in clay host rock; joining the modeling/analysis team for the Gas Permeable Seal Test, GAST, at Grimsel Test Site).
- Additional diffusion studies for engineered and natural barriers (e.g., the Cement-Clay Interaction Test, CI-D at Mont Terri which characterizes diffusion through 10 year old rock-bentonite-cement interface; the upcoming Diffusion in a Thermal Gradient Experiment, DR-C which evaluates diffusion in argillites under a thermal gradient; and the Long-Term Diffusion Experiment, which is ongoing at Grimsel Test Site).
- Adding tunnel, shaft and borehole sealing elements as a priority theme for engineered barriers research (e.g., the upcoming Large-scale Sandwich Experiment, SW-A, which tests a promising layered technology for shaft seals; the upcoming Borehole Sealing Test, SET).

c) *Pursue a more active role in conducting experimental work in international underground research laboratories*

The SFWST campaign will evaluate 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. Recently, SFWST played a leading role in establishing a broad international partnership to conduct the HotBENT in situ heater test, which addresses research needs related to the performance of clay buffers and near-field rock at temperature from 150°C to 200°C. Campaign scientists played a key role in the test design and predictive modeling, and with the start of the heating phase in late 2020 will be involved for years in monitoring and analysis activities for years. More such active collaborations will be considered in the future.

d) *Contribute to integration and confidence building for Generic Disposal System Analysis*

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 performance assessments (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 new PA/UQ/SA benchmarking task in DECOVALEX 2023 compares PA methodologies across multiple international disposal programs.

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. And 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 may be to support site characterization for site screening and site selection, 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 for different host rocks. 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 could 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.

2.7 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 Generic Disposal System Analysis (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.

2.7.1 Accomplishments and Discussion

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

- 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.
- Participation in DECOVALEX 2023, using PFLOTRAN and COMSOL to perform benchmarking simulation of a field scale heater test (at the Grimsel Test Site).
- 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.

Overall, the EBS activities are working to create/implement process models and understand fundamental processes. These activities in the EBS work-scope can be described in broad terms via 3 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.

2.7.2 Summary Discussion of Major Changes to Priorities

Given the accomplishments in this Technical Area, 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,
    - DECOVALEX 2023, Task C, and
    - Integration between hydrothermal experimental methods and cement-host media studies.

- Decreased priority is given to
    - EBS Task Force, Analysis of the FEBEX-DP Test (Task 9),
    - Uranyl complexation (LANL work moved to another Control Account-see Section 2.8), and
    - Spent fuel corrosion (PNNL work also moved to another Control Account-see Section 2.8).

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

2.7.3 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)*

The two 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) also is 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.

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 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 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 provides 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. Additionally, this activity will provide a forum for further integration between EBS research activities undertaken at LANL, LBNL, and SNL. Collaborations will continue with German EBS researchers, focusing on EBS-related aspects of design and evaluation of a generic salt repository. This will include investigations into drift and shaft seal evolution, which evaluates crushed salt reconsolidation and cementitious materials performance. Over the next five years, a new partnership with JAEA researchers at the Horonobe URL in Japan will be developed, aimed at gaining better understanding of the interactions between cementitious EBS materials and the host rock. Collaboration with investigators from IAEC (Israel Atomic Energy Commission) will continue investigating modeling tools/approaches for understanding leaching of cementitious materials in repository conditions.

2.8 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* Technical Area 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 HLW (DHLW) and SNF (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 SNF and HLW glass degradation for use in GDSA, as well as the current suite of testing activities investigation SNF behavior within the DR program and the integrated planning for further testing of CSNF degradation behavior. This Technical Area 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 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.

2.8.1 Accomplishments and Discussion

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

- OWL database activities focused on development and production of both the OWL Change Control Process documentation and the Version Release Process documentation and completing the release of OWL Version 2.0. These processes cover all aspects of changing OWL content and/or structure, as well as the process and schedule for releasing a new version, both with full documentation tracing generated.
- 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. Specifically, information on sodium-bonded spent fuel waste types and wastes forms were collected and added into OWL.
- Initiated evaluation of thermodynamic data updates for zeolites (Zeo19) and clays to conduct EQ3/6 reaction path calculations of HLW glass. The Zeo19 and ALTGLASS™ databases for HLW glass degradation data were used to constrain rate parameters in the reaction path simulation.
- Performed density functional theory (DFT) calculations on the structure and thermodynamics of crystalline clarkeite to evaluate its stability as a function of temperature.

- Development of a thermodynamically based electrochemical model for UO_2 degradation. The objective of this model is to capture electrochemical feedbacks due to changes in solution chemistry.
- Generated a conceptual model for cladding degradation that is to be utilized in both safety assessments and in criticality evaluations for DPC direct disposal.
- Initiated an integrated planning activity to evaluate data gaps and prioritize new testing on SNF within the DR Program. The draft plan is being augmented through multi-National Laboratory workshops (including each of the participating labs in this Technical Area); it is expected that the plan will be finalized in FY22 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.

2.8.2 Summary Discussion of Major Changes to Priorities

Priorities in this area are unchanged, except that the expanded activities have added to both the near-term and longer-term thrust topics. Efforts focused on the OWL remain at the same priority as before. Other activities are still evolving or were initiated recently.

2.8.3 Planned Thrust Topics and Summaries

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

a) *Development of basic interface GDSA scripts to access and read OWL data*
b) *Develop Glass Waste Degradation Expertise*
c) *Finalize SNF testing gap analyses and prioritization*

The primary thrust for the OWL inventory work in the short-term is 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. 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.

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 are being assessed. This effort 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 for additional SNF testing gap analyses and prioritization will focus on a completed testing strategy/plan in the upcoming fiscal year. This work will utilize experts from each of the National Laboratories involved in the DR modeling and testing of SNF to develop a gap analysis and a prioritization of testing activities 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 to address gaps*

The longer-term thrusts in this technical area 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. 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.

2.9 Technical Support for Underground Research Laboratory Activities

The DOE has an inactive underground research laboratory (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 10 years) and all offsite electrical utility power has been disconnected remote 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 ~one year since the previous version of this DR R&D Plan, restoration of power to the URL has been delayed due to the impacts of the COVID-19 pandemic. 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.

2.9.2 Summary Discussion of Major Changes to Priorities

Given the accomplishments in this Technical Area, 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 technical area has two operational objectives and two R&D thrusts at this early 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.

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. 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 activity is to establish a Knowledge Management (KM) program covering the Nuclear Energy Fuel Cycle (NEFC) that is initially focused on relevance/benefit to the SFWST Campaign DR R&D program, with intent to expand coverage to the entire back end of the fuel cycle activities. The loss of senior staff members, who are not only leaders and mentors but also seasoned subject matter experts in nuclear waste management (NWM), necessitates an intentional approach to ensure a more efficient and rigorous approach to capturing, cataloging, archiving, and transferring institutional NWM tacit knowledge to the influx of 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. There is also work underway to design current work processes into database workflows to capture knowledge and information as it is created by current NWM staff. As such, the KM activity cross cuts all the DR R&D areas (and ultimately S&T R&D and beyond), focusing on the larger technical and programmatic aspects of NWM projects.

The KM activity convened focus groups to understand the current state of KM implementation, the most beneficial ways to gather knowledge and the myriad of methods to communicate the knowledge to program staff working in NWM. The focus groups covered technical staff at SNL ranging from junior to most-senior staff grouped by experience levels, as well as a management focus group. A key finding from the focus groups is the need to design a web-based platform as an interactive and living tool for accessing the tacit knowledge captured. A KM workshop was held (December, 2019) to cover primary NWM knowledge from primarily the U.S. radioactive waste disposal programs, with some coverage of the history and regulatory structure of storage and transportation projects, and an overview of the Congressional budgeting and authority structure. The workshop was audio/video recorded as part of the KM collection and was followed by *Information Deep Dives* in key technical areas underpinning the safety case for a repository program. All these knowledge sets have been included in the pilot KM Repository developed in SharePoint on the Sandia restricted (i.e., internal) network (SRN). These materials are kept in various formats (e.g., video presentations, transcripts of video), with referenced materials, linked files, and a discussion board for interaction amongst staff.

2.10.1 Accomplishments and Discussion

In the ~one year since the previous version of this DR R&D Plan, the major accomplishments in the Knowledge Management activities are:

- Conducted a set of two NWM Regulatory Deep Dives
  - March 4, 2021 - *Storage & Transportation: The Regulations* - Kenneth B. Sorenson Lead Speaker.
  - March 9, 2021 - *Nuclear Waste Disposal: The Regulations* - Speakers: Evaristo J. (Tito) Bonano, David Sassani, Donald A. Beckman, and Steve Wagner.
- Conducted a set of two NWM Siting and Requirements Deep Dives
  - May 26, 2021 - *Site Selection for a Future Nuclear Waste Management Facility* – with Speakers: Paul Shoemaker, Peter Swift, Lake Barrett, Ben Belfadhel, Geoff Freeze, Tito Bonano.
  - May 27, 2021 - *Non-Technical Requirements & Processes of a Nuclear Waste Management Project* - Speakers: Nick DiNunzio, Cyrus Nezhad, Peter Swift, Paul Meacham.

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. In particular, coverage of the Storage and Transportation (S&T) regulatory framework helped expand coverage aspects of the S&T R&D program in the KM Repository. In addition, the Knowledge Management activities continued to plan/conduct Knowledge Retention conversations with key staff as they retire to capture some of their tacit knowledge with questions from a range of staff with various experience levels.

2.10.2 Summary Discussion of Major Changes to Priorities

Given the accomplishments in this Technical Area, as well as the changes/drivers on Priorities (e.g., Program Direction; external data/understanding advancements, etc.,), there were no major changes to the priorities for this set of activities. The Thrust Topics in the next Section remain consistent with Knowledge Management priorities.

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 Repository*
b) *Expand topical coverage more fully for disposal programs and to the S&T KM topics*

The primary thrust for KM in the short-term is to maintain and develop the KM Repository, adding more materials relevant to the tacit knowledge for disposal programs, more linked structures, and additional tools for using and transferring this knowledge amongst the current NWM staff. This continues to be the active pursuit with expansion of the topical coverage. A large amount of data/tacit knowledge is already included in the KM Repository, but there are areas that are yet to be mined for relevant experience and linked to key documented resources in the DR arena. Beyond this, expansion of the tacit knowledge content of the KM Repository to the wealth of experience in storage and transportation R&D projects would be the next natural step for this activity and would flesh out the NWM coverage of the back end of the nuclear fuel cycle.

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

a) *Expand KM Repository efficacy to larger portions of the nuclear energy fuel cycle community*
b) *Consider developing training course(s)*

Further development of KM Repository content and capabilities would continue in the long-term as more information is collected and linked. Providing interface capabilities to larger portions of the SFWST Campaign staff, and beyond to all NE-8 staff, would be one focus in the longer-term for KM activities. Additionally, expanding the topical coverage in response to the wider user group would be another focus in the out years. Potential development of explicit training courses using the KM Repository for new/junior NWM staff would be considered in the longer-term as well.

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 disposal R&D programs have focused on the evaluation of the viability of mined repositories in three generic geologic media (salt, clay, 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; NWTRB 2016)[a]. 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.

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 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 Storage and Transportation (S&T) of SNF (e.g., Teague et al., 2020), in addition to Disposal Research. 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., accident tolerant fuels; probable advanced nuclear fuel cycle reactor fuels) may generate additional/new waste forms. Work on the high-level strategy for assessing back-end-of-the-nuclear-fuel-cycle (BENFC)

[a] DOE Campaign R&D for this concept was discontinued in 2017.

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 Integrated Waste Management (IWM) Campaign. 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. 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 Underground Research Laboratories; Engineered Barrier System Representations; and Evaluation of Potential Direct Disposal of Dual Purpose Canisters (DPC).

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 engineered barrier systems (EBS).Within this focus area, efforts include expansion of high-fidelity modeling capability in both the near-field (i.e., source-term and EBS transport) and far-field (i.e, the natural barriers) portions of the system model, as well as integration of multi-fidelity model forms that adequately represent performance-affecting processes while maximizing computational efficiency. For complex coupled chemistry, development of a drift-based model that includes major chemical components reacting with materials over appropriate temperature ranges is also being pursued. Utilization of high-performance computing, advanced computational methods, and enhanced treatment of uncertainty quantification and sensitivity analyses will underpin the tools being expanded. Workflow automation, software verification, and accessibility of these tools for potential use in a regulatory environment is also a key area of development.
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 underground research laboratories (URL) 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. Additionally, a recent effort has been started to apply SFWST R&D expertise in heated experiments in U.S.-based salt host rocks underground, and potentially (next fiscal year) in an unsaturated system tunnel.
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. Additionally, the thermal aspects rooted in the waste form/waste package source term region affect the host rock depending on the timing of disposal and the layout of the repository. This cross-cutting issue was handled well for EBS Concepts in the DR R&D program for those existing systems being investigated around the world, but there were specific gaps related to both waste package (WP) degradation and cladding evolution/failure in the post-closure DR R&D activities identified. Developing, constraining, and implementing models for both waste package degradation and cladding evolution are major goals in this focus area. Additionally, the evaluation of feasibility of direct disposal of DPCs raises some technical issues to more prominent levels, such as thermal effects, including coupled processes, degradation rates of waste forms and other engineered barriers, and evolution of the EBS transport pathways and rates. Consideration of stage III rate processes in glass degradation, as well as potential new waste forms from either accident tolerant fuels or advanced reactor fuel cycle development will become more of a central emphasis. One goal here, as with International Collaboration, is to provide more highly integrated capabilities for analyzing generic repository systems in argillite, crystalline, and salt host rocks, with integrated EBS treatments and GDSA demonstration capabilities

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 dual purpose canisters. 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. Because DPCs tend to be massive both physically and thermally, they present further challenges for operations (e.g., handling) and thermal management. This latter aspect enhances the need to understand coupled thermal-chemical-mechanical-hydrologic (TCMH) processes in all disposal concepts. Additionally, criticality evaluations both prior to closure of a repository and in the post-closure system are an essential part of the considerations. Criticality evaluations include direct disposal without modification (e.g., post-closure criticality consequence analysis, as-loaded reactivity margin analysis) and with modification/mitigation. Mitigation approaches for potential post-closure criticality includes consideration of modifications of the DPC internals, including fillers of both metallic and cementitious compositions. These materials in the EBS add to the considerations of chemical evolution in the near-field environment that applies to waste form degradation, radionuclide release, and EBS transport analyses. Moreover, DPC overpacks designed specifically for post-closure corrosion performance would likely be needed in a number of disposal concepts considered. The DPC would be integral to the EBS so they connect with all near-field studies, and thermal input may affect the damaged zone around the EBS and further into the host rock in terms of mechanical changes. Such effects push the process-level investigations in all areas, as well as the range of conditions considered in GDSA models, to levels higher than previously addressed.

4. SUMMARY AND CONCLUSIONS

In the planning for FY2020 in the U.S. DOE NE-81 Spent Fuel and Waste Science and Technology (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 (Sassani et al., 2020) and represents a strategic guide to the work within the DR R&D technical areas (i.e., the Control Accounts), focusing on the highest priority technical thrusts. This FY2021 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 technical areas (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 technical area, 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 technical area 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. This plan fulfills the Milestone M2SF-21SN010304054 in DR Work Package (WP) SF-21SN01030405 (GDSA - Framework Development – SNL).

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 generic geologic media (salt, clay, 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. Recently, generic unsaturated system mined repository concepts are also being analyzed, especially regarding their capabilities to effectively release heat via ventilation to open emplacement tunnels.

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

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

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 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, 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 Underground Research Laboratories; Engineered Barrier System Representations; and Evaluation of Potential Direct Disposal of Dual Purpose Canisters.

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 Storage and Transportation (S&T) of SNF (e.g., Teague et al., 2020), in addition to Disposal Research. 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., accident tolerant fuels; 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 just 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 back-end-of-the-nuclear-fuel-cycle (BENFC) management processes within the Integrated Waste Management (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, accident tolerant fuels, 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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Appendix A – Roadmap Reassessment and Results Summary

The 2019 Roadmap Reassessment (Sevougian et al., 2019) utilized a systematic process that was similar in many ways to that used in the UFD 2012 Roadmap (DOE 2012), but with important differences in both the definition of the "items" or "quanta" to be prioritized, and in the criteria and process used for prioritization. There were five basic steps in the 2019 process:

1. Identify a set of items to be evaluated (e.g., R&D activities, issues, or options, …)
2. Identify criteria and associated metrics for assessing the set of items, such as:
   a. Importance to the safety case (ISC) (e.g., in this context, important to the post-closure safety assessment or performance assessment (PA) calculations, to technical bases supporting conceptual and numerical model development, and/or to building confidence in design concepts and process understanding)
   b. Potential to reduce key uncertainties, i.e., to advance the state-of-the-art level (SAL) or knowledge
   c. Other factors
3. Evaluate each item (R&D Activity) against the metrics
4. Define a "utility function" (or ranking function) to combine the metric values and produce an overall ranking or score for each item (R&D Activity)
5. Compare rankings of the items (R&D Activities)

The goal was to identify R&D items that provide maximum value to DOE in terms of advancing the program's ability to support future decisions regarding the siting, selection, design, licensing and construction of a geologic repository. For the 2019 R&D Roadmap Reassessment, the SFWST Campaign decided to redefine the R&D items to be prioritized. Instead of using the FEPs list as the basis, the new items to be prioritized were based on ongoing and proposed R&D work scope activities (or tasks) being performed within the SFWST Campaign (i.e., R&D Activities). Additionally, the generic FEP list was used to both map the R&D Activities to the FEP, and to help identify "gap" activities where existing R&D Activities did not fully address a FEP. To ensure that the 2019 Roadmap Reassessment addressed all the R&D Issues identified in the 2012 Roadmap, SWFST staff identified and correlated all the medium- and high-priority FEP from 2012 with the R&D Activities defined for 2019. In this way, the 2012 FEPs list also served as a completeness check on the R&D Activities list and facilitated gap identification.

As noted above, the R&D Activities were assessed from two different perspectives or criteria, and evaluation metrics were defined for these two criteria before the Workshop. Importance to the Safety Case (ISC) was scaled as High, Medium, or Low, with specific definitions of the three scale values being dependent on the importance of the R&D Activity relative to components of a future post-closure safety case. The State-of-the-Art Level (SAL) was assigned to one of five values based on the level of knowledge currently available and what yet needs to be obtained. These two metrics were combined in synthesis work after the Workshop to define a Priority Score: High, Medium-High, Medium, or Low for each R&D Activity.

Consensus on ISC and SAL metric values was obtained within "breakout" sessions comprised of about ten to fifteen experts each, using the provided metric scales, and with guidance by the session chair and the overall Workshop chair. There were six breakout sessions: there were three host-rock (Argillite, Crystalline, Salt) day-long, concurrent sessions; and half-day concurrent sessions on EBS, DPC, and International R&D Activities (cross-cutting sessions relative to the host-rock based sessions). The PA and Other R&D Activities did not have their own separate sessions but were included in the other six sessions. Post-workshop synthesis led to priorities set for the R&D Activities across the entire set of them.

Of the eight topical R&D Activity groupings mentioned above, the DPC R&D Activity group had, by far, the highest percentage of High-Priority Activities (about 70% of its total), primarily because of the recent work to evaluate direct disposal of DPC in generic deep geologic repository concepts, which has led to a number of newly emerging issues that are being addressed by these R&D Activities.

A review of the High- and Medium-High-priority R&D Activities (Sevougian et al., 2019) has led to the identification of a set of "High Impact R&D Topics," including:

- High Temperature Impacts
- Buffer and Seal Studies
- Coupled Processes (Salt)
- Gas Flow in the EBS
- Criticality
- Waste Package Degradation
- In-Package Chemistry
- Generic PA Models
- Radionuclide Transport

These High Impact R&D Topics provide a high-level snapshot of the current and future generic R&D focus. Sevougian et al. (2019) provide the detailed information on how these High Impact Topics relate to specific R&D Activities, as well as elucidating some integration issues involved in generic PA model development. The Gap activities identified included:

- Technical integration between R&D Activities is essential because of the complexity of developing comprehensive technical bases, advanced process modeling capability, and generic repository reference cases for PA demonstration
- The temporal framework (or timeline) for "Generic R&D Needed" appeared to vary a lot between breakout sessions and could improve in the future with more intensive inter-group calibration prior to, and at the beginning of, the Workshop
- "Calibration" on the assignment of ISC and SAL metric values is important to develop prior to, and at the beginning of, the Workshop
- Adding a metric for level of effort (LOE) for individual activities would be very useful
- Integration of DPC-relevant parameters into all modeling activities is needed

Although much has been accomplished since 2012 both through R&D in the U.S. Program and through international collaborations, especially with those countries that operate underground research laboratories (URLs), the 2019 R&D Roadmap Reassessment reflects the need for continuing R&D on many of the 2012 R&D Issues, plus some obvious new priorities, such as R&D on disposal of DPCs (dual purpose canisters), which now contain a significant fraction of the Nation's spent fuel activity. This new 2019 R&D prioritization effort is closely tied to advancement of capabilities in the Campaign's generic performance assessment simulation and analysis toolkit, GDSA Framework.