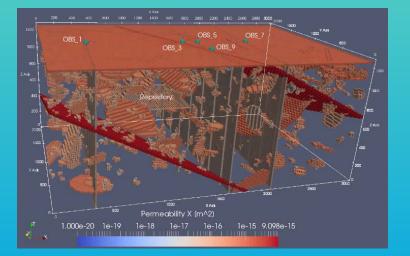


Spent Fuel and Waste Science and Technology (SFWST)









Geologic Disposal Safety Assessment (GDSA) Overview

U.S. Nuclear Waste Technical Review Board Fall Workshop November 3-4, 2021 Emily Stein Sandia National Laboratories

ENERGY

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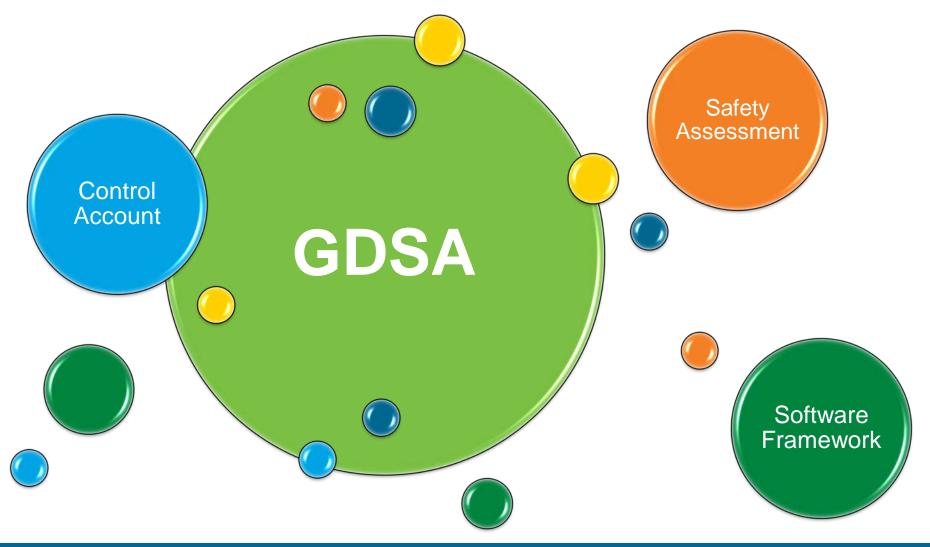
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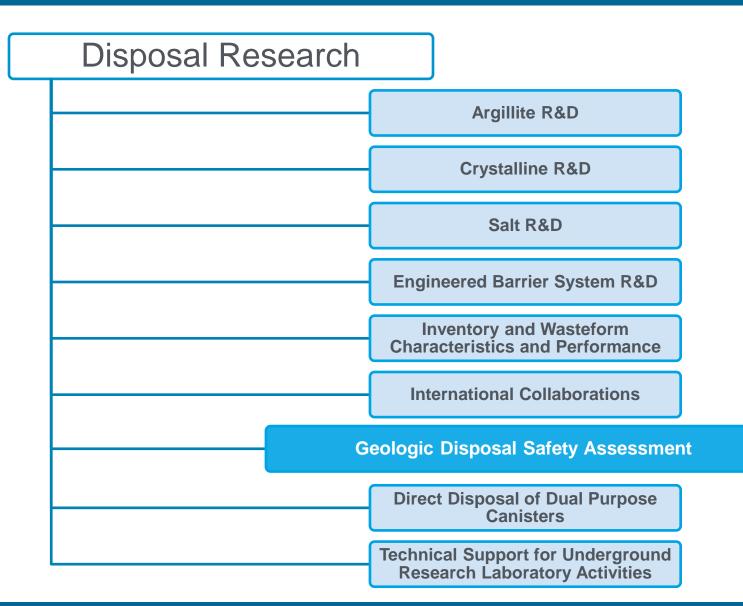


- What is GDSA?
- Objectives
- Prioritization
- Challenges
- 5-year Plan

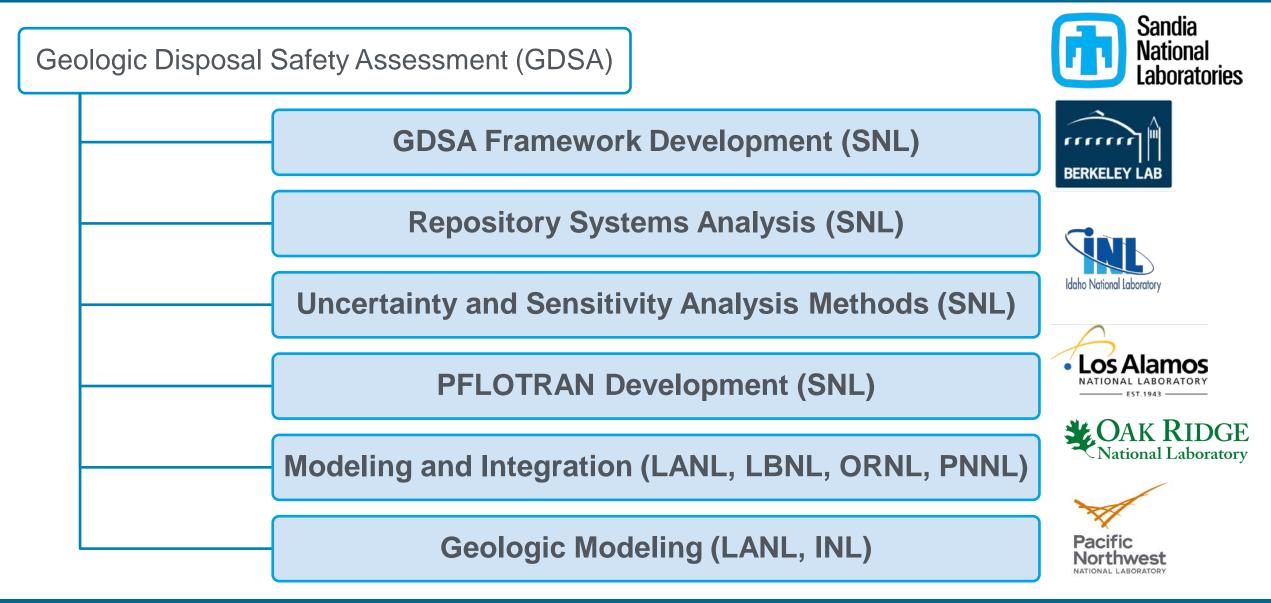
What is Geologic Disposal Safety Assessment or GDSA?



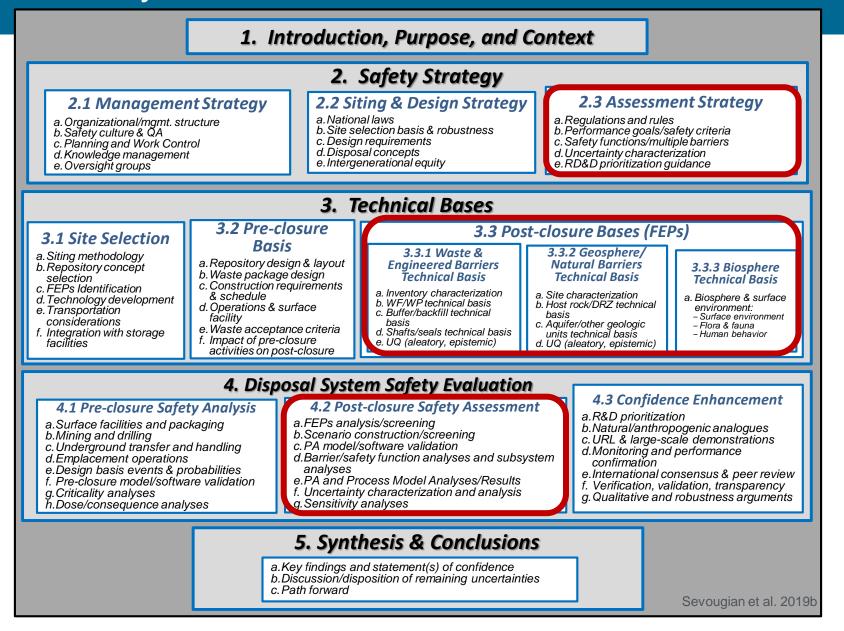
Spent Fuel and Waste Science and Technology Disposal Research Control Accounts



Scope of the GDSA Control Account



Post-closure Safety Assessment



Assumptions for GDSA Development

- Individual performance standard
- Probabilistic risk assessment
- Separation of aleatory and epistemic uncertainty
- Biosphere may be prescribed
- Prioritize features, events, and processes that are likely to occur regardless of site and design specifics
- Provide a quantitative estimate of the performance of the disposal system for comparison to regulatory standards

Assessment Strategy

a. Regulations and rules

C.

- b. Performance goals/safety criteria
 - Safety functions/multiple barriers
- d. Uncertainty characterization
- e. RD&D prioritization guidance

Post-closure Technical Bases

Waste & Engineered Barrier

- a. Inventory characterization
- b. Wasteform and waste package
- c. Buffer and backfill
- d. Shafts and Seals
- e. Aleatory and epistemic uncertainty

Geosphere/Natural Barrier

- a. Site characterization
- b. Host rock and disturbed rock zone
- c. Aquifer and other geologic units
- d. Aleatory and epistemic uncertainty

Biosphere

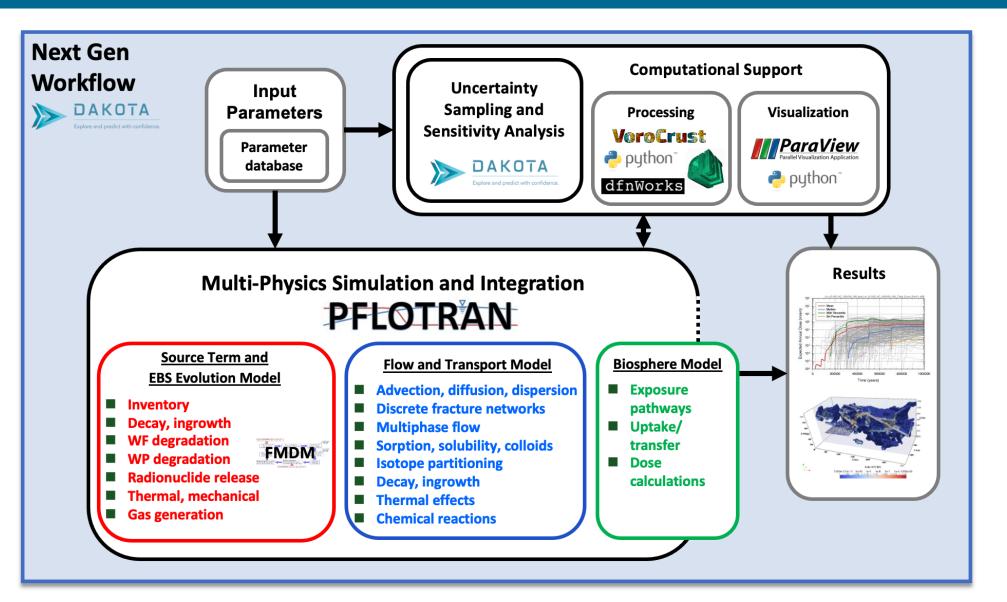
- a. Surface environment
- b. Flora and fauna
- c. Human behavior

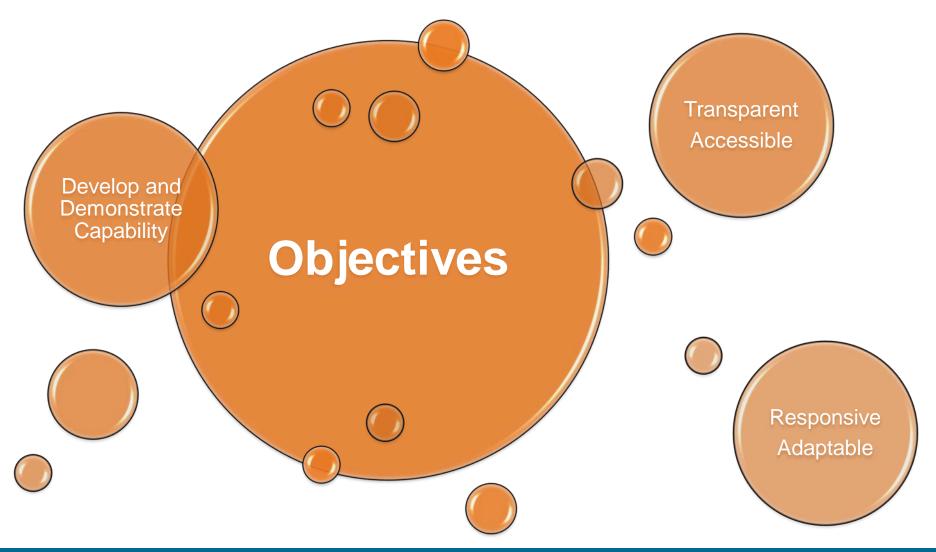
- Post-closure Safety Assessment
- a. FEPs analysis/screening
 - Scenario construction/screening
 - PA model/software validation
- d. Barrier and subsystem analyses
- e. PA and process model analyses
 - Uncertainty characterization and analysis
 - Sensitivity analysis

b.

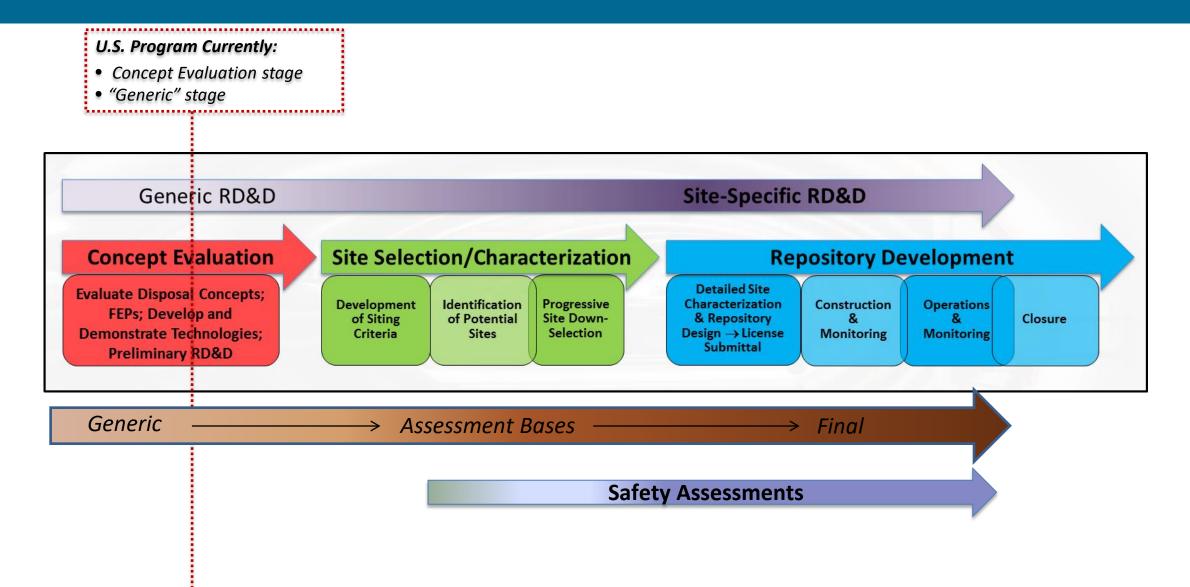
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GDSA Framework

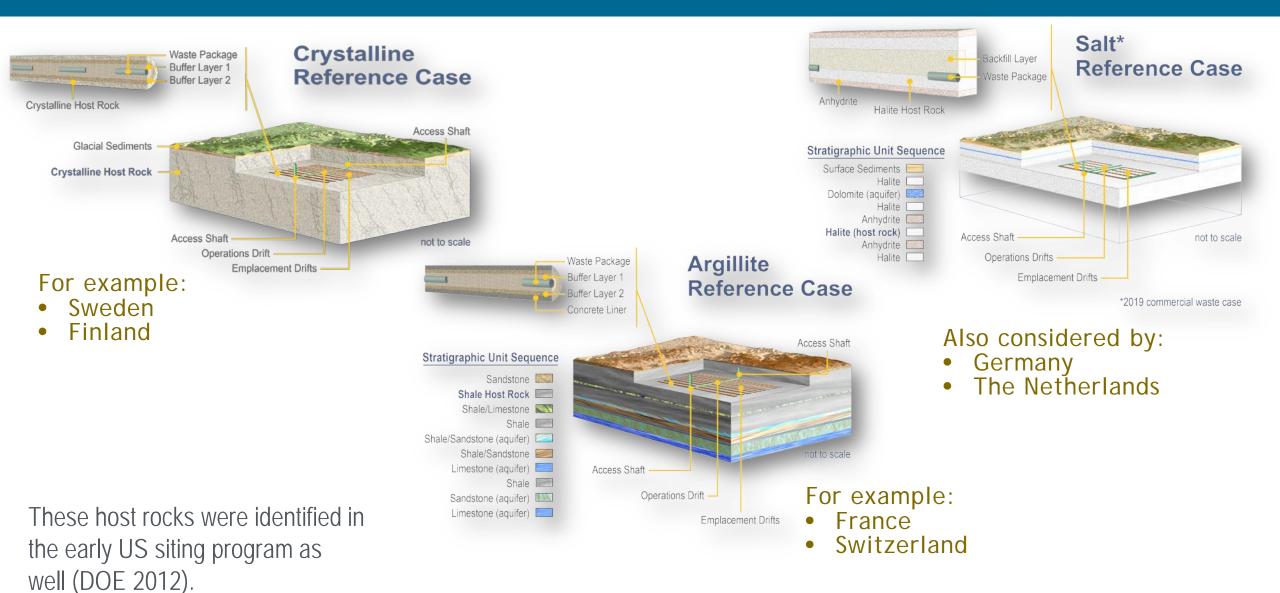




Stages of a Deep Geologic Disposal Program

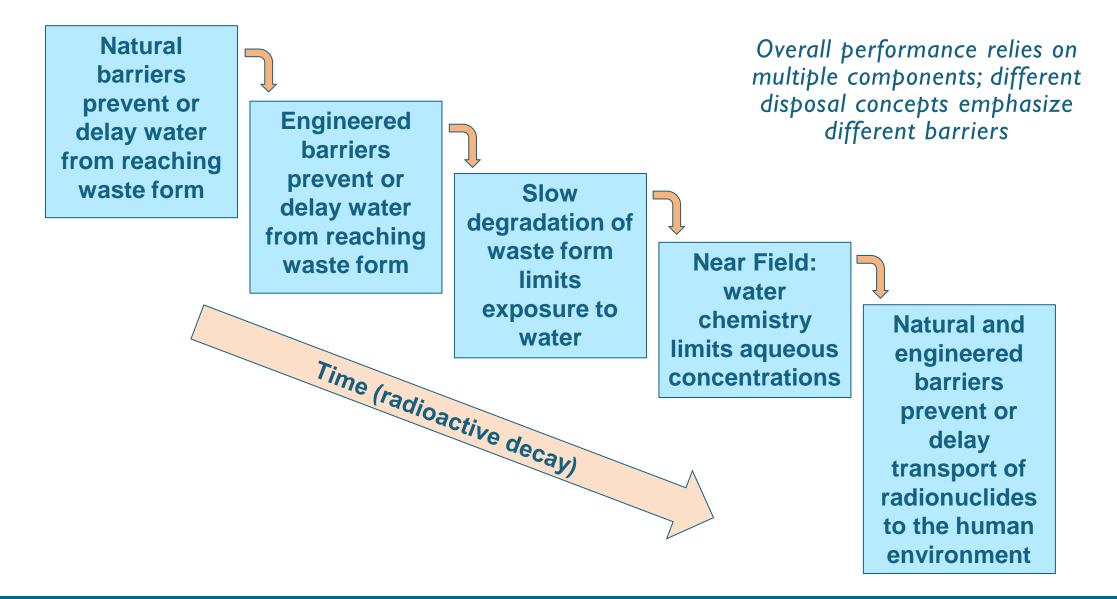


Generic Host Rock Systems



SFWST

Multiple Barriers



Why GDSA Framework?

- Be flexible to changes in design, geometry, or geology
- Represent three-dimensional geometry
- Facilitate two-way coupling
- Integrate process models transparently
- Leverage high-performance computing to
 - Allow more detailed representation
 - Reduce computational costs (of all of the above)
 - Enable probabilistic calculations (given the computational cost)
- State-of-the-art

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Why GDSA Framework?

PFLOTRAN

- High-performance computing
- Open source
- Sequentially coupled flow and transport
- Global implicit reactive transport



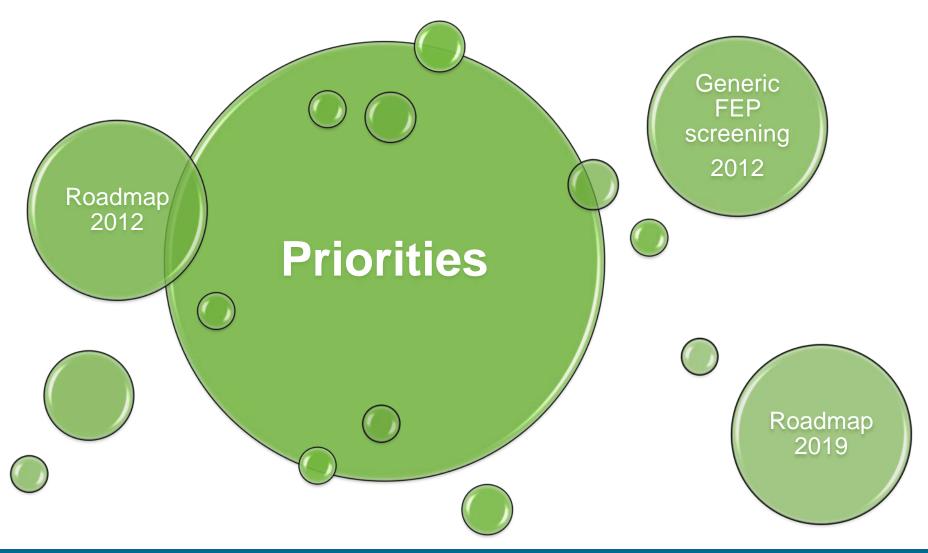
- High-performance computing
- Open source
- Latin hypercube sampling
- Aleatory and epistemic uncertainty

GDSA Objectives

Develop and demonstrate capability

• Geologic modeling, multiphysics simulation, uncertainty and sensitivity analysis, workflow that is

- Responsive to advances in
 - Process understanding, computer hardware and software, simulation and analysis methods
- Adaptable to
 - Generic site and design constraints
 - Site- and design-specific technical bases
 - Evolution of the safety assessment strategy
- Transparent
 - Developed and distributed in an open-source environment with public documentation
- Accessible
 - Laptop, workstation, and high-performance computing



Evolution of GDSA Framework and Reference Cases

with PFL DAKOTA	• Salt reference case with PFLOTRAN & DAKOTA (Freeze et al. 2013)		 Shale reference case Fuel Matrix Degradation (FMD) Glass dissolution (Mariner et al. 2015) 		 Well water ingestion QA test suite Analytical derivatives (Mariner et al. 2017) 		Update al. 2019a) perature ulations stress al. 2019b)	 Dual porosity Criticality (Nole et al. 2021) International sensitivity analysis report (Swiler et al. 2021)
2012 2013 • Roadmap (DOE 2012) • Requirements (Freeze & Vaughn 2012) • Generic FEPs (Vaughn et al. 2012)	• Multiphase added to PFLOTRAN (Sevougian et al	N	 2016 Crystalline reference dfnWorks Isotope pa Wasteforn model (Mariner et al. 2) 	case artitioning n process	 2018 Variance-lisensitivity Stepwise regression Alluvial recase (Mariner et al. 2019) 	analysis linear า ference	 • FMD surre (Mariner et al. • Advanced • Next Gen (Mariner et al. • DECOVAL (LaForce et al. • Biosphere (Condon et al. 	2020a) d solvers Workflow 2020b) LEX Task F . 2020) e model

Planning/Prioritization Disposal Research (DR) Activities Overview

- Used Fuel Disposition (UFD) Campaign 2012 Roadmap
 - Features, Events, and Processes (FEP) gap assessment synthesis
 - Synthesize into High Priority Topics for UFD Campaign work planning
 - 2012 Roadmap Report (Rev. 01; 2012)
- 2019 Roadmap Update
 - Review/prioritize DR Activities for progress, gaps, and recent Program Direction
 - Begin assessment of DR R&D Program in FY2017
 - 2019 Roadmap Update Report (Rev. 01; 2019)
- Development of SFWST Disposal Research Five-year Plan (2020, 2021)
 - Incorporate/address updated priorities
 - Identify short-term primary objectives (1-2 years; relatively certain)
 - Provide longer-term vision (3-5 years; general guide)

2012 Roadmap – Cross Cutting Issues

Disposal System Modeling (High)

- Enable risk-informed, probability-based performance assessment
- Provide a capability for evaluating disposal system performance to inform R&D prioritization
- Support simple and complex integrated generic disposal system models
- Site Screening and Selection Tools (Medium)
 - Unified geospatial database and visualization tool

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2012 Generic FEP screening

Source (Inventory and Waste Form)

- Radionuclide inventory (heat generation, decay and ingrowth)
- Waste form degradation (dissolution processes)
- Gas generation
- Radionuclide release and transport (mobilization, early release [e.g., from gap and grain boundaries], precipitation/dissolution) Near Field (Waste Package, Buffer, Backfill, Seals/Liner, and Disturbed Rock Zone (DRZ))
- Waste package degradation (corrosion processes, mechanical damage, early failures)
- Evolution/degradation of engineered barrier system (EBS) components and DRZ
- Effects from rockfall, drift collapse (e.g., salt creep)
- Fluid flow and radionuclide transport (advection, dispersion, diffusion, sorption, decay and ingrowth)
- Chemical interactions (aqueous speciation, mineral precipitation/dissolution, reaction with degraded materials, surface complexation, radiolysis)
- Thermal effects on flow and chemistry
- Effects from disruptive events (seismicity, human intrusion)

Far Field (Host Rock and Other Units)

- Fluid flow and radionuclide transport (advection, dispersion, diffusion, sorption, decay and ingrowth)
- Effects of fracture flow (e.g., dual porosity/permeability, discrete fracture)
- Groundwater chemistry

Receptor (Biosphere)

- Dilution due to mixing of contaminated and uncontaminated waters
- Receptor characteristics (basis for converting radionuclide concentrations in groundwater to dose)

Vaughn et al. 2012

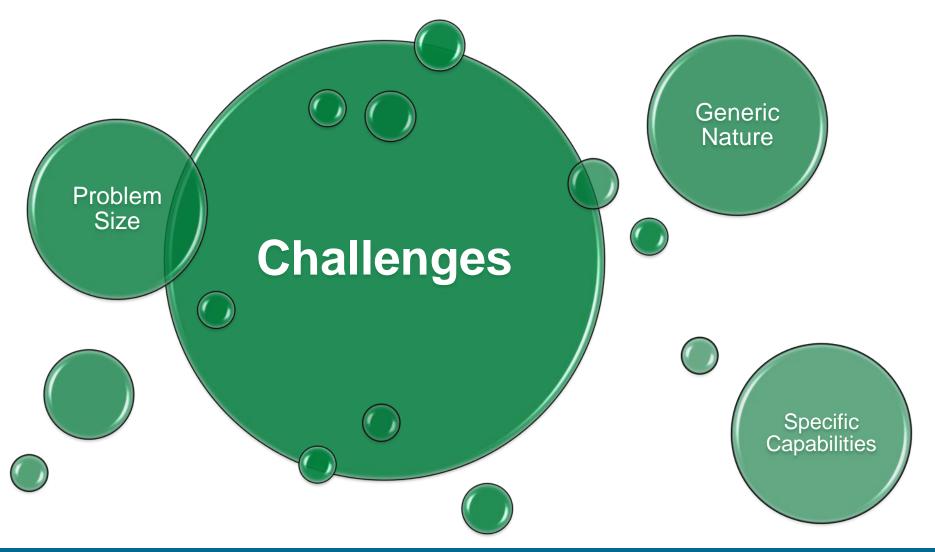
2019 Roadmap Update – High Impact R&D Topics

High-temperature impacts

- Buffer and seal studies
- Coupled processes in salt
- Gas flow in the engineered barrier system
- Criticality
- Waste package degradation
- In-package chemistry
- Generic performance assessment models
- Radionuclide transport

Sevougian et al. 2019

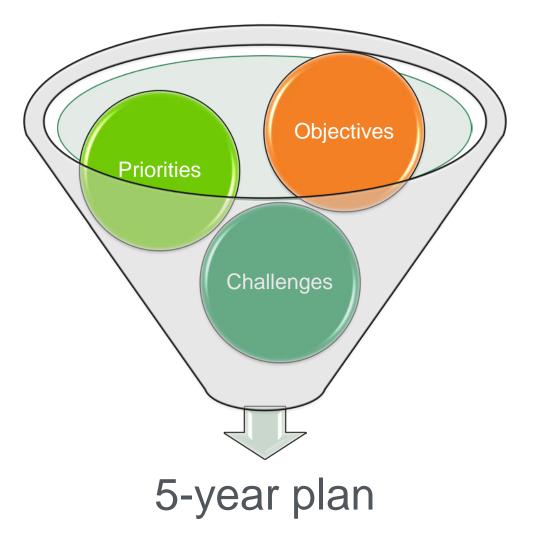
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Challenges

- Generic nature of the problem
- Size of problem
 - 3D comprehensive model domain
 - Long time scale (1 million years)
 - Number of radionuclides
 - Uncertainty propagation
- Resolution of near-field processes
- Specific modeling capabilities
 - High-temperature multiphase flow
 - Computationally efficient implementation of the Fuel Matrix Degradation Model
- Workflow

Objectives, Priorities, and Challenges Shape the 5-year Plan



Research Thrusts in 5-Year Plan

- Advanced simulation capability
- State-of-the-art uncertainty and sensitivity analysis methods
- Traceable, user-friendly workflow
- Repository systems analysis
- Geologic framework modeling



Advanced Simulation Capability

Recent Accomplishments

- Advanced linear and nonlinear solvers
- Waste package criticality
- High-temperature effects
- Fracture-matrix diffusion
- Surrogates for the Fuel Matrix Degradation Model
- Biosphere prototype

Next 1-2 Years

- High-temperature simulation capability
- Material-specific waste package degradation models
- Buffer and backfill evolution
- Biosphere pathways
- dfnWorks capability
- Geologic meshing

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Mariner, Nole, Hyman, & Condon

Uncertainty and Sensitivity Analysis (U/SA)

Recent Accomplishments

- Advance U/SA of crystalline reference case
- Led international comparison of SA methods
- Demonstrate potential of multifidelity methods

Next 1-2 Years

- Increase computational efficiency
- Increase understanding of system behavior
- Metrics for assessing goodness of surrogates
- International best-practices

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Workflow

Recent Accomplishments

- Next Generation Workflow (NGW)
- Expansion of software verification testing ("QA test suite")

- Next 1-2 Years
 - Increase automation through NGW
 - Release the "QA test suite"
 - Develop geologic meshing workflow

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Repository Systems Analysis

Recent Accomplishments

- Conceptual models and simulations that account for high-temperature impacts
- Initiate 4-year international performance assessment comparison (DECOVALEX-2023 Task F)
- Growing collaboration with Germany, Netherlands, and United Kingdom regarding salt FEPs and scenario development

Next 1-2 Years

- Simulation and analysis of salt and crystalline reference cases developed in Task F
- Drive development of process models
 - Bentonite evolution
 - Waste package degradation
 - Salt consolidation and creep

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Topics for this meeting

- GDSA Framework Mariner
- PFLOTRAN Nole
- dfnWorks Hyman
- Fuel Matrix Degradation Model Mariner
- Biosphere Model Condon
- Uncertainty and Sensitivity Analysis Swiler
- Reference Case Simulation LaForce
- DECOVALEX-2023 Task F Stein

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