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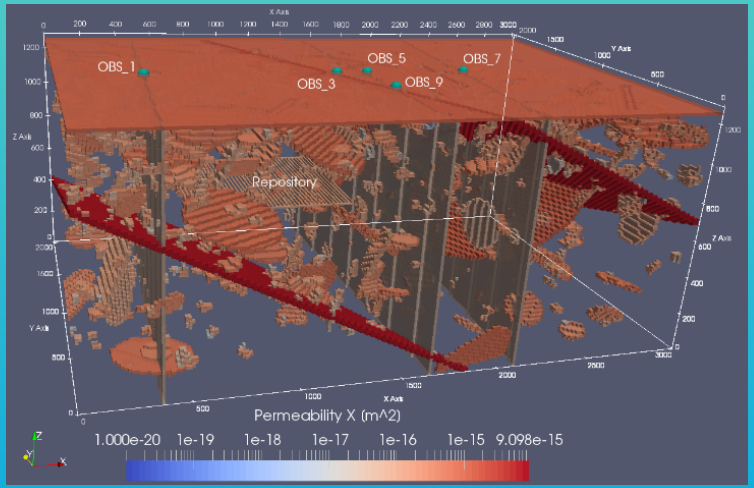
Spent Fuel and Waste Science and Technology (SFWST)



U.S. Nuclear Waste Technical Review Board
Fall 2020 Board Meeting
December 02-03, 2020
Virtual Meeting

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SAND2020-13156 PE

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Disclaimer

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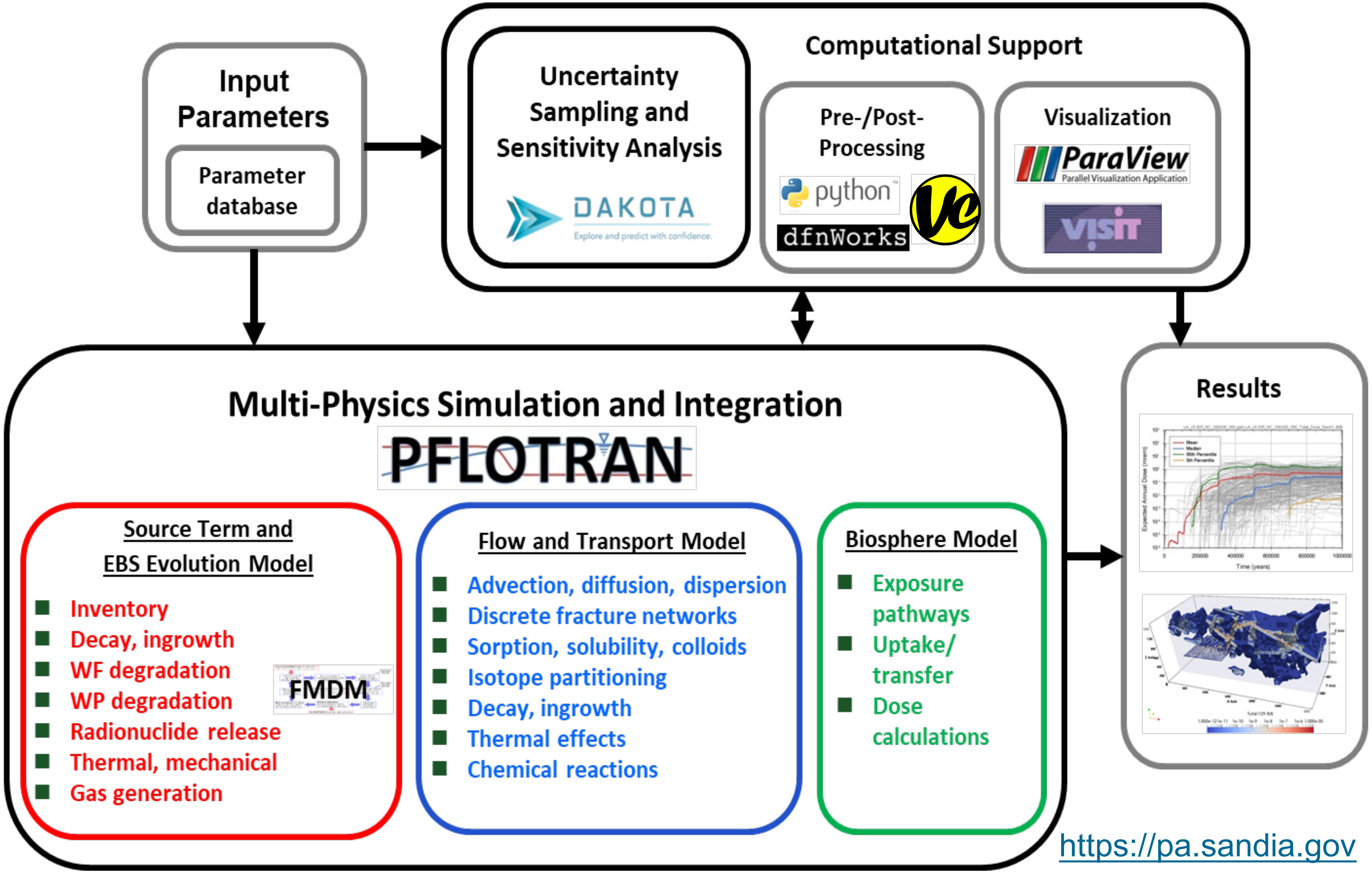
Legal Notice

Outline

- Define Geologic Disposal Safety Assessment (GDSA)
- Introduce the Unsaturated Alluvium Reference Case
- Knowledge and Capability Gaps
- Current Research & Development
  - Criticality Consequence Analysis for Direct Disposal of Dual Purpose Canisters (DPCs)
  - Geologic Framework Modeling
  - Capability Development in GDSA Framework
- Forward Look at GDSA/DPC Integration

Geologic Disposal Safety Assessment (GDSA) Framework

- An open-source, high-performance computing software toolkit for simulation and analysis of the post-closure performance of deep geologic disposal systems



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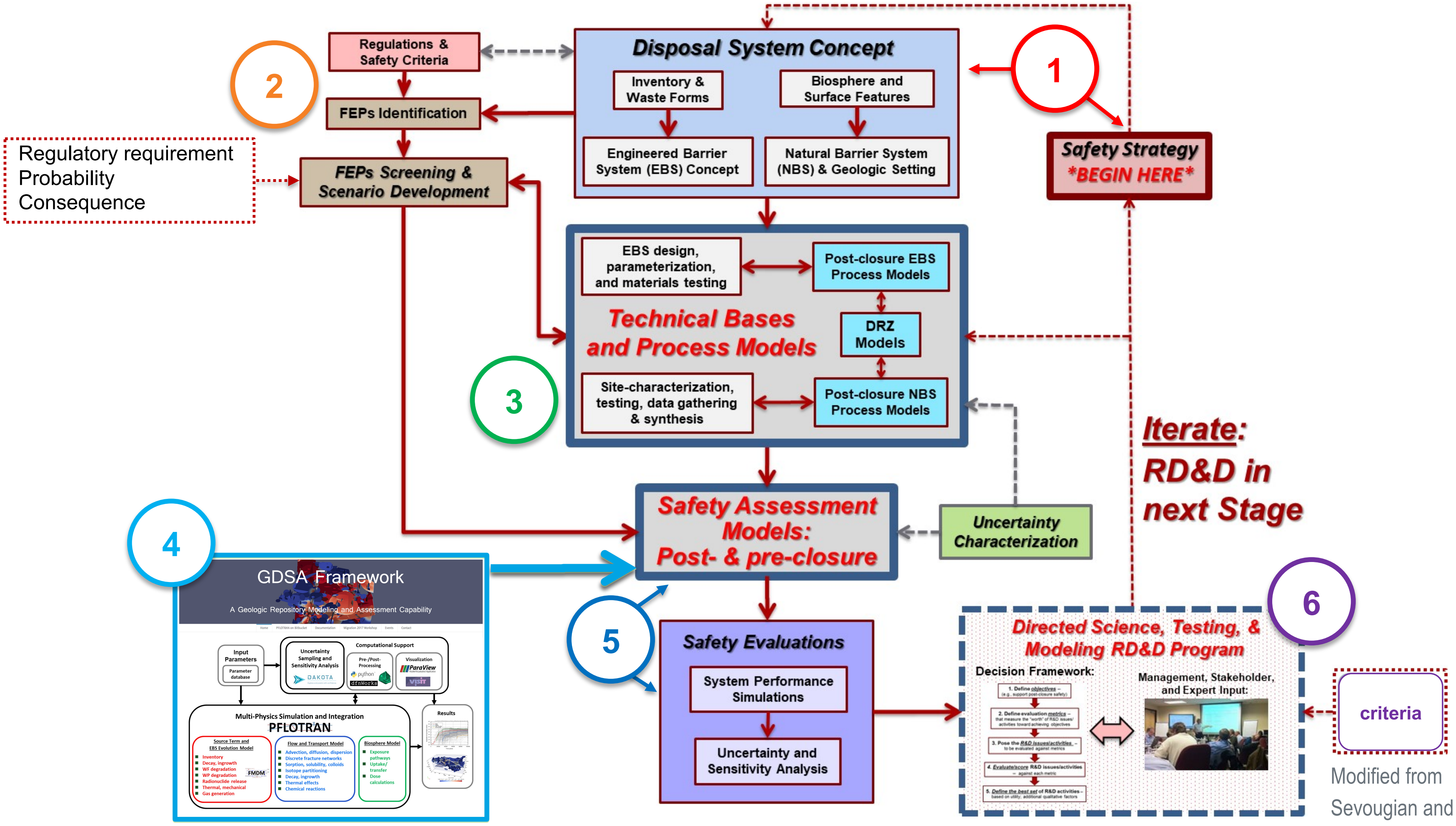
The Safety Assessment Process

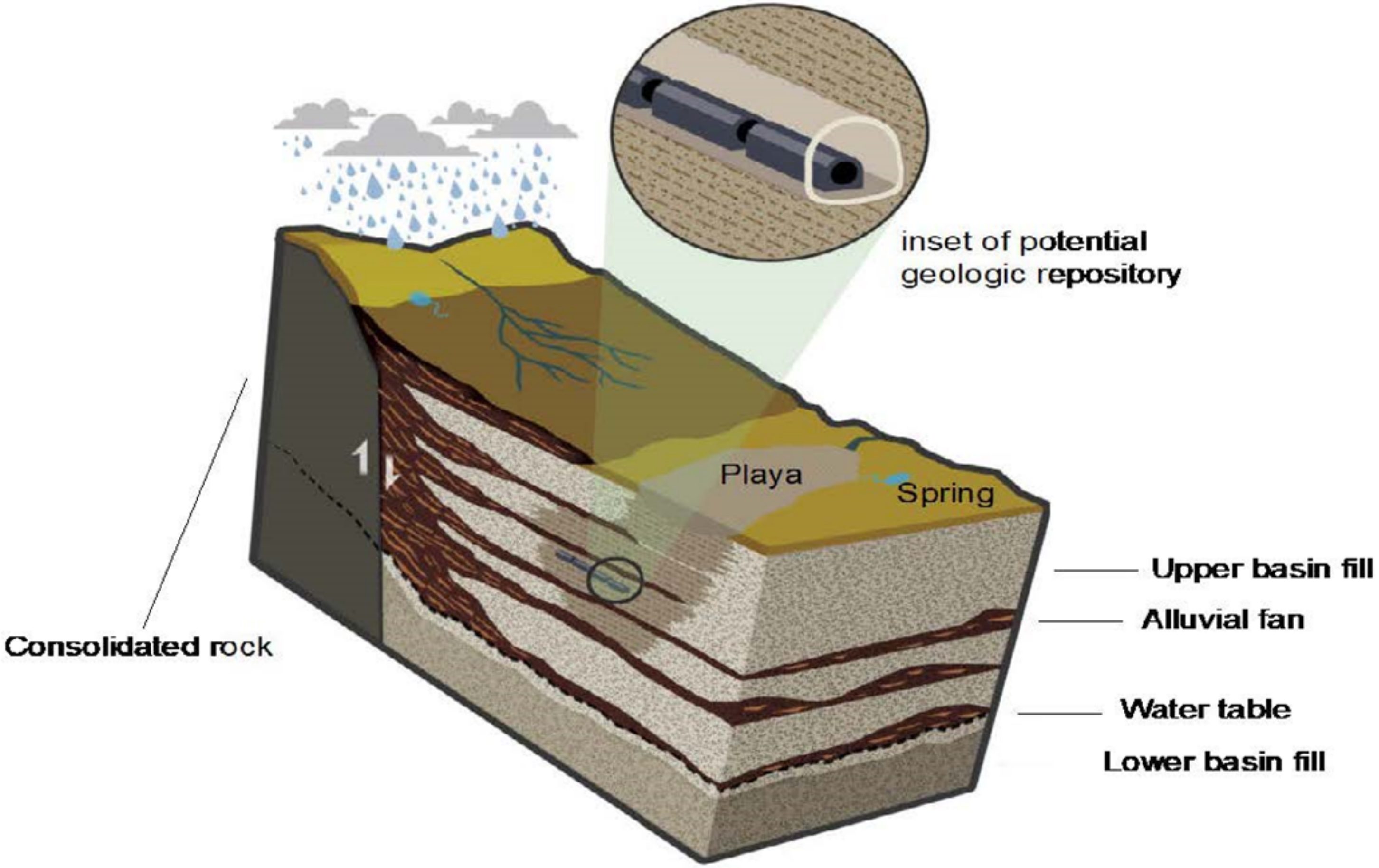


Modified from
Sevougian and MacKinnon (2017)

Unsaturated Alluvium Host Rock Characteristics

1

- Repository in the unsaturated zone (UZ)
- Complex stratigraphy and structure
- Lithologic heterogeneity
- Perched water tables and local aquifers
- Oxidizing in repository; reducing at some depth below water table

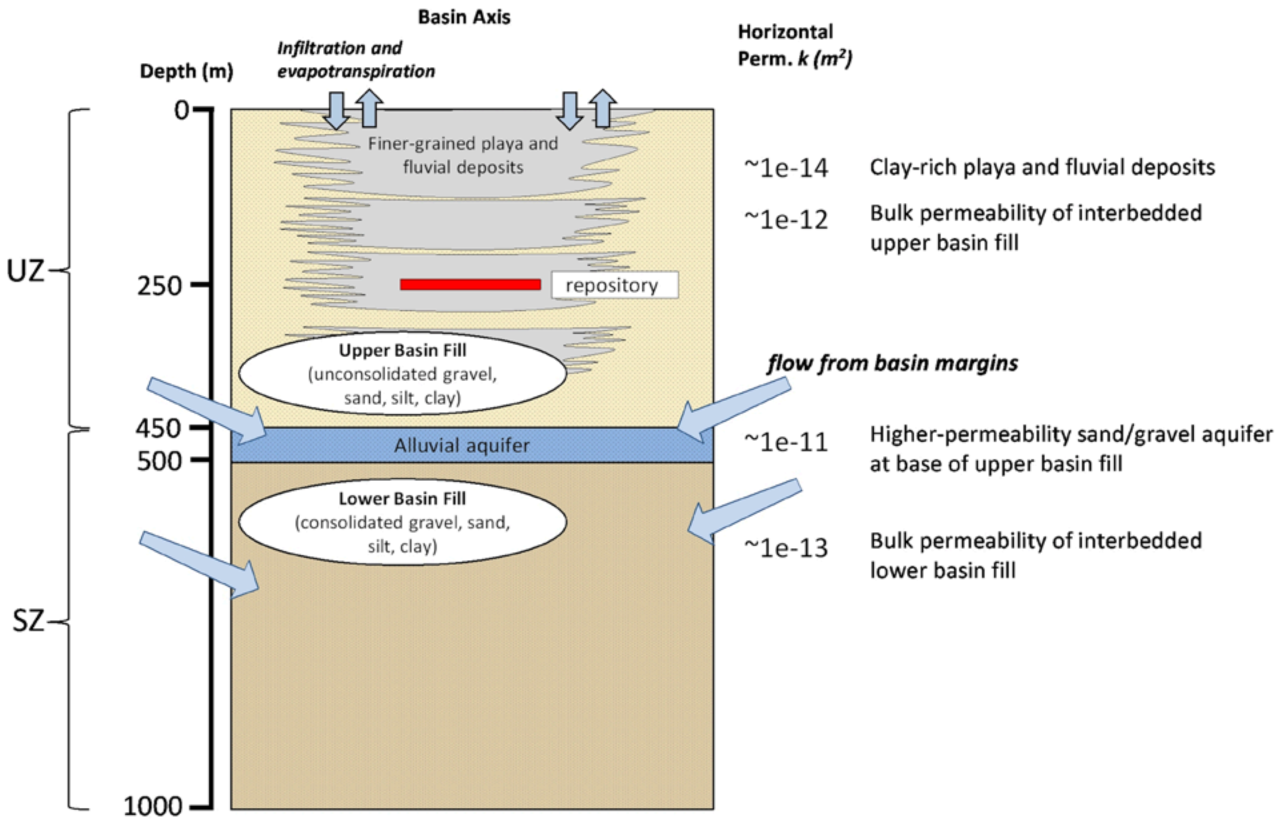


Mariner et al. 2018

Unsaturated Alluvium Post Closure Safety Strategy

1

- Containment
  - Corrosion resistant overpack
  - Low water saturation
- Limited Transport
  - Deep water table
  - Low effective permeability (k_{eff})
- Dilution
  - In saturated zone (SZ)
- Climate variability (arid to pluvial)
  - In some locations recharge has not occurred over the last 100,000 y
  - Under pluvial conditions, downward liquid flux may be 5 to 10 mm/yr
  - Saturation would increase only until k_{eff} balances the infiltration rate

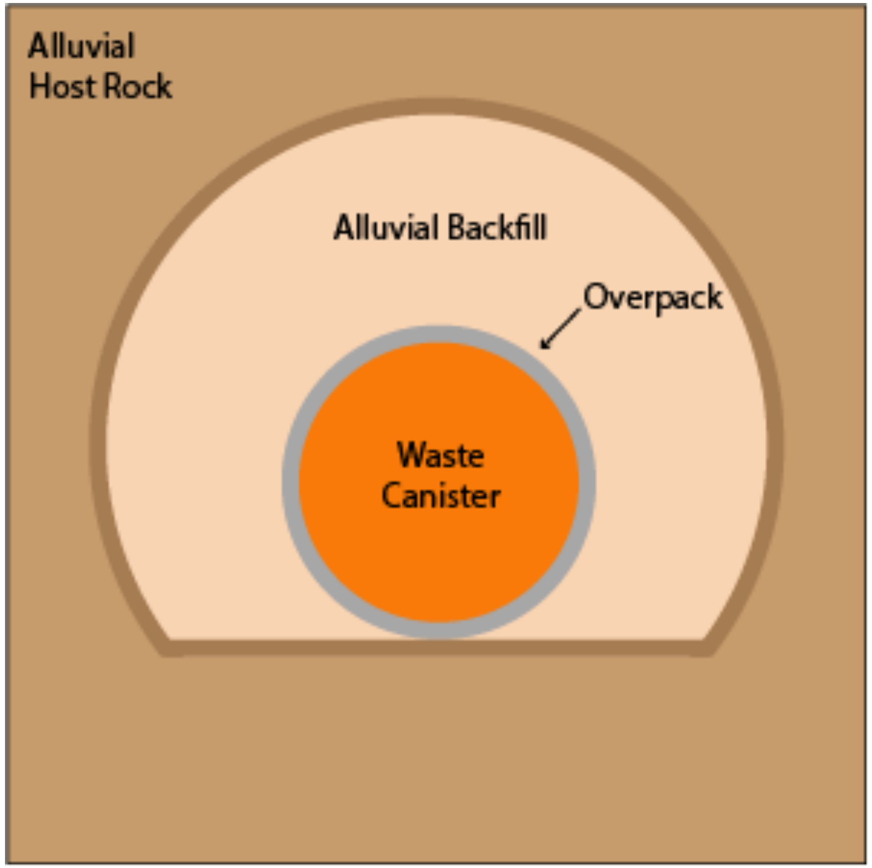


Mariner et al. 2018; Perry et al. 2018

Waste Form and Engineered Barrier in Unsaturated Alluvium

1

- Direct disposal of Dual Purpose Canisters (DPCs)
  - e.g., containing 24 or 37 pressurized water reactor (PWR) assemblies
- Overpack provides mechanical strength and appropriate protection against corrosion
- Crushed alluvium backfill provides shielding and protects against rockfall
- Thermal management achieved through waste package loading, aging, and spacing
- Maintain temperature <100 ºC and liquid saturation > 0 along axes of pillars



Sevougian et al. 2019

Knowledge and Capability Gaps

2 Criticality Consequence Analysis for Direct Disposal of DPCs

- What is the power output that can be sustained before driving water out of the package?
- What are impacts to radionuclide inventory?
- What are impacts to disposal system?

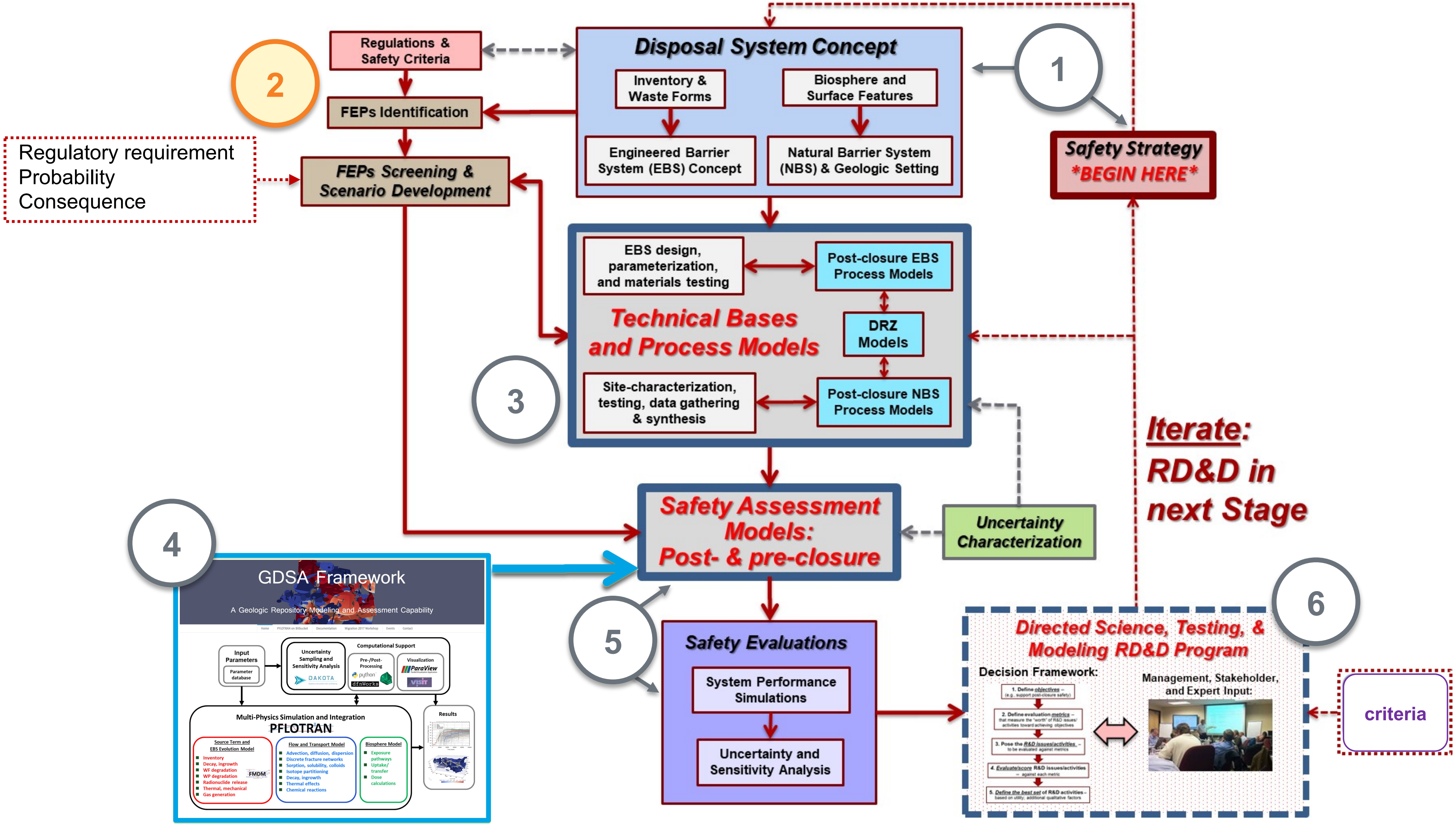
3 Geologic Framework Modeling: From Site Data to Simulation

- Complex structure and stratigraphy
- Spatial heterogeneity
- Geologic meshing

4 Integrated DPC/GDSA Process Model Capability Development

- Numerical methods for solution of highly nonlinear partial differential equations
- Temperature-dependent properties and processes
- Heat and radionuclide source terms associated with criticality event
- Fuel Matrix Degradation Model

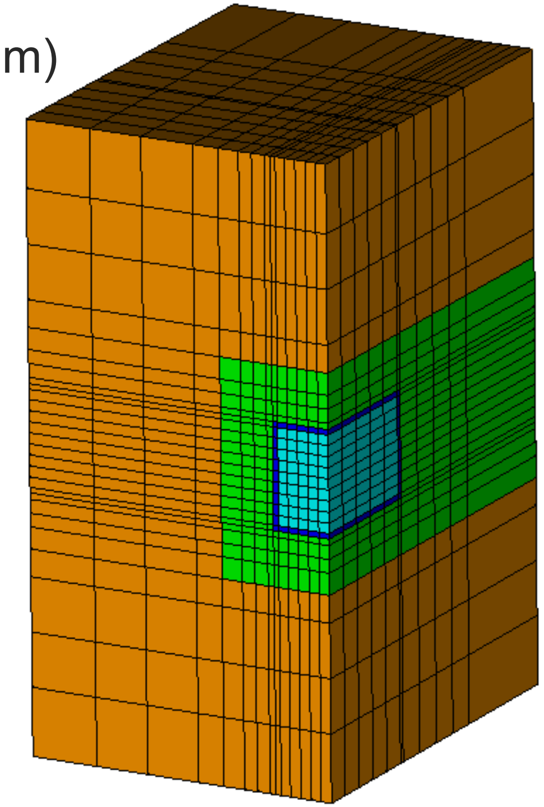
The Safety Assessment Process



Priority R&D – DPC Criticality Consequence Analysis

2

- Geometry
  - Consistent with GDSA Unsaturated Alluvium reference case (Sevougian 2019; Hardin and Kalinina 2016)
  - 40 m drift spacing, 40 m center-to-center spacing within drift
  - Square cross-section for drift (4m x 4m) and DPC (1.67 m x 5 m x 1.67 m)
  - 0.1 m overpack/shell
- Properties
  - Permeability 10^{-14} m^2 (alluvium) 10^{-13} m^2 (backfill)
  - Thermal conductivity = 1 W/(m·K) (dry) and 2 W/(m·K) (wet)
  - Canister internals = hydraulic properties of backfill
- Scenario
  - Postclosure with 37-PWR DPC and backfilled drifts
  - Top of DPC shell breached at 9000 years allowing water to enter
  - Initiate criticality event when canister is filled with water
- Cases
  - 10 mm/year and 2 mm/year percolation into waste package
  - Range of power outputs for criticality event

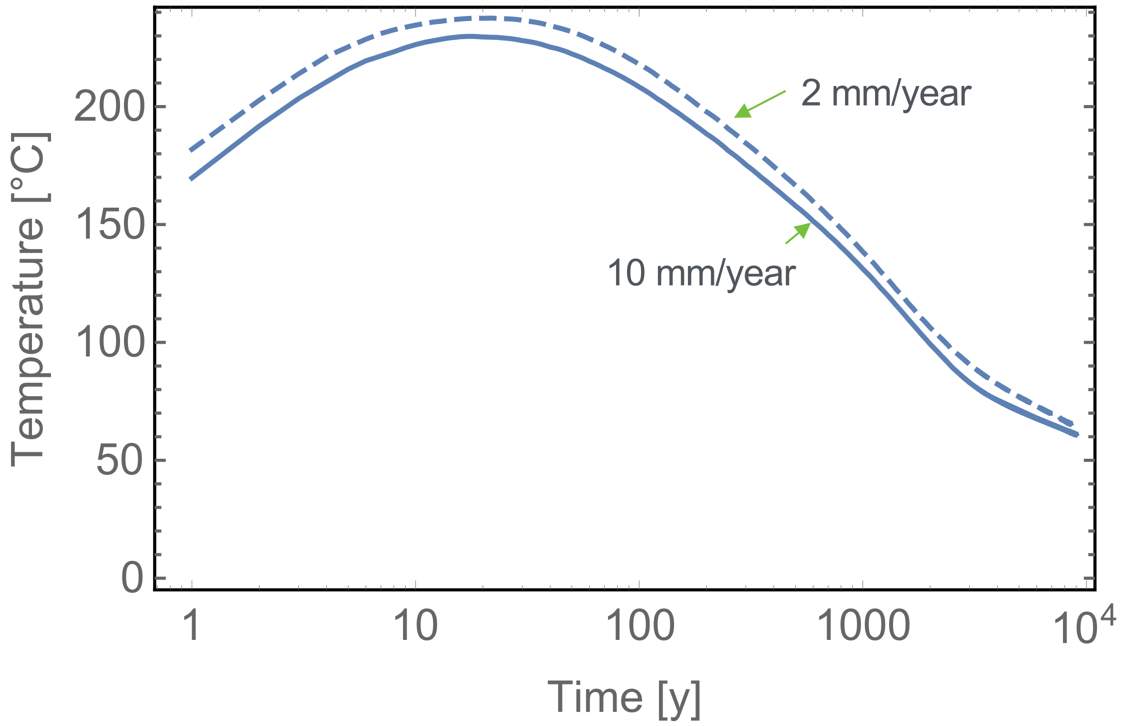


Price et al. 2019; Price 2020

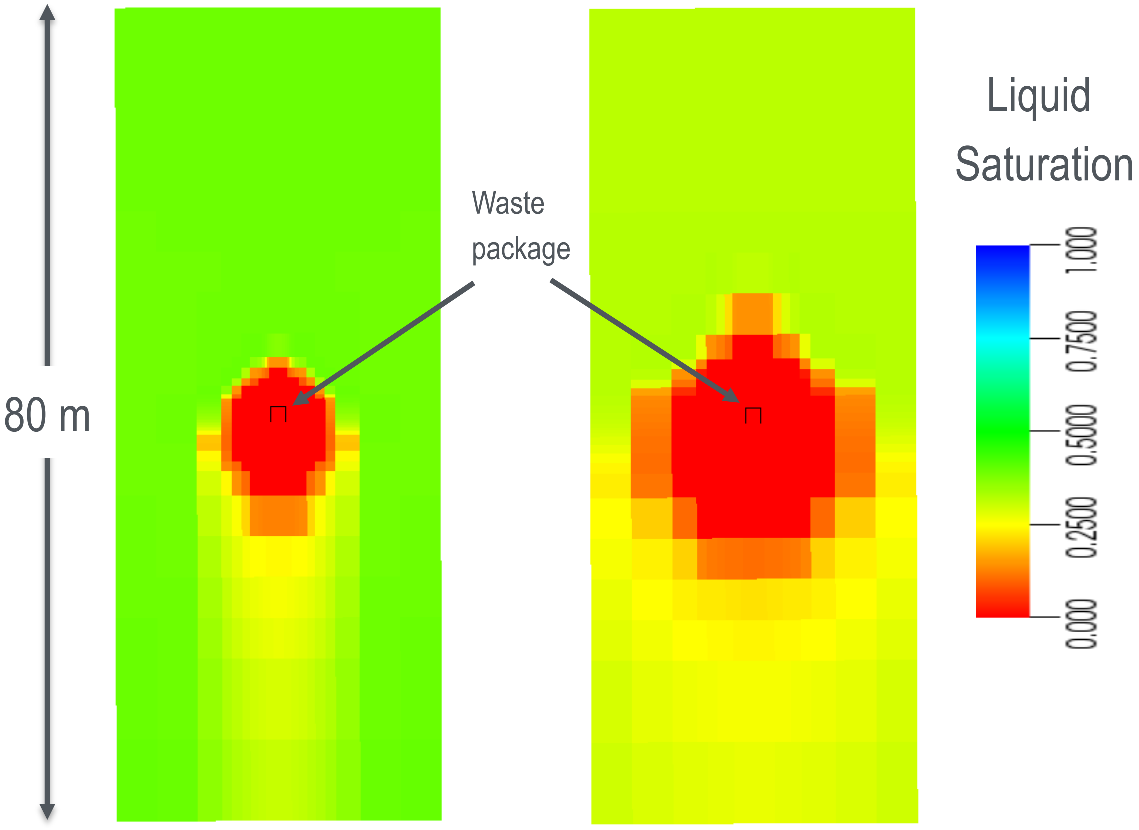
37-PWR DPC in Unsaturated Alluvium: Before Breach

2

Temperature up to 9000 y



Maximum dryout
40 m x 80 m vertical cross sections



10 mm/year
500 y postclosure

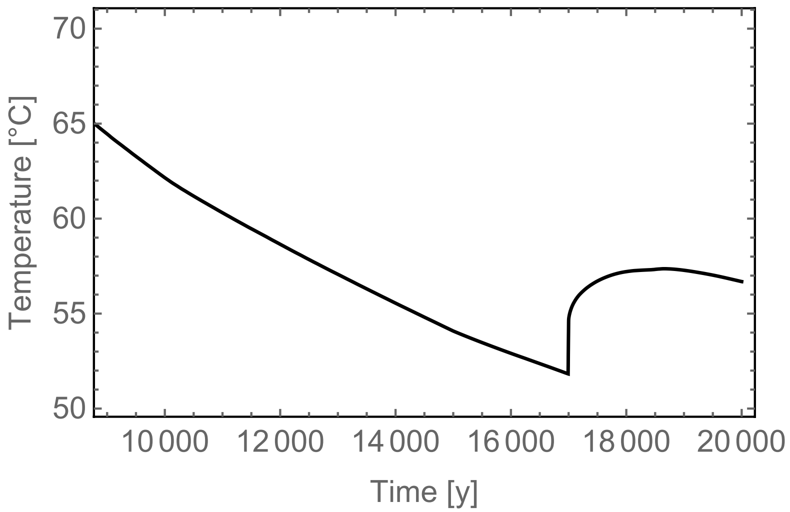
2 mm/year
750 y postclosure

Price et al. 2019; Price 2020

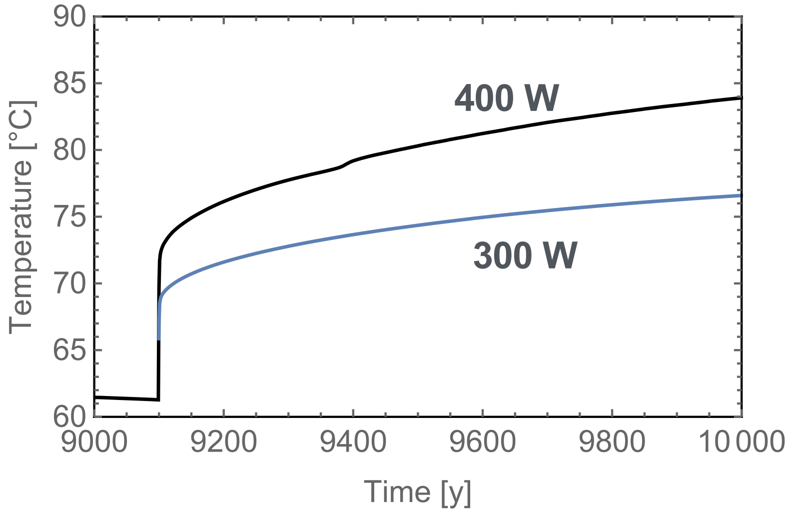
37-PWR DPC Hypothetical Criticality Events

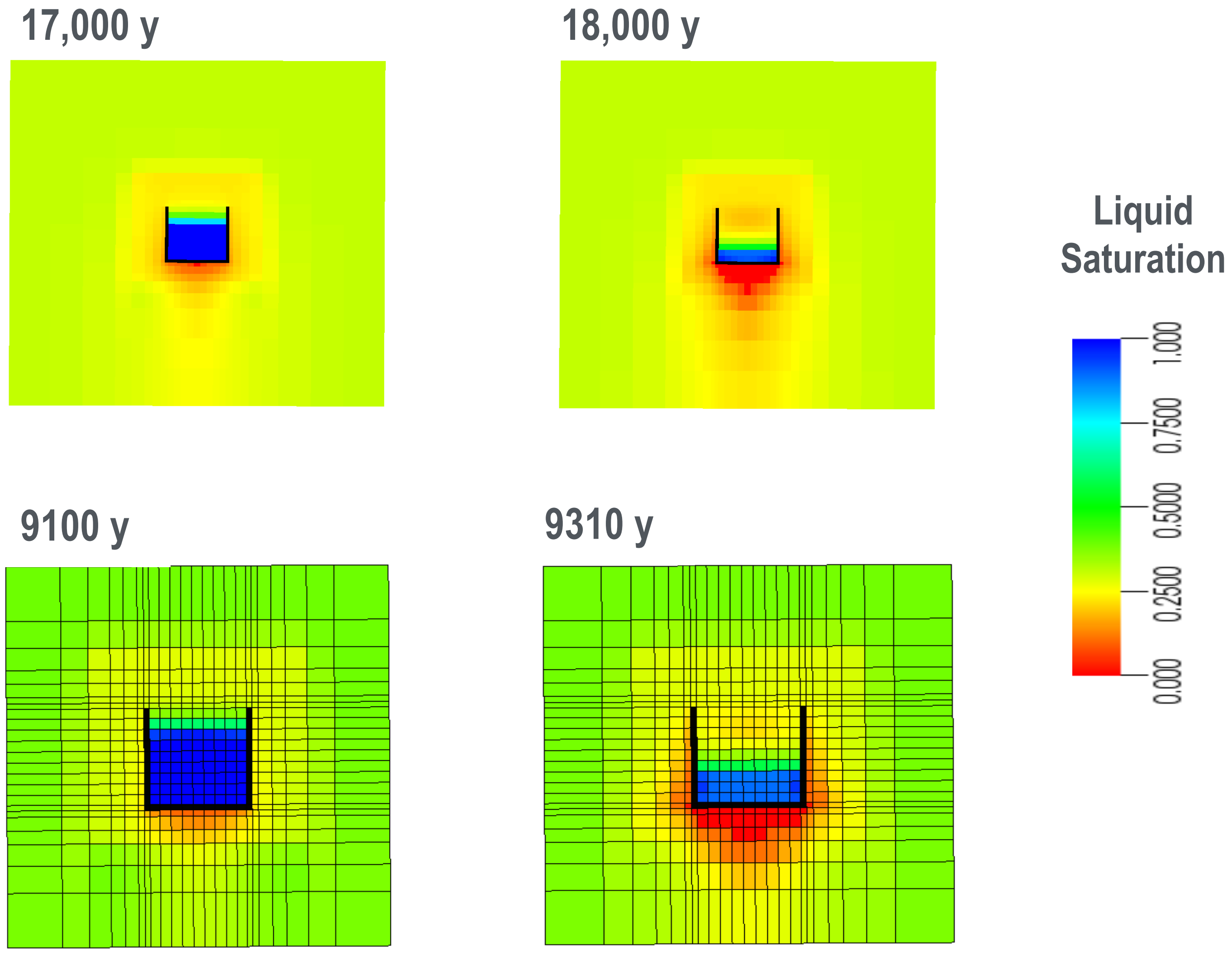
2

2 mm/year
100 W event



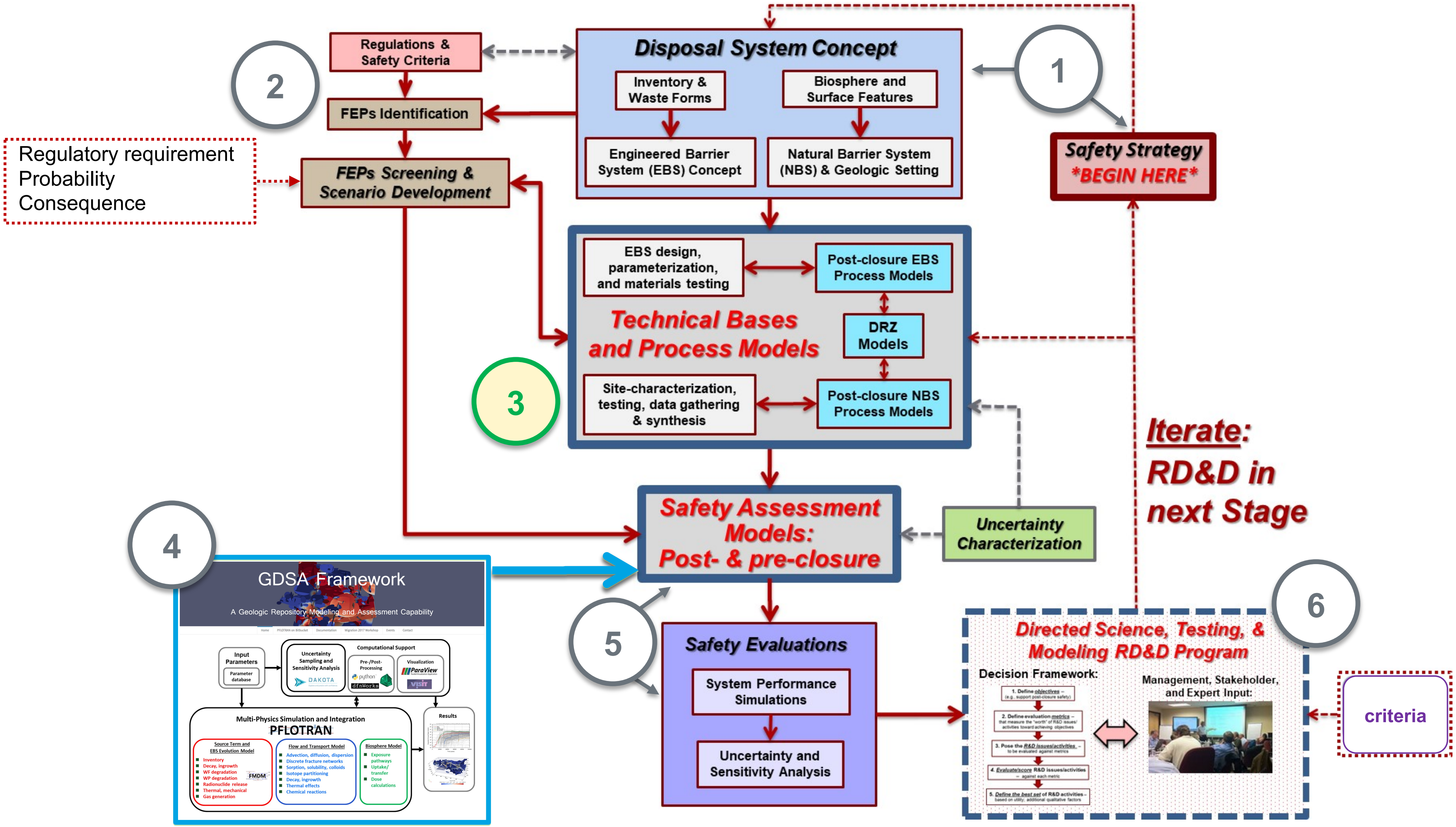
10 mm/year
400 W event





Price et al. 2019; Price 2020

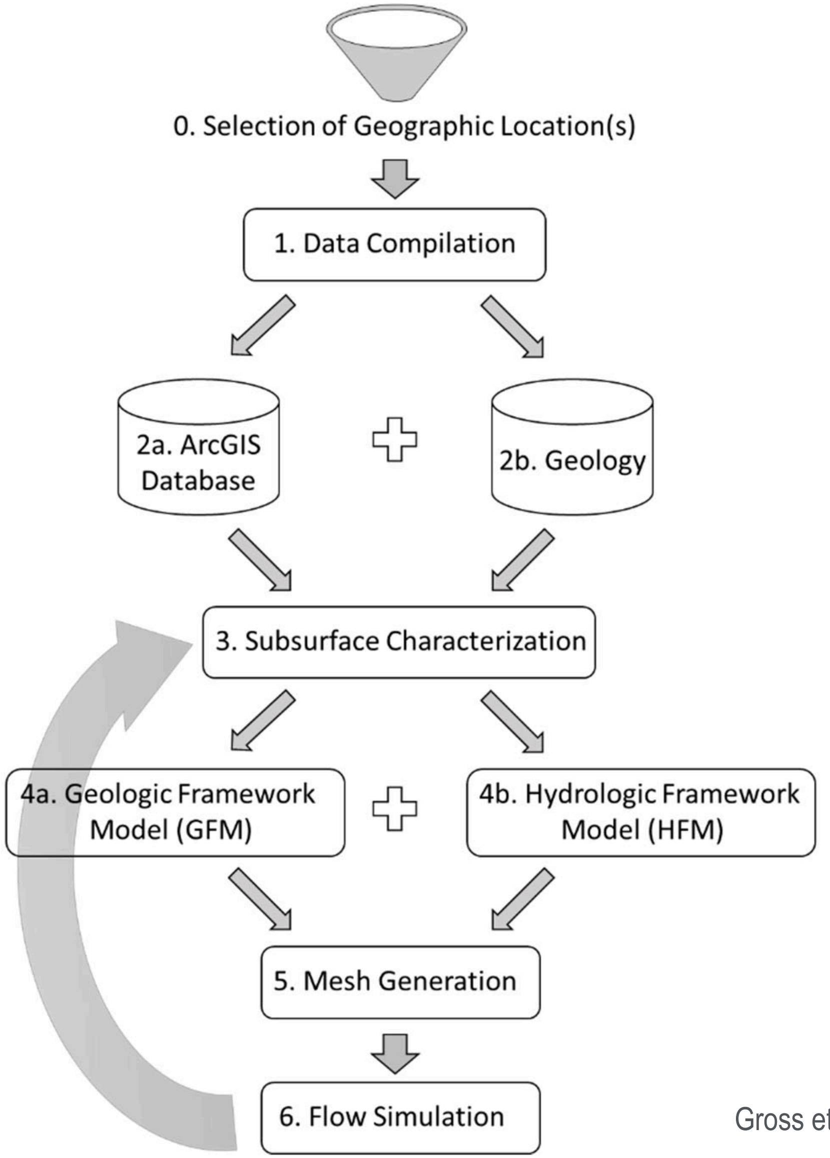
The Safety Assessment Process



Priority R&D – 3-Dimensional Geologic Framework Model (GFM)

3

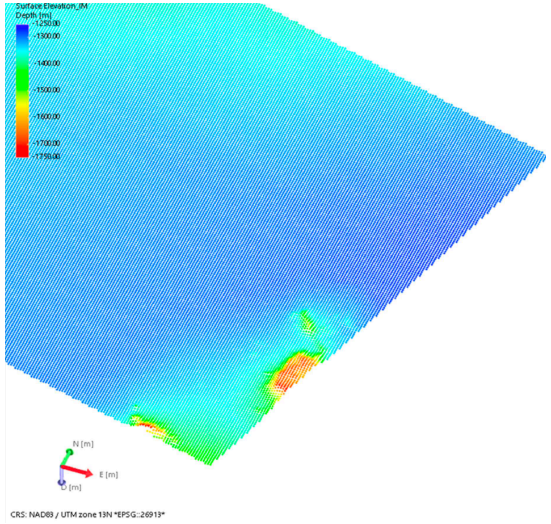
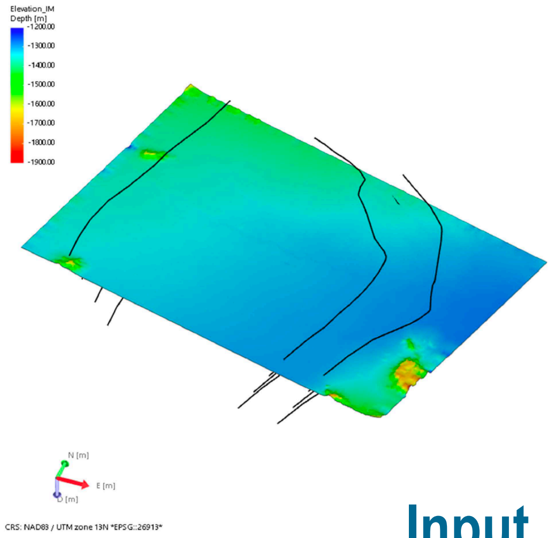
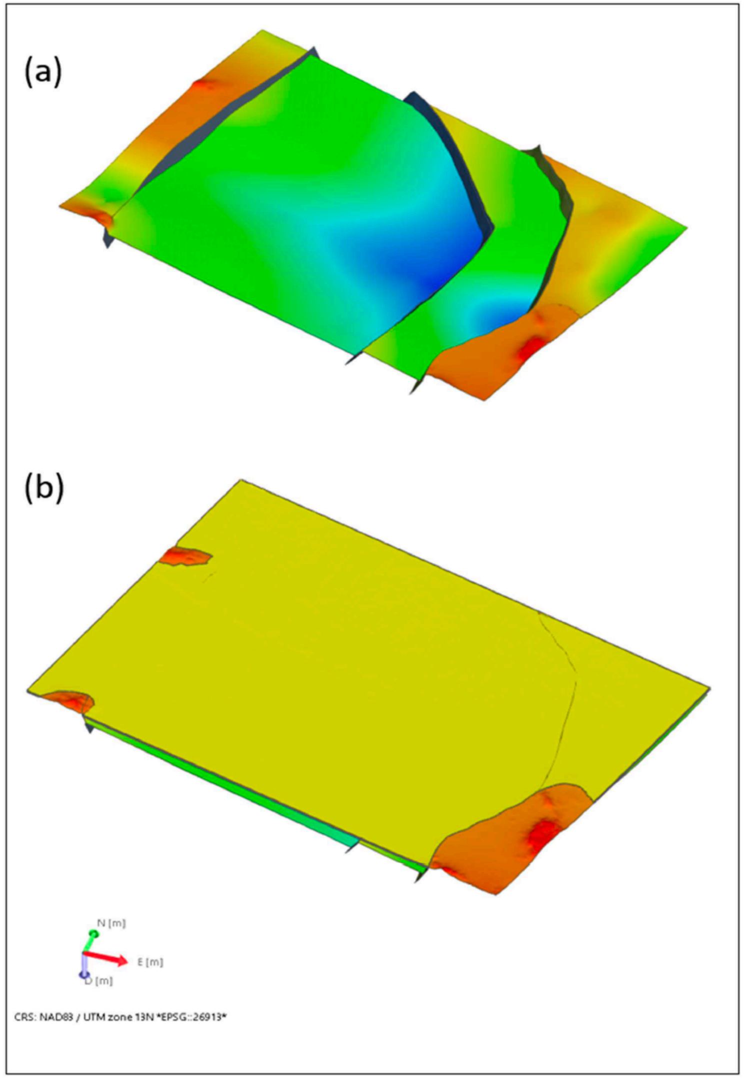
- Constructed from surfaces (stratigraphic horizons, faults) derived from 3D seismic surveys and borehole data
- Informed by digital elevation maps, geologic maps, cross sections, and conceptual models
- May also hold lithologic data, hydrologic data
- Iteration improves subsurface characterization

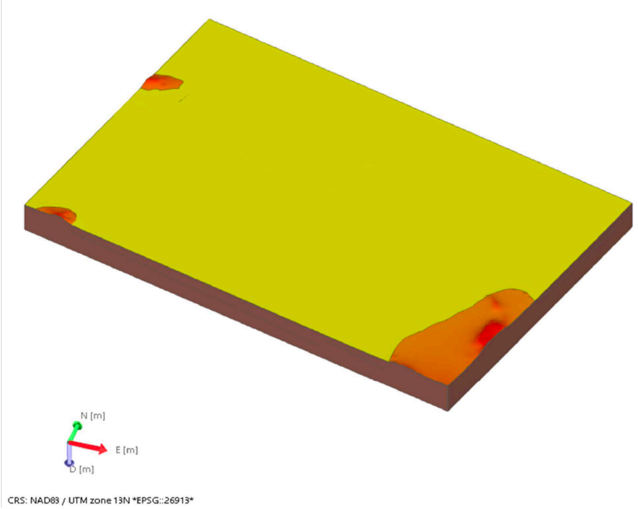
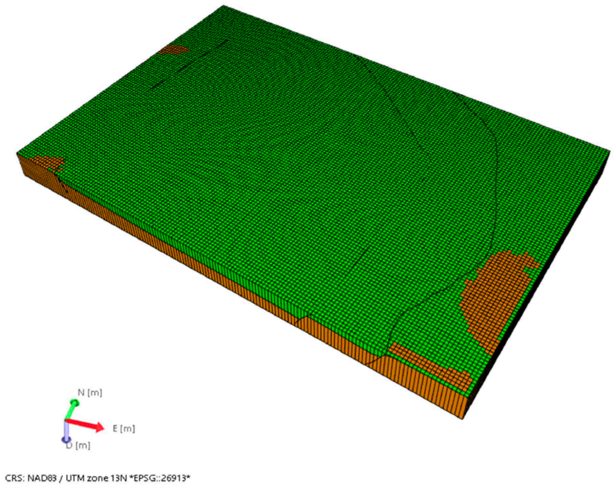


Gross et al. 2019

Complexity Makes Alluvial Basin GFM a Useful Test Case

3

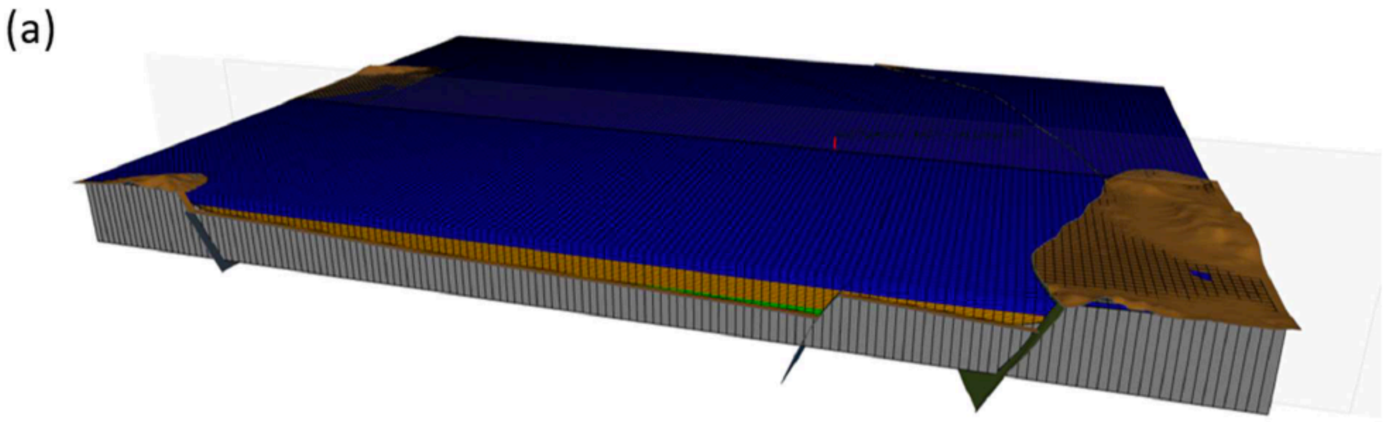



Input → → Surfaces → → Volumes

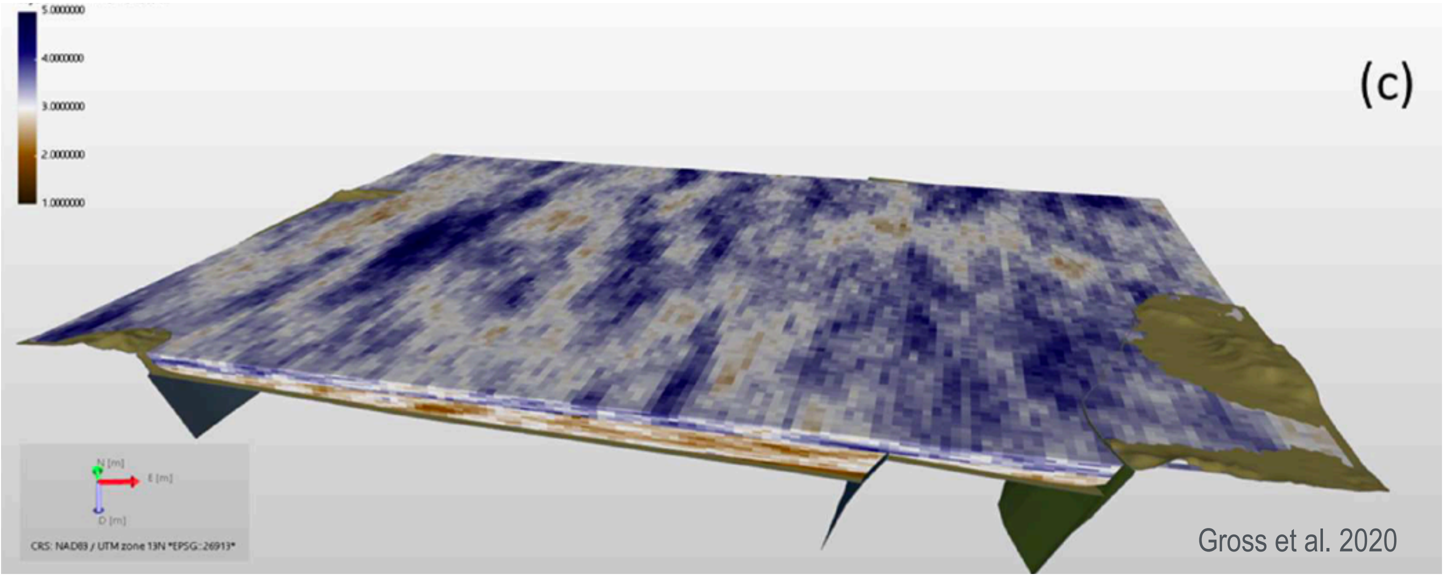
Gross et al. 2020

Adding Lithofacies and Hydrologic Properties

- Lithofacies
  - 3 alluvial facies
  - Bedrock



- Geostatistical distributions describe hydrologic properties
  - Porosity
  - Permeability

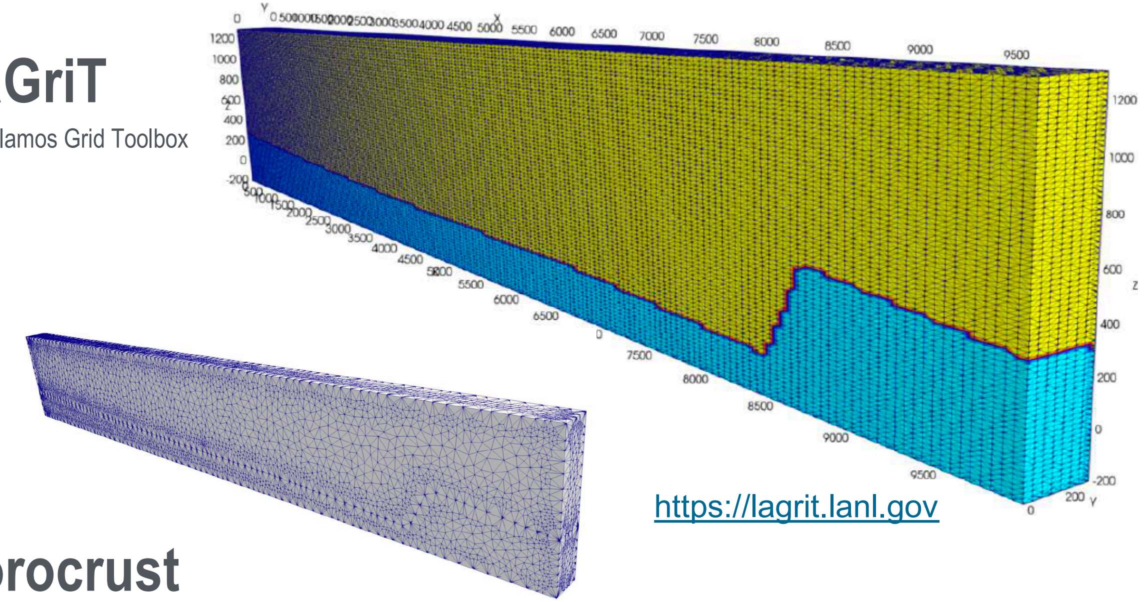


GFM to Computational Mesh

3

- LaGriT
  - Automate information processing and workflow to create computational mesh from GFM
  - Versatile tools for user-controlled generation of Voronoi mesh using Delauney triangulation
- VoroCrust
  - The first provably correct algorithm for conforming Voronoi tessellation
  - Automated algorithm simplifies meshing
  - Developing: User-specified features, parallel processing, anisotropic cells

LaGriT
Los Alamos Grid Toolbox



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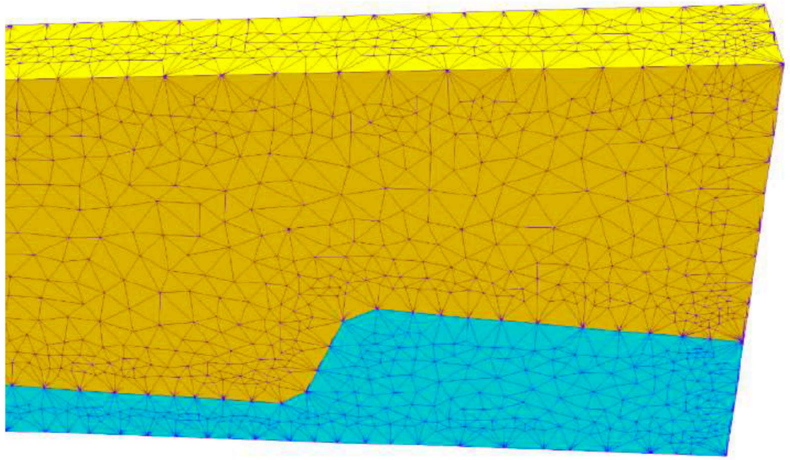
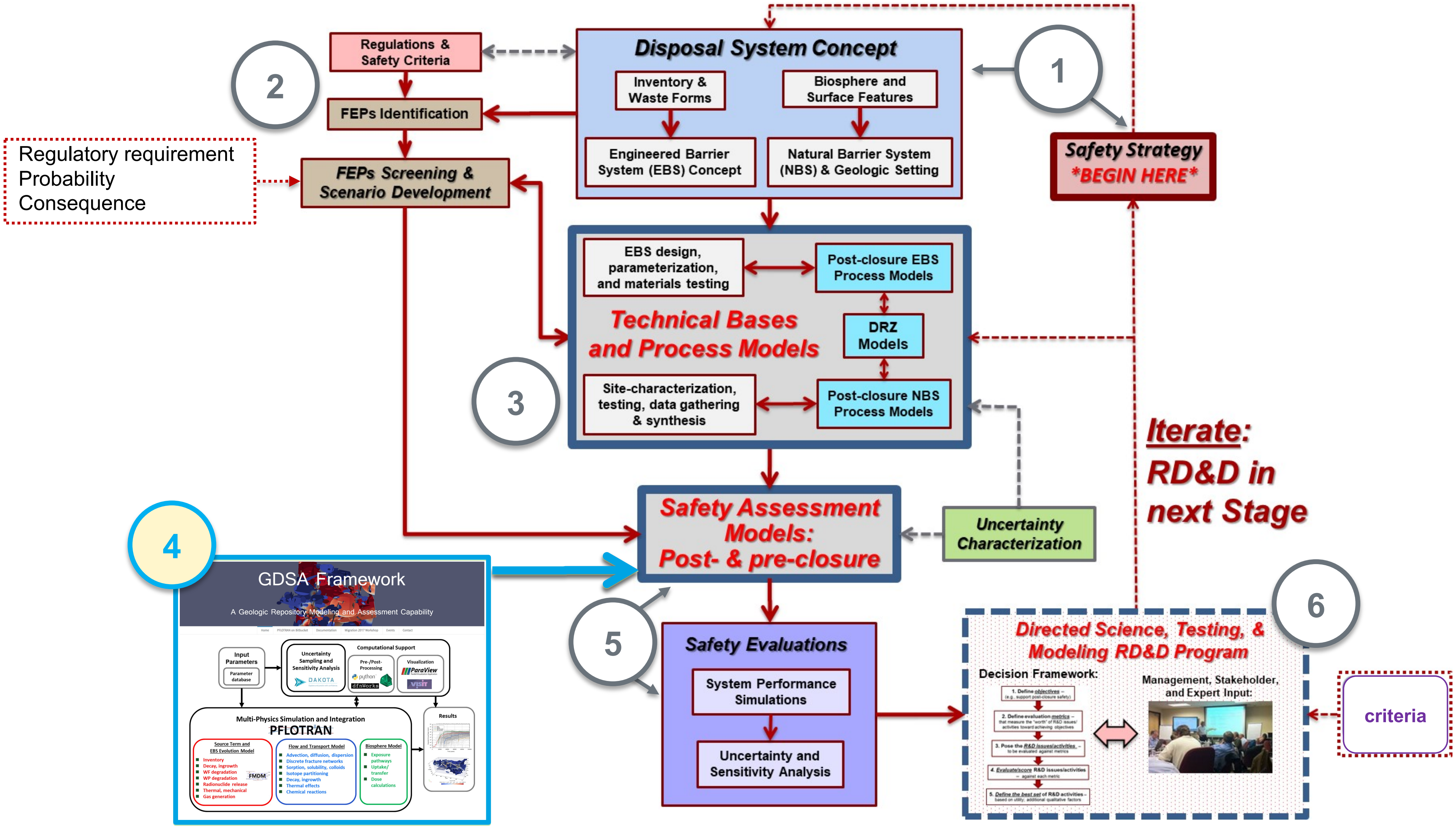
Vorocrust



https://vorocrust.sandia.gov Gross et al. 2020

The Safety Assessment Process

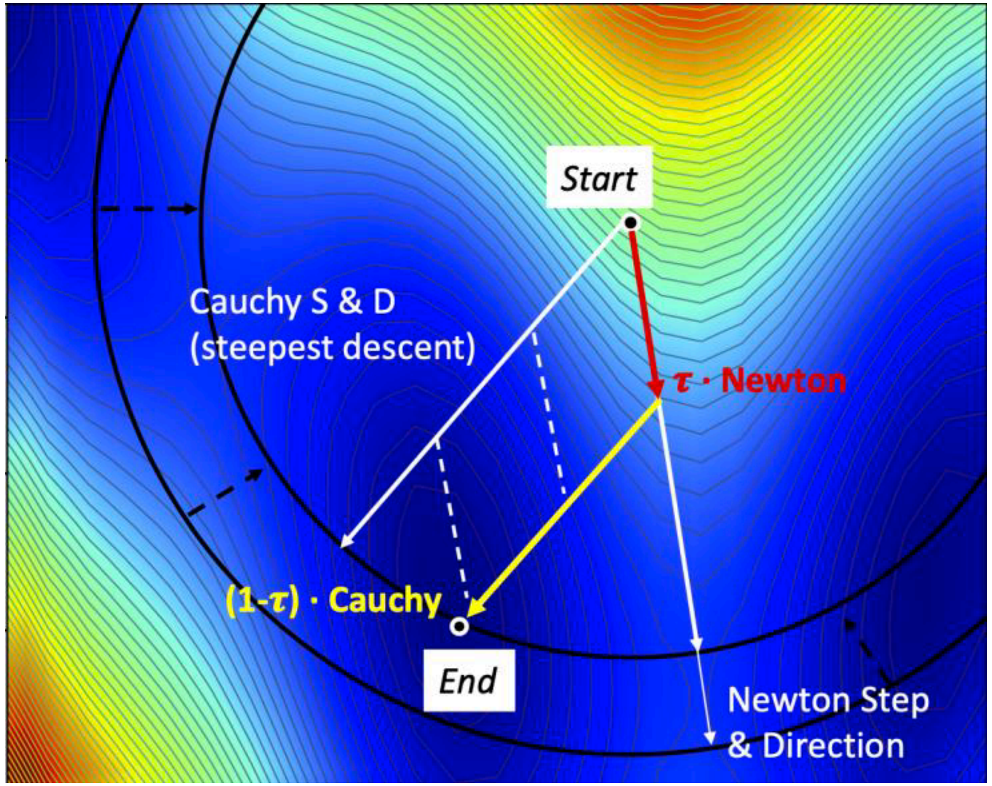


Advanced Nonlinear Solvers

Minimize the residual of a multi-dimensional function

1. Newton Step and Direction overshoots.
2. Newton Trust Region (NTR) truncates the step to keep it within the region in which minimum is predicted to exist.
3. Cauchy Step and Direction follows the steepest descent.
4. Newton Trust Region Dogleg Cauchy (NTRDC) combines NTR with Cauchy to find the minimum in a single iteration.

NTRDC reduces computation time by a factor of approximately 35.

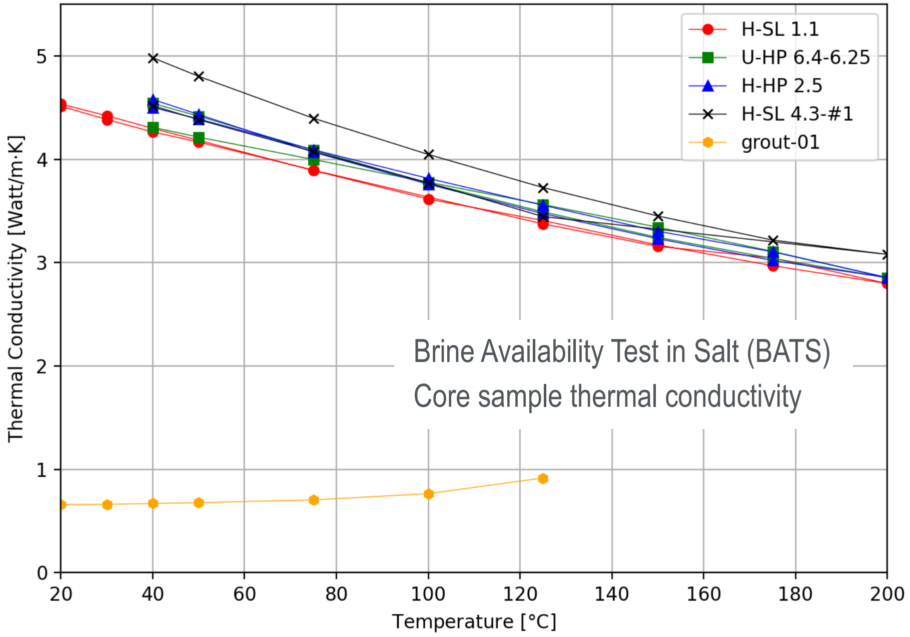


A demonstration of the NTRDC method. The algorithm corrects the appropriate Newton step-and-direction by reducing the trust region and adds Cauchy step-and-direction if the solution update can be improved further in the same iteration.

Mariner et al. 2020

Temperature-Dependent Thermal Conductivity

- Temperature-dependent processes
  - Corrosion
  - Mineralogical changes
  - Aqueous speciation (radionuclide solubilities)
  - Thermal expansion of solids
  - Buoyancy-driven fluid flow



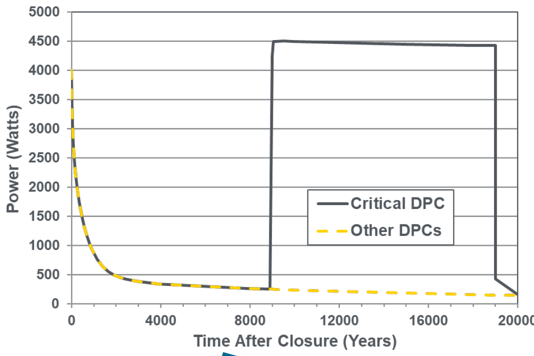
Kuhlman et al. 2020;
LaForce et al. 2020

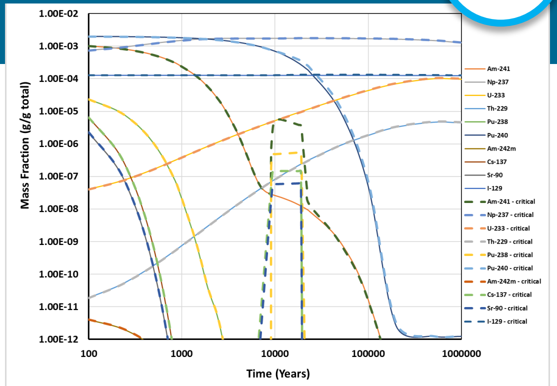
Name	Function
Default	$\kappa_T^D(S_l)=\kappa_T^{dry}+\sqrt{S_l}\left(\kappa_T^{wet}-\kappa_T^{dry}\right)$ (24)
Constant	$\kappa_T=\kappa_T^C$ (25)
Linear Resistivity	$\kappa_T(S_l,T)=\frac{\kappa_T^D(S_l)}{a_1+a_2(T-T_{ref})}$ (26) Granite, basalt, shale, and salt
Cubic Polynomial	$\kappa_T(S_l,T)=\kappa_T^D(S_l)\left[1+\beta_1(T-T_{ref})+\beta_2(T-T_{ref})^2+\beta_3(T-T_{ref})^3\right]$ (27) Various soils at temperatures up to 1700 °C
Power Law	$\kappa_T(S_l,T)=\kappa_T^D(S_l)\left(\frac{T-T_{ref}}{300}\right)^{\gamma}$ (28) Crystals, ceramics, and engineering materials

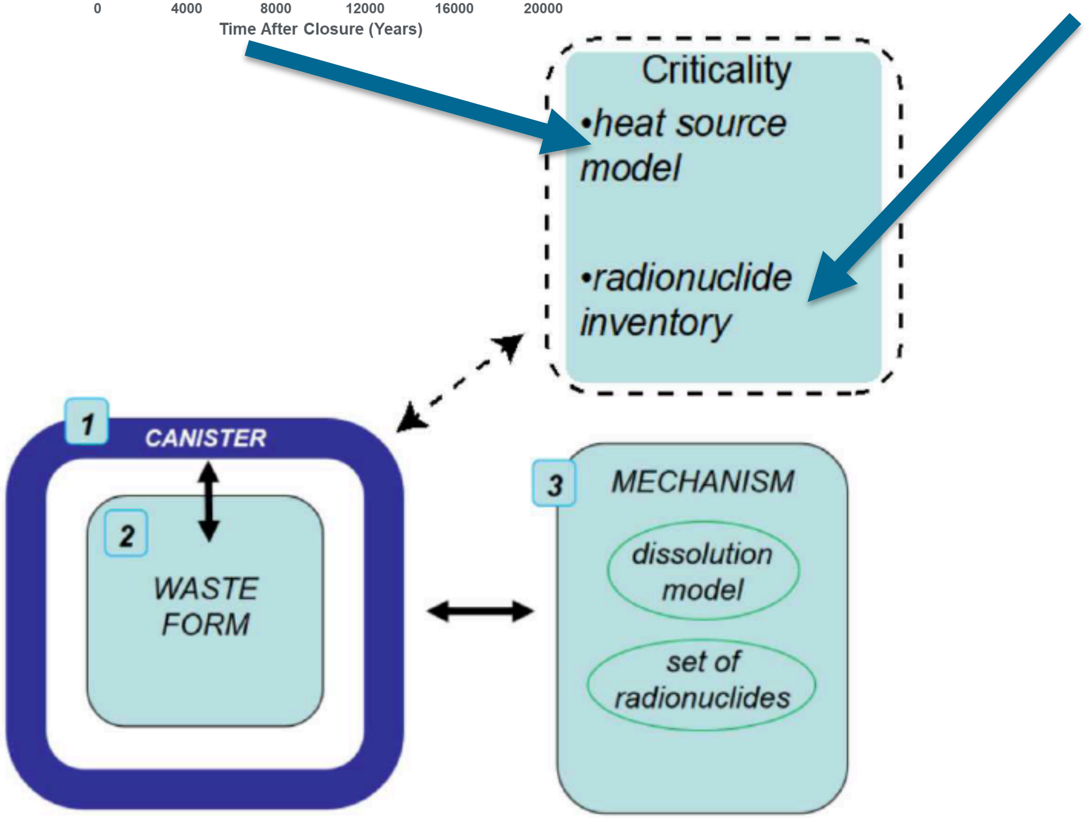
Criticality Submodule

4

- Capability added to PFLOTRAN's Waste Form Process Model
- Reads files containing
  - Power as function of time
  - Radionuclide inventory as function of time
- Future: integrate with neutronics calculations to model criticality power output as a function of water saturation





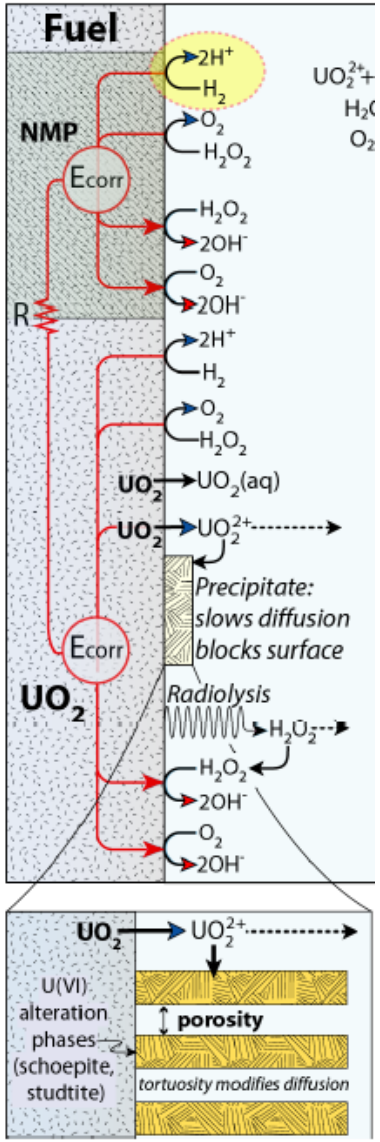


Price et al. 2019

Fuel Matrix Degradation Model (FMDM)

4

- 1-D reactive transport model to simulate dissolution of spent nuclear fuel (SNF) as a function of
  - Radiolysis
  - Diffusion of reactants through growing alteration layer
  - Interfacial corrosion potential
- GDSA Framework integration:
  - Implement efficient numerical methods for mechanistic coupling
  - Speed computation using machine-learned surrogate models
  - Future: Couple to evolution of in-package chemistry given specific conditions
  - Future: Model validation against SNF dissolution experiments



(Jerden et al. 2018; Mariner et al. 2020)

Priority R&D – Forward Look at GDSA-DPC Integration

Prioritization of Cross-Cutting Research & Development Activities:
High-Temperature Shale Reference Case, Disposal of Dual Purpose Canisters, and Geologic Disposal Safety Assessment

- Representative waste package loading from database at Oak Ridge National Laboratory
  - UNF ST&DARDS (Used Nuclear Fuel Storage, Transportation & Disposal Analysis Resource and Data System)
- Temperature dependent reactions
  - Bentonite mineralogy and porewater chemistry
  - Radionuclide solubility and sorption
- Corrosion models
  - Temperature-dependent, material-specific
  - Waste package
  - Cladding
  - Neutron absorbers
- Thermal-Hydrological-Mechanical evolution of the near field

Price 2020;
Freeze and Howard 2020;
Stein et al. 2020

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