SAND2018-5483PE

Spent Fuel and Waste Science and Technology

SFWST – Disposal in Argillite R&D

PFLOTRAN THC Model
3D Single Waste Package Test Case

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Sandia National Laboratories (SNL)

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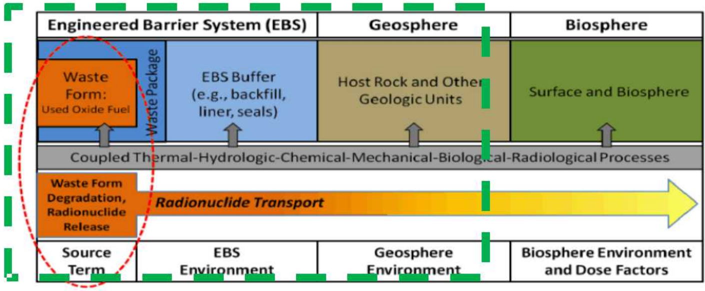
Argillite Disposal R&D

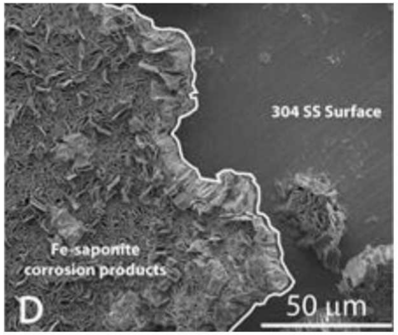
- **Reactive-transport modeling (THC) with decay heat effects**
  - 1D → 3D EBS Representation
- **Engineered barrier system (EBS) model integration with performance assessment (PA)**
- **Thermodynamic modeling of barrier material interactions (clay, cement, metal) and thermodynamic database (TDB) development**
- **Clay interaction experiments:**
  - **High temperature mineral phase stability, clay – metal interactions (waste package material (steel) corrosion)**
  - **Low-T RN sorption/diffusion in bentonite & modeling**
- **High temperature coupled thermal-hydrological-mechanical-chemical (THMC) modeling**
- **Spent fuel matrix degradation model development**
- **International collaborations: FEBEX-DP (GRIMSEL URL), DECOVALEX19, SKB EBS Task Force, Mont Terri/Bure URLs (France)**

GDSA PA Level Of Integration



International Collaboration: FEBEX-DP

Clay-Metal Interactions



Steel Corrosion

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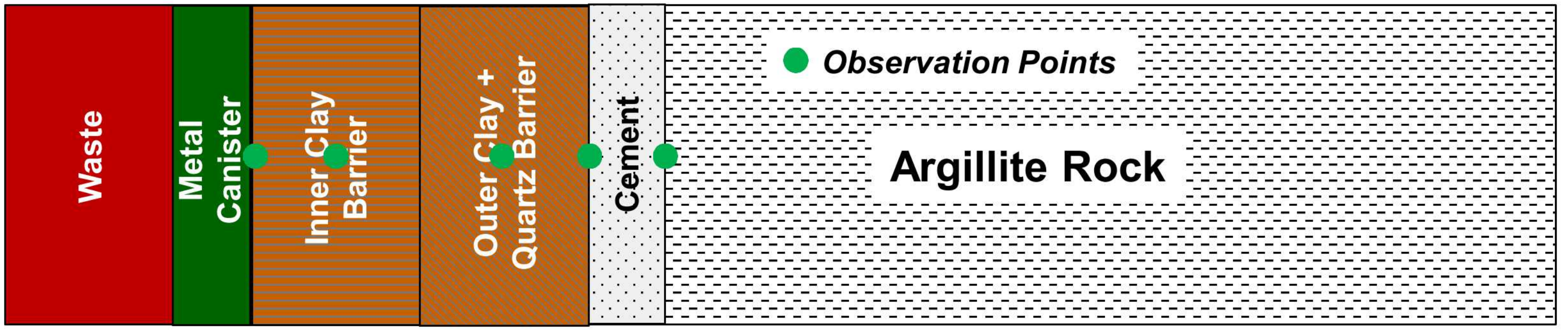
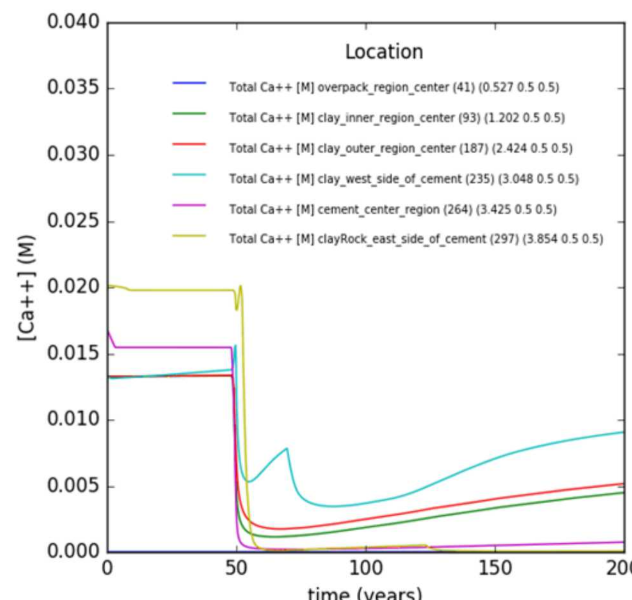
PFLOTRAN EBS High-T Reactive Transport Simulations (THC): 1D Layered EBS



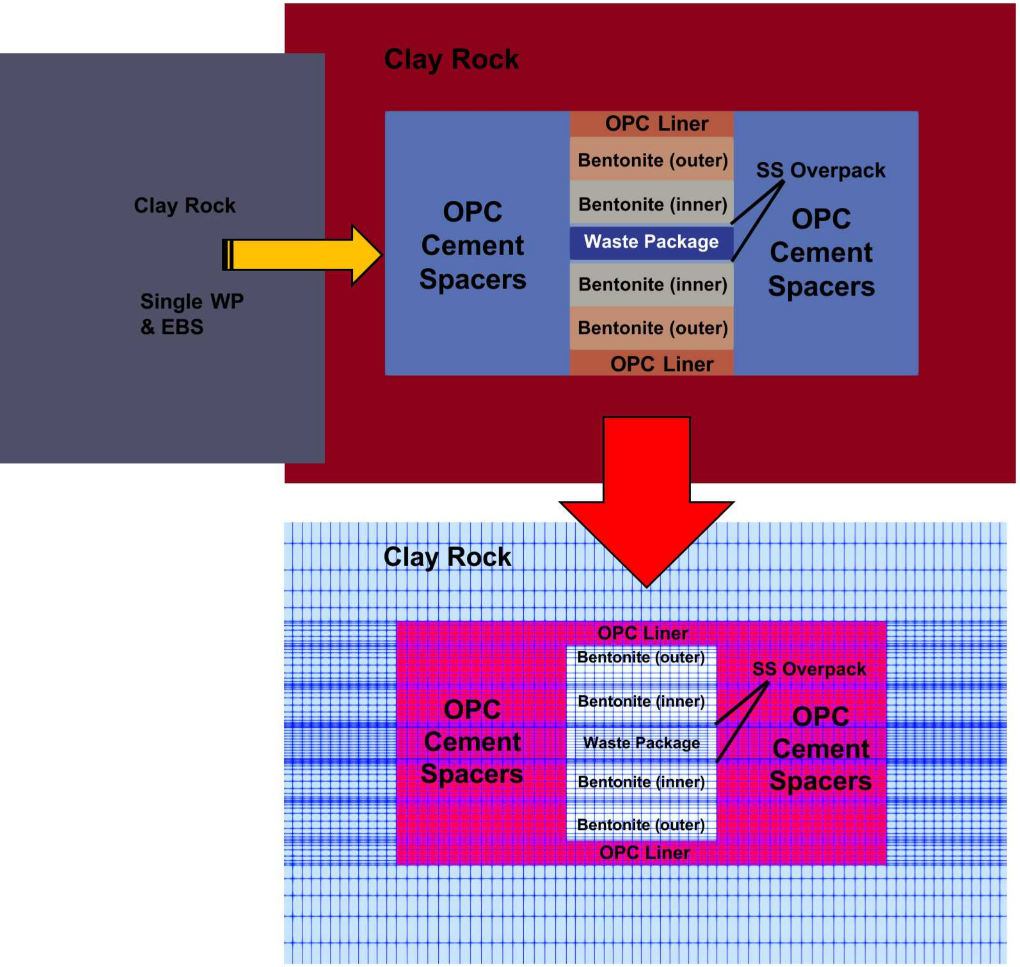
0.475 m 0.1 m 1.24 m 1.24 m 0.75 m >>10 m (RED Font: Domains Considered)

- **1D reactive transport (RT) PFLOTRAN calculations:**
  - 24 minerals, 4 initial pore solution chemistries
  - Efficient model scoping in High Performance Computing (HPC) platforms
  - Evolution of mineral volume fraction and aqueous speciation with time: equilibrium & kinetics
- **Temperature effects case:**
  - SNF decay heat profile
  - Capture mineral phase transitions:

  gypsum → anhydrite + 2 H_2O

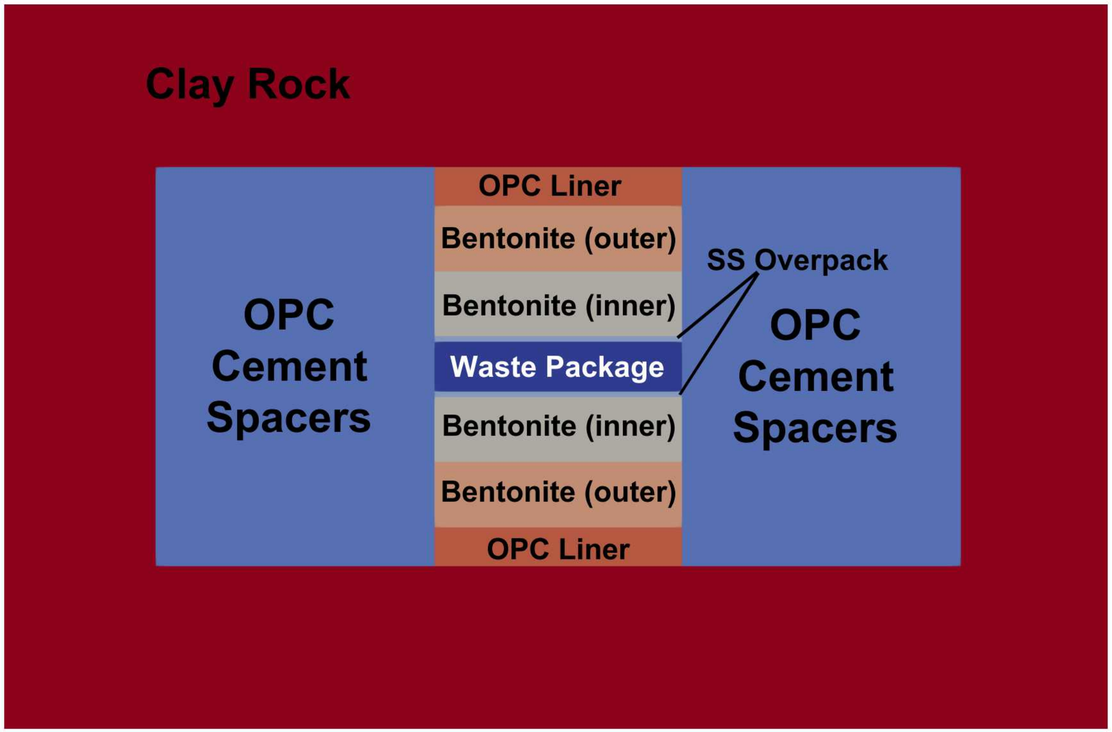


PFLOTRAN EBS High-T Reactive Transport Simulations (THC): 3D Layered EBS



- **3D THC Simulations**
- **Unstructured Mesh**
- ***Dimensions***
  - *Waste Canister Length: 4.7 m*
  - *Waste Canister diameter: 1.15 m*
  - *Overpack Thickness: 0.1 m*
  - *Buffer Layer 1 & 2 Thicknesses: 1.24 m*
  - *Spacer Cement Length: 5.3 m*

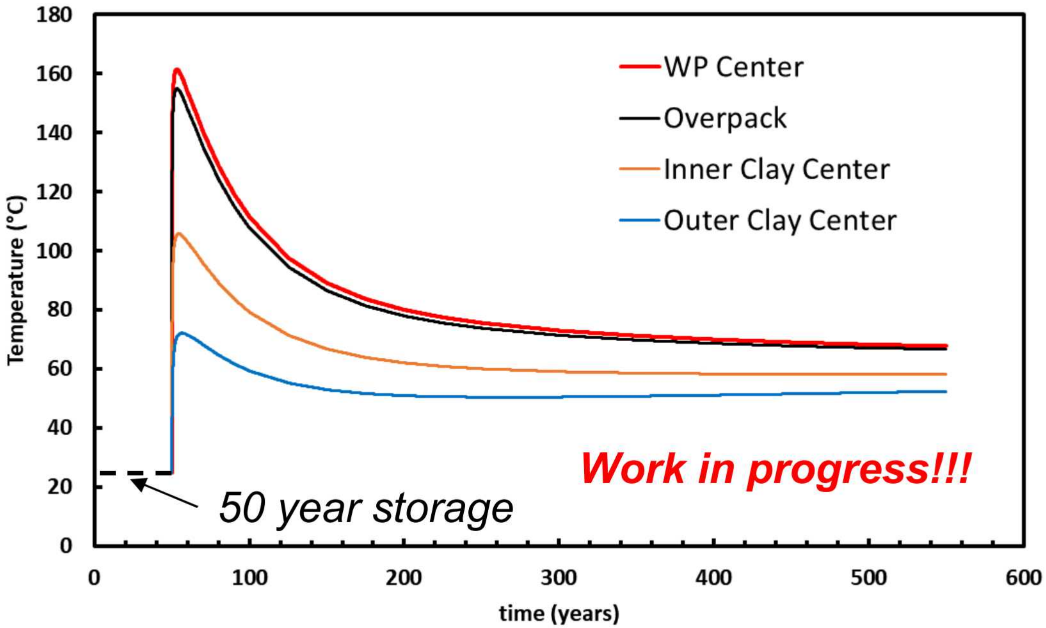
PFLOTRAN EBS Reactive Transport Simulations: Multilayered EBS Case

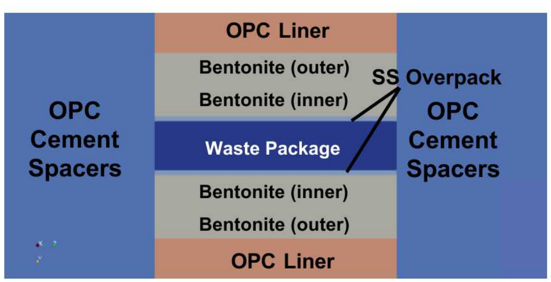


- Multicomponent aqueous & mineral system
  - 26 minerals + kinetic parameters
  - 31 aqueous species (primary & secondary) and gas species

- **EBS configuration**
  - 2-layer bentonite clay (inner w/ quartz; outer w/o quartz)
  - OPC spacers bet. WP's
  - OPC drift wall liner
  - WP w/ stainless steel (SS) overpack
  - Waste degradation not considered at this moment
- **PFLOTRAN Simulation:**
  - TH mode (saturated)
  - Thermal load:
    - 50 year storage
    - 12 PWR
    - Burnup: 40 GWd per SNF assembly
    - Porosity/permeability constrains
  - Pore solution chemistries (natural & engineered barriers) based on URL/bentonite studies

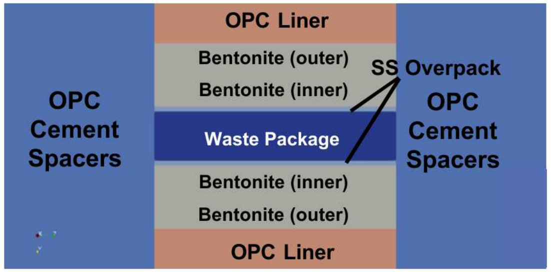
PFLOTRAN EBS Reactive Transport Simulations: Peak Temperature

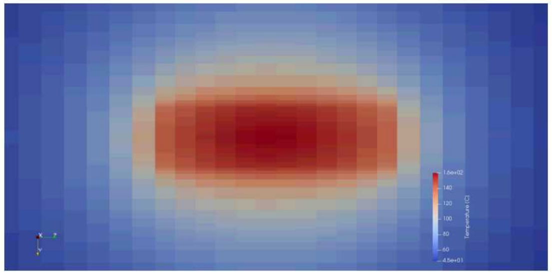


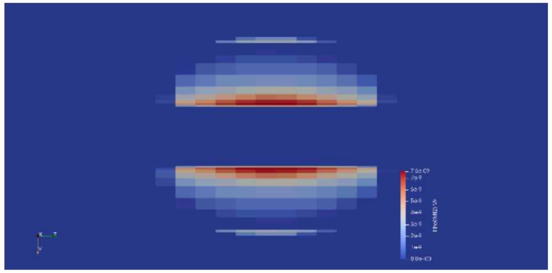


- **Thermal load:**
  - 50 year storage
  - 12 PWR
  - Burnup: 40 GWd per SNF assembly
- **Focus On Thermal Period**
  - Overpack Peak T → ~163°C
  - Inner Clay Peak T → ~103°C
  - Outer Clay Peak T → ~72°C
- **TODO**
  - Explore higher peak thermal conditions with larger SNF burnup → code stability with chemistry
  - Sensitivity analysis (SA) on thermal, transport, & chemical parameters

PFLOTRAN EBS Reactive Transport Simulations: Illite Formation?







- **Illite Formation**
  - Forms at the bentonite / overpack interface – High T for clay buffer
  - Spatially tracks peak temperatures
  - Predicted volume fractions are extremely small (unrealistic?)
  - However, useful in the evaluation of bentonite alteration mineral assemblage
  - **CAUTION: Still work in Progress!!!**
- **TODO**
  - Evaluate aqueous speciation at peak thermal locations between metal and bentonite barriers
  - Sensitivity analysis (SA) of chemical (e.g., initial pore solution chemistry) and kinetic parameters
  - SA on thermodynamic database parameters: minerals & aqueous species

Work in progress!!!

Integration with GDSA/PA (Disposal in Argillite R&D)

- **Understanding thermal effects on bentonite barrier to evaluate constrains on the extent of the *sacrificial zone* away from the heater. This could place constrains in EBS design according to thermal loads.**

- **Single drift / waste package baseline: 3D Simulations of barrier interactions and transport to evaluate performance**
  - Effects of thermal loads on barrier phase stability coupled with changes in fluid chemistry
  - Provide PA with more realistic representations of barrier chemical and transport properties
  - Inform PA on the effects of canister degradation and SNF interactions

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Future Outlook and Accomplishments

- **Future Outlook:**

  3D Reactive Transport (RT) modeling of EBS:

  - Expand 3D single waste package (WP) RT modeling to include more waste packages (WP's)
  - Consider larger WP's / barriers geometries with increased number of SNF assemblies / burnup
  - 3D simulation of unsaturated flow and transport in response to heating and eventual resaturation

- **Thermodynamic Database Development (TDB)**
  - Thermodynamic description of barrier material interactions on reaction with cementitious materials
  - Extend thermodynamic analysis of EBS material interactions to in-package chemistry & waste form (WF)
  - IAPWS H_2O EoS incorporation into SUPCRT92 → Consistency with key H_2O-bearing reactions at elevated T,P → inputs in RT model (LLNL lead)

- **Accomplishments:**
  - 1D-3D reactive-transport (RT) modeling of EBS in PFLOTRAN
    - Leveraging High Performance Computing (HPC)
    - Comprehensive RT chemical system representation of barrier components
    - Decay heat effects → high temperature interactions with barrier materials
  - Thermodynamic Database Development (TDB)
    - Updates: clay, zeolite system relevant to bentonite → Inputs to RT model
    - H_2O EoS update to the current IAPWS standard

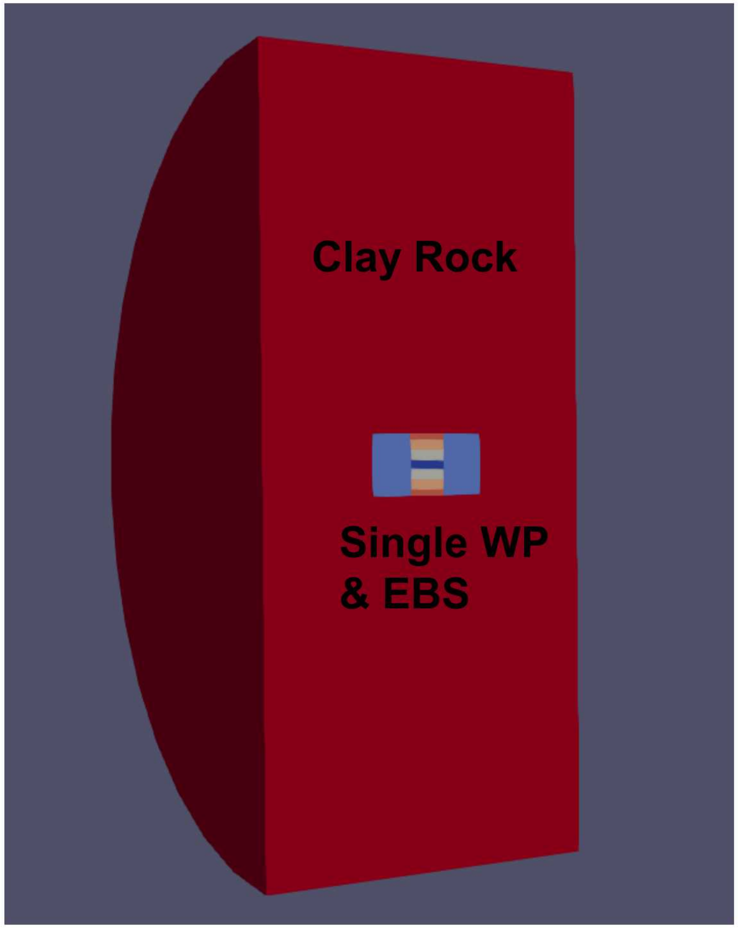
Questions?

Acknowledgements

- **This work supported by the DOE-NE Spent Fuel Waste Science and Technology campaign, Fuel Cycle Technologies R&D program.**

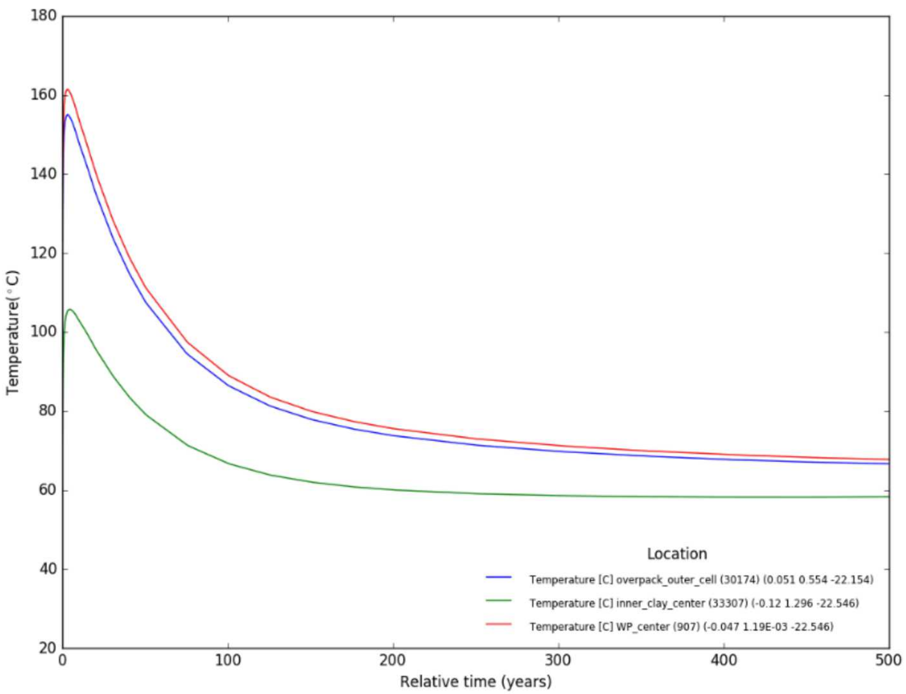
Backup Slides

PFLOTRAN EBS Reactive Transport Simulations: 3D unstructured mesh of Single Waste Package with Spacers



- **3D unstructured Mesh**
- **Large radial domain**
- **Dimensions:**
  - Waste Canister Length: 4.7 m
  - Waste Canister diameter: 1.15 m
  - Buffer Layer 1 & 2 Thickness: 1.24 m each
  - Cement Liner Thickness: 0.75 cm
  - Spacer Cement Length: 5.3 m
  - Spacer Cement Diameter: 7.6 m

PFLOTRAN EBS Reactive Transport Simulations: Peak Temperature



- **Thermal load:**
  - 50 year storage
  - 12 PWR
  - Burnup: 40 GWd per SNF assembly
- **Focus On Thermal Period**
  - Overpack Peak T → ~163°C
  - Inner Clay Peak T → ~103°C
  - Wall Rock Peak T → ~~~°C
- **TODO**
  - Explore higher peak thermal conditions with larger SNF burnup → code stability
  -

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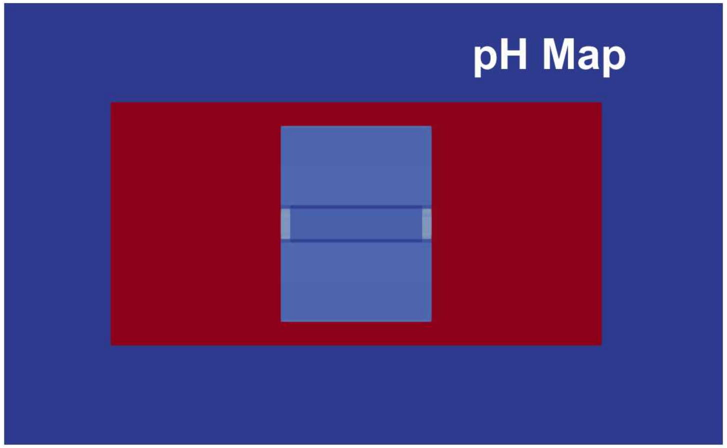
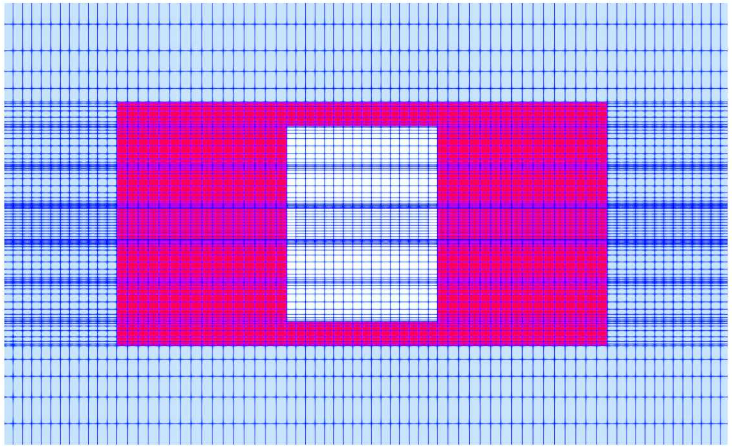
PFLOTRAN EBS Reactive Transport Simulations





- **3D Unstructured Mesh**
- **Single Waste Package with Spacers**
- ***Dimensions:***
  - *Waste Canister Length: 4.7 m*
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