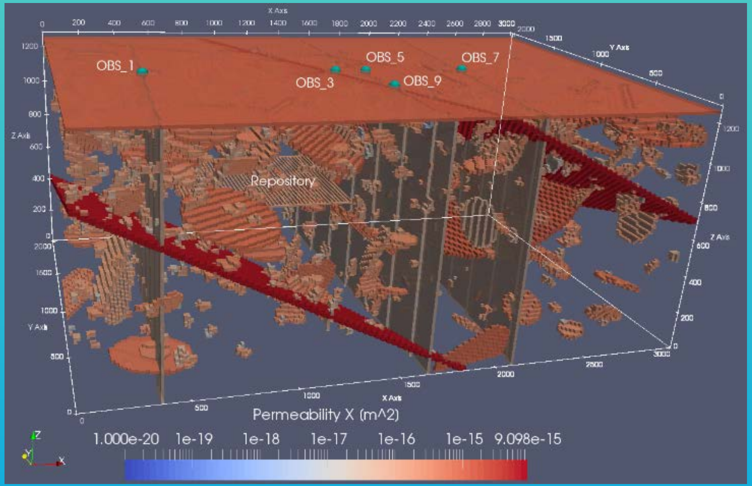
U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

Spent Fuel and Waste Science and Technology (SFWST)

Clean. Reliable. Nuclear.



Integration into Geologic Disposal Safety Assessment (GDSA) Framework for models related to Clay-Bearing Host Rocks and Engineered Barriers

U.S. Nuclear Waste Technical Review Board

Summer 2022 Board Meeting

Sept 14, 2022

SAND2022-11698 PE

Tara LaForce

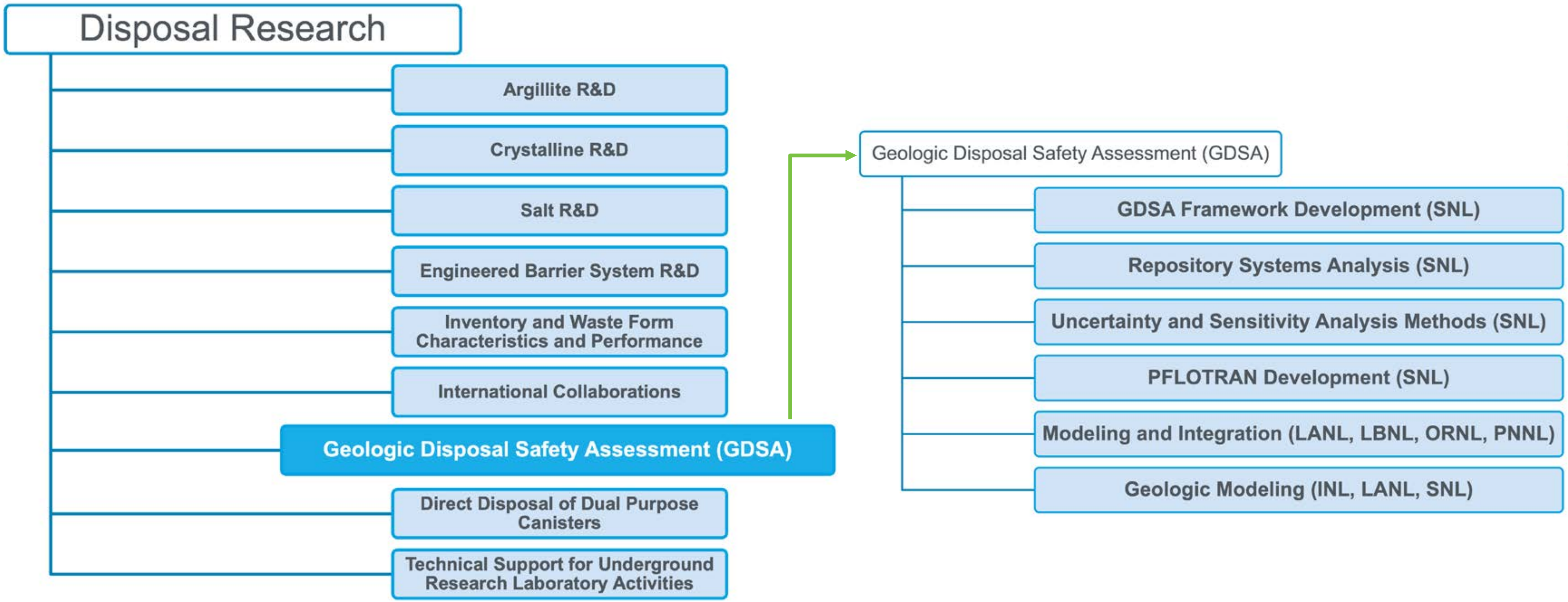
Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

NNSA

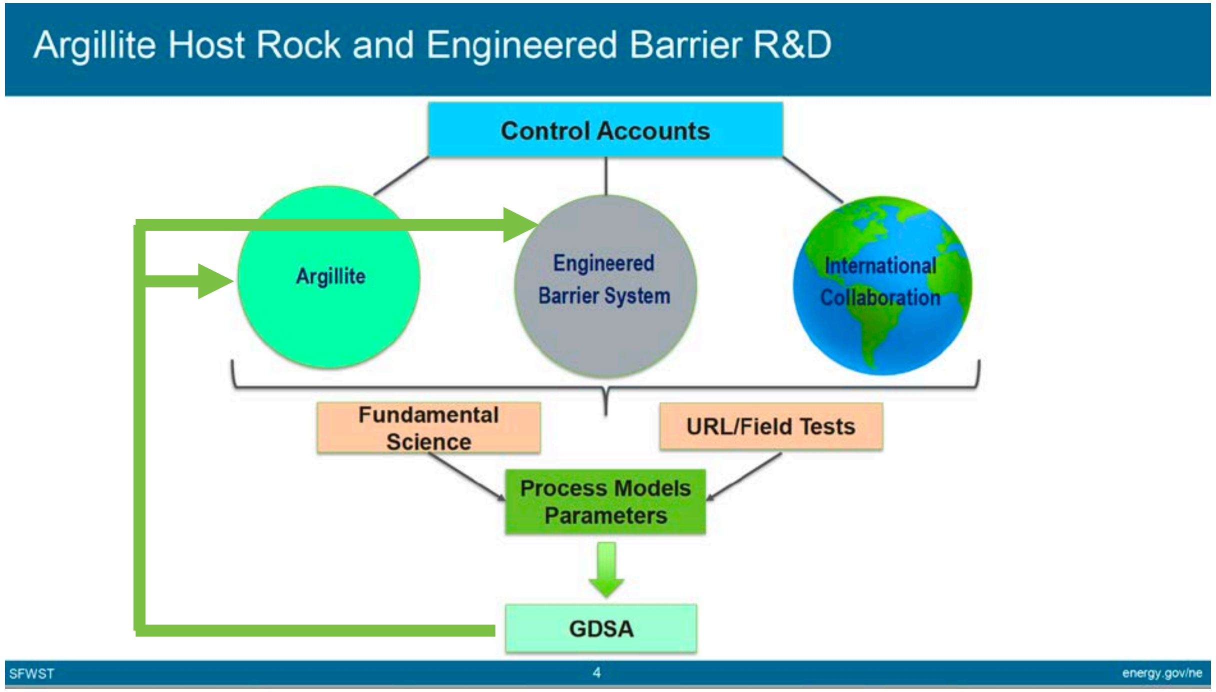
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

SFWST Disposal Research Control Accounts



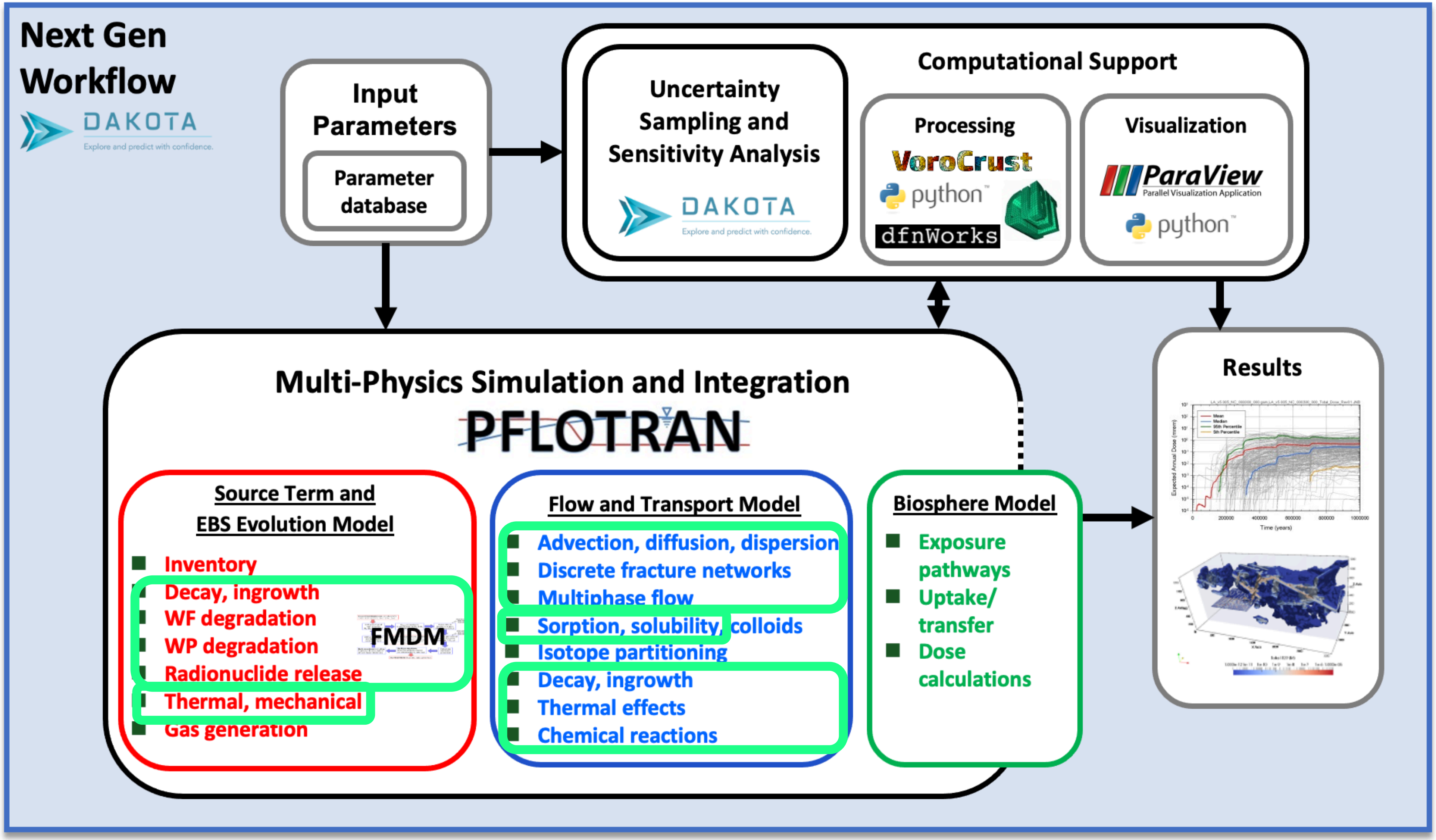
Where does GDSA Framework fit in?

- Overarching goal: Develop and demonstrate numerical modelling and analysis capability to provide a sound technical basis for multiple disposal options
  - Three potential host rocks
  - Find gaps and enhance capability in process models, workflow, etc.
  - Drive development of process models
  - Recent focus on high-temperature waste package disposal
- In all performance assessment (PA) cases
  - Only undisturbed scenarios
  - Generic features, events, and processes (FEPs) screening (Vaughn, 2012)
  - Dakota uncertainty and sensitivity analysis
  - Main performance metric is peak I-129



(Camphouse, 2022)

GDSA Framework

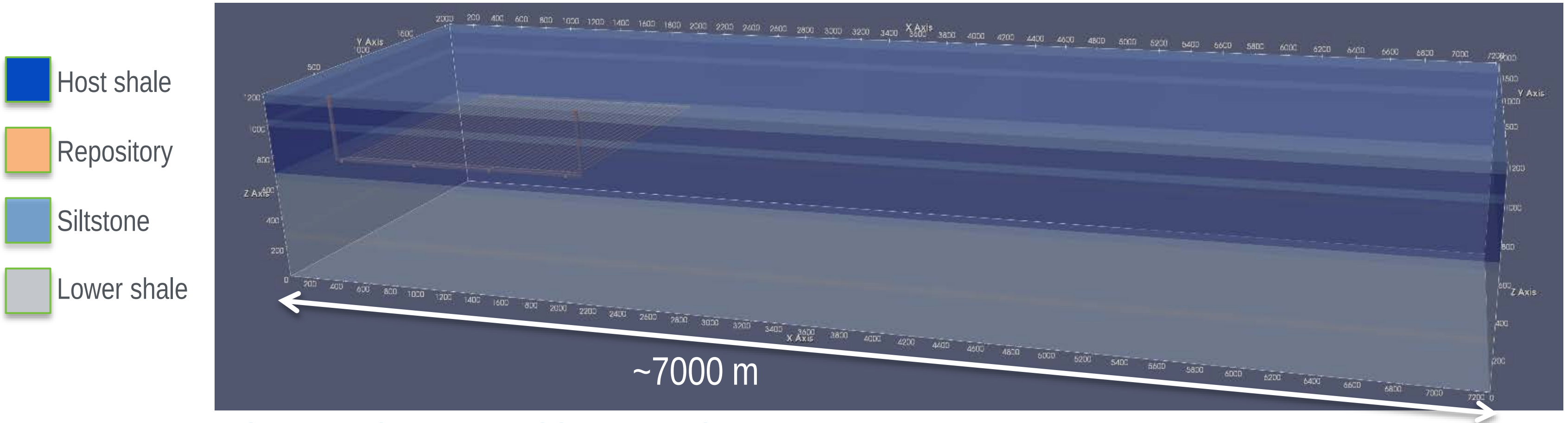


Processes in all performance assessment models

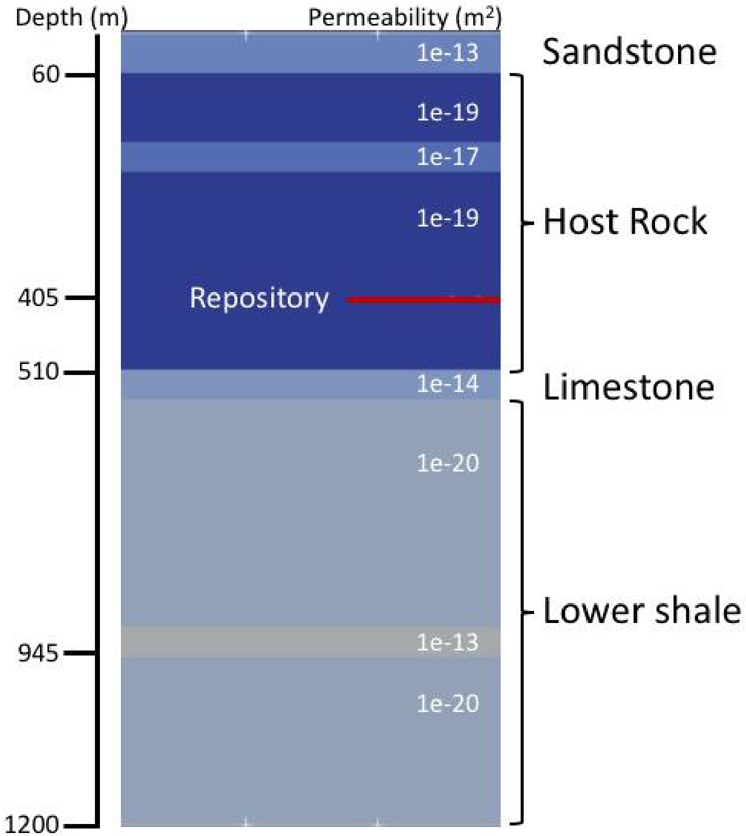
- Coupled heat and fluid flow
- Radionuclide
  - Transport via advection and diffusion
  - Sorption using linear distribution coefficients (K_d)
  - Precipitation/dissolution
- Radioactive decay and ingrowth in all phases
- Waste package degradation
- Waste form dissolution

Argillite reference case PA model

- 3150 24-Pressurized water reactor (PWR) waste packages (WPs) and 2000 37-PWR WPs in 84 drifts
- Numerical model is a half-symmetry domain with 6.9 million grid cells
- Geological features:
  - 0.0013 (m/m) head gradient from west to east
  - Sandstone aquifer above the repository
  - Limestone aquifer below the repository



Numerical model colored by material type.

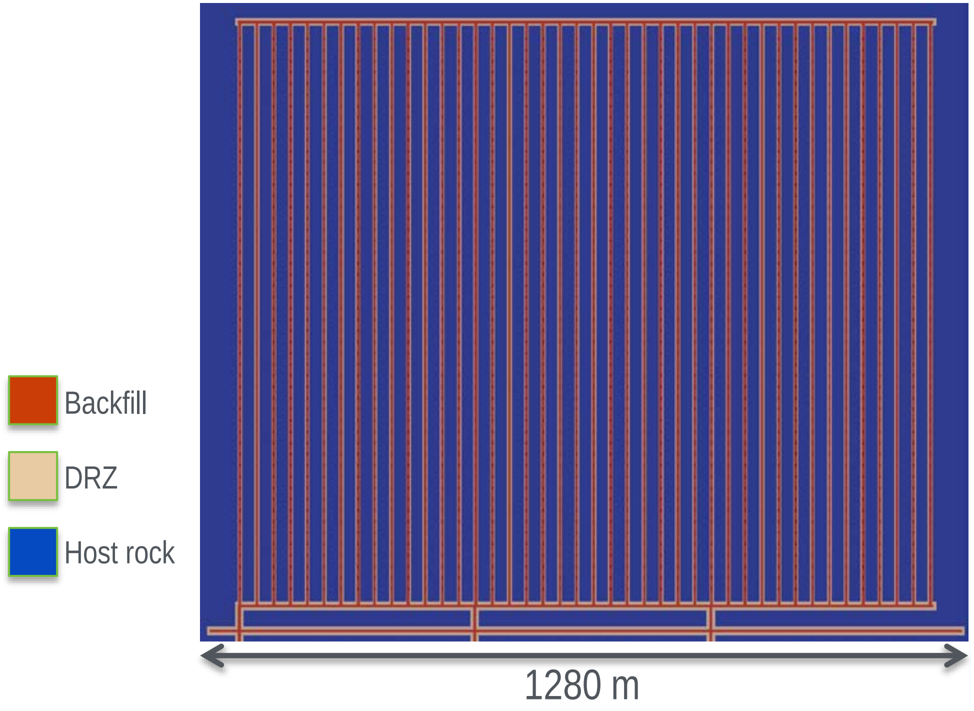


Schematic of repository in geological model.

(Sevougian et al. 2019; Swiler et al. 2019)

Argillite reference case PA model

- Repository features
  - Bentonite backfill
  - Instant-release fraction for I-129 of 0.10 and fractional dissolution of SNF



Map view of half of the repository colored by material type.

- Incremental Latin Hypercube Sampling (LHS) of uncertain parameters with a final sample size of 200
- Quantity of interest is maximum I-129 in aquifers

Input	Description	Range	Units	Distribution
rateSNF	SNF Dissolution Rate	$10^{-8} – 10^{-6}$	yr^{-1}	log uniform
rateWP	Mean Waste Package Degradation Rate	$10^{-5.5} – 10^{-4.5}$	yr^{-1}	log uniform
kSand	Upper Sandstone Permeability	$10^{-15} – 10^{-13}$	m^2	log uniform
kLime	Limestone Permeability	$10^{-17} – 10^{-14}$	m^2	log uniform
kLSand	Lower Sandstone Permeability	$10^{-14} – 10^{-12}$	m^2	log uniform
kBuffer	Buffer Permeability	$10^{-20} – 10^{-16}$	m^2	log uniform
kDRZ	DRZ Permeability	$10^{-18} – 10^{-16}$	m^2	log uniform
pShale	Host Rock (Shale) Porosity	0.1 – 0.25	-	uniform
bNpKd	Np K_d Buffer	0.1 – 702	m^3kg^{-1}	log uniform
sNpKd	Np K_d Shale	0.047 – 20	m^3kg^{-1}	log uniform

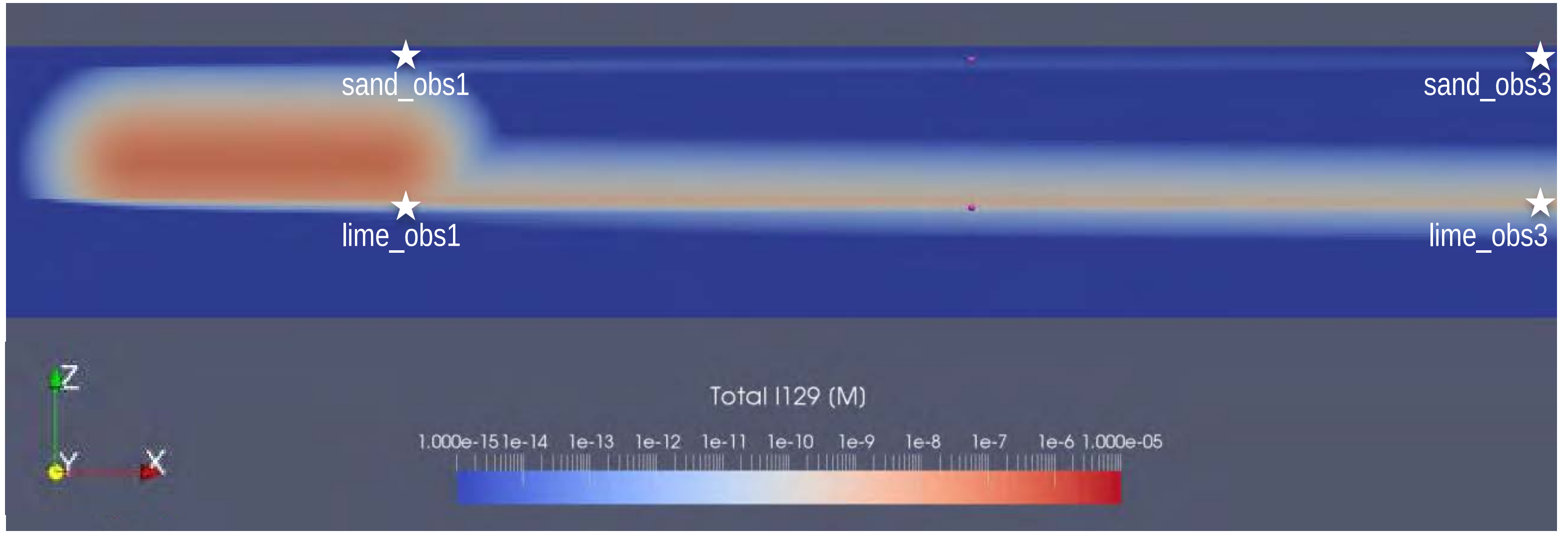
10 sampled parameters (Np not used)

(Sevougian et al. 2019; Swiler et al. 2019)

Argillite reference case results

- At 10,000 years
  - Impact of sampled waste package breach on near repository I-129 is clear.
  - Diffusive transport of I-129
- At 1,000,000 years
  - In the shale host rock I-129 transport is mainly diffusive
  - Advection of I-129 in the sandstone and limestone aquifer is evident.

I-129 concentration at 10,000 y plotted in a horizontal slice at the Z-midpoint of the repository.



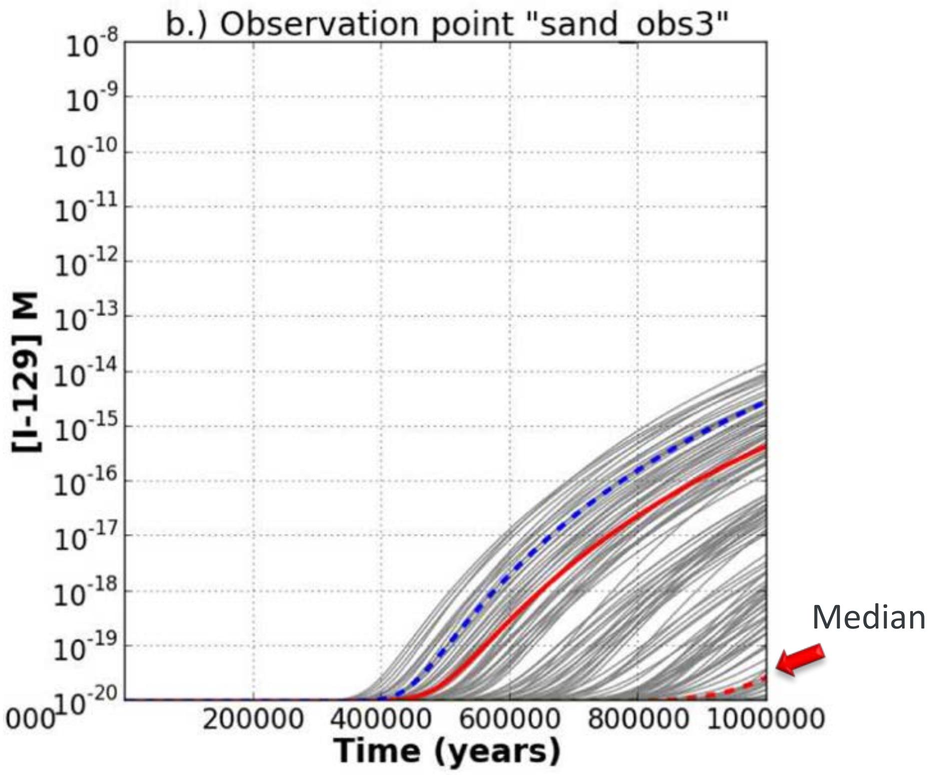
I-129 concentration at 1,000,000 y plotted in a vertical slice at the Y-midpoint of the repository.

(Sevougian et al. 2019)

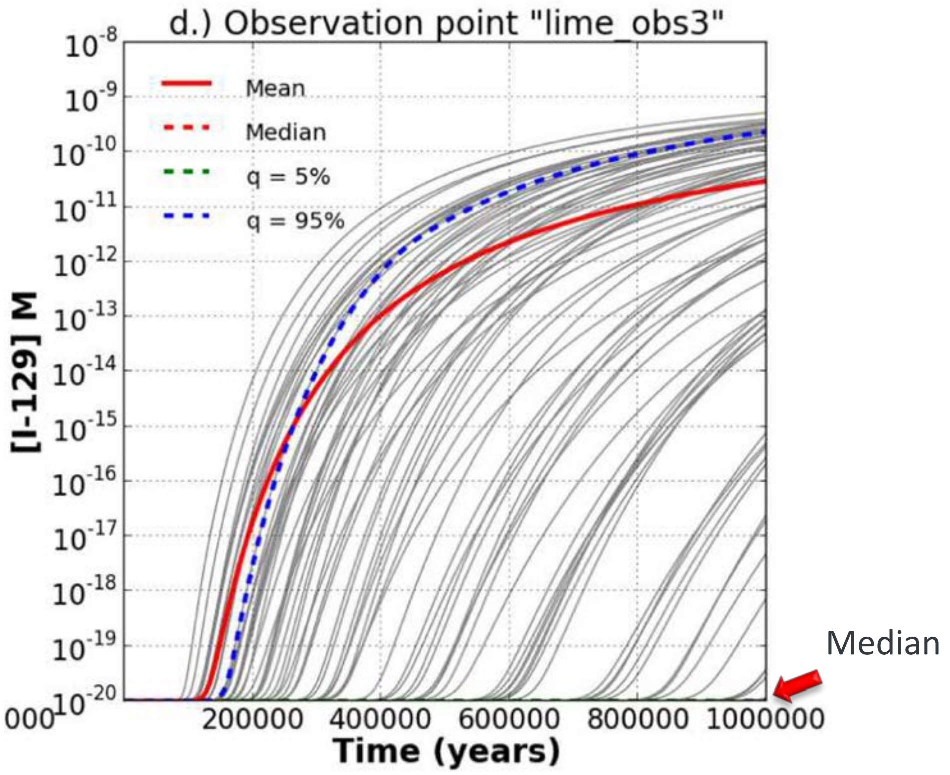
Argillite reference case results

(Stein et al., 2019; Swiler et al., 2019)

- Significant spread in I-129 breakthrough curves
- Mean is much higher than median



I-129 concentration versus time for 200 realizations at sandstone aquifer downstream observation point.

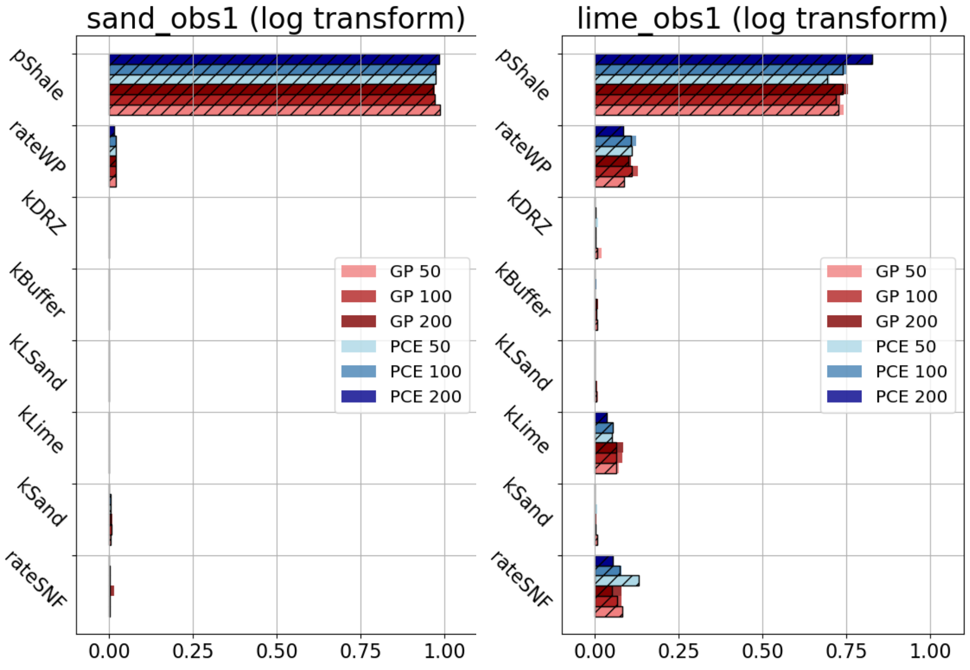


I-129 concentration versus time for 200 realizations at limestone aquifer downstream observation point.

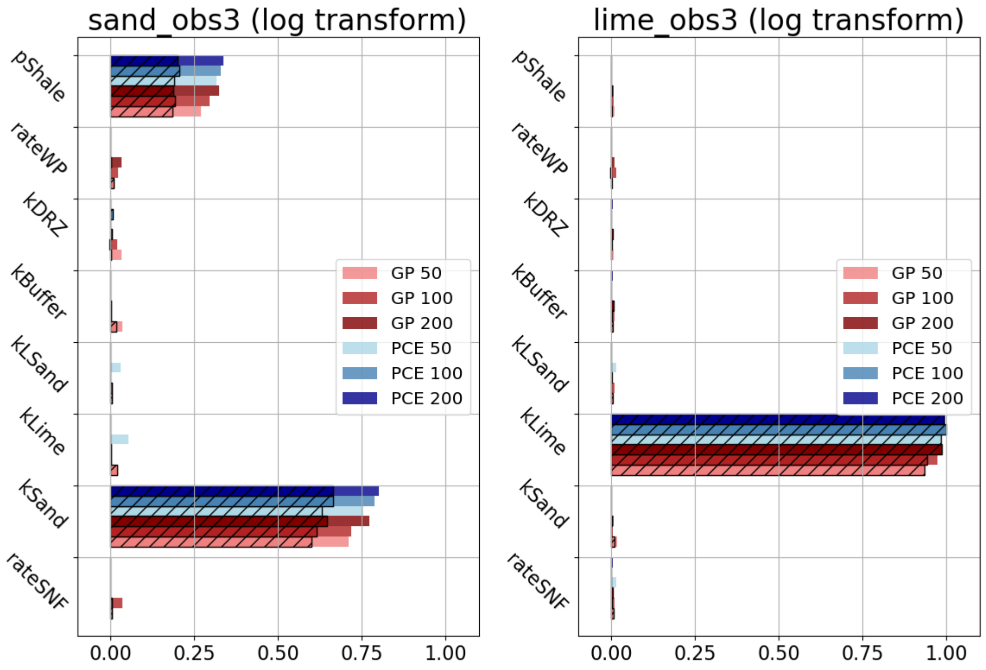
Argillite reference case results

(Stein et al., 2019; Swiler et al., 2019)

- Sensitivity indices: how much variance in the output is due to variance in an uncertain input
- Max [I-129] is sensitive to
  - Porosity of the shale host rock near the repository (pShale).
  - Aquifer permeability 5km downstream (kLime or kSand).
  - Rate of waste-form and waste package dissolution (lime_obs1)



Sandstone aquifer sensitivity indices.



Limestone aquifer sensitivity indices.

Disturbed Rock Zone (DRZ) Evolution Modelling

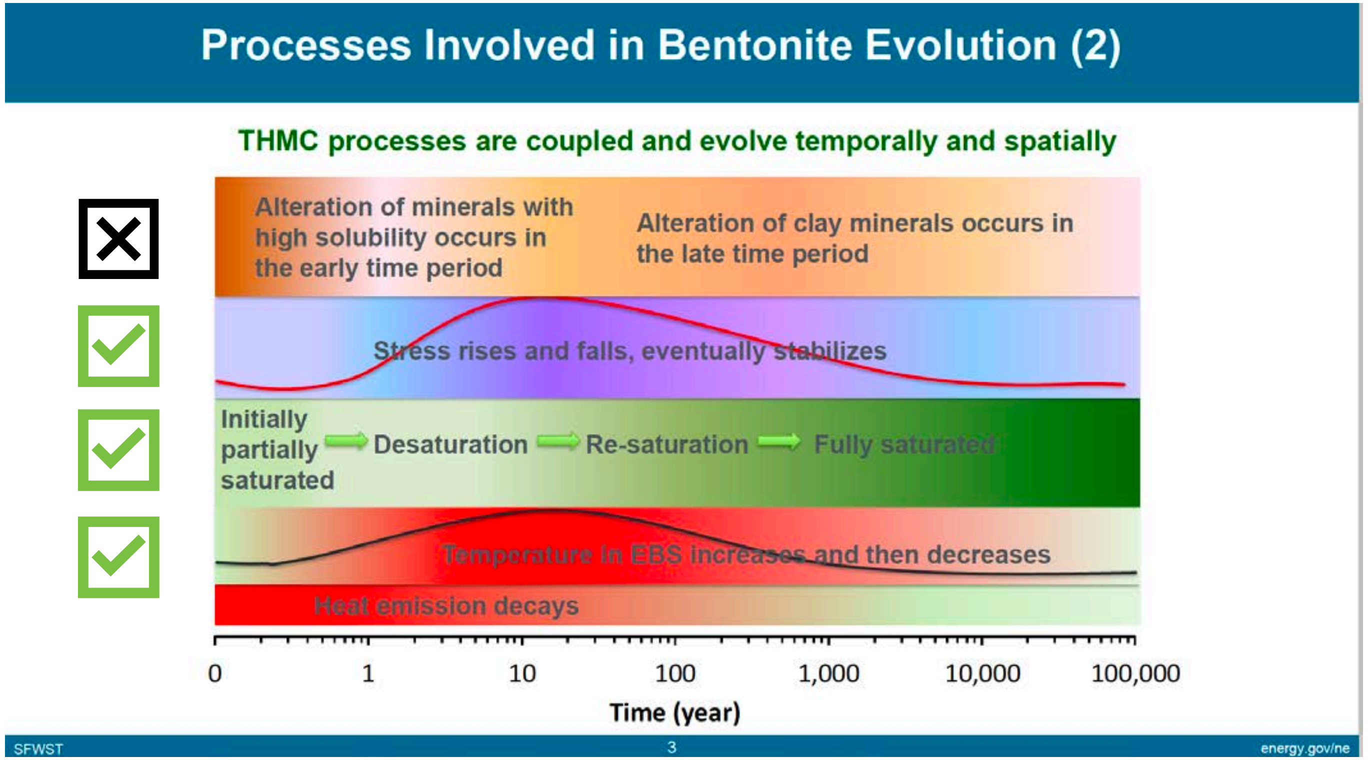
Buffer swelling and DRZ evolution: Goals set in 2019

Collaboration with LBNL

- Sandia GDSA PFLOTRAN Development and Repository Systems Analysis work packages
- Adapt an increasingly mechanistic modeling approach to PA-scale simulations without sacrificing computational efficiency

Questions:

- How can coupled Thermal HydroMechanical Chemical (THMC) simulations affect PA-scale assessments?
- What can we learn from high-resolution nearfield models that we can use to upscale to PA-scale?
- What are the process/scale relationships that dictate whether a simple functional form is appropriate for approximating a particular process?



(Nole and Chang, 2019)

(Zheng et al., 2022)

Buffer swelling and DRZ evolution: 2019 proposed workflow

- Use TOUGH-FLAC to derive functional relationships between water saturation and bentonite swelling stress

We are here

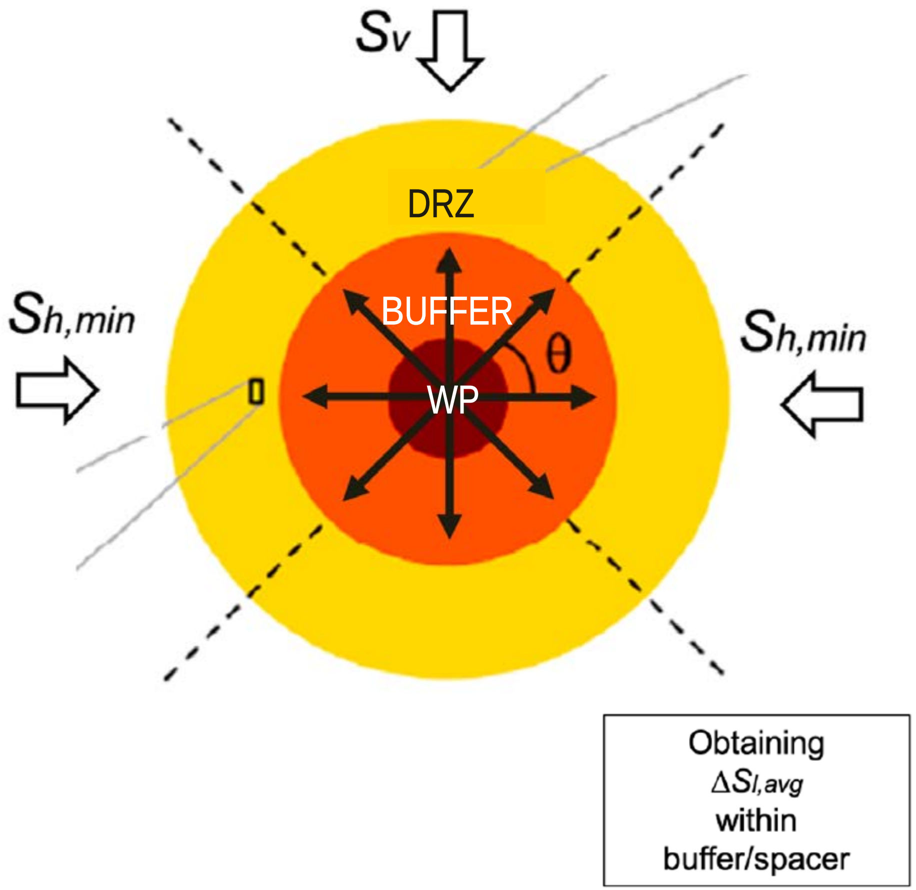
- Relate permeability in the disturbed rock zone (DRZ) to swelling stress in the bentonite through calculation of reduced order model for effective stress in the DRZ (Chang et al., 2021)

- Compare nearfield PFLOTRAN models with reference cases (e.g DECOVALEX Mont Terri) in TOUGH-FLAC

- Use models in a PA-scale simulation and compare results back to nearfield simulations

(Nole and Chang, 2019)

Buffer swelling and DRZ evolution: Conceptual model



Simplified model for DRZ evolution study.

Assume stress on DRZ is radial and isotropic

Assume in swelling stress is a linear function of the change in average liquid saturation in the buffer

Two Part Hooke's Law (TPHM) model from Zheng et al. (2015) gives total permeability as a exponential function of stress

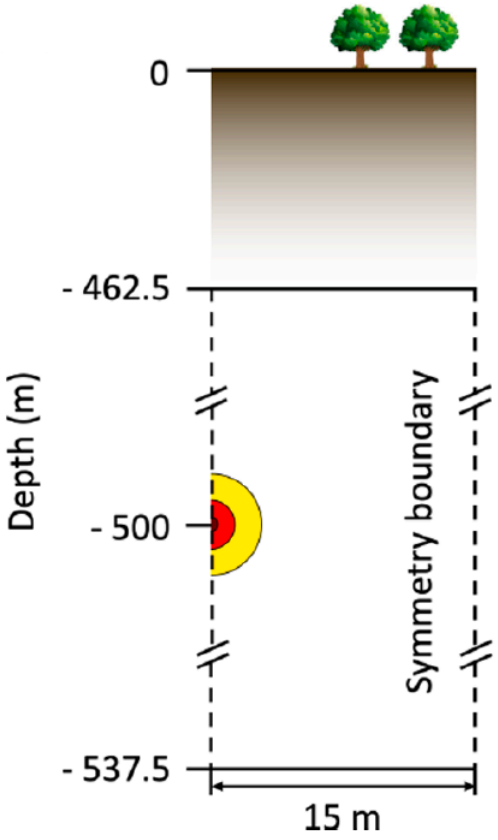
(Chang et al., 2021)

Buffer swelling and DRZ evolution

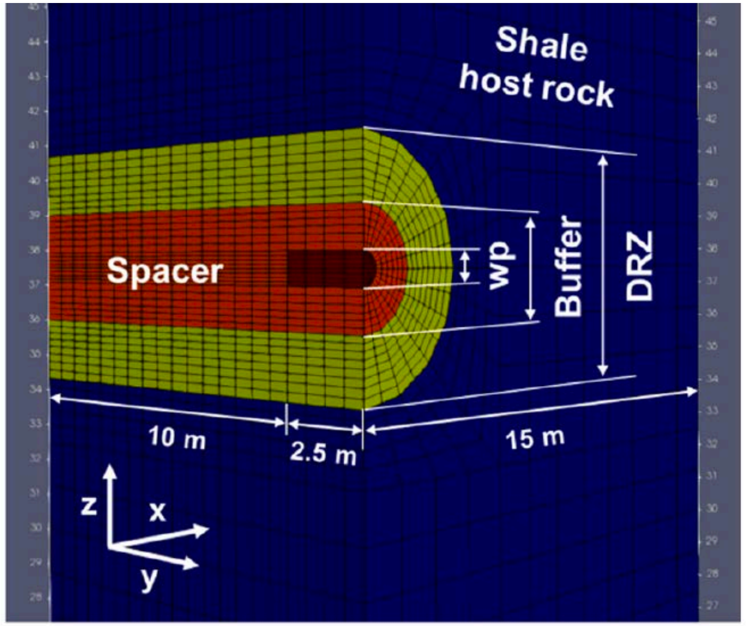
(Chang et al., 2021)

- Model is ¼ of one waste package
- All lateral boundaries closed to create reflective boundaries
- Hydrostatic initial pressure and temperature
- Inside buffer and DRZ S_L=0.65 and S_L=1.0 elsewhere

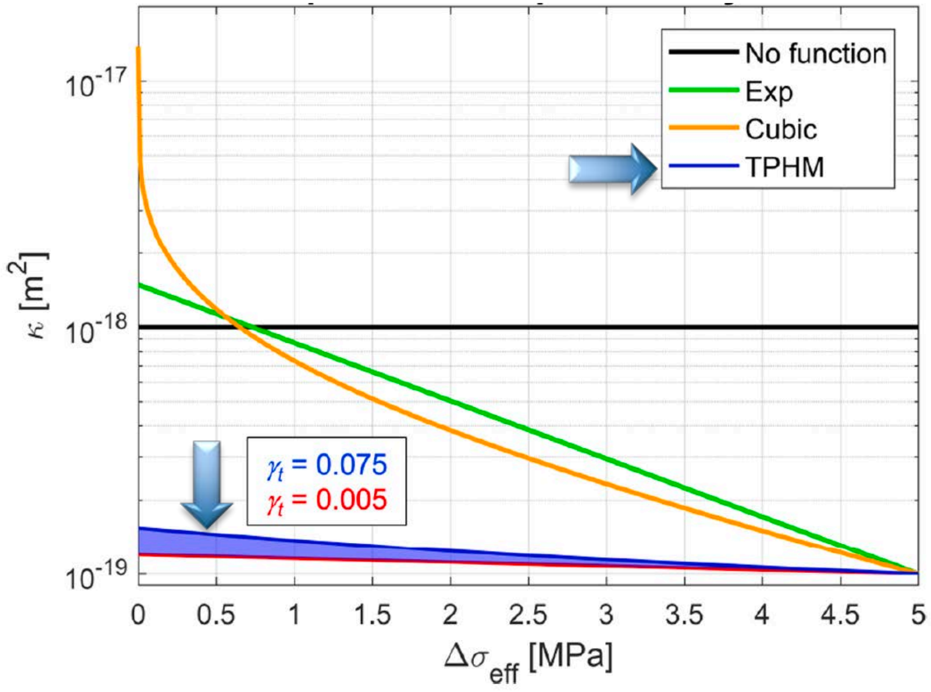
Model domain.



Simulation mesh near the waste package.

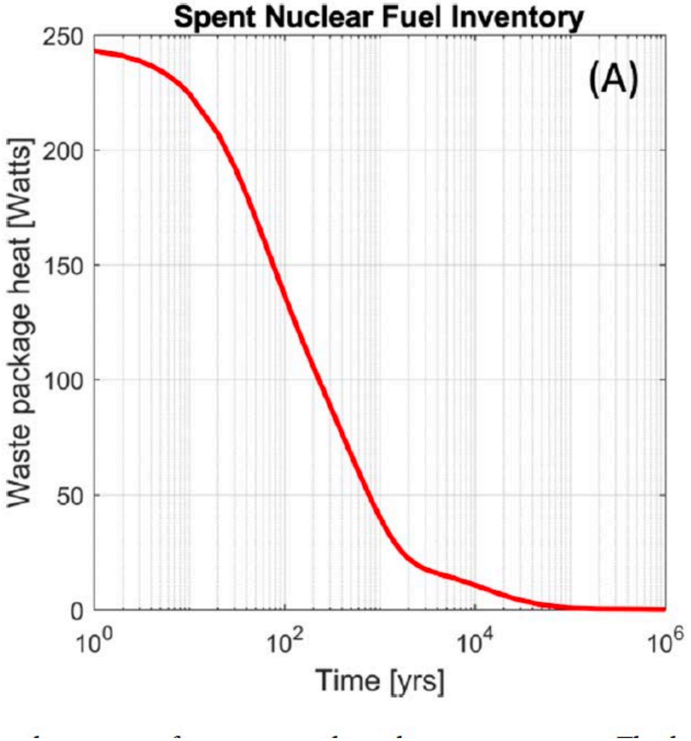


Stress-dependent DRZ permeability as a function of effective stress.

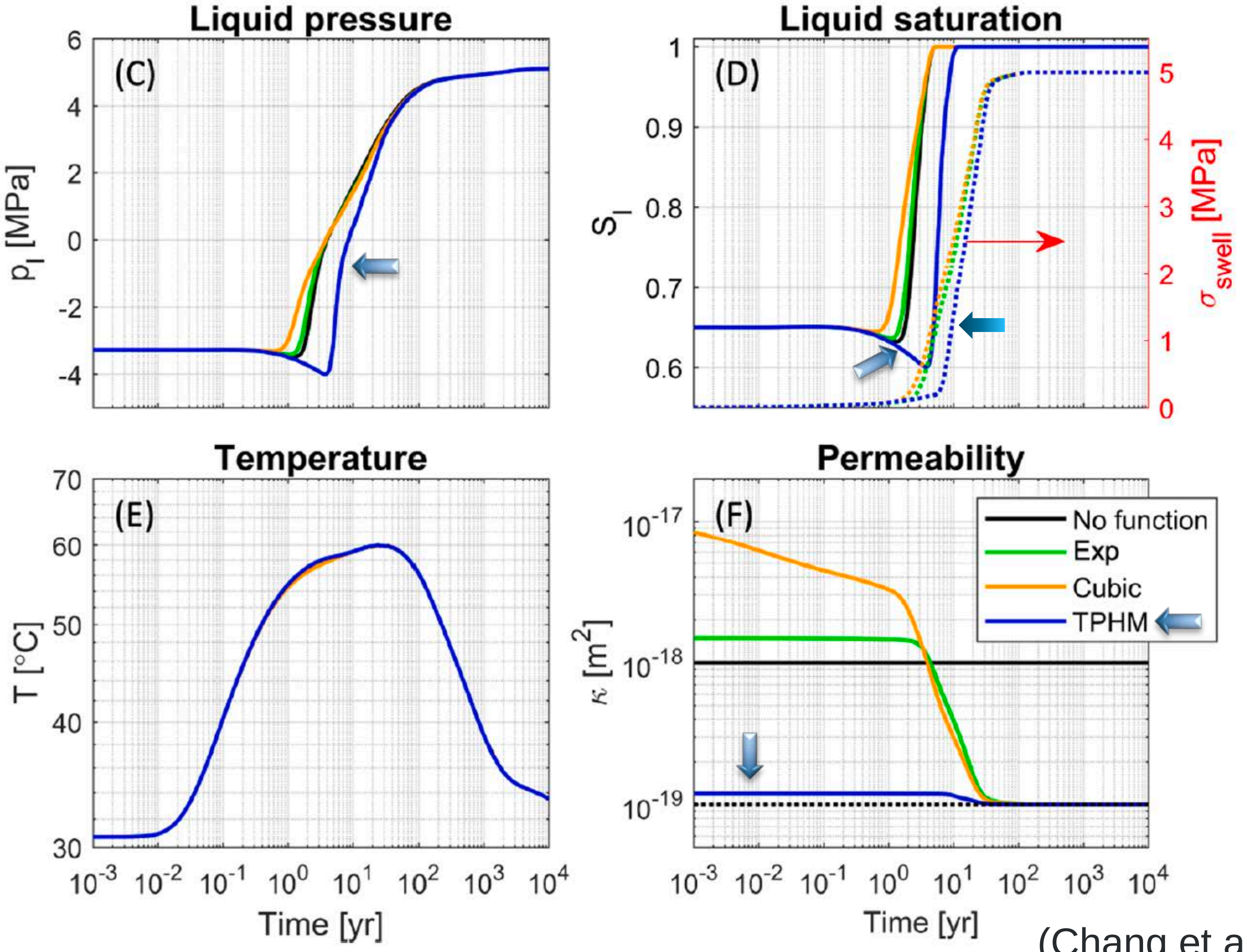


Buffer swelling and DRZ evolution

Waste package heat and temperature in the repository as a function of log time.



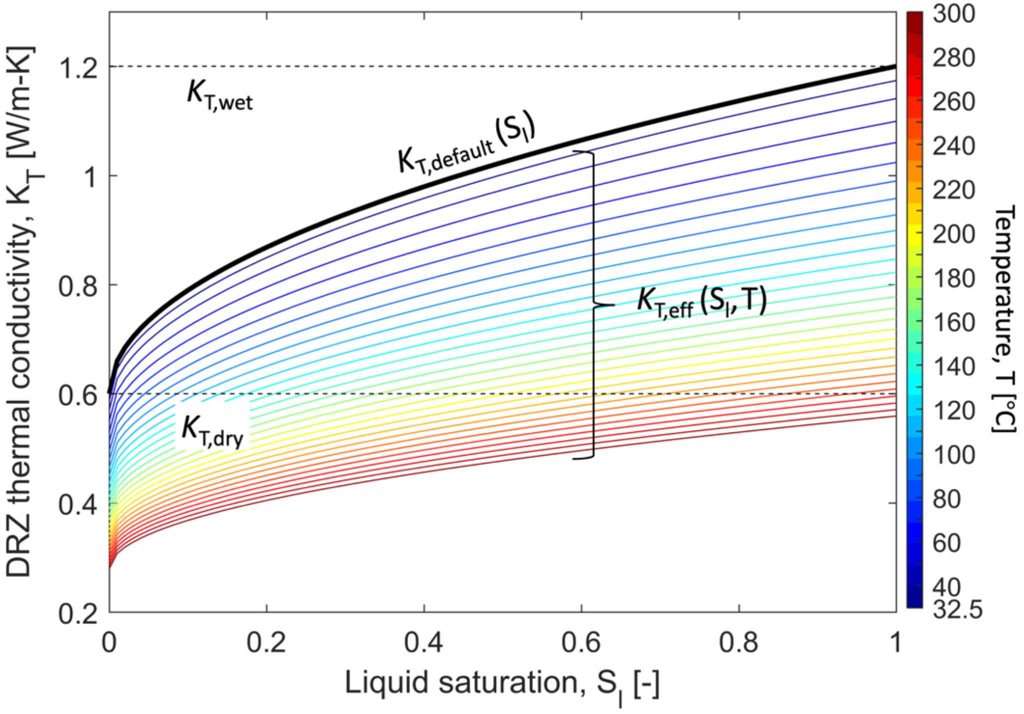
Simulated quantities in the DRZ next to the buffer as a function of log time.



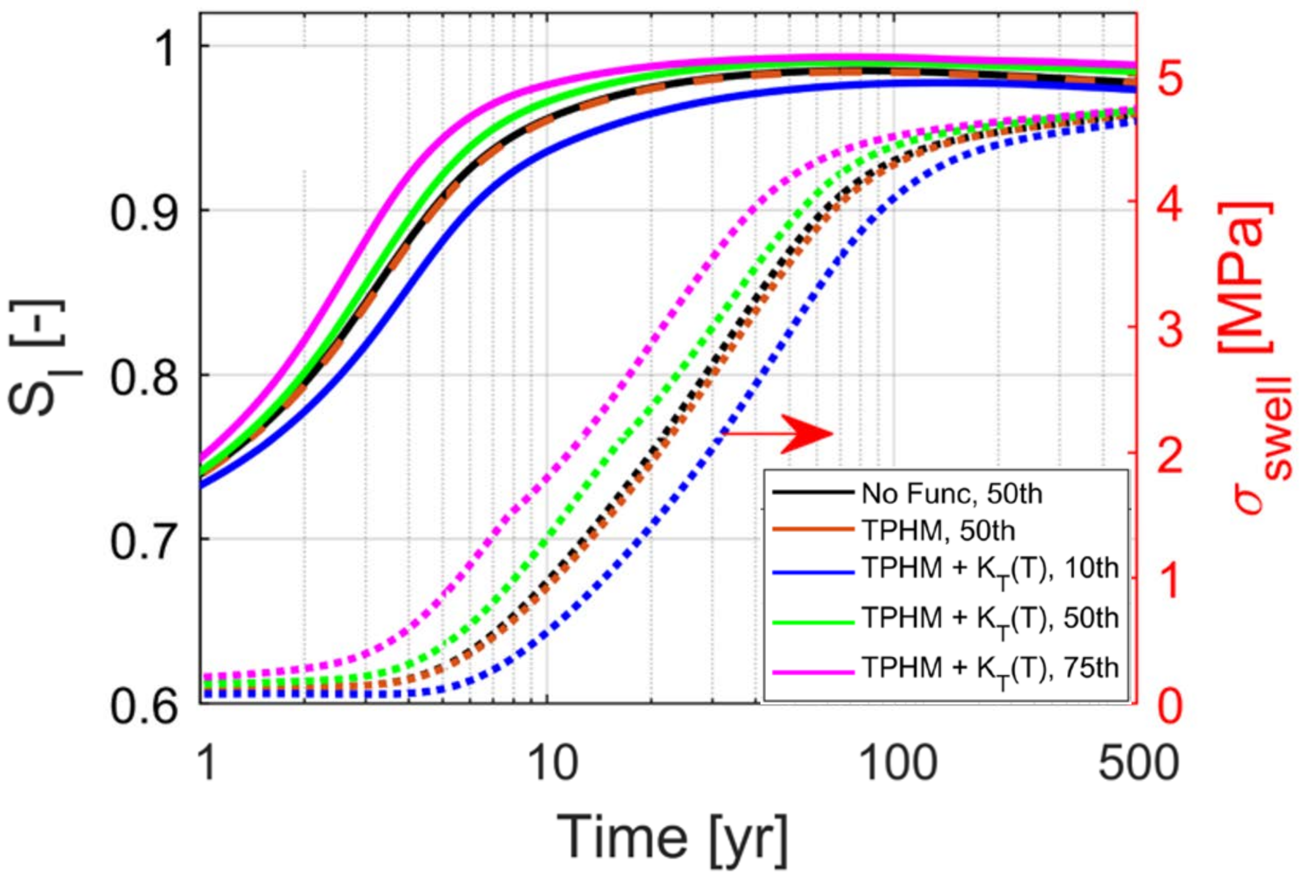
(Chang et al., 2021)

Buffer swelling and DRZ evolution

- Thermal conductivity (K_T) is saturation-weighted combination of wet and dry properties
- Add temperature dependence in K_T to the model
- Looking at hotter waste packages



DRZ thermal conductivity as a function of liquid saturation at temperature from 32.5 to 300 ^{o}C.



Average liquid saturation in the DRZ as a function of log time.

(LaForce et al., 2022-in preparation)

Results to date

- Performance assessment modelling
  - Statistical analysis over 200 simulations has been conducted using DAKOTA and PFLOTRAN for generic argillite host rock.
  - Model behavior appears realistic and methods are robust.
  - Aquifer and shale properties have significant impact on peak I-129 results.
- Small-scale modelling:
  - Model for DRZ evolution in response to buffer swelling has been implemented.
  - Simulations indicate that buffer swelling has impact on near-waste package flow.
  - Temperature-dependence of thermal conductivity added to the model.

Next steps

- Next 1-2 Years
  - Drive development of process models
    - Bentonite evolution
    - Waste package degradation
  - New shale PA cases
    - Add uncertainty in waste package heat and inventory
    - Add realism/uncertainty in geological structure
    - Explore sensitivity to new quantities of interest (e.g. mean residence time in the repository)
  - Small-scale modelling
    - Smectite to illite material transform module
    - Anisotropic permeability and/or thermal conductivity
- Longer term
  - Gas generation
  - Disruptive events (e.g. induced seismicity)
  - New material transform modules (e.g. reduced order K_ds)
  - Explore sensitivity as a function of time

References

- Camphouse, C. 2022. *Overview of DOE R&D Efforts Related to a Clay-Based Repository and Clay Based Engineered Barriers.* Presented at the 2022 U.S. Nuclear Waste Technical Review Board Fact Finding Meeting July 19, 2022.
- Chang, K. W., M. Nole, M., & E.R. Stein. 2021. Reduced-order modeling of near-field THMC coupled processes for nuclear waste repositories in shale. *Computers and Geotechnics*, *138*, 104326.
- LaForce, T., E. Basurto, K.W. Chang, M. Ebeida, W. Eymold, C. Faucett, R. Jayne, N. Kucinski, R. Leone, P. Mariner, F.V. Perry. 2022-in preparation. *GDSA Repository Systems Analysis Investigations in FY 2022.* SAND2022-XXXXR, Sandia National Laboratories, Albuquerque, NM
- Nole, M. and K.W Chang, 2019 SFWST 2019. *GDSA/LBNL Nearfield Modeling Integration*. Paper presented at the 2019 SFWD Annual Working Group Meeting. May 21-23, 2019.
- Sevougian, S. D., E. R. Stein, T. LaForce, F. V. Perry, M. Nole, C. B. Haukwa, and K. W. Chang, 2019. *GDSA Repository Systems Analysis FY19 Update*. M3SF-19SN010304052 SAND2019-11942R, Sandia National Laboratories, Albuquerque, NM
- Stein, E. R., L.P Swiler. S.D and Sevougian, 2019. *Methods of Sensitivity Analysis in Geologic Disposal Safety Assessment Framework.* Paper presented at the 2019 International High-Level Radioactive Waste Management Conference, April 14-18, 2019,
- Swiler, L. P., J. C. Helton, E. Basurto, D. M. Brooks, P. E. Mariner, L. M. Moore, S. Mohanty, S. D. Sevougian and E. R. Stein, 2019. *Status Report on Uncertainty Quantification and Sensitivity Analysis Tools in the Geologic Disposal Safety Assessment (GDSA) Framework*. SAND2019-13835 R, Sandia National Laboratories, Albuquerque, NM
- Vaughn et al., 2012, *Generic Disposal System Model: Architecture, Implementation, and Demonstration*, Sandia National Laboratories, Albuquerque, NM
- Zheng, L., C. Chang, S. Yoon, S. Borglin, C. Chou, J. Rutqvist, T. Kneafsey, Y. Wu, S. Nakagawa, L. Peruzzo, and J. Birkholzer. 2022. *Coupled THMC Processes under High Temperature in bentonite buffer: Laboratory Experiments, Field Tests, and Modeling*. Presented at the 2022 U.S. Nuclear Waste Technical Review Board Fact Finding Meeting July 19, 2022.
- Zheng, J., L. Zheng, H.H. Liu, and Y. Ju. 2015. Relationships between permeability, porosity and effective stress for low-permeability sedimentary rock. *International Journal of Rock Mechanics and Mining Sciences*, *78*, pp.304-318.

Questions?