Key Accomplishments & Priorities for Geologic Disposal Safety Assessment (GDSA)

Paul Mariner

Sandia National Laboratories

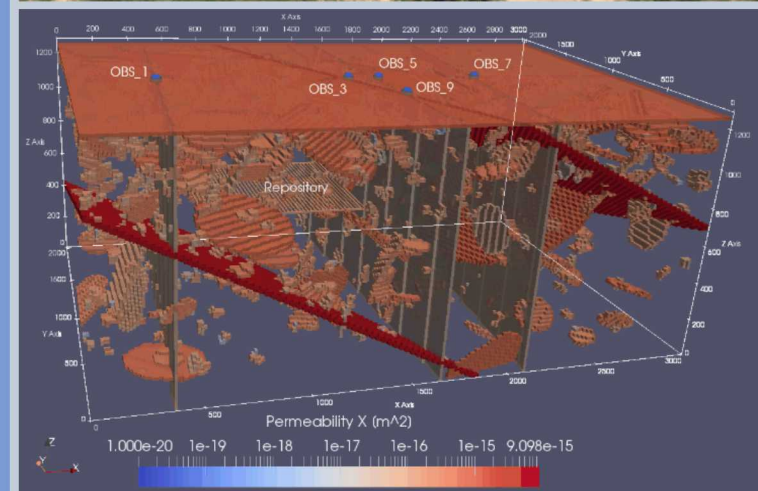SAND2019-5607PE

SFWD

Spent Fuel & Waste Disposition

Annual Working Group Meeting
UNLV-SEB – *Las Vegas, Nevada*
May 21-23, 2019

ACKNOWLEDGEMENTS

- GDSA modeling accomplishments over the past decade were made possible by the support and direction of DOE and the ingenuity and collaboration of scientists and engineers across the UFD and SWFST campaigns.

- Major contributors in the PA group alone since 2012 include (alphabetical by first name)
  - Bob MacKinnon, David Dobson, David Sevougian, Eduardo Basurto, Emily Stein, Geoff Freeze, Glenn Hammond, Heeho Park, Jennifer Frederick, Leigh Cunningham, Michael Nole, Mike Wallace, Palmer Vaughn, Paul Mariner, Payton Gardner, Ralph Rogers, Spencer Jordan, Tara LaForce, Tom Lowry, Vince Mousseau

UFD Campaign Priorities

- Highest cross-cutting R&D issues from the 2011 UFD disposal R&D roadmap
  - Design concept development
  - Disposal system modeling

Table 6. Synopsis of the Results of Cross-Cutting R&D Issues

DESIGN CONCEPT DEVELOPMENT	High
DISPOSAL SYSTEM MODELING	High
OPERATIONS-RELATED RESEARCH AND TECHNOLOGY DEVELOPMENT	Low
KNOWLEDGE MANAGEMENT	Medium
SITE SCREENING AND SELECTION TOOLS	Medium
EXPERIMENTAL AND ANALYTICAL TECHNIQUES FOR SITE CHARACTERIZATION	Medium
UNDERGROUND RESEARCH LABORATORIES	Medium
RESEARCH AND DEVELOPMENT CAPABILITIES EVALUATION	Medium

DOE (2011). Used Fuel Disposition Campaign Disposal Research and Development Roadmap. FCRD-USED-2011-000065 REV 0.

- New PA Framework – **GDSA Framework**
 - Genesis in 2013
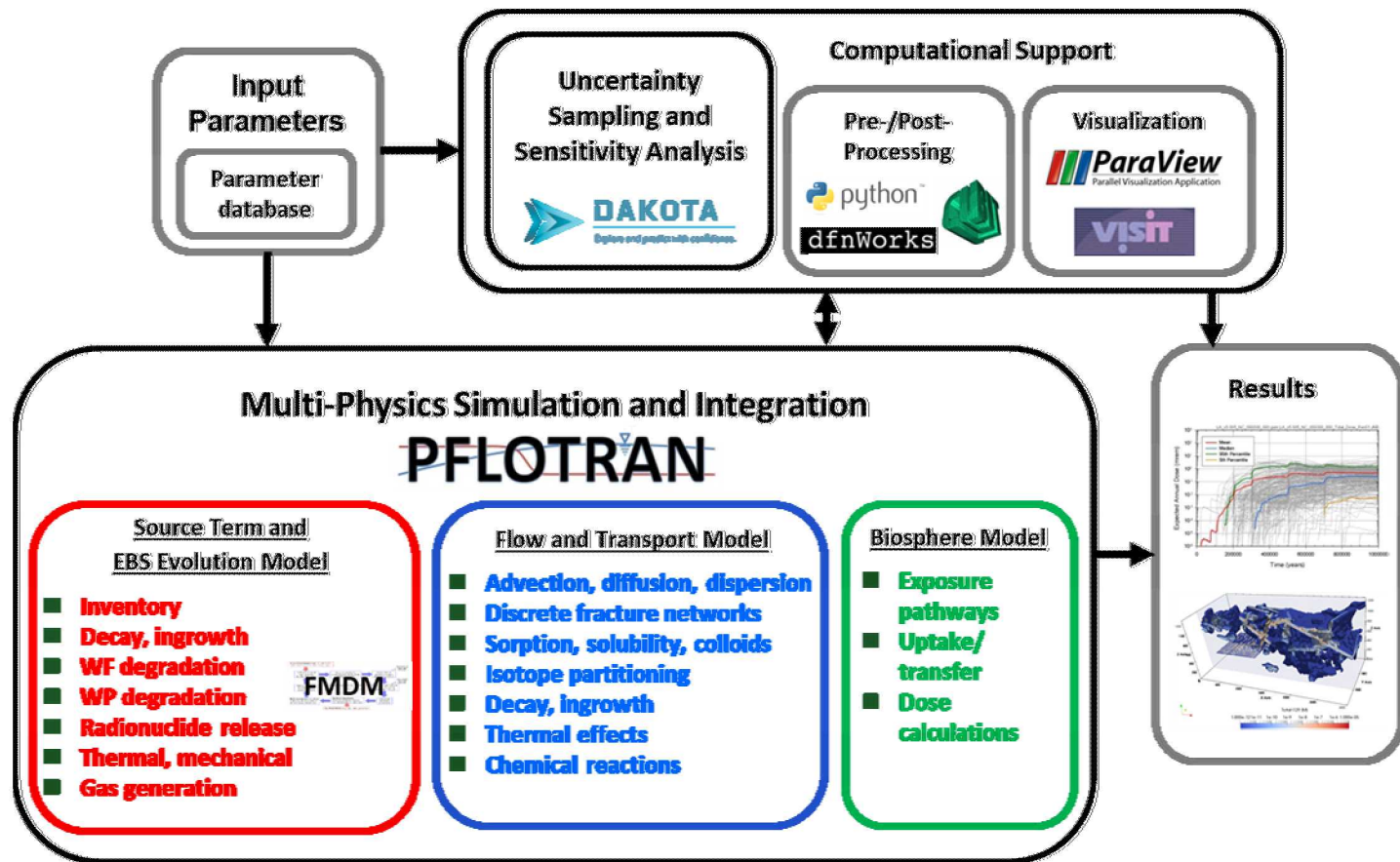
KEY ACCOMPLISHMENTS

- Importance of PFLOTRAN-based framework
    - More mechanistic
        - Improved coupling and representation of processes and domains
    - Ability to include more FEPs
        - Reduces the need for FEP exclusion analyses
    - Built for high-performance computing (HPC)
        - Allows for higher fidelity probabilistic simulations
    - Open source is advantageous for
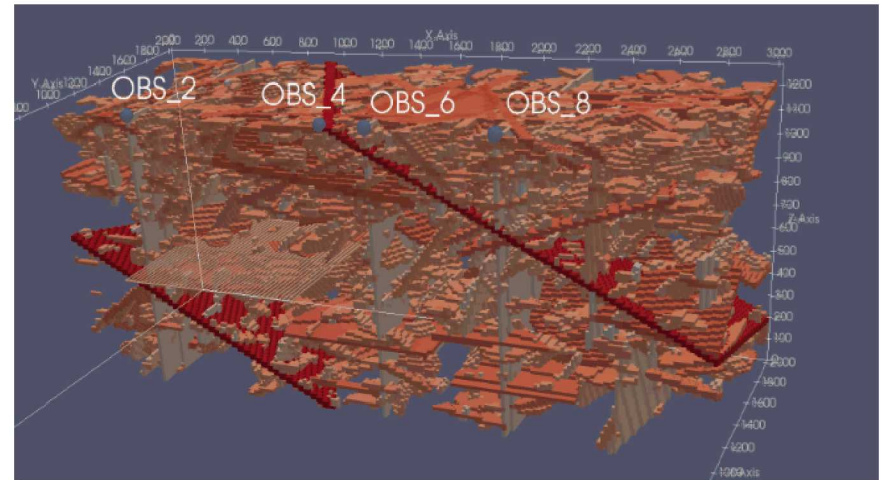   - Expanding the user base
        - Code development
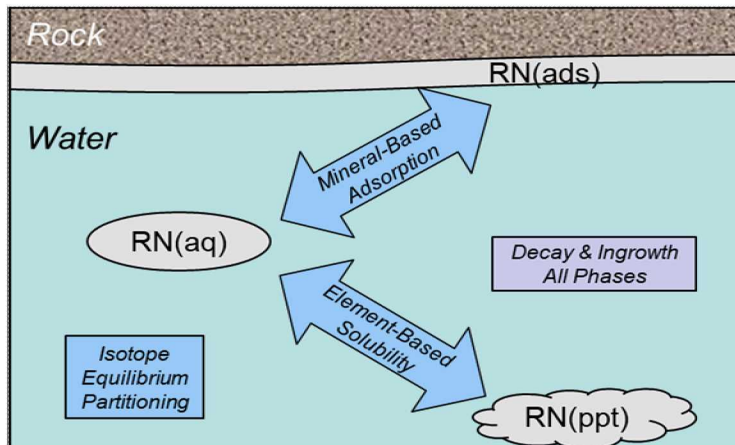   - Vetting the code
        - Code acceptance

Key Accomplishments

- PFLOTRAN source term developed for GDSA
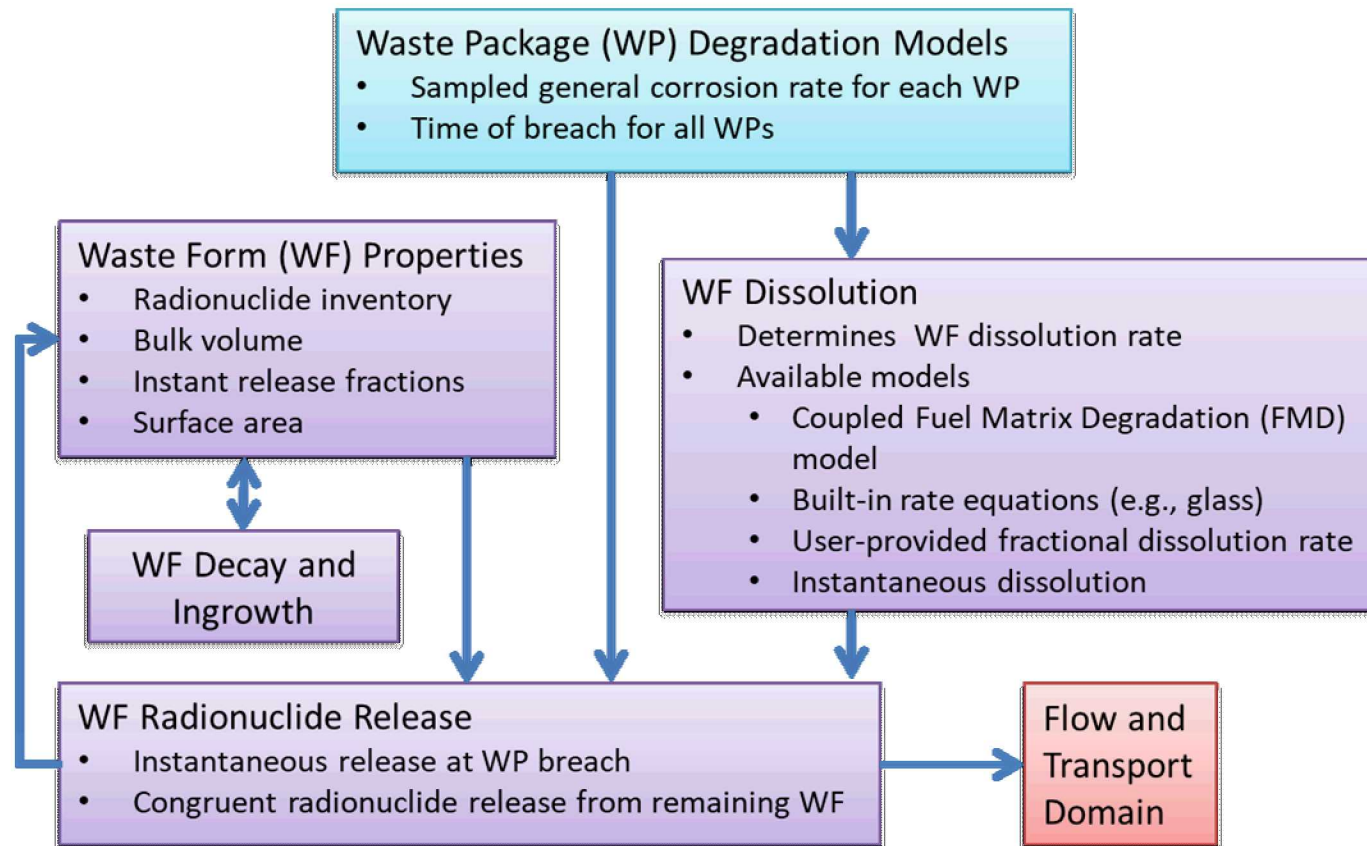
Key Accomplishments

- ## GDSA Framework development for flow and transport

  - Decay/ingrowth all phases
  - Mineral-based adsorption
  - Element-based solubility
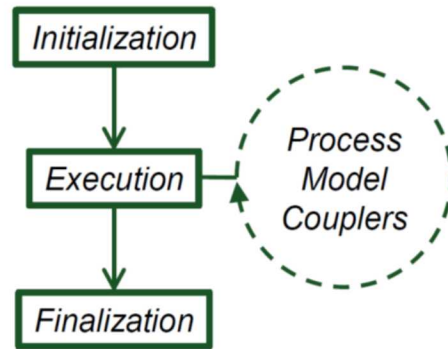 - Isotope equilibrium partitioning

  - dfnWorks – for generating DFNs
  - mapDFN – for mapping DFNs to porous continuum meshes
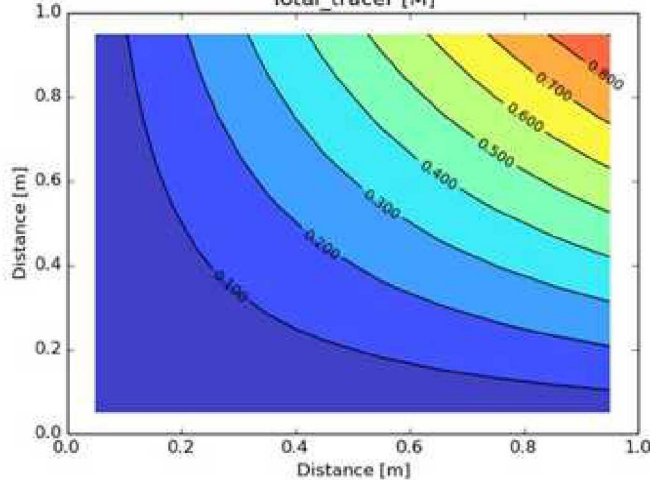 - Reference biosphere model (dose from water ingestion)

KEY ACCOMPLISHMENTS

- PFLOTRAN code infrastructure for GDSA

- Developed process model coupling infrastructure
  - Used to couple Fuel Matrix Degradation (FMD) model
- Convergence and efficiency improvements
  - Added analytical derivatives
  - Added multiphase solution controls
  - Automated mapping of boundary and initial conditions
- Verification testing
- Online code documentation
- QA software documentation drafted

KEY ACCOMPLISHMENTS

- Dakota tools integrated
  - Sampling uncertain inputs to define realizations
    - Latin Hypercube sampling
    - Simple random sampling
  - Sensitivity analysis
    - Scatter plots
    - Simple and partial correlation coefficients (and rank transformed equivalents)
    - Stepwise linear regression
    - Main and total sensitivity indices calculated via polynomial chaos expansion (PCE) and Gaussian process (GP) metamodels
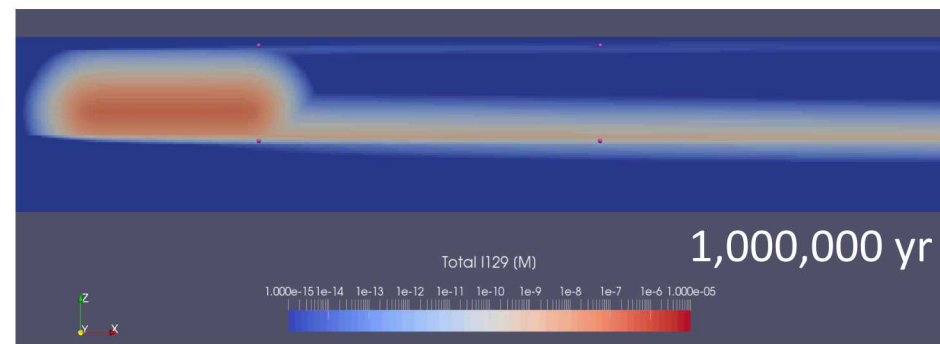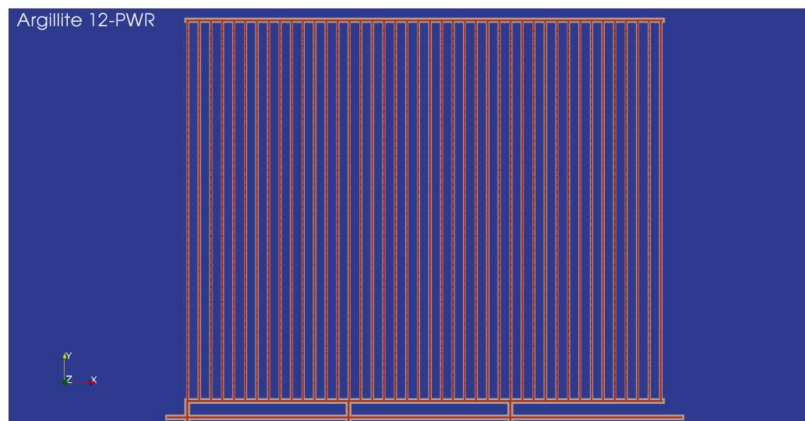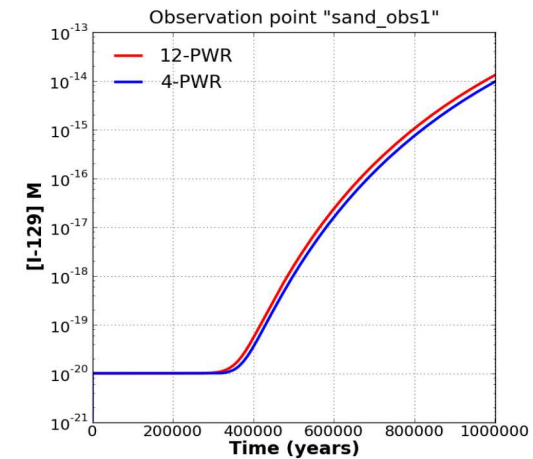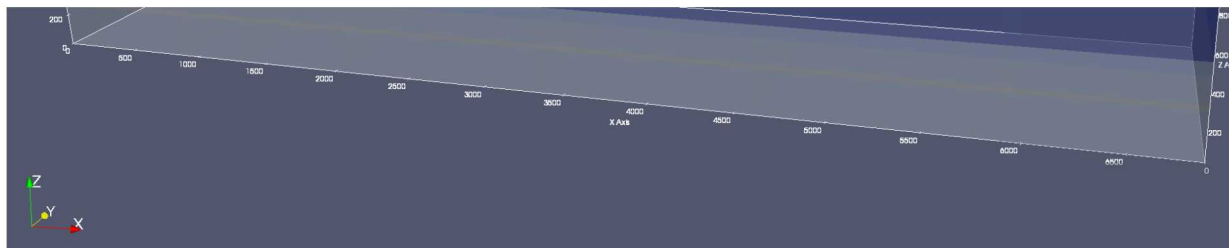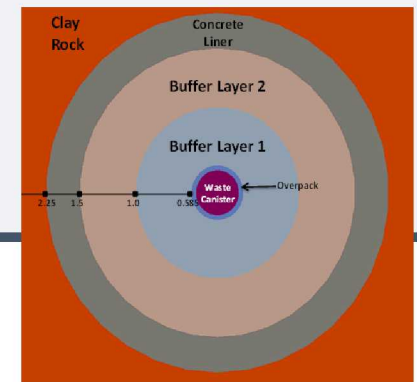
KEY ACCOMPLISHMENTS

- Integration of Disposal Research (DR) R&D

| FY	GDSA Integration Activities
2015	• Fuel Matrix Degradation process model coupled to PFLOTRAN • 18 process model templates from DR R&D work packages • Model Integration Table (new)
2016	• Informal FEP gap analysis • Lightning talks at annual meeting • Discrete fracture network integration • Model Integration Table expanded to include level of effort, level of readiness, and integration timeframe
2017	• Planning for GDSA Framework to be ready for a site by 2020 • Identification of capabilities to add, prioritization of these capabilities, and consideration of the timeline
2018	• Annual Working Group Meeting driven by GDSA group to enhance integration across the campaign; "evaluation" sessions held to assess level-of-effort, state-of-art, etc.
2019	• DR R&D Roadmap Update workshop held, Roadmap Update report completed • DR R&D activities and gaps identified, mapped to FEPs, and prioritized • Access database developed for tracking integration efforts and FEP coverage • Began surrogate model development to facilitate integration of process models • Built SFWD Document Archive for milestones

KEY ACCOMPLISHMENTS

- ## Shale Reference Case

KEY ACCOMPLISHMENTS

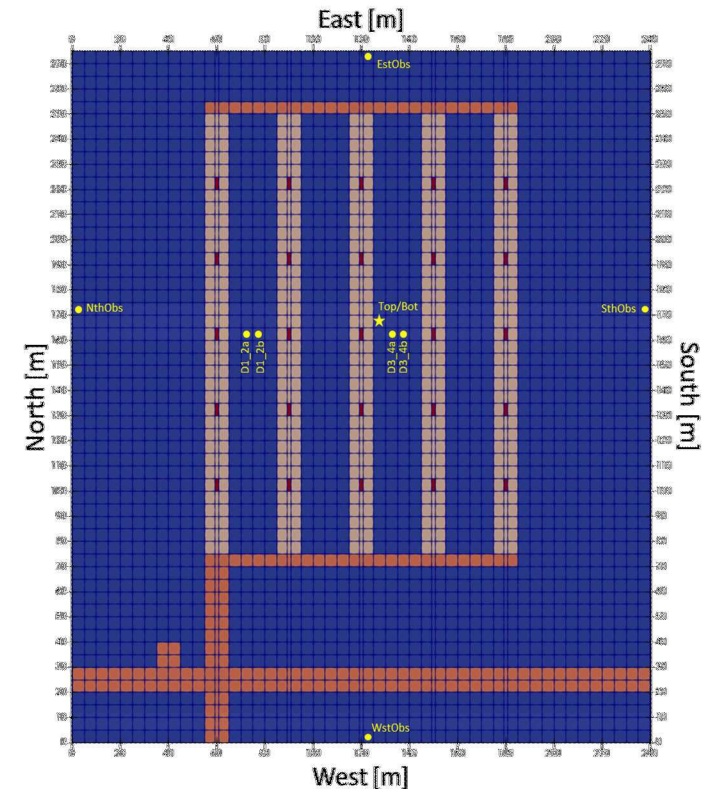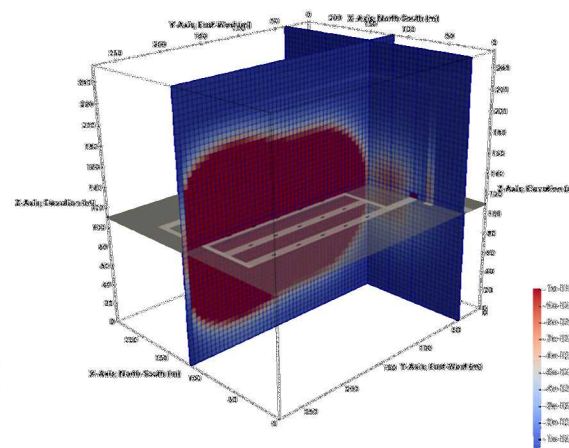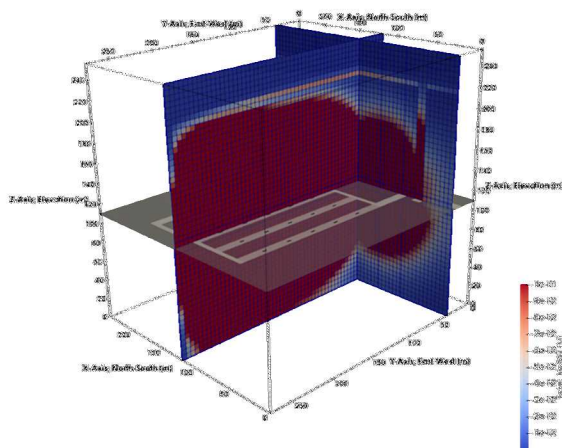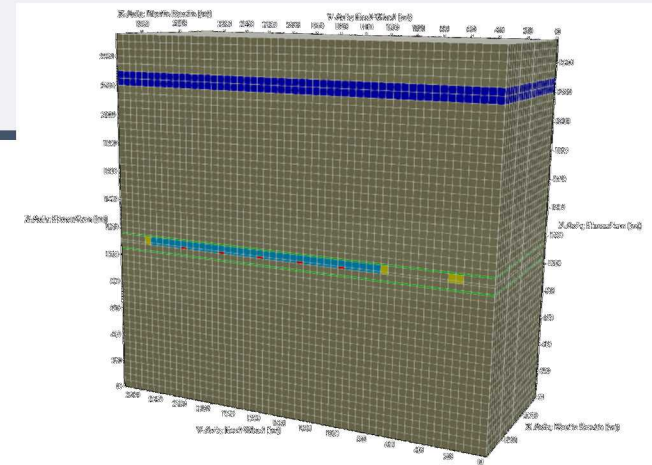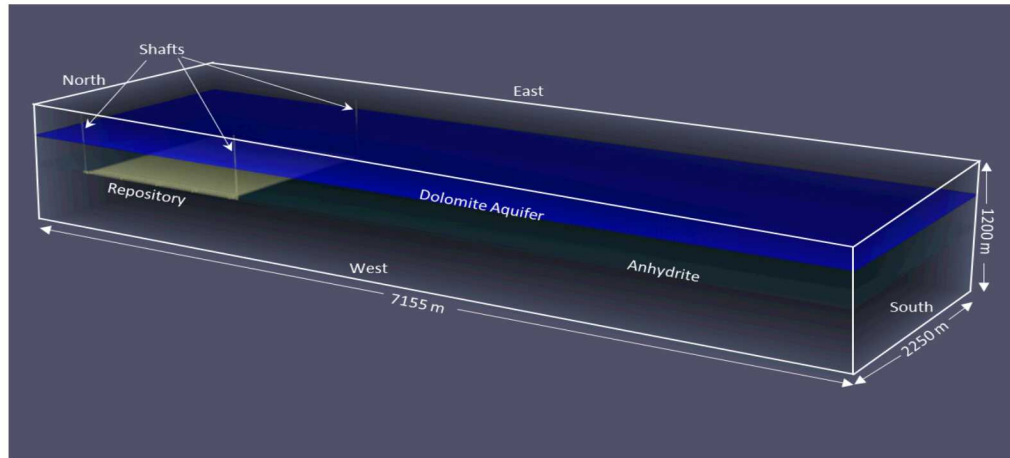- Crystalline Reference Case
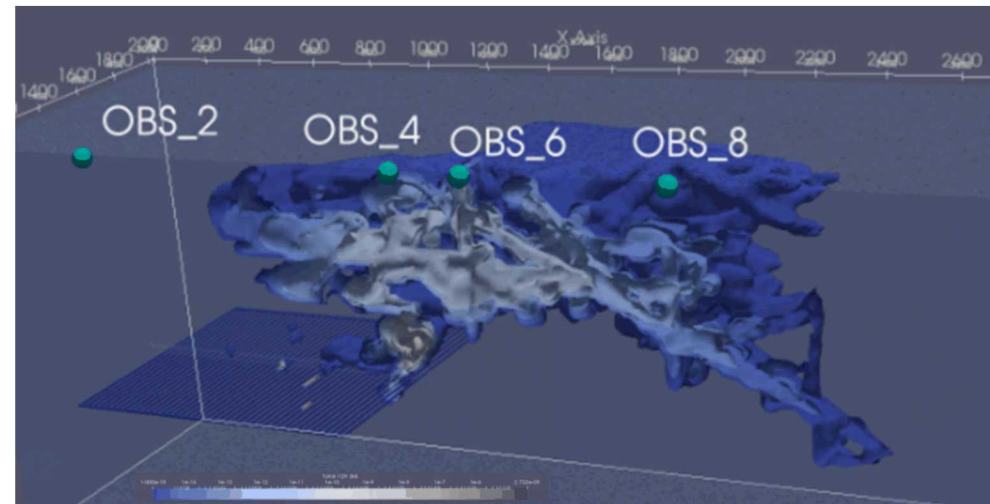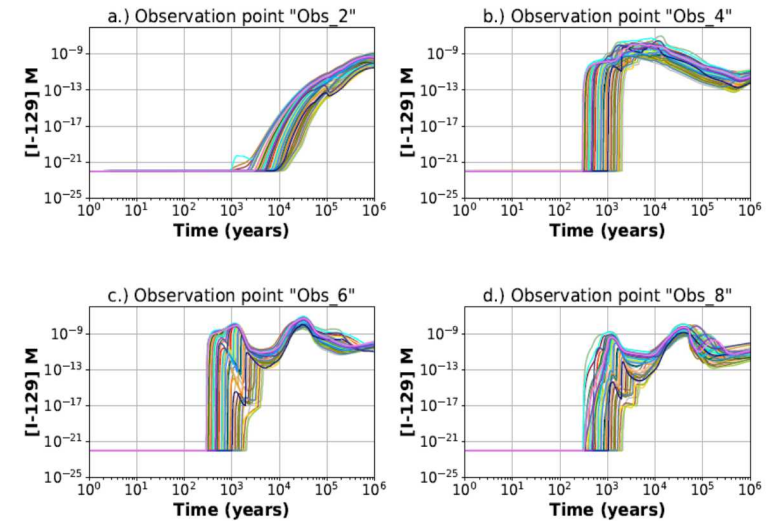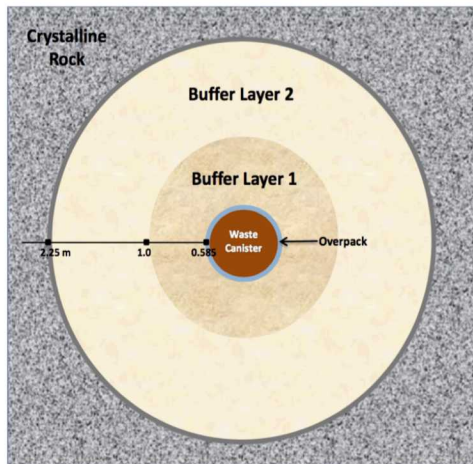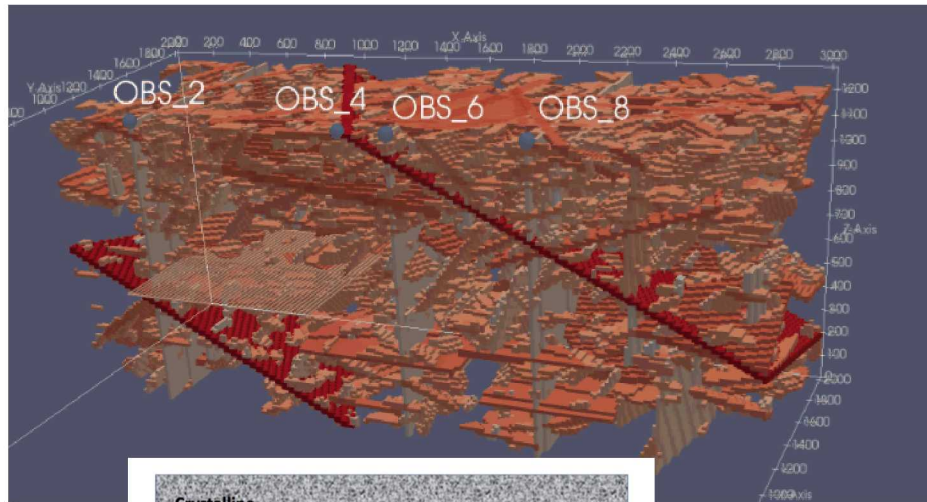
KEY ACCOMPLISHMENTS

- ## Salt Reference Case

KEY ACCOMPLISHMENTS

- ## Unsaturated Alluvium Reference Case

inset of potential geologic repository

Playa

Spring

Upper basin fill

Alluvial fan

Water table

Lower basin fill

Consolidated rock
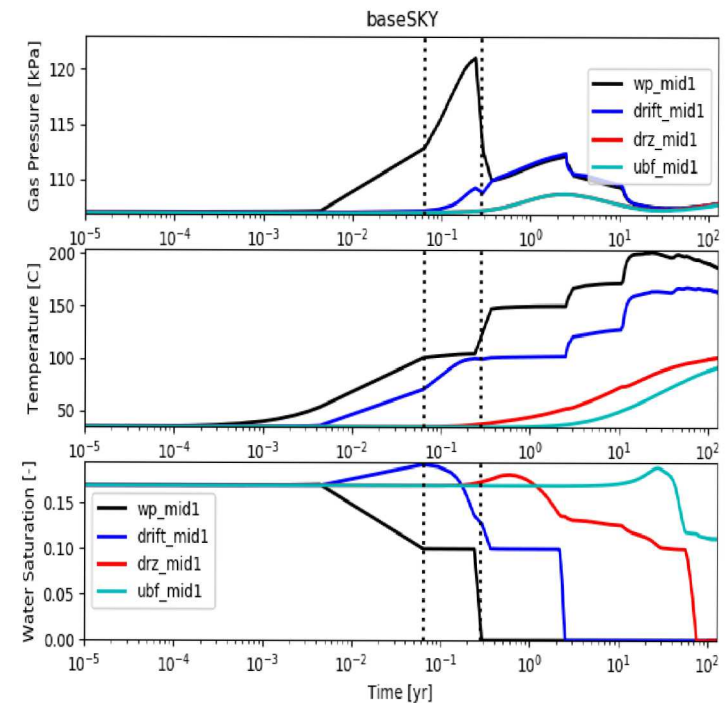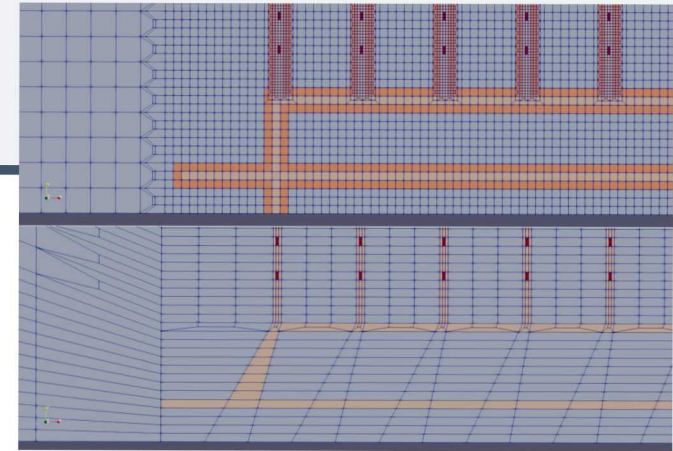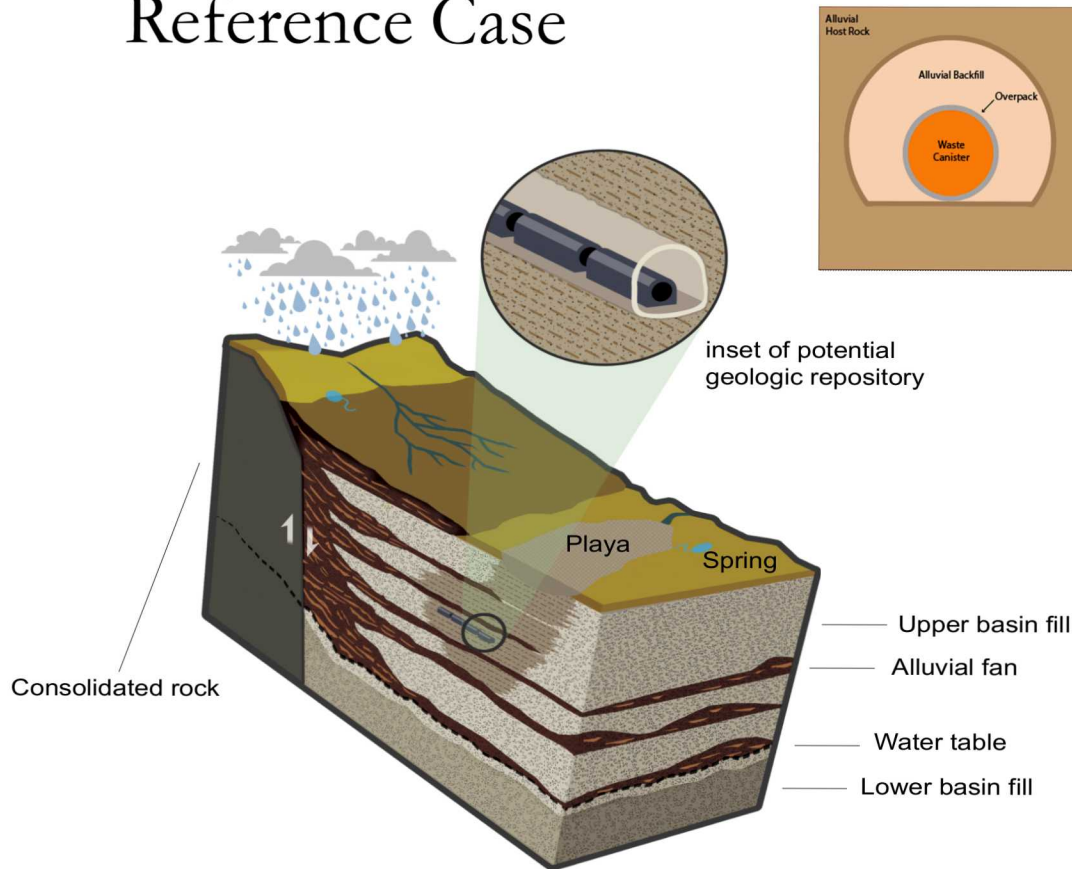
KEY ACCOMPLISHMENTS

- Conducted PFLOTRAN short courses

Year	Participants / Event (Location)
2017	• Sandia (Albuquerque) • Migration 2017 (Barcelona) • Performance & Risk Assessment Community of Practice (Albuquerque)
2018	• TaiPower (Taipei)
2019	• Vanderbilt Univ. (Albuquerque) • CSIRO (Adelaide) – not DOE funded • IHLRWM (Knoxville) • Uni Bern (Bern)

GDSA PRIORITIES GOING FORWARD

- ## High Priority
  - P-12 WP Degradation Model Framework

- ## Medium-High Priority
  - P-1 CSNF repository argillite reference case
  - P-2 CSNF repository crystalline reference case
  - P-4 CSNF repository unsaturated alluvium reference case
  - P-11 Pitzer model
  - P-13 Full Representation of Chemical processes in PA
  - P-14 Generic Capability Development for PFLOTRAN
  - P-15 Species and element properties
  - P-16 Solid solution model
  - P-17 Multi-Component Gas Transport

QUESTIONS?

SFWD

SPENT FUEL & WASTE DISPOSITION

Annual Working Group Meeting
May 21-23, 2019

UNLV-SEV – *Las Vegas, Nevada*