Exceptional service in the national interest

SAND2014-1331C

Performance Assessment Modeling of a Generic UNF/HLW Repository in Salt

Geoff Freeze, W. Payton Gardner, Palmer Vaughn,
S. David Sevougian, Paul Mariner,
Glenn Hammond, and Vince Mousseau

WM 2014 Conference
Phoenix, AZ, USA
March 4, 2014

Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. This presentation is approved as SAND2014-1331C.

Outline

- **Objectives**
- **Enhanced Performance Assessment (PA) Analysis Capabilities**
- **Enhanced PA Demonstration**
  - Generic Salt Repository for Used Nuclear Fuel (UNF) and High-Level Radioactive Waste (HLW)
- **PA Demonstration Results**
- **Conclusions**

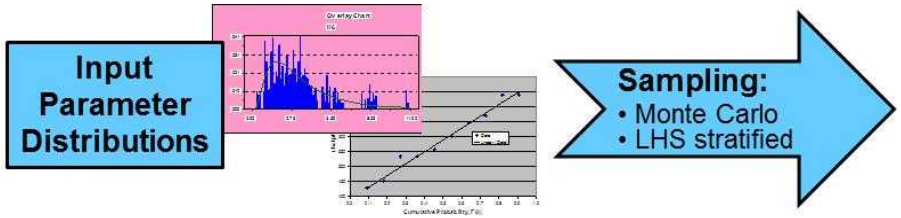
Objectives

- **Develop an enhanced UNF/HLW repository PA modeling and analysis capability that supports:**
  - Science-based PA-scale representation of important coupled multi-physics processes
  - A range of disposal options (e.g., salt, clay, granite, deep borehole)
  - Sensitivity and uncertainty analyses to enhance system understanding

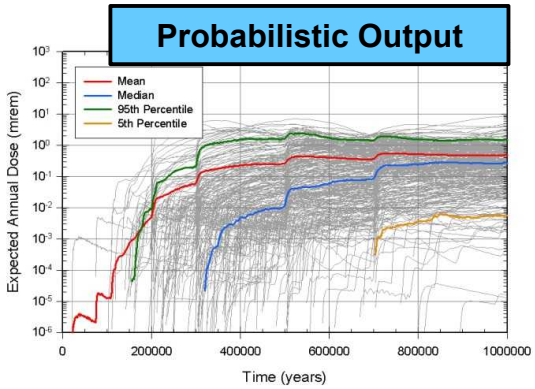
- **Support the Department of Energy, Office of Nuclear Energy (DOE-NE), Used Nuclear Fuel Disposition Campaign (UFDC)**
  - Analysis capability evolves commensurate with UFDC needs throughout program lifecycle
    - e.g., evaluation of disposal options, consent-based site selection, site characterization, stakeholder communication, safety case development, licensing, and operation

Enhanced PA Analysis Capabilities

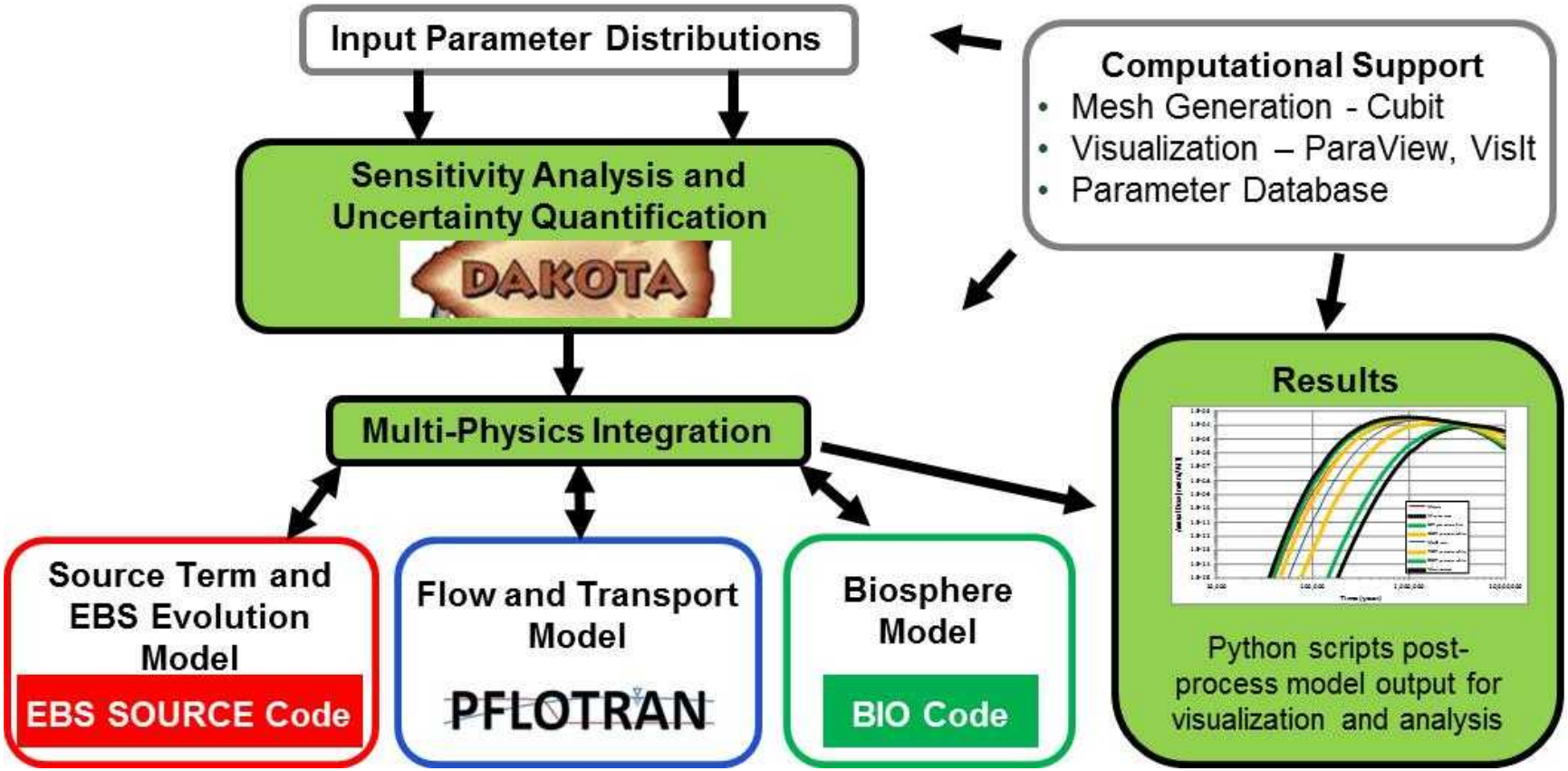
- **Science-based PA-scale representation of important coupled multi-physics processes**
  - Direct implementation of important thermal-hydrologic-chemical-mechanical (THCM) multi-physics processes and couplings, where necessary
    - Minimize use of conservative assumptions, simplifications, and process abstractions
  - Appropriate spatial and temporal representation of geometry, features, events, and processes (FEPs), and uncertainty (i.e., 3D probabilistic simulation)
    - Engineered barrier system (EBS): spatial variability in degradation processes and THCM behavior
    - Natural barrier system (NBS): spatial heterogeneity in stratigraphy and pathways



- **High-performance computing (HPC) architecture**
  - Facilitates reasonable probabilistic PA-model runtimes for science-based, 3D multi-physics

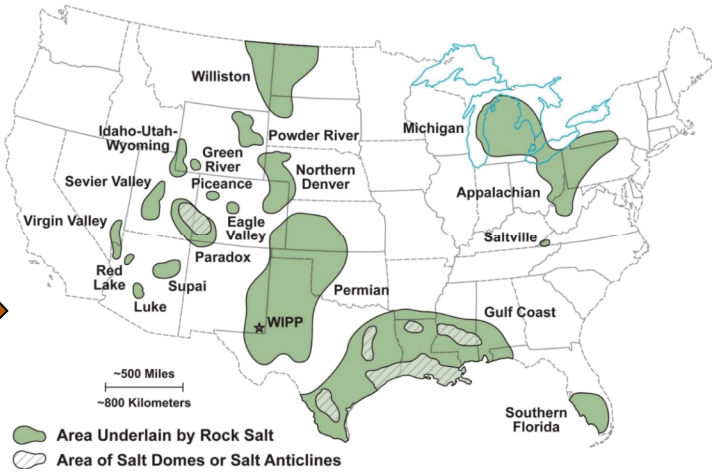


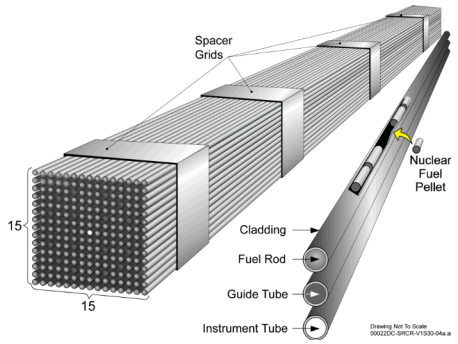
Enhanced PA Analysis Code Integration



Enhanced PA Demonstration – Generic Salt Repository Reference Case

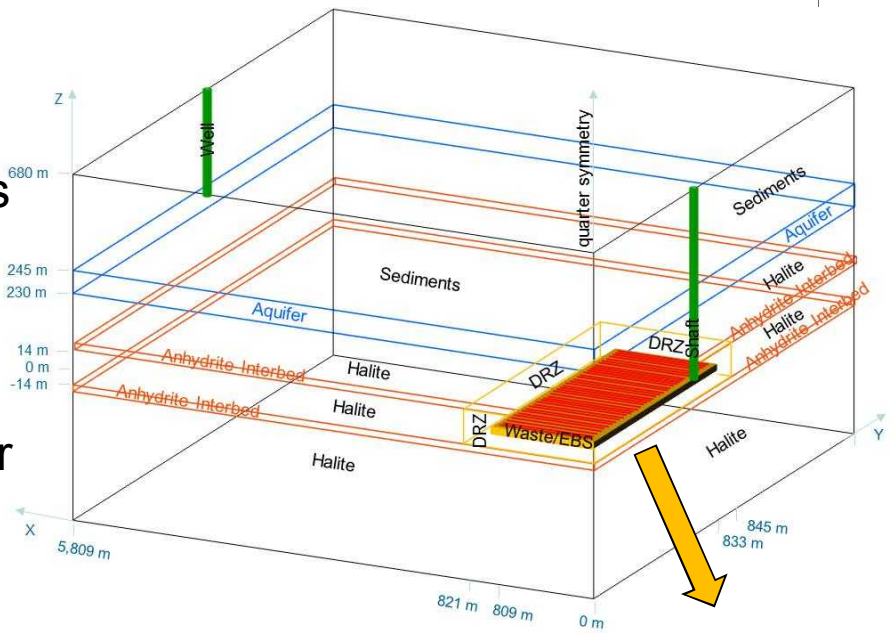
- **Assumptions are needed to describe a generic repository system**
  - Surrogate for site- and design-specific information from an actual location
- **Generic NBS characteristics are representative of major bedded salt basins in the United States**
  - Stratigraphy – e.g., depth, thickness, extent
  - Formation properties – e.g., hydraulic gradient, permeability, porosity, diffusivity, sorption
  - Fluid (brine) chemistry
- **Generic EBS layout and properties**
  - Waste Inventory – 70,000 MTHM (~ 13,400 waste packages (WP) of UNF)
    - 12 PWR assemblies/WP: 60 GWd/MT burnup, 7.5 kW/WP
  - Geometry – layout of waste emplacement drifts/tunnels and shafts
    - Drift spacing and WP loading based on 200˚ thermal limit for salt

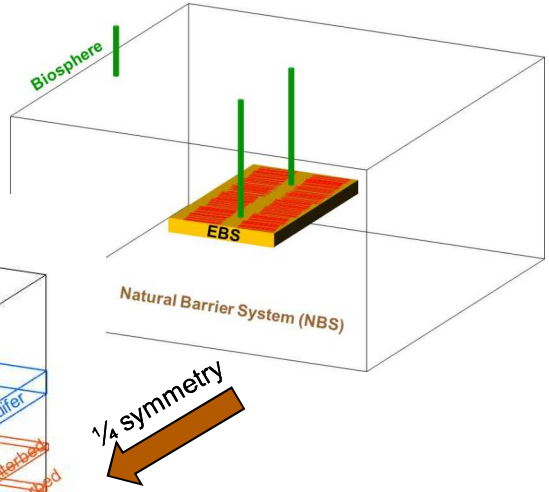




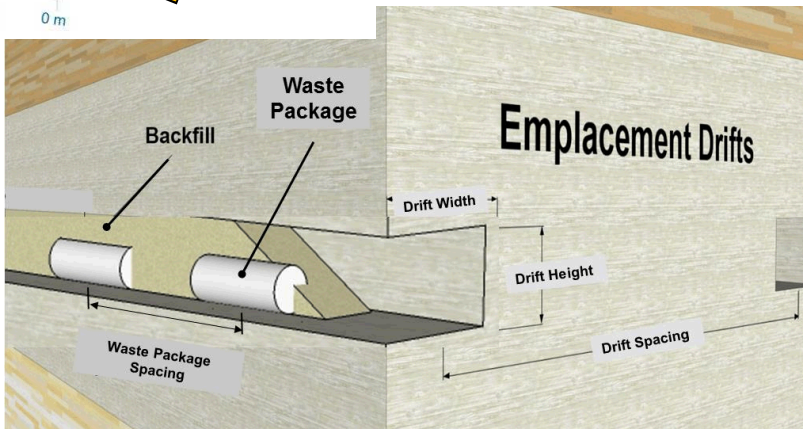
Enhanced PA Demonstration – Generic Salt Repository Reference Case

- **Generic NBS**
  - Halite host rock
  - Anhydrite interbeds
  - Disturbed rock zone (DRZ)
  - Overlying aquifer
  - 5,000 m to receptor well

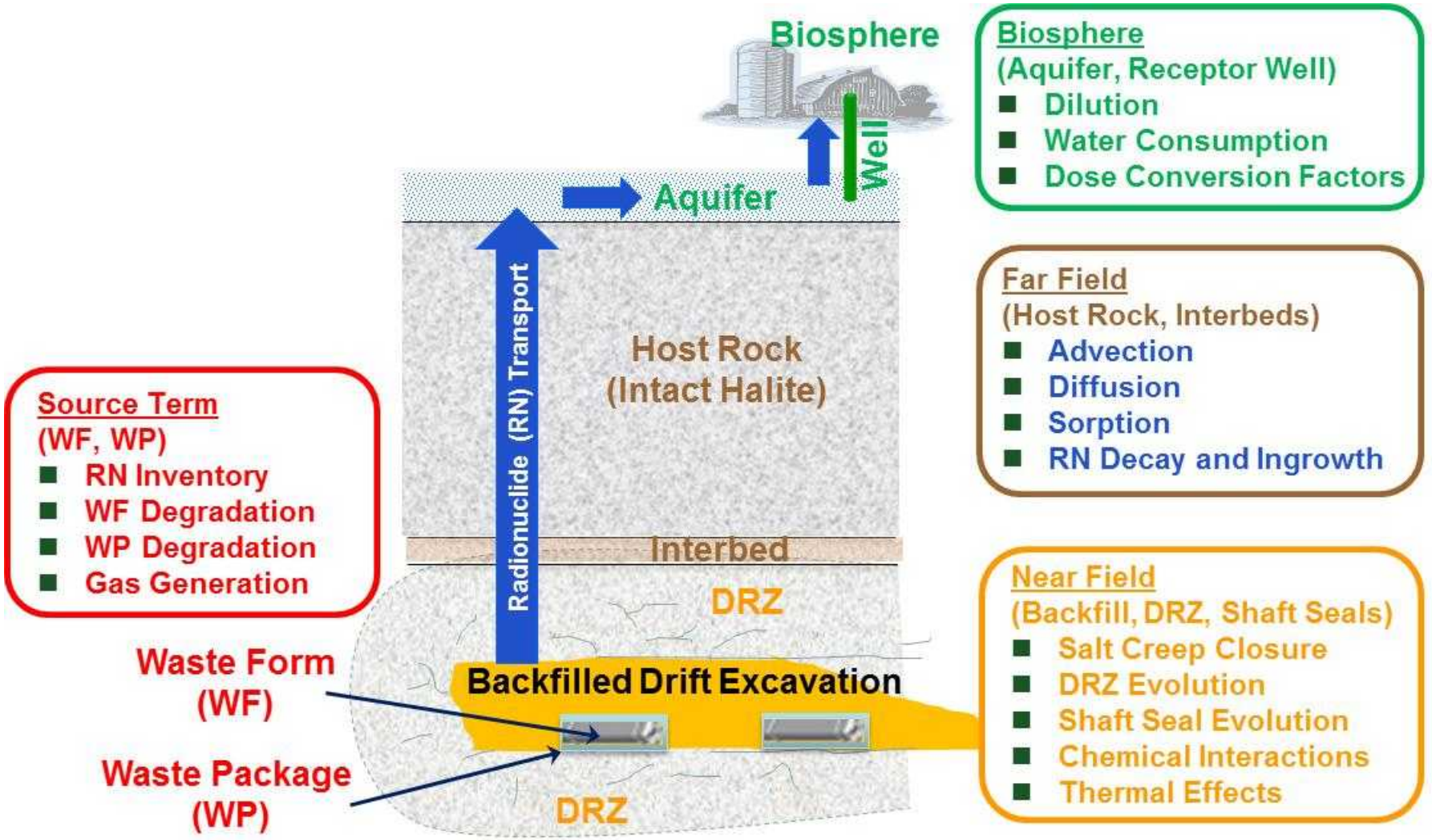




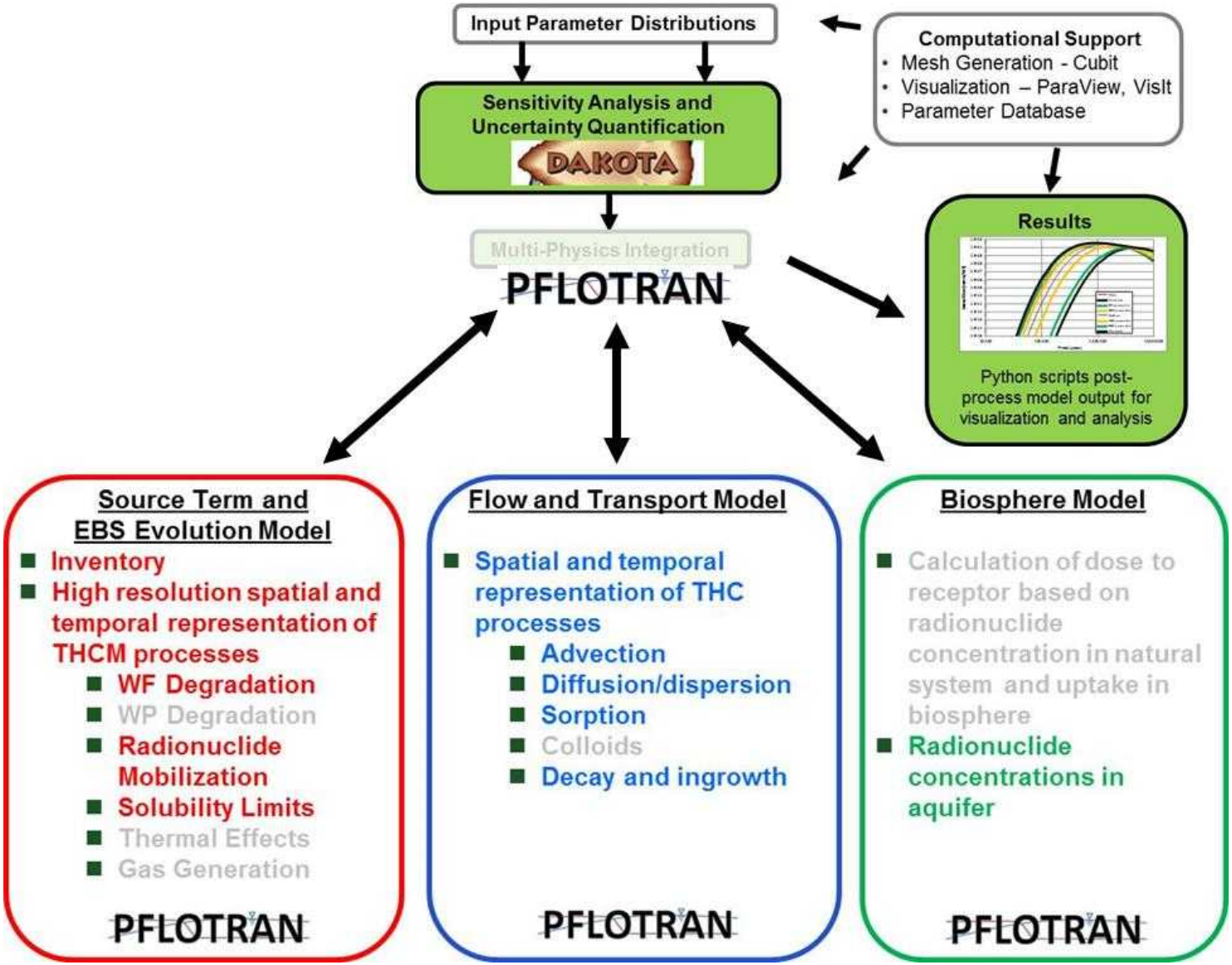
- **Generic EBS**
  - 84 pairs of 800-m emplacement drifts
    - 20-m spacing between drifts
    - 80 WPs/drift with 10-m spacing
  - Crushed salt backfill in drifts
  - Sealed shafts



Generic Salt Repository Reference Case – Components and FEPs (Undisturbed Scenario)



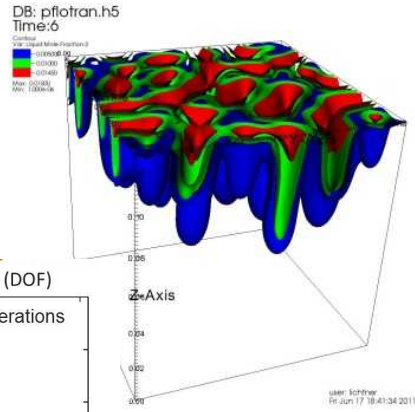
Enhanced PA Demonstration – Code Integration

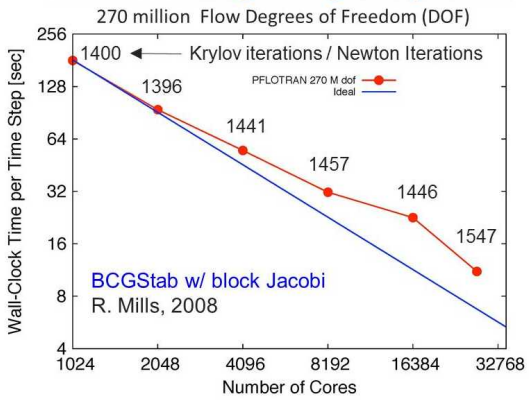


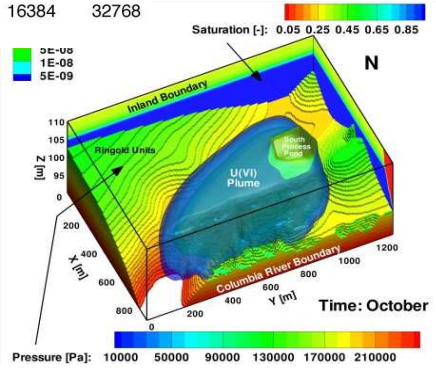
PFLOTRAN Code Capabilities

- **Multi-physics**
  - Multi-phase fluid and heat flow
  - Multi-component transport
  - Biogeochemical processes
- **High-Performance Computing (HPC)**
  - Built on PETSc – parallel solver library
  - Highly refined 3D discretizations
  - Massively parallel probabilistic runs
    - Rapid turnaround (minutes to hours)
- **Open Source**
  - Freely available
  - Leverages diverse scientific community
  - Scalable from laptop to supercomputer
- **Object-Oriented Fortran (2003/2008)**
  - Modular code framework for adding new capabilities

PFLOTRAN



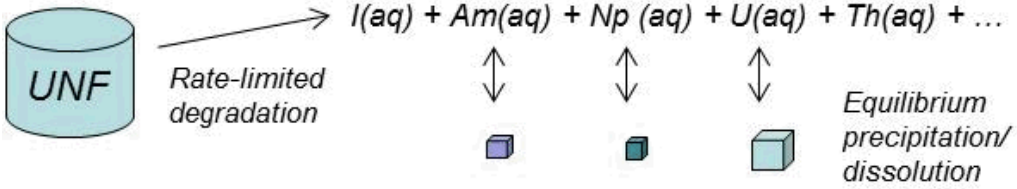




Hammond and Lichtner, WRR, 2010

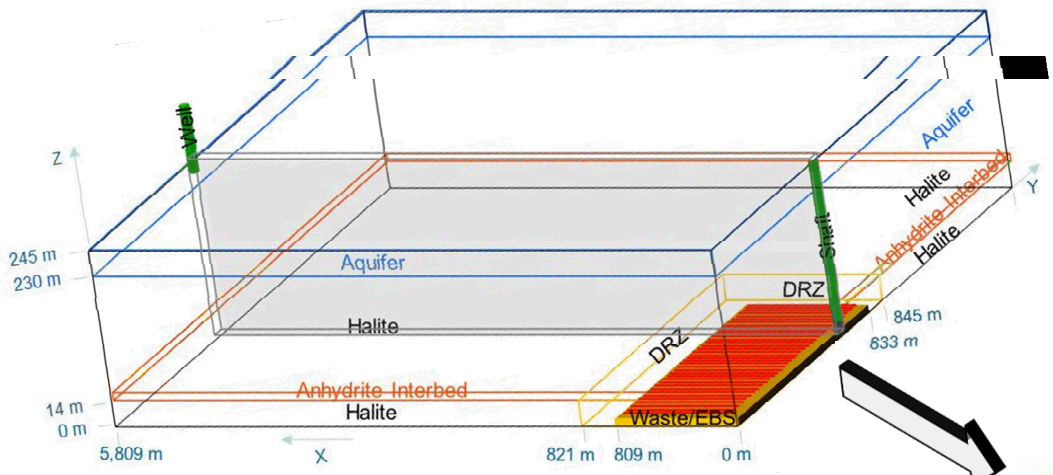
Generic Salt Repository PA Demonstration

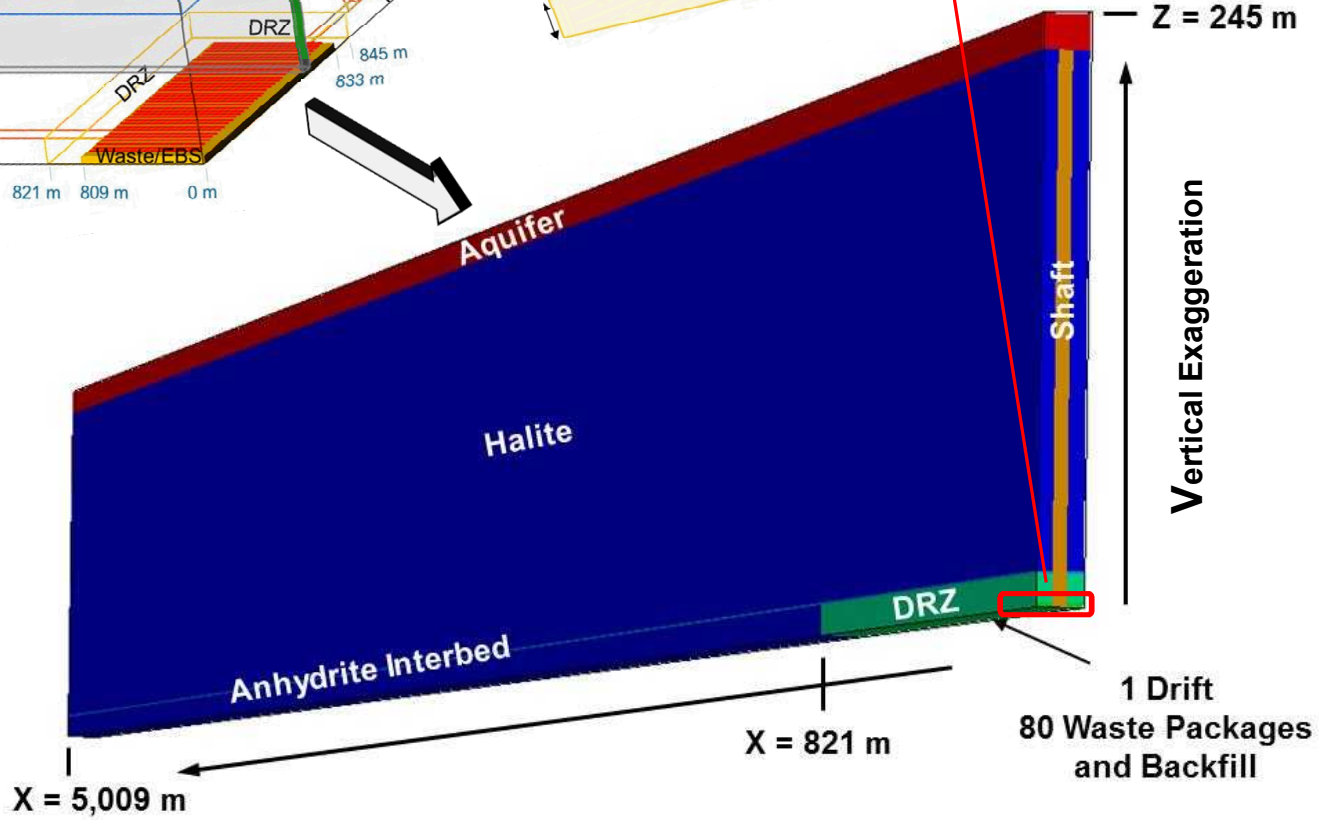
- **Undisturbed scenario only (i.e., no human intrusion)**
- **Coupled multi-physics (PFLOTRAN)**
  - **EBS:** source term
    - 5 radionuclides:
      - ^{129}I, ^{241}Am, ^{237}Np, ^{233}U, ^{229}Th



    - Waste form (UNF) degradation rate controlled by kinetic rate of reaction
      - *Complete degradation in approximately 10,000 years (for demonstration purposes)*
    - Solubility limits
      - *Dissolved radionuclides that reach solubility precipitate*
  - **NBS:** 3D fluid (brine) flow and radionuclide transport
    - Diffusion through DRZ and bedded salt
    - Advection through aquifer
- **Uncertainty quantification with DAKOTA**
  - Latin Hypercube sampling (LHS) of input parameter distributions
  - Sensitivity Analysis

Generic Salt Repository PA Demonstration – 3D Model Domain (Vertical Slice)

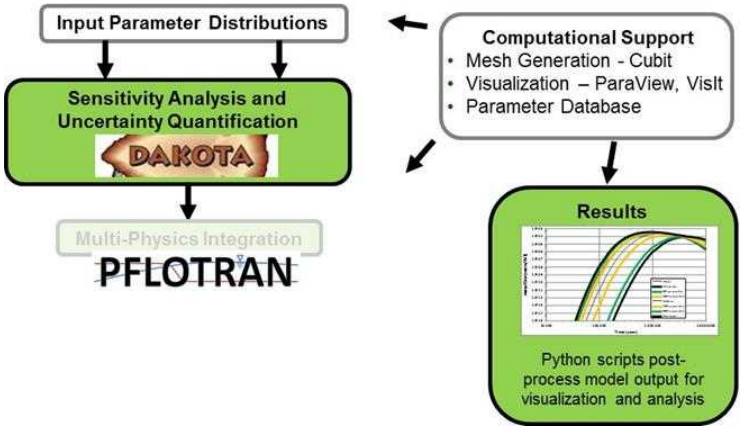




NX = 242 (x = 5,009 m)
NY = 5 (y = 20 m)
NZ = 38 (z = 245 m)
Cells = 45,980

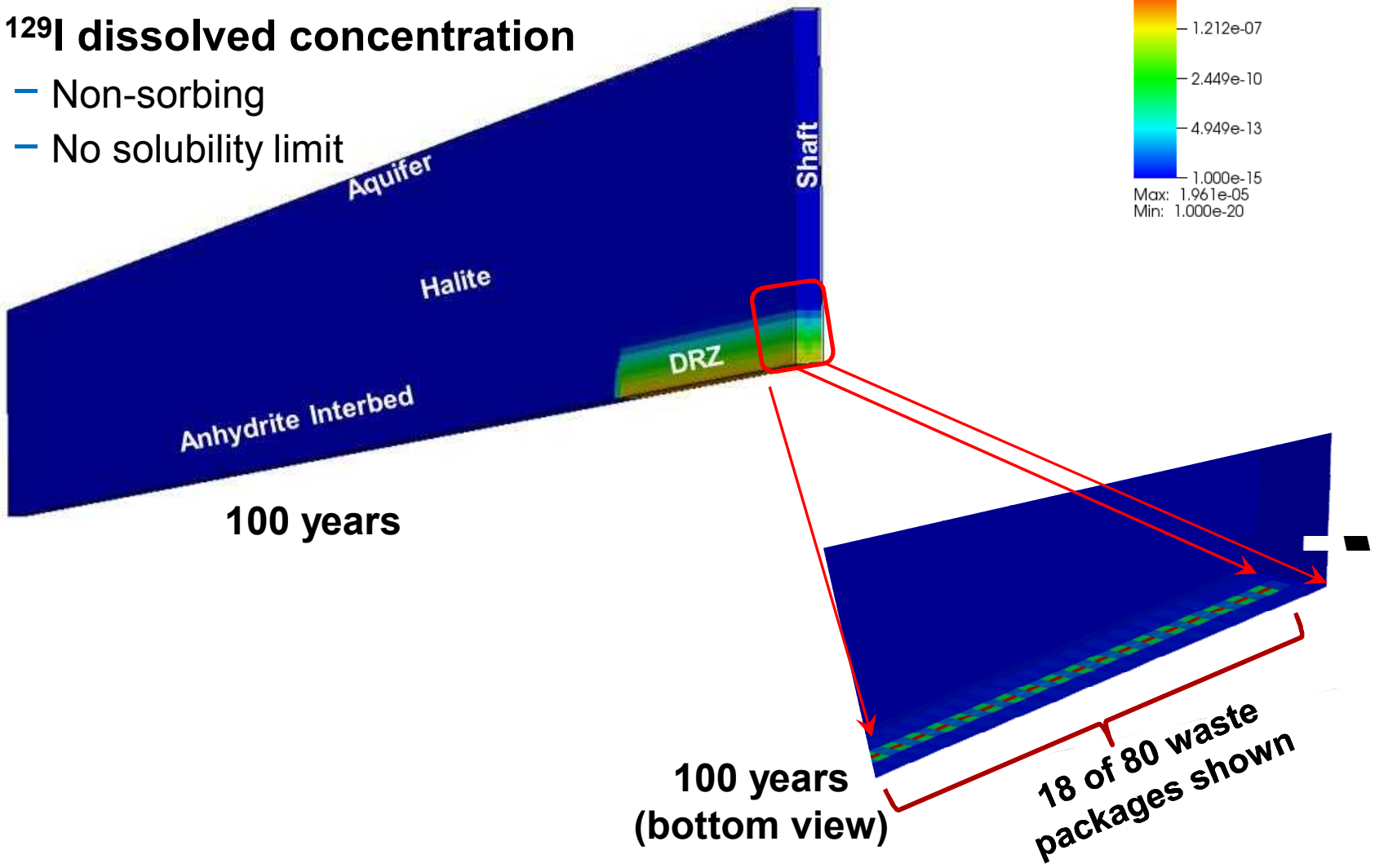
Generic Salt Repository PA Demonstration – Simulations

- **PFLOTRAN / DAKOTA**
  - Direct representations of source term, flow, and transport processes
    - 3D spatial and temporal heterogeneity/variability
    - 80 individual waste packages
    - 45,980 cells x 9 radionuclides/mineral phases = 413,820 degrees of freedom
  - Deterministic simulation with mean values
  - Probabilistic simulation with 9 sampled parameters
  - Run on SNL Red Sky HPC cluster
    - Nested parallelism
    - Many concurrent realizations
    - Each realization distributed across many processors
    - Multi-realization problem run in short wall clock time



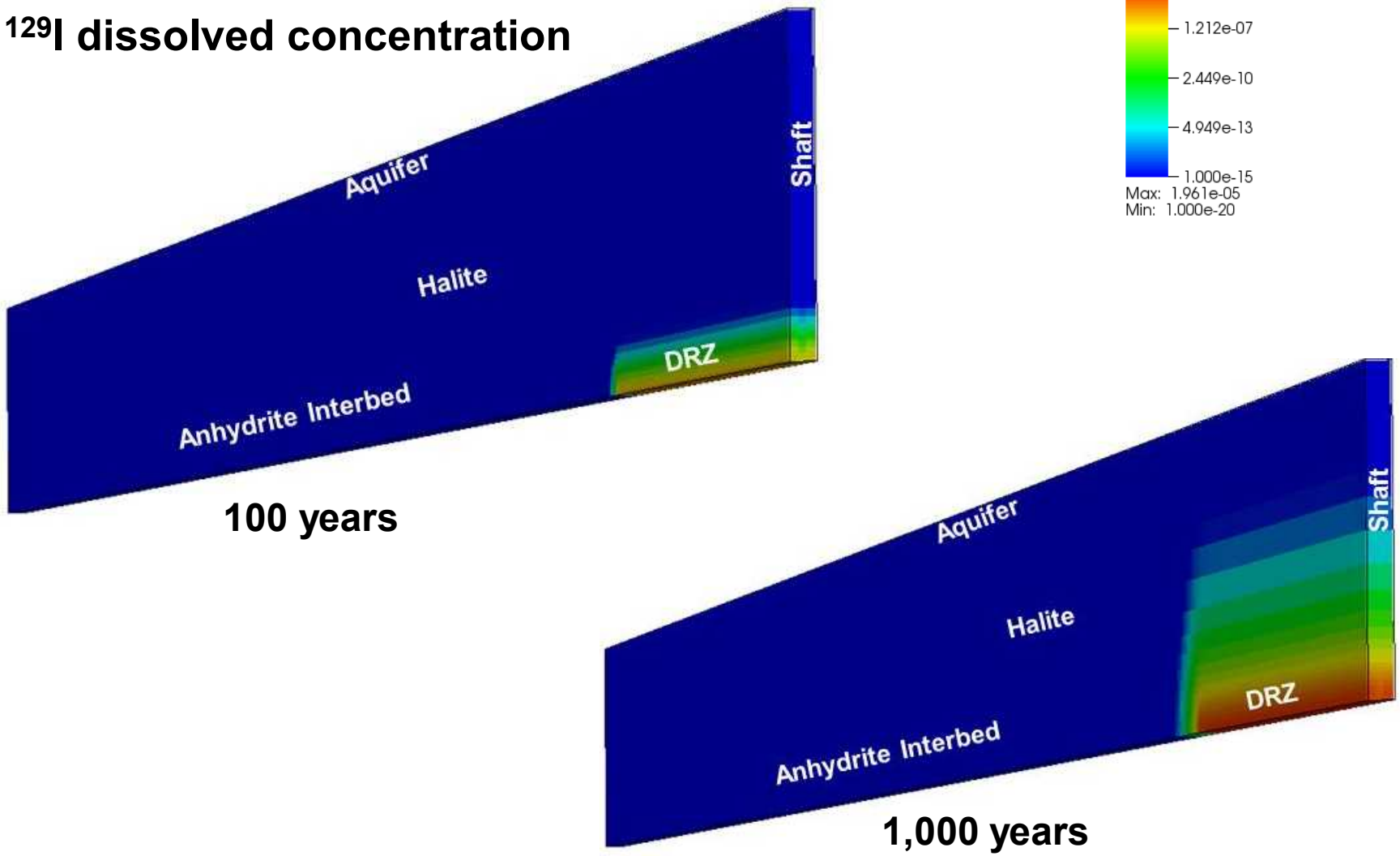
Generic Salt Repository PA Demonstration – Deterministic Simulation Results

- **^{129}I dissolved concentration**
  - Non-sorbing
  - No solubility limit



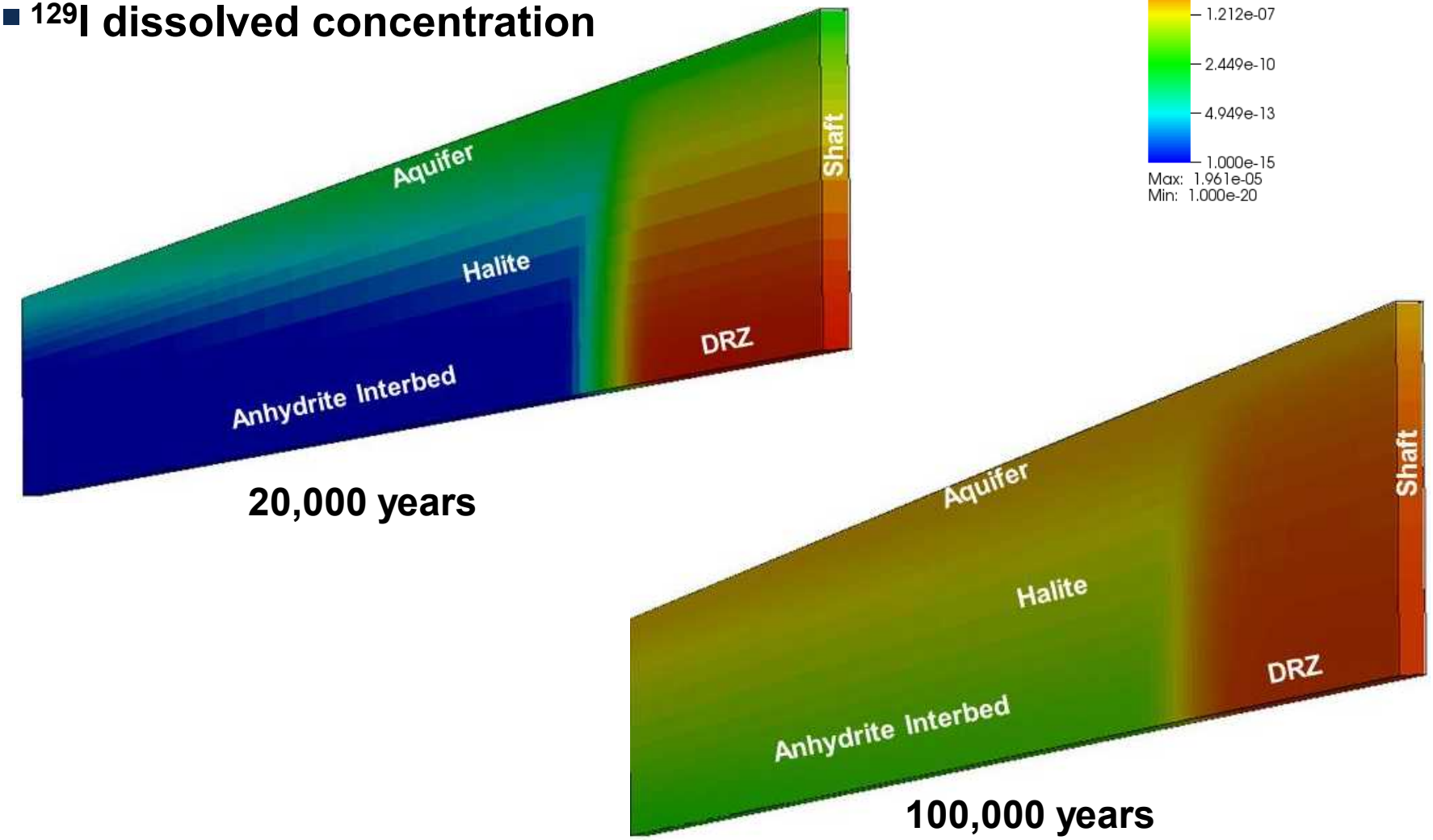
Generic Salt Repository PA Demonstration – Deterministic Simulation Results

- ^{129}I dissolved concentration



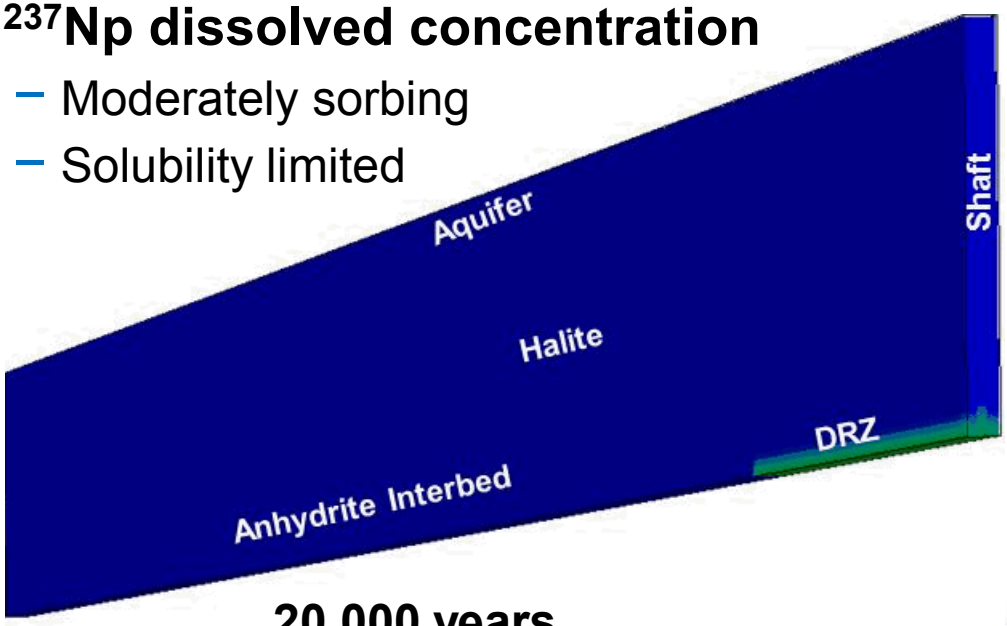
Generic Salt Repository PA Demonstration – Deterministic Simulation Results

- ^{129}I dissolved concentration

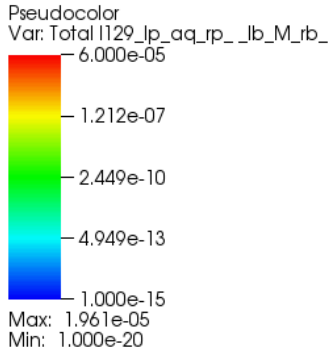


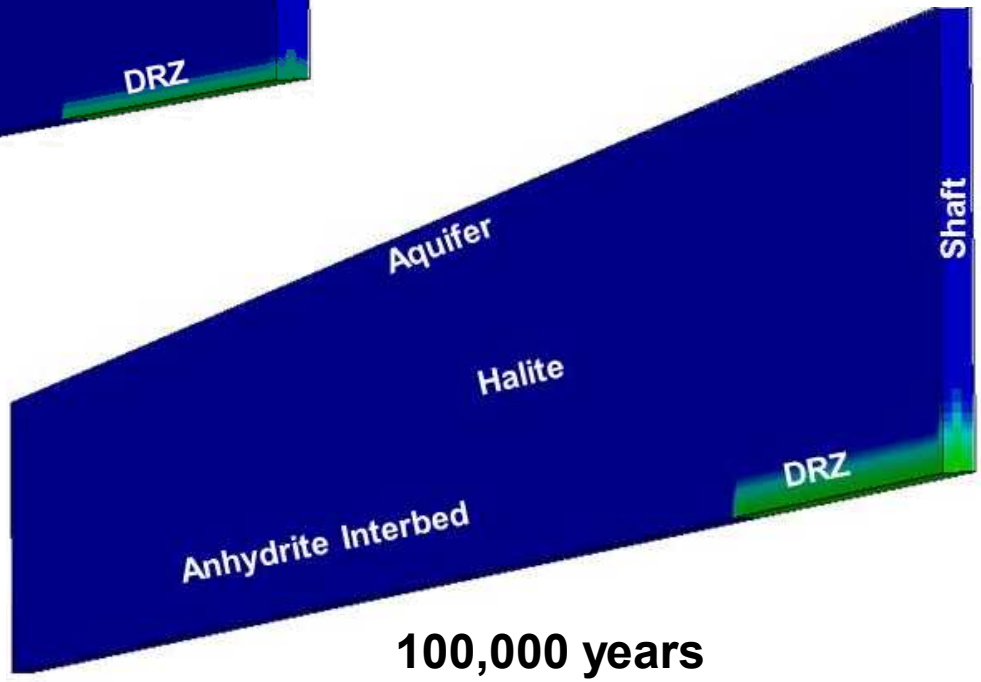
Generic Salt Repository PA Demonstration – Deterministic Simulation Results

- **^{237}Np dissolved concentration**
  - Moderately sorbing
  - Solubility limited



20,000 years

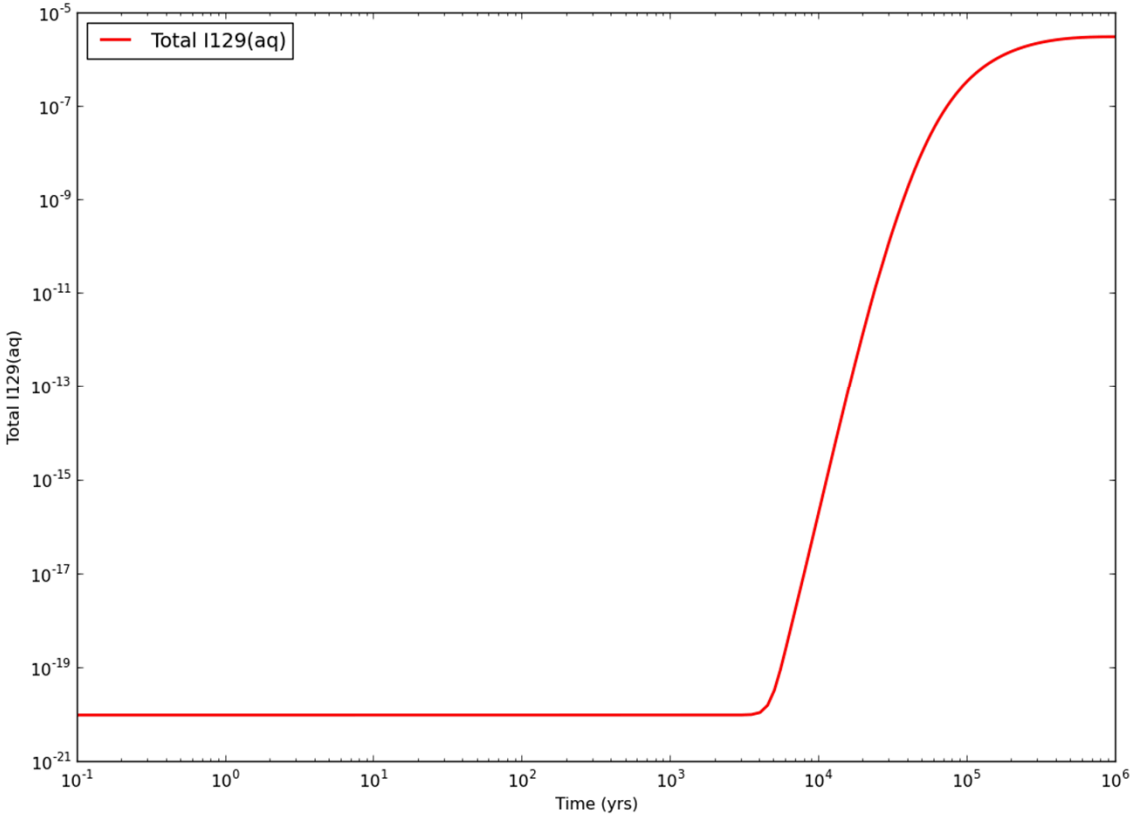


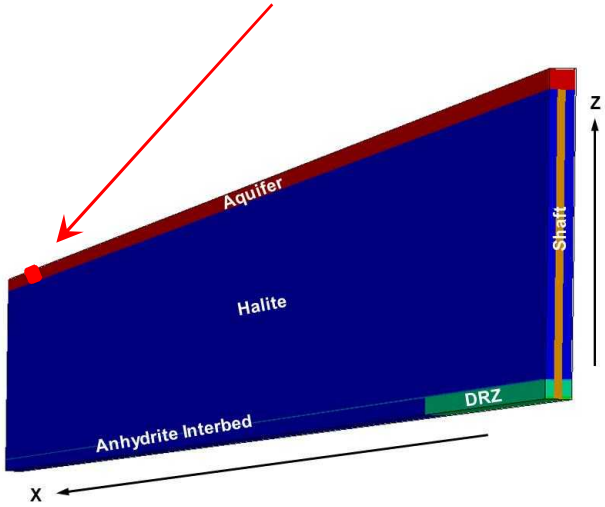


100,000 years

Generic Salt Repository PA Demonstration – Deterministic Simulation Results

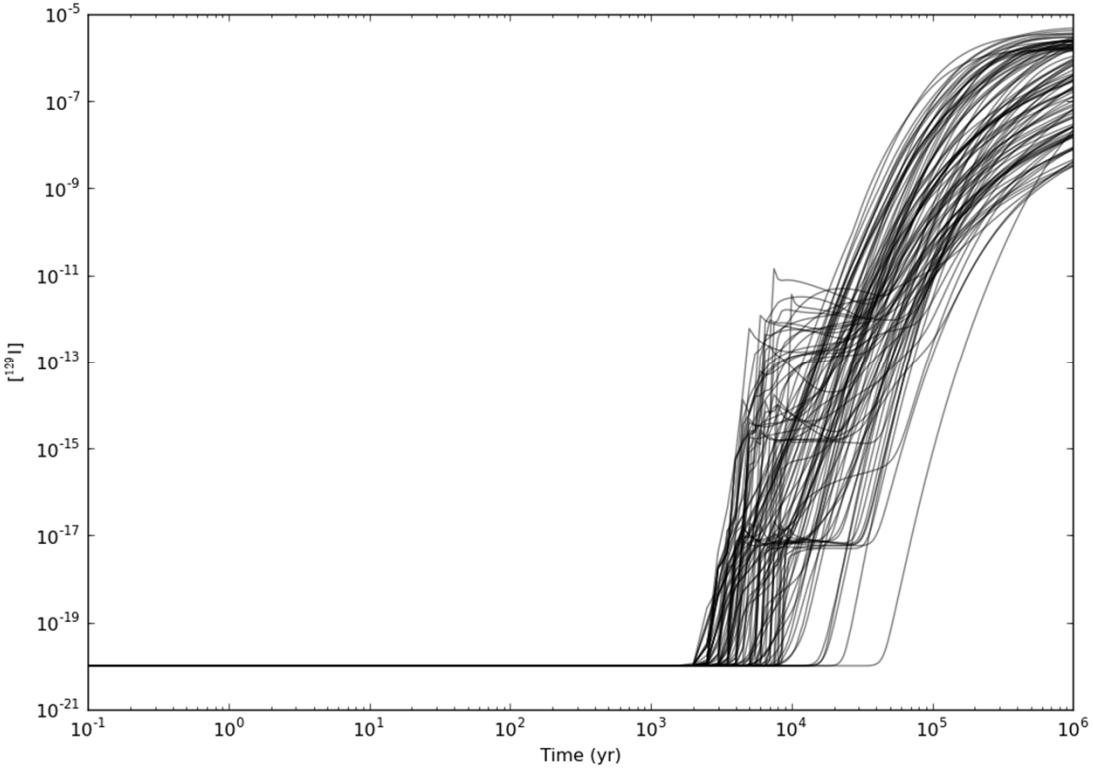
- ^{129}I dissolved concentration vs. time in aquifer at x = 4,900 m

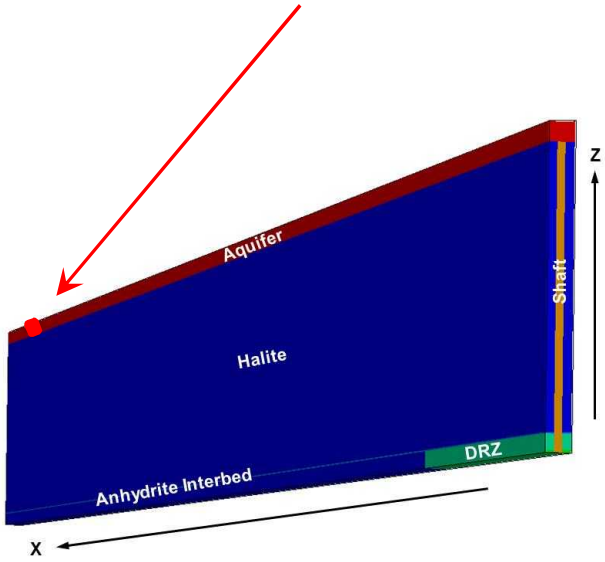




Generic Salt Repository PA Demonstration – Probabilistic Simulation Results

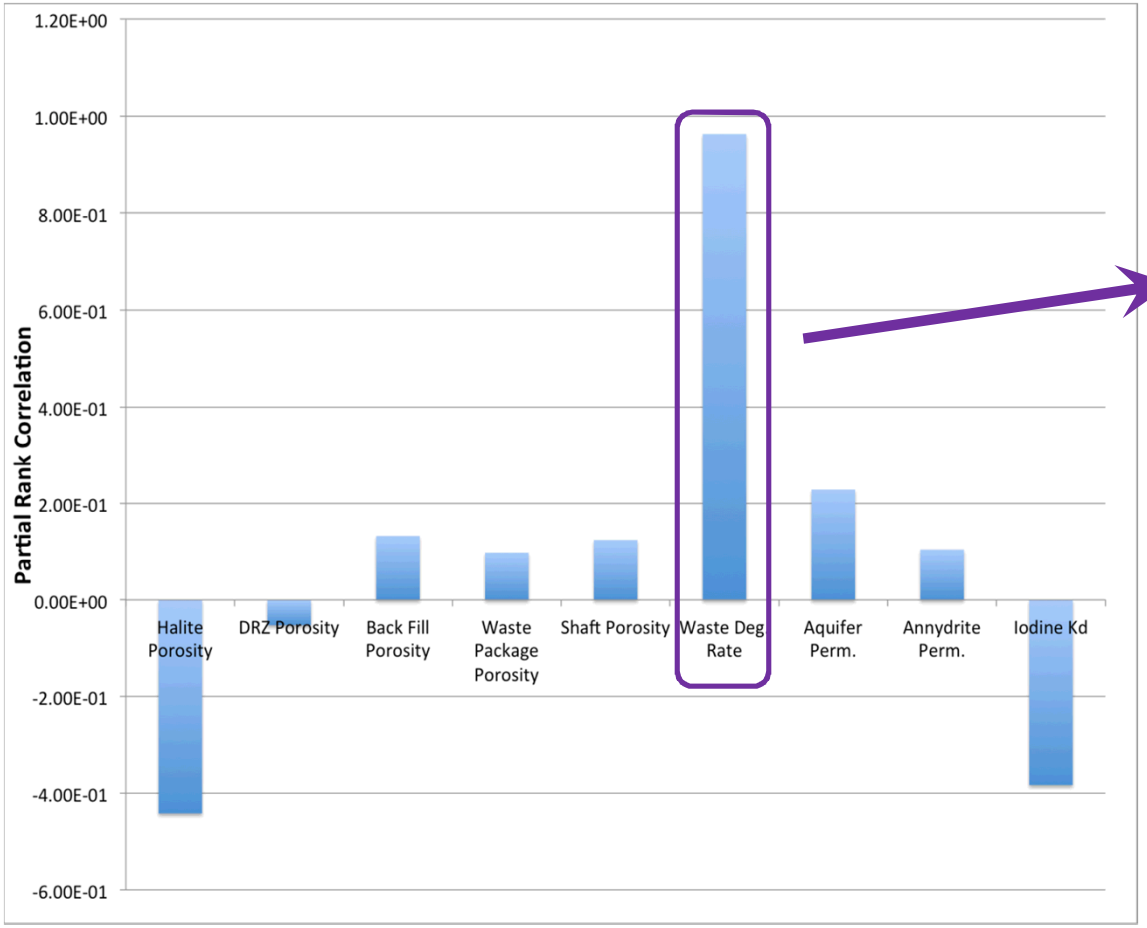
- **^{129}I dissolved concentration vs. time in aquifer at x = 4,900 m**
  - Probabilistic output
    - 100 realizations with 9 sampled parameters

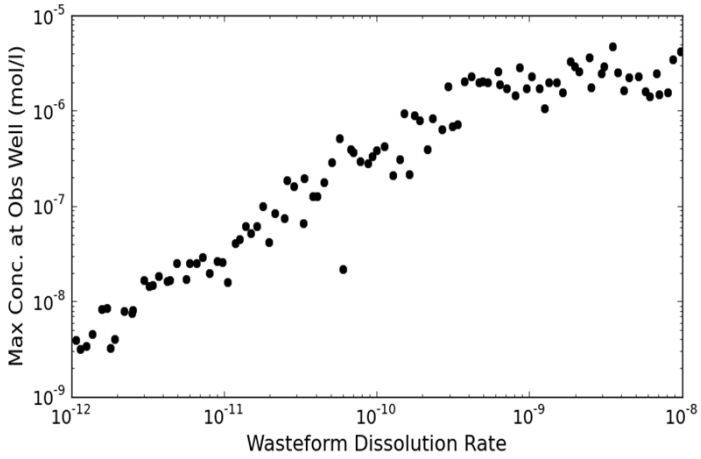




Generic Salt Repository PA Demonstration – Sensitivity Analysis

- **DAKOTA partial rank correlation analysis and scatterplot of uncertain parameters**





Conclusions

- **An HPC-based PA modeling and analysis capability was demonstrated by application to a generic salt repository**
  - Science-based PA-scale representation of important coupled multi-physics processes
    - Direct source term (inventory, WF degradation) representation
  - Realistic spatial and temporal representation of geometry and FEPs
    - 80 individual waste packages
  - Sensitivity and uncertainty analyses to enhance system understanding
    - Reasonable probabilistic PA model runtimes