SAND2015-4527PE

Used Fuel Disposition Campaign

Generic Disposal System Analysis (GDSA): Development, Coupling, Application, and Integration

Paul Mariner, Payton Gardner, Glenn Hammond, David Sassani, David Sevougian, and Emily Stein

Sandia National Laboratories

UFD Annual Working Group Meeting

UNLV, Las Vegas, NV

June 10, 2015

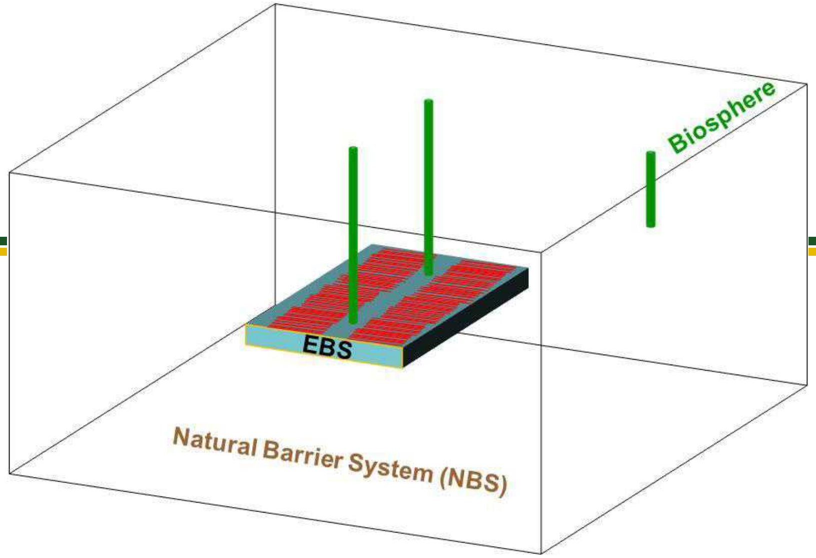
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND2014-4697P.

Sandia National Laboratories

GDSA Work Package Participants

- **DOE**
  - Mark Tynan
- **SNL (Code Development, PA Model Implementation)**
  - Paul Mariner, Glenn Hammond, Dave Sevougian, Payton Gardner, Emily Stein, Geoff Freeze, Bob MacKinnon, Peter Lichtner (contractor)
- **Contributors of special mention**
  - SNL: David Sassani, Carlos Jove-Colon, Yifeng Wang
  - ANL: Jim Jerden, Jackie Copple
  - PNNL: Edgar Buck, Rick Wittman

Outline



- **GDSA Overview**
  - Scope and Methodology
  - Code Capabilities
- **Code Development**
  - Coupling the Fuel Matrix Degradation Model (FMDM)
- **GDSA PA Model Simulations in Salt and Clay**
  - Implementation of the UFD clay repository reference case
  - Effects of WP temperature, clay vs. salt, expanded spatial domains
- **Insights for Coupling Process Models to a PA System Model**
  - Insights from the process model side
- **GDSA Integration Efforts**
  - Identification of UFD process models for future coupling and integration
- **Future Plans**
- **Open Discussion**

Used Fuel Disposition Campaign

Generic Disposal System Analysis (GDSA): Overview

Paul Mariner

Sandia National Laboratories

UFD Annual Working Group Meeting

UNLV, Las Vegas, NV

June 10, 2015

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND2014-4697P.

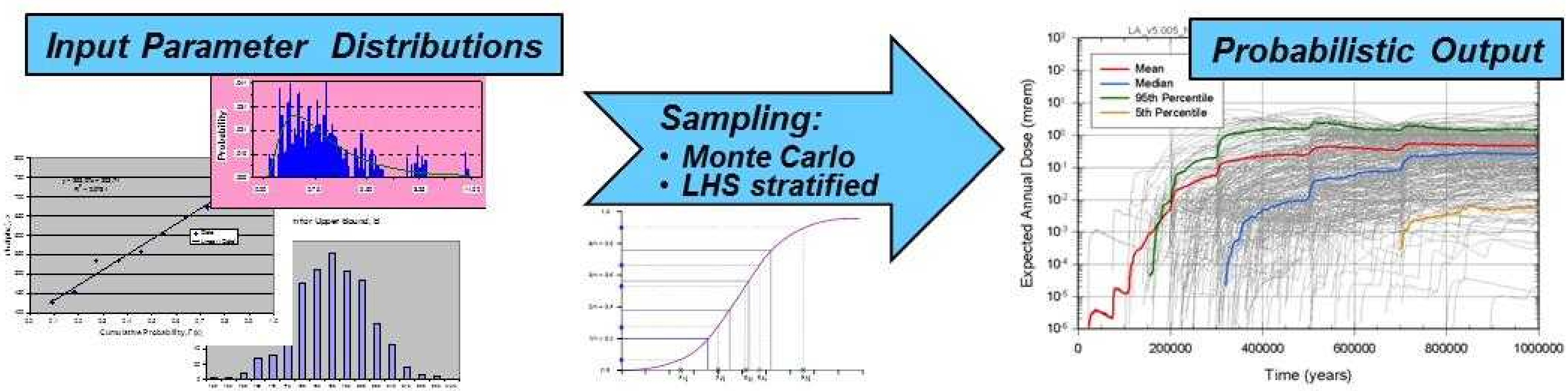
Sandia National Laboratories

GDSA Scope (WBS 1.02.08.08)

- **Objectives**
  - Develop a disposal system modeling and analysis capability that supports the prioritization of Disposal Research R&D and the evaluation of disposal system performance, including uncertainty, for a range of disposal options (e.g., salt, argillite, crystalline, deep borehole)
- **FY15 tasks**
  - Integrate source term, decay, and solubility modeling capabilities for isotopes
  - Integrate updated subsystem conceptual models into the system model architecture
  - Develop and perform simulations of selected repository reference cases to evaluate the importance of various system components and configurations (e.g., waste form, DPCs, EBS features, host rock features) and to inform R&D planning

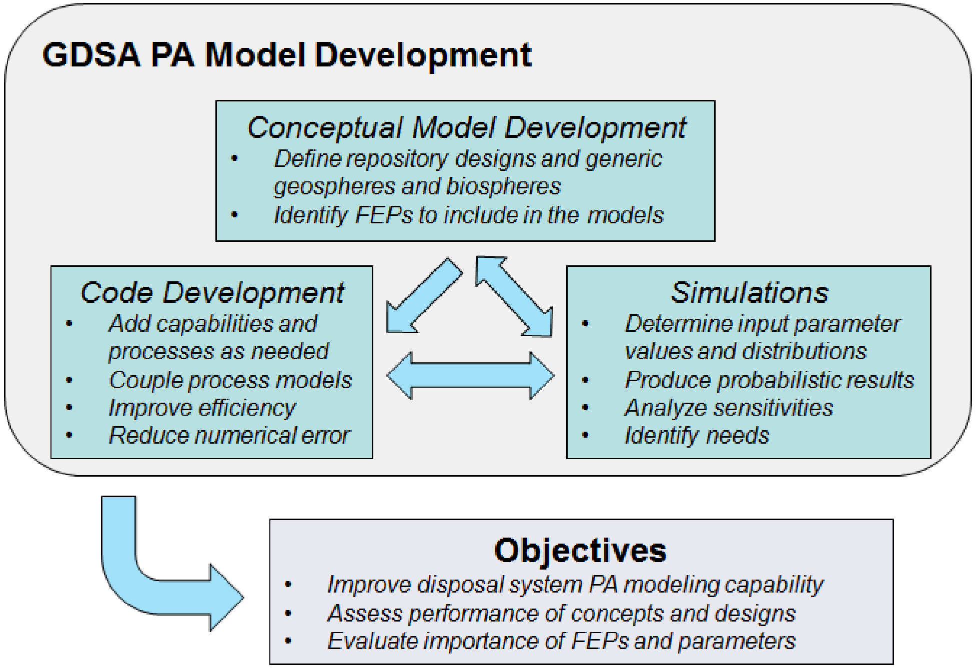
GDSA Objectives

- **Improve disposal system PA modeling capability**
  - *Provide a tool for realistic spatial-temporal probabilistic representation of radionuclide release and transport in 3D*
  - *Reduce the use of conservative assumptions and process abstractions*
  - *Improve the coupling of multi-physics processes*
  - *Minimize numerical error and error due to model form*
  - *Enhance transparency in process modeling*
  - *Provide useful tools for sensitivity analysis and uncertainty quantification*
- **Assess performance of generic concepts/designs (salt, clay, DBH, …)**
- **Evaluate importance of FEPs and model parameters**



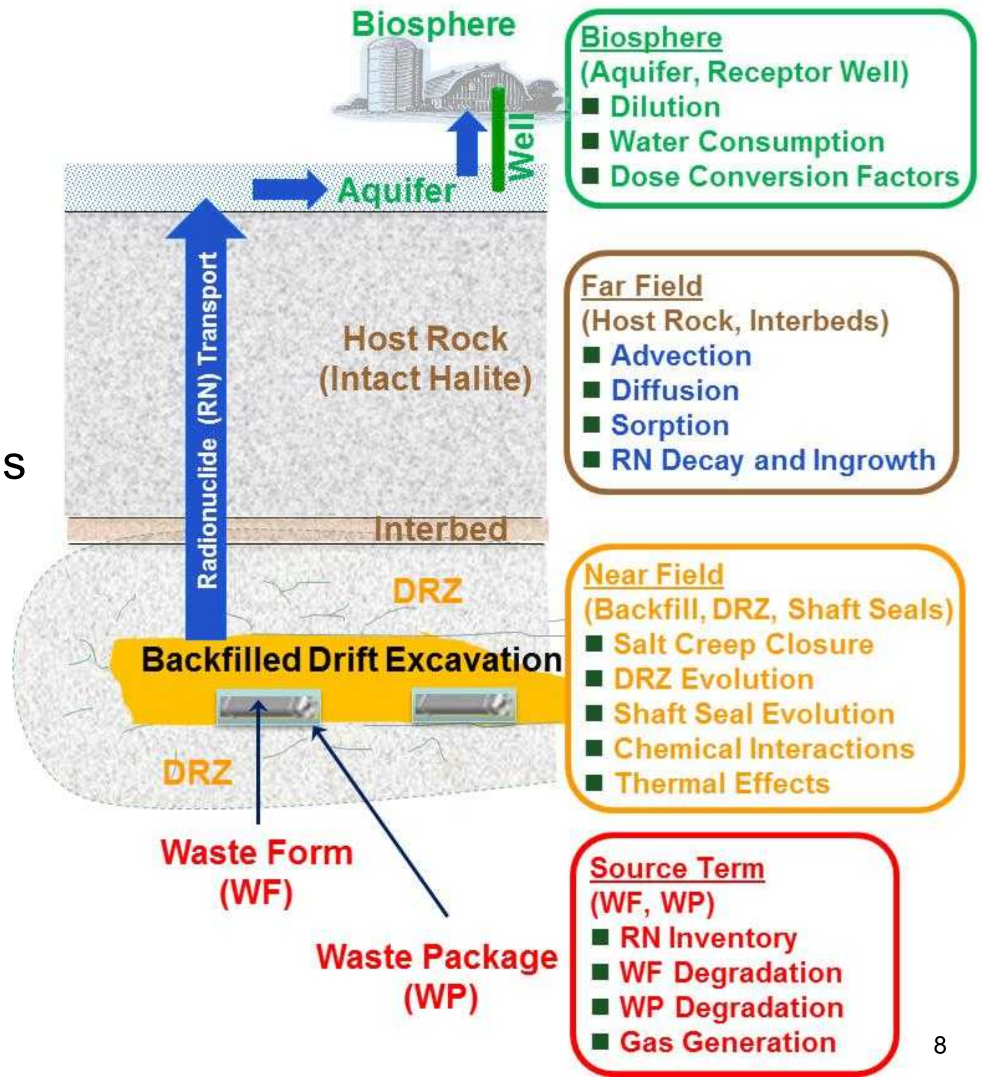
GDSA PA Model Development Methodology

- **Conceptual model development (e.g., repository in salt, clay, granite, etc.)**
  - *Define dimensions of the generic geosphere and biosphere*
  - *Define full-scale layout of the generic repository, guided by generic reference cases developed in UFD Campaign*
  - *Identify Features, Events, and Processes (FEPs) to include in the PA model*
- **Code development**
  - *Add capabilities as needed to simulate the conceptual model*
- **Simulations**
  - *Assess importance of FEPs and parameters on Rn migration and safety*
  - *Evaluate code performance*
- **Iterate**
  - *Learn from simulations*
  - *Improve code and model to achieve overall objectives*



GDSA Repository Evolution – Feature, Event, and Process (FEP) Analysis

- **FEP analysis informs the reference case**
  - Necessary properties and parameter values
- **FEP analysis supports PAs and safety cases**
  - Development of system models
  - Prioritization of research
  - Licensing/safety case (completeness)



GDSA Current Code Capabilities

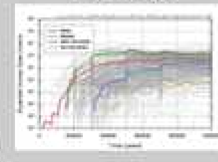
Input Parameter Distributions

Sensitivity Analysis and Uncertainty Quantification
DAKOTA

Computational Support
- Mesh Generation - Cubit
- Visualization – ParaView, VisIt
- Parameter Database

Multi-Physics Simulation and Integration
PFLOTRAN

Results



Source Term and EBS Evolution Model
- Inventory
- High resolution of spatial and temporal representation of processes and couplings:
  - WF Degradation

Fuel Matrix Degradation Model
FMDM

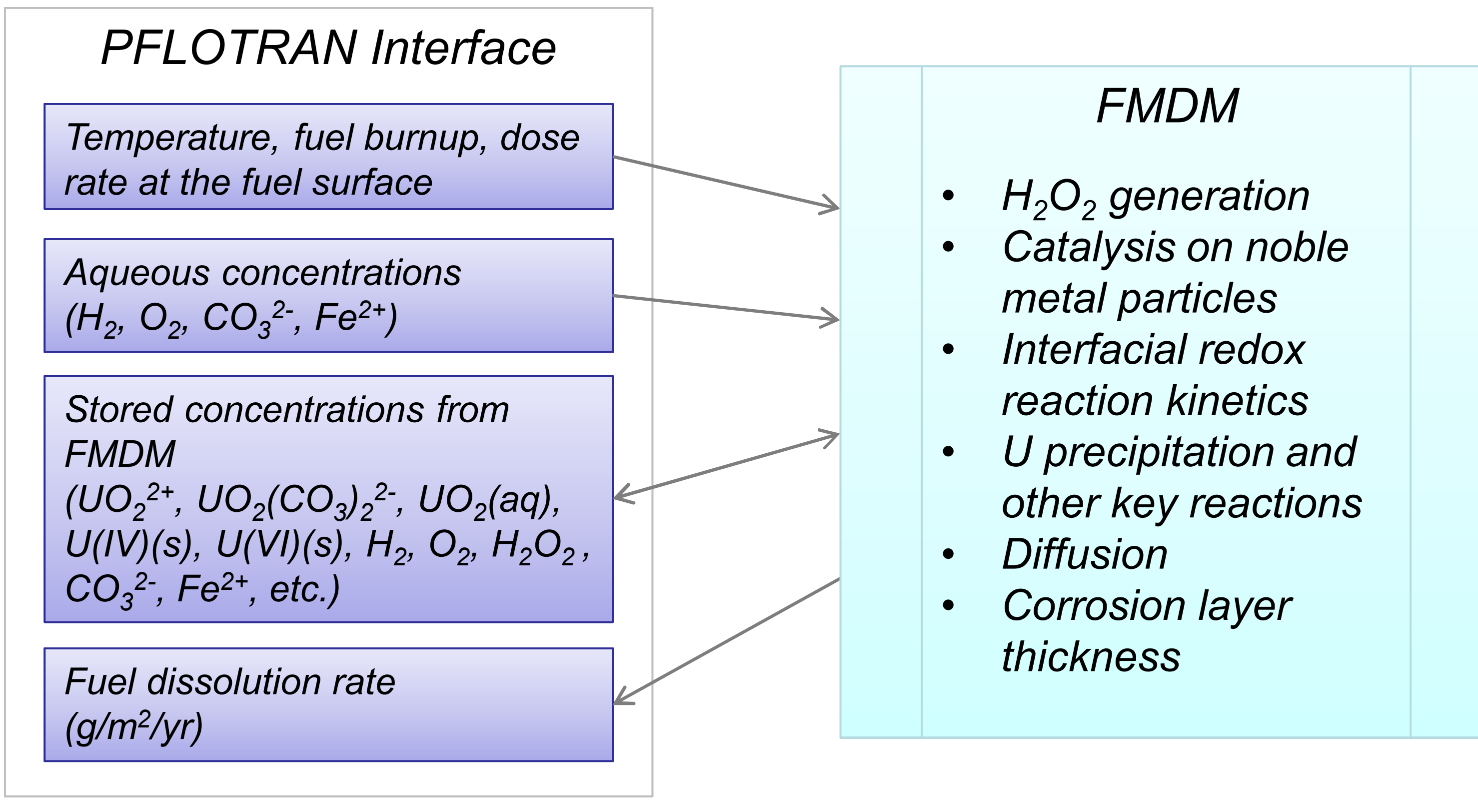
  - WP Degradation
  - Radionuclide Mobilization
  - Solubility Limits
  - Thermal Effects
  - Gas Generation

Flow and Transport Model
- Spatial and temporal representation of THC processes
  - Advection
  - Diffusion/dispersion
  - Sorption
  - Colloids
  - Decay and ingrowth
  - Homogeneous/heterogeneous chemical reactions

Biosphere Model
- Exposure pathways
- Uptake/transfer factors
- Radionuclide concentrations in aquifer

Source Term – UNF Waste Form Degradation

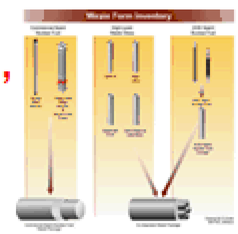
- **Fuel Matrix Degradation Model (FMDM) coupled to PFLOTRAN**
  - Developed by ANL (Jerden, Copple, Frey, Ebert), PNNL (Buck, Wittman), and SNL (Sassani, Hammond (coupling))
  - Calculates fuel dissolution rate from burnup, dose rate, temperature, and solution chemistry



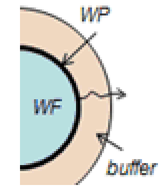
Source Term and Coupling Currently Implemented in GDSA Models

Radionuclide Inventory

- UNF: enrichment, aging, burn-up, partial stoichiometry
- No HLW
- No decay and ingrowth



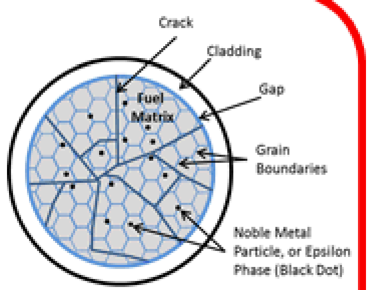
Radionuclide Mobilization



- No corrosion layer
- No colloids
- No adsorption in WF cell
- Solubility Limits (isotope needs)
- Decay and ingrowth (not in solid)

UNF Waste Form and Cladding Degradation

- Gap and grain boundary release (at cladding failure)
- UO_2 matrix dissolution (FMDM)



Fuel Pellet

HLW Waste Form Degradation

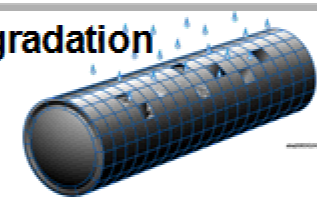
- Glass dissolution model needed

EBS Near-Field Environment

- Changing temperature
- Fixed chemistry
- Fluid saturated

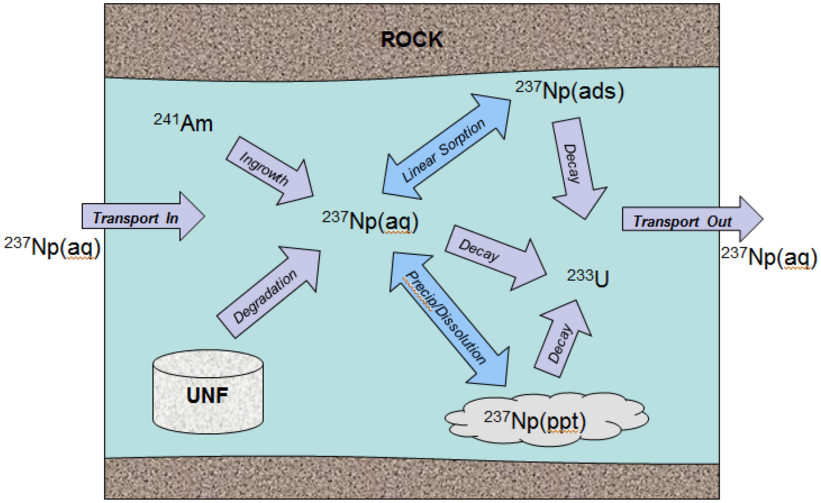
Waste Package Degradation

- Instantaneous
- Models needed



Additional Process Modeling

- **Process models under development in GDSA**
  - *Decay in precipitate phase and in waste form*
  - *Equilibrium isotope solubility and partitioning*
  - *Waste package degradation, user-defined*
  - *Solution density model*
  - *Generic aquifer transport and capture*
  - *Pitzer ion-interaction model*
  - *Solid solution model*
  - *(Nested meshing)*



- **Process models available or under development elsewhere in UFD Campaign**
  - *Discrete fracture network model, THMC model for buffer materials, clay deformation, non-Darcy flow, PBNP RD model, kinetic multiple site sorption, colloid stability, colloid transport, in-package chemistry, EBS chemistry, biosphere dose model, waste package degradation*

GDSA – FY15 Deliverables

- **Sep 2015: M2FT-15SN0808011 Application of Generic Disposal System Models**
  - Updated salt reference case simulations
  - New clay reference case simulations
  - Integration of source term model capabilities
    - *Coupled fuel matrix degradation model (FMDM), decay in precipitate phase, isotope solubility*
  - Evaluations of the importance of specific system components
  - Integration across UFD
    - *Documentation of results of integration activities with process modelers and with data collection efforts within the UFD Campaign*

Used Fuel Disposition Campaign

Generic Disposal System Analysis (GDSA): Coupling of PFLOTRAN to ANL's Fuel Matrix Degradation Model (FMDM)

Glenn Hammond

Sandia National Laboratories

UFDC Annual Working Group Meeting

UNLV, Las Vegas, NV

June 10, 2015

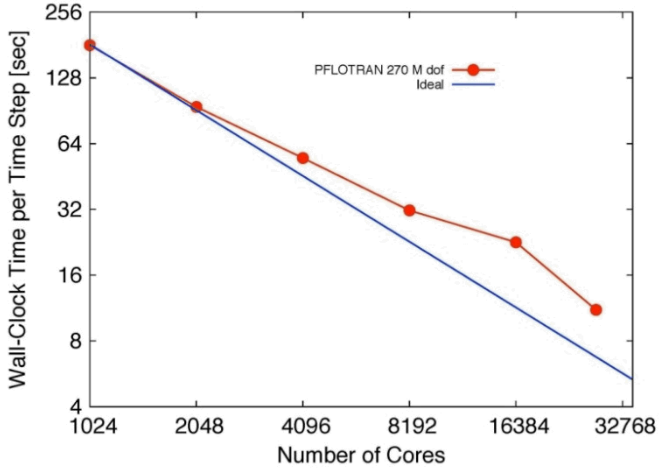
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND2014-4697P.

Sandia National Laboratories

Used Fuel Disposition

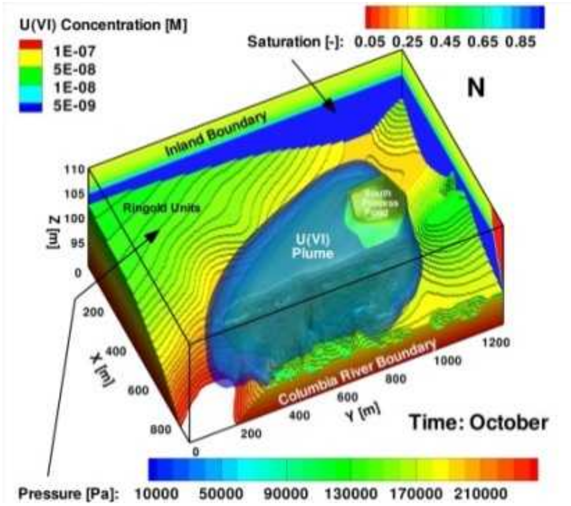
PFLOTRAN

- **Petascale reactive multiphase flow and transport code**
- **Open source license (GNU LGPL 2.0)**
- **Object-oriented Fortran 2003/2008**
  - Pointers to procedures
  - Classes (extendable derived types with member procedures)
- **Founded upon PETSc parallel framework**
  - Parallel communication through MPI
  - Parallel I/O through binary HDF5
  - Unstructured domain decomposition through METIS/ParMETIS (Cmake)
- **Demonstrated performance**
  - Maximum # processor cores: 262,144 (Jaguar supercomputer)
  - Maximum problem size 3.34 billion degrees of freedom
  - Scales to over 10K cores



Application of PFLOTRAN

- **Nuclear waste disposal**
  - Waste Isolation Pilot Plant (WIPP) in Carlsbad, NM
  - DOE Used Fuel Disposition Program
  - SKB Forsmark Spent Fuel Nuclear Waste Repository (Sweden, Amphos[21])
- **Climate: coupled overland/groundwater flow; CLM**
  - Next Generation Ecosystem Experiments (NGEE) Arctic
  - DOE Earth System Modeling (ESM) Program
- **Fate and transport of contaminants**
  - U(VI) at Hanford 300 Area
- **CO_2 sequestration**
- **Enhanced geothermal energy**
- **Radioisotope tracers**
- **Colloid-facilitated transport**
- **Cement degradation**



Hammond and Lichtner, WRR, 2010

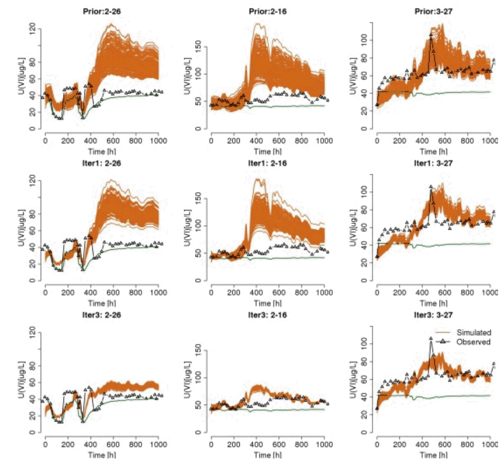
PFLOTRAN Process Models

- **Flow**
  - Single phase, variably-saturated
  - Multiphase gas-liquid
  - Interchangeable constitutive models and equations of state
- **Energy**
  - Thermal conduction and convection
- **Multi-Component Transport**
  - Advection
  - Hydrodynamic dispersion
- **Chemical Reaction**
  - Aqueous speciation
    - *Ion activity models*
  - Mineral precipitation-dissolution
  - Sorption
    - *Isotherm-based*
    - *Ion exchange*
    - *Surface complexation*
      - Equilibrium
      - Kinetic / multirate kinetic
  - Microbiological
    - *Biomass*
    - *Inhibition*
  - Radioactive decay with daughter products

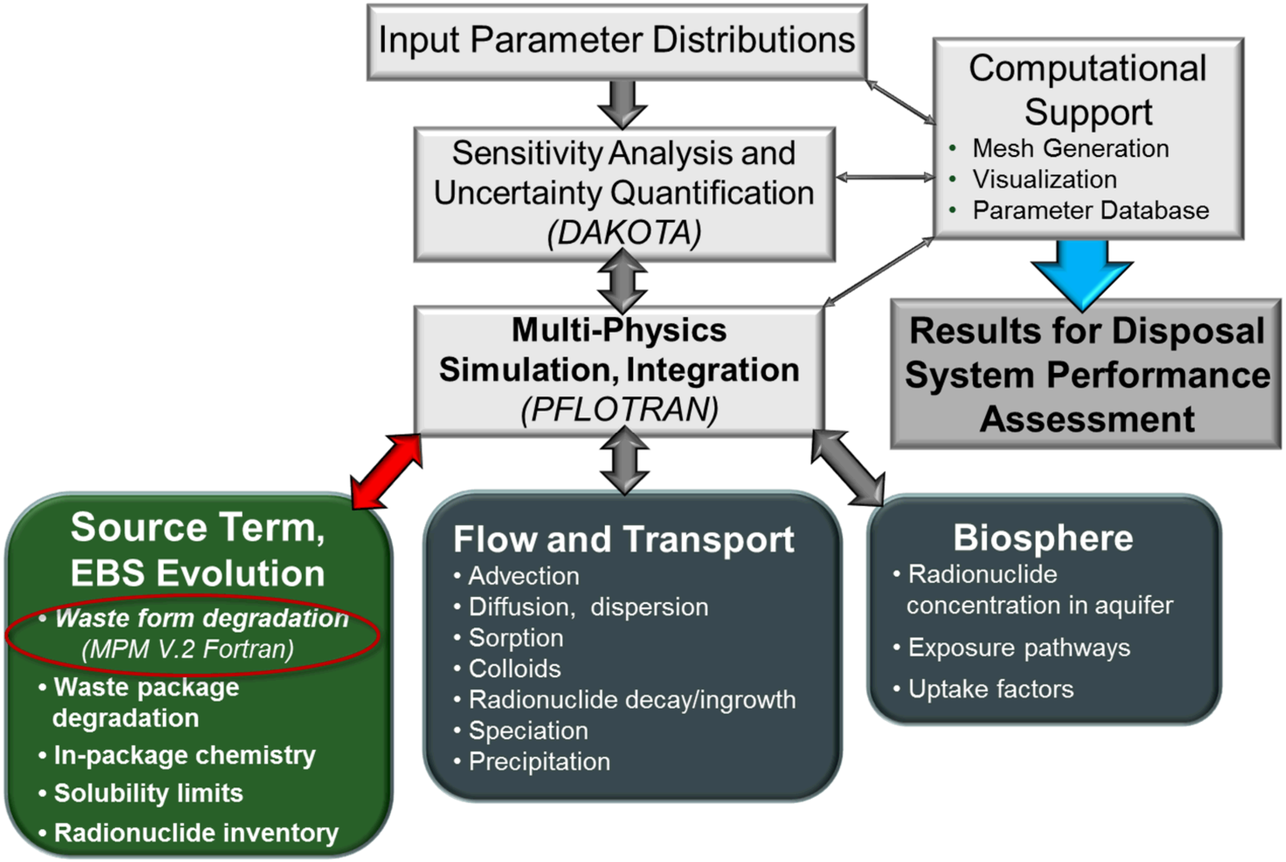
PFLOTRAN Computing Capability

- **High-Performance Computing (HPC)**
  - Increasingly mechanistic process models
  - Highly-refined 3D discretizations
  - Massive probabilistic runs
- **Open Source Collaboration**
  - Leverages a diverse scientific community
  - Sharing among subject matter experts and stakeholders from labs/universities
- **Modern Fortran (2003/2008)**
  - Domain scientists remain engaged
  - Modular framework for customization
- **Leverages Existing Capabilities**
  - Meshing, visualization, HPC solvers, etc.
  - Configuration management, testing, and QA

Data Assimilation



Waste Form Degradation within GDSA Modeling Framework



Schematic of GDSA modeling framework (Figure 2 from Jerden et al., 2015, an adaptation of Figure 2-6 from Sevougian et al., 2014).

Workflow between PFLOTRAN and Fuel Matrix Degradation Model

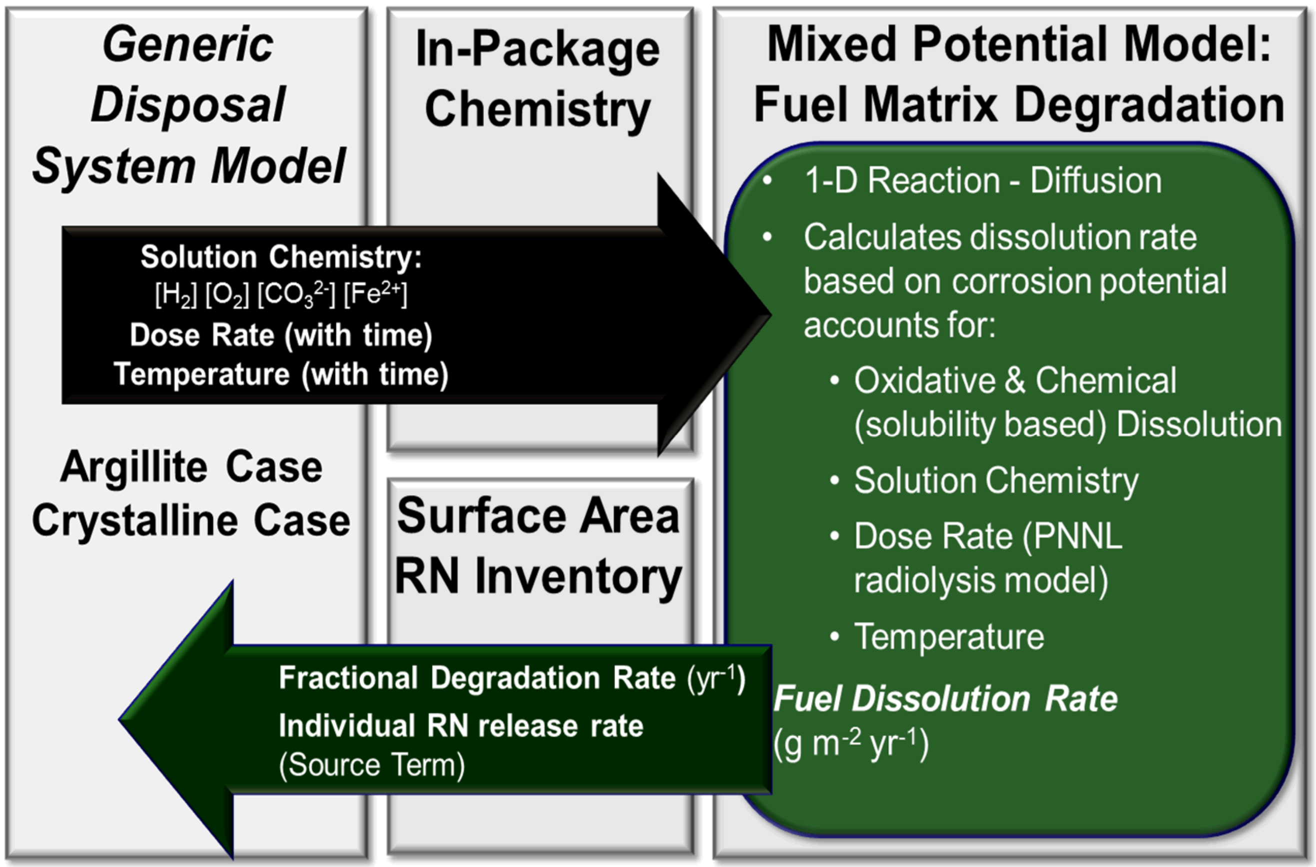
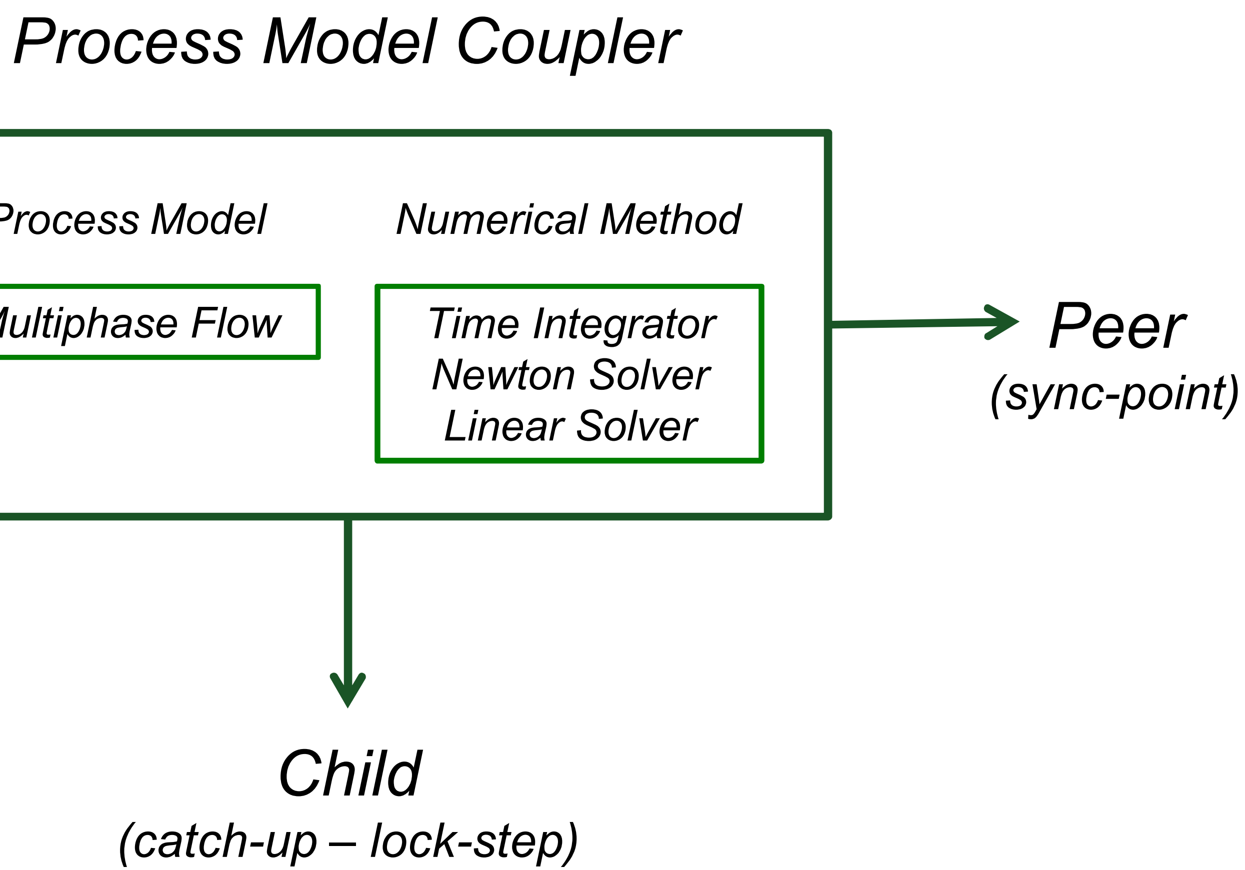
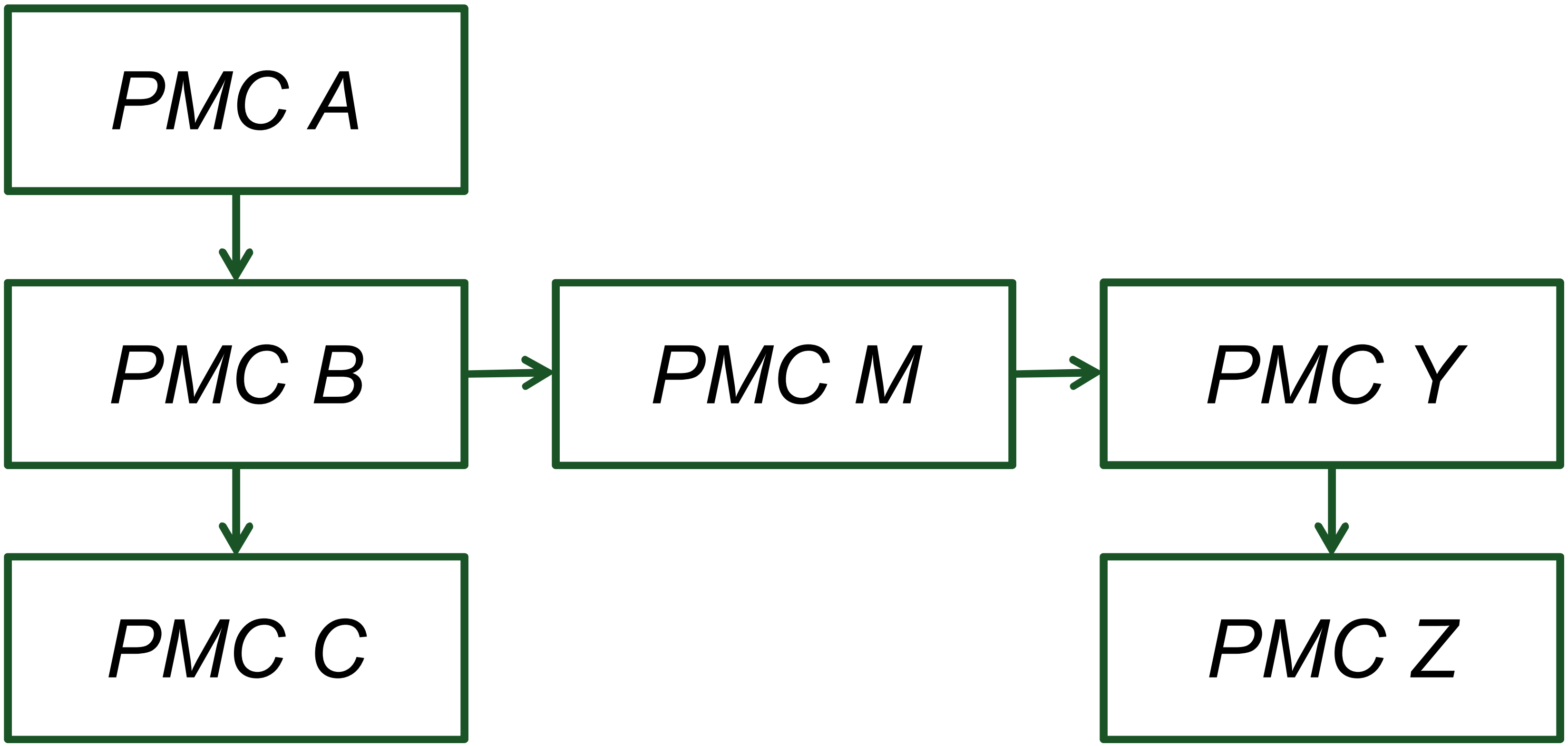


Figure 3 from Jerden et al., 2015.

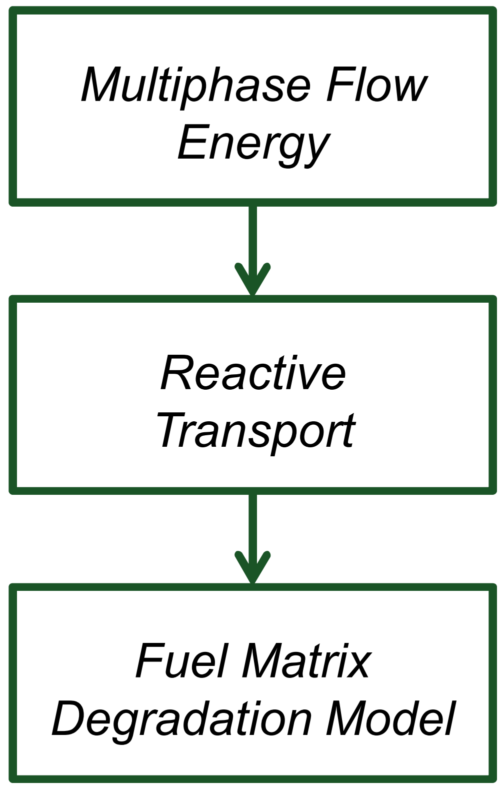
PFLOTRAN Process Model Couplers (PMCs)



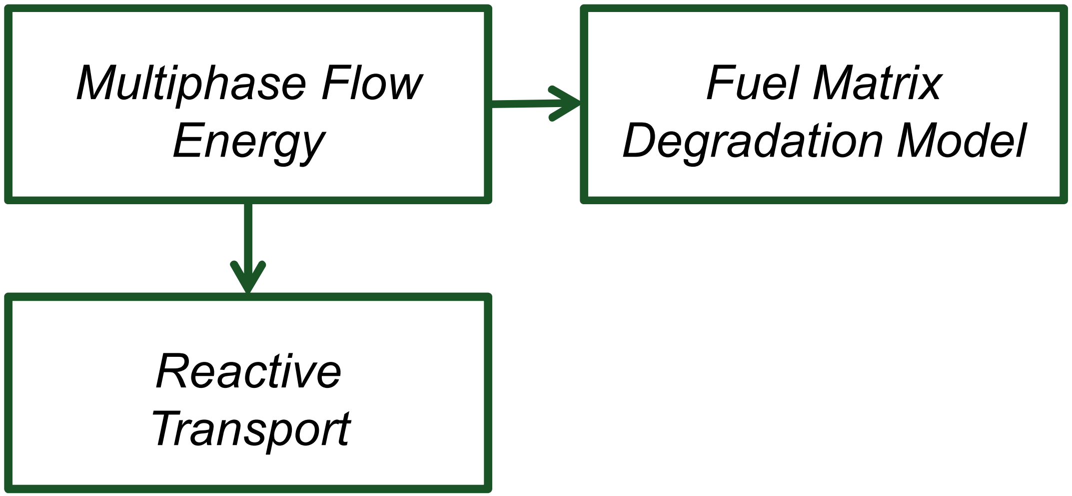
Hypothetical PMC Hierarchy



PFLOTRAN-FMDM Process Model Coupling



PFLOTRAN-FMDM Process Model Coupling (Alternative Approach)



PFLOTRAN-FMDM Pseudocode

PFLOTRAN

FMDM Process Model Wrapper

- *Read (FMDM) Block*
- *Set Up Infrastructure*
- *Initialize Waste Forms*
- *For Each Timestep*
    - *For Each Waste Form*
        - *Solve Waste Form*
    - *Update Source Terms*
- *Destroy Waste Forms*

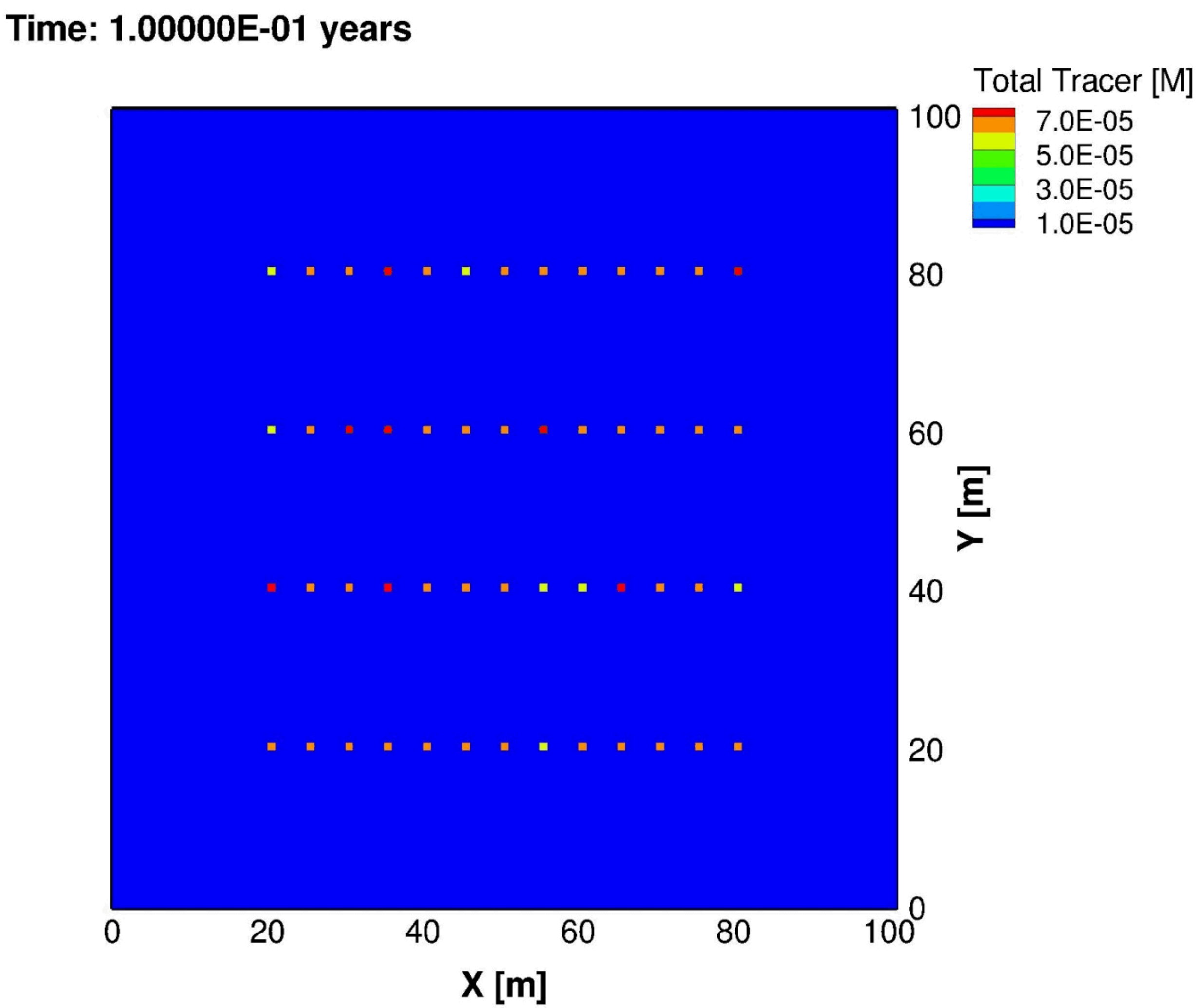
Fuel Matrix Degradation Model

AMP_Step(…)

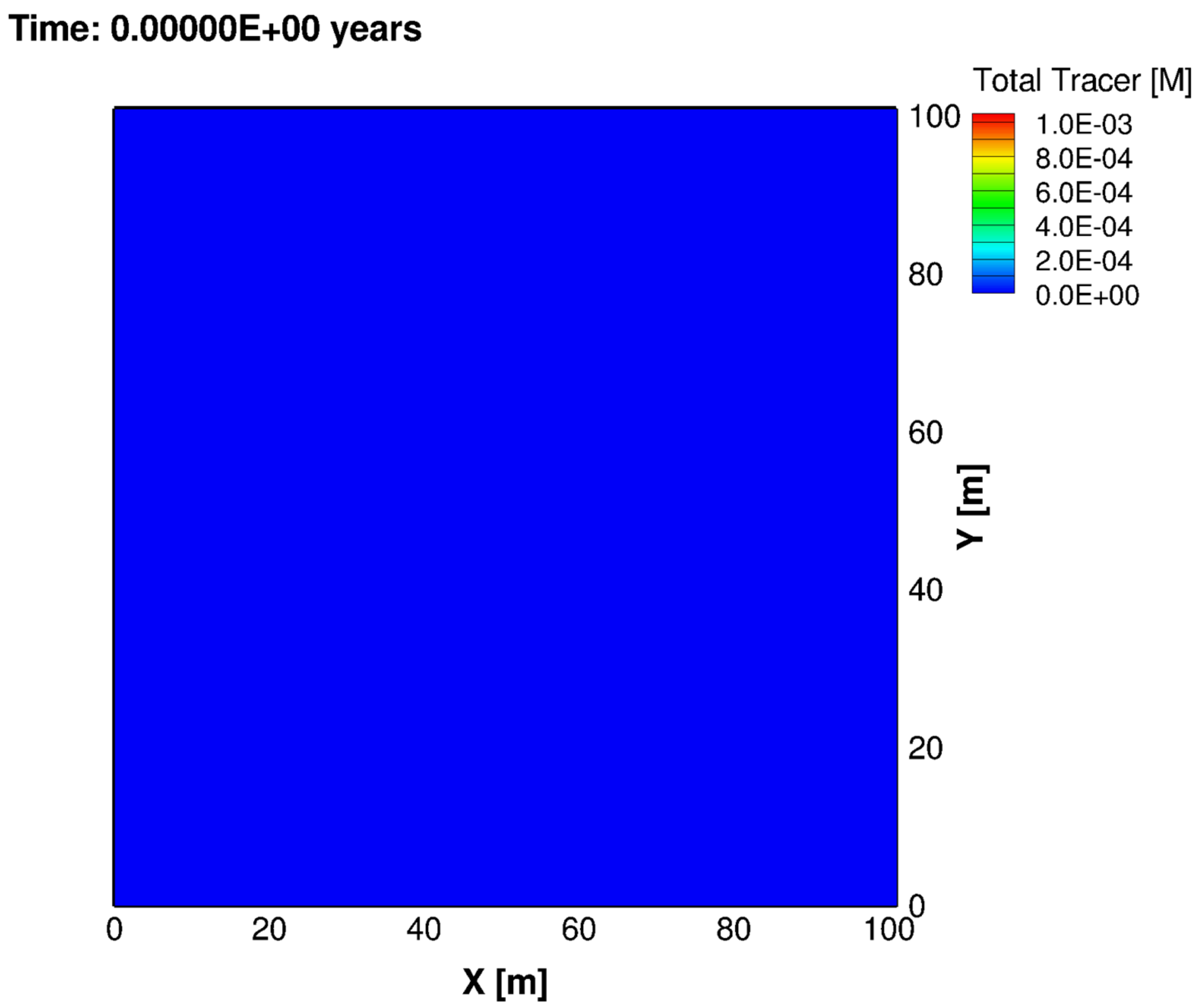
PFLOTRAN-FMDM Demonstration

- **Spatial Discretization**
  - 101 $\times$101$\times$21m @ 1m resolution (~214K grid cells)
- **Temporal Discretization**
  - 100 years @ 1 year time step (10^{-6} y initial)
- **Waste Package Spacing**
  - 5m (X), 20m (Y) between 20-80 m (X,Y)
- **Prescribed Concentrations [M]:**
  - O2(aq), HCO_3^-, $H_{2(aq)}$, Fe^{++}: 10^{-3}
- **Waste Package Burnup [y]:**
  - 55-65 (random)
- **Waste Package Reactive Surface Area [m^2]:**
  - 0.8-1 (random)
- **Pore Water Velocity [m/y]:**
  - 1 (X), 0.14 (Y)
- **Performance**
  - 66% of total time spent (31 minutes) in FMDM

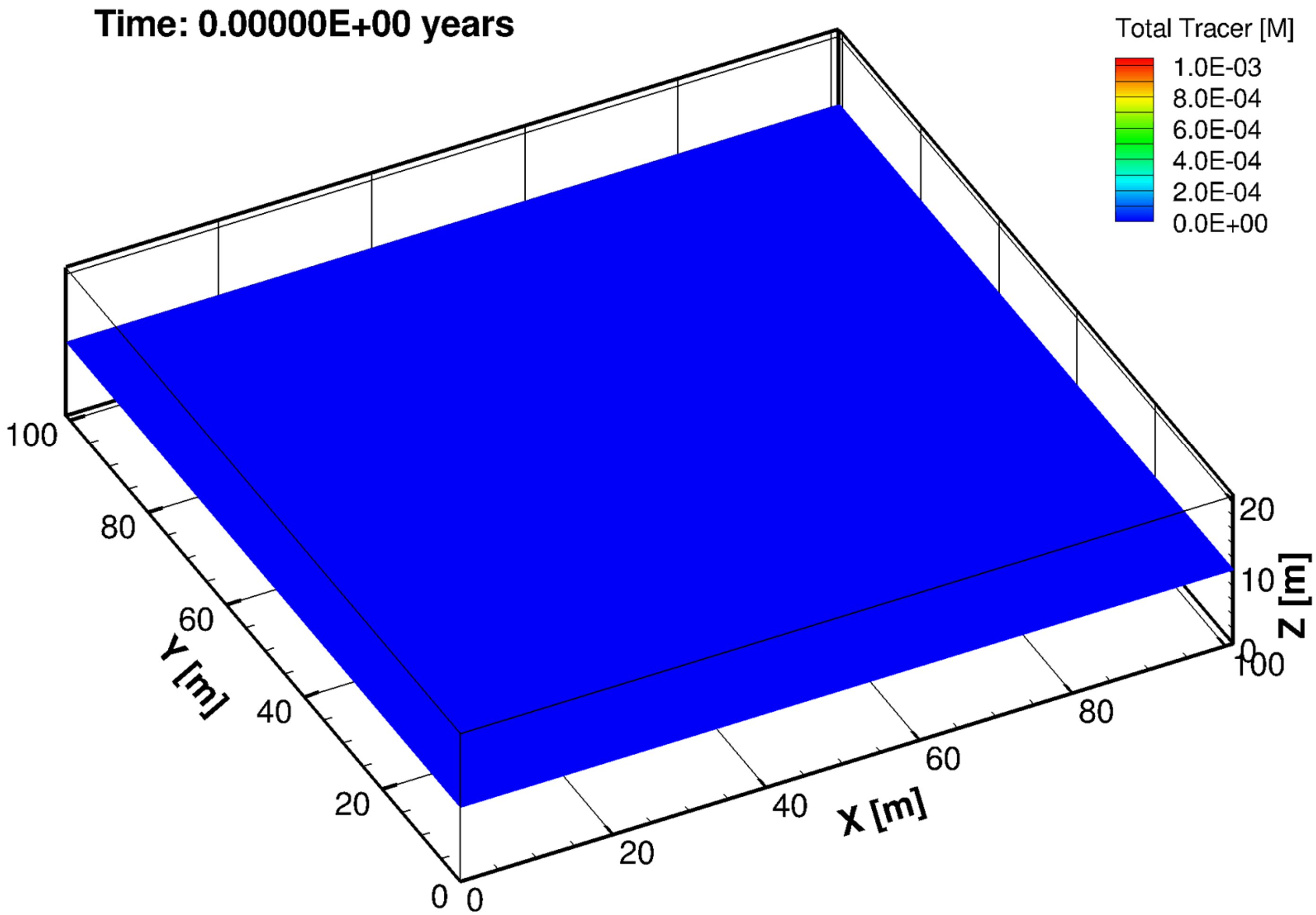
Radionuclide Concentration in Waste Form Cells with Random Burnups and Surface Areas



Radionuclide Concentration Over Time



Radionuclide Concentration Over Time



PFLOTRAN-FMDM: Future Directions

- **Increase flexibility of coupling**
  - Ability to customize FMDM discretization from PFLOTRAN side
  - Load balancing (uniform distribution of waste forms to all processes)
- **Update to MPM v.3**
- **Add increasingly mechanistic geochemistry (i.e. within the repository conceptual model)**
- **Optimized FMDM serial performance**

Used Fuel Disposition Campaign

Generic Disposal System Analysis (GDSA): Salt and Clay Repository PA Model Results

Payton Gardner and Emily Stein
Sandia National Laboratories

UFDC Annual Working Group Meeting
UNLV, Las Vegas, NV
June 10, 2015

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND2014-4697P.

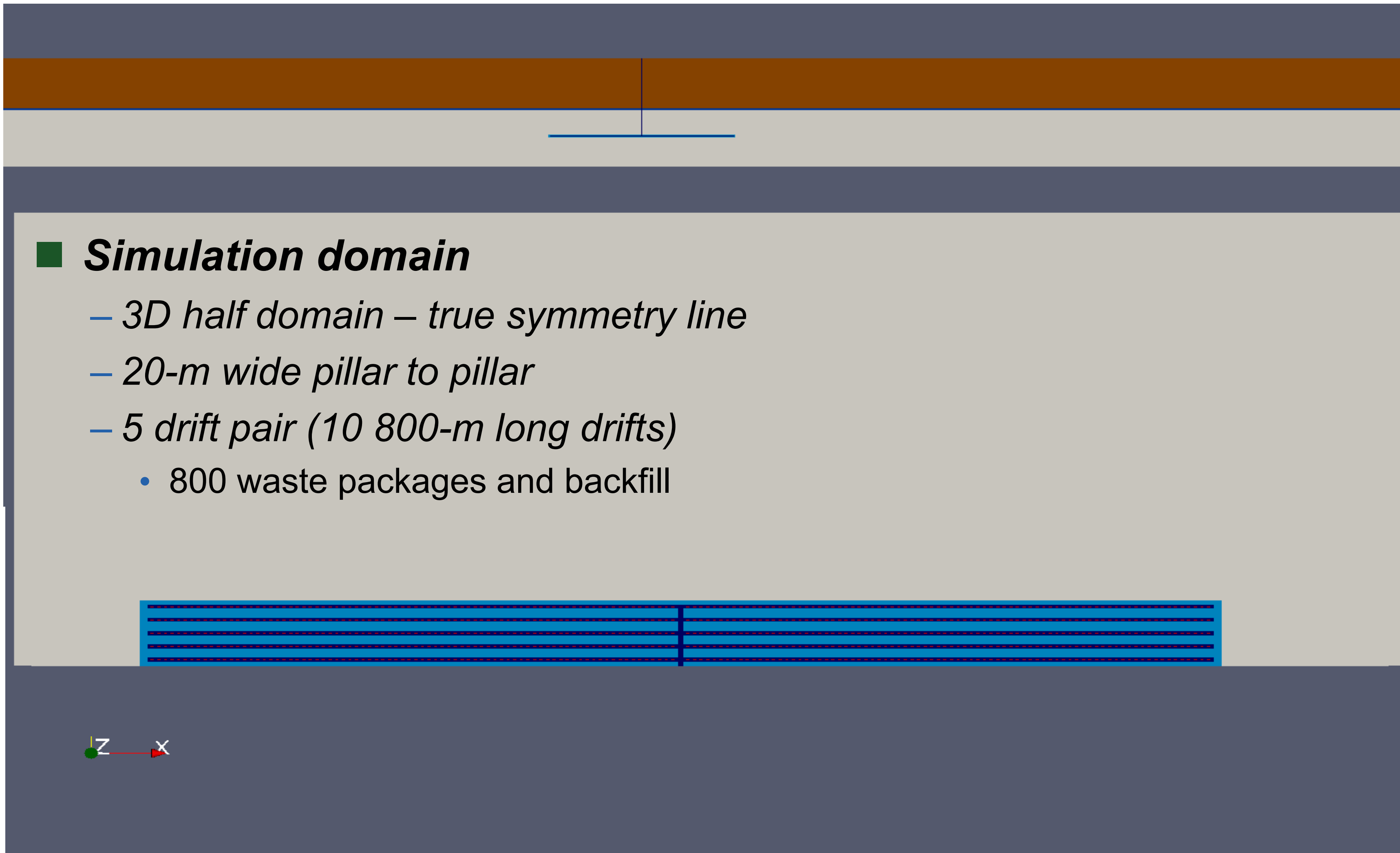
Sandia National Laboratories

Generic Salt Repository PA Model Updates

- **Salt reference case full 3d PA Isothermal**
  - 3D, single-phase, isothermal, HC (radionuclide source term, flow and transport)
  - 1,000,000 years
    - *Deterministic*
    - *Probabilistic*
  - 3D multi-drift vs. single drift comparison
- **Salt reference case full 3d PA Thermal**
  - 3D THC (radionuclide source term, coupled heat, fluid flow and transport)
  - 1,000,000 years
    - *Deterministic*
    - *Probabilistic*
  - Comparison of thermal vs. isothermal results

Used Fuel Disposition

Generic Salt Repository PA Model – Isothermal 3d Multi-drift Deterministic Simulation Results

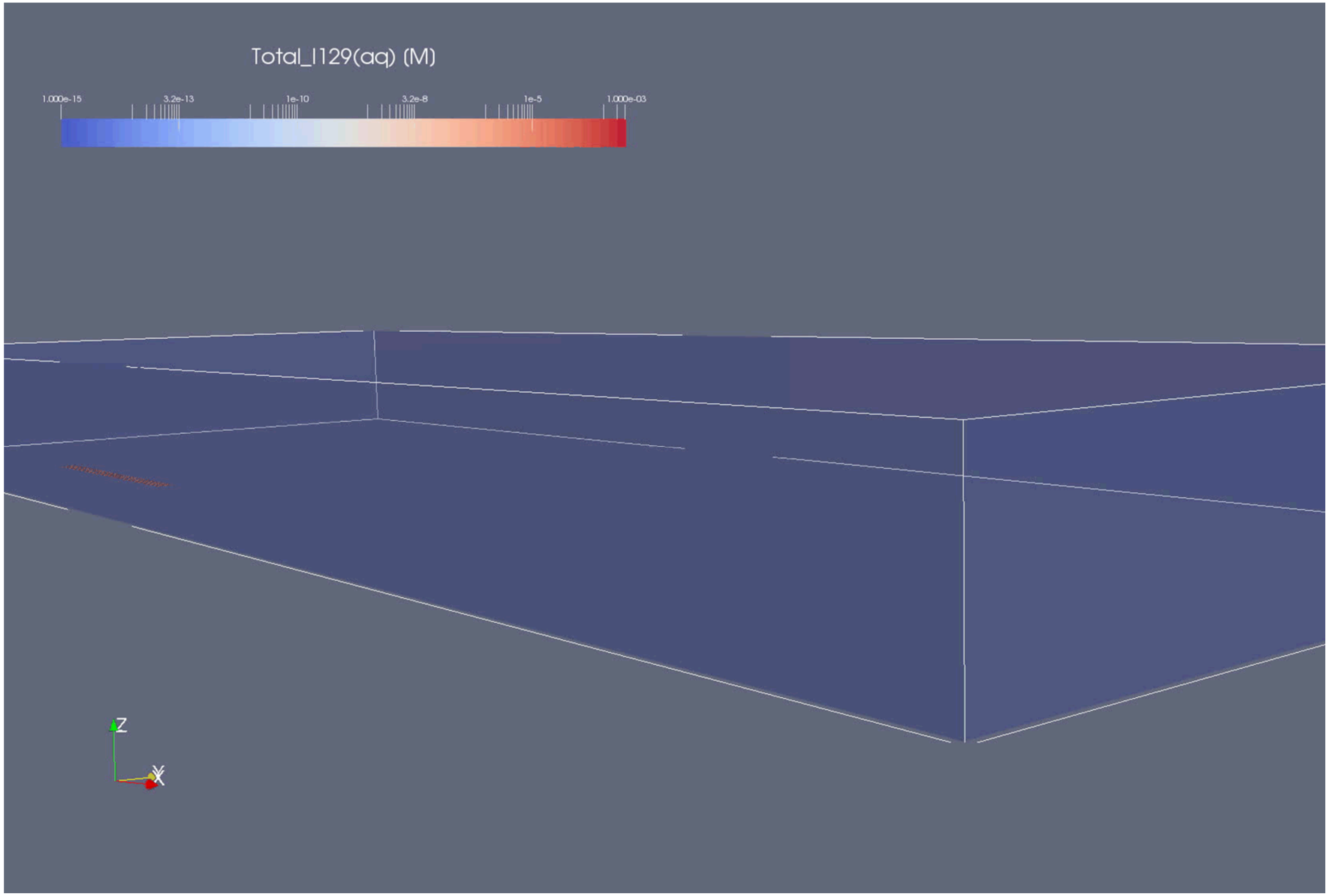


- ***Simulation domain***
  - *3D half domain – true symmetry line*
  - *20-m wide pillar to pillar*
  - *5 drift pair (10 800-m long drifts)*
    - 800 waste packages and backfill

Generic Salt Repository PA Model – Isothermal 3d Multidrift Deterministic Simulation Results

- ^{129}I dissolved concentration time history

Repository domain ~ 3,000 m



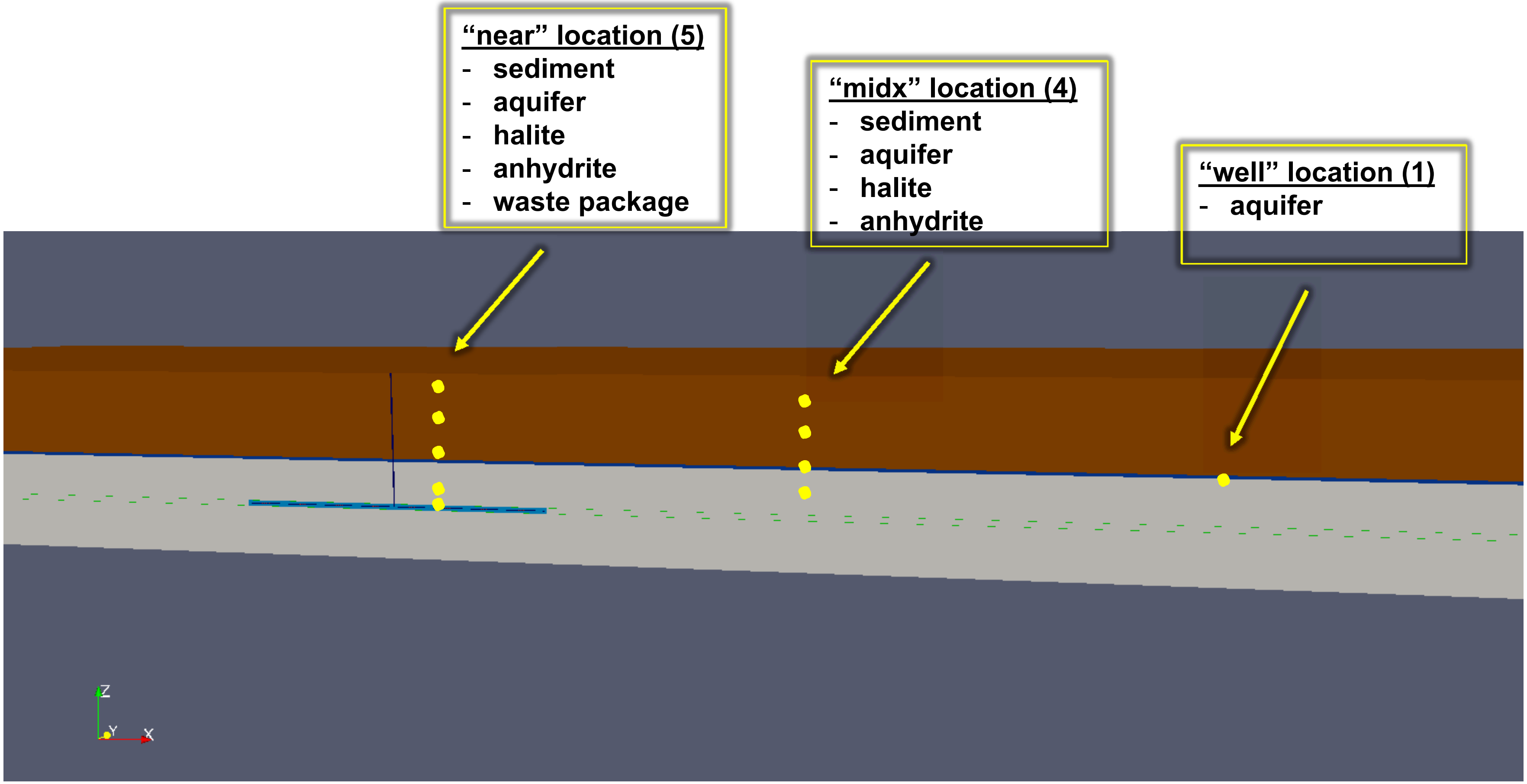
Generic Salt Repository PA Model – 3d Isothermal Probabilistic Simulations

- **50 realizations with 10 sampled (Monte Carlo) parameters**

Model Parameter	Deterministic Value	Probability Range	Distribution Type
Waste Form Degradation Rate (time for 99% degradation) (yrs)	7,000	700 – 700,000	Log uniform
^{129}I K_d^P (ml/g)	0.0	0.0 – 1.0	Uniform
^{237}Np K_d^P (ml/g)	5.5	1.0 – 10.0	Uniform
Waste Package Porosity	0.30	0.05 – 0.50	Uniform
Backfill Porosity	0.113	0.010 – 0.200	Uniform
Shaft Porosity	0.113	0.010 – 0.200	Uniform
DRZ Porosity	0.0129	0.0010 – 0.1000	Uniform
Halite Porosity	0.0182	0.0010 – 0.0519	Uniform
Interbed Permeability (m^2)	1.26×10^{-19}	1.00×10^{-21} - 1.00×10^{-17}	Log uniform
Aquifer Permeability (m^2)	1.00×10^{-13}	1.00×10^{-14} - 1.00×10^{-12}	Log uniform

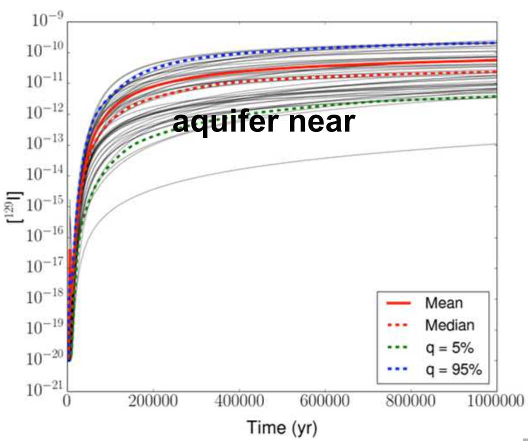
Generic Salt Repository PA Model – Probabilistic Simulations

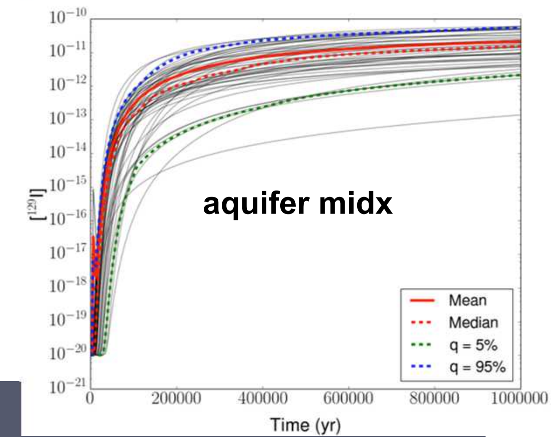
- **Sensitivity analysis (partial rank correlation) at 10 locations**

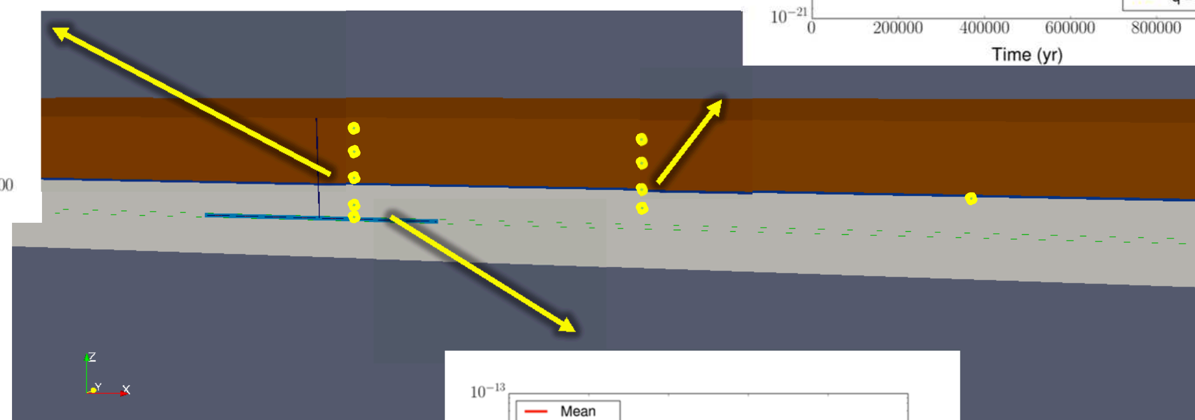


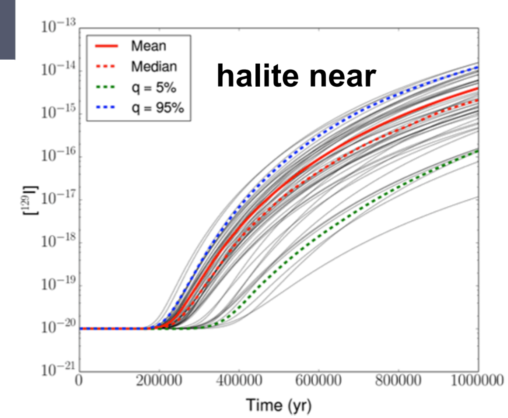
Generic Salt Repository PA Model – Multi-Realization Analysis

- ^{129}I dissolved concentration vs. time
  - (DAKOTA probabilistic output of 100 realizations)



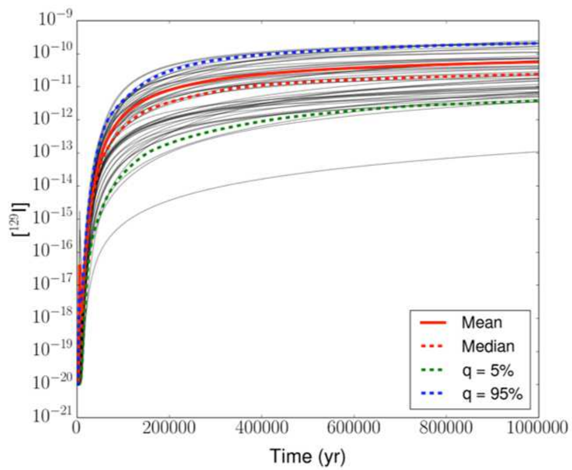


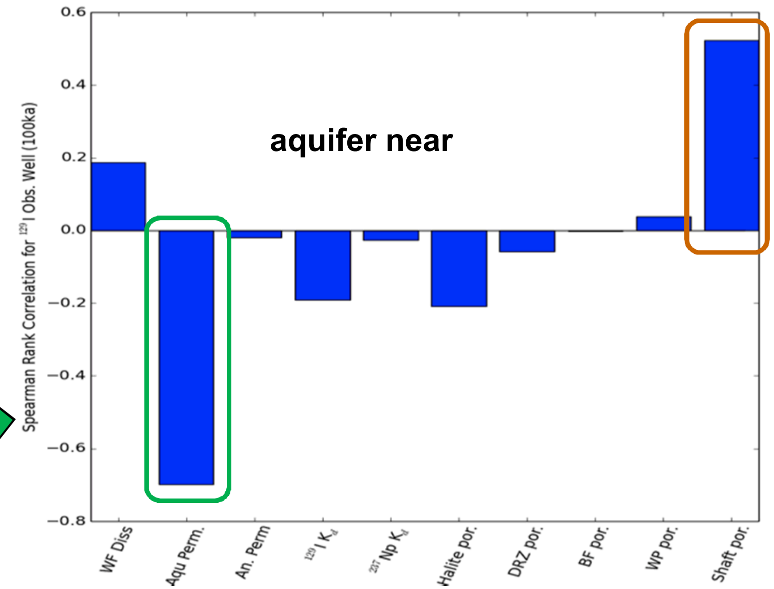


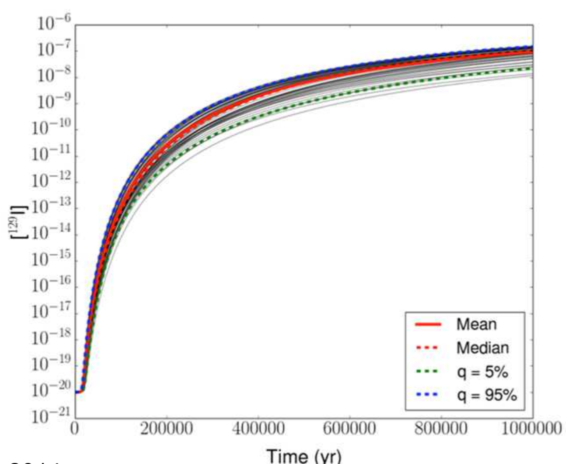


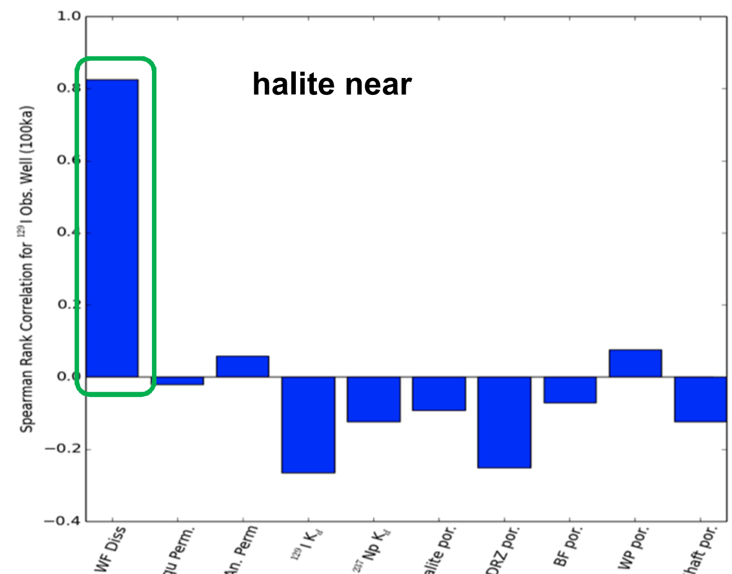
Generic Salt Repository PA Model – Multi-Realization Analysis

- **Partial rank correlation**
  - Peak ^{129}I concentration vs. time



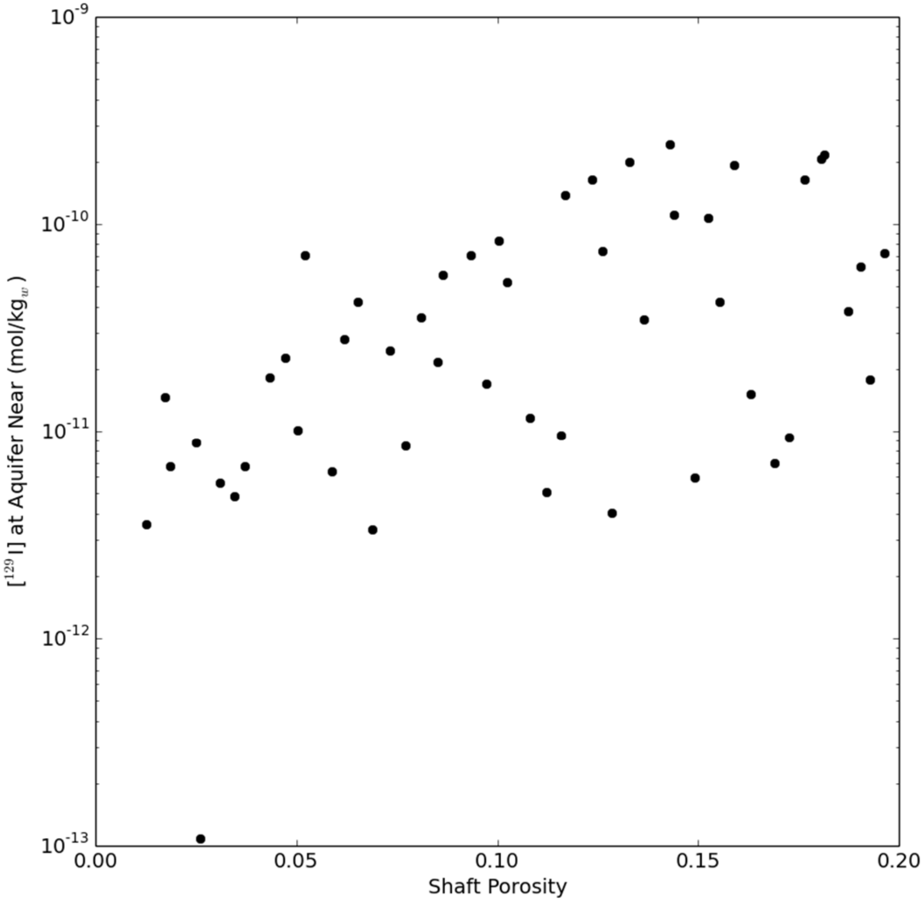


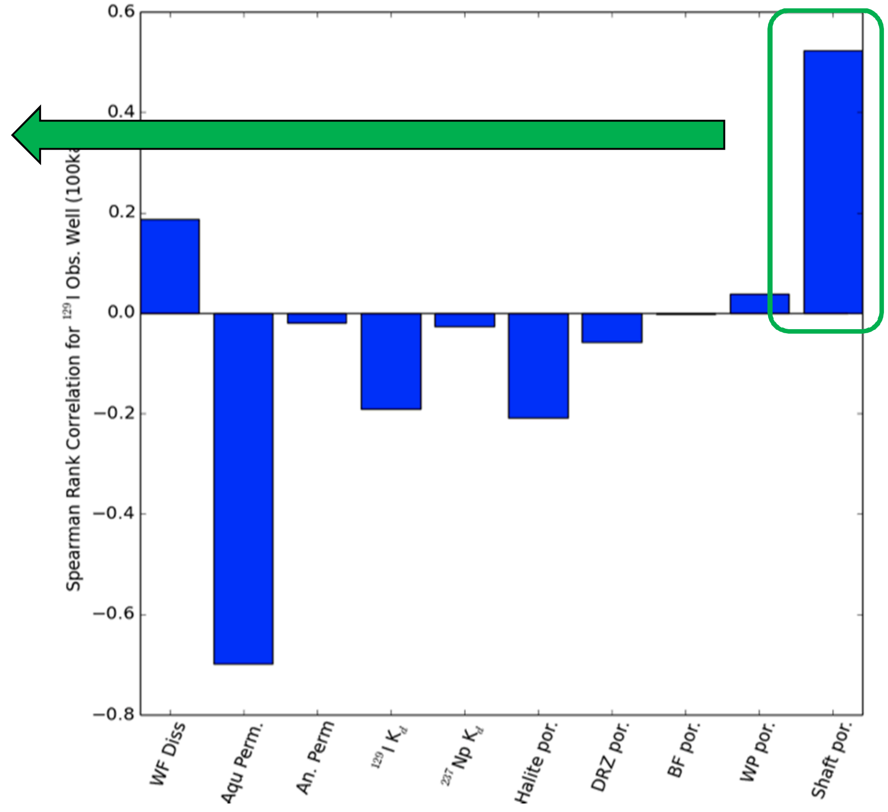




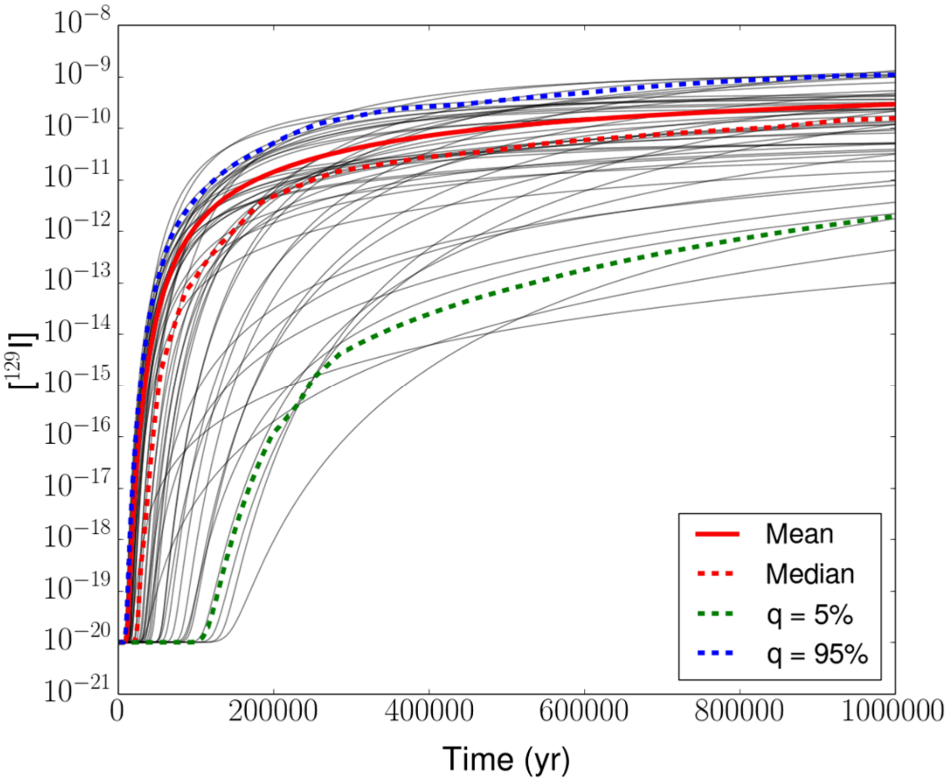
Generic Salt Repository PA Model – Multi-Realization Analysis

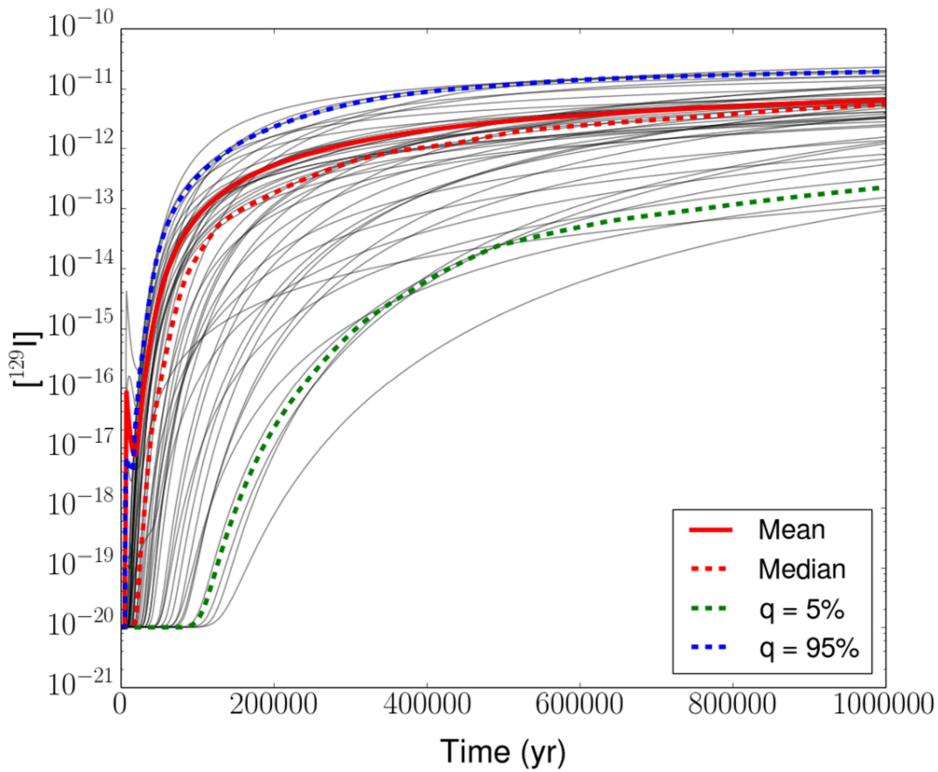
- **DAKOTA scatterplot analysis**
  - Max ^{129}I concentration at "aquifer near" at 100,000 years versus shaft porosity





Generic Salt Repository PA Model – Single Drift vs. 3d Isothermal

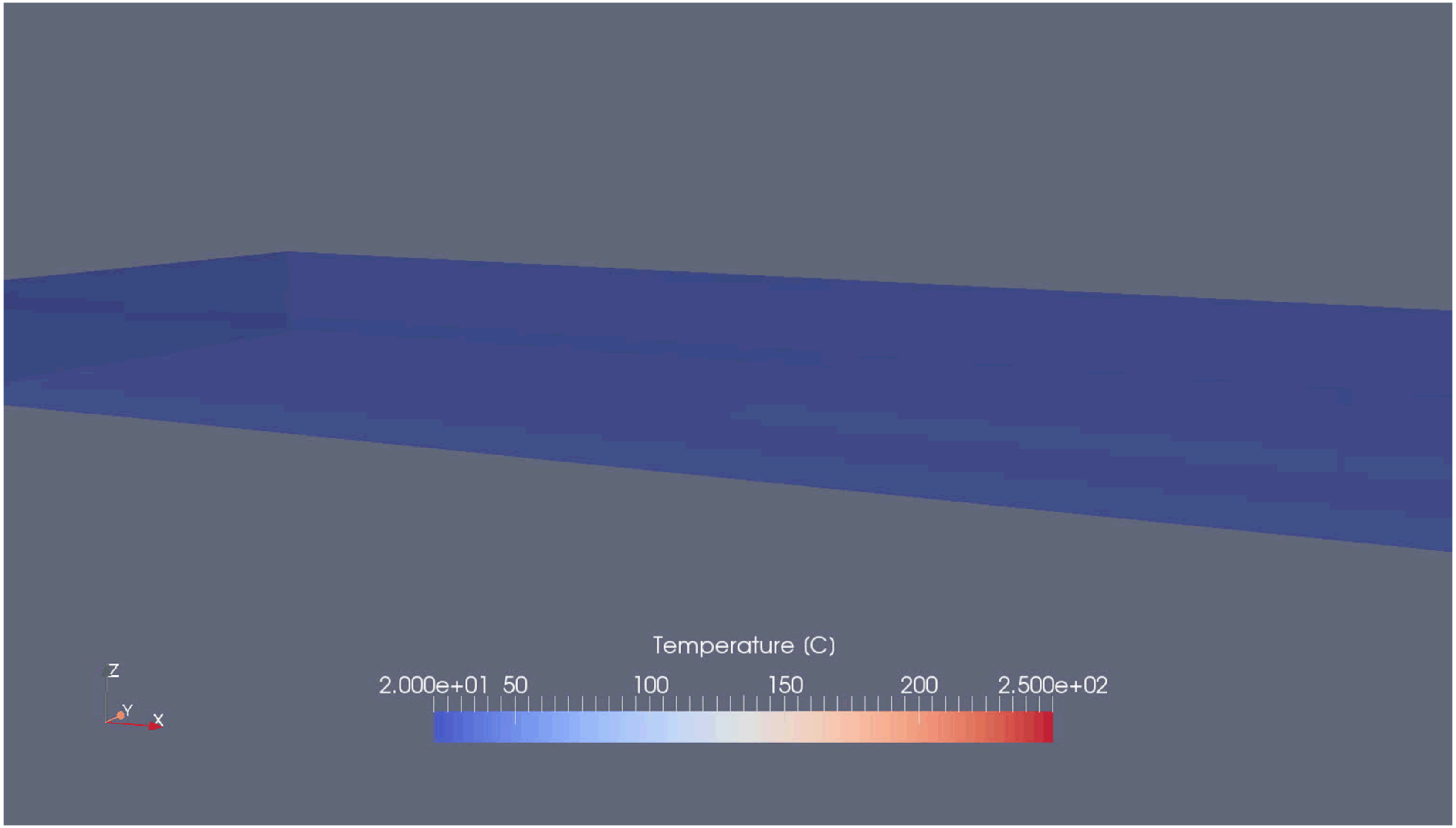




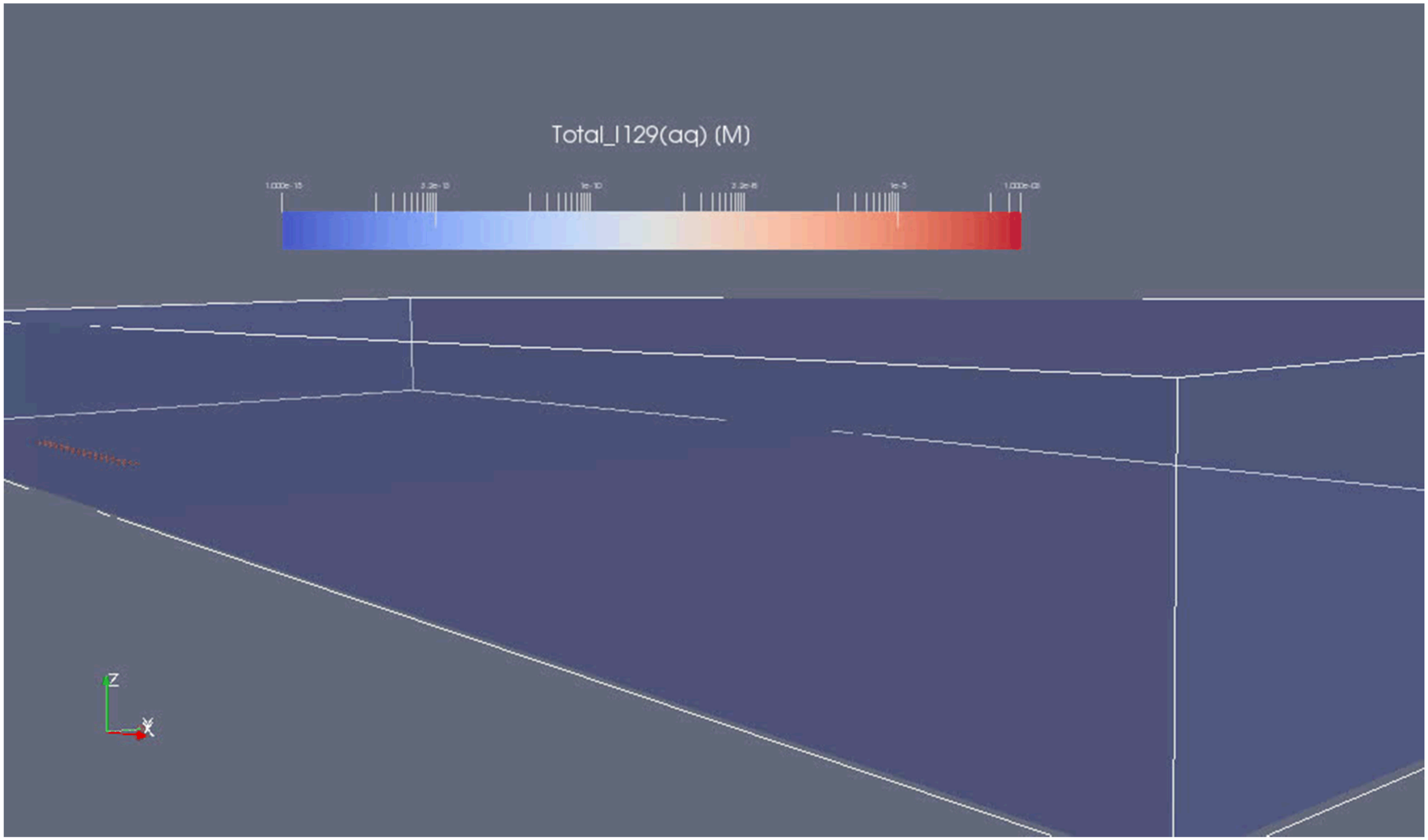
Generic Salt Repository PA Model Updates

- **Salt reference case mesh refinement results**
- **Salt reference case full 3d PA Isothermal**
  - 3D, single-phase, isothermal, HC (radionuclide source term, flow and transport)
  - 1,000,000 years
    - *Deterministic*
    - *Probabilistic*
  - 3D multi-drift vs. single drift comparison
- **Salt reference case full 3d PA Thermal**
  - 3D THC (radionuclide source term, coupled heat, fluid flow and transport)
  - 1,000,000 years
    - *Deterministic*
    - *Probabilistic*
  - Comparison of thermal vs. isothermal results

Generic Salt Repository PA Model – 3d Thermal Simulation Results



Generic Salt Repository PA Model – 3d Thermal Simulation Results



Generic Salt Repository PA Model – 3d Thermal Probabilistic Simulations

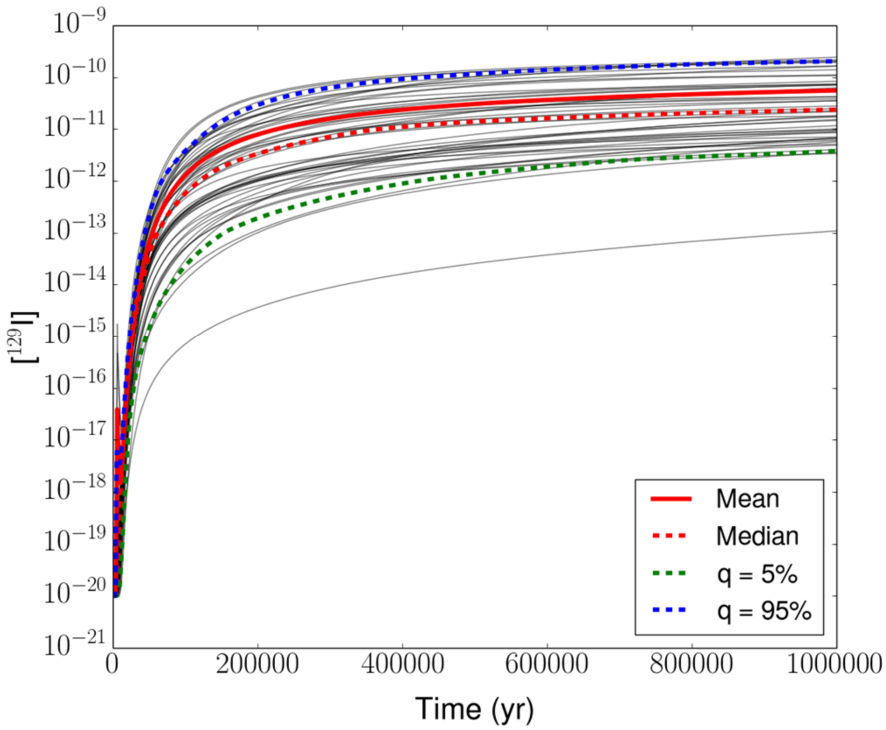
- **40 realizations with 10 sampled (Monte Carlo) parameters**

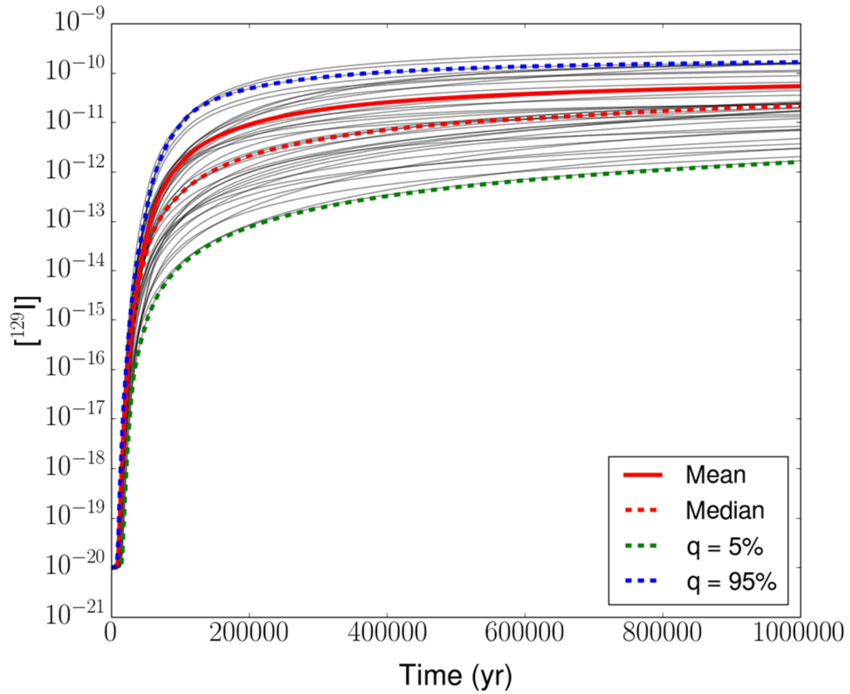
Model Parameter	Deterministic Value	Probability Range	Distribution Type
Waste Form Degradation Rate (time for 99% degradation) (yrs)	7,000	700 – 700,000	Log uniform
^{129}I K_d^P (ml/g)	0.0	0.0 – 1.0	Uniform
^{237}Np K_d^P (ml/g)	5.5	1.0 – 10.0	Uniform
Waste Package Porosity	0.30	0.05 – 0.50	Uniform
Backfill Porosity	0.113	0.010 – 0.200	Uniform
Shaft Porosity	0.113	0.010 – 0.200	Uniform
DRZ Porosity	0.0129	0.0010 – 0.1000	Uniform
Halite Porosity	0.0182	0.0010 – 0.0519	Uniform
Interbed Permeability (m^2)	1.26×10^{-19}	1.00×10^{-21} - 1.00×10^{-17}	Log uniform
Aquifer Permeability (m^2)	1.00×10^{-13}	1.00×10^{-14} - 1.00×10^{-12}	Log uniform

Used Fuel Disposition

Generic Salt Repository PA Model – 3d Isothermal vs. Thermal

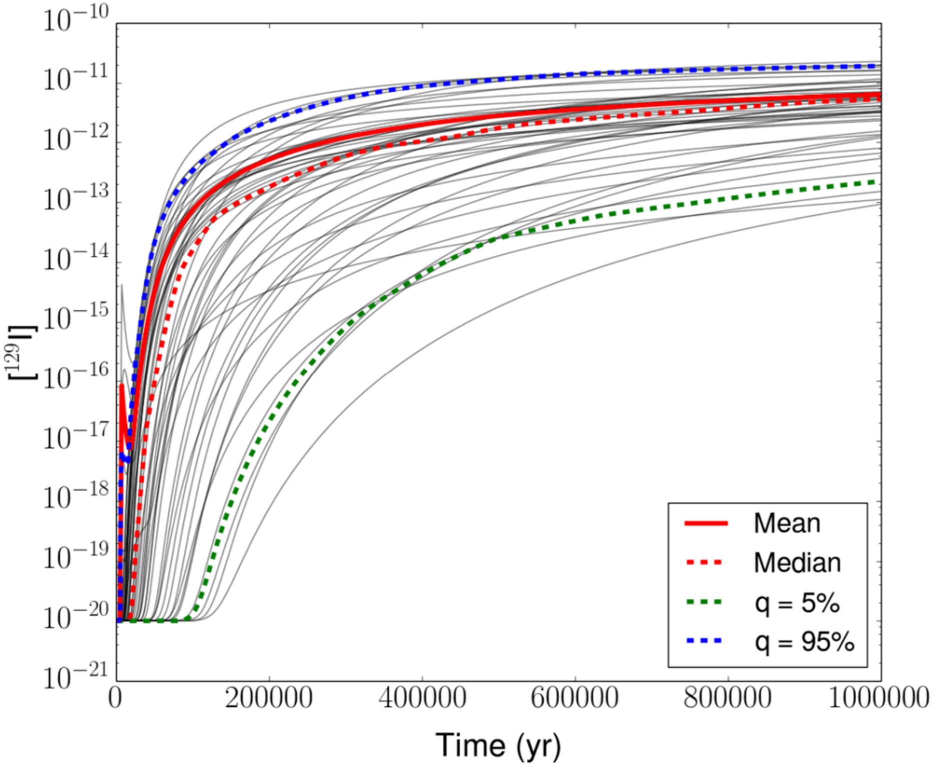
aquifer near

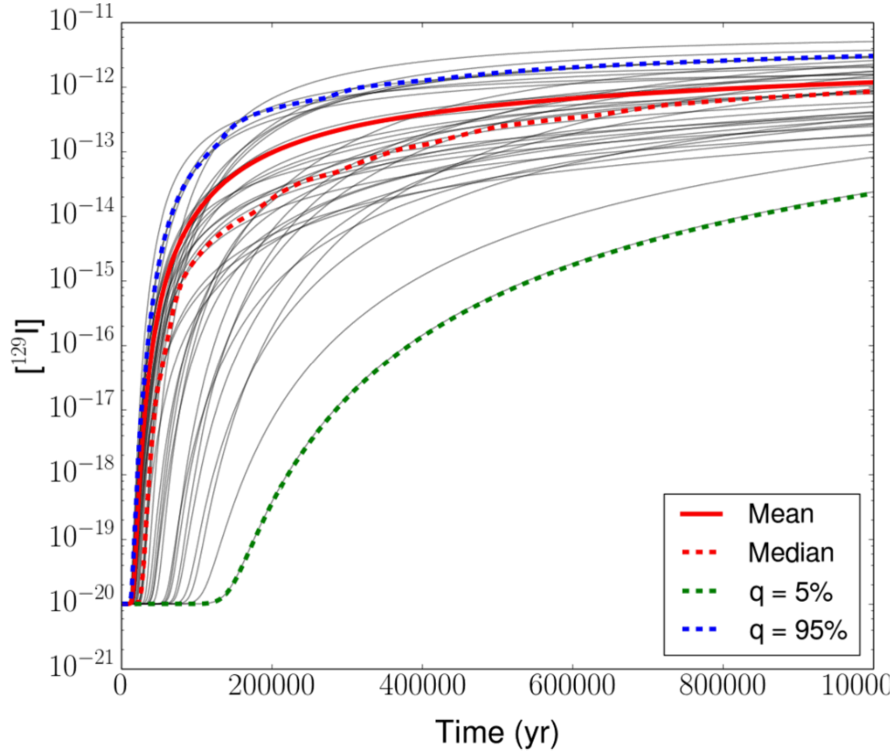




Generic Salt Repository PA Model – 3d Isothermal vs. 3d Thermal

Extraction well





Used Fuel Disposition Campaign

Generic Disposal System Analysis (GDSA): Clay Repository PA Model Results

Payton Gardner and Emily Stein
Sandia National Laboratories

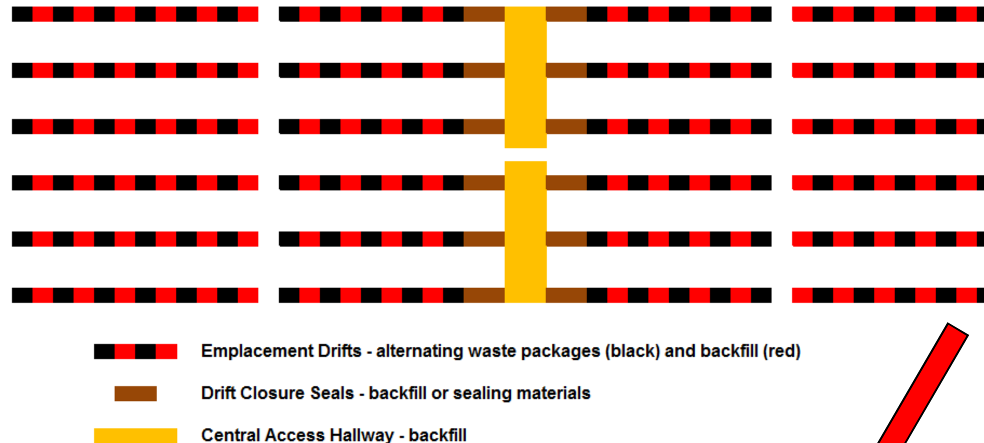
UFDC Annual Working Group Meeting
UNLV, Las Vegas, NV
June 10, 2015

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND2014-4697P.

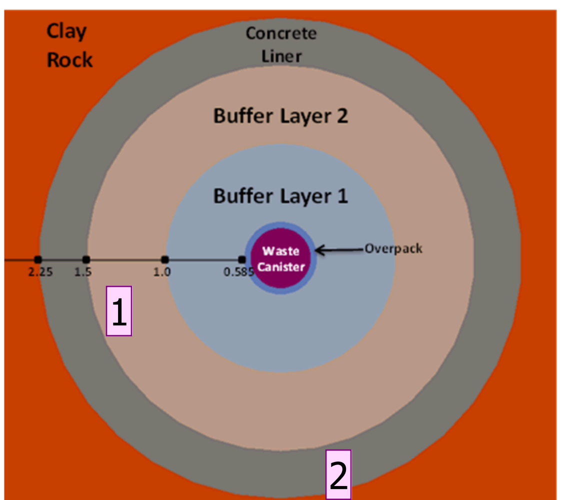
Sandia National Laboratories

Generic Clay Reference Case – Concept of Operations

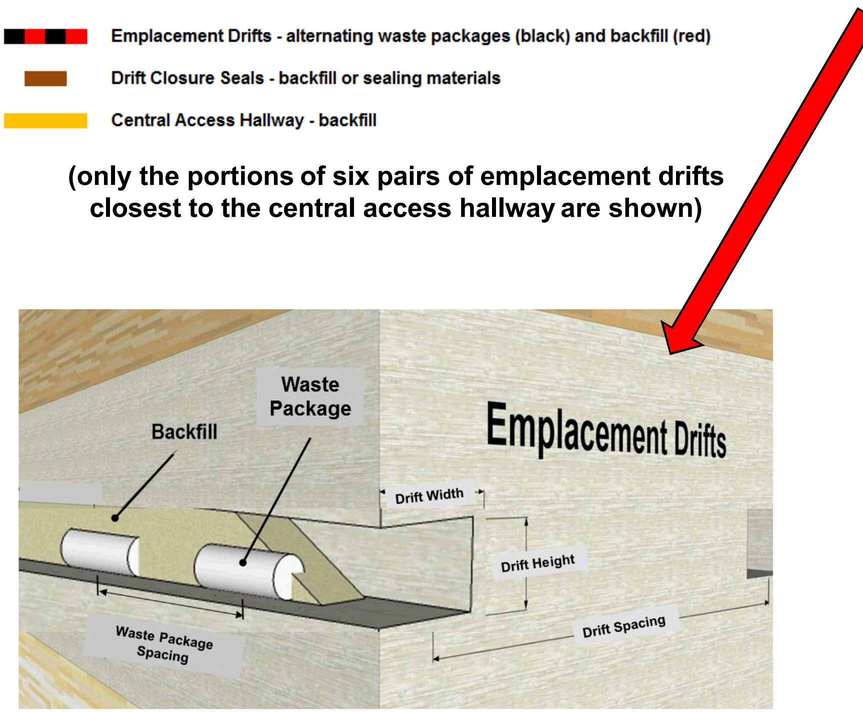
- **Concept of Operations**
  - Horizontal end-to-end emplacement of waste packages in drifts separated by intact host rock "pillars"
  - Drifts and access hallways backfilled with 2-layer buffer immediately after package emplacement
  - Shafts are sealed with bentonite
  - Ground support includes concrete liners in drifts and hallways



(only the portions of six pairs of emplacement drifts closest to the central access hallway are shown)



Jové Colón et al., 2014



Slide 48

1 bentonite, cement, and asphalt?

Emily Stein, 6/3/2015

2 though this may not be a good assumption for clay.

Emily Stein, 6/3/2015

3 Emily Stein, 6/3/2015

Generic Clay Reference Case – Inventory

- **Decay heat**

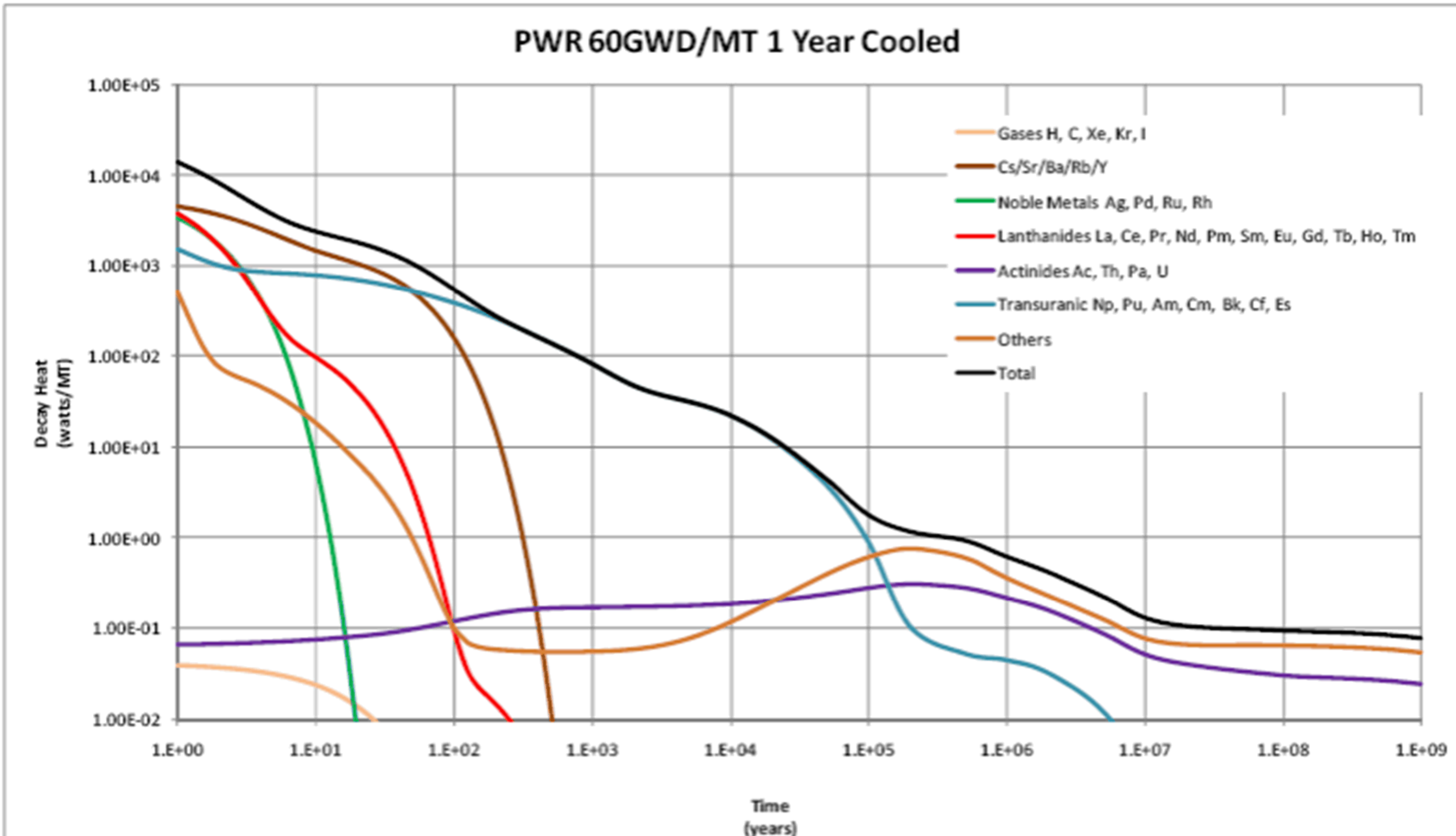


Figure 3-11 PWR 60 GWd/MT Used Fuel Decay Heat

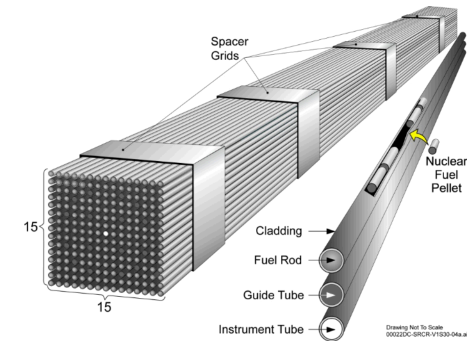
Generic Clay Reference Case – Repository Layout

- **Number, dimensions, and spacing of drifts determined by total inventory, waste package size, and mechanical design considerations**
  - 12-PWR UNF waste packages
    - *5.225 MTHM / WP, 3.1 kW / WP*
  - ~ 13,400 waste package for 70,000 MTHM repository
  - No ventilation
  - In future, consider thermal constraint, if appropriate

Parameters	Value
Waste Package	
WP center-to-center spacing in-drift (m)	10.0
Approx. number of WPs for 70,000 MTHM	13,397
Emplacement Drift	
Drift height (m)	4.0
Drift width (m)	4.0
Drift center-to-center spacing (m)	20.0
Number of WPs per drift	80
Drift length, including seals (m)	805.0
Repository	
Number of drift pairs (rounded up)	84
Repository length (m)	1,618.0
Repository width (m)	1,666.0

84 pairs of 805-m long emplacement drifts
80 WPs per drift

Generic Clay Reference Case – Geologic Disposal System EBS: Waste Form



- **Waste Form**
  - PWR assemblies composed mainly of UO_2 and zircaloy
    - *solid volume = 0.057 m^3 per assembly*
  - Instant release fraction for I^{129}
    - *triangular: most likely = 0.11, min = 0.02, max = 0.27 (SNL 2008 – YMP)*
  - Fractional waste form degradation rate [$M = M_0 \exp(-\lambda t)$]
    - *from Gorleben salt dome (Keinzler et al. 2014)*

Case	**λ (d^{-1})**	**λ (yr^{-1})**	**Time for 50% Degrad (yrs)**	**Time for 99% Degrad (yrs)**
Deterministic	10^{-6}	3.6525×10^{-4}	~ 1,900	~ 12,500
Probabilistic – Lower	10^{-8}	3.6525×10^{-6}	~ 190,000	~ 1,250,000
Probabilistic – Upper	10^{-5}	3.6525×10^{-3}	~ 190	~ 1,250

* Uniform distribution

Slide 51

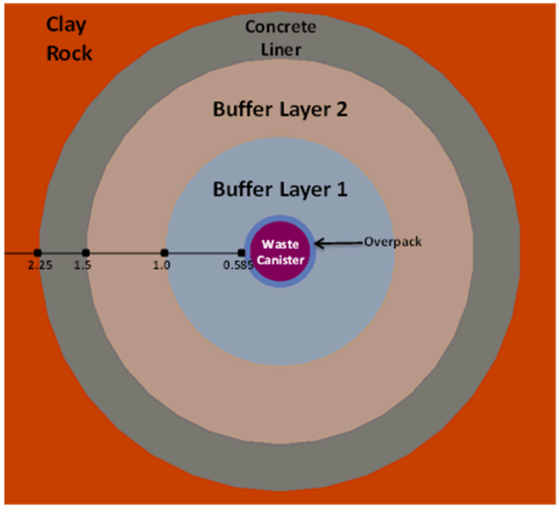
4 keeping salt brine values here would be conservative assumption, because they are much faster. have no idea how skb came up wtih these values for granite deep porewaters.
Emily Stein, 6/3/2015

Generic Clay Reference Case – Geologic Disposal System EBS: Waste Package

- **Waste Package**
  - Stainless steel canister sealed at point of origin, enclosed in a low-alloy carbon steel overpack for handling and emplacement
  - Currently using 12 PWR waste package loading, based on repository layout considerations
    - *length = 5.0 m, diameter = 1.29 m, overpack thickness = 5 cm (Hardin et al. 2012)*
    - *volume = 6.53 m^3*
  - Volume of UNF waste (12 PWR) = 0.68 m^3; Volume of internals and overpack = 2.6 m^3
    - *Initial void fraction = 0.5*
    - *Waste form volume fraction = 0.104*
  - Thermal output: 5.225 MTHM / WP (100 yr OoR) $\rightarrow$ 3.1 kW / WP
  - Currently assume instantaneous degradation (i.e., no barrier function)
  - In future, consider gas generation from carbon steel overpack, if appropriate
  - Simulation parameters for a crushed waste package
    - *Porosity = 0.3; permeability (m^2) = 10^{-13}; tortuosity = 1*

Generic Clay Reference Case – Geologic Disposal System EBS: Buffers

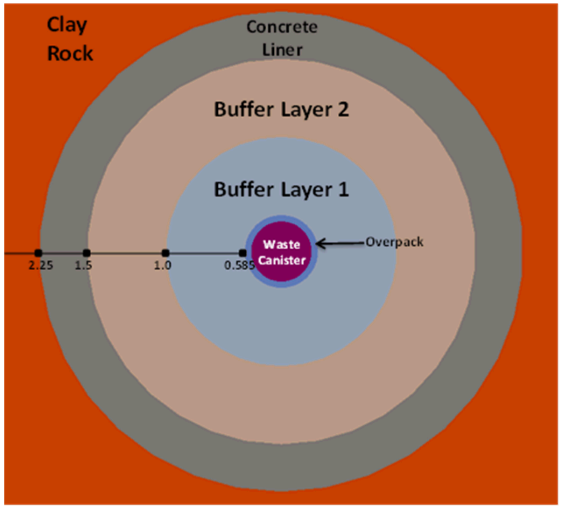
- **Buffer 1**
  - Bentonite/quartz sand mixture
  - Porosity = 0.35 (min = 0.25, max = 0.45)
  - Permeability (m^2) = 10^{-16}
  - Tortuosity = Porosity
- **Buffer 2**
  - Bentonite: Properties based on FEBEX and MX-80 bentonites
  - Porosity = 0.25 (min = 0.10, max = 0.40)
  - Permeability (m^2): 10^{-20}
  - Tortuosity = Porosity



Jové Colón et al., 2014

Generic Clay Reference Case – Geologic Disposal System EBS: Shaft and Drift Seals; Liners

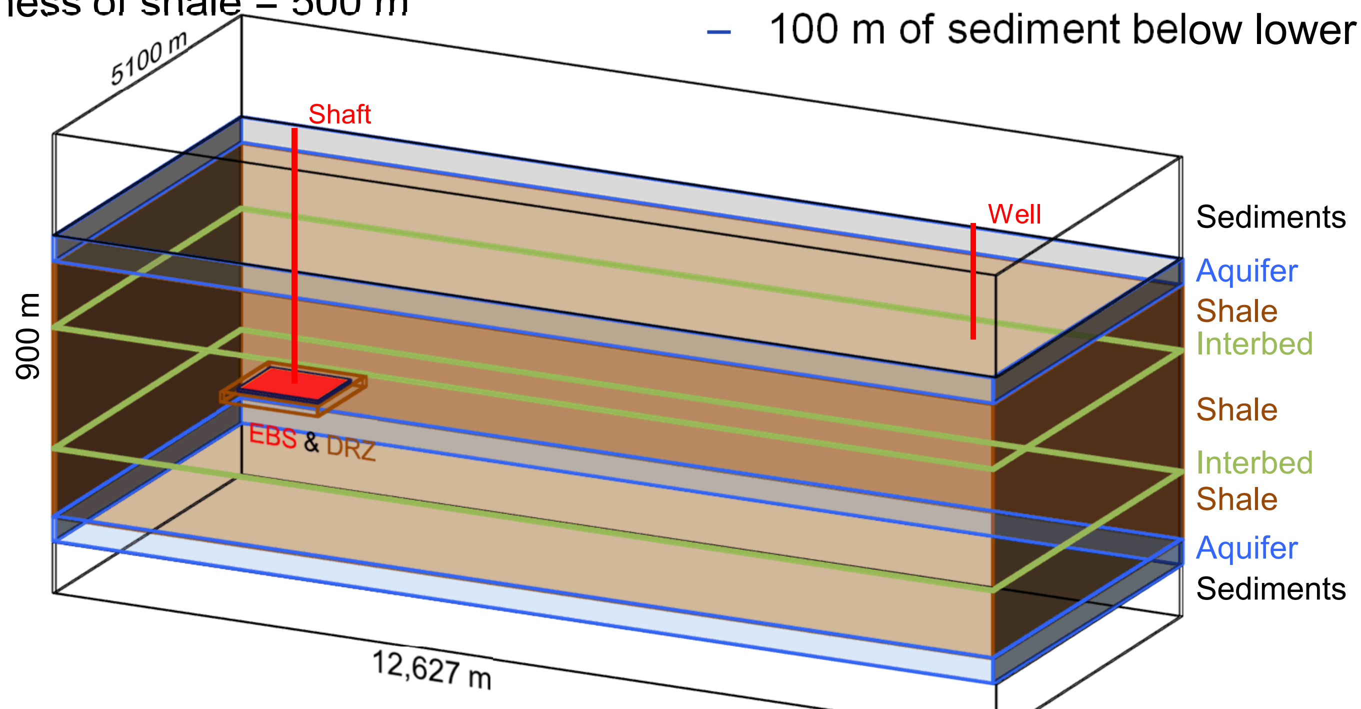
- **Shaft and Drift Seals**
  - Bentonite: Properties based on FEBEX and MX-80 bentonites (same as buffer)
  - In future, consider a multi-component shaft seal of bentonite, concrete, and asphalt.
- **Liners**
  - Concrete (0.75 m thick) lines drifts and hallways
  - Porosity = 0.15
  - Permeability = 10^{-17}
  - Tortuosity = Porosity



Jové Colón et al., 2014

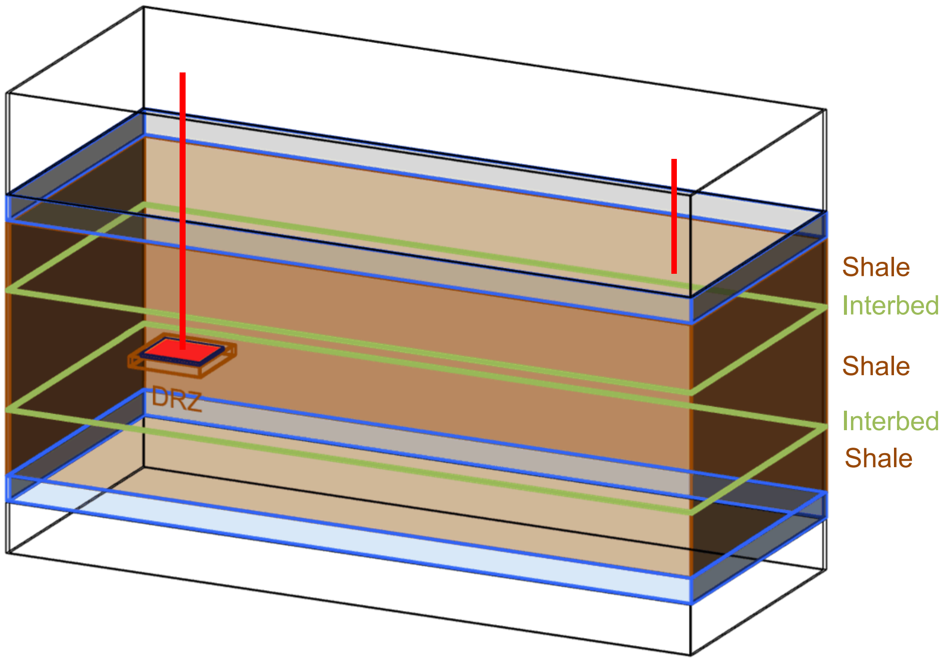
Generic Clay Reference Case – Geologic Disposal System NBS: Stratigraphy

- **Stratigraphy – based on shale formations in interior U.S.**
  - Laterally extensive formation
  - Dip angle < 5° (0° in simulation)
  - Minimal topography (none in simulation)
  - Depth to top of shale = 250 m
  - Thickness of shale = 500 m
  - Repository centered in shale @ 500 m below surface
  - High-k interbeds (5 m thick) within shale, 125 m above and below repository
  - Aquifers (50 m thick) above and below shale
  - 200 m of sediment above upper aquifer
  - 100 m of sediment below lower aquifer



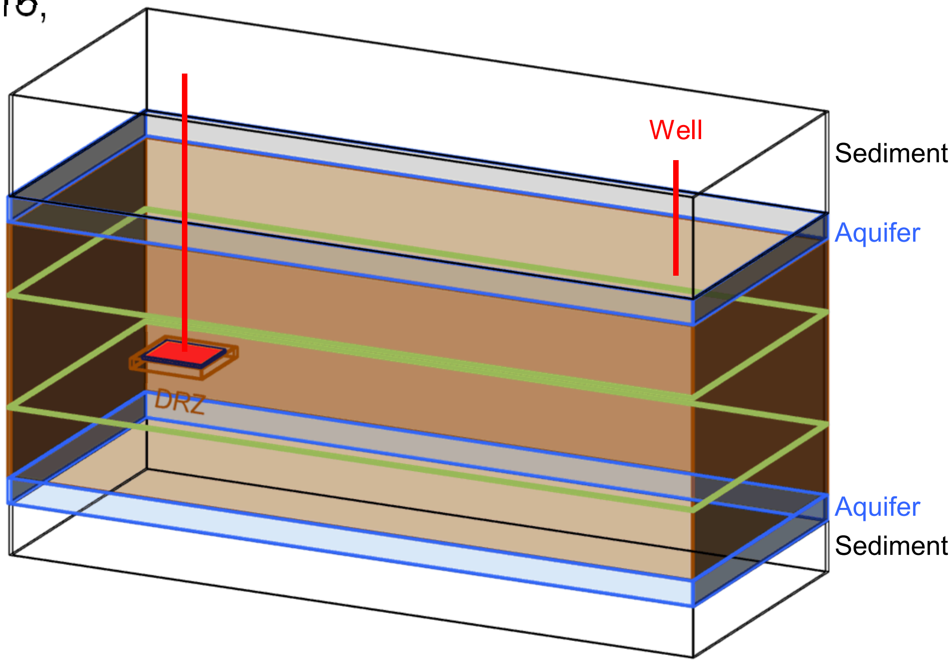
Generic Clay Reference Case – Geologic Disposal System NBS: Shale, DRZ, and Interbeds

- **Shale**
  - 500-m thick
  - Porosity = 0.25 (min = 0.10, max = 0.40)
  - Log permeability (m^2) = -19.5 (min = -22, max = -17)
  - Tortuosity = Porosity
- **Disturbed Rock Zone (DRZ)**
  - 9-m thick on all sides of excavation
  - Porosity = 0.25 (min = 0.10, max = 0.40)
  - Log permeability (m^2) = -18 (min = -20, max = -16)
  - Tortuosity = Porosity
- **High-k Interbeds**
  - 5-m thick
  - Porosity = 0.20
  - Log permeability (m^2) = -16 (min = -18, max = -14)
  - Tortuosity = Porosity



Generic Clay Reference Case – Geologic Disposal System NBS: Aquifers, Sediments; Path to Biosphere

- **Aquifers**
  - 50-m thick
  - Porosity = 0.20 (min = 0.10, max = 0.30)
  - Log permeability (m^2) = -14.5 (min = -16, max = -13)
  - Tortuosity = Porosity
- **Sediments**
  - 200-m thick above
  - 100-m thick below
  - Porosity = 0.20
  - Log permeability (m^2) = -15
  - Tortuosity = Porosity
- **Path to Biosphere**
  - 5 km lateral extent from repository edge to a groundwater well
  - Regional hydraulic gradient = 0.0013



Generic Clay Reference Case – Geologic Disposal System Deterministic Properties

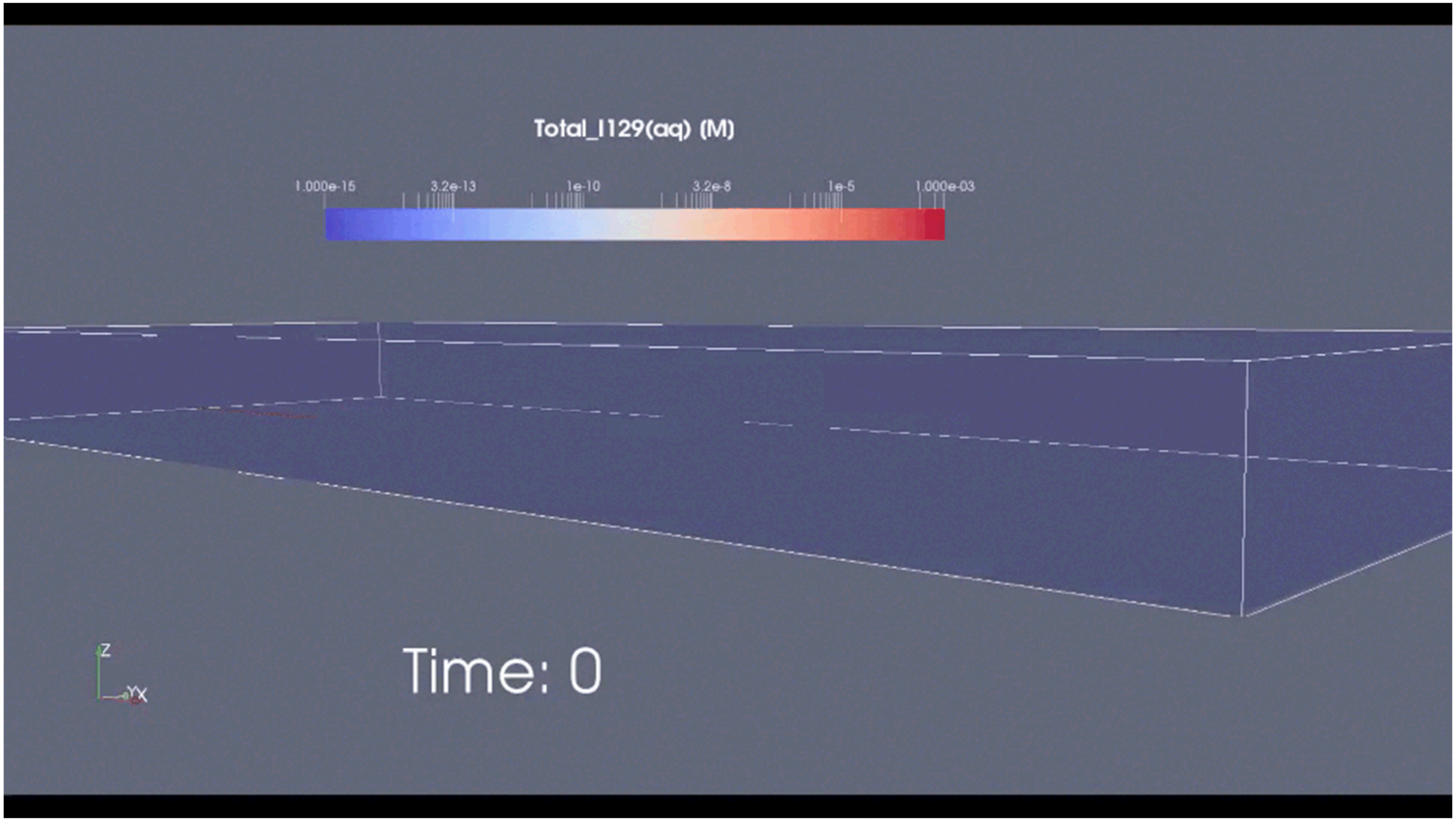
Model Region	Permeability (m^2)	Porosity	Tortuosity[1]	Effective Diffusion Coefficient[2] (m^2/s)	Longitudinal Dispersivity (m)	Thermal Conductivity[3] (W/m·°K)	Specific Heat Capacity[4] (J/kg·°K)
Waste Package	1.00×10^{-13}	0.300	1.00	6.90×10^{-10}	0.5	16.7	466
Buffer1	1.00×10^{-16}	0.35	0.35	2.82×10^{-10}	0.0	1.75	920
Buffer2 (also shaft, seals)	1.00×10^{-20}	0.25	0.48	1.44×10^{-10}	0.0	1.6/1.3	920
Liners	1.00×10^{-17} 3.5×10^{-21}	0.15	0.15/1	5.18×10^{-11}	0.0	1.7	1550
DRZ	1.00×10^{-17}	0.25	0.25	1.44×10^{-10}	0.0	1.8/1.2	1000
Shale	3.16×10^{-20}	0.25	0.25	1.44×10^{-10}	0.0	1.8/1.2	1000
High-k Interbed	1.00×10^{-16}	0.20	0.20	9.20×10^{-11}	50.0	1.5	927
Aquifer	3.16×10^{-15}	0.20	0.20	9.20×10^{-11}	50.0	1.5	927
Sediments[5,6]	1.00×10^{-15}	0.20	0.58	9.20×10^{-11}	50.0	1.5	927

[1] Tortuosity = Porosity, except for WP
[2] Effective diffusion coefficient = (free water diffusion coefficient) x (tortuosity) x (porosity)
[3] Hardin et al. 2012, Tables D-1, D-2, and D-5
[4] Hardin et al. 2012, Table D-3
[5] Freeze and Cherry 1979, Tables 2.2 and 2.4
[6] Hardin et al. 2012, Tables D-1, D-3, and D-5 (alluvium)

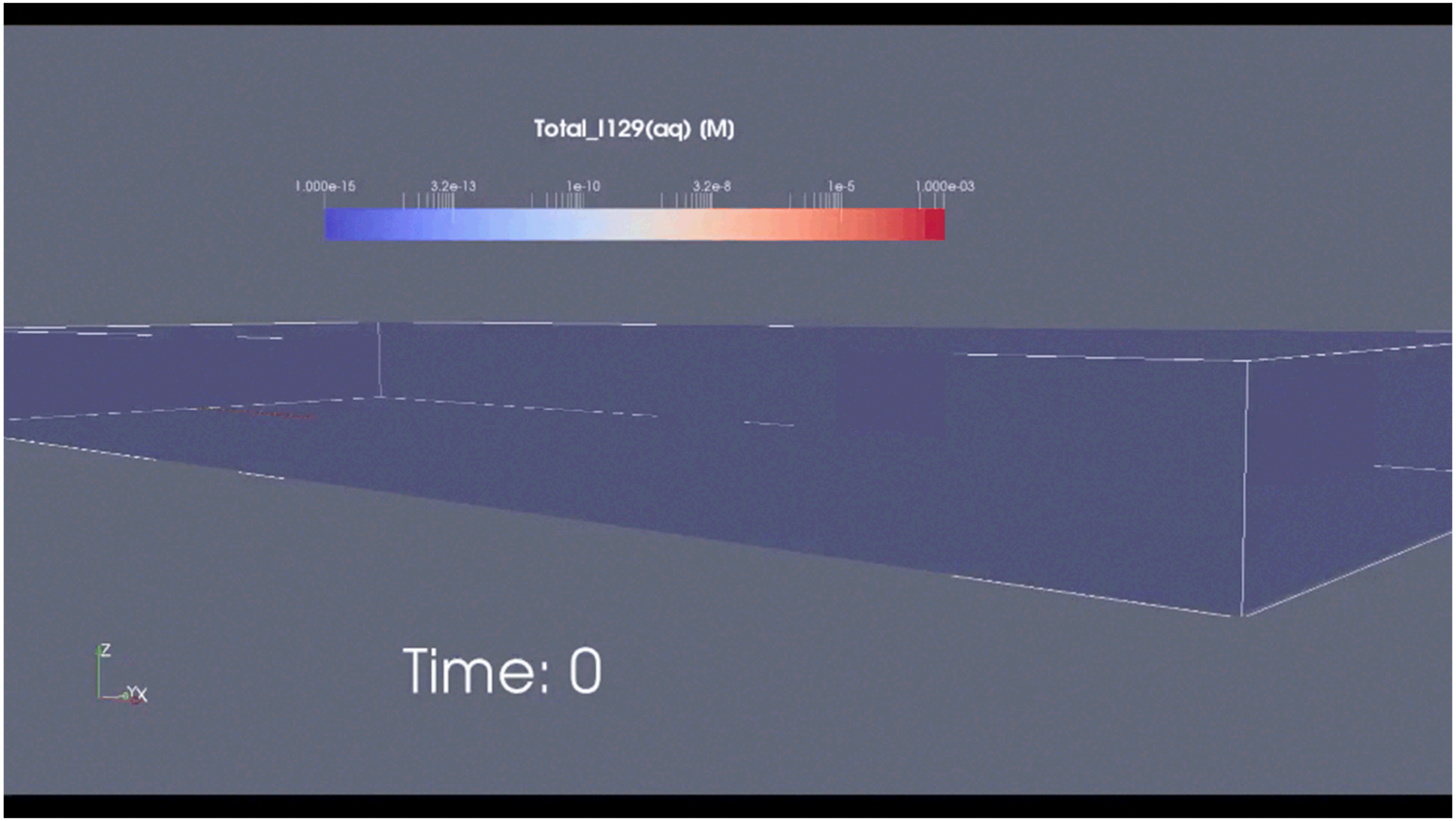
Generic Clay Repository PA Model Updates

- **Clay reference single drift**
  - 3D multi-drift, isothermal
    - *1,000,000 years*
      - Deterministic
      - Probabilistic
- **Thermal simulation results**
  - 3D THC (radionuclide source term, coupled heat, fluid flow and transport)
  - 1,000,000 years
    - *Deterministic*

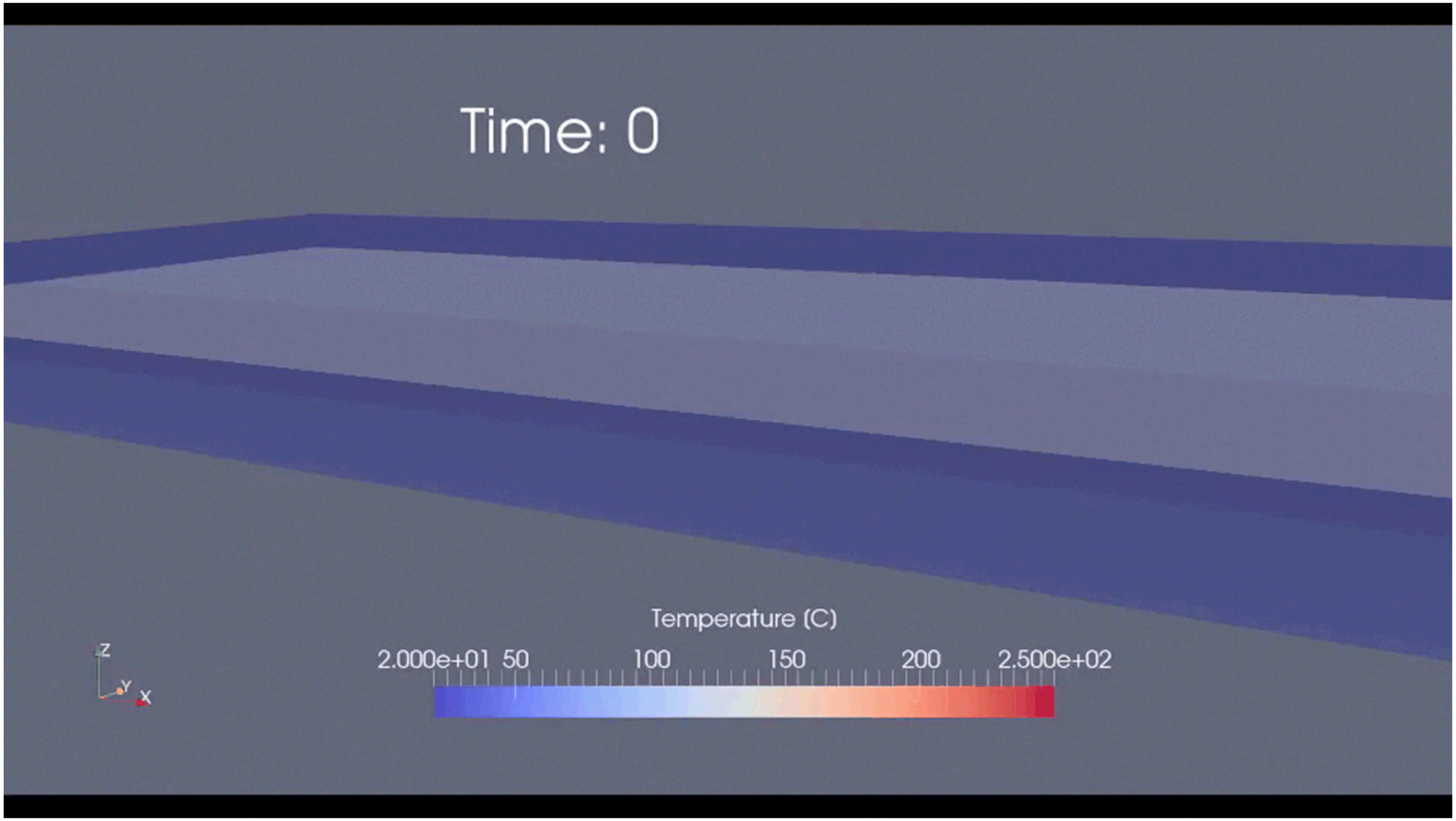
Generic Clay Repository PA Model – 3d iso-thermal Simulation Results



Generic Clay Repository PA Model – 3d Thermal Simulation Results

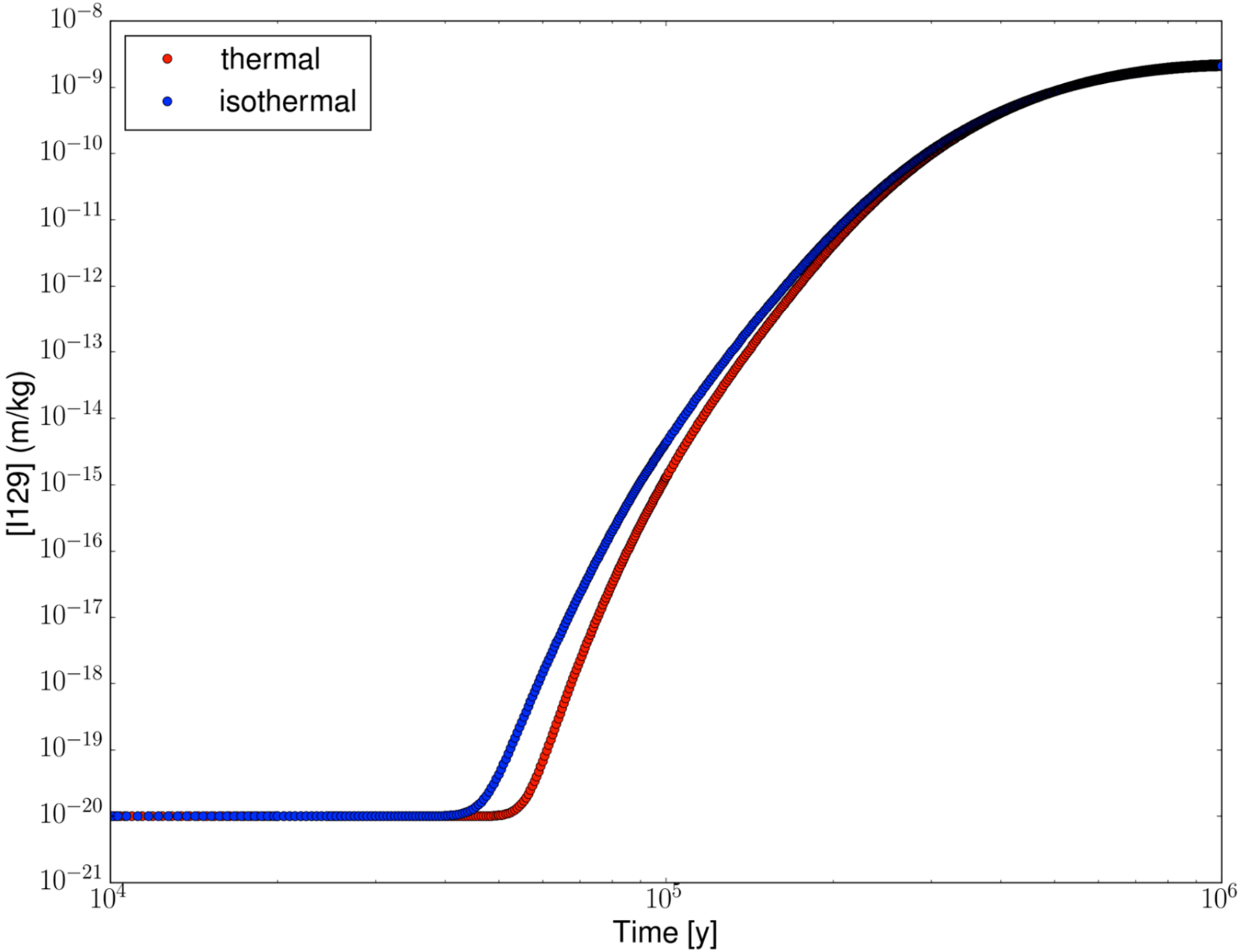


Generic Clay Repository PA Model – 3d Thermal Simulation Results



Used Fuel Disposition

Generic Clay Repository PA Model – 3d Thermal Simulation Results



GDSA Results Summary

- **Full 3d non-isothermal simulations run for the salt reference case developed last year**
  - 3d case shows somewhat decreased concentration from the single drift
  - Isothermal case shows slightly higher concentrations over all but probably within error.
    - *Do we need thermal simulation in the far field for long term transport prediction?*
- **Full 3d isothermal and non-isothermal simulation run for the newly developed clay reference case**
  - Deterministic results for non-isothermal case only
  - Thermal simulation shows slightly early breakthrough, but maximum concentration very similar
    - *Given the computational overhead, do we need thermal effects for long term prediction*
  - Probabilistic results for isothermal simulation?
- **Capability is improving, and being exercised on more problems.**
  - Further improvement will allow more detailed investigation of may important questions facing PA

Used Fuel Disposition Campaign

Insights for Coupling Process Models into Performance Assessment System Models

David C. Sassani
Sandia National Laboratories

UFD Campaign Annual Working Group Meeting
UNLV, Las Vegas, NV
June 10, 2015

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND2014-4697P.

Sandia National Laboratories

Presentation Outline

- **Coupling Insights**
  - Process and PA Model Perspectives
- **Schedule Insights**

Coupling Insights

- **Ideal Start Includes both Bottoms-Up and Top-Down Approaches**
- **Process modelers**
  - Identify the “what” that is to be augmented in the PA model
    - *For example, sampled distribution for fuel degradation rate*
- **PA modelers**
  - Identify where process detail is desired
    - *For example, bases for degrading fuel based on physical and chemical processes*
- **Early Targeting of Parameter Hooks**
  - Feeds from the process model output
  - Connections within PA Model

Coupling Insights Nuts and Bolts

- **Process Model Intended Use vs Use in PA Model**
  - Conceptual model definition
  - Model limitations
- **Uncertainty Approach**
  - Conceptual
    - *State variables driving output variation*
    - *Capture major driving processes*
  - Parameter
- **Scaling Aspects**
  - Comparative process model to PA model
    - *Temporal*
    - *Spatial*
- **External Process Model Couplings**
  - Awareness of environment process connections
  - Cross fertilization among process-PA staff

Schedule Insights

- Start *YESTERDAY*
- Expect Issues
- Be Resilient and Flexible

Used Fuel Disposition Campaign

Integration Efforts in GDSA

S. David Sevougian
Sandia National Laboratories

2015 UFDC Annual Working Group Meeting
GDSA Session, June 10, 2015
Las Vegas, NV

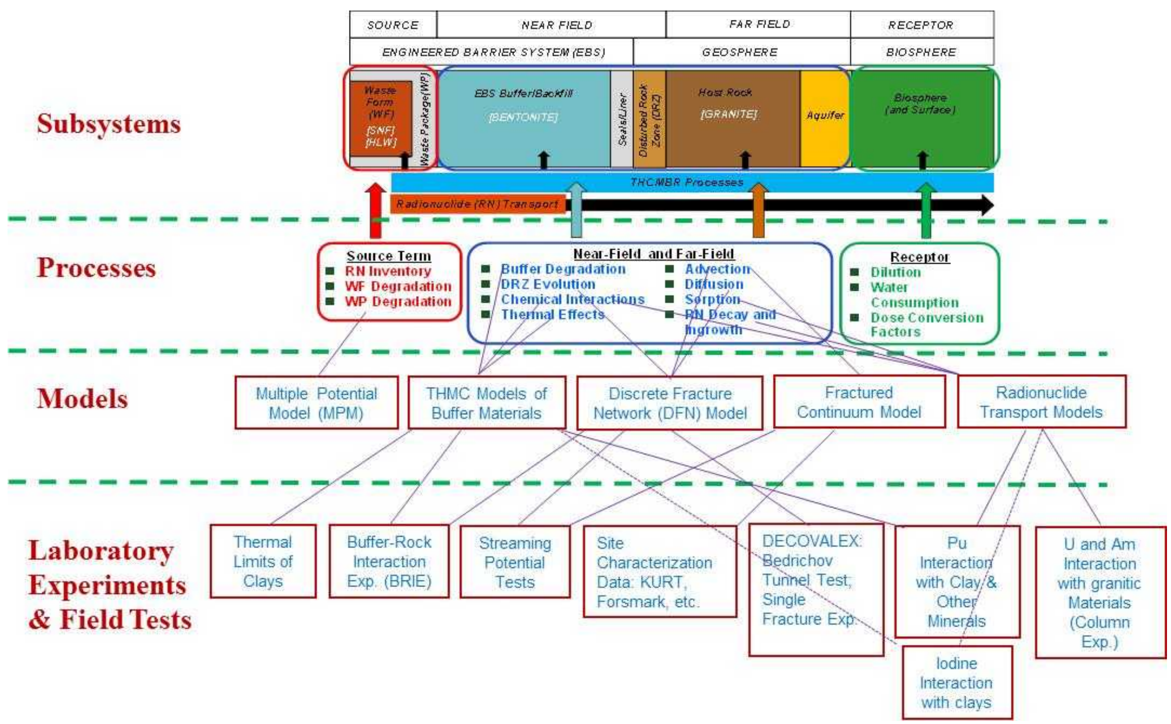
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND2014-4697P.

Sandia National Laboratories

Evolution of FY15 Integration Effort

- **December: "Inspiration" from DOE (Mark Tynan) following monthly crystalline-argillite telecon:**
  - Need more detailed schedule for completion of the advanced PA system model, which will rely much less on "abstractions"
  - How can UFD program R&D be integrated with PA and vice-versa
- **January: First integration meeting between GDSA, Argillite, Crystalline WP managers:**
  - Review of argillite and crystalline workscope and its importance to PA

Wang: Crystalline workscope pyramid



Evolution of FY15 Integration Effort (continued)

- **February thru May: Monthly GDSA-Crystalline-Argillite integration telecons:**
  - Development of [Process] Model Integration Template
  - Development of Process Model Summary Table (laundry list of models & experiments; x-Salt)
- **April: Second integration meeting between GDSA, Argillite, Crystalline WP managers:**
  - Developed Model Integration Table (process models most suitable for integration)
  - Develop an initial consensus on ease of integration of each process model
  - Develop an initial consensus on expected coupling method for each process model (e.g., directly coupled, used to develop a reduced-order model, or used only for FEPs screening)
  - Determine which processes and models are needed by PA but are not currently being developed by UFD (i.e., they are "missing")
  - Sent out e-mail request to process modelers on April 15, requesting completion of Model Integration Template for their particular model
- **May: Received completed Model Integration Templates**
  - Based on template responses, determined need for more info at UFD Working Group meeting in the form of 10 "lightning talks" (at the session just following this one)
- **"Inspiration" based in part on the successful integration of PFLOTRAN with the FMDM (from ANL and PNNL)**

Goals of Integration Session
(to follow this session)

- **Facilitate the integration of UFD process modeling with GDSA**
- **Ten process-model, five-minute "lightning" talks that explain:**
  - (1) *WHY* the given process model is important to PA and
  - (2) *HOW* it can be coupled to the GDSA-PA in the next year or two

3:50 – 4:05 Introduction and Objectives (Sevougian)

4:05 – 4:15 PFLOTRAN: Process Model Coupling/Abstraction Options (**Hammond**)

4:15 – 5:10 Lightning Round (5 min per talk)

- Colloid-facilitated transport model – granite, clay (**Reimus**)
- Desorption of radionuclides from pseudocolloids – clay, granite (**Zavarin**)
- Non-Darcy Flow model – clay (**Wang**)
- RBSN model – clay (**Houseworth**)
- THMC model for EBS bentonite – clay illitization – (**Zheng**)
- BBM/BExM/TOUGH-FLAC model – clay (**Rutqvist**)
- DFN model – granite (**Viswanathan**)
- Coupled THC processes in salt – (**Stauffer**)
- Salt Coupled THM processes (TOUGH-FLAC) – (**Rutqvist**)
- Nesting of domains – all media (**Hammond**)

5:10 – 5:40 Integration discussion (**all**)

Goals of Integration Session (cont.)

- **Update "Model Integration Table"**
- **Tentative schedule (priority) and L.O.E. for integration**

Used Fuel Disposition Campaign

Future Plans for GDSA

Paul Mariner
Sandia National Laboratories

UFD Annual Working Group Meeting
UNLV, Las Vegas, NV
June 10, 2015

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND2014-4697P.

Sandia National Laboratories

GDSA Future Plans – Generic Reference Case Development

- **Generic crystalline/granite repository**
  - Develop generic conceptual model based on UFD crystalline reference case
  - Simulate fracture flow in PA model using dual continuum model
- **Generic deep borehole disposal**
  - Collaborate with deep borehole work package
- **Additional concepts**
  - Large capacity dual purpose canisters (DPCs)

GDSA Future Plans – Model and Code Development and Integration

- **Improved process modeling**
  - Source term decay
  - Waste package degradation
  - New process model(s) from integration activities
- **Improved code efficiency**
  - Nested modeling for EBS

GDSA Future Plans – PA Model Application

- Crystalline/granite PA model
- Updated salt and argillite PA models
- Support Salt R&D Work Package
- Support Deep Borehole Work Package

Generic Disposal System Analysis (GDSA): Open Discussion

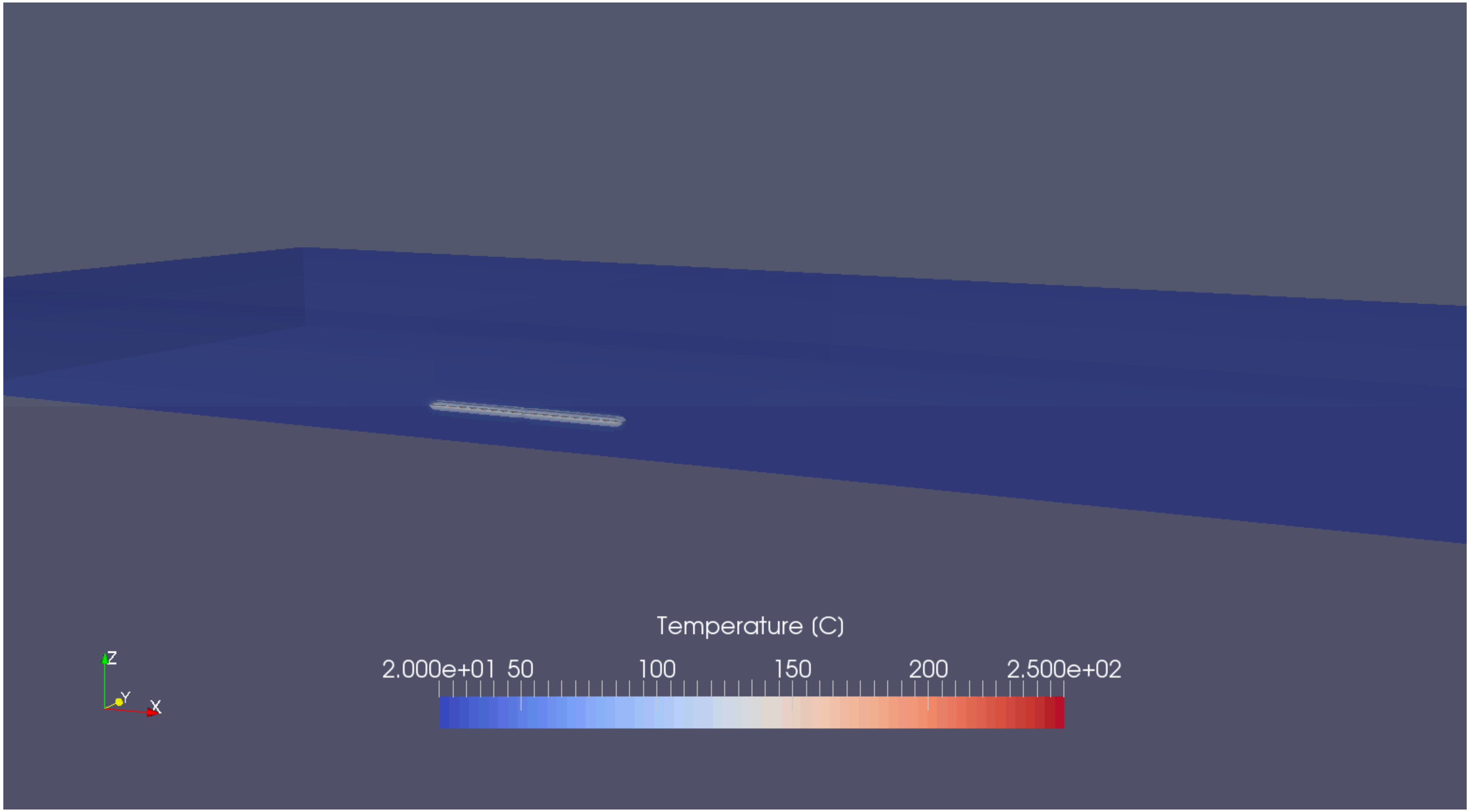
Used Fuel Disposition Campaign

Backup Sides

Generic Disposal System Analysis (GDSA) Results:
Extra slides

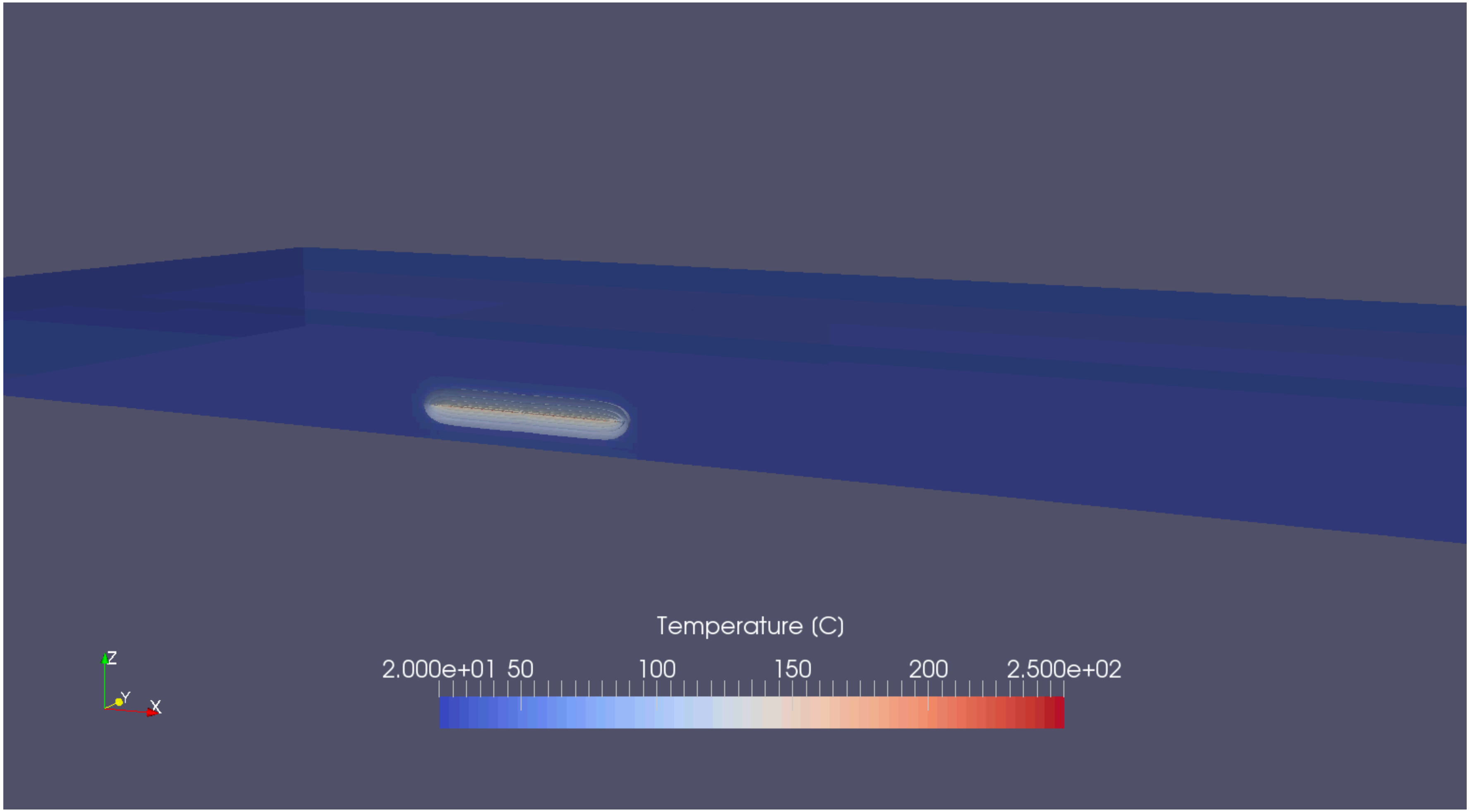
Generic Salt Repository PA Model – 3d Thermal Simulation Results

- Thermal results - temperature field 10 yr



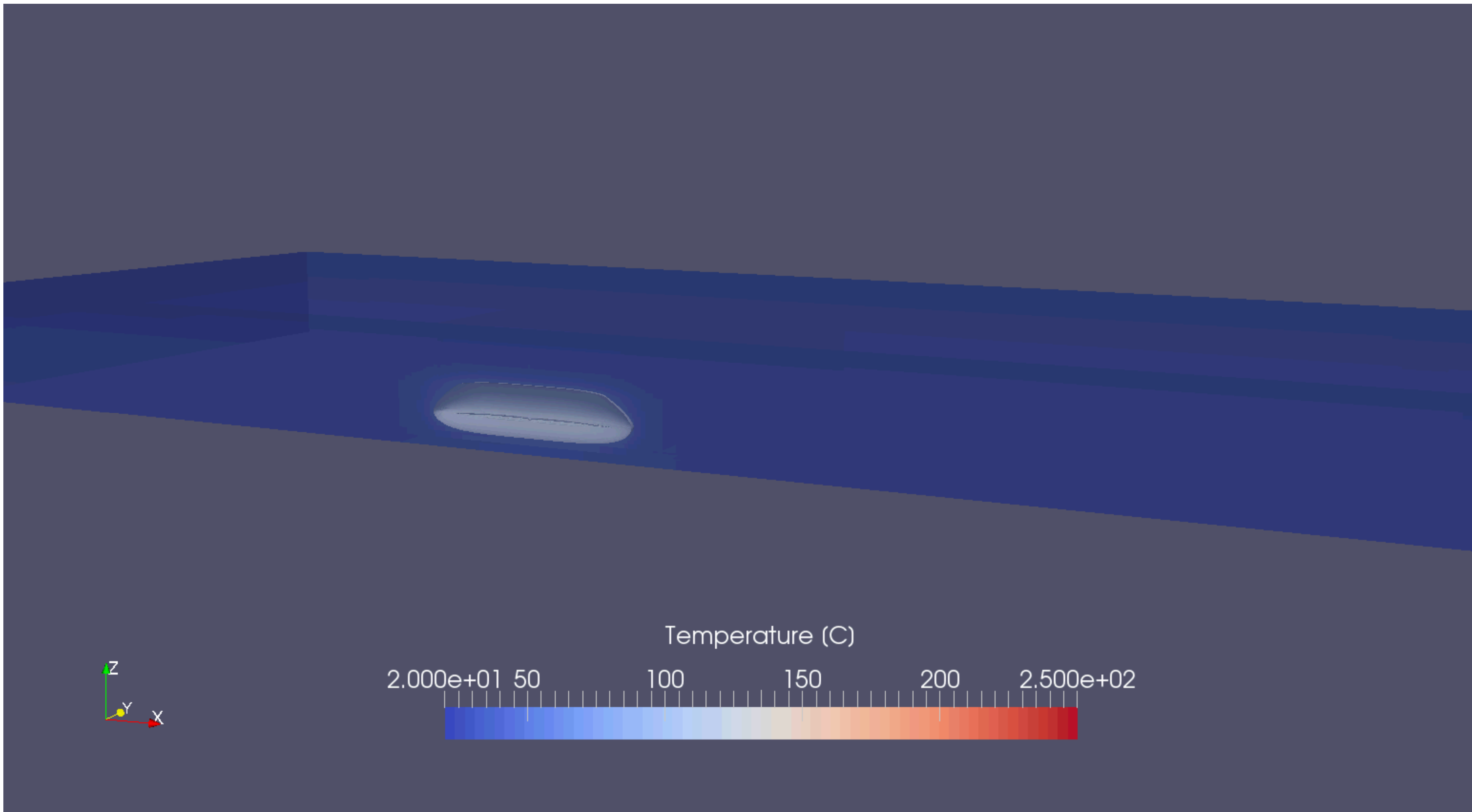
Generic Salt Repository PA Model – 3d Thermal Simulation Results

- Thermal results - temperature field 100 yr



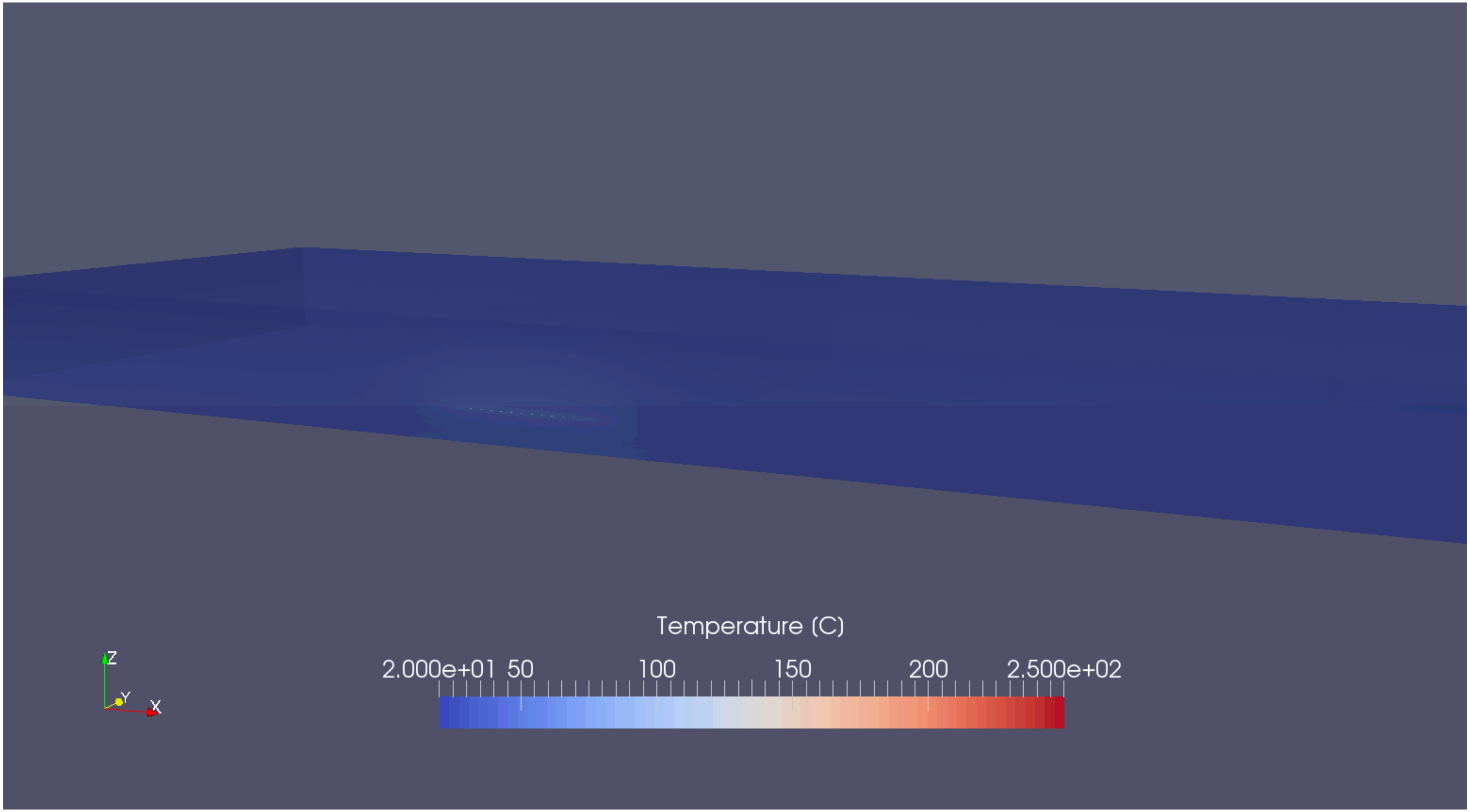
Generic Salt Repository PA Model – 3d Thermal Simulation Results

- **Thermal results - temperature field 1000 yr**



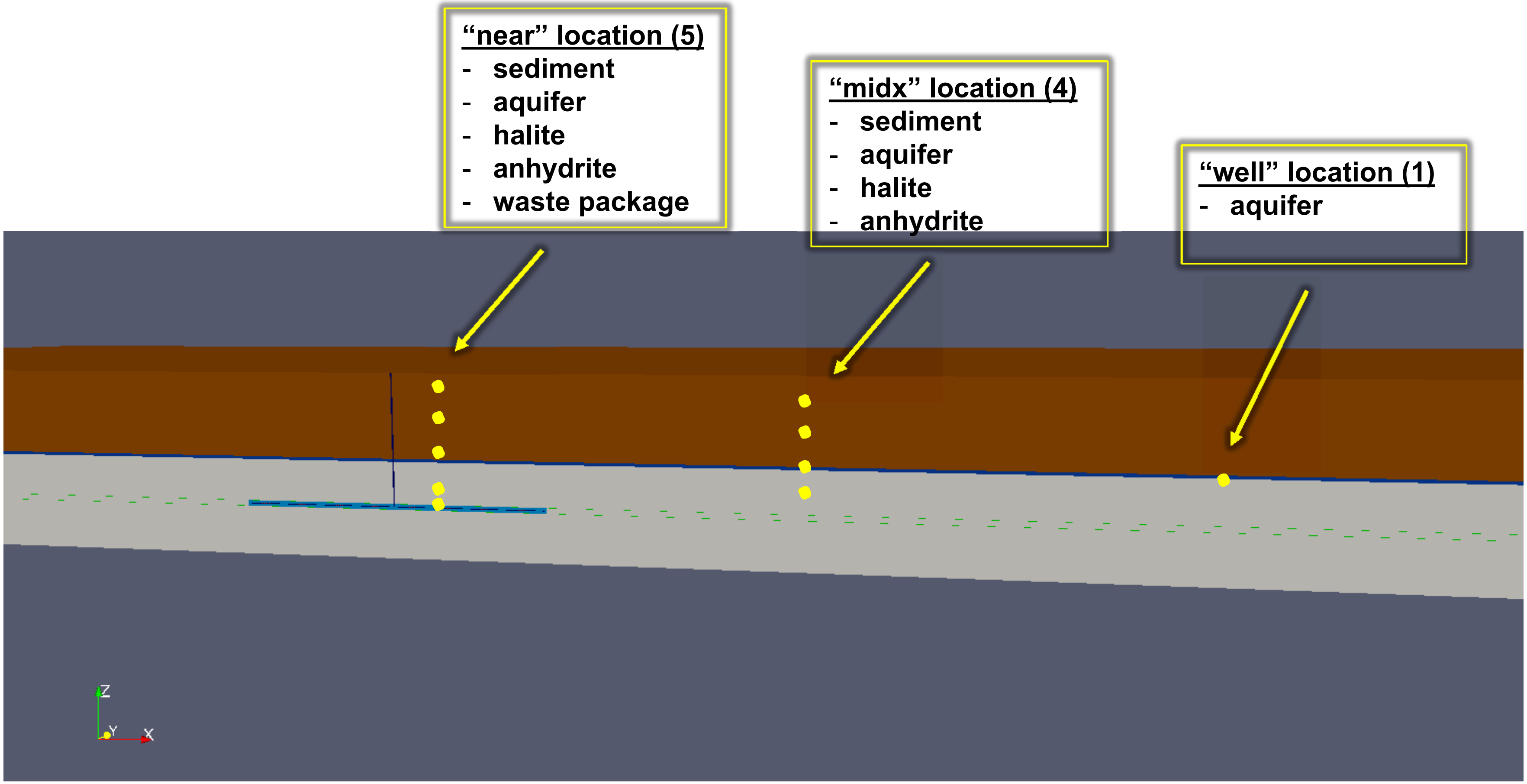
Generic Salt Repository PA Model – 3d Thermal Simulation Results

- **Thermal results - temperature field 5000 yr**



Generic Salt Repository PA Model – Thermal Probabilistic Simulations

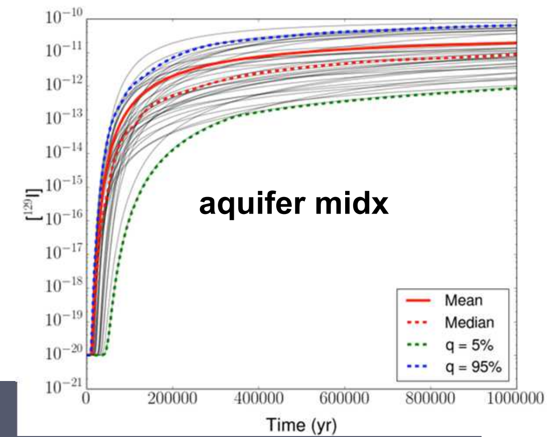
- Sensitivity analysis (partial rank correlation) at 10 locations

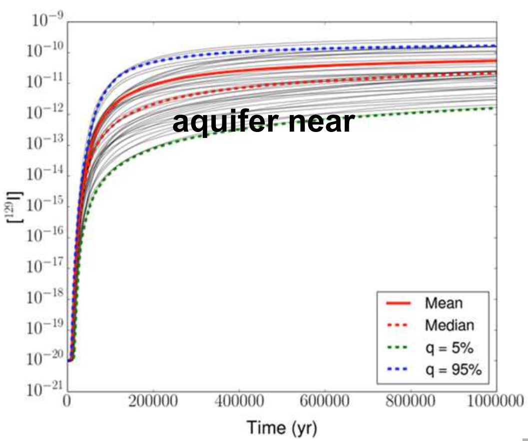


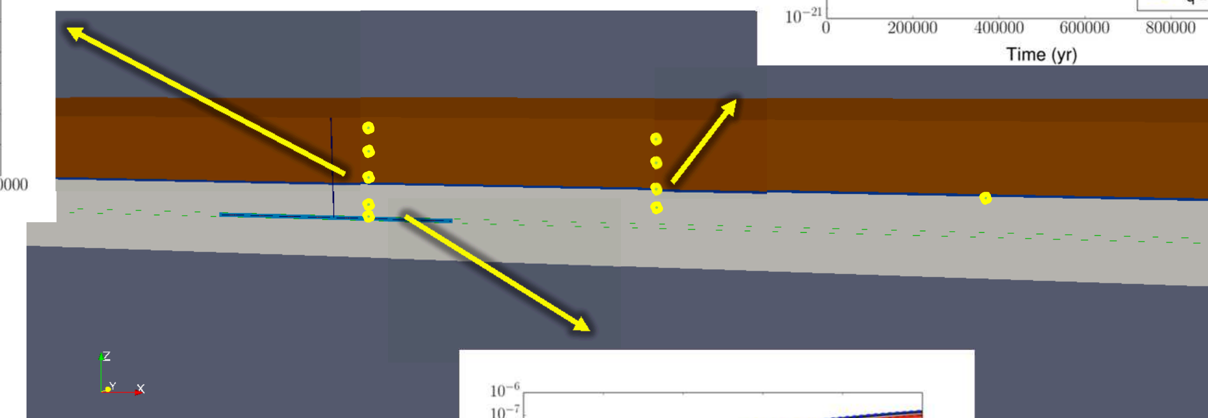
Used Fuel Disposition

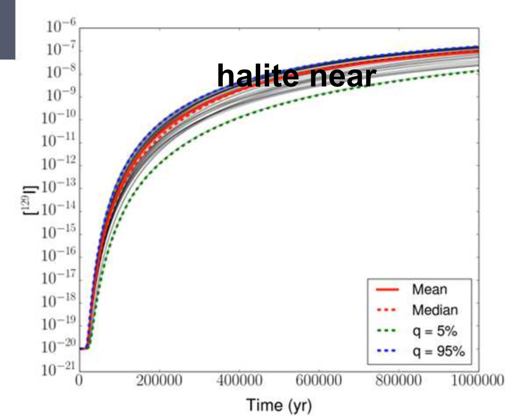
Generic Salt Repository PA Model – Multi-Realization Analysis

- ^{129}I dissolved concentration vs. time
  - (DAKOTA probabilistic output of 100 realizations)



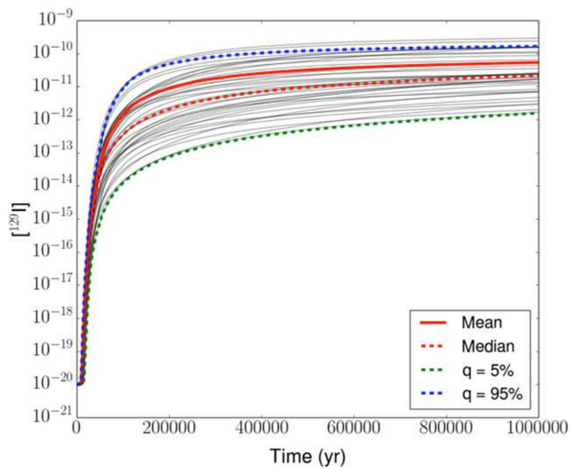


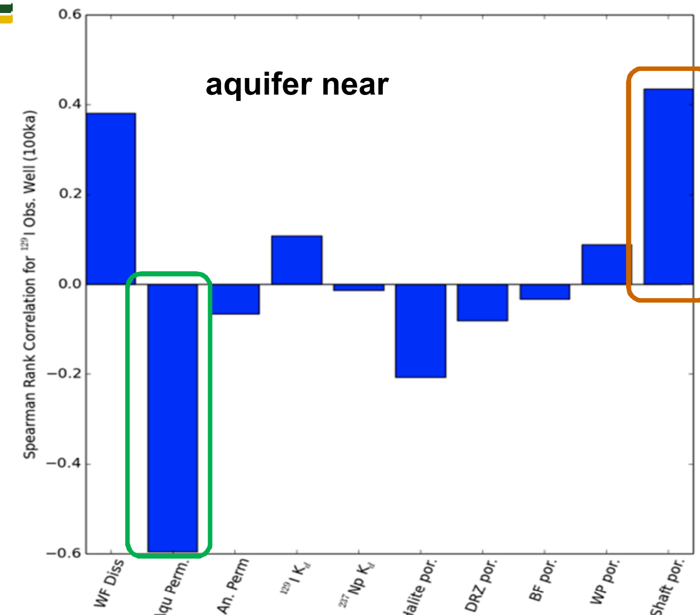


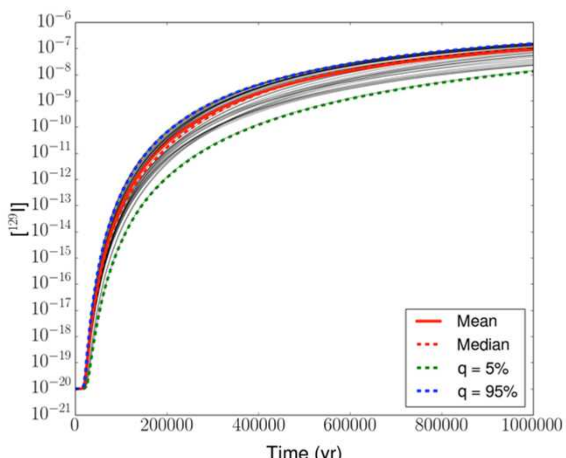


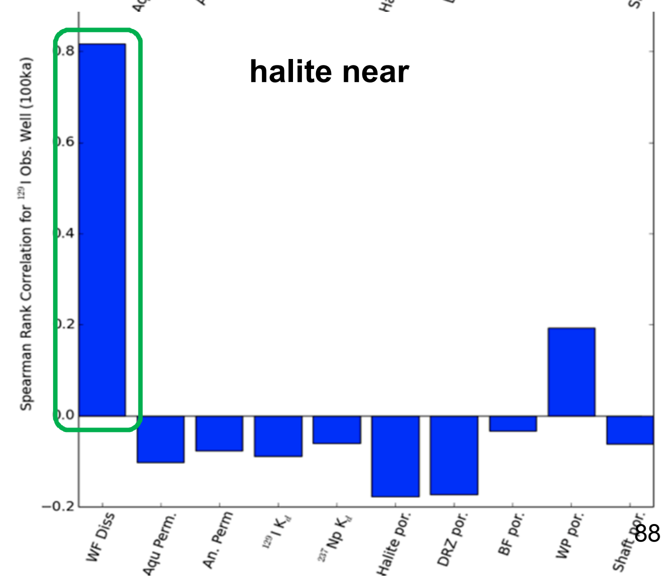
Generic Salt Repository PA Model – Multi-Realization Analysis

- **Partial rank correlation**
  - Peak ^{129}I concentration vs. time



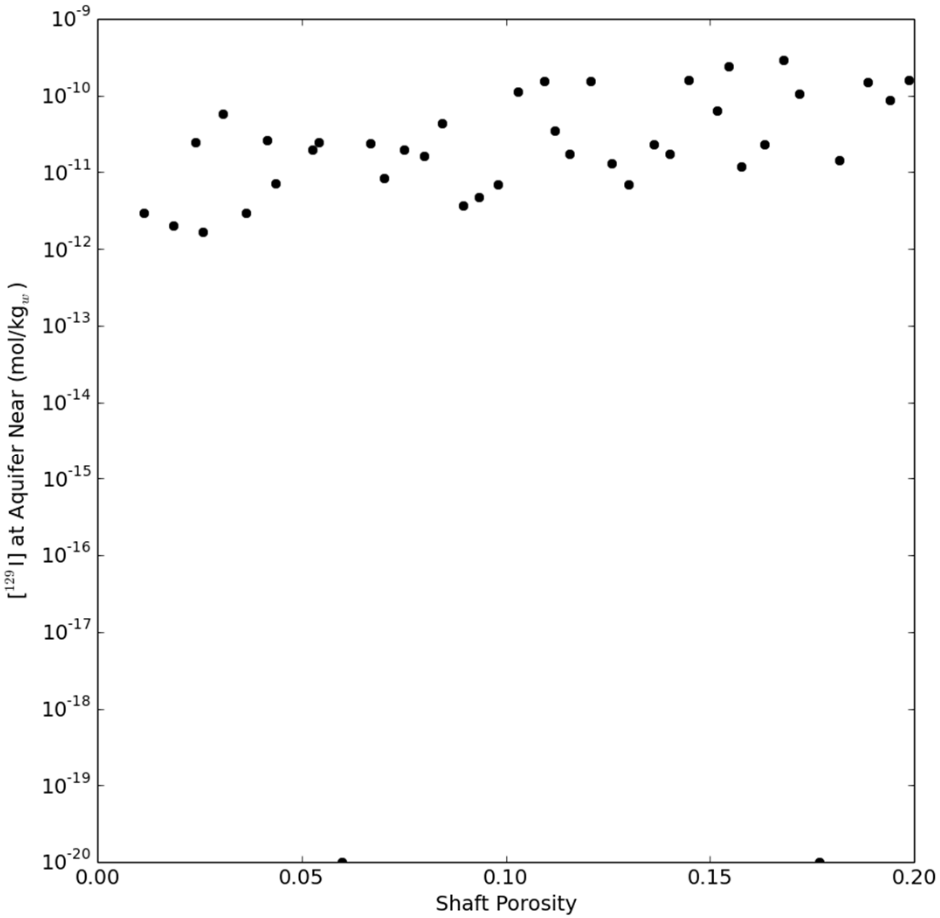


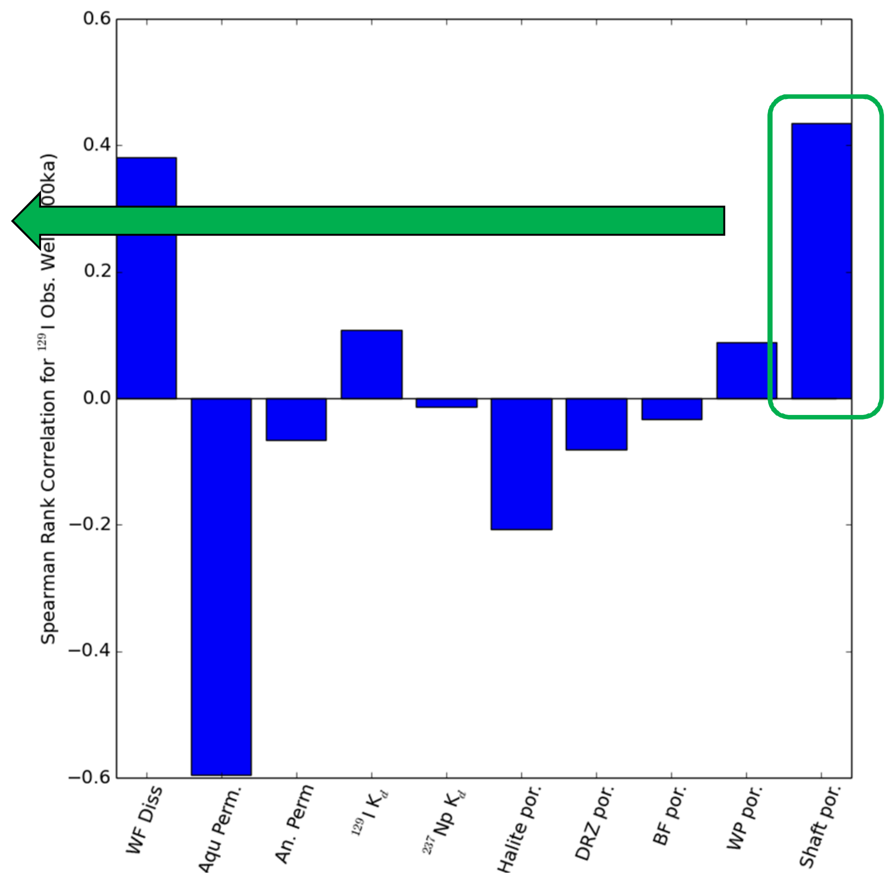




Generic Salt Repository PA Model – Multi-Realization Analysis

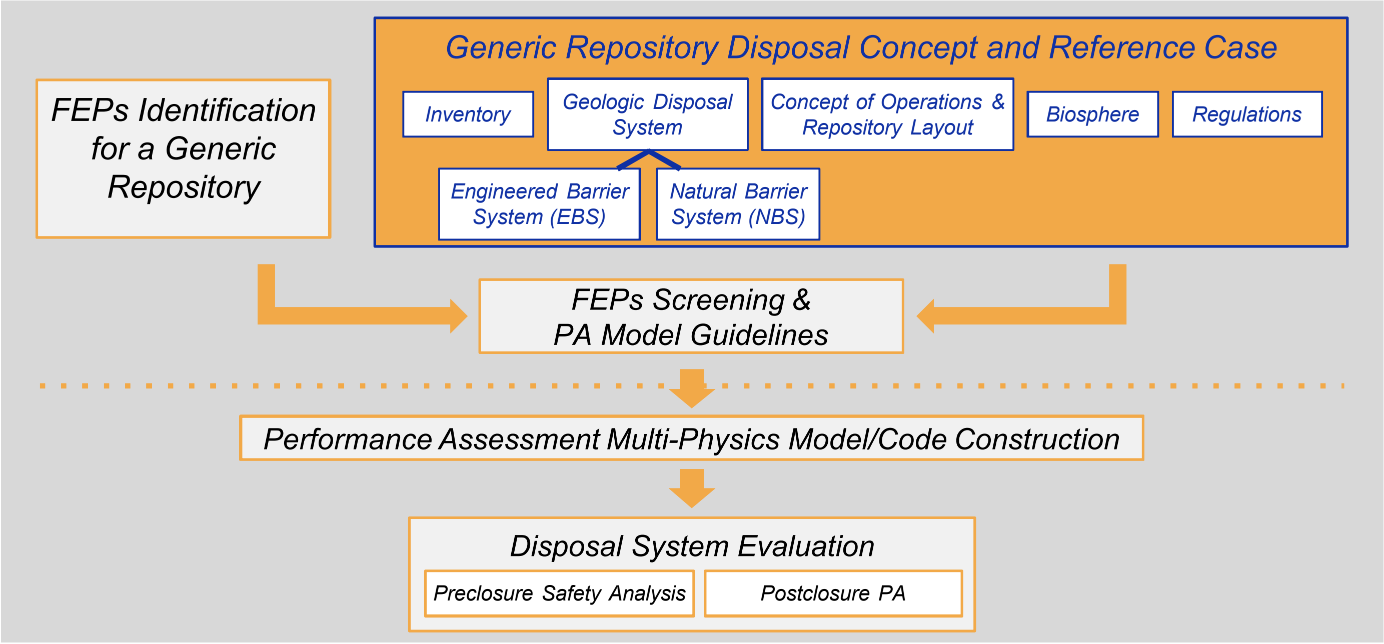
- **DAKOTA scatterplot analysis**
  - Max ^{129}I concentration at "aquifer near" at 100,000 years versus shaft porosity





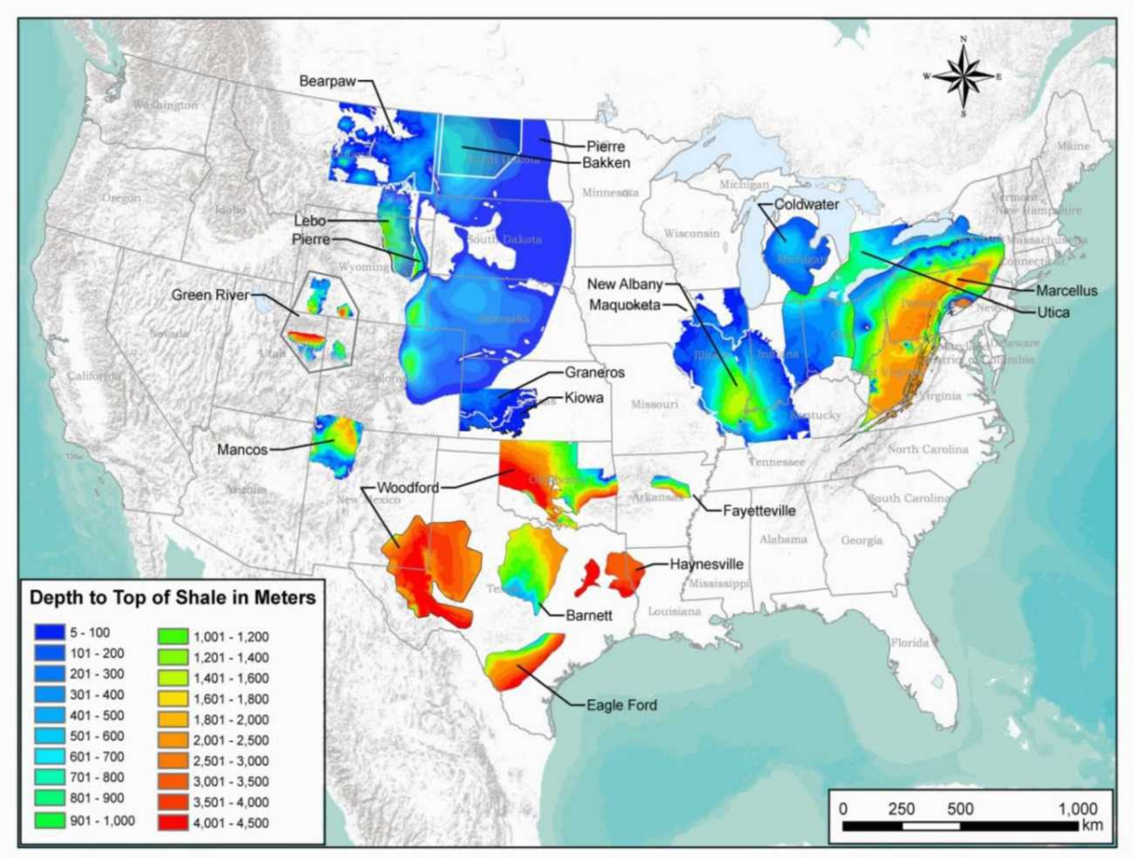
Generic Repository Reference Case

- **Reference Case is a surrogate for site- and design-specific information**
  - Documents information and assumptions needed for generic disposal system models
  - Helps ensure consistency across analyses (e.g., process modeling, PA, uncertainty and sensitivity analysis)



Generic Clay Reference Case – Disposal Concept

- **Disposal Concept**
  - Waste capacity of 70,000 MTHM
  - Repository located in a relatively homogeneous, vertically and laterally extensive, clay-rich formation (e.g., mudstone, shale, or argillite)
  - Homogeneous thickness is preferably ≥150 m



U.S. shale formations in GIS database of Perry et al., 2014

Slide 91

5 bentonite, cement, and asphalt?

Emily Stein, 6/3/2015

6 though this may not be a good assumption for clay.

Emily Stein, 6/3/2015

7 Emily Stein, 6/3/2015

Generic Clay Reference Case – Inventory

- **“No replacement nuclear generation” scenario (Carter et al. 2012)**
  - Commercial UNF (PWR and BWR) reaches 140,000 MTHM by 2055
  - Only PWR considered in reference case, with a conservative burn-up of 60 GWd/MT
  - 100-year OoR decay storage, initial enrichment of 4.73%
  - 450 isotopes with a total mass of total mass of 1.44×10^{6} g/MTHM

Isotope	Waste inventory mass (g/MTHM)	Mass fraction (g / g UNF)	Half-Life (yrs)
^{238}U	9.10×10^{5}	6.32×10^{-1}	4,470,000,000
^{237}Np	1.24×10^{3}	8.61×10^{-4}	2,140,000
^{241}Am	1.25×10^{3}	8.68×10^{-4}	432.7
^{242}Pu	8.17×10^{2}	5.68×10^{-4}	375,000
^{129}I	3.13×10^{2}	2.17×10^{-4}	15,700,000
^{234}U	3.06×10^{2}	2.13×10^{-4}	246,000
^{230}Th	2.28×10^{-2}	1.58×10^{-8}	75,400
^{233}U	1.40×10^{-2}	9.73×10^{-9}	159,300
^{229}Th	6.37×10^{-6}	4.43×10^{-12}	7,300
^{226}Ra	3.18×10^{-6}	2.21×10^{-12}	1,599

- **Smaller set of radionuclides for current PA model development:**
  - Neptunium series α-decay chain: ($^{241}Am \rightarrow {}^{237}Np \rightarrow {}^{233}Pa \rightarrow {}^{233}U \rightarrow {}^{229}Th$)
  - ^{129}I, a non-sorbing radionuclide with a long half-life

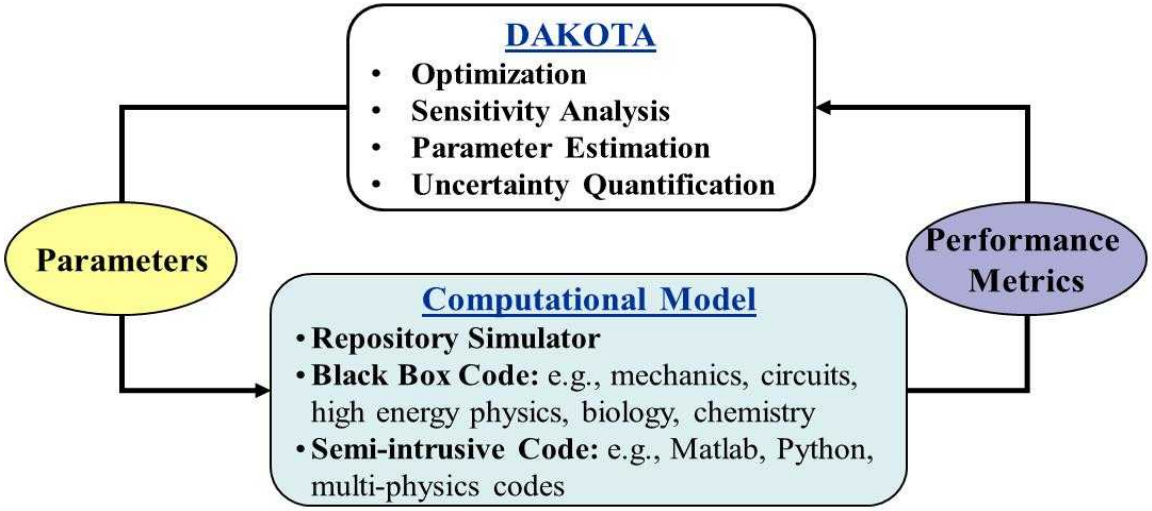
Slide 92

8 change these numbers for 100-year OoR
Emily Stein, 6/3/2015

9 update this table
Emily Stein, 6/3/2015

DAKOTA Modeling Capabilities

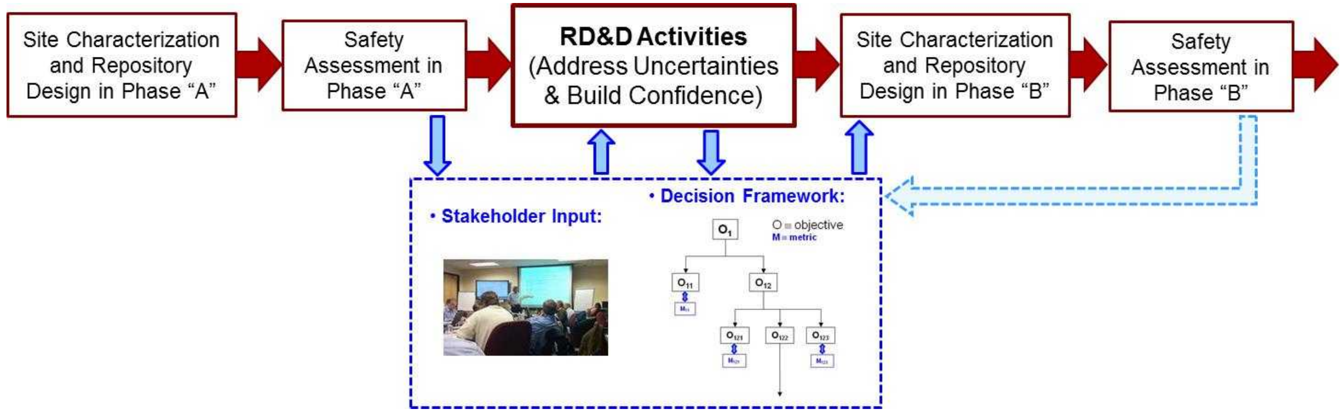
- **Manages uncertainty quantification (UQ), sensitivity analyses (SA), optimization, and calibration**
  - Generic interface to simulations
  - Extensive library of time-tested and advanced algorithms
  - Mixed deterministic / probabilistic analysis
  - Supports scalable parallel computations on clusters
  - Object-oriented code; modern software quality practices

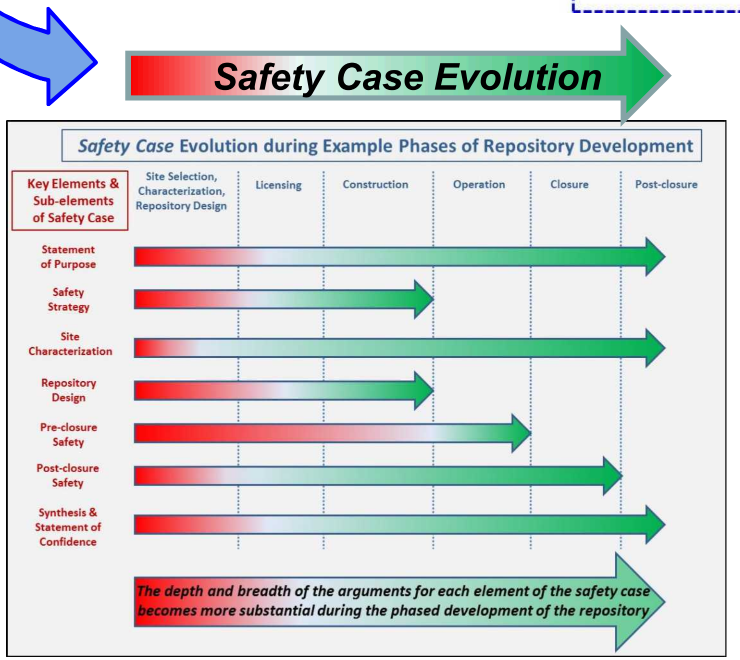


http://dakota.sandia.gov/

Role of RD&D in Evolution of the Safety Case

- **Iteration of Safety Assessment and Site Characterization/Design**





- Safety case provides a structured framework to assist in prioritizing the technical work in the next phase, to reduce uncertainties and enhance confidence
- Safety understanding and the associated technical bases evolve with phases of repository development, via RD&D

- **Calculation of concentration in each cell, $C_{i,j,k}(t+\Delta t)$**
  - i = isotope, j = element, k = phase

Initial concentrations, $C_{i,j,k}(t)$

Newton Solve

- Rate of change of concentrations $r_{i,j,k,n}$ for n time-dependent processes
  - Waste form degradation
  - Mass transport in/out
    - Advection and hydrodynamic dispersion
  - Radioactive decay/ingrowth
    - Use PFLOTRAN sandbox
- Non-equilibrated isotope concentrations at time $t+\Delta t$

$$\tilde{C}_{i,j,k}(t+\Delta t) = C_{i,j,k}\ (t) + \sum_n r_{i,j,k,n}\ \Delta t$$

Equilibrium Partitioning

- Partition isotopes among all phases
  - Aqueous
  - Adsorbed (K_d)
  - Precipitate (limited by elemental solubility)
- Assume that daughter products are not trapped within parent precipitate phases
- Isotope mole fractions within each phase are set equal to the overall isotope mole fractions within the cell

Updated concentrations, $C_{i,j,k}(t+\Delta t)$