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Waste IPSC: Thermal-Hydrologic-Chemical-Mechanical (THCM) Modeling and Simulation

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NEAMS Fall 2010 Principal Investigators' Meeting

October 19, 2010

THCM Modeling Overview

- **Waste IPSC Objective**
  - Develop an integrated suite of high performance computing capabilities to simulate radionuclide movement through the engineered components and geosphere of a radioactive waste storage or disposal system
    - *with robust thermal-hydrologic-chemical-mechanical (THCM) coupling*
    - *for a range of disposal system alternatives (concepts, waste form types, engineered designs, geologic settings)*
    - *for long time scales and associated large uncertainties*
    - *at multiple model fidelities (sub-continuum, high-fidelity continuum, PA)*
    - *in accordance with V&V and software quality requirements*
- **THCM Modeling collaborates with:**
  - Other Waste IPSC activities: Sub-Continuum Processes (and FMM), Frameworks and Infrastructure (and VU, ECT, and CT)
  - Waste Form Campaign
  - Used Fuel Disposition (UFD) Campaign
  - ASCEM

THCM Modeling Scope

- **8 preliminary repository environment categories**
  - combinations of concept and geologic setting

Group Number	Disposal Concept / Geologic Setting	Description
1	Surface Storage	Long-term interim storage at reactors or at centralized sites
2	Shallow Disposal	e.g., near-surface disposal, LTHLW sites (Depths <= 100 m)
3	Mined Geologic Disposal (Hard Rock, Unsaturated)	Granite/crystalline or tuff (Depths > 100 m)
4	Mined Geologic Disposal (Hard Rock, Saturated)	Granite/crystalline or tuff (Depths > 100 m)
5	Mined Geologic Disposal (Clay/Shale, Saturated)	Clay/shale (Depths > 100 m)
6	Mined Geologic Disposal (Salt, Saturated)	Bedded or domal salt (Depths > 100 m)
7	Deep Borehole Disposal	Granite/crystalline (Depths~ 1000 m)
8	Other	Sub-seabed, carbonate formations, etc.

THCM Modeling Scope

- **6 preliminary repository waste form / inventory categories**

Group Number	Waste Form Type	Description
1	Used Nuclear Fuel (UNF)	e.g., Commercial, DOE-Owned, HTGR
2	High-Level Waste (HLW) Glass	Current (e.g., borosilicate) and future (e.g., no minor actinides)
3	High-Level Waste (HLW) Glass Ceramic / Ceramic	Current (glass bonded sodalite) and future (e.g., from electrochemical processing)
4	High-Level Waste (HLW) Metal Alloy	From electrochemical or aqueous reprocessing, cermets
5	Lower Than HLW (LTHLW)	Class A, B, and C, and GTCC
6	Other	Molten salt, electro-chemical refining waste, etc.

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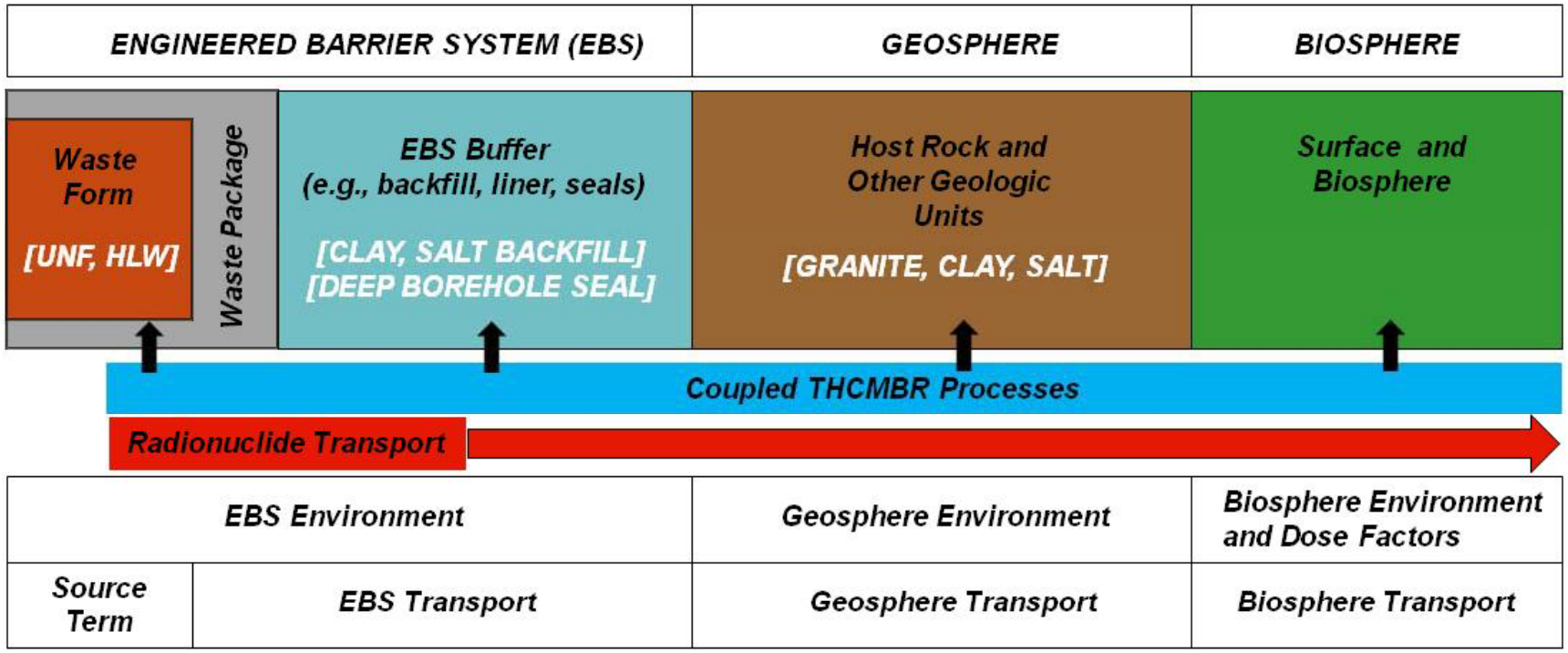
THCM Modeling Scope

- **Initial Focus on long-term disposal of UNF and HLW**
  - **20 disposal alternatives**
    - ***5 repository environments (Mined and Deep Borehole Disposal)***
    - ***4 waste forms types (UNF and HLW)***

- **Surface interim storage (for up to 300 years) being evaluated by UFD**
  - Is being added to Waste IPSC scope

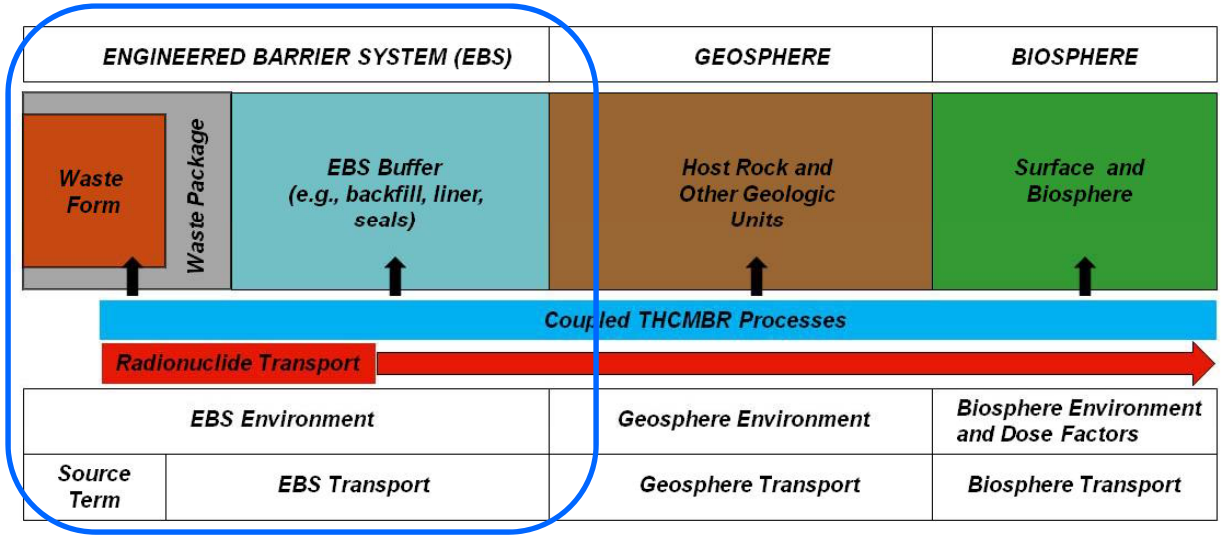
THCM Modeling Scope

- **1D schematic of generic disposal system domains and phenomena**
  - Informed by feature, event, and process (FEP) analysis
  - Applicable to a range of disposal system concepts
  - Applicable to high-fidelity continuum scale and to PA scale models



THCM Modeling Scope

- **Initial Focus on coupled THCM processes in the EBS (and adjacent near-field host rock)**
  - Radionuclide Source Term
    - *WF degradation, interaction with EBS environment, radionuclide solubility*
  - Radionuclide Transport in EBS
    - *advection, diffusion, sorption of dissolved and colloidal radionuclides*
  - EBS/Near-Field Environment
    - *temperature, fluid movement, fluid chemistry, component degradation*

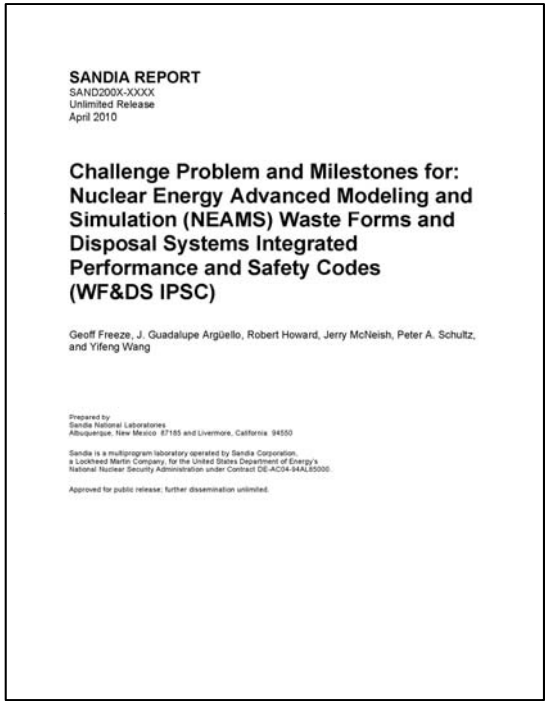


THCM Modeling
FY10 Accomplishments

- **Specification of Challenge Problem**
  - 5 challenge milestones
    - *Storage milestone to be added*
  - 1 disposal alternative
    - *HLW glass in Mined salt*

	Milestone	Source Term	Near-Field Environ-ment	Near-Field Transport
1	Chemical Equilibrium Calculation	T=C	T=C	N/A
2	HLW Glass Degradation	T=H=C=M	T=H=C	N/A
3	Tunnel Closure (Salt Creep)	N/A	T=M-H	N/A
4	Heat and Fluid Movement in the EBS and Salt	N/A	T=H=C	N/A
5	Radionuclide Mobilization and Transport in the EBS and Salt	T=H=C=M	T=H=C=M	T=H=C=M

Note: Strong multi-physics coupling is represented by =;
Weak multi-physics coupling is represented by -


SANDIA REPORT
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April 2010

Challenge Problem and Milestones for: Nuclear Energy Advanced Modeling and Simulation (NEAMS) Waste Forms and Disposal Systems Integrated Performance and Safety Codes (WF&DS IPSC)

Geoff Freeze, J. Guadalupe Argüello, Robert Howard, Jerry McNeish, Peter A. Schultz, and Yifeng Wang

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

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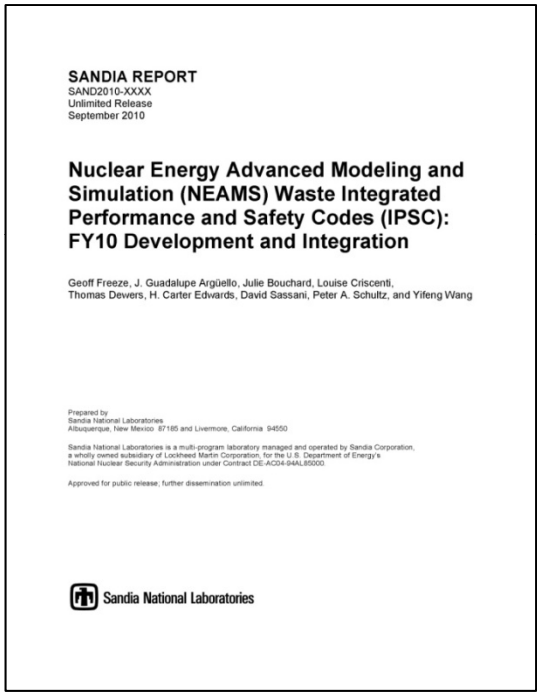
THCM Modeling
FY10 Accomplishments

- **Specification of THCM Code Capabilities**
  - Sub-Continuum Processes
    - *HLW Glass Degradation*
  - Continuum Processes
    - *THC Processes (Reactive Transport)*
    - *TM and THM Processes (Salt Creep)*
  - Frameworks and Infrastructure
- **Gap Analysis**
  - THC and THM codes that can be applied to both high-fidelity-scale and PA-scale



SANDIA REPORT
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September 2010

Nuclear Energy Advanced Modeling and Simulation (NEAMS) Waste Integrated Performance and Safety Codes (IPSC): FY10 Development and Integration

Geoff Freeze, J. Guadalupe Argüello, Julie Bouchard, Louise Criscenti, Thomas Dewers, H. Carter Edwards, David Sassani, Peter A. Schultz, and Yifeng Wang

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THCM Modeling FY11 Activities

- **Gap analysis of THCM code capabilities**
  - Expand and refine FY10 gap analysis
  - Level 3 deliverable – March 2011

- **Development and integration of THCM code capabilities to apply to challenge problem milestones**
  - Code selection informed by gap analysis
  - THC modeling (complete milestone #1, initiate milestones #2 and #4)
  - THM modeling (initiate milestone #3)
  - at high-fidelity continuum scale and PA scale
  - Level 2 deliverable – September 2011

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THCM Continuum Modeling – Needs

- **Basic thermal, hydrological, chemical, (i.e., reactive transport) and mechanical capabilities are needed**
- **For HLW glass in mined salt (as well as for other disposal options), the mechanical effect will be significant**
- **Waste IPSC problems will likely result in relatively large computational models, implying a need for:**
  - compact memory-usage footprint
  - fast/robust solution procedures
  - robust massively parallel processing (MPP) capability
- **Waste IPSC problems entail multiple physics, hence an effective and robust framework to allow efficient coupling of various physics is needed**
  - assortment of time-stepping and physics-coupling algorithms
  - permit physics of disparate time-scales and length scales to be solved efficiently

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THCM Continuum Modeling – Preliminary Code Assessment

- Conducted a preliminary assessment of several existing high-fidelity simulators for use in modeling THCM coupled processes
- Preliminary assessment performed on basis of limited available public information
- May be other capability available in the simulators that was not listed in those sources; hence not included or acknowledged
- Intent is to acquire various simulators in the near-future and perform a more complete hands-on assessment
- Said assessment may change the outcome of our preliminary assessment discussed here

THC Continuum Modeling – Preliminary Code Assessment – TOUGHREACT

- **Nmerical simulation program for chemically reactive non-isothermal flows of multiphase fluids in porous and fractured media**
- **Developed by introducing reactive chemistry into the multiphase flow code TOUGH2 V2**
- **Gas phase is considered active for multiphase fluid flow, species transport, and chemical reactions**
- **Applicable to porous media as well as to fractured rocks**
- **Integral finite difference (IFD) technique is employed for space discretization**
- **Non-isothermal effects are considered, including**
  - water-vapor phase change and air partitioning between the liquid and gas phases,
  - temperature-dependence of thermophysical properties such as phase density and viscosity, and chemical properties such as thermodynamic and kinetic parameters.
- **Chemical reactions considered under the local equilibrium assumption include**
  - aqueous complexation,
  - acid-base,
  - Redox,
  - gas dissolution/exsolution,
  - cation exchange, and
  - surface complexation
- **Mineral dissolution/precipitation can proceed either subject to local equilibrium or kinetic conditions**
- **Applicable to one-, two-, or three-dimensional geologic domains with physical and chemical heterogeneity**
- **Can be applied to a wide range of subsurface conditions**
  - Temperature can range from 0 to 300 0C, limited at present by available geochemical databases such as EQ3/6
  - Pressures can be from 1 bar (atmospheric pressure) to several hundred bars (at several thousand meter depth)
  - Water saturation can range from completely dry to fully water saturated
  - Can deal with ionic strength from diluted to saline waters with up to 6 mol/kg H2O for NaCl dominant solution

THCM Continuum Modeling – Preliminary Code Assessment – FEHM

- Numerical simulation code for subsurface transport processes
- Models 3-D, time-dependent, multiphase, multi-component, non-isothermal, reactive flow through porous and fractured media
- Flow of gas, water, oil and heat
- Flow of air, water, and heat
- Flow of CO2, water, and heat
- Simulation of gas hydrates
- Multiple chemically reactive and sorbing tracers
- Finite element/finite volume formulation
- Coupled stress module
- Saturated and unsaturated media
- Preconditioned conjugate gradient solution of coupled linear equations
- Fully implicit, fully coupled Newton Raphson solution of nonlinear equations
- Double porosity and double porosity/double permeability capabilities
- Complex geometries with unstructured grids

THC Continuum Modeling – Preliminary Code Assessment – STOMP

- Fundamental purpose is to produce numerical predictions of thermal and hydro-geologic flow and transport phenomena in variably saturated subsurface environments contaminated with volatile or non-volatile organic compounds
- Simulator utilizes a variable source code configuration, which allows the execution memory and speed be tailored to the problem specifics
- Predictions of solute transport processes including reactive transport
- Quantitative predictions generated from the numerical solution of PDEs that describe subsurface environment transport phenomena
- Description of subsurface environment is founded on governing conservation equations and constitutive functions
- Governing coupled flow equations are PDEs for the conservation of water mass, air mass, CO_2 mass, CH_4 mass, volatile organic compound mass, salt mass, and thermal energy
- Constitutive functions relate primary variables to secondary variables
- Solution of the governing PDEs occurs by the integral volume finite difference method
- The governing equations that describe thermal and hydrogeologic flow processes are solved simultaneously using Newton-Raphson iteration to resolve the non-linearities in the governing equations
- Governing transport equations are PDEs for the conservation of solute mass
- Solute mass conservation governing equations are solved sequentially, following the solution of the coupled flow equations

THCM Continuum Modeling – Preliminary Code Assessment – SIERRA

- **Goal is the development of massively parallel multi-physics capabilities to support the SNL engineering sciences mission**
- **Designed and developed from its inception to run on the latest and most sophisticated massively parallel computing hardware**
- **Foundational toolkit provides code services such as:**
  - mesh and field data management, both parallel and distributed,
  - transfer operators for mapping field variables from one mechanics application to another,
  - a solution controller for code coupling, and
  - included third party libraries (e.g. solver libraries, MPI communications package, etc.)
- **Code suite is comprised of application codes that address specific physics regimes**
  - thermal and fluid mechanics analysis codes
  - solid mechanics and structural dynamics codes
  - and software development tools used by the SIERRA Mechanics codes for configuration management, software builds, and release management.
- **The two SIERRA Mechanics codes which are used in the THCM coupling are SIERRA/FD (Aria) and SIERRA/SM (Adagio)**
- **The suite of physics currently supported by SIERRA/FD (Aria) includes**
  - the incompressible Navier-Stokes equations
  - the energy transport equation
  - species transport equations
  - generalized scalar, vector and tensor transport equations
  - A saturated porous flow capability is a recent addition
  - multiphase porous flow is under development
  - some basic geochemistry functionality available through existing chemistry packages such as Chemeq and Cantera.
- **The solid mechanics portion of the THCM coupling is handled by SIERRA/SM (Adagio) which solves for the quasistatic, large deformation, large strain behavior of nonlinear solids in three-dimensions**
  - has some discriminating technology that has been developed at SNL for analyzing problems in solid mechanics
  - involves the use of matrix-free iterative solution algorithms that allow extremely large and highly nonlinear problems to be solved efficiently
  - technology also lends itself to effective and scalable implementation on massively parallel computers
- **The THCM coupling is done through a solution controller within SIERRA Mechanics called Arpeggio**

THCM Continuum Modeling – Preliminary Code Assessment – Conclusions

- **Simulators have significant, but varying degrees, of capability in terms of reactive transport, from fledgling (SIERRA) to advanced (TOUGHREACT)**
- **Lack of complete coupling of mechanical capability in all but one (SIERRA)**
  - TOUGH+/Hydrate variant coupled to a commercial geomechanics (FLAC) code, but unknown if this coupling extends to TOUGHREACT
  - FEHM website lists “coupled stress module” but not clear what behavior this module is capable of modeling on mechanical side
  - SIERRA suite of codes designed to seamlessly permit multiple physics to be coupled (has been demonstrated)
- **Capability of the codes to perform in a MPP environment is unclear in all but one case (SIERRA)**
  - TOUGH2-MP available and intended for large-scale, high-performance simulations, but unclear if this capability extends to TOUGHREACT
  - An effort in this direction may be underway for FEHM, based on “research priorities” identified in a Zyvoloski publication
  - MPP capability designed and developed into SIERRA from its inception (has been demonstrated)

THM Modeling – Coupled Processes

- **Thermal processes**
  - Decay heat
  - Geothermal gradient (deep borehole disposal)
  - Conduction
  - Convection
  - Radiation

- **Mechanical processes**
  - Quasi-static
  - Large strain/deformation
  - Inelastic material response (e.g., creep, plasticity, cap-plasticity, etc.)
  - Contacting surfaces
  - Fracturing
  - Fracture healing
  - Consolidation/re-solidification

- **Hydrologic processes**
  - Multiphase flow
    - *Unsaturated flow*
  - Boiling & condensation
  - Density flow
  - Darcy's flow
  - Fracture flow
  - Open channel flow
  - Density flow
  - Advection & diffusion

- **Chemical processes**

Reactive transport

THM Modeling – Coupled Processes

- **Tunnel closure due to salt creep (Milestone #3)**
  - Near-field salt (roof, ribs, floor) large strains/deformations, damage/healing, mechanical (& thermal) contact during large deformations, backfill consolidation/re-solidification, etc.
  - Creep of salt is highly temperature-dependent; creep rate will be accelerated due to heat load induced by HLW
  - Heat load will cause movement/migration of moisture in tunnel, backfill, EDZ, surrounding salt and other geologic strata

- **Demonstration using SIERRA**
  - Coupled TM simulation of salt creep

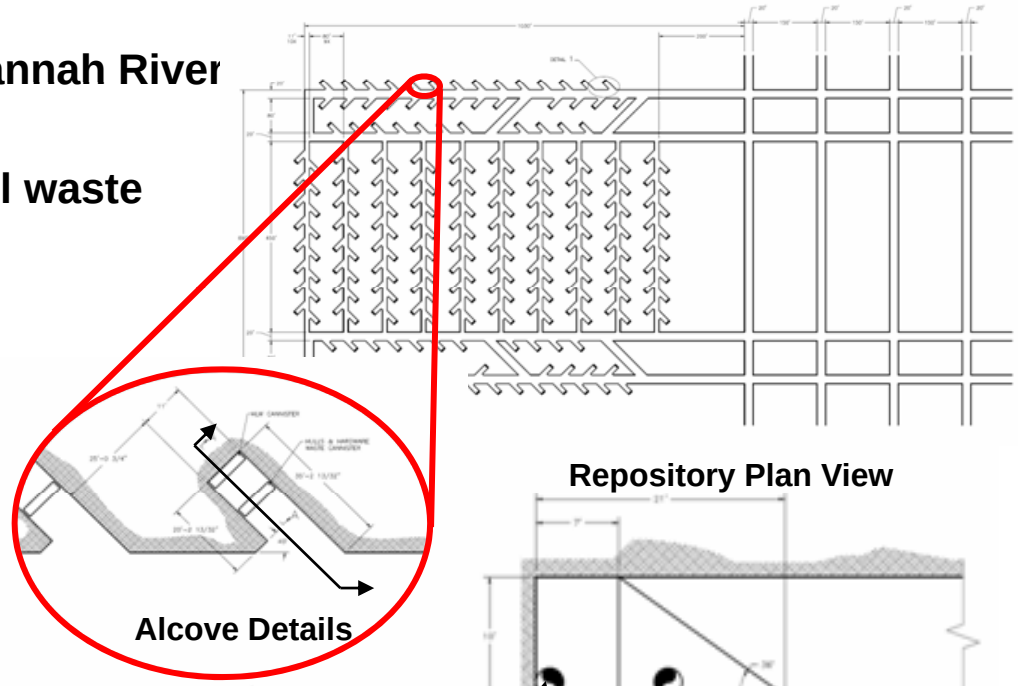
Demonstration: Coupled Thermal-Mechanical Simulation of Generic Salt Repository

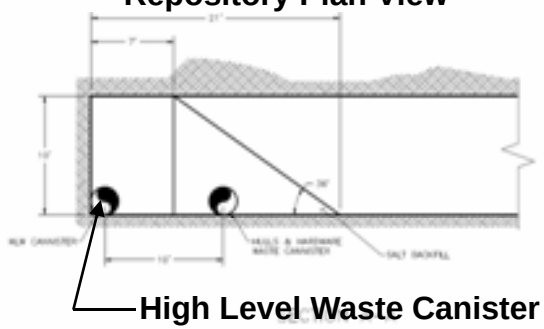
Sample Geometry:

- Configuration based on a 2008 Savannah River study
- Vitrified borosilicate glass high level waste canister with output 8.4 kW

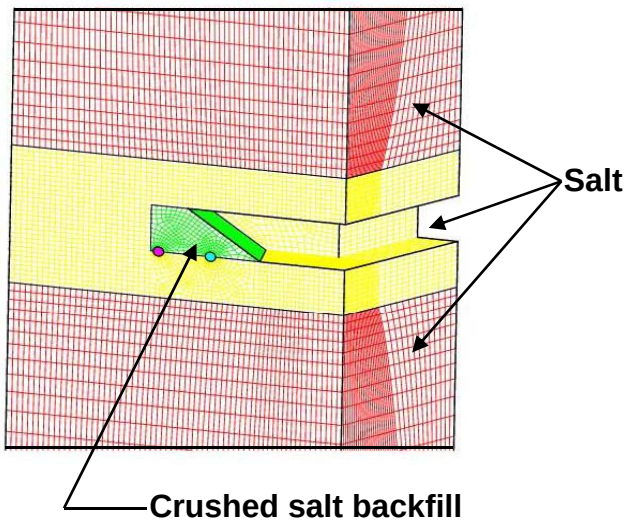
Technical challenges:

- High Thermal Gradients
- Temperature dependent material properties
- Large Deformation Salt Creep behavior
- Contact modeling with heat conduction and load transfer
- Long duration simulation to room closure





Demonstration: Coupled Thermal-Mechanical Simulation of Generic Salt Repository (Cont'd)



- Three-dimensional fully coupled thermal/mechanical analysis
- Massively Parallel Calculation - 96 processors
- Dissimilar meshes and domains for thermal and structural mechanics
- Contact surfaces used for both thermal and structural problems

Thermal Analysis Features:

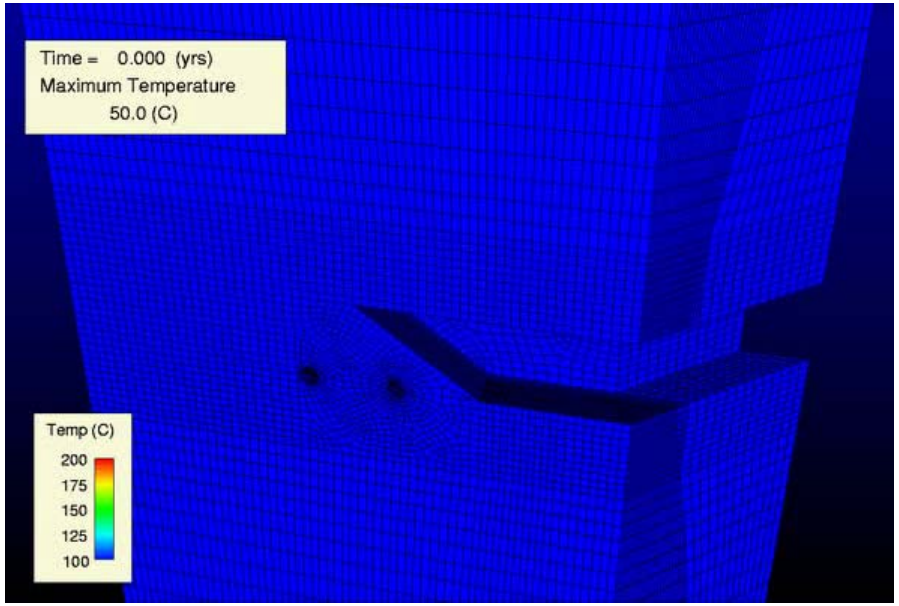
- 904736 nodes / 864927 elements
- Contact surfaces used to accommodate heat conduction between contacting surfaces (alcove and haulage way)
- Re-computation of radiation view factors for deforming heated room surfaces

Structural Analysis Features:

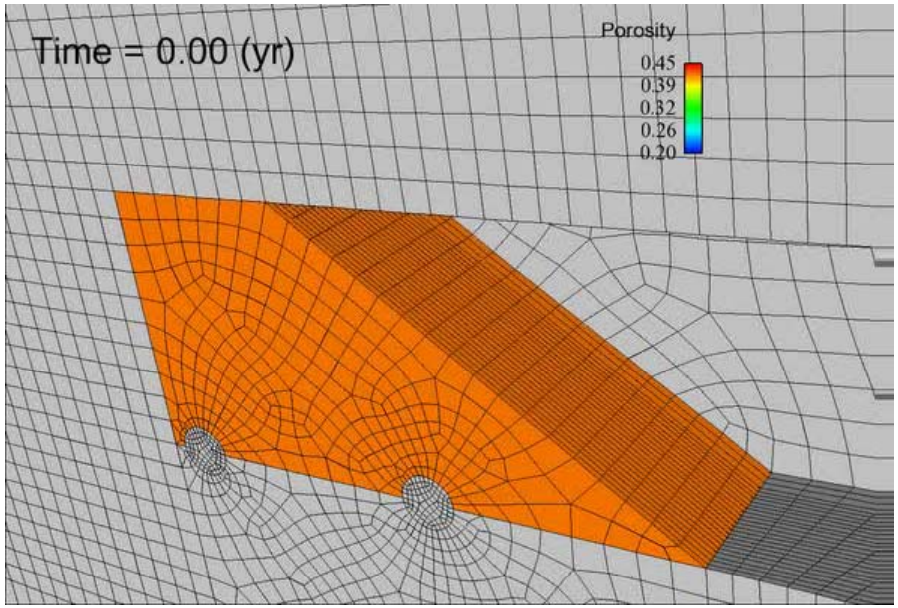
- Quasistatic analysis with 294698 nodes / 279537 elements
- Large deformation, large strain formulation
- Nonlinear power law secondary creep model for salt
- Volumetric compaction model for the crushed salt
- Contact surfaces defined to allow arbitrary roof, rib, and floor contact
- Temperature dependent material properties

Demonstration: Coupled Thermal-Mechanical Simulation of Generic Salt Repository (Cont'd)

- Maximum salt temperature 407 C (canister/salt interface)
- Haulage way floor/ceiling contact at 21 years
- Closure modes are different for haulage way and alcove
- Full closure predicted by 27 years
- Minimum crushed salt porosity at 27 years 12.4% (original 42%)



Repository Temperature Contours



Crushed Salt Backfill Porosity Contours

THC Modeling – Coupled Processes

- **Thermal processes**
  - Decay heat
  - Geothermal gradient (deep borehole disposal)
  - Conduction
  - Convection
  - Radiation

- **Mechanical processes**

- **Hydrologic processes**
  - Multiphase flow
    - *Unsaturated flow*
  - Boiling & condensation
  - Density flow
  - Darcy's flow
  - Fracture flow
  - Open channel flow
  - Density flow
  - Advection & diffusion

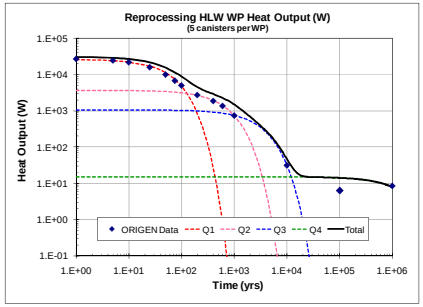
Reactive transport

- **Chemical processes**
  - Phase transition
  - Dissolution & precipitation
  - Waste form degradation
  - Waste package corrosion
  - Backfill reactions
  - Chemical speciation
  - Redox reactions
  - Radiolysis
  - Radionuclide sorption
  - Colloid generation & suspension
  - Microbial reactions
  - Radionuclide decay & ingrowth

THC Modeling – Mathematical Formulation

Heat transfer

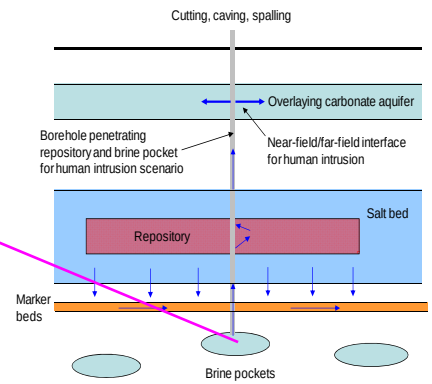
$$\frac{\partial}{\partial t}\left[(1-\phi)\rho_s e_s + \phi(\rho_l S_l e_l + \rho_g S_g e_g)\right] + \vec{\nabla}\bullet\vec{\mathbf{q}}_e = Q_e$$



Flows

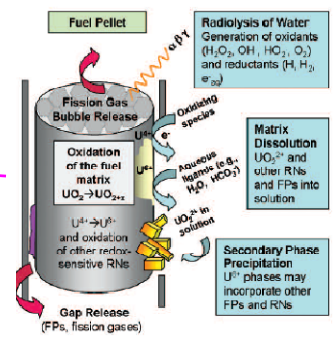
$$\frac{\partial}{\partial t}\phi(Y_{il}\rho_l S_l + Y_{ig}\rho_g S_g) + \vec{\nabla}\bullet(Y_{il}\rho_l\vec{\mathbf{v}}_l + Y_{ig}\rho_g\vec{\mathbf{v}}_g - \vec{\mathrm{J}}_{ig}) = Q_i$$

$$\vec{\mathbf{v}}_j = -\frac{k_{rj}}{\mu_j}k\bullet(\vec{\nabla}P_j + \rho_j\vec{\mathbf{g}})$$



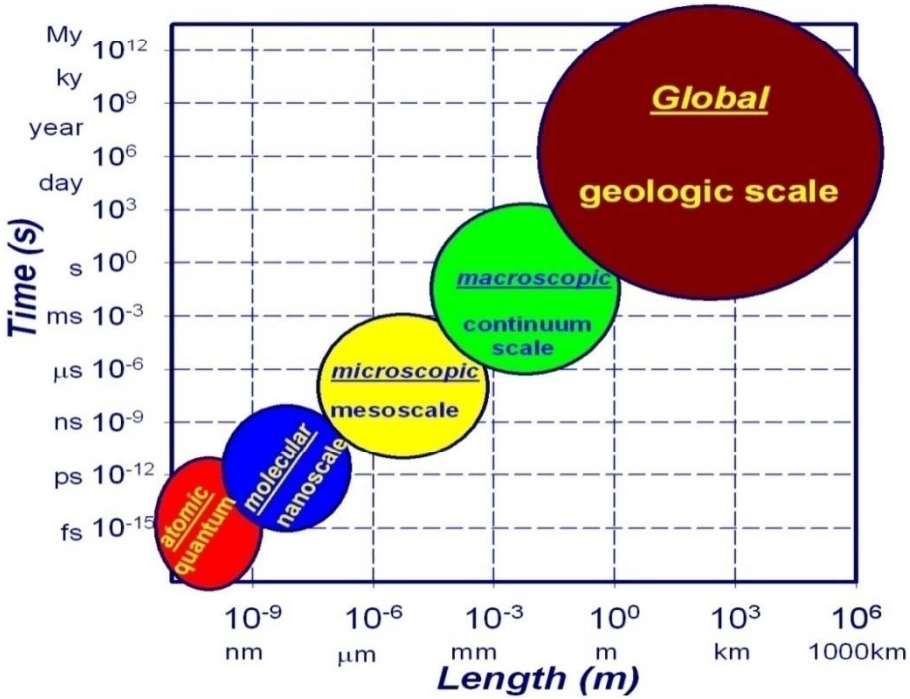
Reactive transport

$$\frac{\partial}{\partial t}\left(\phi s_{\pi_i} c_i\right) + \vec{\nabla}\cdot\vec{J}_i = \sum_{r=1}^{N_r}\upsilon_{ir} I_r \quad (i = 1,\ldots N)$$



THC Modeling - Complexity

- **Time scales**
  - Regulatory time scale: Up to 1 million years
  - Laboratory measurements & field observation: mostly days or shorter, at best decades
  - Disparity in reaction rates
- **Spatial scales**
  - Nanometers to kilometers
  - Heterogeneity of geologic media/repository configuration
  - Scale-dependent properties (e.g., matrix diffusion coefficients, reaction rates)
- **Initial conditions**
  - Different waste forms
  - Different radionuclide inventories
- **Boundary conditions**
  - Different disposal environments



THC Modeling – Preliminary Gap Analysis

- **Identification of specific functional requirements**
  - Dimensions
  - Flow types
  - Thermal calculation
  - Number of chemical components for transport
  - Types of chemical reactions
  - Activity calculations
  - Types of sorption models
  - Numerical solvers
  - Meshes
- **Literature survey of the existing codes**
- **Comparison of the existing codes against the identified functionalities**
- **Identifying gaps**

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THC Modeling – Preliminary Gap Analysis – Reactive Transport Codes (partial list)

Table A-1. Reactive Transport Codes with THC Capabilities Potentially Relevant to the Waste IPSC

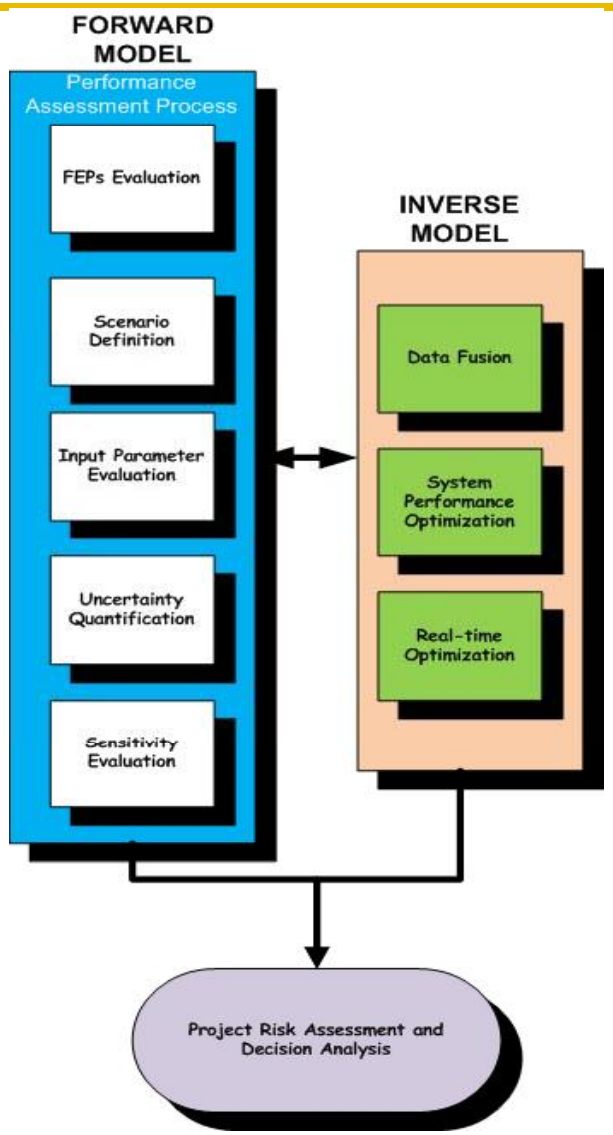
Model Name	Dim.	Processes and Approaches							Activity models	Sorption models	Solver Appr.	Num. Meth.	Notes
		Flow	Ther-mal	Chem. Tran-sport	Reactions								
					Aq. Com-plex	Sorp	P/D	Bio					
CRUNCH	2D/ 3D	VF	Yes	MC	EQ	EQ	KI	Yes	extended Debye-Huckel	DLM, NEM, IE	DSA, SIA	IFV	Based on codes OS3D and GIMRT. Implements radioactive decay chains. OS3D simulations are up to 3D and implement SIA; GIMRT simulations are up to 2D, and implement DSA (global implicit). Restricted to orthogonal grids.
FEHM (LANL)	1D/ 2D/ 3D	MF, VF	Yes	MC*	EK*	Emp.	KI	Yes[d]	All activities assumed to be unity?	LI and NLI, with kinetics	?	CVFE	Uses particle tracking to model transport. *Up to 10 solutes with chemical reactions between each. Reactions can be kinetic (e.g., biodegradation).
FEMWATER (WES)	3D	VF	No	SC	No	Emp	No	KI	N/A	LI, NLI	SIA	FE/ FE-LE	
FRACHEM (CGR)	3D	SF	Yes	MC	EQ	No	EK	No	Pitzer	N/A	SNIA	FE	Based on CHEMTOUGH2 (chemistry) and FRACTure (flow in fractured, porous rock)
GeoSysBRNS (Centler et al. 2010)	1D/ 2D/ 3D	MF, VF	Yes	MC	EK?	EK?	EK	EK	?	?	SNIA	FE	Couples Biogeochemical Reaction Network Simulator (BRNS) with GeoSys, a THM flow and transport simulator. Current version does not account for changes in porosity due to mineral prrecipitation. Parallel version available.
GWB professional	1D/ 2D	No*	Yes	MC	EK	?	EK	?	Debye Huckel, Pitzer	?	?	?	*Flow fields imported as a table or from MODFLOW
HYDROGEOCHEM 4.1/5.1	2D/ 3D	VF	Yes	MC	EK	EK	EK	EK	Davies equation, and ?	CCM, DLM, TLM	DSA, SIA	FE, FE-LE	Version 4.1 is 2D; version 5.1 is 3D. These versions of HYDROGEOCHEM appear to incorporate all capabilities of earlier versions, as well as of of the codes developed in parallel (LEHGC, HYDROBIOGEOCHEM and HGBC123). Note that (1) applications are limited to single fluid phase flows and (2) dual-porosity media cannot be effectively dealt with.
HYDRUS (2D/3D)	2D/ 3D	VF	Yes	MC	No*	Emp-KI	No	Yes[d]	N/A	EI; LI and NLI; uses two-site sorption (fast-slow) for sorption kinetics	SNIA	FE	Includes colloidal transport.

THC Modeling – Preliminary Gap Analysis – Conclusions

- **Total 38 codes surveyed**
- **Existing capabilities and gaps**
  - Existing codes have significant capabilities in THC modeling, which can be leveraged for the waste IPSC.
  - No single existing code is able to take into account all physical chemical processes involved in the near-field of a disposal system.
  - Historically, most reactive transport codes have been developed by ad hoc marriage of hydrological codes with chemical reaction codes. A code that emphasizes equally on both flows and chemical reactions and fully accounting for their couplings needs to be further developed.
  - Functions needed for waste IPSC are scattered in various codes. Coupling these functions by simple code linkage (usually called stove-pipe approach) may not be adequate for disposal system performance assessments. The mechanism for seamless coupling of multiple physics is still lacking.
  - Very few reactive transport codes are finite-element-based, which makes the coupling of these codes to flow or mechanical codes inherently difficult.
  - Most of existing reactive transport codes were developed for non-radioactive contaminants, and they need to be adapted to account for radionuclide decay and ingrowth.
  - Massively parallel processing (MPP) capability is lacking for many reactive transport codes.
  - Numerical robustness (e.g., compact memory-usage footprint and fast/robust solution procedure) of existing codes are not fully demonstrated.
  - Some important supporting technical data are not available, especially those for extreme chemical and physical environments.

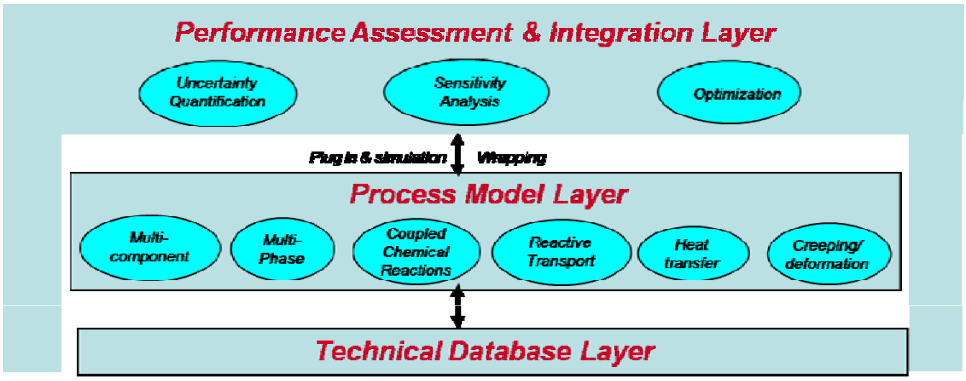
PA Methodology

- **PA intends to answer**
  - Scenario identification – What can happen?
  - Likelihood of scenarios – How likely is it to happen?
  - Consequences of scenarios – What are the consequences if it does happen?
  - Credibility – How much confidence do we have in the answers to the first three questions?

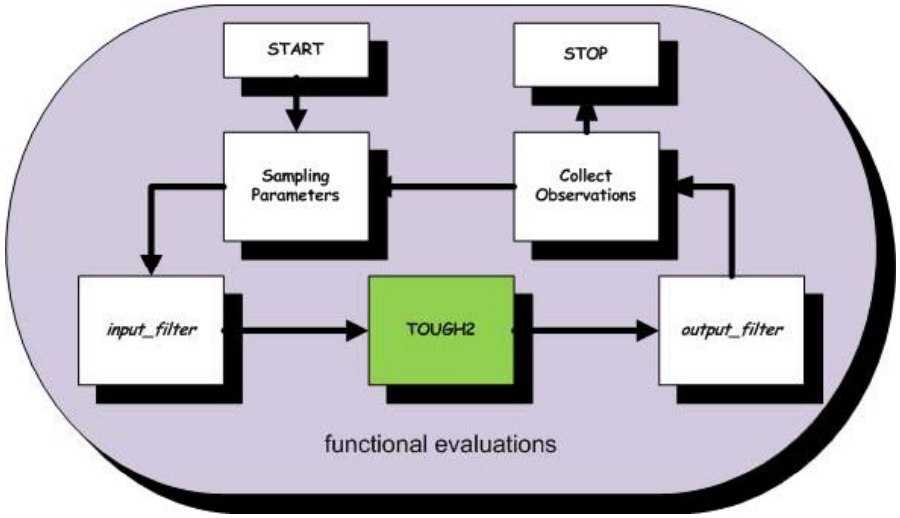


PA Methodology: Example Architecture

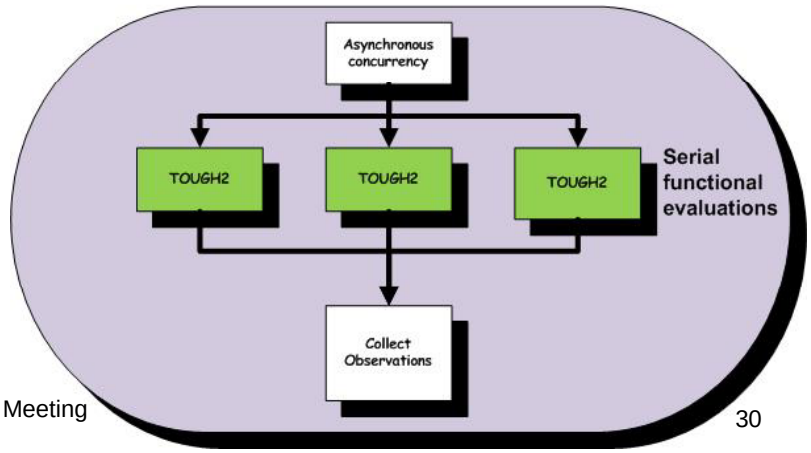
- **Enhanced PA system (EPAS) for CO_2 sequestration (Wang et al. 2010)**
  - DAKOTA (Design Analysis Kit for Optimization and Terascale Applications) is used as a PA driver.
  - TOUGH2 is chosen as a reservoir simulator.



DAKOTA SAMPLING SCHEME

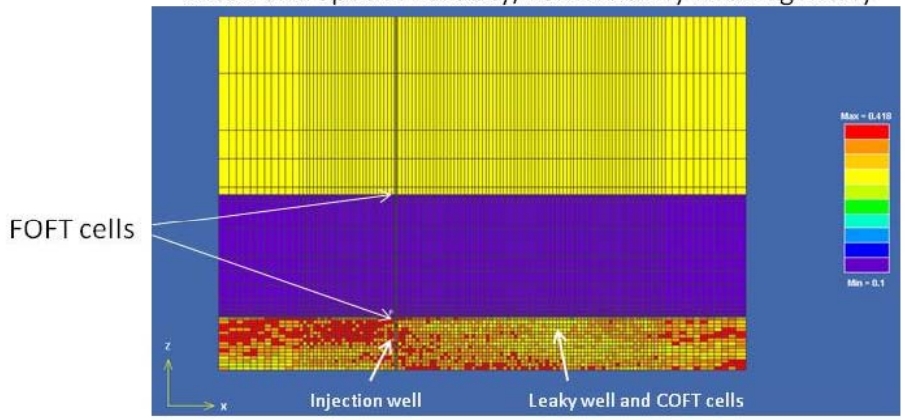


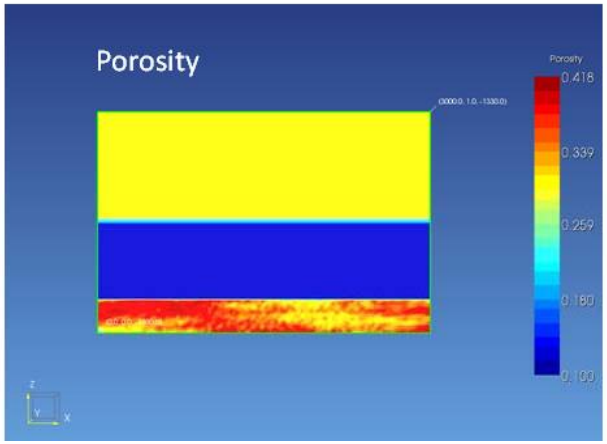
DAKOTA – TOUGH2
HYBRID PARALLELISM

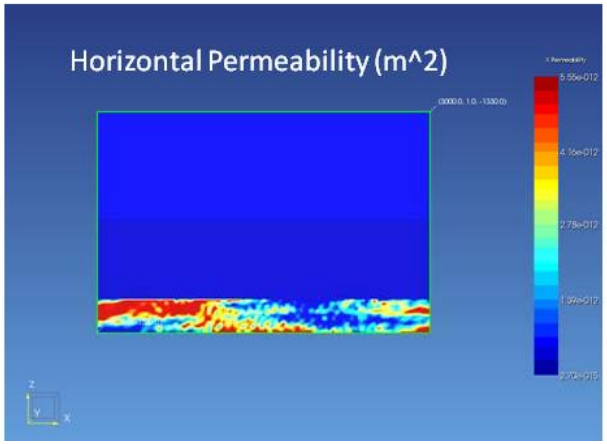


PA Model Setup: Meshing and Hydrologic Heterogeneity

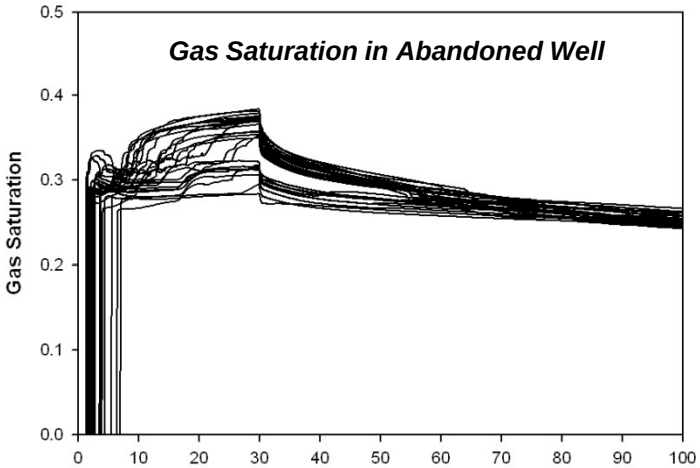
Mesh and Spatial Porosity/Permeability Heterogeneity

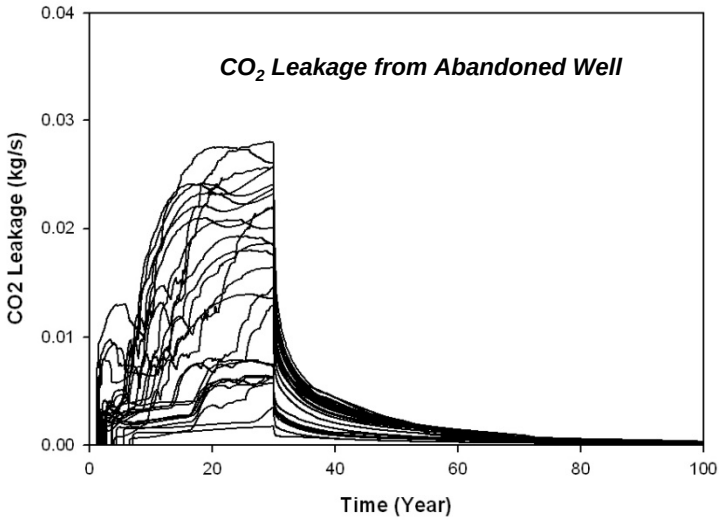


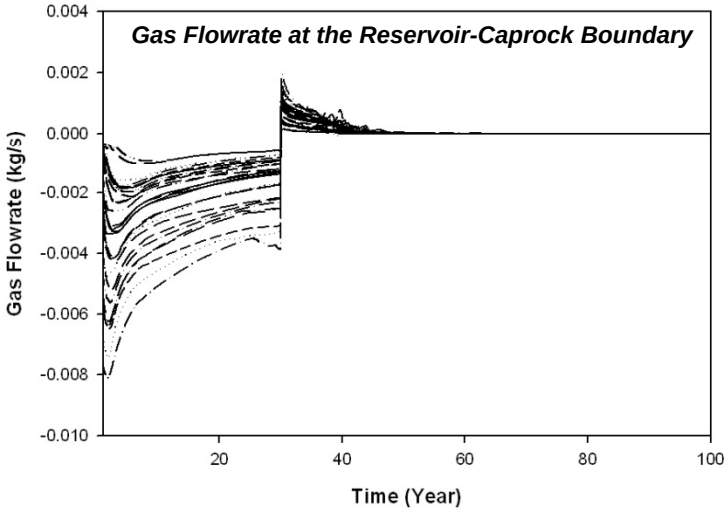


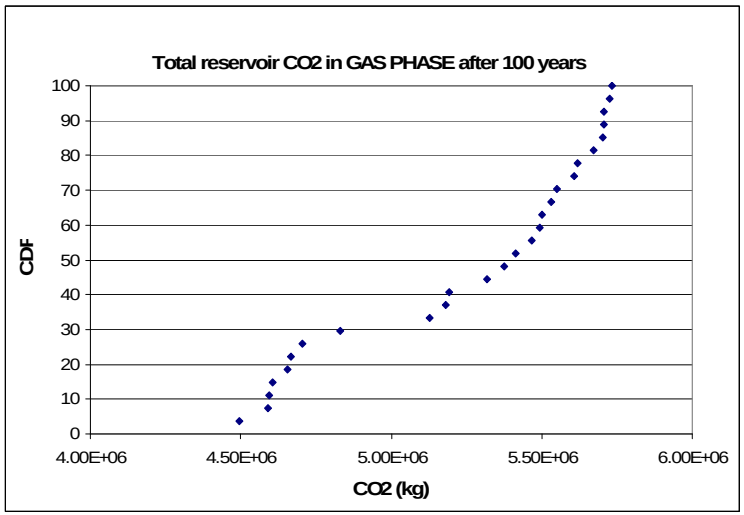


PA Simulation Results: Multiple Realizations









PA Code Requirements

- **Process codes**
  - Robust numerical schemes
    - *27 of 30 realizations succeeded for EPAS CO_2 sequestration*
  - Reasonable computational time
    - *~ 4 hours for each realization on 1 processor*

- **PA driver (DAKOTA)**
  - Statistical sampling
  - Multiple realizations
  - Code coupling/linking
  - Uncertainty quantification
  - Sensitivity analysis
  - Optimization

- **Credibility of PA results**
  - Time scale
  - Extrapolation vs. interpolation
  - Mechanistic vs. empirical models
  - Dangers of over-simplification or abstraction
    - *Internal consistency*
    - *Meaningful sensitivity analysis*
  - Facilitating public communication

- **Backup Slides**

THC Modeling - Needs

- **Continuum THC models should be able to**
  - **Capture relevant thermal, hydrologic and chemical processes, features & events (FEPs)**
    - *Different disposal environments*
  - **Allow seamless couplings among different processes**
    - *THCM*
    - *Flexibility for couplings (e.g., modular structures)*
  - **Be validated for the models and model input parameters**
    - *Reliable constitutive models*
    - *Chemical parameters for elevated temperatures*
  - **Accommodate various computational needs**
    - *From simple FEP screening calculations to total system analyses*
    - *Optimization of disposal system design*
  - **Efficiently simulate multiple temporal & spatial scale processes**
    - *Numerical stiffness related to moving reaction fronts*
    - *Computational time*
  - **Capture specific features related to radionuclide release and migration**
    - *Radionuclide decay & ingrowth*

Interfaces Between UFD and NEAMS Radioactive Waste Models

- **UFD Model Timeline**
- **Short time horizon (2-3 yrs)**
  - Simplified generic system models (i.e., PA-fidelity)
  - Current computing capabilities
  - Minimal multi-physics coupling
  - Sufficient for scoping studies and high-level comparison of options
- **Intermediate time horizon (~5 yrs)**
  - More advanced system models developed in parallel with NEAMS WF IPSC
- **Long time horizon (~10 yrs)**
  - Mature models based on NEAMS WF IPSC experience

- **R&D (UFD and NEAMS)**
  - Informs process and PA model development

- **NEAMS Waste IPSC Timeline**
- **Long time horizon (~ 10 yrs)**
  - Fully coupled multi-physics (THCMBR) models from first principles (i.e., high-fidelity)
  - PA-fidelity system model abstracted from high-fidelity model
  - Advanced high-performance computing capabilities
  - Models capable of detailed analyses of a range of disposal options, sufficient for licensing