SAND2011-4715C

Used Fuel Disposition Campaign

FY11 YTD Status Update
Disposal Research (DR) Control Account

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Wasteforms/Used Fuel Disposition Working Group

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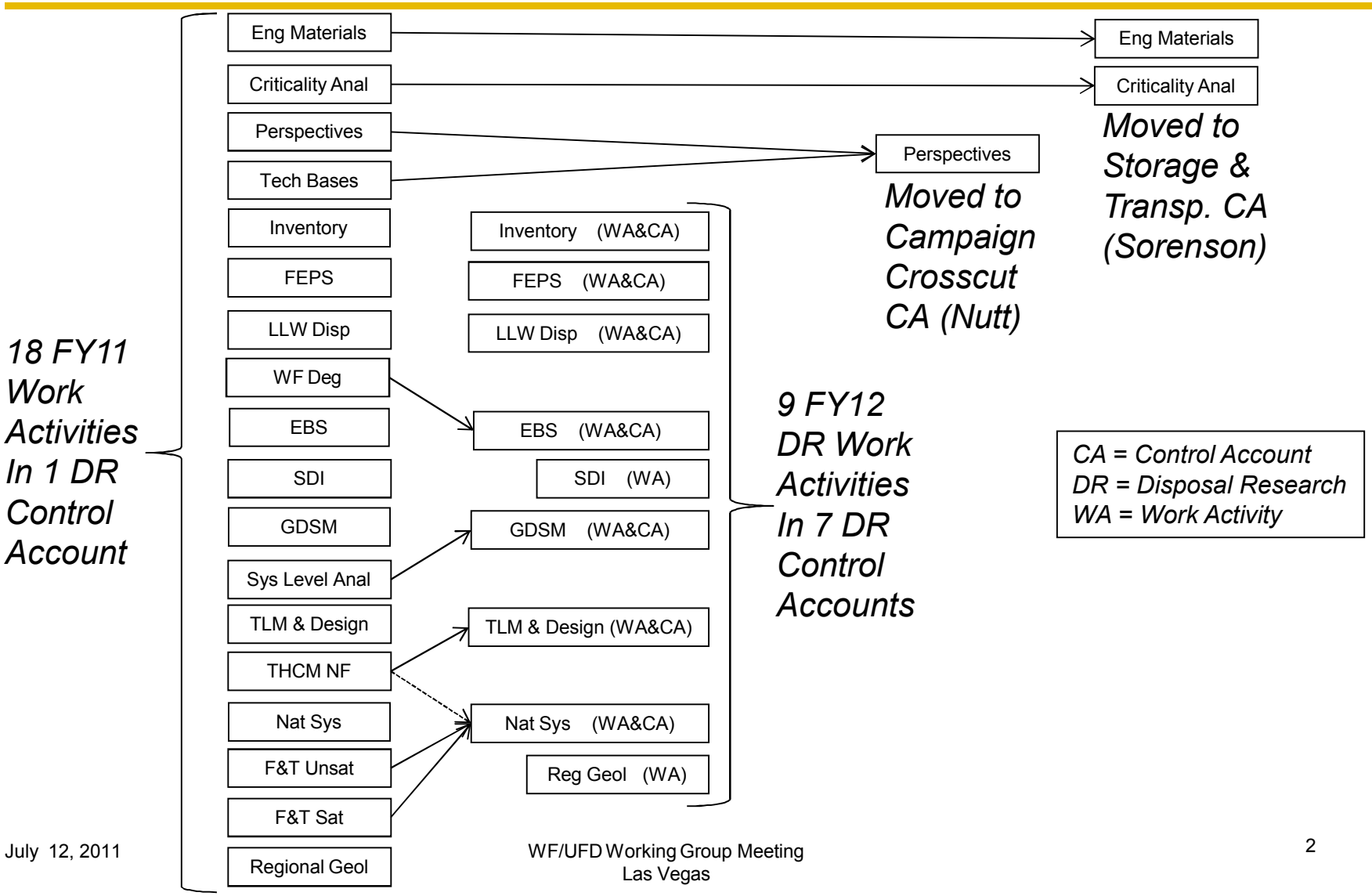
Used Fuel Disposition

UFD Disposal Research
FY11 vs. FY12 Work Activity Structure



Used Fuel Disposition

Generic Disposal System Modeling (GDSM) Accomplishments

- **Completed GDSM work Plan.**
- **Completed first iteration generic models for clay, granite, salt, and deep borehole repository concepts for incorporation into the Generic Performance Assessment Model (GPAM).**
- **Initiated development of the GPAM.**
  - *Identified common model components and parameters from each of the 4 generic models*
  - *Began development of the integrated GPAM model and data input structure in GoldSim.*
  - *Tested GoldSim capabilities of contaminant transport using test problems.*
- **Developed schedule and annotated outline for Level 2 milestone report**
- **Initiated Level 4 milestone reports for 4 individual generic models and diffusion process in clay. These are feeds to the level 2.**
- **Initiated a generic repository design concept and EBS model architecture for ultimate use in the GPAM.**
  - *Tabulated design parameters for the 4 repository types.*
  - *Identified modularity in parameters and functions/processes.*
- **Completed FEPs mapping work plan and mapping tool and imitated mapping**

Generic Disposal System Modeling Future Plans

- Complete Level 4 milestone reports (7/11/2011): 4 generic model descriptions; feeds Level 2 report.
- Complete level 2 milestone report (8/11/2011): GPAM description.
- Exercise/Benchmark the 4 generic models to demonstrate capability and confidence building. Document in Level 4 reports.
- Initiate sensitivity analyses using the clay and granite repository model options.
- Document generic repository design concept and EBS model architecture in Level 2 report.
- Finalize FEPs mapping on first iteration generic models. In Level 2 report.
- Complete first iteration of GPAM development.
- Initiate Generic PA Model Safety Case by developing safety case strategies and considering international guidance.

System Level Analysis Accomplishments

- **Initiated development of external computational database for GPAM.**
  - Completed database work plan.
  - Developed requirements and architecture for computational database.
  - Developed integrated parameter list based on first iteration models.
  - Implemented interim Excel database version for initial use.
- **Completed development of LHS sampling software (broader capabilities, more robust, input from external database).**
  - Tested stand-alone version.
  - Converted to dll for interface to GPAM and database.
  - Developed linkage for GPAM/database interface.

Systems Level Analysis Future Plans

- **Continue development of external database:**
  - Refine requirements
  - Populate with parameters for GPAM
- **Implement first iteration of configuration management to support model calculations and sensitivity analyses.**
- **Initiate development of structure and process for results archiving .**
- **Complete separation of aleatory and epistemic uncertainty in sampling software.**
- **Complete L4 milestone report for sampling software: (6/30/2011).**
- **Complete L4 milestone report on database and GPAM architecture (9/15/2011).**

Inventory Accomplishments

- **Reports Completed/Updated**
  - Fuel Cycle Potential Waste Inventory for Disposition (Revisions 3)
    - *Updated commercial UNF inventory estimates thru Dec 2010*
    - *Included additional dry storage inventory estimates thru Dec 2010*
    - *Provides isotopic composition of 100 GWd/MT Burn-up fuel as an example of continuous improvement of the existing once thru fuel cycle*
    - *Provides decay heat as a function of time for LWR UOX, MOX fuel (from LWR reprocessing) and Sodium fast Reactor Fuels*
    - *Provides decay heat as a function of time for heat generating waste forms*
  - Issued "LLW Inventory from MOX Fuel Fabrication" FRCD-USED-000059 Rev 0
    - *Provides secondary waste from MOX fuel fabrication activities*
  - Issued "U.S. Radioactive Waste Inventory and Characteristics Related to Potential Future Nuclear Energy Systems" FCRD-USED-2011-00068 Rev 0, 1 and 2
    - *Summary report requested by the Blue Ribbon Commission*
  - Issued "Low Level Waste Disposition-Quantity and Inventory" (FCRD-USED-2010-000033,Rev 2)
    - *Initiated to eliminate the metal waste stream estimates. Estimates of the metal waste stream are already provided in the report, Fuel Cycle Potential Waste Inventory for Disposition, FCR&D-USED-2010-000031. The duplicate waste estimates have caused confusion.*

Inventory Current Work in Progress

- **Fuel Cycle Potential Waste Inventory for Disposition (Revision 4)**
  - *Reviewing minor element additions to support repository modeling*
  - *Update for Additional Alternative Fuel Cycles*
    - Modified Open Cycle Alternatives
      - *Th-U* — *SNL*
      - *Traveling Wave / Candle*
      - *Energy Multiplier Mod.*
      - *Ultra Long Life Core (Battery)*
      - *Small Modular Reactor*
      - *Toshiba 4S*

      } *INL* *Choose 1*
      - *HTGR* — *PNNL*
    - *Full Recycling*
      - *Th-U with recycle* — *SNL*
      - *Th-U Molten Salt* — *PNNL*
      - *U Molten Salt* — *PNNL*
- **Comparison with Industry**
  - *Objective: Understand the differences in process and secondary waste estimated volumes, masses and activity*
  - *Task Order drafted, DOE Comments Incorporated, Approval Delayed*
  - *Target completion 30 weeks after approval*
- **Milestone Deleted (until it can be rescheduled)**

FEPs Work Package Accomplishments

- **Existing FEP List and Evaluations**
  - 208 FEPs relevant to 20 different disposal alternatives
    - *20 alternatives = 4 WF types x 5 geologic settings/concepts*
  - 104 preliminary FEP evaluations documented in FY10 progress report
- **Ongoing Evaluations**
  - Performing preliminary evaluations on 28 additional FEPs
  - Continuing to compile relevant existing information from U.S. and foreign programs to augment existing evaluations
    - *Collaborative with EBS, Natural Systems, and Generic Modeling*
- **Sharepoint Website**
  - Continuing development and use of collaborative website to share evaluation information and produce consistent formats for documentation
- **Summary Tracking Tool developed**
  - Updated Excel spreadsheet/database to include latest information

FEPs Work Package Future Plans

- **Expand/enhance FEP Evaluations**
  - Initiate preliminary evaluations for 76 yet-to-be-addressed FEPs
  - Continue to identify new information to augment existing evaluations
- **Collaborate with FEP work in other UFD work packages**
  - Support FEP screening for generic models (salt, clay, granite, deep BH)
  - Support LLW FEPs identification and screening
- **Enhance FEP Tools**
  - Evaluate web-based database applications as a repository for Sharepoint and Tracking Tool information
- **Milestones**
  - Level 3: FY11 Progress Report (Aug 19, 2011)

LLW Disposition Accomplishments

- **Draft report on prior LLW performance assessment models issued for team review**
  - Take advantage of prior work, avoid duplication of effort
  - Identify model features relevant to the UFD model
  - Five models identified for review
- **List of applicable Features, Events and Processes (FEPs) developed**
  - Compiled from a variety of domestic and international sources
  - 1,194 FEPs contained in initial list
  - Workshop held May 17-18 in Las Vegas to screen the FEPs for the UFD Generic LLW Disposal Model
  - Final FEP list reduced to 469 FEPs (226 Included FEPs and 243 Excluded FEPs)
- **Initiated modeling efforts**

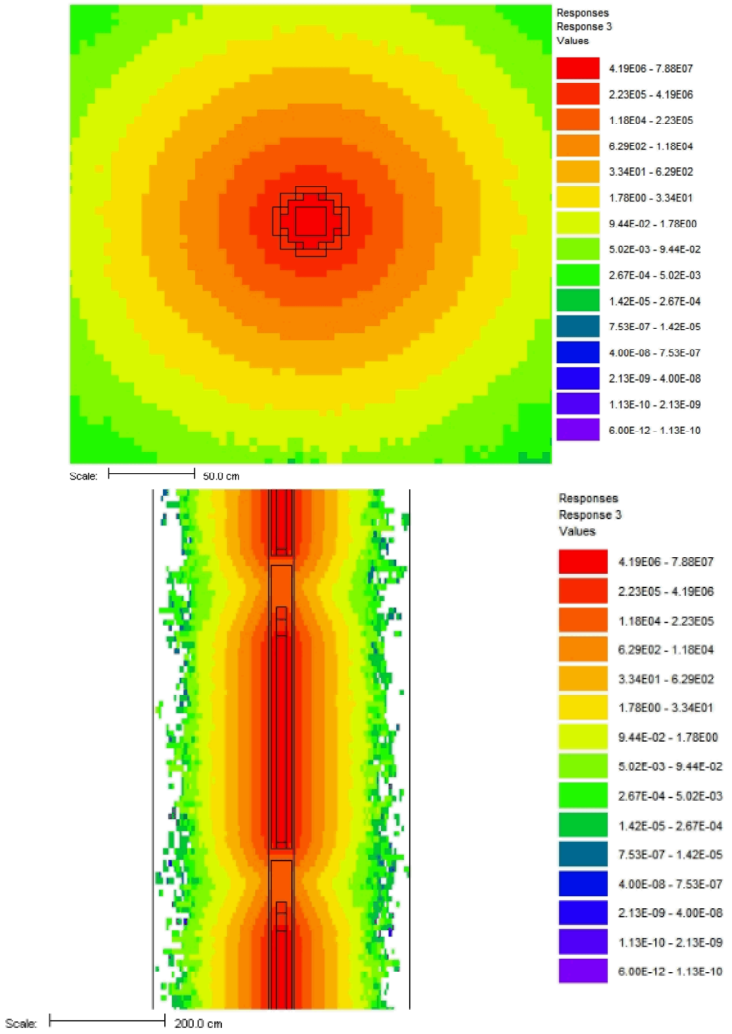
LLW Disposition
Future Plans

- **Finalize assessment of prior models and prepare report**
- **Additional work remains to complete the FEP list:**
  - Finalize FEPs as required to suit the generic model (e.g. remove facility specific terminology, ensure the content of “Subsumed” FEPs are captured by the text of the subsuming FEPs, etc.)
  - Final team review of FEP list
  - Prepare report
- **Develop model concepts**
- **Continue modeling efforts for the identified concepts based on the final FEP list**
- **Prepare year-end report on model development**
  - Reference prior modeling assessment report
  - Reference final FEP list report
  - Provide status of model development
  - Identify tasks to be completed in FY 2012
- **Prepare update to the LLW disposal history for significant events from FY 2011**
- **Anticipated FY 2012 Tasks**
  - Complete initial UFD Generic LLW Disposal Models for near-surface and borehole configurations
  - Develop scenarios to evaluate with the models (inventory, configuration, environmental parameters, etc.)
  - Update history as needed

Criticality Analysis Accomplishments YTD

- **Completed**
  - Spent Fuel Benchmark Evaluation (3/31/11)
  - Criticality Consequence Whitepaper (6/30/11)
- **In-process Activities**
  - Degraded Model Benchmark Applicability
    - Several degraded configuration models developed
  - Radiation Transport Evaluation
    - alpha particle source module prototype developed for ORIGEN
    - Time and burnup dependent neutron and gamma source terms generated
    - SCALE/MAVRIC models and preliminary results generated for Dry storage, Borehole, and Clay/Shale configurations
  - Computational Analysis of New Radiochemical Assays
    - Additional design and operating data needs identified
    - NDA being processed for acquisition and use

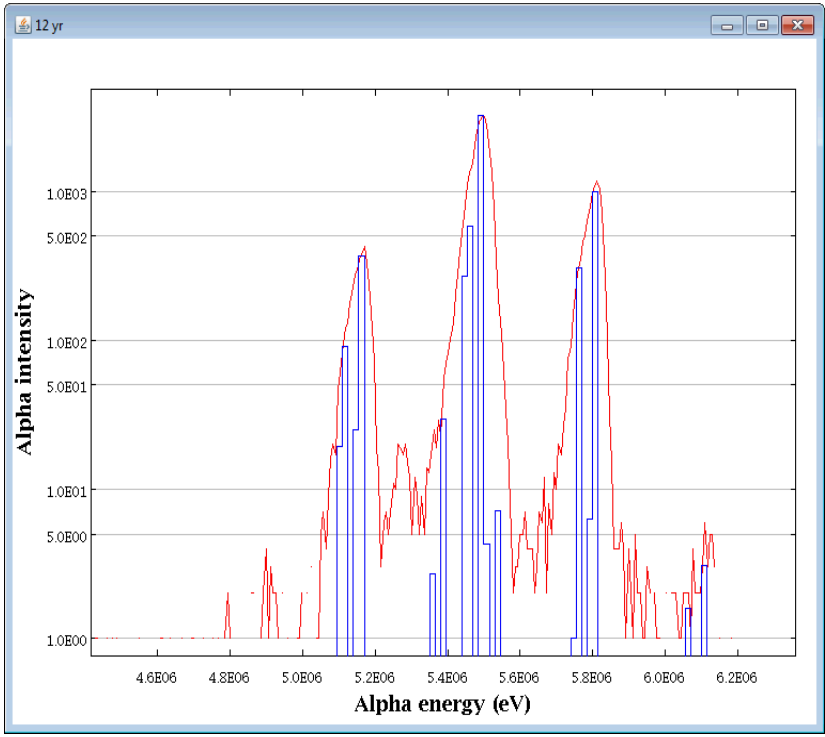
Dose rate values in rad/h



Example dose map for borehole

Criticality Analysis Plans for Future

- **Radiation Transport Evaluation**
  - Develop time- and burnup dependent beta and alpha particle source terms
  - Complete the calculations for fuel storage and disposal configurations
  - Perform energy deposition calculations in support of water radiolysis analyses
  - Formalize alpha and beta source term modules as part of ORIGEN for distribution with SCALE (post FY11)
- **Degraded Model Benchmark Applicability**
  - Perform sensitivity/uncertainty analysis comparison with SCALE/TSUNAMI
- **Radiochemical Assays**
  - Finalize NDA so additional operating and design information can be used in model development
  - Complete computational analysis comparison to experimental results



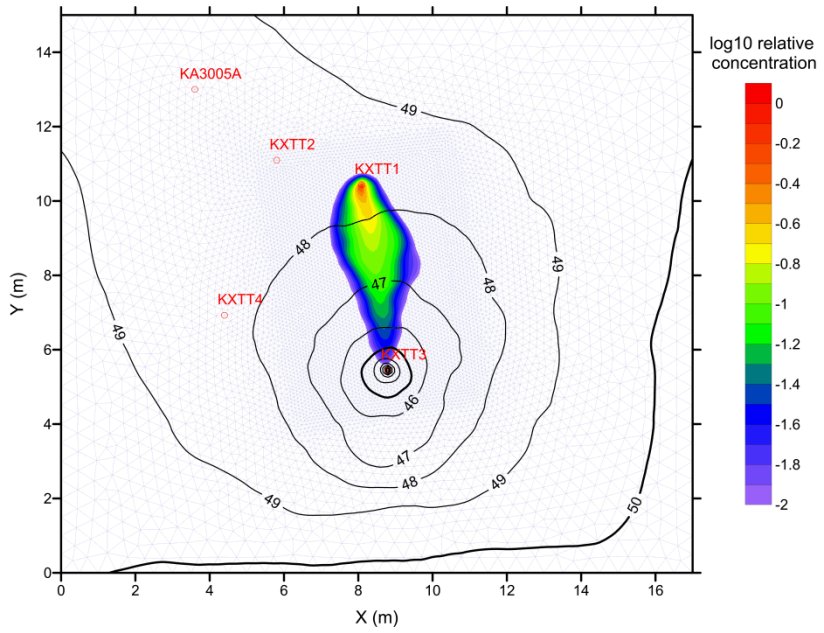
Comparison of predicted (blue)alpha source against measured (red)

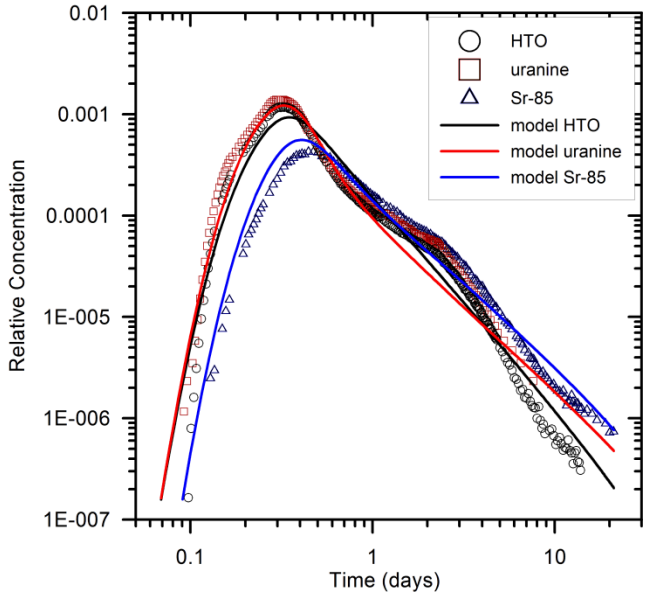
Flow & Transport - Saturated

Uncertainty Analysis of Saturated Flow and Transport Parameters Derived from Field-Scale Testing

- *Data from the TRUE radionuclide transport SST-1b test at the Äspö Hard Rock Laboratory used in the analysis*
- *Test conducted using multiple tracers in a single fracture with a convergent flow field*
- *Model of flow and transport incorporates spatially variable multi-rate matrix diffusion, heterogeneous transmissivity, sorption, and decay using the FEHM software code*

- *Uncertainties in parameters derived from the tracer test are being quantitatively analyzed through simultaneous optimization to breakthrough curves using the PEST and Dakota software codes*
- *Linear and non-linear confidence limits on parameter values are estimated using a variety of formal methods, including null-space Monte Carlo analysis*
- *Both gradient-based and non-gradient methods will be assessed for use in optimization and sensitivity analyses*





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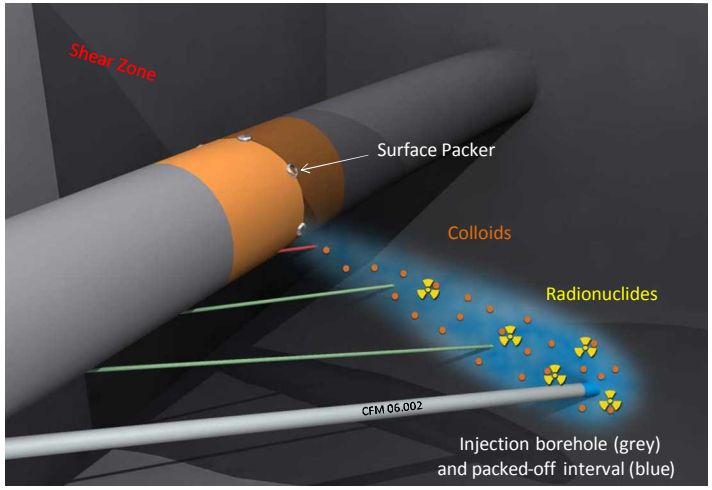
Flow & Transport – Saturated

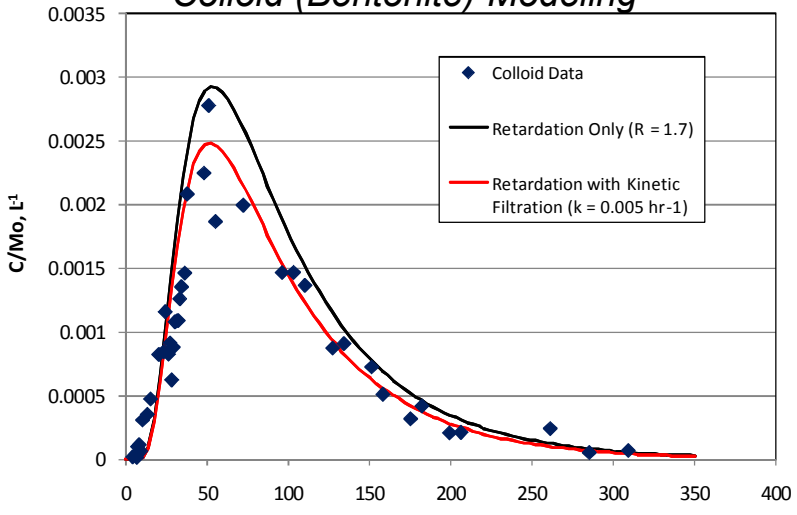
Interpretation of Colloid-Facilitated Radionuclide Transport Field Experiments Conducted at the Grimsel Test Site



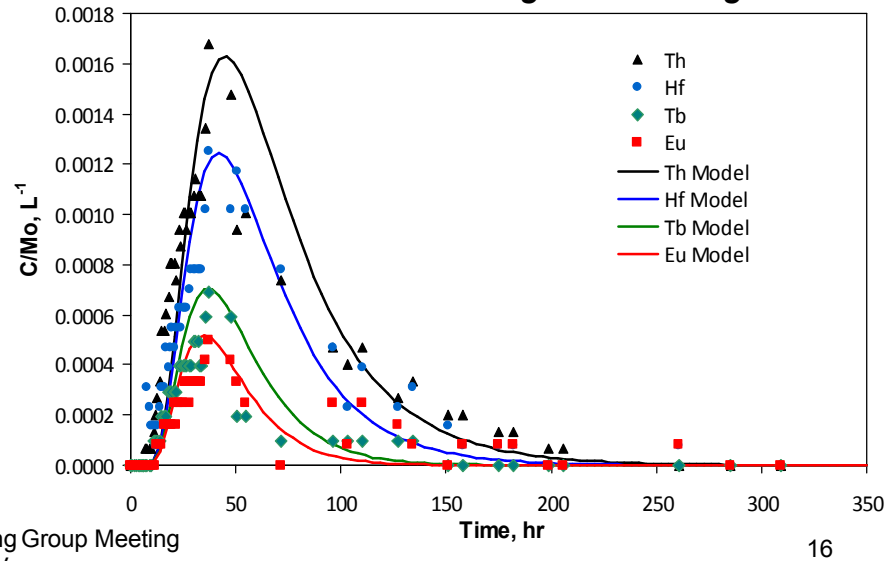
Highlights

- *Injection of "homologues" of actinides (Th, Hf, Tb, Eu) pre-sorbed onto bentonite colloids*
- *Observed both colloid filtration and desorption of homologues from colloids*
- *Desorption rate constant for Th in good agreement with lab measurements (only homologue measured in lab to date)*
- *Future injection of radionuclide cocktail with bentonite colloids, followed by emplacement of a RN-doped bentonite plug (NBS and EBS)*

Colloid (Bentonite) Modeling



Radionuclide Homologue Modeling



Thermal Load Mgmt & Design Concepts Analysis FY11 Accomplishments

- **Selected Reference Repository Design Concepts:**
  - Granite (SKB), Clay/shale (ANDRA), Salt (GSR), Deep Borehole (SNL, MIT, others)
- **Developed Inventory/Heat Output for Major Radwaste Streams for Three Fuel Cycles:**
  - LWR 60 GW-d/t once-through
  - Reprocess LWR 50 GW-d/t → Pu-MOX 50 GW-d/t once-through
  - Reprocess LWR 50 GW-d/t → SFR w/ E-Chem. reprocessing, "closed"
- **Evaluated Peak Temperature for Combinations of Decay Storage, Waste Package Size, and Waste Type**
- **Results Overview:**
  - Waste forms from advanced fuel cycles can be relatively hot
  - "Enclosed" emplacement requires smaller packages and/or decay storage (vs. "open")
  - Repository concepts can accommodate all major radwaste streams

Thermal Load Mgmt & Design Concepts Analysis FY12 Planned Activities

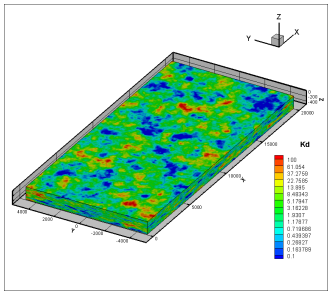
- **Refine Reference Repository Design Concepts**
  - Disposal of multiple waste streams
  - Estimate scale of facilities needed for reference cases
  - Refine estimates for cost of disposal
- **Develop Inventory/Heat Output for Additional Advanced Fuel Cycles**
  - Support NE System Engineering/System Analysis fuel cycle studies
- **Evaluate Peak Temperatures and Demonstrate FEM Capability**
- **Evaluate Future Operational and Multi-Purpose UNF Container Strategies**

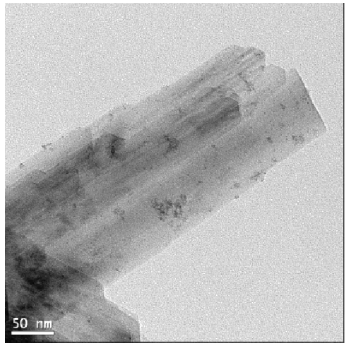
Thermal Load Mgmt & Design Concepts

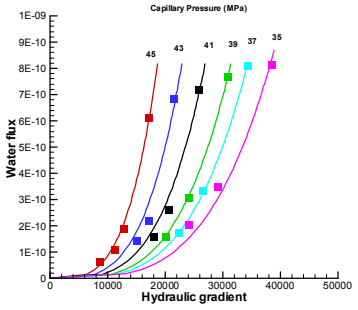
Used Fuel Disposition

Natural System Evaluation: FY11 Accomplishments

- Developed a detailed R&D work plan for next 5 years.
- Completed the analysis for Discrete Fracture Network (DFN) model development.
- Evaluated the effect of spatial heterogeneity in Kd on radionuclide transport.
- Performed a comprehensive review on radionuclide interaction with clays.
- Continued experimental studies on Pu interaction with minerals under wide chemical & physical conditions.
- Developed new constitutive relationships for clay deformation and non-Newtonian flow.
- Continued model development & demonstration for THM and THC couplings.
- Continued conceptual model development & experimental testing for direct disposal of ER salt.
- Identified potential areas & approaches for international collaboration.
- Initiated database development for natural system knowledge management.

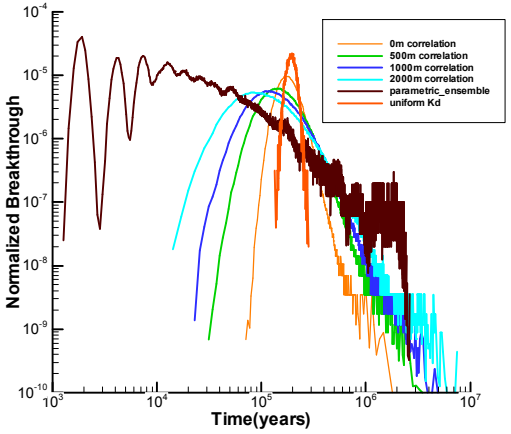


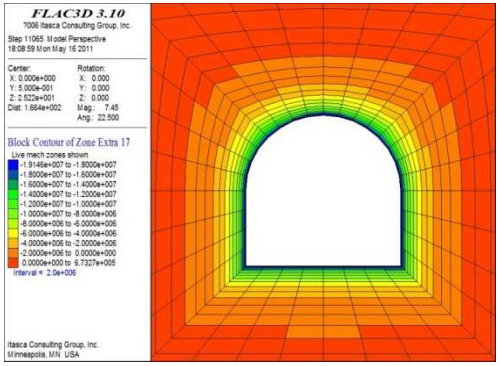




Natural System Evaluation: FY12 Work

- **Continue existing work**
  - Development of direct disposal electrochemical refinery waste: Concept development & testing
  - Natural system knowledge management : Database development
  - Modeling hydrologic flows in representative geologic media : Saturated and unsaturated flow (e.g. non-Newtonian flow)
  - Continued evaluation of radionuclide transport in heterogeneous subsurface environments
  - Mechanistic understanding of radionuclide interactions with geologic media in repository performance assessments: Colloid formation & stability, radionuclide interaction with clays
  - Modeling THMC couplings in the near field: Clay salt repository
- **Additional work**
  - Initiating disposal concept development for natural systems
  - Initiating development of a performance assessment model for natural system
  - Initiating development of critical field testing and site characterization techniques
  - Exploring international collaboration





Used Fuel Disposition

Salt Disposal Investigations YTD Accomplishments

- **LABORATORY STUDIES**
  - Completed Test Plan TP SNL-FCT-TP-11-0001: *Consolidation of Crushed Salt at Temperatures up to 250°C, Under Hydrostatic and Shear Stresses* by Frank Hansen
  - Conducted First Test at 100°C
    - *The sample assembly system works well. Jacketing worked well (we developed a jacket leak at the end of the test at about 40% axial shortening). Loading by advancing the piston worked well. Calculated force is close to load cell force. A fairly constant load rate was achieved. Unload-reload capability.*

- **FIELD STUDIES**
  - Issued the SDI Quality Assurance Program Document (DOE/CBFO-11-3465)
  - Issued the SDI Management Proposal (DOE/CBFO-11-3470)
    - *Incorporated technical and programmatic comments received from the UFD, EM, and others.*
  - Drafted the SDI Functional and Operational Requirements document (LCO-SDI-001)
    - *Completing formal review with a milestone submission date planned for 9/1/2011.*
  - Drafted Planned Change Notice for EPA Notification to support FY 2012 mining start of test drifts
    - *Completing formal review for submission to EPA in August*

Salt Disposal Investigations Plans for the Future

LABORATORY STUDIES AND MODELING

- Future Plans—This Year
  - *Continue matrix of consolidation experiments*
  - *Begin optical and scanning electron microscopy*
- Future Plans—Next Year
  - *Complete matrix of consolidation experiments and summarize investigations*
  - *Complete optical and scanning electron microscopy of consolidated samples*
  - *Write a Test Plan for thermal conductivity as a function of porosity*
  - *Develop a test plan and begin measuring the effect of temperature on radionuclide solubility in the laboratory*
  - *Develop a test plan and begin studying repository interactions with waste container and constituent materials*
  - *Evaluate and use coupled multiphysics modeling capability for field test configuration and analysis*

FIELD STUDIES

- Future Plans—This Year
  - *Complete and issue SDI Functional and Operational Requirements document (LCO-SDI-001)*
  - *Continue development of quality and technical procedures for the field test*
- Future Plans—Next Year
  - *Develop and review the detailed field test plan*
  - *Begin mining underground access drifts to the test bed location*
  - *Begin instrumentation research and development*

Waste Form Degradation and Radionuclide Mobilization Accomplishments

- **ANL, PNNL, SNL**
  - Developed chemical-radiolysis model for predicting the dissolution rate of used fuel
    - *enhanced the model for in-package chemical conditions*
    - *investigated the sensitivity of model parameters to find where model uncertainty may be reduced most effectively*
    - *validated model through comparisons with the AECL model*
  - Evaluated flow through testing data to identify data sets relevant to fuel dissolution in a radiolytic field
    - *obtained and evaluated MOX material for sufficient for testing dissolution with alpha-radiation*
    - *developed compositions for synthetic used fuel preparation*
  - Conducted Literature review/gap analysis on UOX and MOX degradation rates
    - *prepared draft report*
  - Electrochemical studies of fuel matrix and radionuclide oxidation and dissolution
    - *conducted shakedown testing of micro-electrochemical cell*
  - Produced draft set of milestones for FY12 planning
  - Produced draft 3-5 year plan

Waste Form Degradation and Radionuclide Mobilization Look Ahead

- **Gap analysis will continue**
  - Include additional literature and expanded topics as needed
- **Experimental work will be initiated**
  - Based on gap analysis and for validation and testing models
  - Develop test plans and testing matrix
  - Begin executing testing matrix
- **Implementation of degradation rate model**
  - Develop specific scenarios for analyses
    - *create detailed integration with Generic repository models*
  - Include radiolysis model
  - Develop targeted enhancements for rate model
    - *role of* H_2
    - *epsilon phase catalytic properties*
- **Produce results for use by Generic repository models**
  - Initiate analyses for highest priority scenarios

Flow and Transport Unsaturated Zone

Objective

Continue to investigate unsaturated flow and transport processes and contribute to evaluating clay/shale formations as alternative repositories.

FY11 Tasks

- Development of a new theory for preferential flow in unsaturated media.
- Investigation of clay/shale caprock leakage using petroleum analogues.
- Survey of clay/shale formations in the US.

Milestone

The tasks started from Jan 2011. A milestone report (Level: M4; QA Rigor: QRL 3) entitled “FY11 Report on UZ Flow and Transport” will be delivered by Aug. 30, 2011.

Flow and Transport Unsaturated Zone

Major Accomplishments

- Developed and validated a new theory for unsaturated flow in porous media based on optimality (that unsaturated flow pattern is formed in such a way that flow resistance in the whole domain in minimized).
- Analyses are being conducted to investigate the potential effects of a discrete preferential pathway, in the context of natural disturbances, on radionuclide transport from a repository in a clay/shale host rock.
- Surveyed public literature for shale/clay distributions in the US.

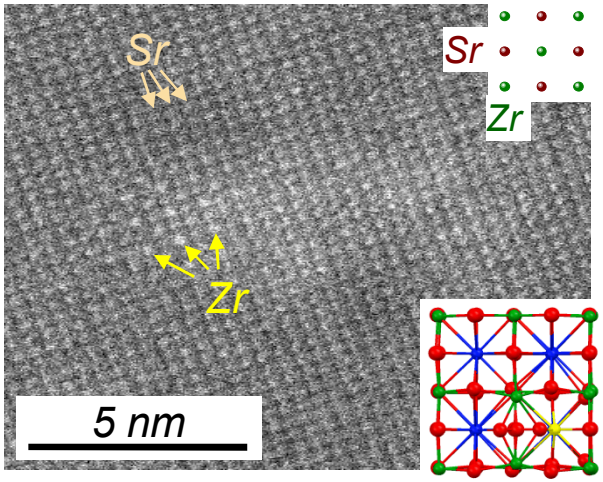
Future work

- Incorporate the new unsaturated flow theory into TOUGH2 and extend it to the multiphase flow region in the near field.
- Extend current analyses of natural analogues to consider the effects of episodic flow through discrete preferential pathways on radionuclide transport through the host rock.
- Compile the data from the literature survey of shale/clay distributions and related properties.

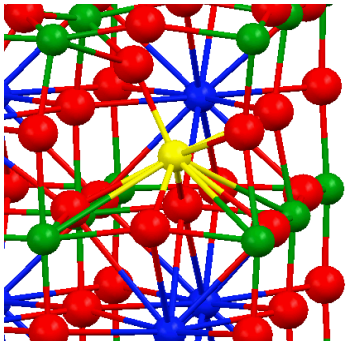
Used Fuel Disposition

Model Waste Form I: ^{90}Sr Decay in $SrTiO_3$

- **Combined theory and experimental study of $^{90}Sr^{2+}$ to $^{90}Zr^{4+}$ decay**
  - Density Functional Theory (DFT) applied to charged defects
  - Implantation of $^{16}O^{+}$ and $^{90}Zr^{+}$ and analyses with RBS, PIXE, SIMS, XRD and TEM
- **Results show**
  - Implanted structure for Zr in $SrTiO_3$
  - Zr resides at or near alternating Sr sites
  - The superlattice structure is stable ≥ 1423 K
  - Zr charge compensation by:
    - *Reduction of Ti*
    - *e- donation to other defects*
    - *(for co-implantation) oxidation*



- **Consistency in Theory & Experiment**
  - Metal interstitial configurations
  - Lattice expansion
  - Location and immobility of Zr
- **Work in progress for FY 2011**
  - Complete experimental & theoretical analyses of novel phases
  - Prepare manuscript for publication



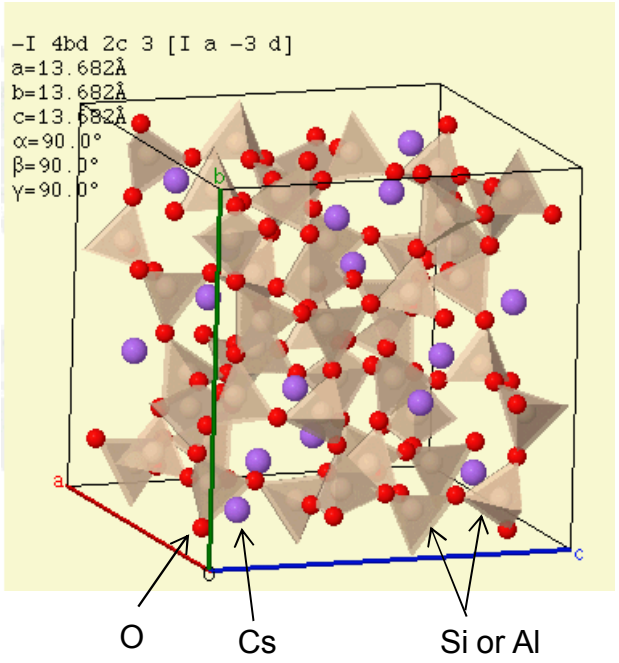
- **Level II Milestone Completed March 2011**

W. Jiang, R. Van Ginhoven, D. Strachan. 2011 FCRD WAST-2011-000070, Pacific Northwest National Laboratory, Richland, WA.
W. Jiang, *et al*. 2011. *Defects and Minor Phases in O^{+} and Zr^{+} Ion Co-implanted $SrTiO_3$ (invited)*. Industrial & Engineering Chemistry Research (in press, 2011, DOI:10.1021/ie200267n).
J. Jaffe, R. Van Ginhoven, W. Jiang *Interstitial and substitutional zirconium in $SrTiO_3$.* Comp. Mater. Sci. (submitted).

Model Waste Form II: ^{137}Cs Decay in Pollucite $CsAlSi_2O_6$

Cs^+ in pollucite is compensated by network Al. What happens when Cs^+ becomes Ba^{2+}?

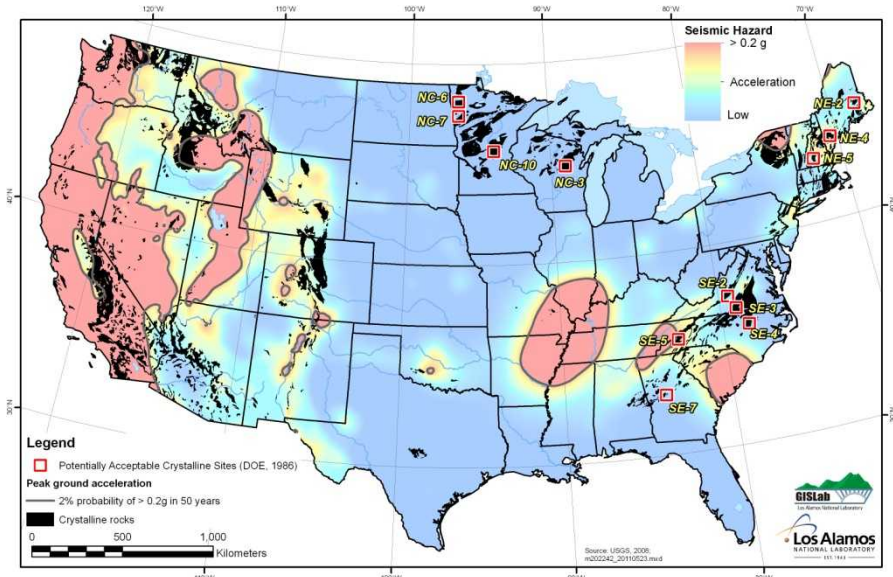
- **Combined theory and experimental study of $^{137}Cs^+$ to $^{137}Ba^{2+}$ decay**
  - Density Functional Theory (DFT) applied to neutral and charged defects
  - Investigation of undoped and Ba-doped samples provided by collaboration with Sandia National Laboratory
  - Investigation of natural mineral samples
  - Implantation of $^{16}O^+$ and Ba^+ and analyses with spectroscopy and microscopy techniques
- **Work planned/in progress for FY 2011 - FY 2012**
  - Samples received: initial characterization performed
  - Experimental plans
    - *Characterize and evaluate all samples*
    - *Complete preparation and testing of BaO cathode*
    - *Implantation of Ba in undoped samples*
    - *Characterization of irradiated samples*
  - Simulation series designed
    - *Sampling of Al distributions*
    - *Charged and neutral defects*
    - *Iterate simulation steps in conjunction with experiments*



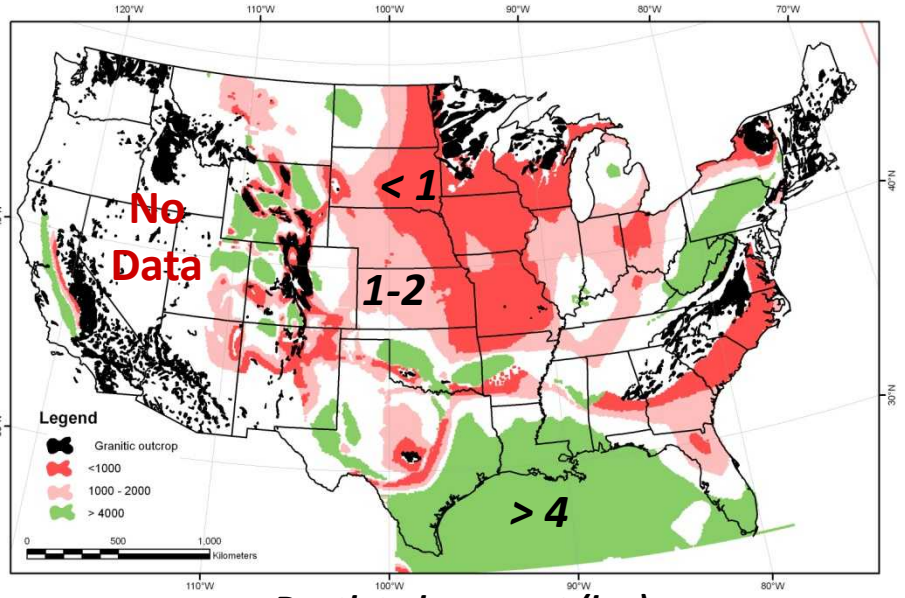
Pollucite is a zeolite with a cubic structure, having 160 atoms in the unit cell. There is a random substitution of Al on 33% of the Si sites.

Regional Geology and Tectonic Hazards

- **Initial focus on creating spatial database for crystalline (granitic and gneissic) rock**
  - **Populated GIS database with modern digital data (USGS 2009) for crystalline rock exposures**
  - **Found and incorporated location data into GIS for Potentially Acceptable Crystalline Sites from DOE Crystalline Repository Program (DOE 1986)**
  - **Obtained digital data from SMU for depth to basement (sediment thickness) presented in MIT-led geothermal report (MIT 2006)**
  - **Began developing capability to assess potential siting factors (e.g., seismic hazard, mineral resources, topographic slope, population) against distribution of crystalline rocks**



Crystalline rock exposures, DOE crystalline rock sites, and seismic hazard



Depth to basement (km)

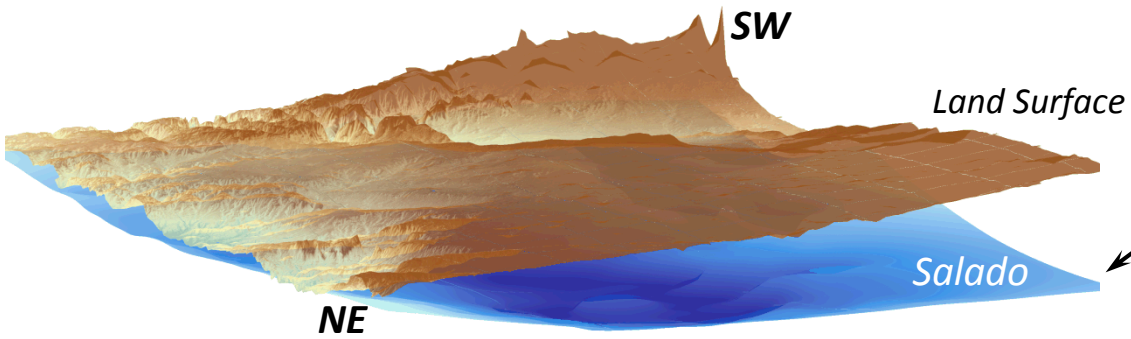
Used Fuel Disposition

Regional Geology and Tectonic Hazards

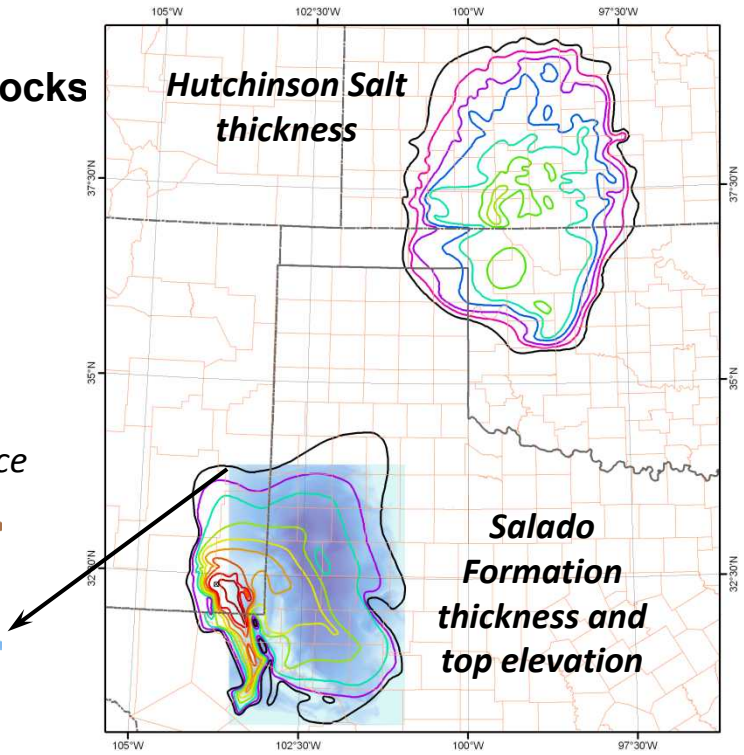
- Compiled data on salt distribution at the formation level for major basins in U.S.
- Began populating GIS with salt data to identify potential host rocks of appropriate thickness and depth for mined repository
- Initiated collaboration with LBL (Pat Dobson) to identify potential shale host rock units for incorporation into GIS database
- Have begun assessing impact of potential siting guidelines against distribution of alternative host rocks

Future Plans

- Continue populating GIS database with appropriate geologic, hydrologic and siting data
- Continue assessment of siting factors and potential impact on repository siting and complexity of site characterization efforts



Visualization of top of Salado and surface topography in West Texas



Regional salt formations

Engineered Barrier System (EBS) Evaluation – Accomplishments

- **Accomplishments**
  - Milestone report M21UF033901 (submitted June 15, 2011)
  - Representation of generic EBS design concepts
  - THMC coupled processes:
    - *Expanded applications of the Barcelona Basic Model (BBM) to clay barriers using TOUGH-FLAC simulator:*
      - Simulation of THM phenomena in the barrier/buffer at temperatures above 100°C
      - Modeling scenarios involve variable tunnel and canister spacing to evaluate peak temperatures
      - Use of anisotropic strength properties of host rock to evaluate failure in layered rock
  - Reactive diffusion in bentonite (single and double type pore model)
  - Thermodynamic modeling and database development (cement, clay)
    - *Consolidation and evaluation of thermodynamic data for cement solids (CEMDATA07 and YMP databases)*
    - *Initiated evaluation of thermodynamic data and modeling approaches for clay*
  - Disposal System Evaluation Framework (DSEF) version 1.0 and thermal analysis

Engineered Barrier System (EBS) Evaluation – Future Plans

- **Future Plans**
  - Barrier phase properties and interactions with EBS materials (cement and clay):
    - *Experimental and characterization studies on clay stability and interactions with barrier materials at high temperatures*
    - *Thermodynamic, sorption, and ion exchange properties of cement and clay*
    - *Seal material (e.g., cement) stability and modeling tool development (EQ3/6 & Cantera)*
      - Development of solid-solution model for cementitious materials
  - Molecular dynamics (MD) evaluation of clay:
    - *Characterization of swelling and mechanical properties of clay using MD and High Performance Computing (HPC)*
  - THCM coupled processes modeling for EBS NW salt disposal at elevated temperatures:
    - *Focus on potential transport in crushed salt*
    - *Evaluation of site characterization data (e.g., Deaf Smith County site)*
  - Continued development of THCM coupled processes modeling of EBS processes in clay
    - *Implementation of Double Structure constitutive model for bentonite in TOUGH-FLAC3D*
  - Diffusive transport experiments in clay
  - Continued development of the Disposal System Evaluation Framework (DSEF) and thermal analysis
  - Establishment of international collaborations and engagements for EBS research in NW disposal