

Spent Fuel Waste Science & Technology

Key Integration Aspects of Crystalline Process Models and Testing

Yifeng Wang

Sandia National Laboratories

SFWST Crystalline-GDSA Integration

May 25, 2017

Used Fuel Disposition

Crystalline Disposal R&D Work Packages

■ Objectives

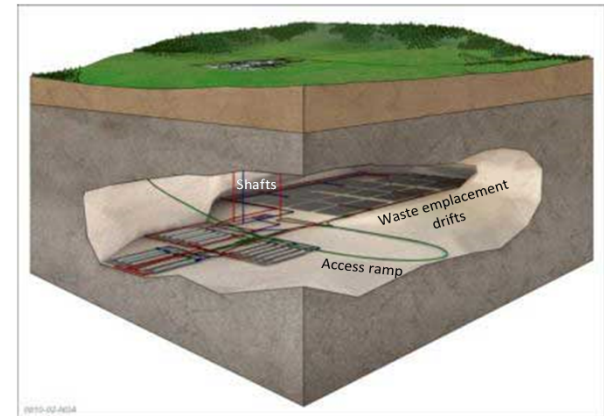
- Advance our understanding of long-term disposal of used fuel in crystalline rocks;
- Develop experimental and computational capabilities to evaluate various disposal concepts in such media.

■ Focus on two key components of deep geologic repository in crystalline rocks

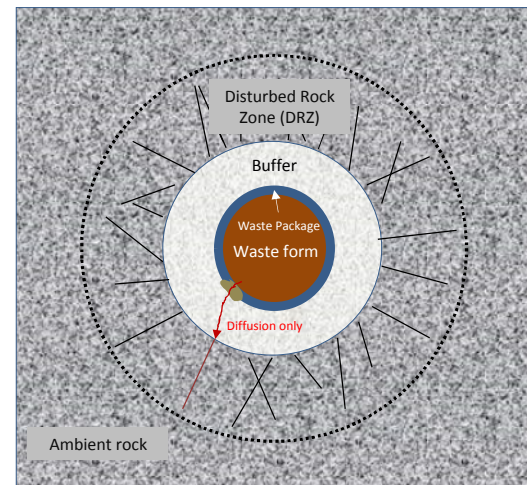
- Better characterization and understanding of fractured media and fluid flow and transport in such media
- Designing effective engineered barrier systems for waste isolation
- Assisting GDSA to develop a TSPA model for a reference case

■ Fully leverage international collaborations

- Korean Atomic Energy Research Institute (joint with DBH)
- Äspö Hard Rock Laboratory (Sweden)
- DECOVALEX (UK, France, Japan, Switzerland, etc.)
- Colloid Formation & Migration Project (Switzerland)
- Others



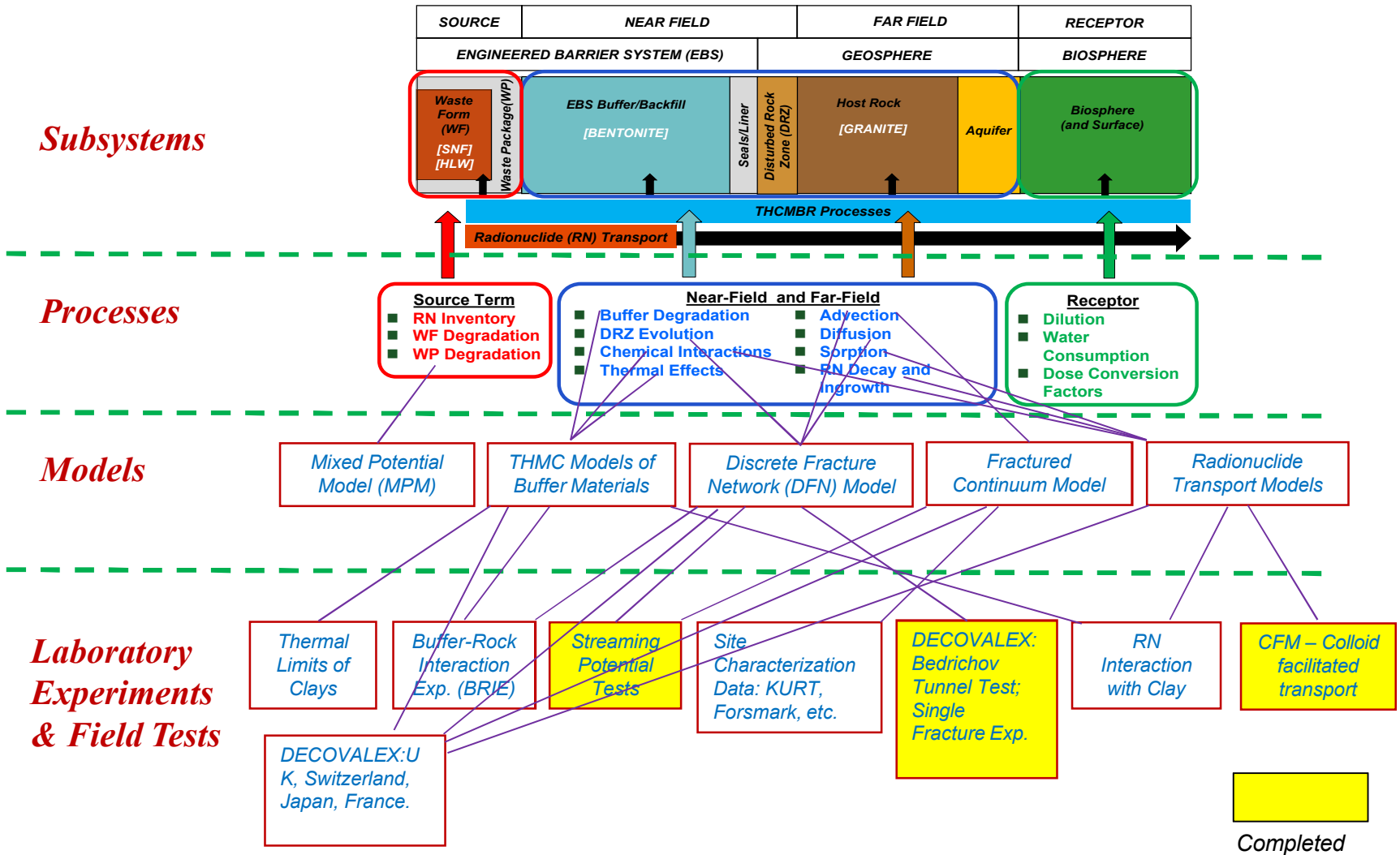
Modified from <http://www.bbc.com/news/uk-england-cumbria-21253673>



Institutions involved: ANL, LANL, LBNL, LLNL, SNL

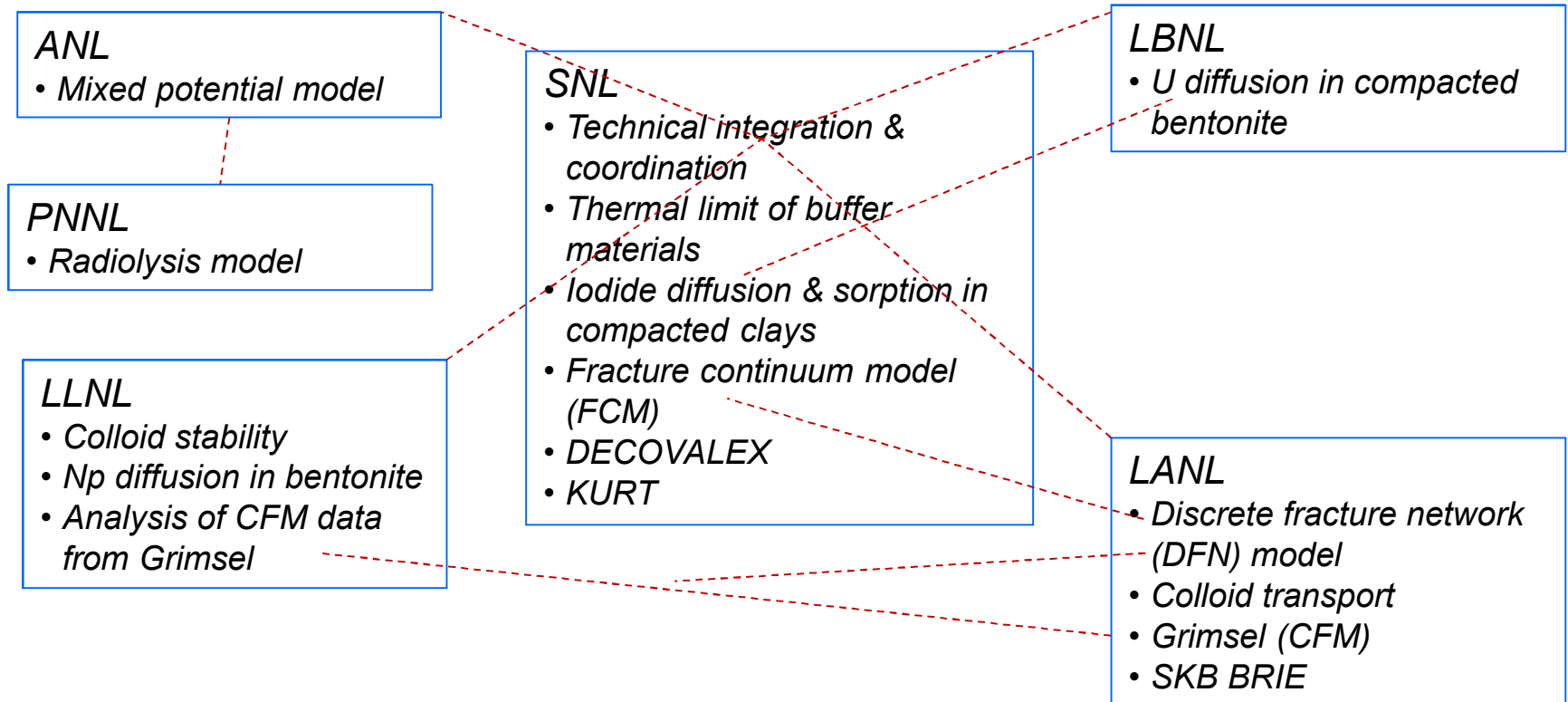
Used Fuel Disposition

Experimental & modeling activities for used fuel disposition in crystalline rocks



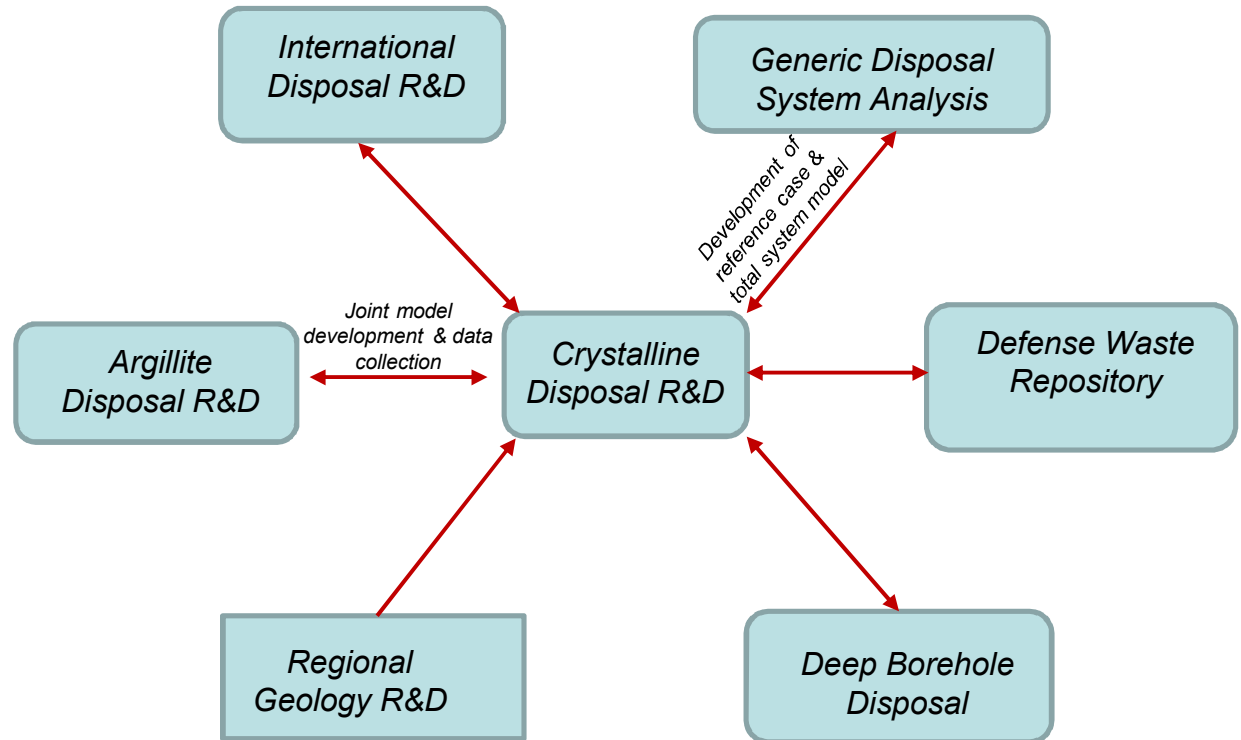
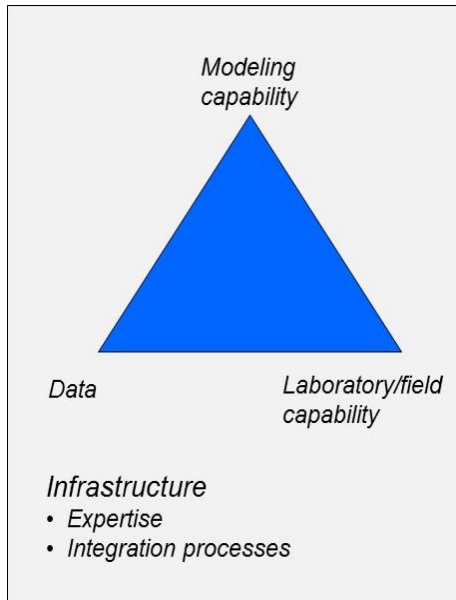
Used Fuel Disposition

Integration & coordination among institutions

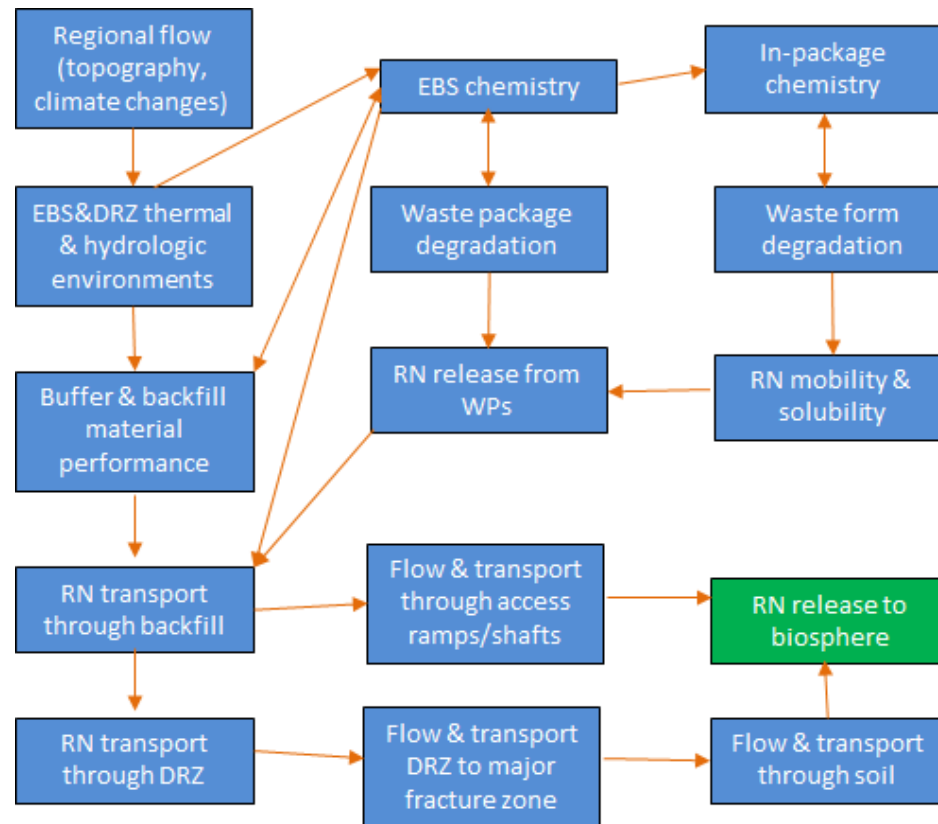


Used Fuel Disposition

Integration & coordination



Institutions involved: ANL, LANL, LBNL, LLNL, SNL



Key features:

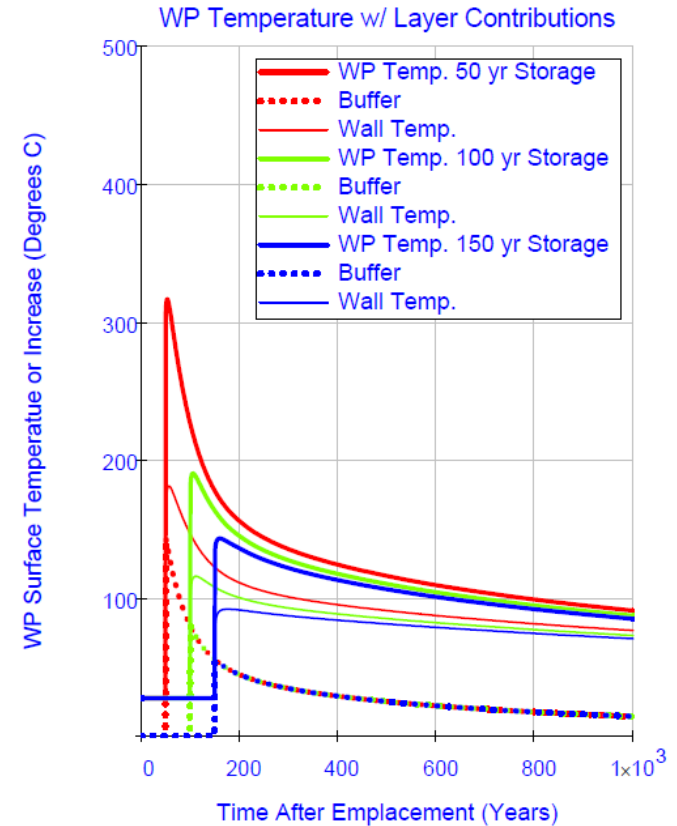
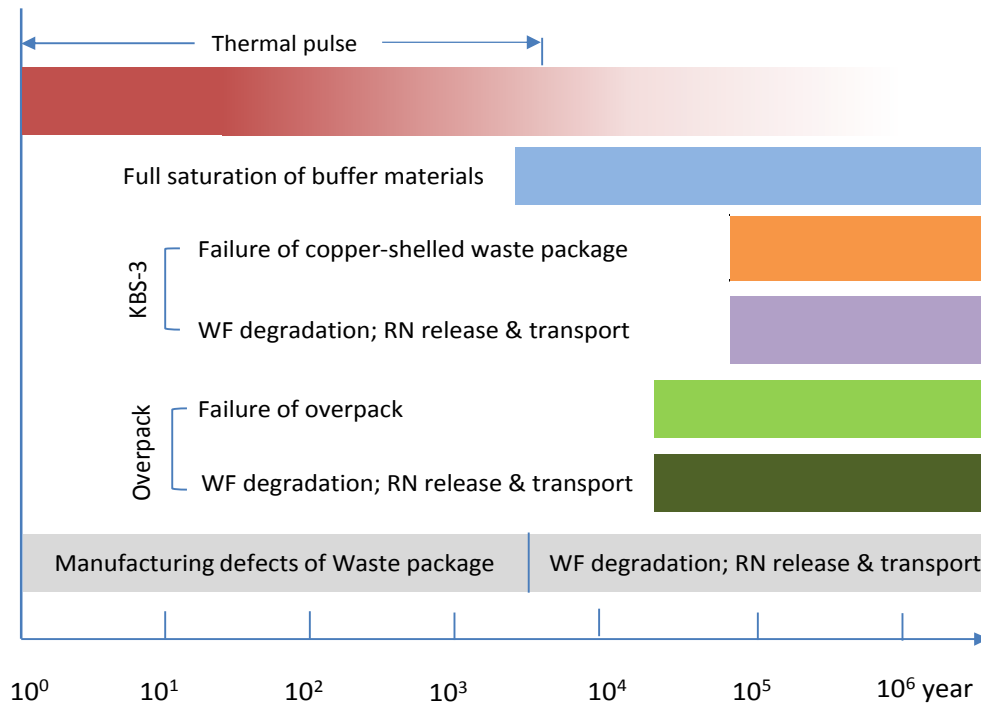
- *Fractured media: DFN vs. continuum*
- *Engineered barrier system*
- *WP failure*
- *Level of details for modeling WPs*

Codes used for UFD in crystalline media

- **PFLOTRAN: Parallel reactive transport code for simulating far and near field flow and transport**
- **FMDM: Fortran code for fuel matrix degradation, incorporated in PFLOTRAN**
- **MCNPX/ORIGEN: Calculating the buildup, decay, thermal loading of radioactive materials**
- **FEHM: Simulating subsurface multi-phase multi-fluid heat and mass transfer**
- **CrunchFlow: Reactive transport code for column experiments**
- **PEST: Optimization code for parameter estimation from experimental measurements**
- **DAKOTA: Optimization and uncertainty quantification code as a performance assessment driver**
- **DENWORKS: Simulating flow and transport in discrete fracture network**
- **FCM: Using a stochastic method to estimate effective permeability fields from site characterization data.**
- **TOUGHREACT: Multiphase reactive transport simulator for studying near-field evolution**
- **FLAC3D: Geochemical code coupled with TOUGHREACT for studying near-field evolution**
- **LAMMPS: Molecular dynamics modeling for mechanistic understanding of radionuclide interaction with clay materials**
- **PHREEQC: Chemical equilibrium code for interpretation of sorption data**
- **RELAP: Reactive transport Laplace transform code for model fitting to conservative tracer experiments**
- **EQ3/6: Chemical equilibrium code for water chemistry and solubility calculations**

Used Fuel Disposition

Relevant Physical & Chemical Conditions



UOX fuel (40 GW-d/MT), 32-PWRs (Hardin & Voegelé, 2013)

- **Realistic representation of fracture networks in both the far field and the DRZ, preferably using a continuum modeling approach**
 - Honor measured fracture distributions
- **Capability for capturing the THMC evolution of the near field**
- **Reasonable representation of EBS**
 - Buffer materials
 - Waste package failure
 - Credit for cladding
- **Reasonable representation of source terms**
 - In-package chemistry).
 - Waste form degradation
 - Radionuclide decay and in-growth
 - Solubility control
 - Sorption
 - Colloid-facilitated transport