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Overview of Crystalline Work Packages

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Sandia National Laboratories

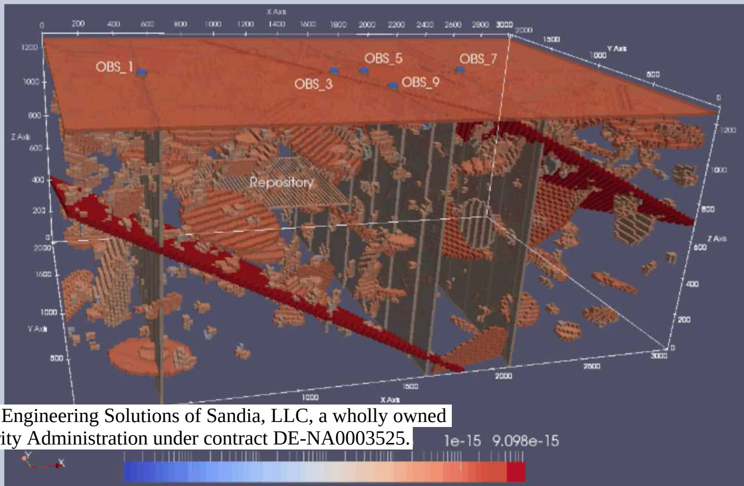
SFWD

Spent Fuel & Waste Disposition

Annual Working Group Meeting

UNLV-SEB – *Las Vegas, Nevada*

May 21-23, 2019



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OBJECTIVES

Advance understanding of long-term disposal of used fuel in crystalline rocks (granitic or metamorphic rocks) and develop experimental and computational capabilities to evaluate various disposal concepts in such media.

- Assist the geologic disposal safety assessment (GDSA) team to develop a robust repository performance assessment model by 2020.
- Provide the GDSA with a basic "minimal" set of process models and model feeds in next two years to support the GDSA 2020 goal.
- Develop basis for process modeling that enables streamlined integration with system modeling resulting in feeds to GDSA.
- Consolidate model parameter data, especially thermodynamic data, to ensure more consistent usage of the data across the project.
- With the existence of different approaches taken by various researchers there is a need to understand how well the models are developed in terms of pedigree and rigor.
- Fully leverage international collaborations for data collection and model development and validation.
- Closely collaborate with other work packages, especially those on disposal in argillite and engineered barrier system design.

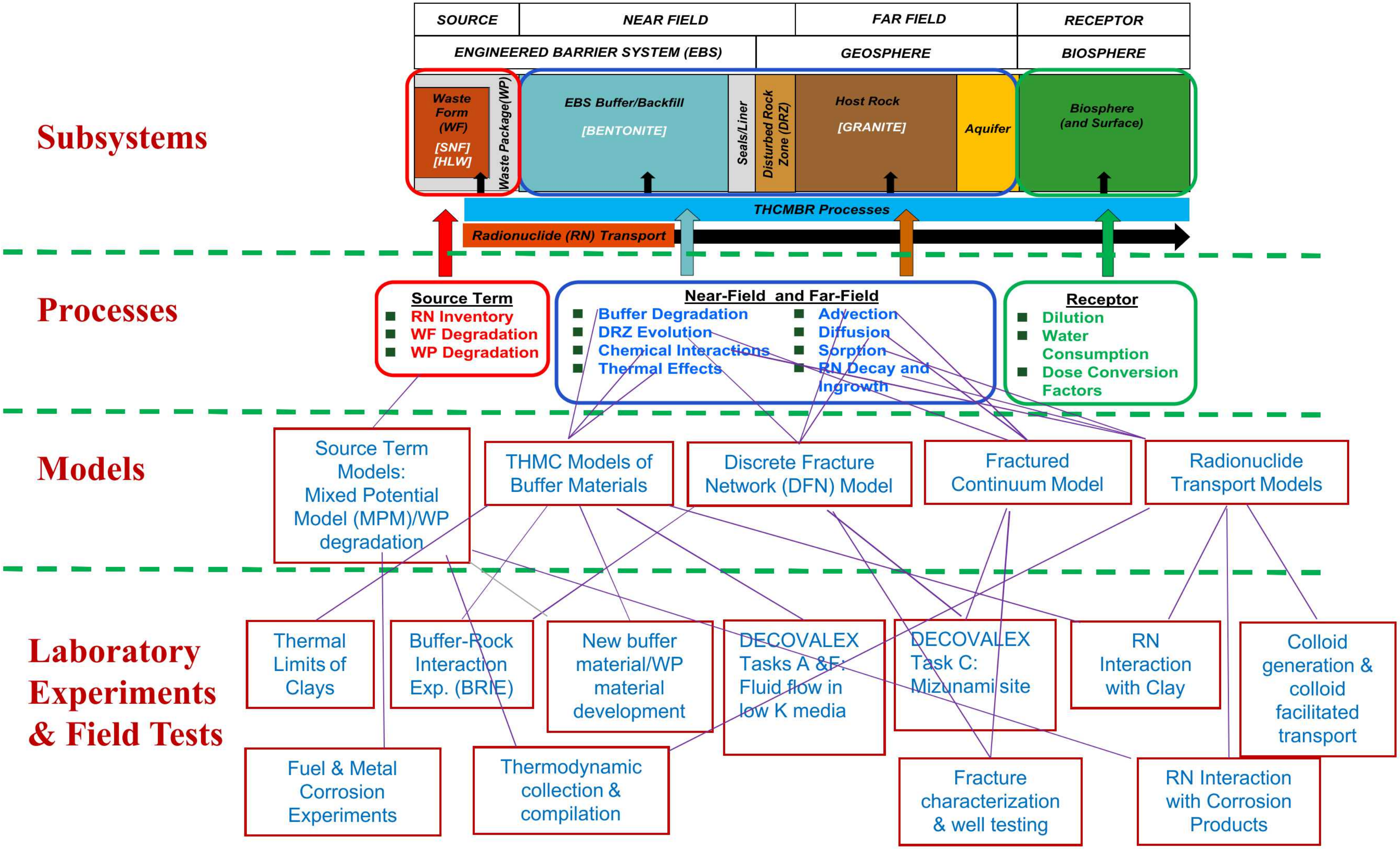
The FY19 work will focus: (1) better characterization and understanding of fractured media and fluid flow and transport in such media, and (2) designing effective engineered barrier systems (EBS) for waste isolation.

FY19 Activities

- Refine and optimization of the fuel matrix degradation model (FMDM). Account for the effect of metal corrosion (jointed with argillite work package). (ANL)
- Understand and quantify radionuclide interactions with corrosion products, especially Pu sorption and incorporation into magnetite and green rust. (LLNL)
- Understand and quantify bentonite erosion and colloid generation and their impact on radionuclide transport. (LANL)
- Understand fluid flows in low-permeability media. (SNL, LBNL)
- Conduct long-term (up to months) temperature-controlled (up to ~200°C) flow and mechanical (and chemical) experiments on multiple core-scale samples; understand U interaction with bentonite. (LBNL)
- Continue development of new-generation buffer materials/waste package materials; understand thermal limits of buffer materials (SNL)
- Continue development of the discrete fracture network (DFN) model; especially develop a reduced order model for GDSA. (LANL)
- Continue development and demonstration of a workflow for field data synthesis and flow modeling in fractured media. (SNL)
- Develop geophysical and well-testing techniques for characterizing fractures and inflows; reduce the uncertainties of key flow parameters in the EDZ. (LBNL)

Many of these activities include international collaboration components.

EXPERIMENTAL & MODELING ACTIVITIES FOR USED FUEL DISPOSITION IN CRYSTALLINE ROCKS

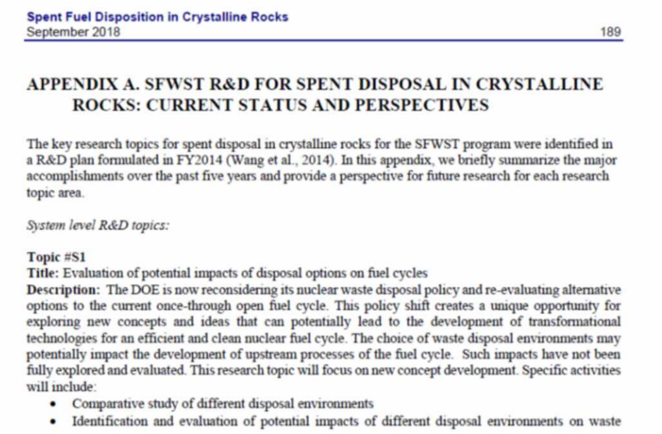


FY19 Activities mapped to safety case & roadmap

- Refine and optimization of the fuel matrix degradation model (FMDM). Account for the effect of metal corrosion (jointed with argillite work package). (SC 3.3.1a, 4.2e-g) (H: D-05, E-14)
- Understand and quantify radionuclide interactions with corrosion products, especially Pu sorption and incorporation into magnetite and green rust. (SC 3.3.1a, 4.2e-g) (H: D-05, E-14)
- Understand and quantify bentonite erosion and colloid generation and their impact on radionuclide transport. (SC 3.3.1b,c, 4.2e-g) (H: C-15, M-H: E-20)
- Understand fluid flows in low-permeability media. (SC 3.3.1c, 4.2e-g) (H: I-08, M-H: C-11)
- Conduct long-term (up to months) temperature-controlled (up to ~200°C) flow and mechanical (and chemical) experiments on multiple core-scale samples; understand U interaction with bentonite. (LBNL) (SC 3.3.1c, 3.3.2b, 4.2e-g) (H: C-15, M: C-08)
- Continue development of new-generation buffer materials/waste package materials; understand thermal limits of buffer materials (SC 3.3.1b,c,d, 4.2e-g) (H: C-15, C-16, E-11, E-17)
- Continue development of the discrete fracture network (DFN) model; especially develop a reduced order model for GDSA. (SC 3.3.2, 4.2e-g) (M-H: C-01, P-02)
- Continue development and demonstration of a workflow for field data synthesis and flow modeling in fractured media. (SC 3.3.2, 4.2e-g) (M-H: C-01, M-H: C-13, P-02)
- Develop geophysical and well-testing techniques for characterizing fractures and inflows; reduce the uncertainties of key flow parameters in the EDZ. (SC 3.3.2, 4.2e-g) (M-H: E-03)

Highlights of accomplishments since 2010

- Developed a reference case for the disposal concept.
- Implemented a preliminary reference case in GDSA.
- Significantly advanced flow and transport modeling in fractured media.
- Advanced THMC modeling capability for buffer materials.
- Developed new models for waste form degradation
- Advanced mechanistic understanding of RN interactions with both engineered and natural materials.
- Leverage materials science for engineered material development.
- Established strong international collaborations.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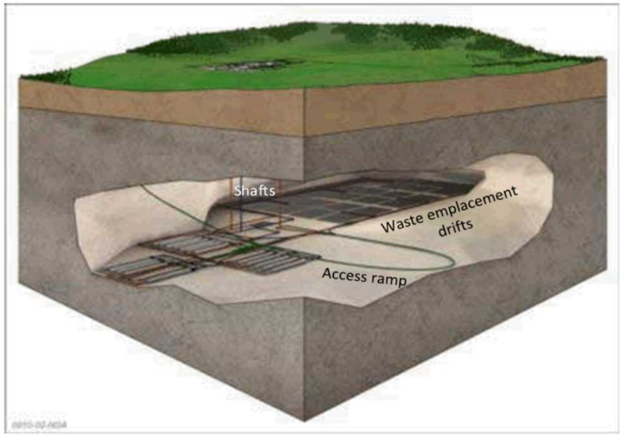
APPENDIX A. SFWST R&D FOR SPENT DISPOSAL IN CRYSTALLINE ROCKS: CURRENT STATUS AND PERSPECTIVES

The key research topics for spent disposal in crystalline rocks for the SFWST program were identified in a R&D plan formulated in FY2014 (Wang et al., 2014). In this appendix, we briefly summarize the major accomplishments over the past five years and provide a perspective for future research for each research topic area.

System level R&D topics:

Topic #S1
Title: Evaluation of potential impacts of disposal options on fuel cycles
Description: The DOE is now reconsidering its nuclear waste disposal policy and re-evaluating alternative options to the current once-through open fuel cycle. This policy shift creates a unique opportunity for exploring new concepts and ideas that can potentially lead to the development of transformational technologies for an efficient and clean nuclear fuel cycle. The choice of waste disposal environments may potentially impact the development of upstream processes of the fuel cycle. Such impacts have not been fully explored and evaluated. This research topic will focus on new concept development. Specific activities will include:

- Comparative study of different disposal environments
- Identification and evaluation of potential impacts of different disposal environments on waste



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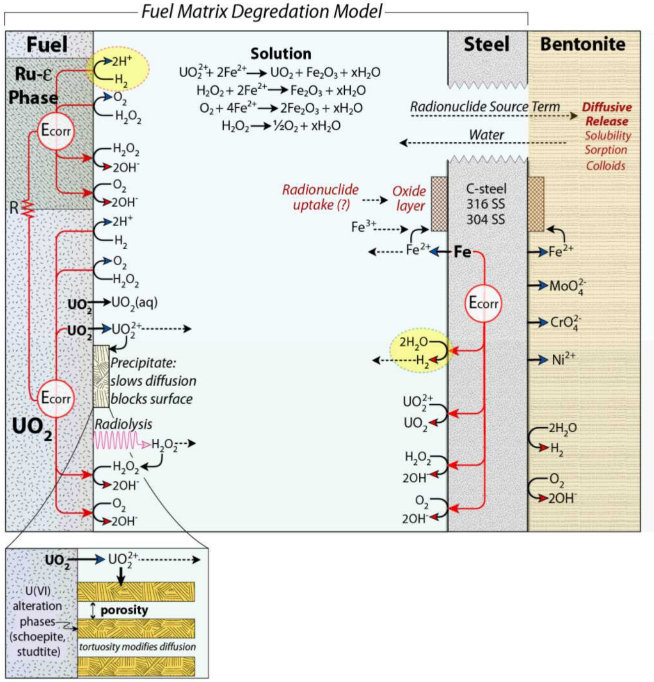
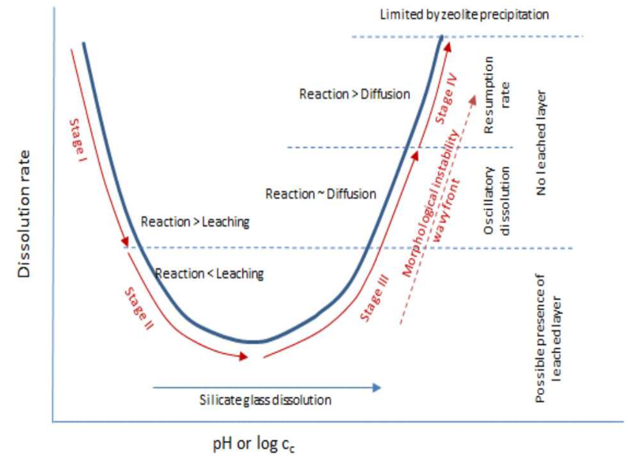
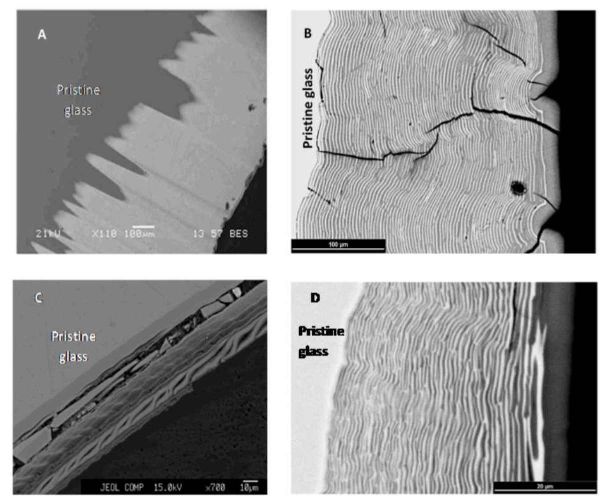
WASTE FORM DEGRADATION



Fuel matrix degradation model





Nonlinear glass corrosion model

Effect of an initial micro-molar concentration of Fe(II) on H_2O_2 generation.

Comparison of with and without dose rate (red and black). Comparison of with and without Fe(II) (solid and dashed curves).

PU INTERACTION WITH GOETHITE AND CLAY

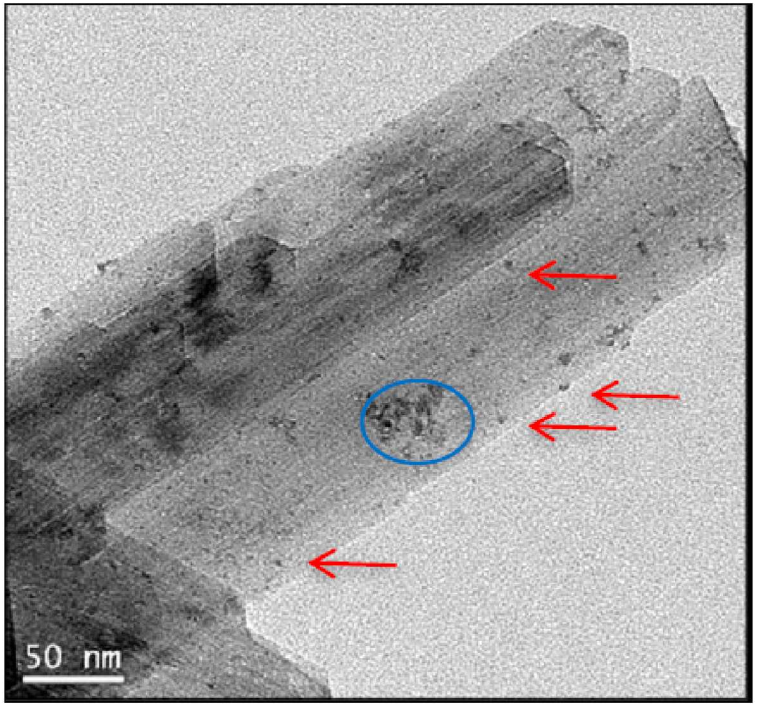


Figure 2-11. Both PuO_2 aggregates (blue) and dispersed Pu_4O_7 (red) on the goethite surface were observed at 25°C in high concentration samples. 8900 ppm Pu on goethite.

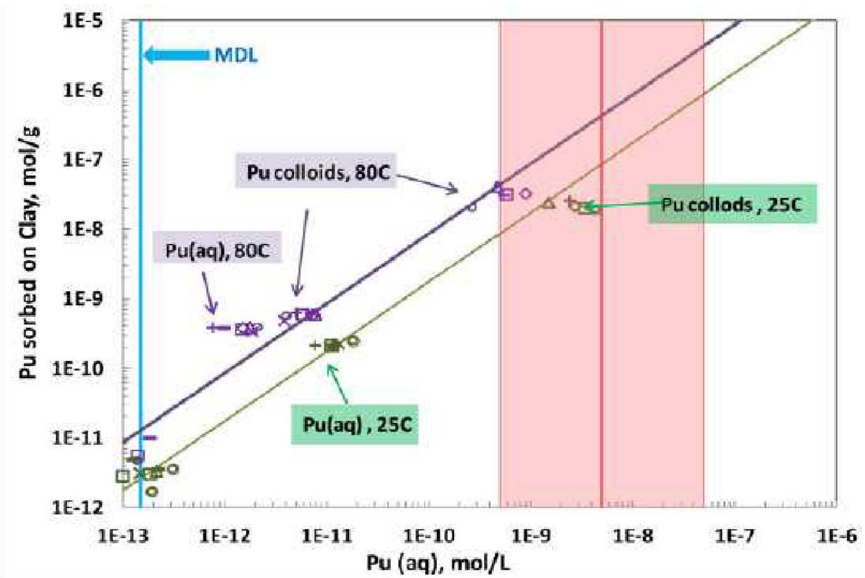
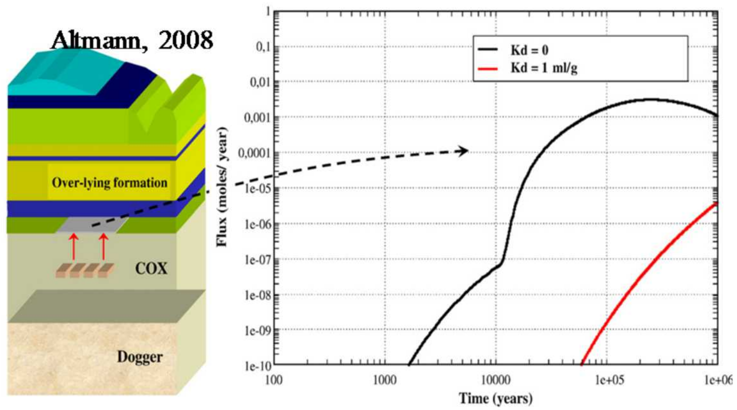
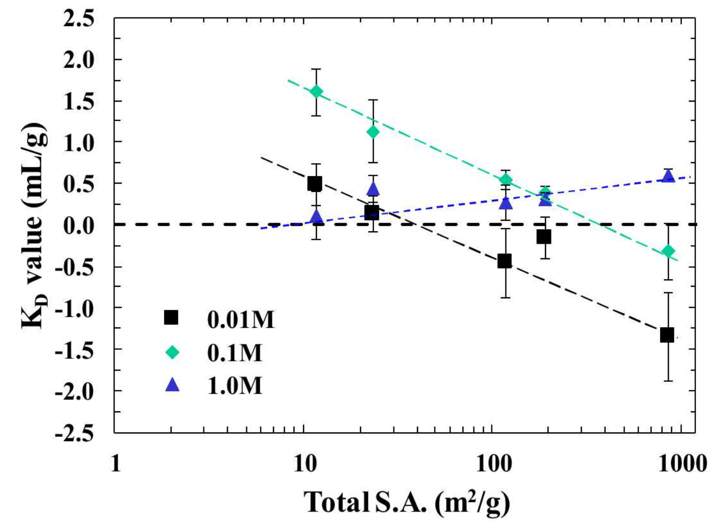


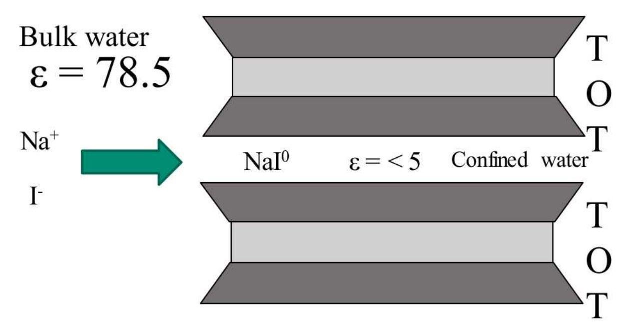
Figure 3-7. Summary of Pu sorption data at 25°C (green points) and 80°C(purple points). Shift between the 25 and 80°C isotherm is indicative of increasing Kd with temperature.

I-129 INTERACTION WITH CLAYS





Clay Mineral	Column K_D Value (mL/g)	Batch K_D Value (mL/g)	Ref.
Opalinus (Illite)	0.008-0.02		Van Loon et al., 2003
Montmorillonite	0.57		Sato et al., 1992
Callovo-Oxfordian (Interstratified illite/smectite)		0.15-0.37	Bazer-Bachi et al., 2006
Illite		27.7	Kaplan et al., 2000
Montmorillonite		-0.33	Kaplan et al., 2000



ELECTRICAL DOUBLE LAYER SPILLOVER EFFECT

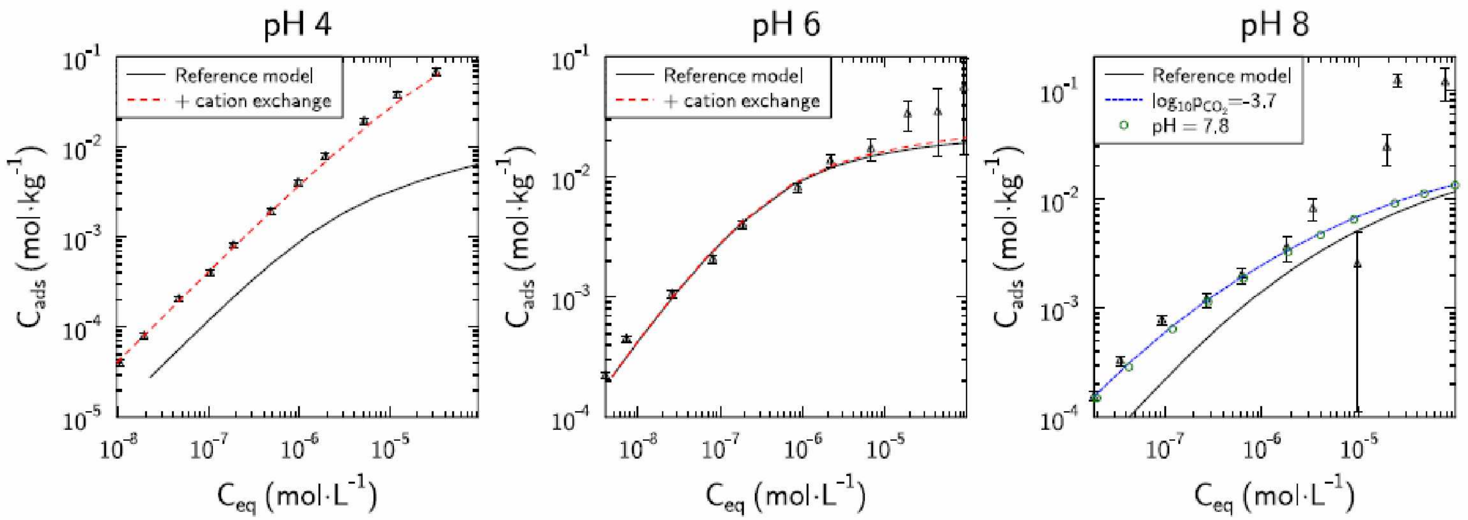
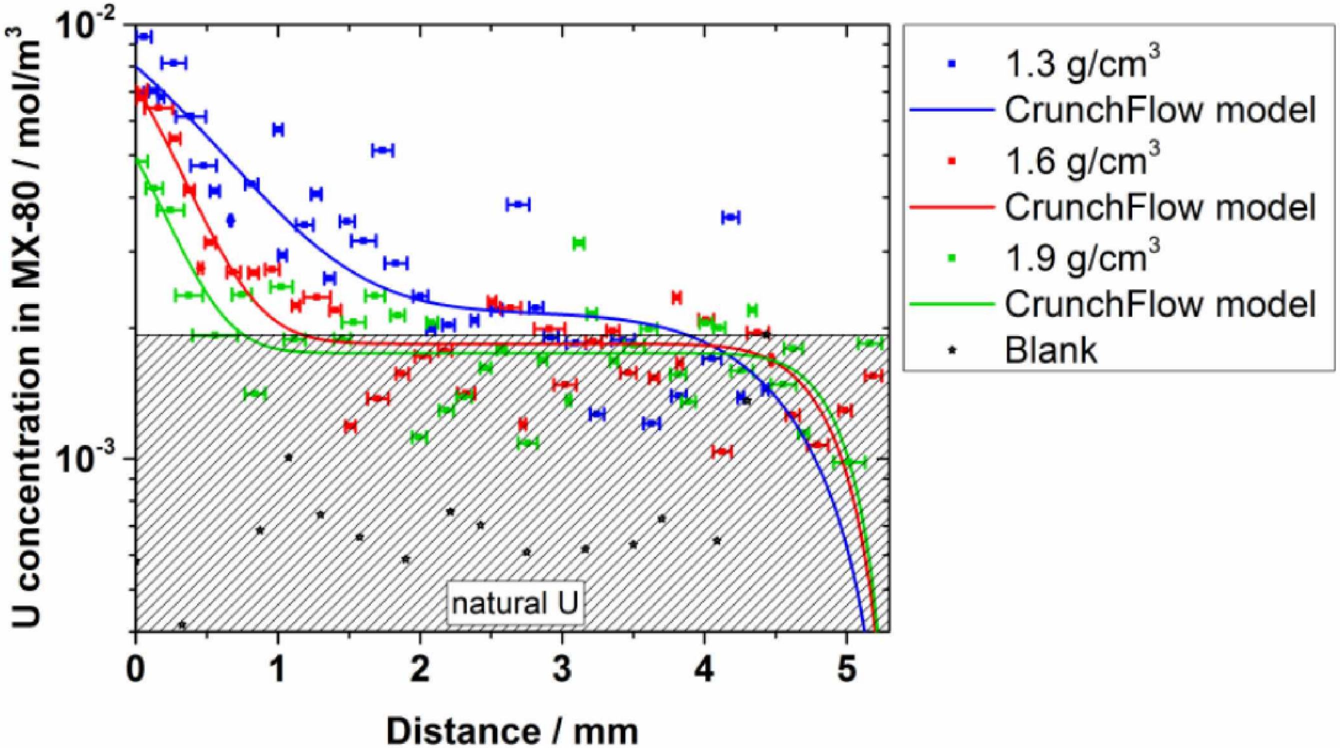


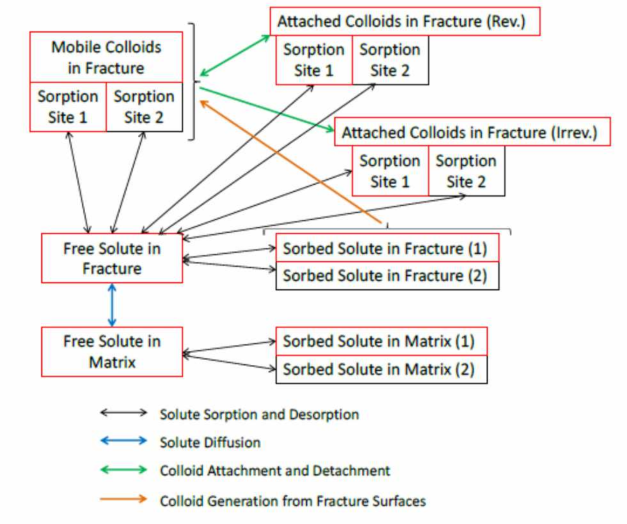
Figure 4-9. Comparison of model predictions with the U(VI) adsorption data on montmorillonite by Troyer et al. (2016).

LONG-TERM PARTITION COEFFICIENTS



Kd values obtained from batch sorption experiments are ~ one order of magnitude higher than those from the long-term (6 years) column diffusion experiments.

Multiple rate colloid-facilitated transport model



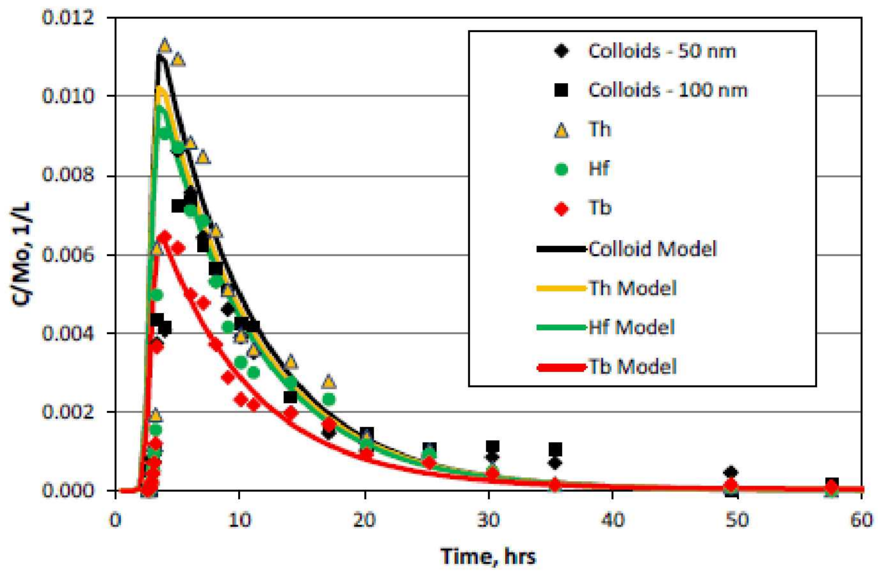
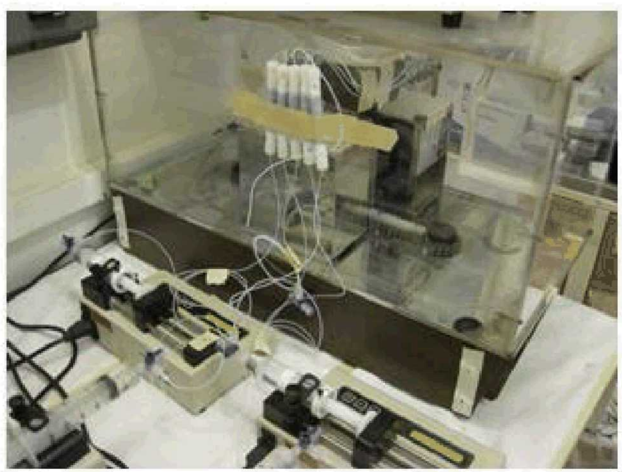
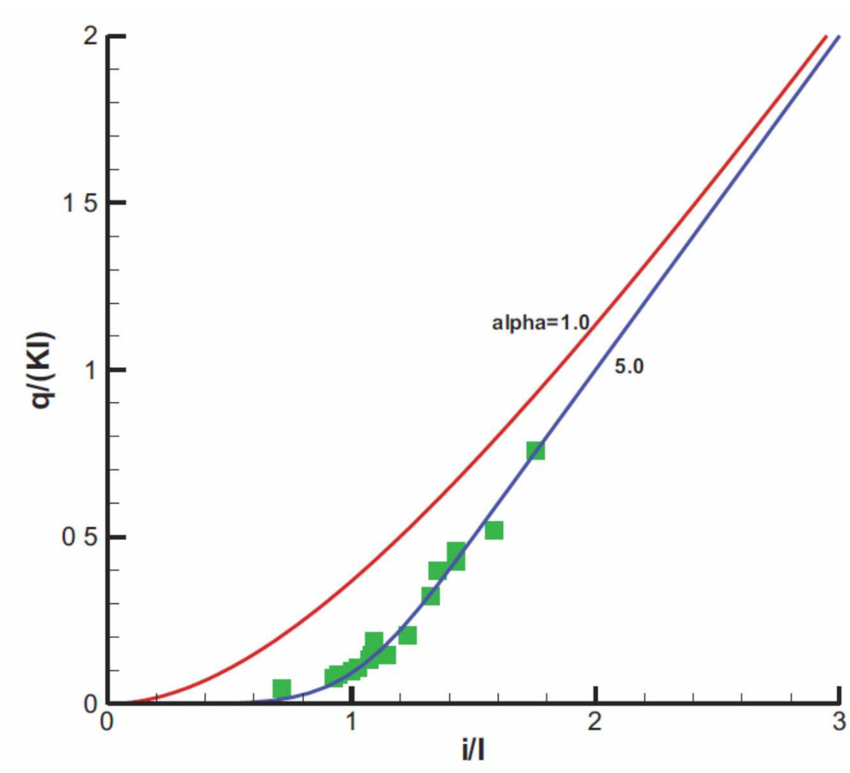
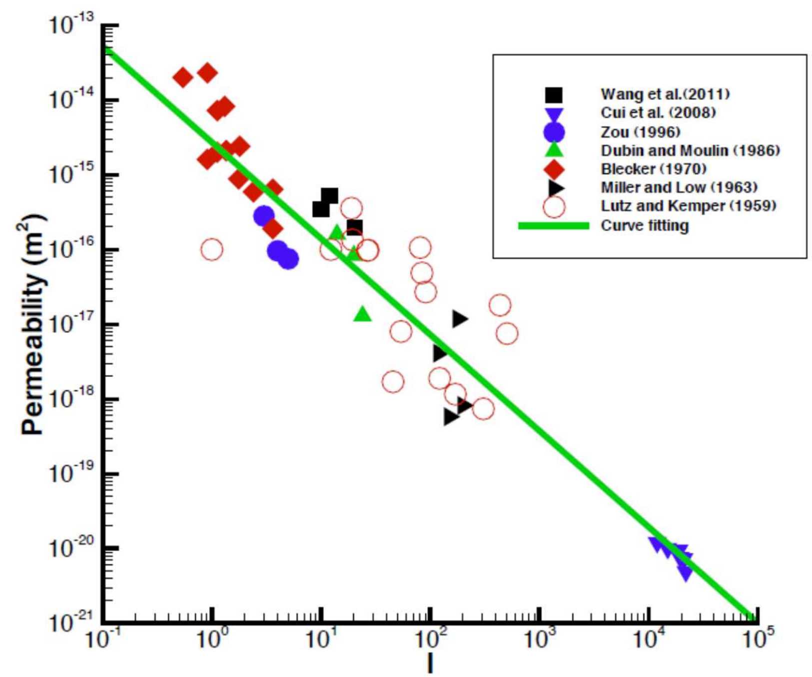


Figure 2-11. Model matches to the extraction breakthrough curves of test 08-01.

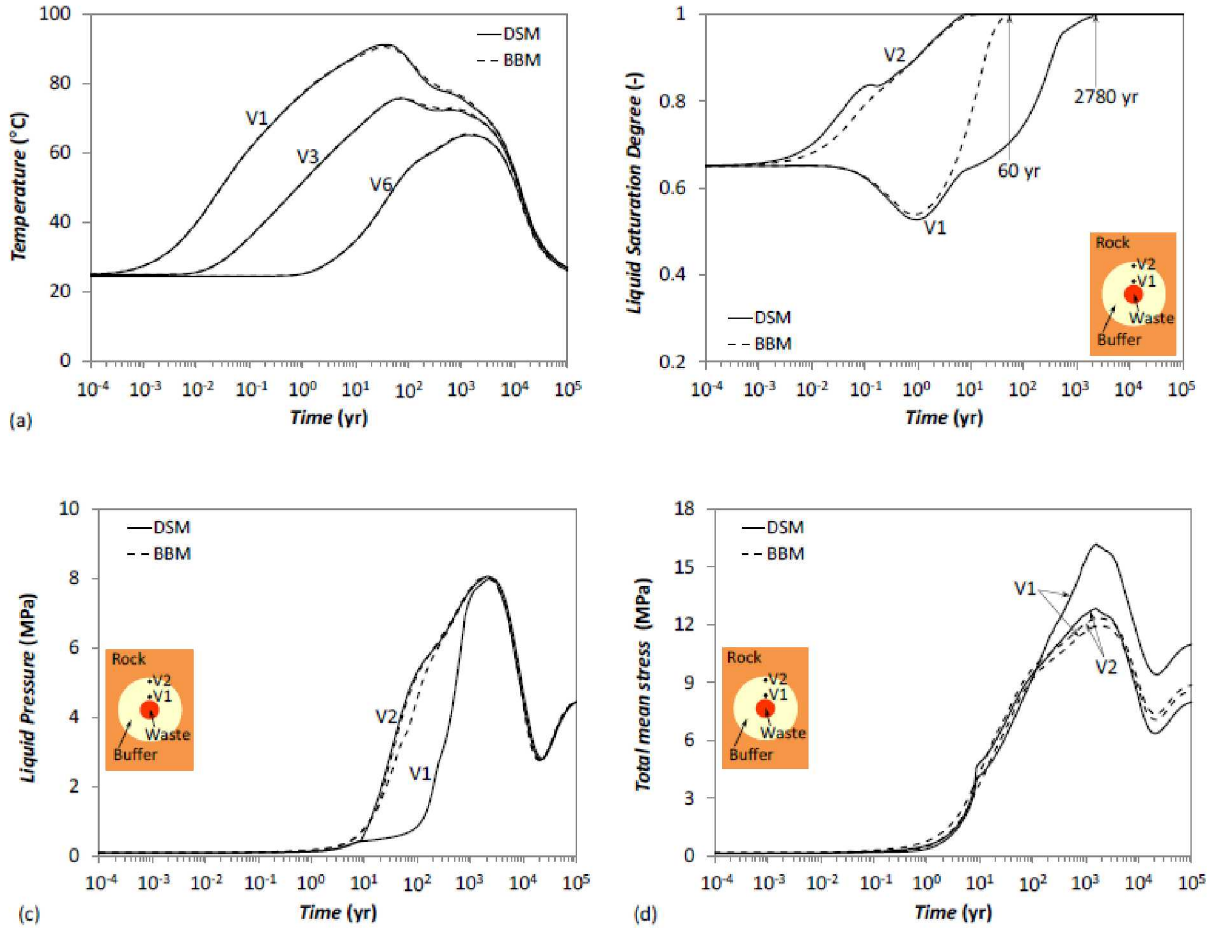


NON-DARCIAN FLOW IN LOW-K MEDIA



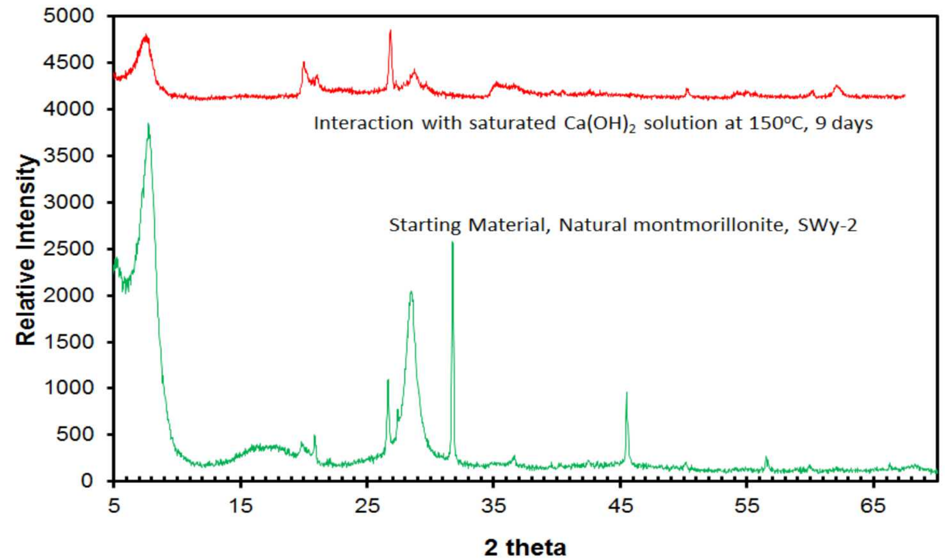


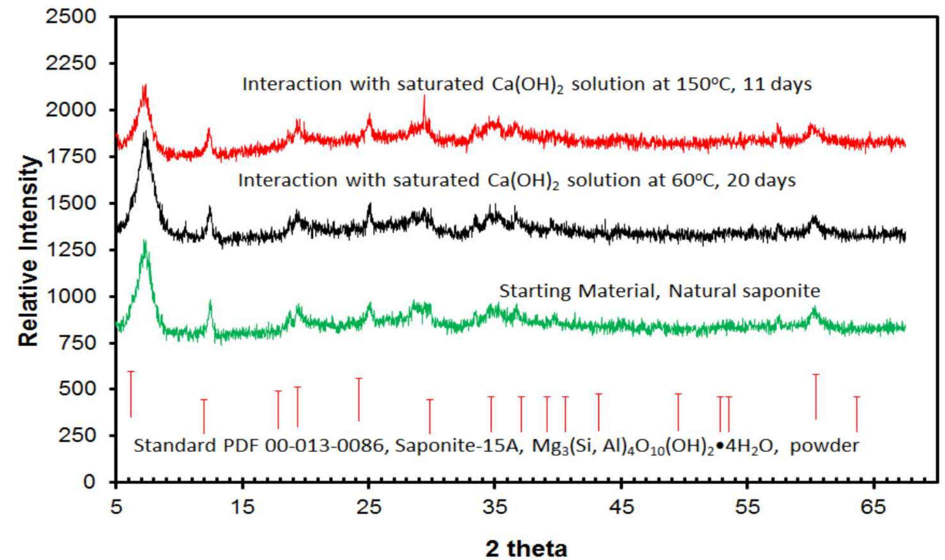
THMC MODELING OF BUFFER MATERIALS



THERMAL/CHEMICAL STABILITY OF BUFFER MATERIALS

- HTXRD data show that no significant mineralogic change in Na-montmorillonite takes place under 500 ^{o}C upon dry heating.
- Solid/water ratio plays a significant role in smectite-to-illite transformation.
- Interlayer cations play a critical role in clay stability.





RIGID-BODY-SPRING NETWORK MODEL FOR SIMULATING FRACTURE PATTERNS

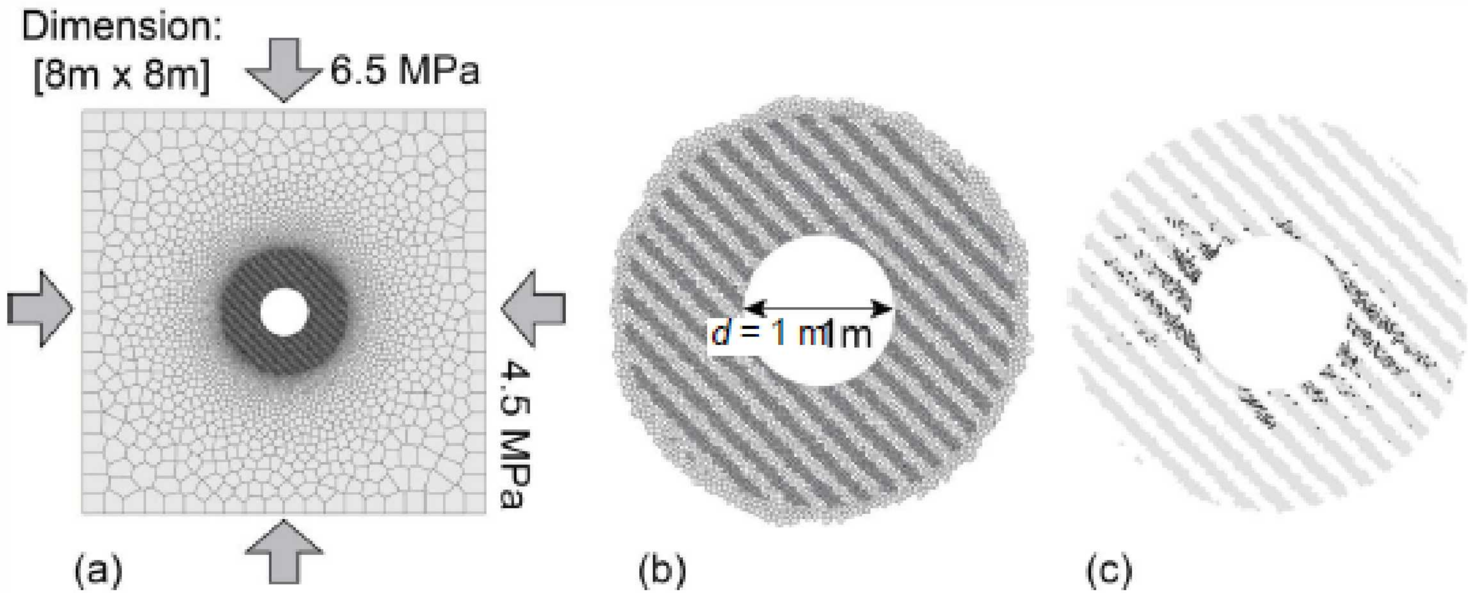
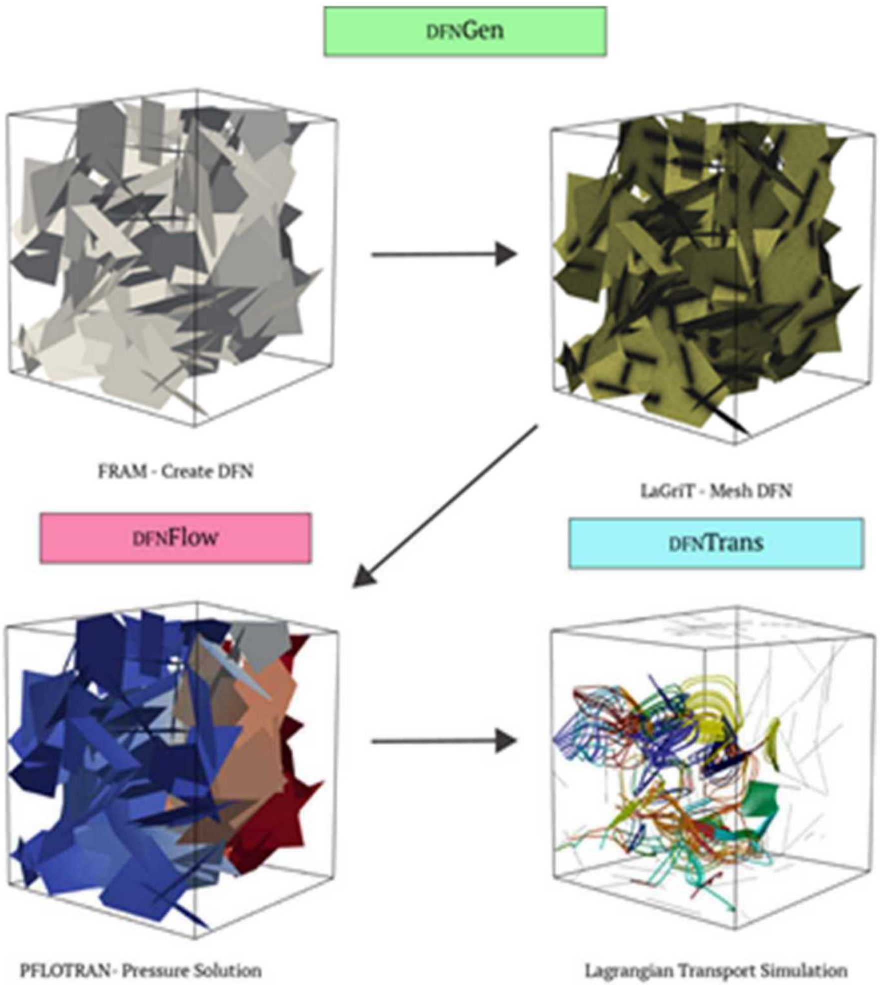
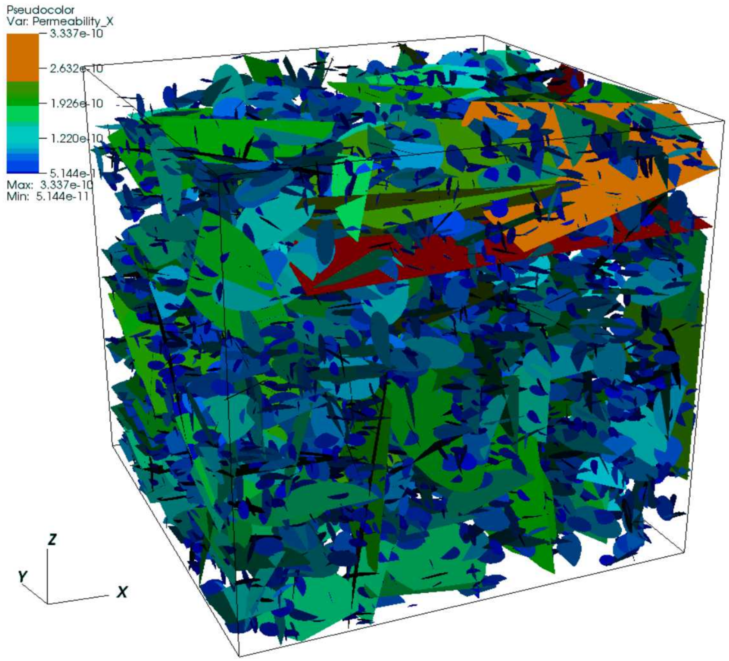


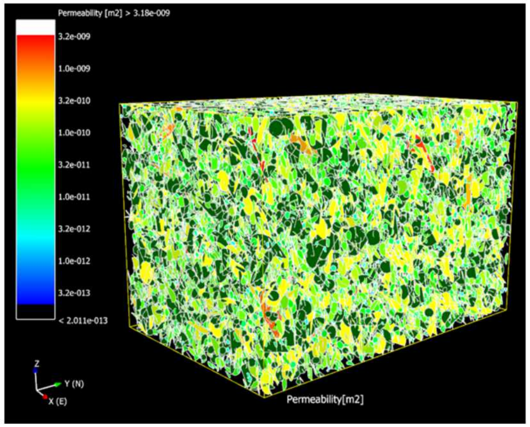
Figure 3-53. (a) Computational grid used for the RBSN simulator (10248 nodes), (b) enlarged view around the borehole, and (c) simulated fracture pattern.

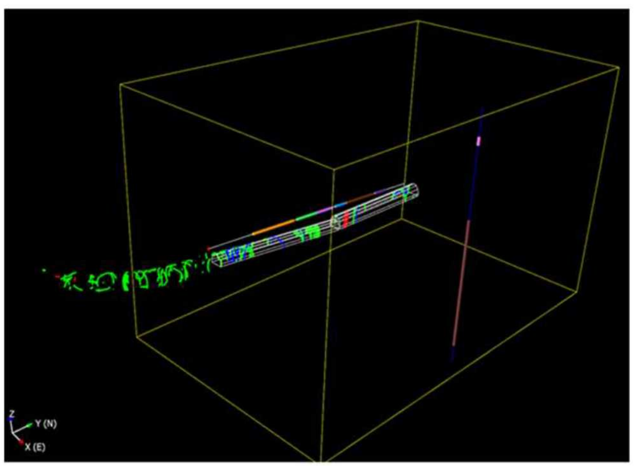
DEVELOPMENT OF DISCRETE FRACTURE NETWORK MODEL

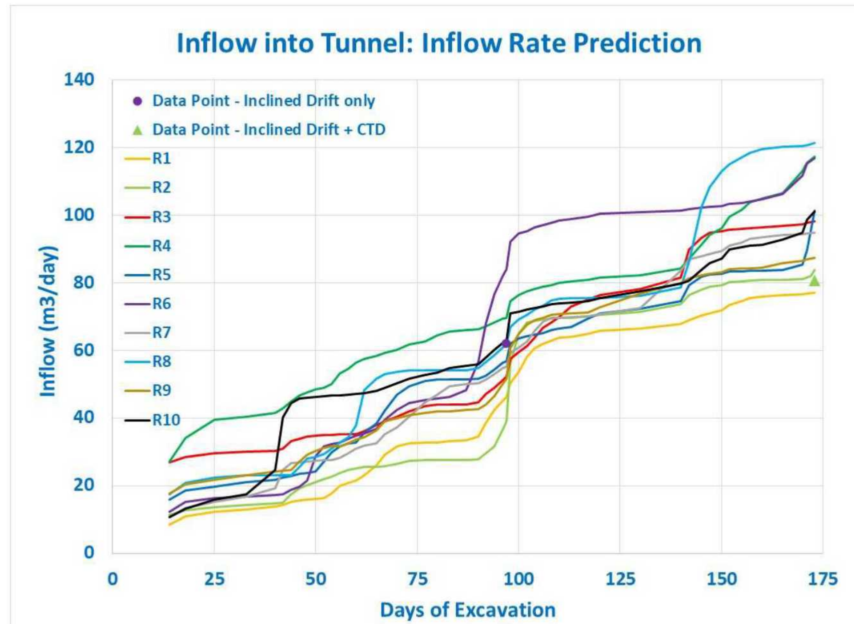




DEVELOPMENT OF A WORKFLOW FOR SYNTHESIZING FIELD DATA INTO A FRACTURE NETWORK MODEL

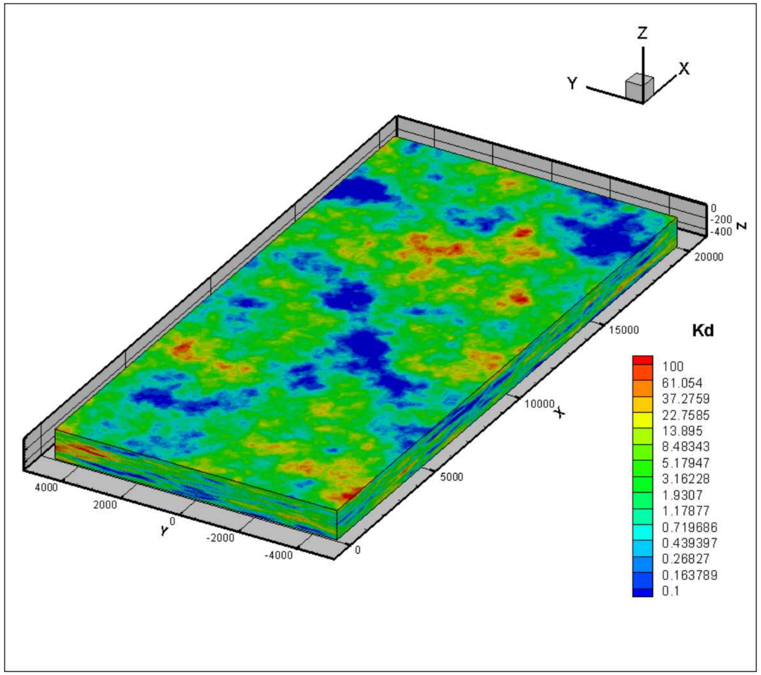


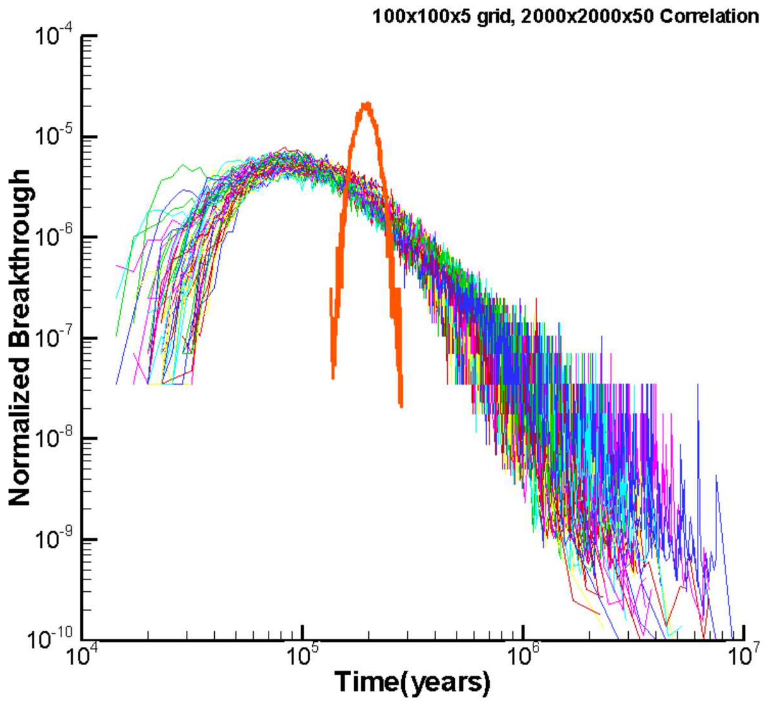




Statistical stability of fracture networks?

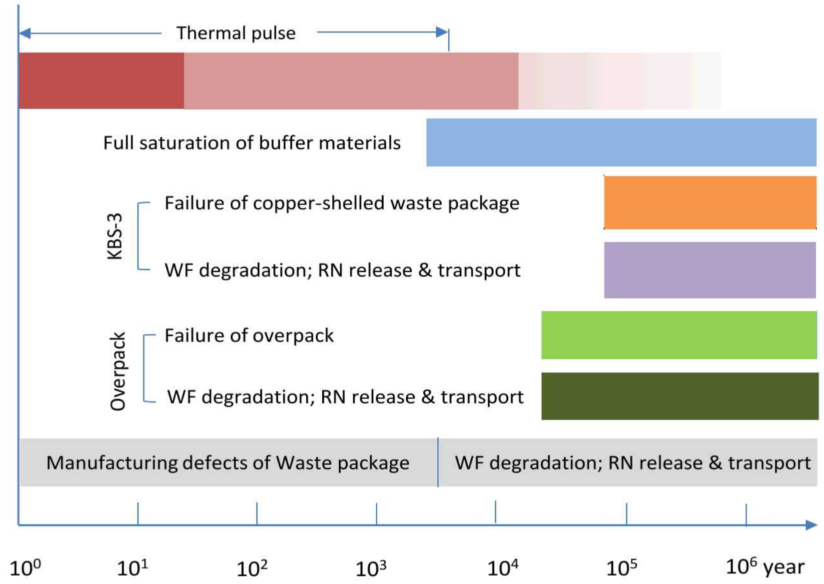
EFFECT OF HETEROGENEOUS PARTITION COEFFICIENT ON RADIONUCLIDE BREAKTHROUGH





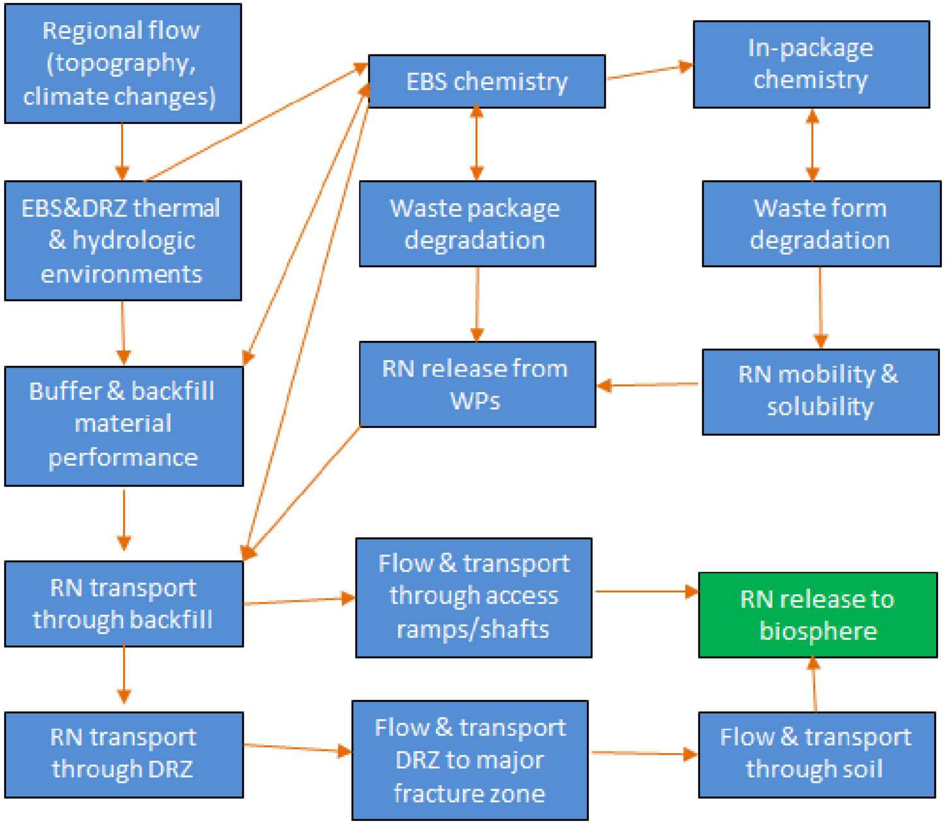
NEXT STEPS

- Develop a sensible GDSA model for sensitivity analyses.
  - Provide a minimum set of process models to GDSA (FY20)
- Move model development more towards model validation with real data.
- Develop reduced order models for incorporation into the GDSA model.
- Continue with buffer material development.
- Develop and refine EBS models, especially WP degradation models.



Towards a more realistic perception (then representation) of fluid flows in crystalline rocks

PERFORMANCE ASSESSMENT SYSTEM FOR UFD IN CRYSTALLINE ROCKS



Key features:

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

QUESTIONS?

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