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Flow and Transport in Fractured Granite: Modeling Studies involving the BRIE, GREET, and LTDE Experiments

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LA-UR-19-21112

Crystalline Rock Team

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Underground Research Labs (URLs):

Bentonite Rock Interaction Experiment (BRIE)

Groundwater Recovery Experiment in Tunnel (GREET)

Long Term Diffusion Experiment (LTDE)

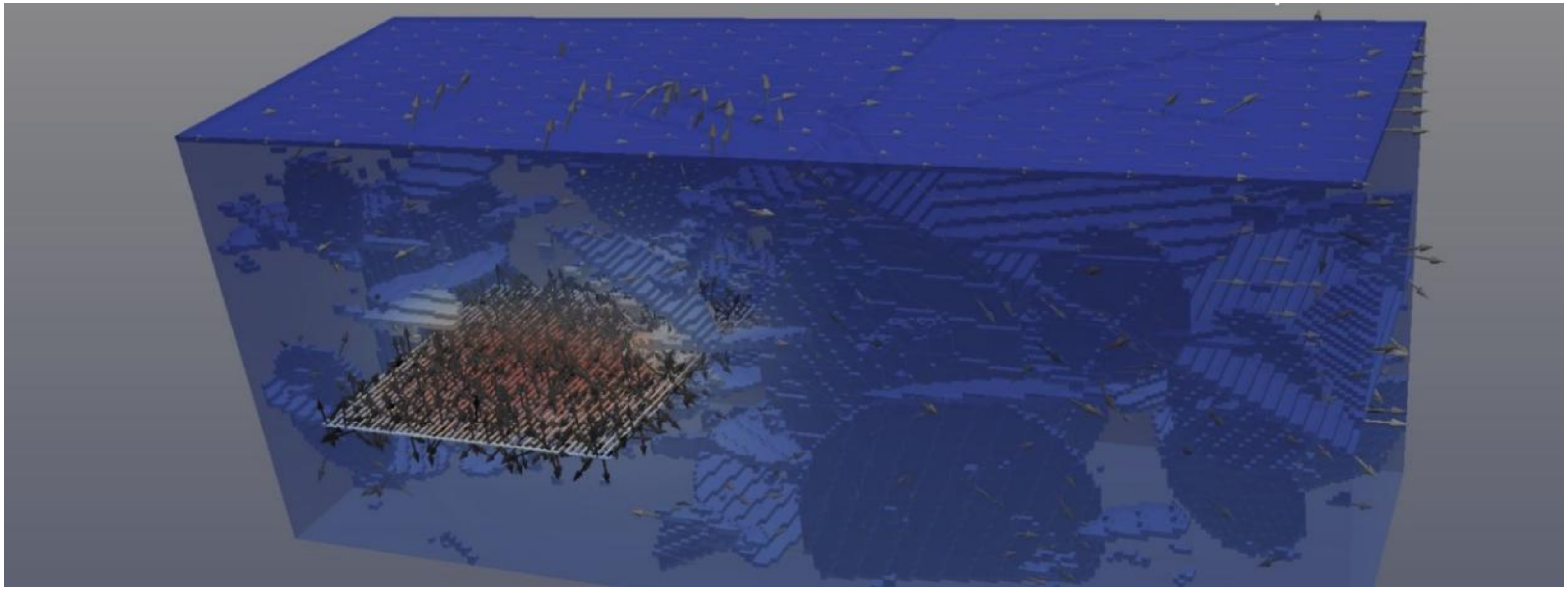
Los Alamos NATIONAL LABORATORY EST.1943

Sandia National Laboratories

SKB

Importance to Geologic Repository Post-Closure Safety

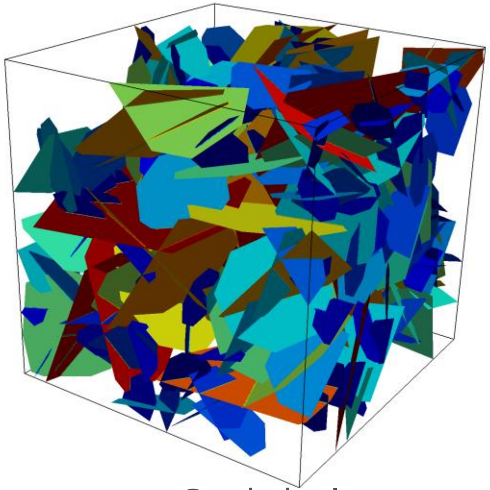
Generic Geologic Disposal Safety Assessment in Crystalline Rock



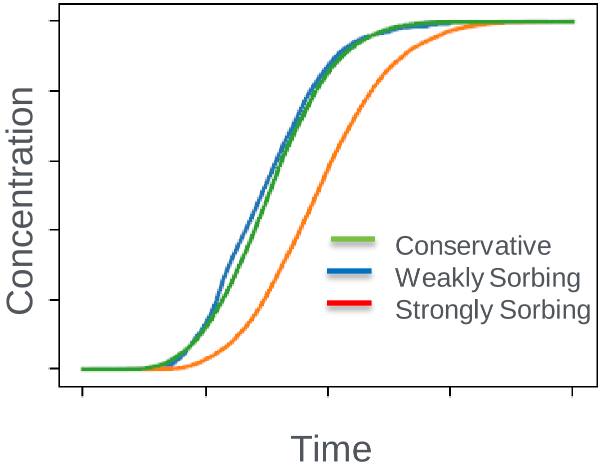
- Post-closure, fractures are primary pathways into bentonite filled deposition holes (BRIE) and drive resaturation around tunnels (GREET)
- Fracture networks are one of the primary pathways for radionuclides to transport from the near field to the far field in crystalline rock (LTDE)

Conceptual Model

Fractured Rock
Outcrop at Field Site
50 m x 50 m



Statistical
Discrete Fracture
Network Model



Typical Quantity of Interest

How these processes affect repository performance: potential for high permeability pathways to accessible environment

Fracture data needs: fracture orientation, spacing, aperture distributions, matrix diffusion

Transport data needs: same as non fractured systems, fracture roughness, surface area

R&D Context: State of the Art for Flow and Transport in Fractured Rock Systems

- Fractures are the primary flow and transport mechanism in crystalline rocks
- Discrete fracture network models, complex continuum approaches, and pipe flow models have been used to simulate these systems
- These models have evolved to include complex meshing, physics and chemistry for mechanistic representations of flow and transport in fractures

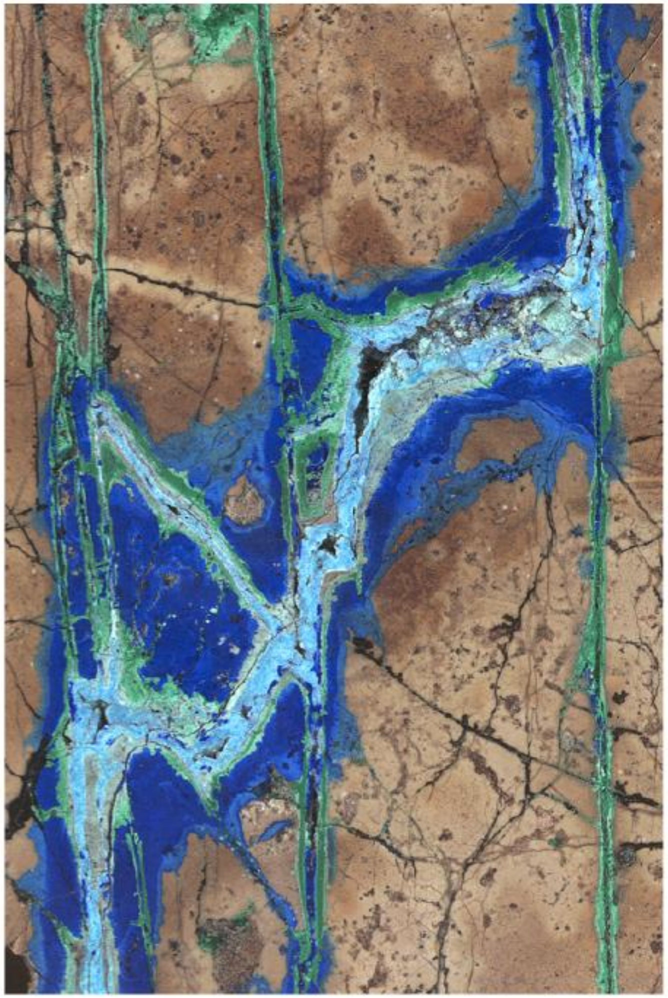


Image Courtesy of Dr. Barb Dutrow

R&D Context: Representative Literature on Transport in Fractured Rock Systems

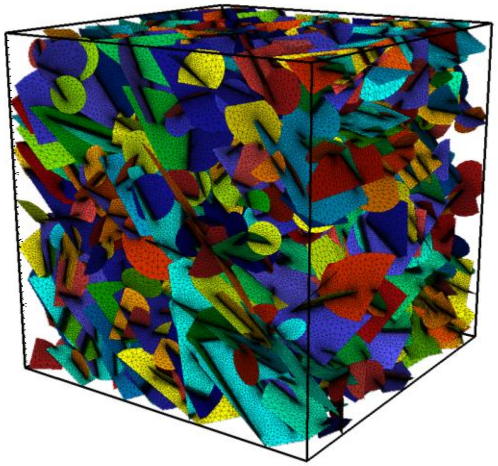
- Complex Continuum
  - Barenblatt et al., 1960
  - Neuman 2005
- Discrete Fracture Networks
  - Dershowitz et al. 1998
  - Dreuzy et al. 2014
  - Hyman et al. 2015*
- Graph-based Machine Learning Reduced Order Models
  - Viswanathan et al. 2018*
  - Srinivasan et al. 2018*

Photo by Lee Lau

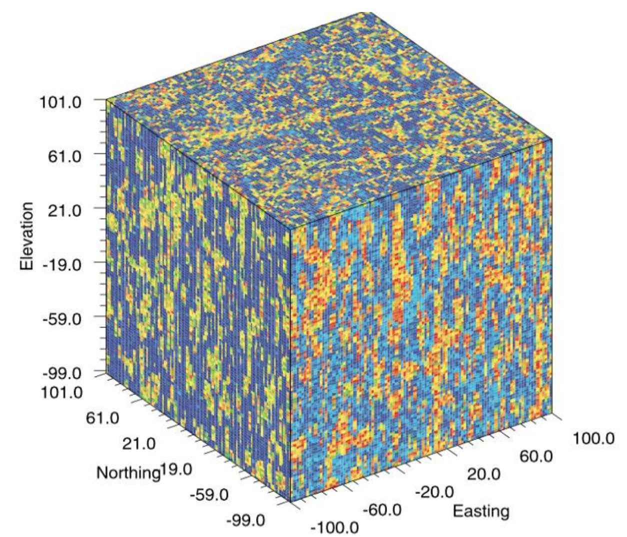
*** Our team's publications**

R&D Context: Outstanding Questions for Transport in Fractured Rock Systems

- Discrete fracture networks can explicitly account for topology of the fracture network but topology in the field is typically only known statistically so is this complexity warranted?
- Continuum models ”smooth” out the structure but for large scale problems are they sufficient?
- Are reduced order models (e.g. graph-based machine learning emulators) sufficient and necessary for uncertainty quantification?



LANL Discrete Fracture Network



SNL Fractured Continuum Model

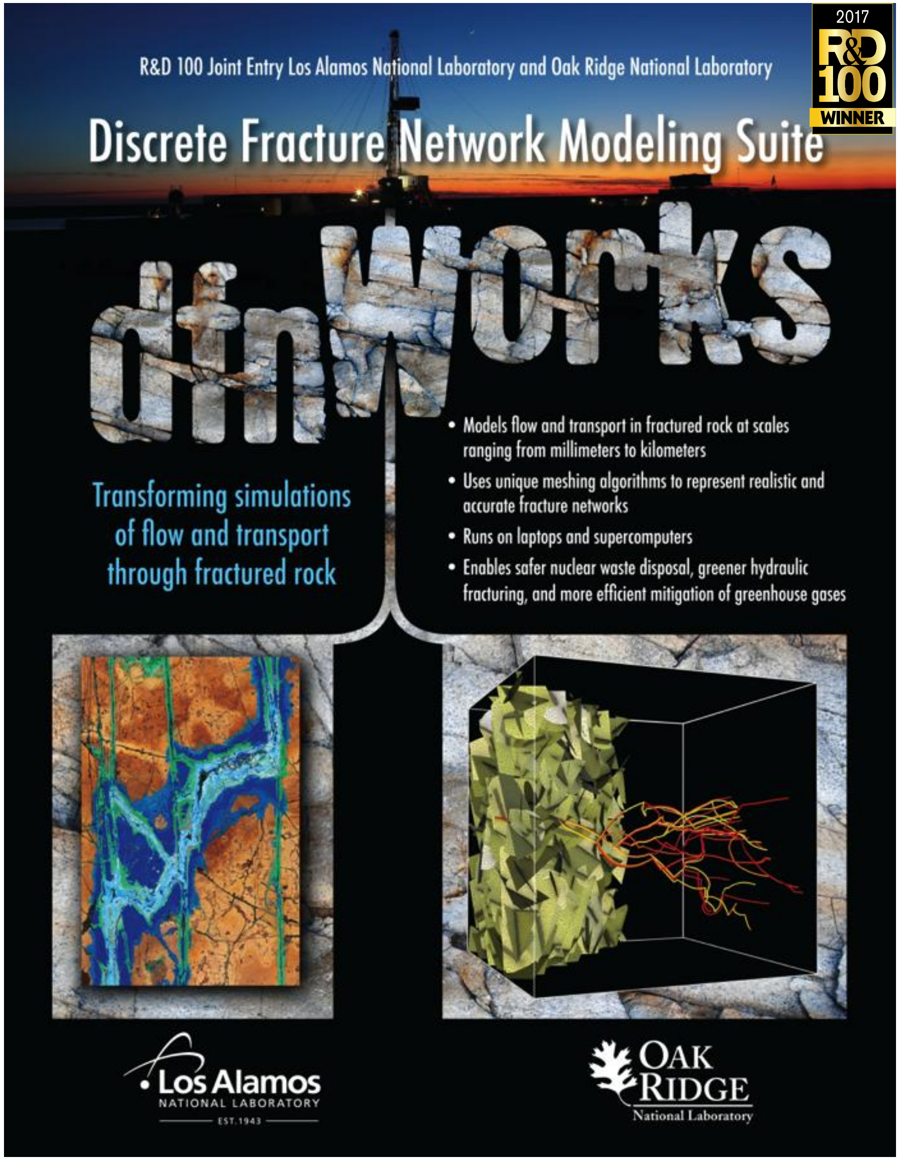
Field tests are key for validation and International work has been critical

R&D Context: R&D gap and needs for Flow and Transport in Fractured Rock Systems

- During last decade observations at field sites improved providing rock and fracture network characteristics.
- This created a need for an advanced modeling tool for numerical representation of fracture networks, followed by accurate flow & transport simulations.
- SKB Laboratory, Sweden, provided fracture network characteristics data needed to validate numerical simulations of flow and transport through fracture networks.
- Development started in 2013 under UFD and R&D100 winner in 2017

JD Hyman, S Karra, N Makedonska, CW Gable, SL Painter, HS Viswanathan, dfnWorks: A discrete fracture network framework for modeling subsurface flow and transport, Computers & Geosciences 84, 10-19, 2015.

dfnWorks.lanl.gov



International Experiment Participation

Bentonite Rock Interaction Experiment (BRIE):

Characterize bentonite inflow and erosion questions

Groundwater Recovery Experiment in Tunnel (GREET):

Study resaturation and chemical effects

Long Term Diffusion Experiment (LTDE):

Measure radionuclide transport and matrix diffusion

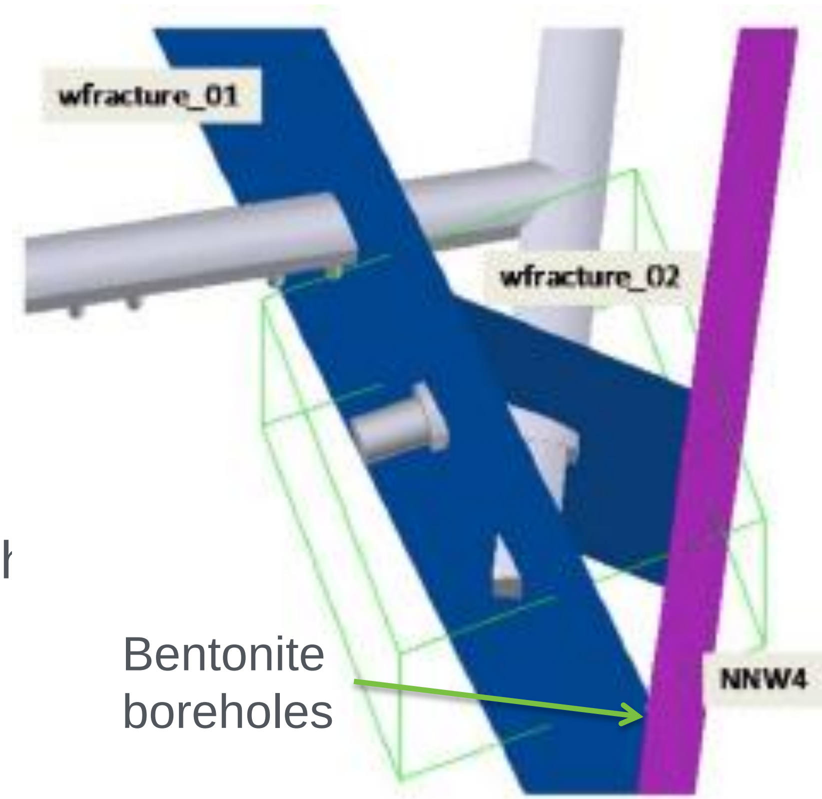
Field Tests: Bentonite Rock Interaction Experiment (BRIE), Sweden, 2013-2015

How water flows from surrounding fracture network into bentonite-filled boreholes?

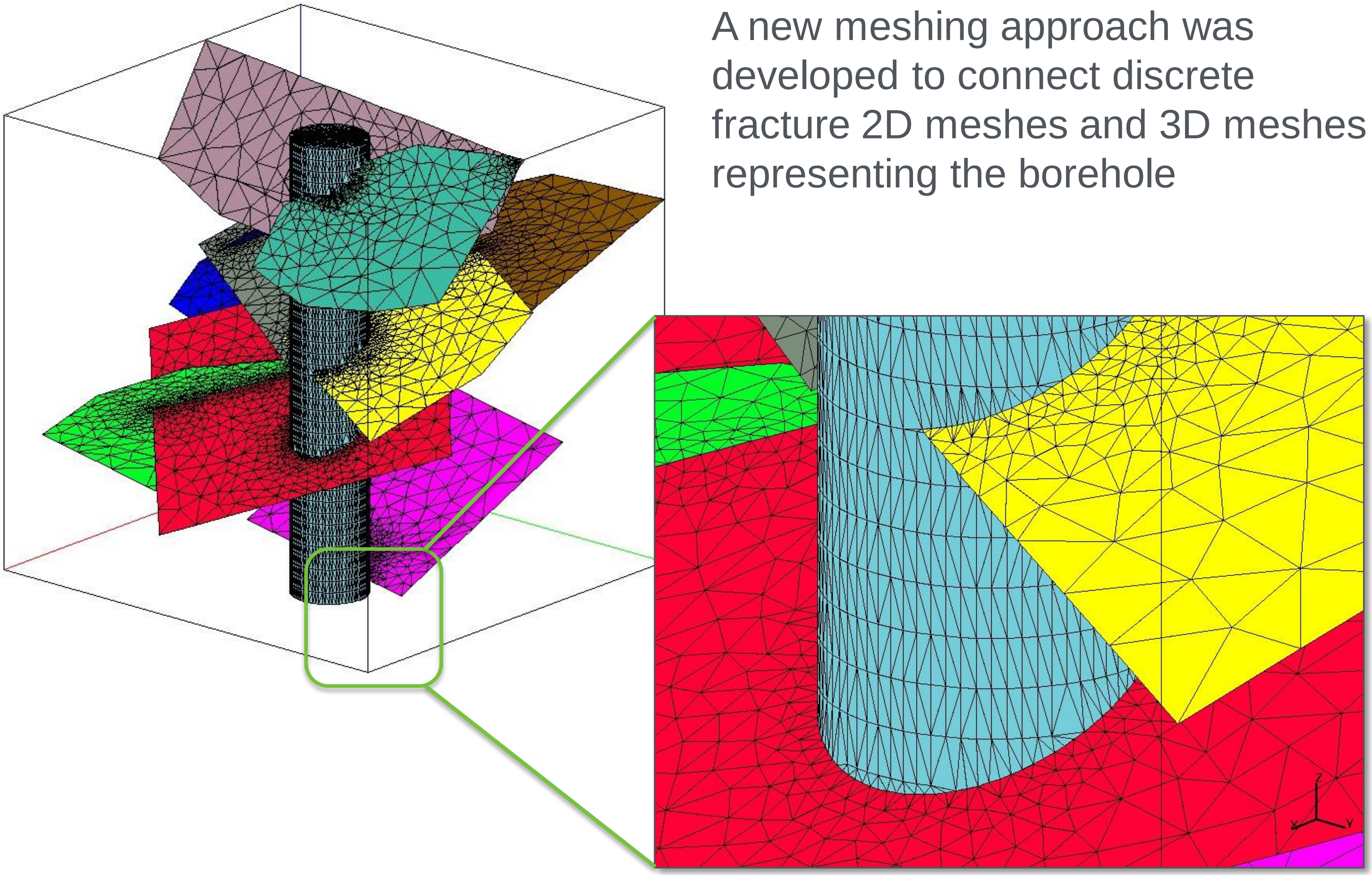
Discrete Fracture Network is used to represent the fractures around borehole *(2D triangular mesh)*

3D volume mesh at the cylinder represents the borehole

DOE shaped a more integrated effort witl a move toward uncertainty quantification



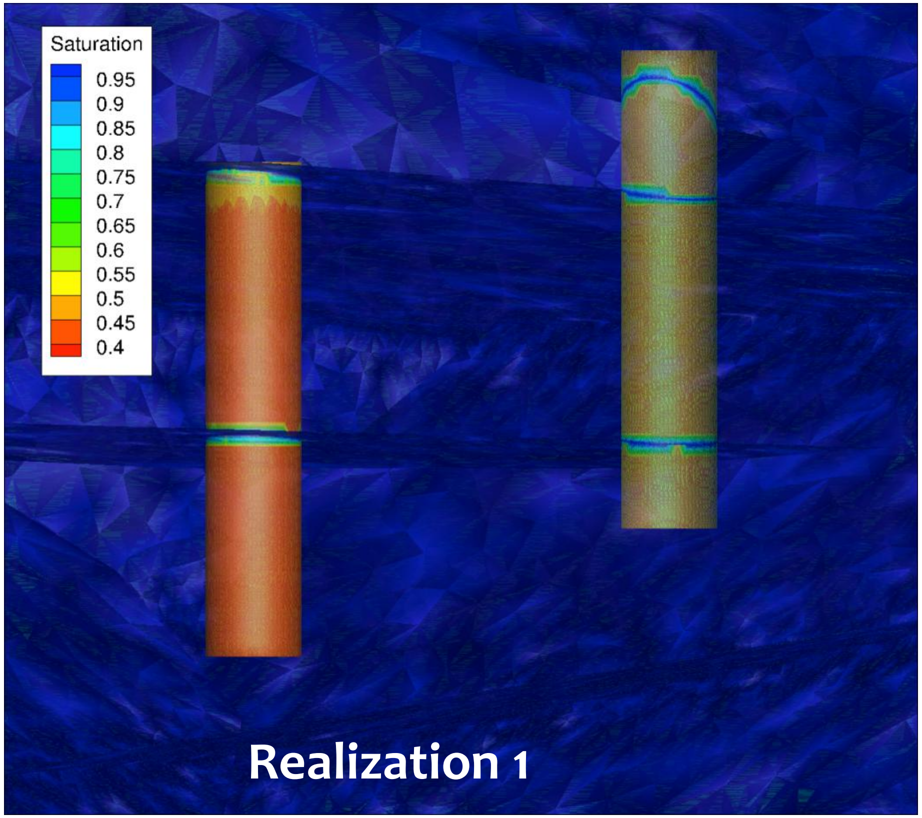
Field Tests: Bentonite Rock Interaction Experiment (BRIE)

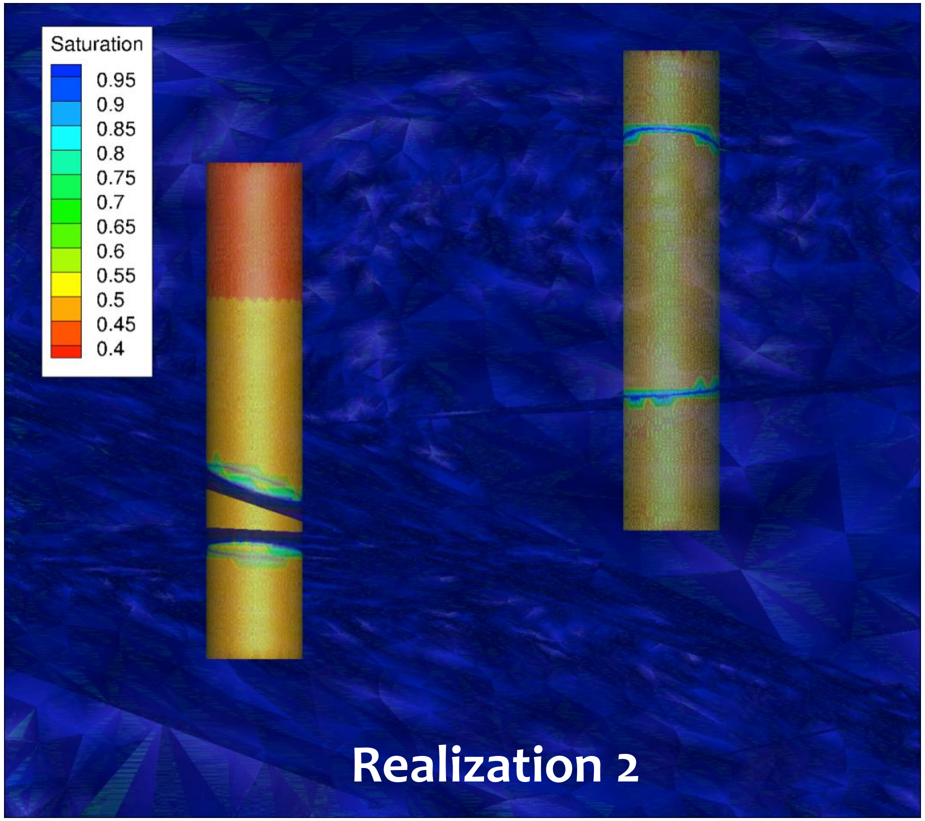


A new meshing approach was developed to connect discrete fracture 2D meshes and 3D meshes representing the borehole

Field Tests: Bentonite Rock Interaction Experiment (BRIE)

Two phases (air and water) solution 3 months



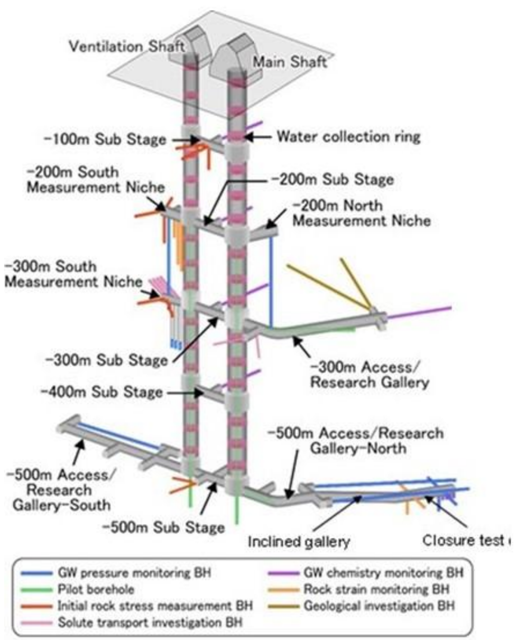


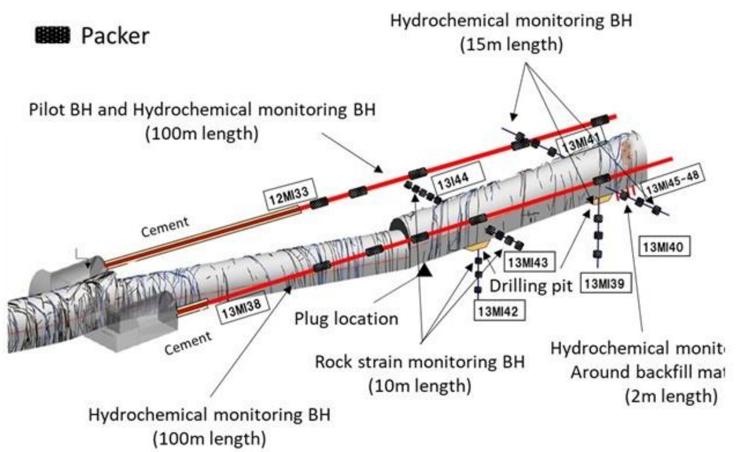
- Steep gradient in liquid saturation in the bentonite near where it intersects with fractures as observed in the field
- Bentonite rewets uniformly

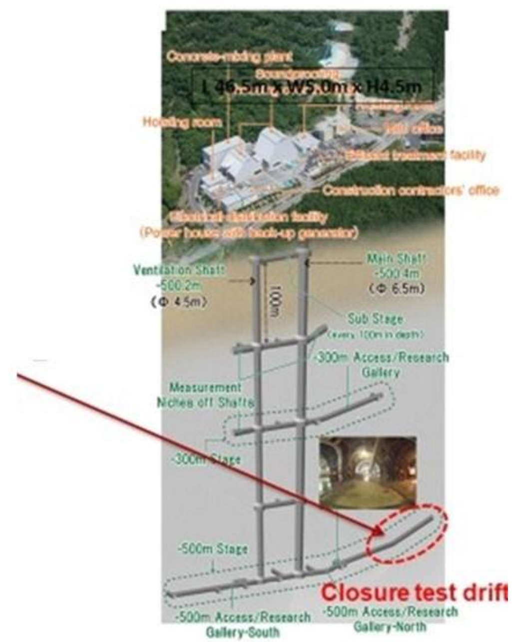
First dfnWorks application to a field site in 2014

DECOVALEX19 Task C: GREET (Groundwater Recovery Experiment in Tunnel), Japan, 2014-Present

- GREET provided field experimental data on fractures, hydrology and transport supporting the study of nuclear waste disposal in crystalline rock.
- Experiments conducted by Japan Atomic Energy Agency (JAEA) at the Mizunami Underground Research Laboratory
- URL located at Tono area (Central Japan)



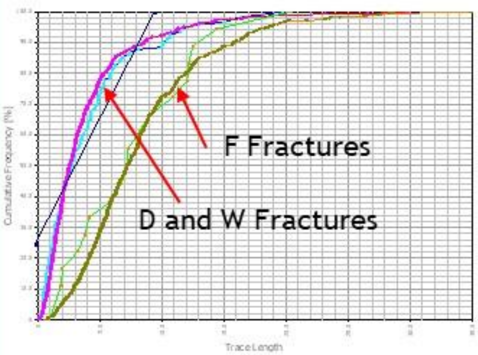




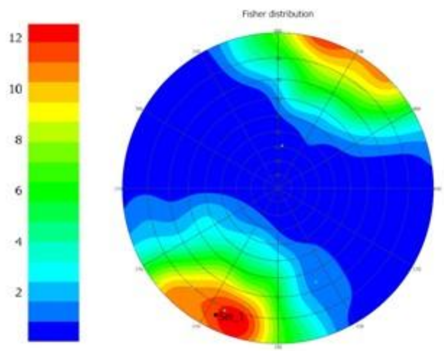
GREET: Development of DFN and FCM

Fracture data:
- 2,023 fractures in the tunnel; 146 included in the model
- 297 fractures in borehole 12MI33; 17 included in the model

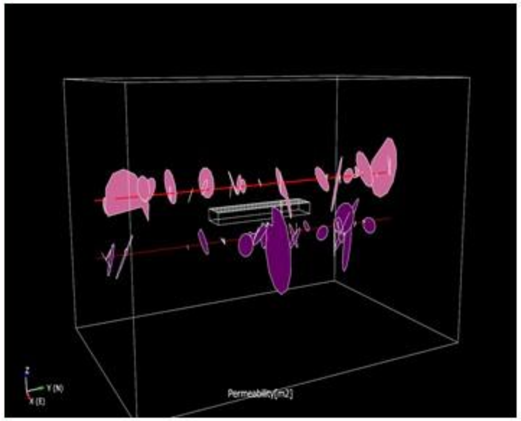
Fracture Size Distribution



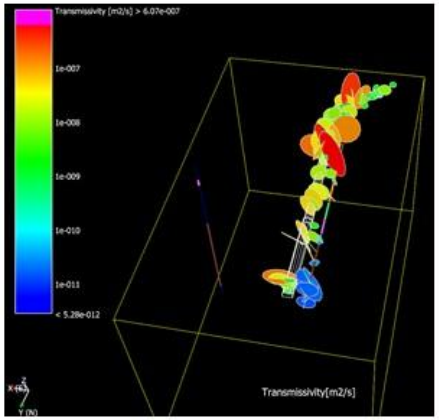
Fracture Orientation



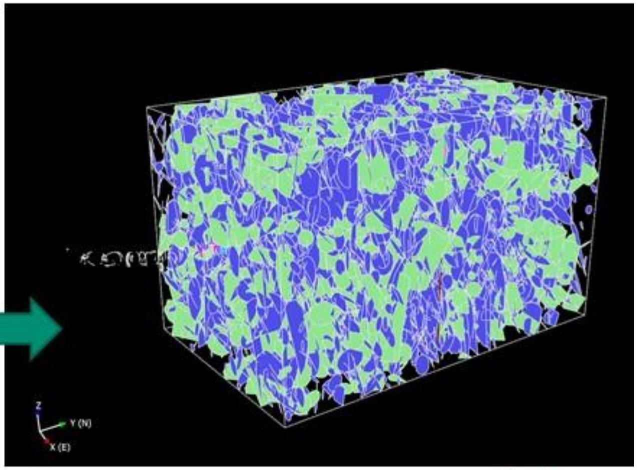
Fracture Intensity



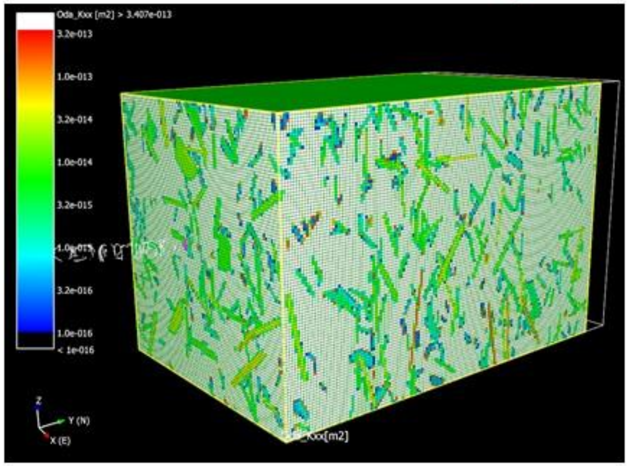
Fracture Transmissivity



DFN Model



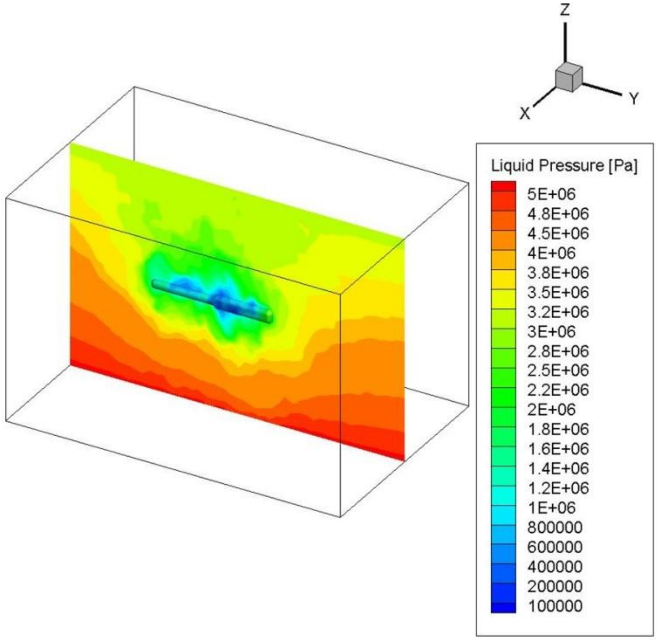
FCM Model

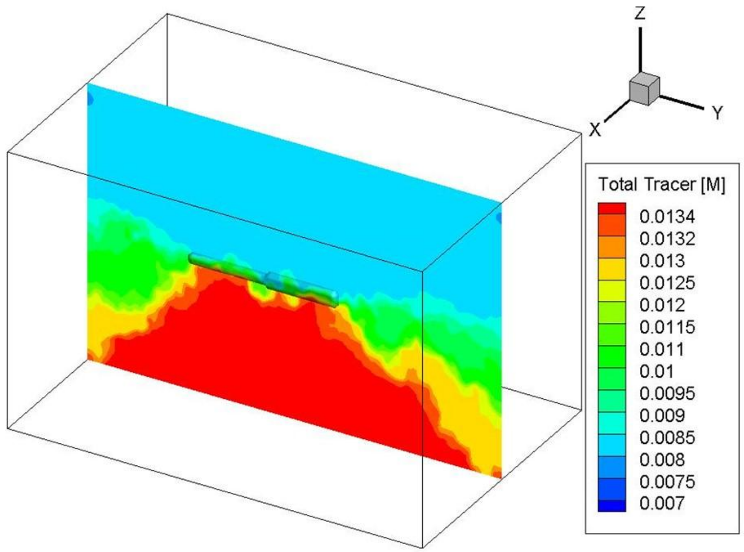


GREET: Simulation of Flow and Non-Reactive Transport During Excavation

- JAEA project experimental data was used to conduct simulation of flow and transport using a site-scale domain.
- Upscaled permeability and porosity used in simulations.
- Pressure and chloride concentration initial and boundary conditions based on measure data.

Simulation results for pressure and chloride concentration at end of excavation:

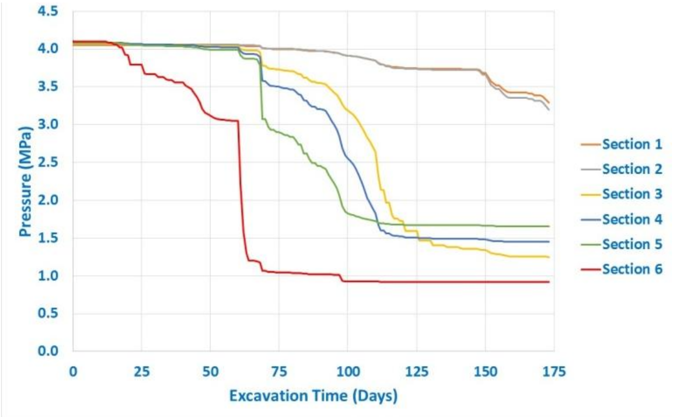




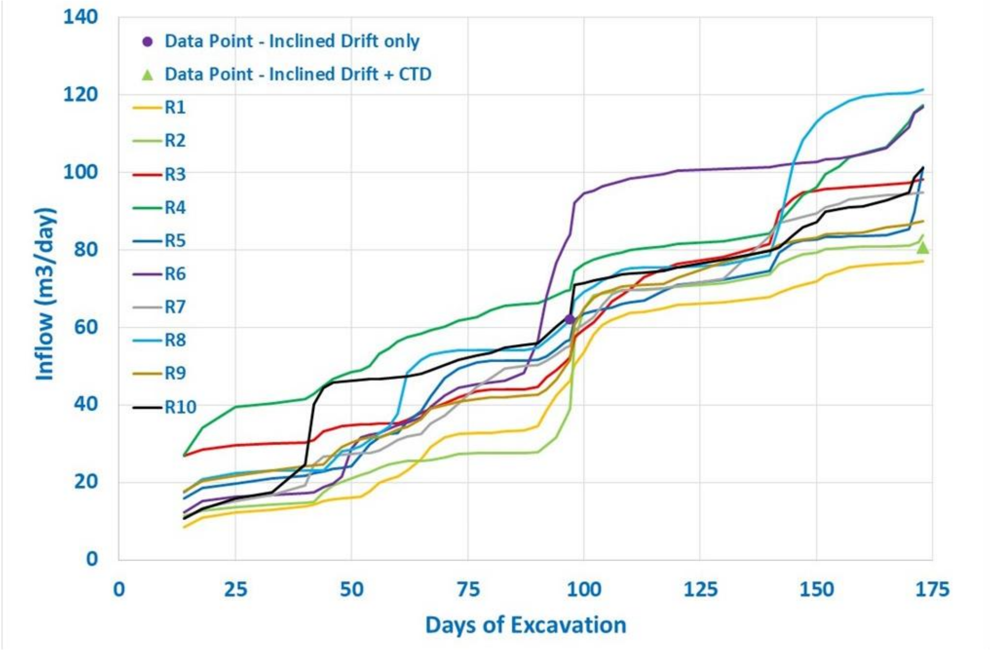
GREET: Predictions of Inflow and Pressure and Chloride at Observation Points in a Monitoring Borehole

- Tunnel Excavation progress data and location of observation points used in simulations

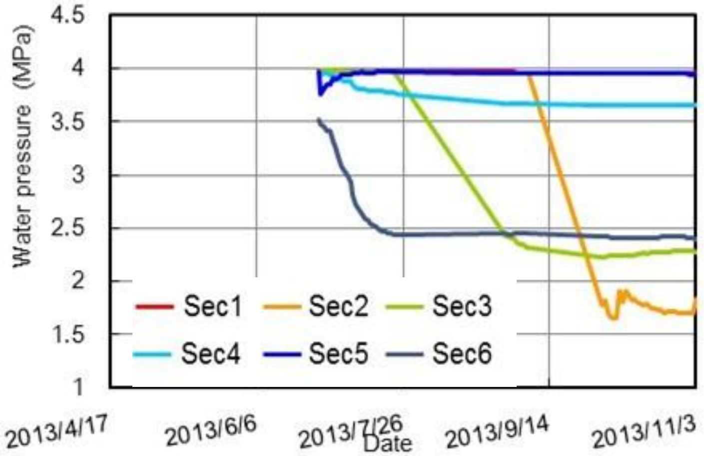
Pressure prediction



Inflow rate predictions and experimental data



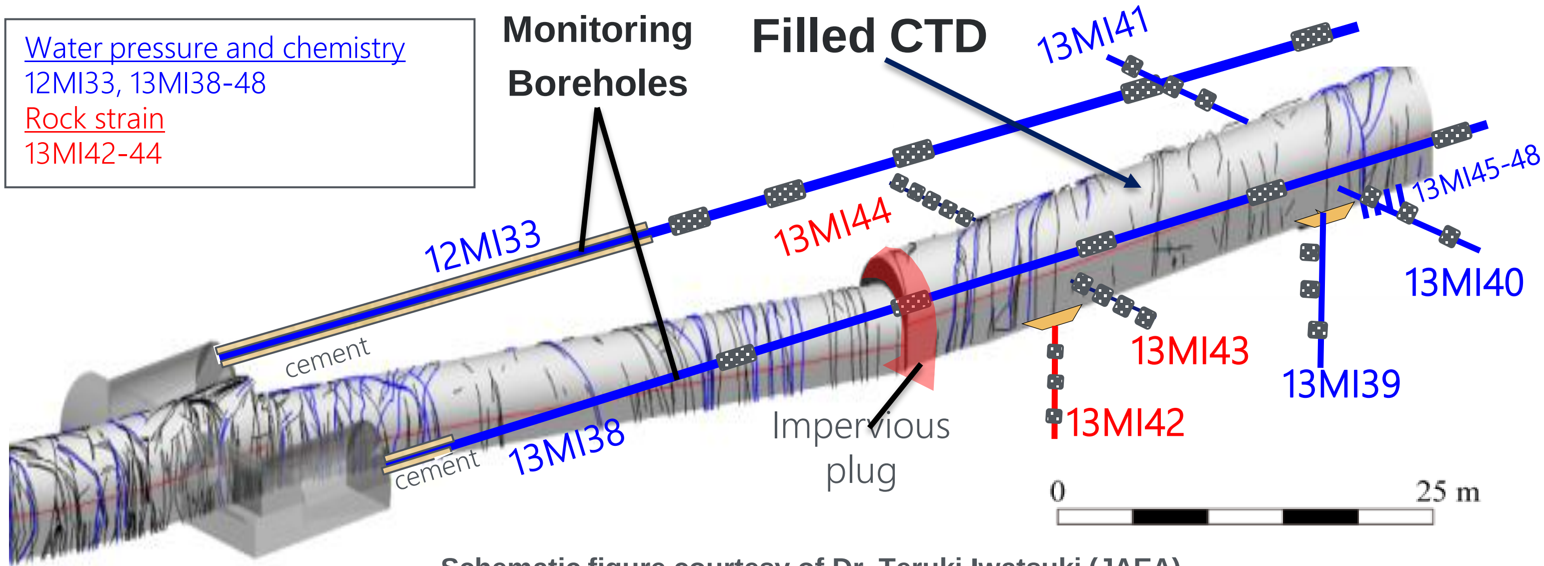
Observation data



DECOVALEX19 GREET Task C: Closure Test Drift (CTD) Geochemistry & Reactive Transport Modeling

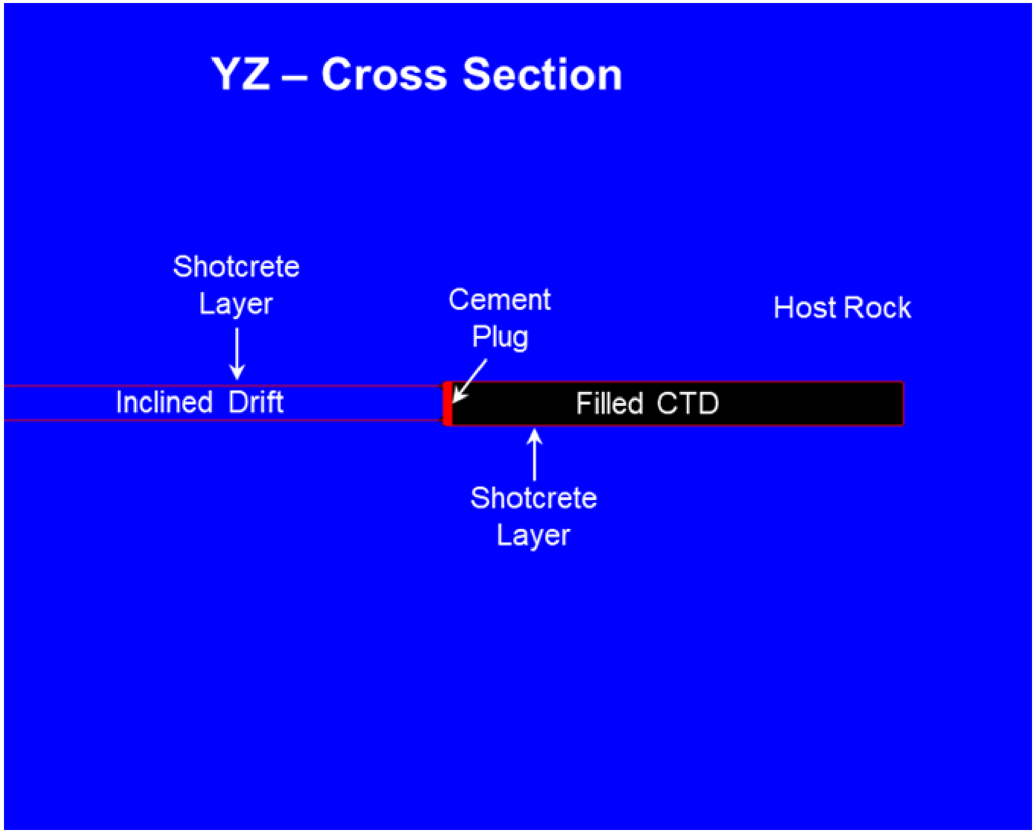
– Step 2a-b Preliminary Reactive Transport Simulations

- **Focus**: Predictions of filled CTD water chemistry resulting from interactions with cementitious materials under saturated conditions
- PFLOTRAN reactive transport simulation code (Lichtner et al. 2017):
  - » Adopted structured mesh of flow and transport simulations (Hadgu) but with shotcrete layer (0.1 m thick) surrounding tunnel
  - » Using transition state theory (TST) mineral kinetics expressions for portlandite



Schematic figure courtesy of Dr. Teruki Iwatsuki (JAEA)

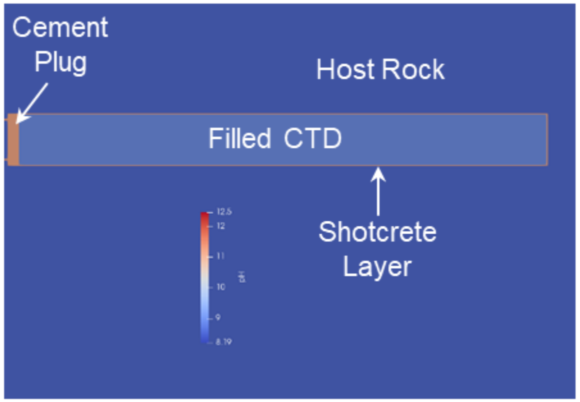
DECOVALEX19 GREET Task C (Step 2b): PFLOTRAN Reactive Transport (RT) Model Domain



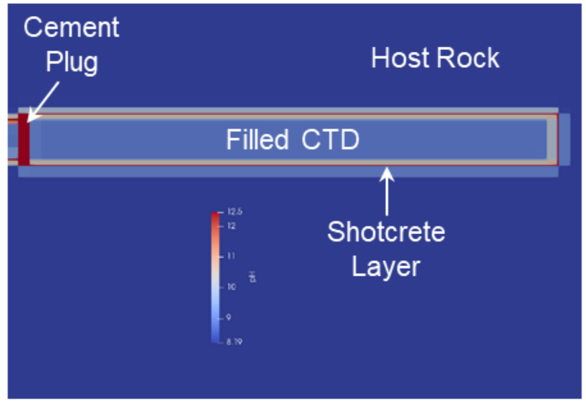
- **PFLOTRAN Reactive Transport (RT) Simulation**
  - **3D structured mesh**
  - **Focused on filled CTD with dilute groundwater**
  - **Starting pH 8.9**
  - **Shotcrete: generic (no brucite)**
  - **Diffusion only problem**
  - **400-600 days simulation**

DECOVALEX19 Task C (Step 2b): PFLOTRAN 3D Reactive Transport (RT) Model

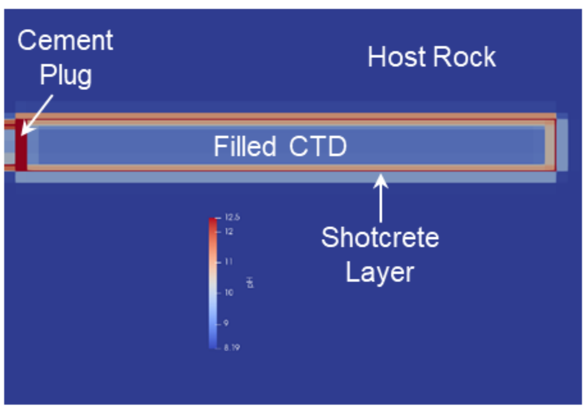
Filled CTD → pH Mapping (Prelim. Results)



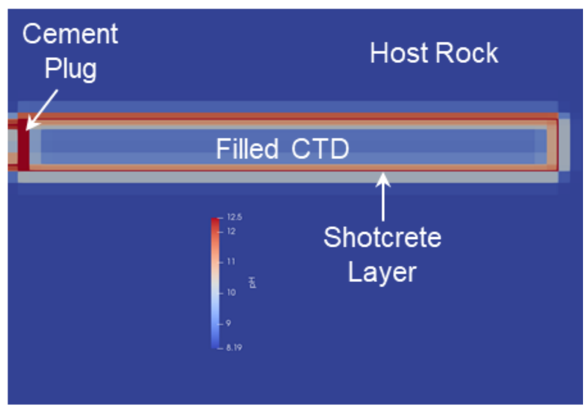
0 days



60 days



150 days

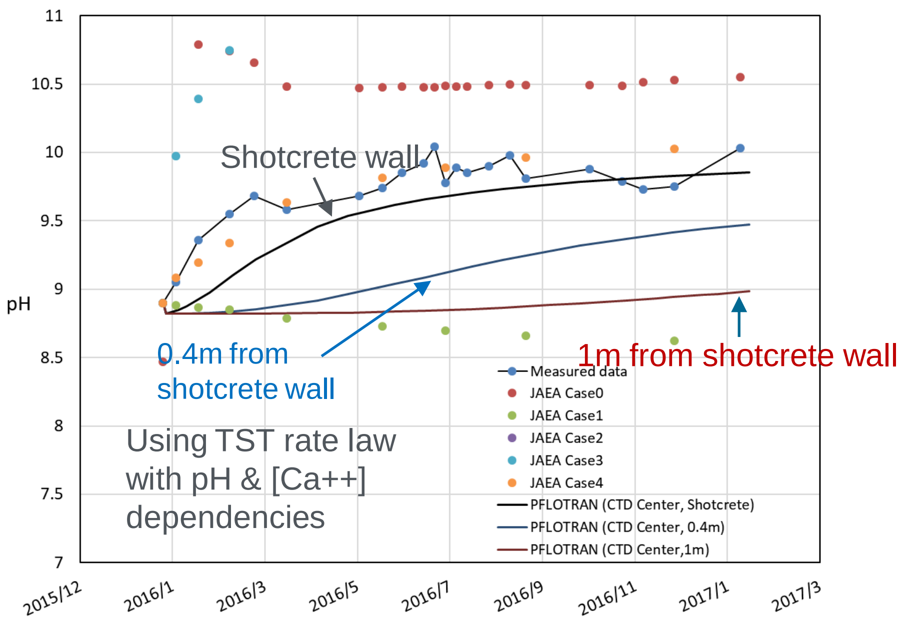


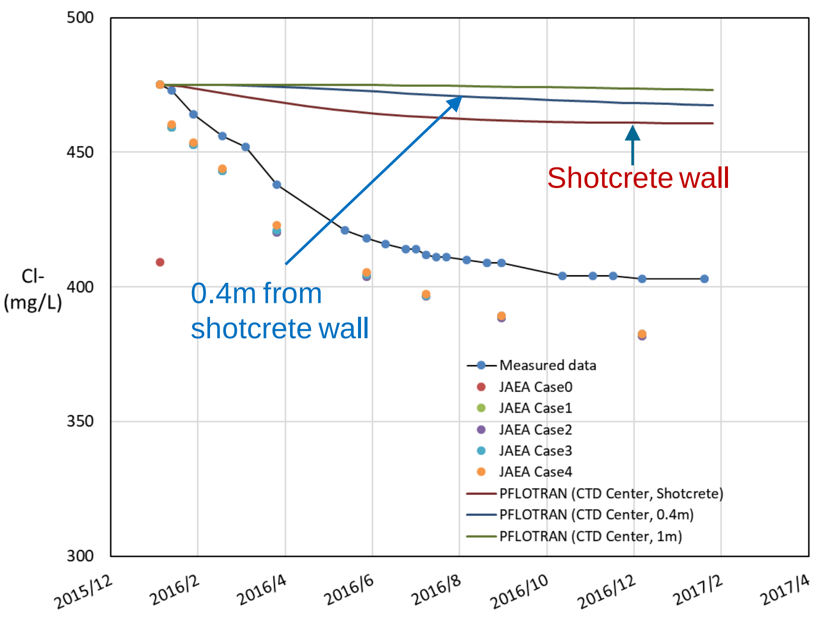
300 days

WORK IN PROGRESS!!!

- ❑ **Reaction Front Simulation**
  - **pH increases with time within CTD**
  - **Diffusion front migration towards inner CTD center**
  - **[Cl-] decreases with time**
- ❑ **Questions?**
  - **Deviations from measured data – both pH and [Cl-]**
  - **Diffusive transport effects? – Not likely**
  - **Kinetic rate treatment?**
    - **Using TST rate law expression for portlandite with [Ca] dependencies**
  - **Consideration of Cl-bearing cement phases**

DECOVALEX19 Task C (Step2b): PFLOTRAN 3D Reactive Transport (RT) Model





WORK IN PROGRESS!!!

❑ Filled CTD RT Simulation

- Increase in pH with time → Improved pH representation using extended TST rate law expression – Still, need to resolve discrepancies at early times
- Predicted small decrease in [Cl-] concentration → CTD [Cl$^-$] measurement show large drop with time – Considering inclusion of Cl-bearing solids (e.g., Friedl's salt) in the model
- Focus on TST kinetic rate law parameters & sensitivity analysis in modeling geochemical profiles

GREET Summary

- The modeling analysis supported by field data resulted in better fracture characterization and prediction of flow and transport. Comparison of modeling results with other DECOVALEX19 Task C teams also helped refine prediction methods.
- The simulation results showed that:
  - Upscaled fracture model provides better representation of the fractured rock compared to continuum porous medium assumption.
  - Upscaling methods are grid block size dependent.
  - Domain size is one of the important variables. A smaller domain size affects accuracy of boundary conditions and may not capture all important features.
- It was demonstrated that including fractures observed in the tunnel and in the boreholes in the DFN model results in better predictions of flow and transport with the corresponding upscaled FCM.

Comparison of Discrete Fracture Network (DFN) and Fractured Continuum Models (FCM)

Step 1: Generate fracture networks using dfnWorks

- Three fracture sets are generated based on Forsmark site fracture characteristics (Table 6-75 SKB report TR10-52)

Set	Mean trend (deg)	Mean plunge (deg)	κ	a	R_u	R_0	Number of fractures in 1 km^3
NS	90	0	22	2.5	500	15	2100
EW	0	0	22	2.7	500	15	2000
HZ	360	90	10	2.4	500	15	2300

- Fracture transmissivity is defined as function of fracture size

$$\log(\sigma) = \log\left(\gamma \cdot R^{\omega}\right) \qquad \gamma=1.6\times10^{-9},\ \omega=0.8.$$

- Fracture aperture is correlated to fracture size and calculated from transmissivity using cubic law

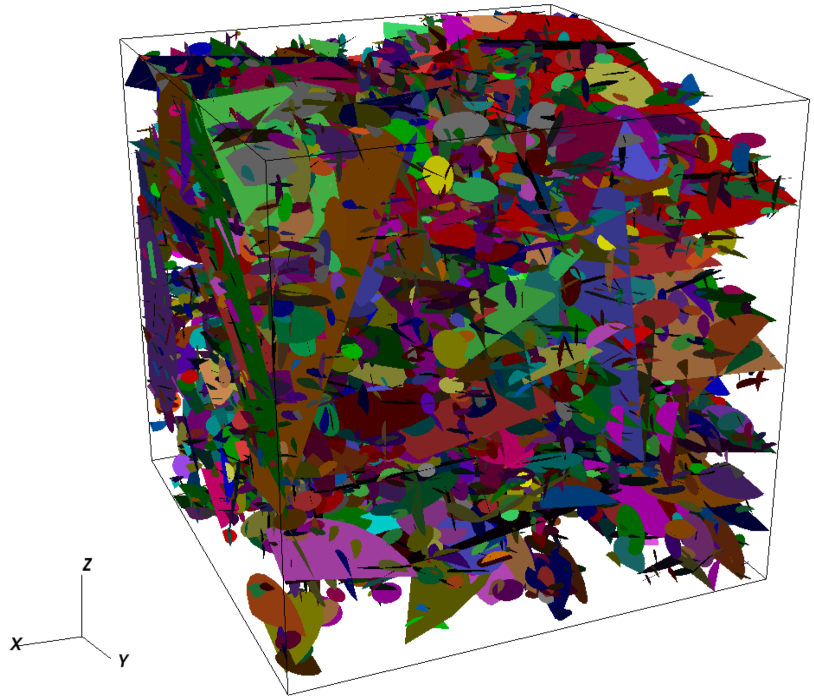
$$\sigma = \frac{b^3}{12}\frac{\rho g}{\mu}$$

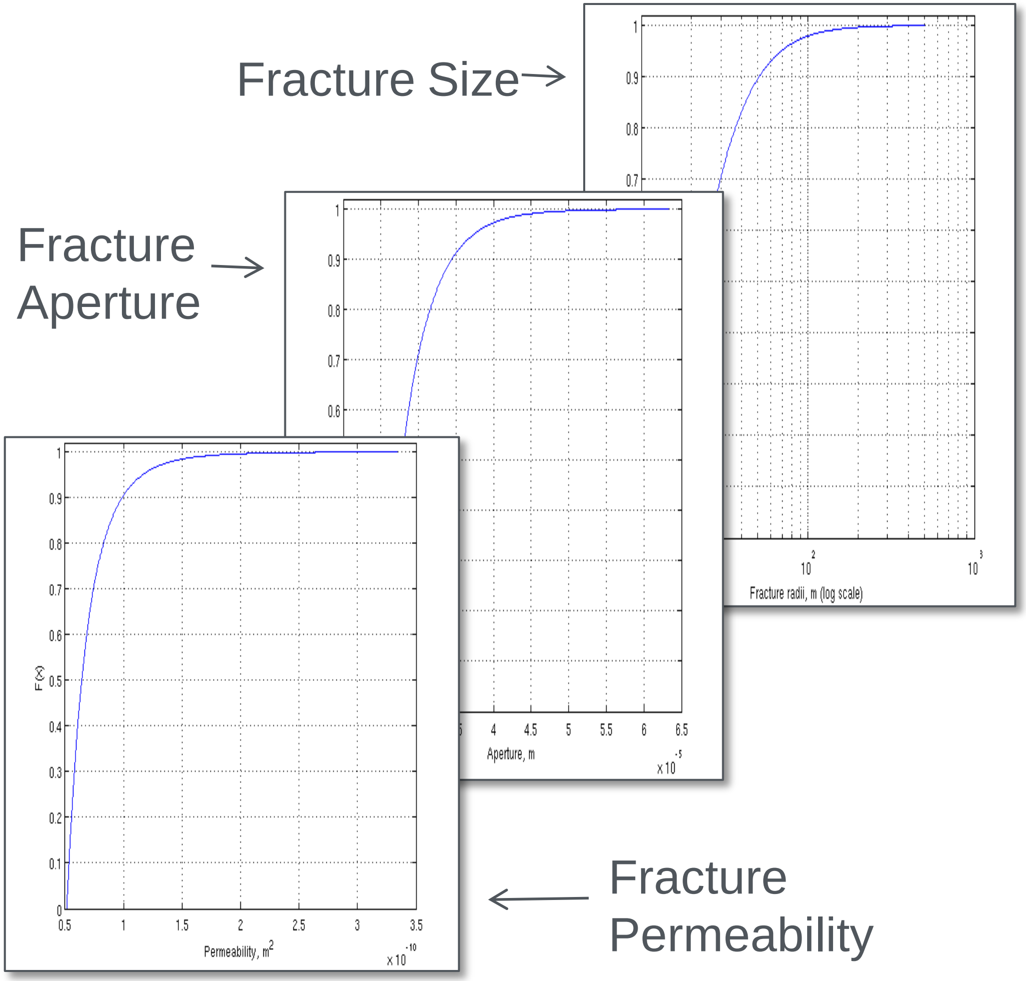
Comparison of Discrete Fracture Network (DFN) and Fractured Continuum Models (FCM)

Step 1: Generate fracture networks using dfnWorks

Statistical distributions of fracture network:

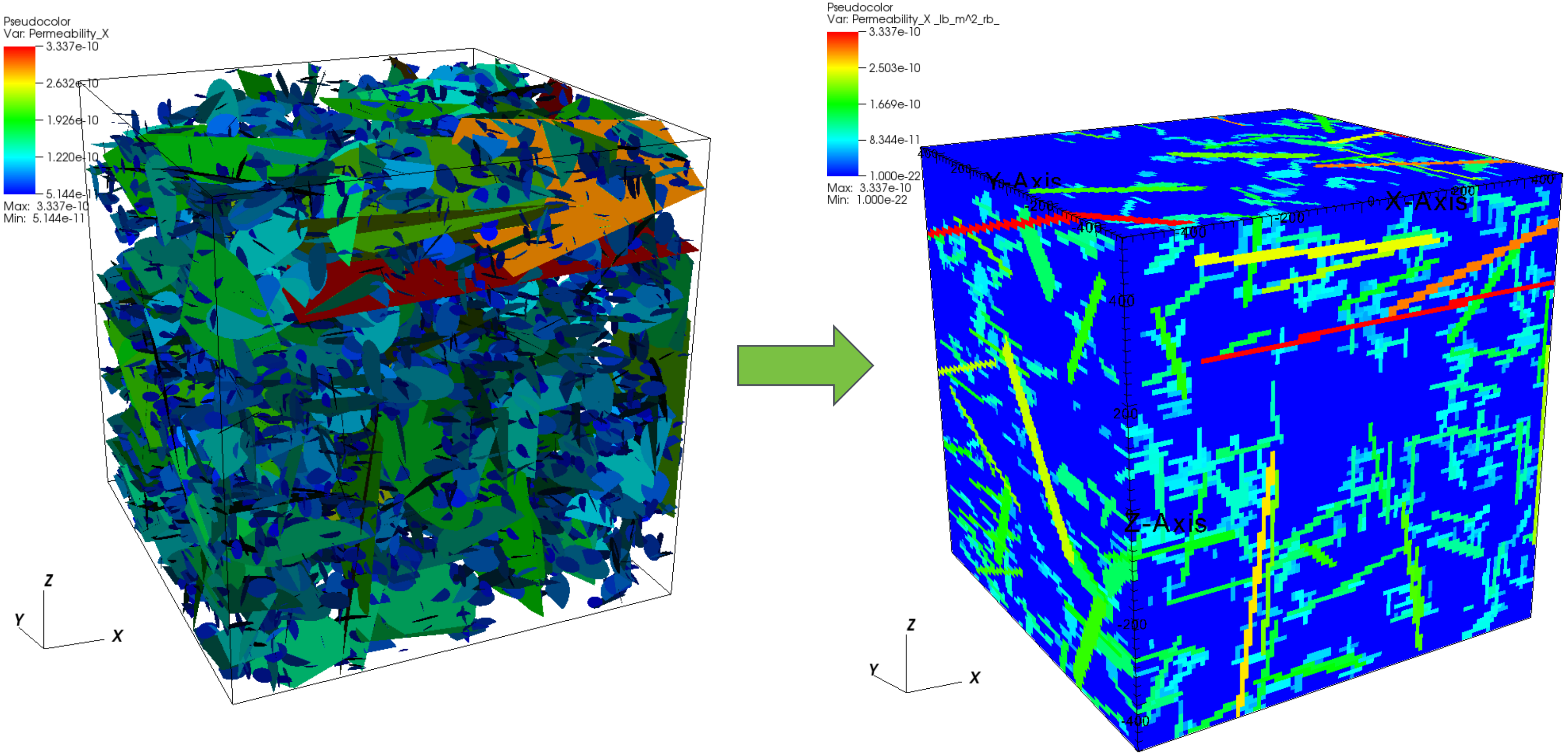
Example of DFN realization





Comparison of Discrete Fracture Network (DFN) and Fractured Continuum Models (FCM)

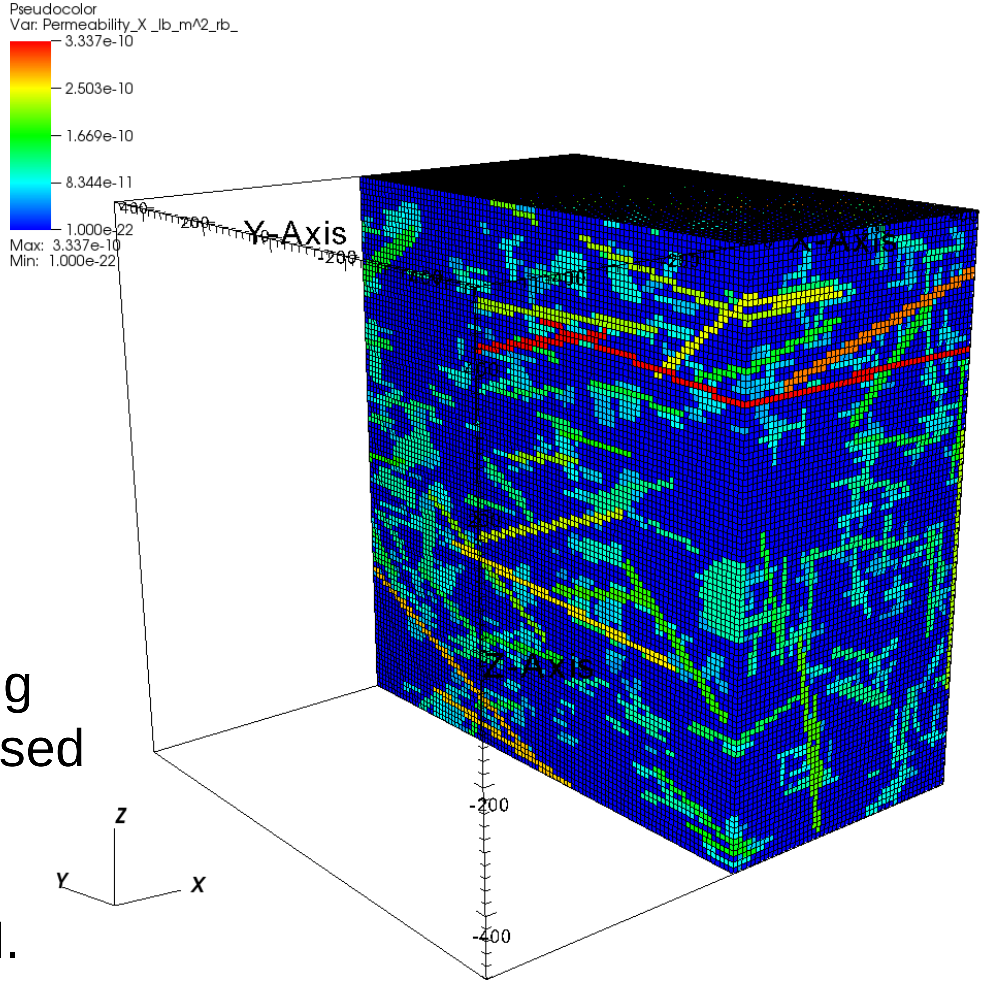
Step 2: Mapping DFN into Continuum



Comparison of Discrete Fracture Network (DFN) and Fractured Continuum Models (FCM)

Step 2: Mapping DFN into Continuum

- The fracture network structure of the DFN is mapped into regular voxel mesh.
- Each voxel in the hexahedral mesh has dimensions of 10 m.



- The list of fractures intersecting each voxel is created and passed to FCM team.
- DFN team proceeds with DFN.

Comparison of Discrete Fracture Network (DFN) and Fractured Continuum Models (FCM)

Step 3: Compare Effective permeability of DFN and FCM

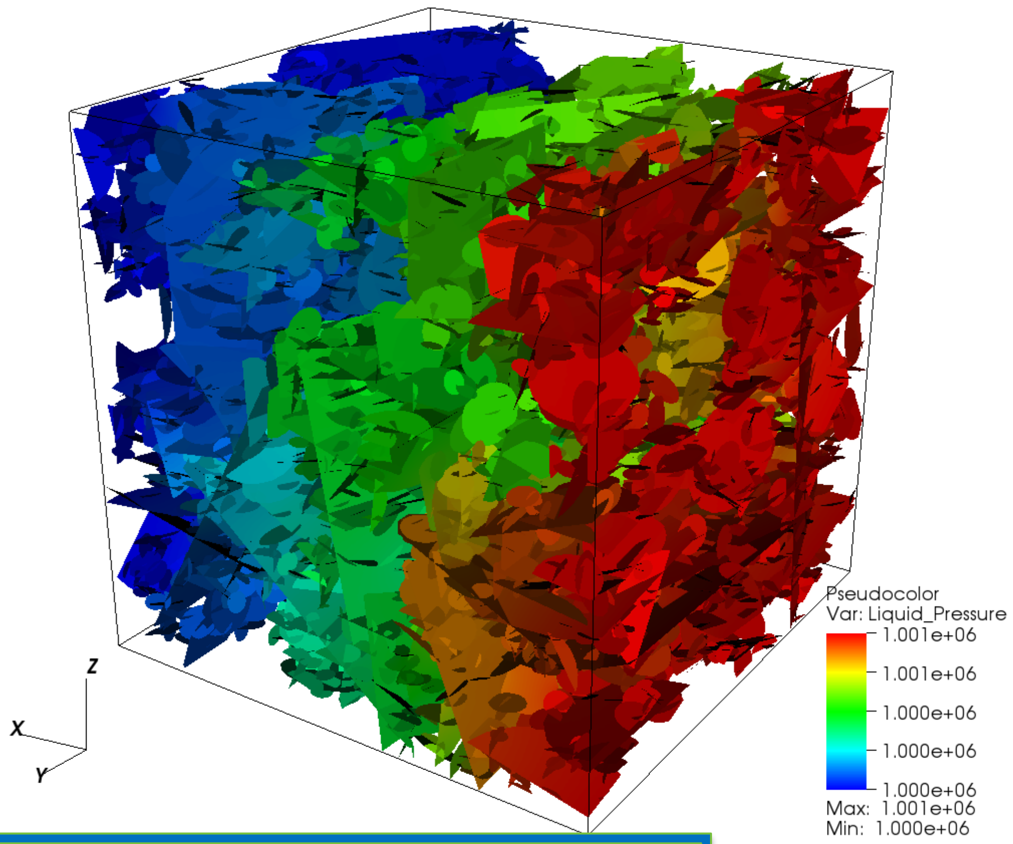
Flow direction:
West-East

Pressure gradient:
10^3 Pa

Compare Effective Permeability of DFNs and FCM:

Effective permeability of 5 realizations is in the range:

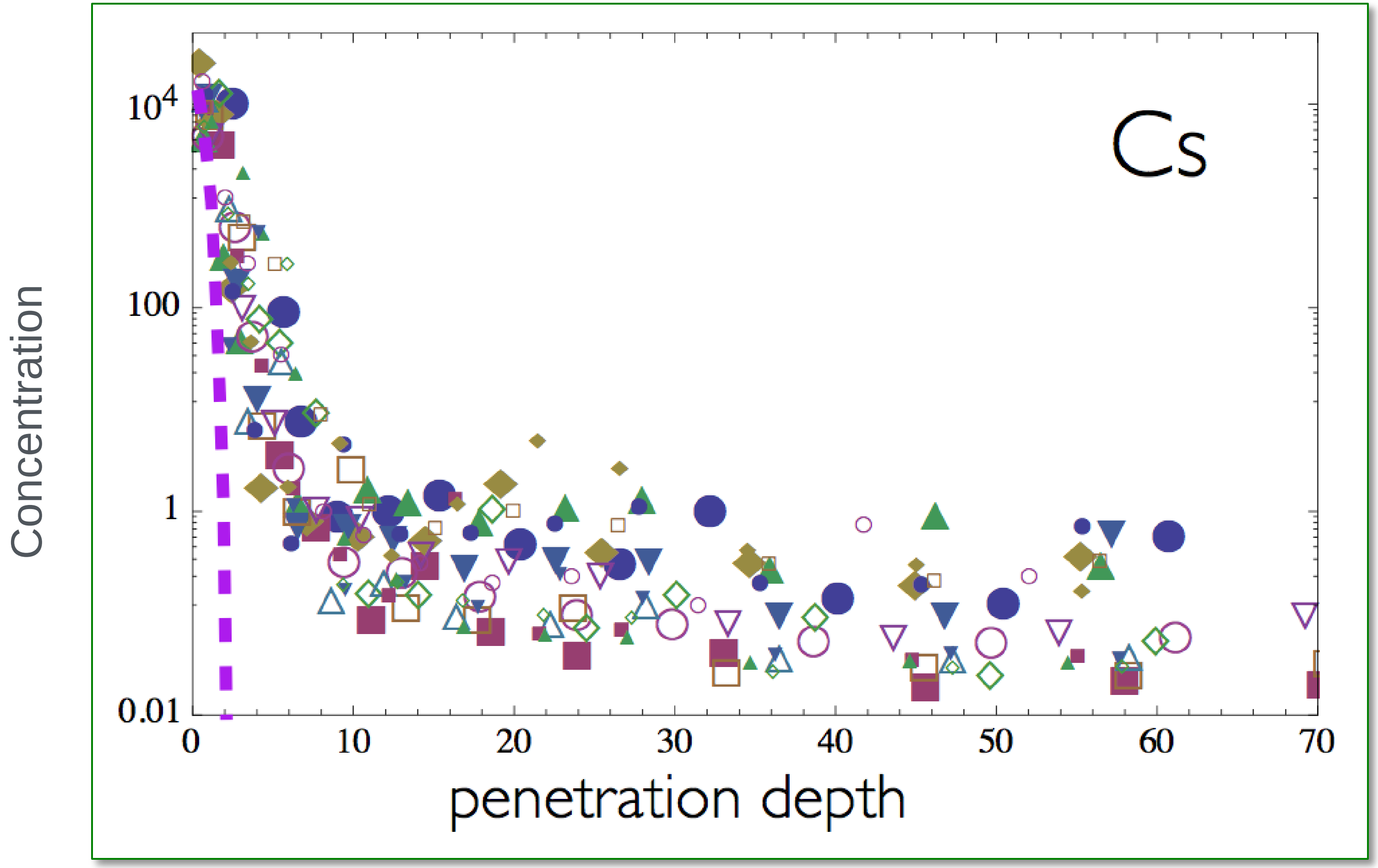
DFN 3.347 e-17 – 4.242 e-17 m^2
FCM 3.68 e-17 – 4.67 e-17 m^2



Both models result in similar effective permeabilities

Field Tests: Long Term Diffusion Experiment (LTDE), Sweden, 2015-Present

Penetration Profile in Long-Term Diffusion Experiment



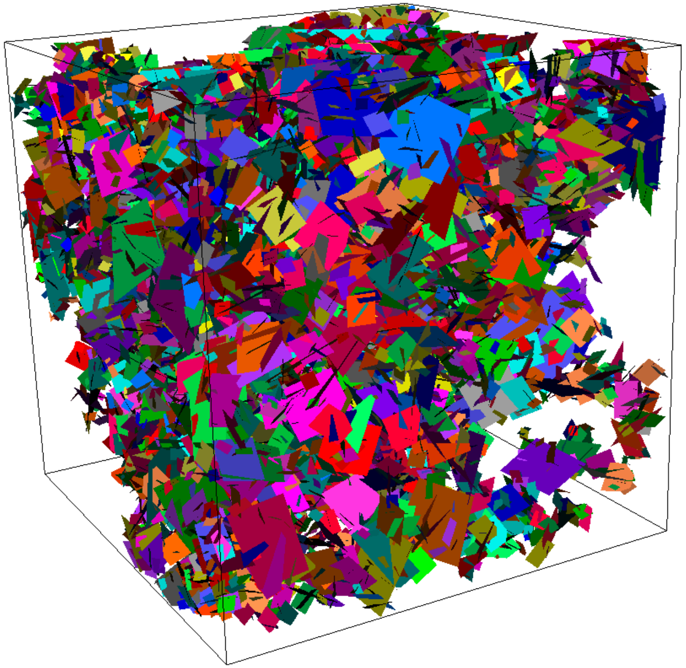
Enhanced penetration of cesium was measured into the crystalline rock

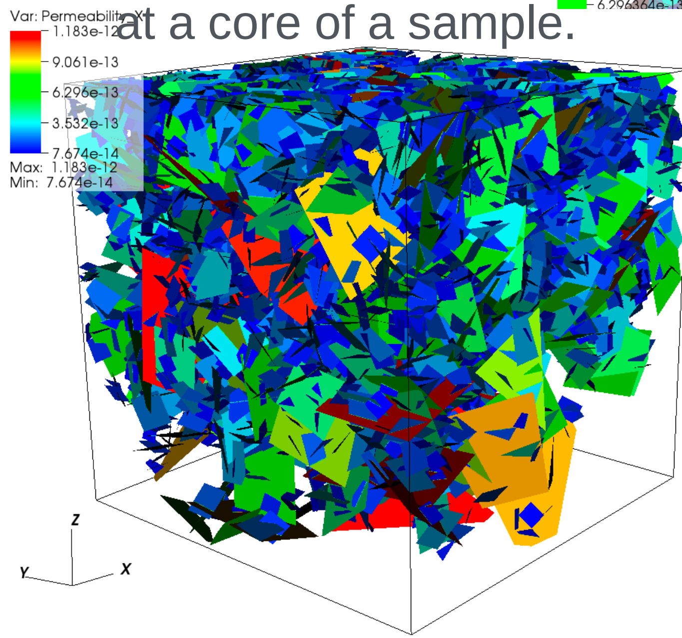
Field Tests: Long Term Diffusion Experiment (LTDE)

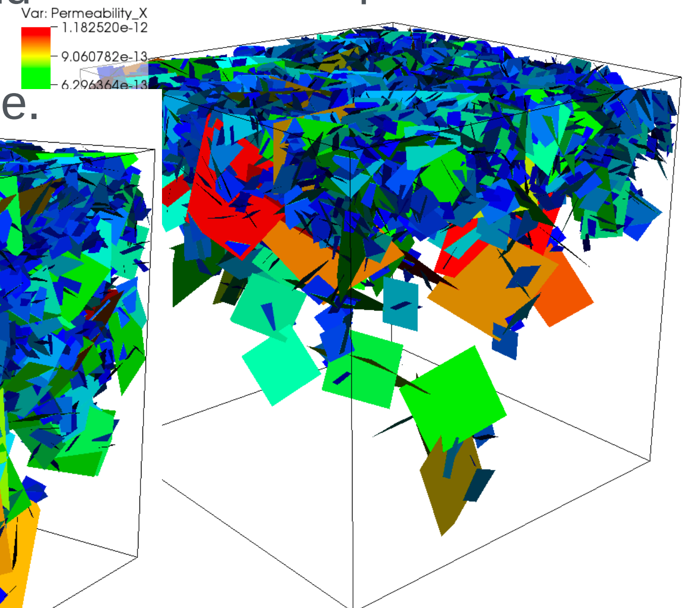
1. DFN of high uniform micro-fracture intensity

2. DFN of high micro-fracture intensity at a surface of a sample (top) and decreased P_{32} at a core of a sample.

3. DFN of significantly low intensity at a core of a sample







Three DFN configurations

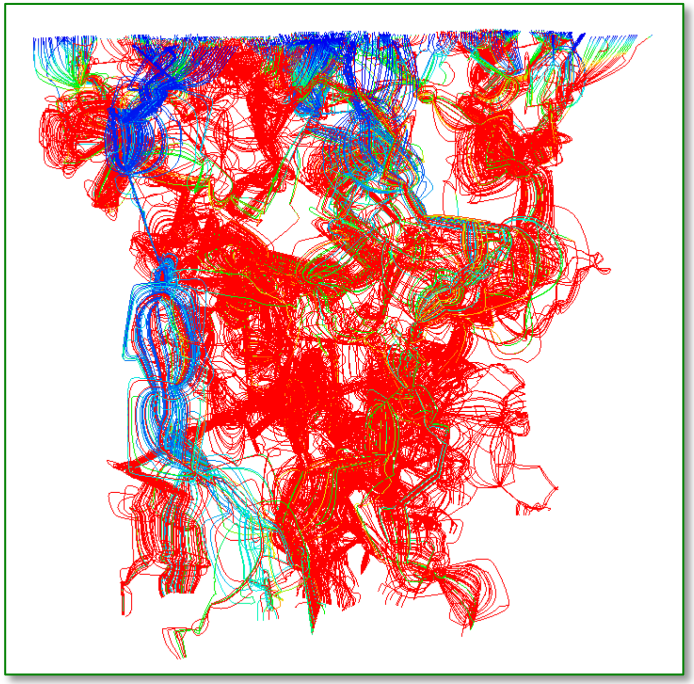
Field Tests: Long Term Diffusion Experiment (LTDE)

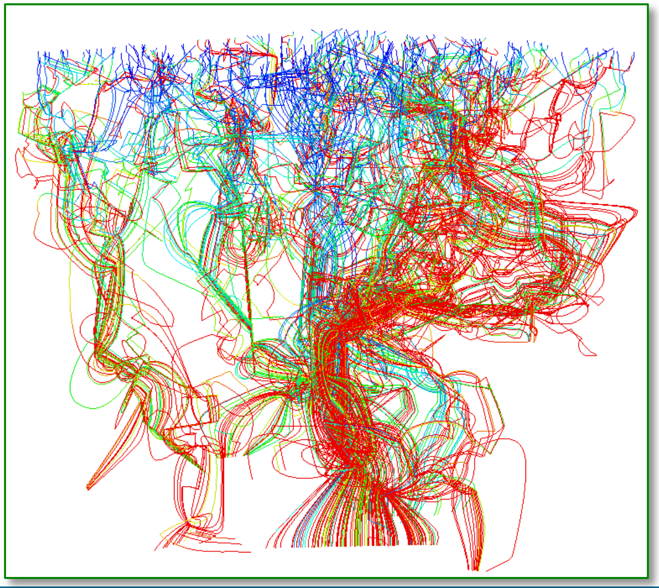
1. DFN of high uniform micro-fracture intensity

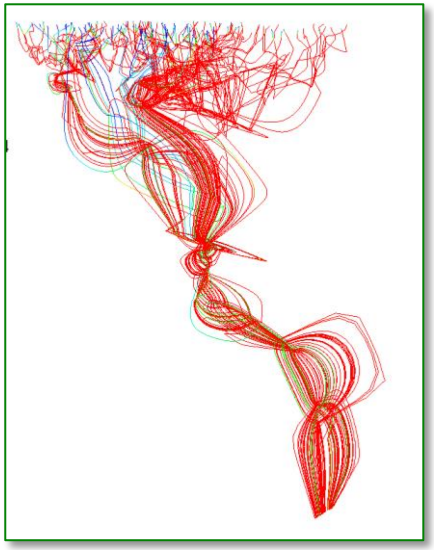
2. DFN of high micro-fracture intensity at a surface of a sample (top) and decreased P_{32} at a core of a sample.

3. DFN of significantly low intensity at a core of a sample

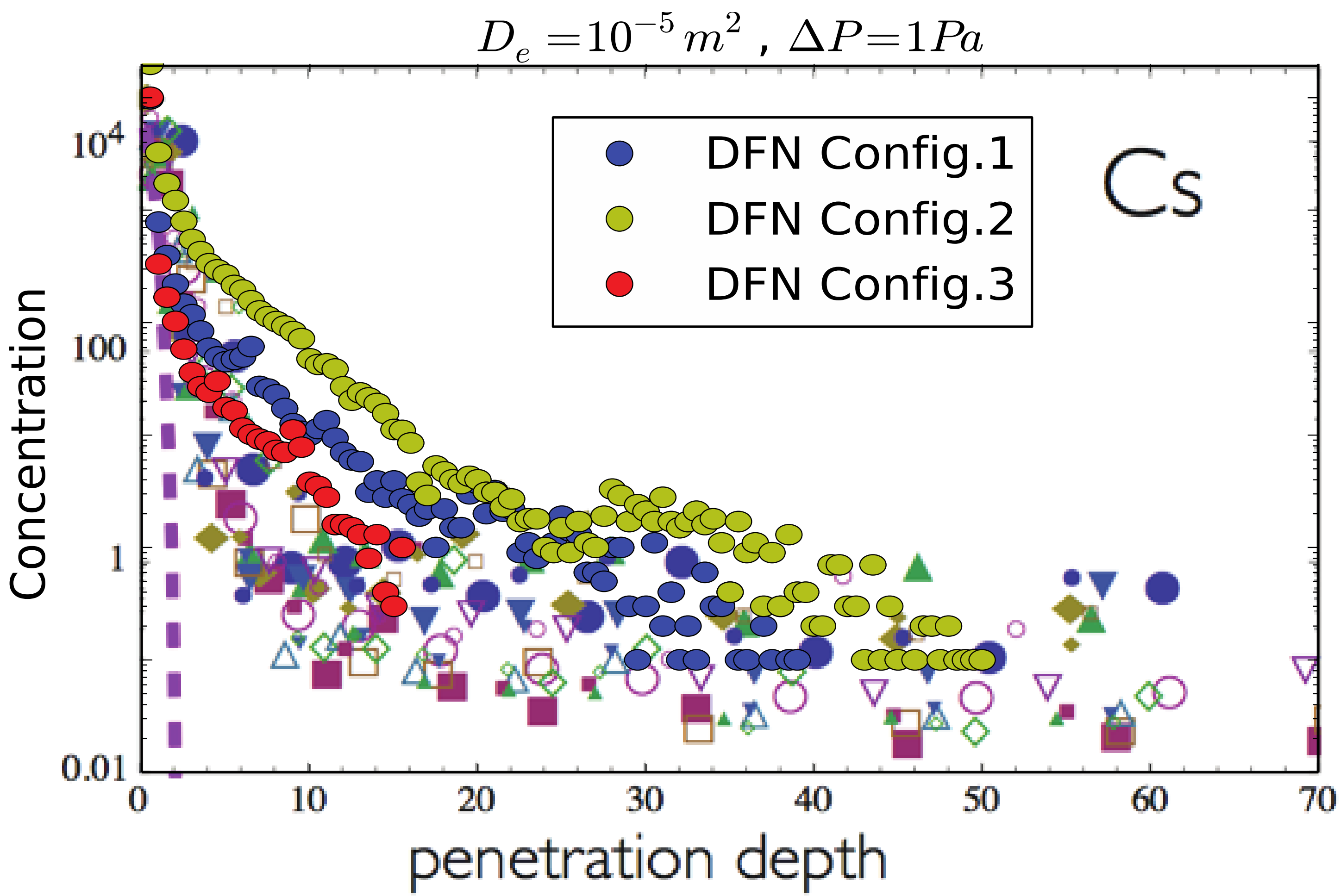
Perform Particle Tracking Simulations







Field Tests: Long Term Diffusion Experiment (LTDE)

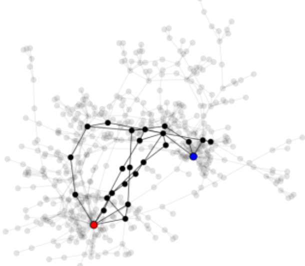


Microstructure can explain increased Rn penetration

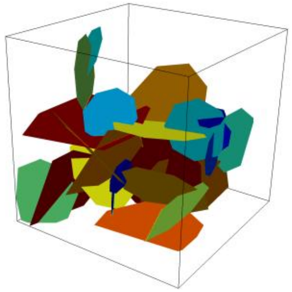
Incorporation into GDSA and the Safety Case

Fractured Rock at Field Site

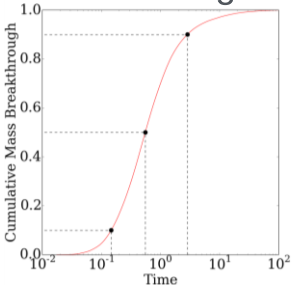
Pruned Graph



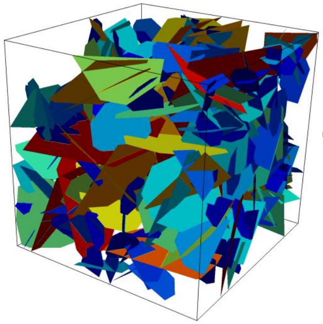
Pruned DFN



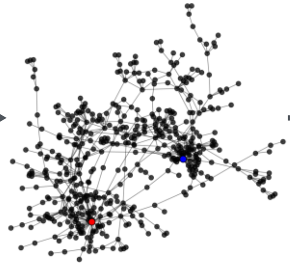
QOI - Breakthrough



ML / Physics Informed Pruning

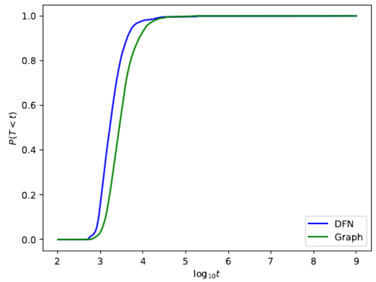


High Fidelity DFN



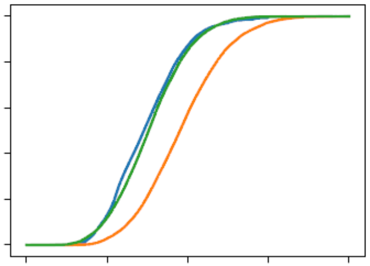
Graph Representation

Physics on Graph



QOI - Breakthrough

UQ / Bias Correction

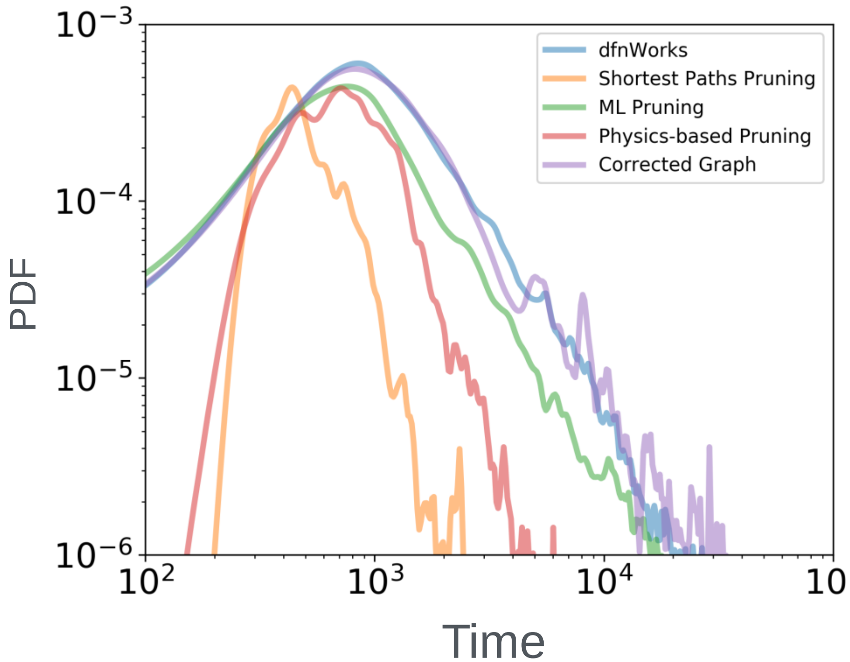


Corrected Breakthrough

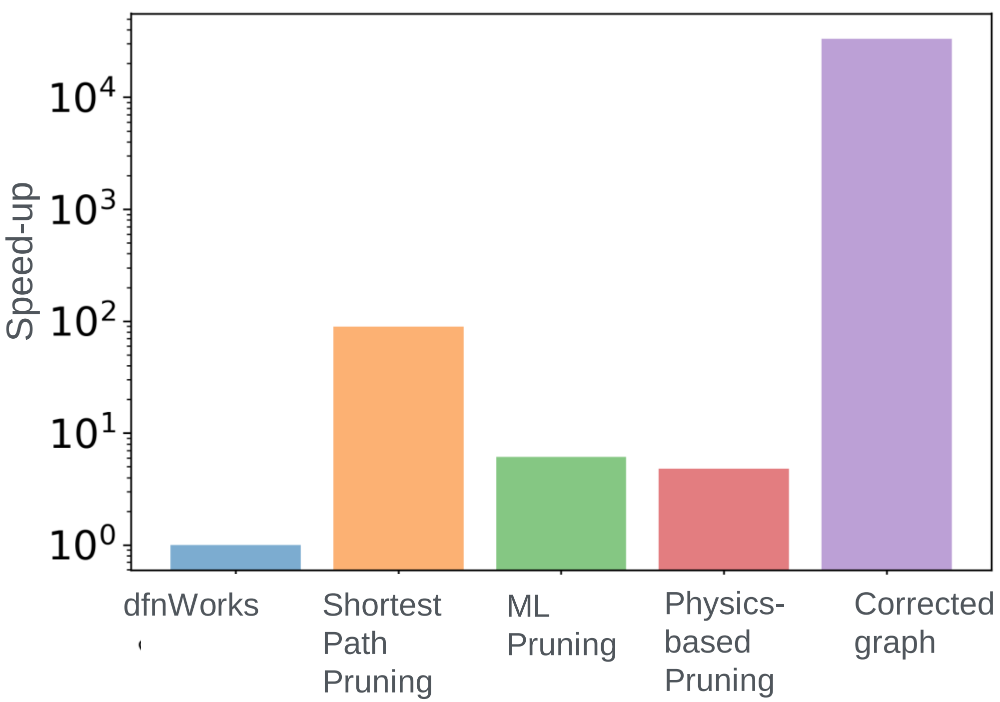
Reduced order models of fracture flow and transport using machine learning

Incorporation into GDSA and the Safety Case

QOI: Breakthrough Curves



Computational Performance



We can tailor the reduced order model depending on the QOI:

- Quick shortest path calculation if only early arrival is needed
- ML or physics-based pruning is effective but still requires mapping back to DFN(10X-100X speedup)
- Transport on the graph is 4 orders of magnitude faster but accurate for more complex cases?

Incorporation into GDSA and the Safety Case

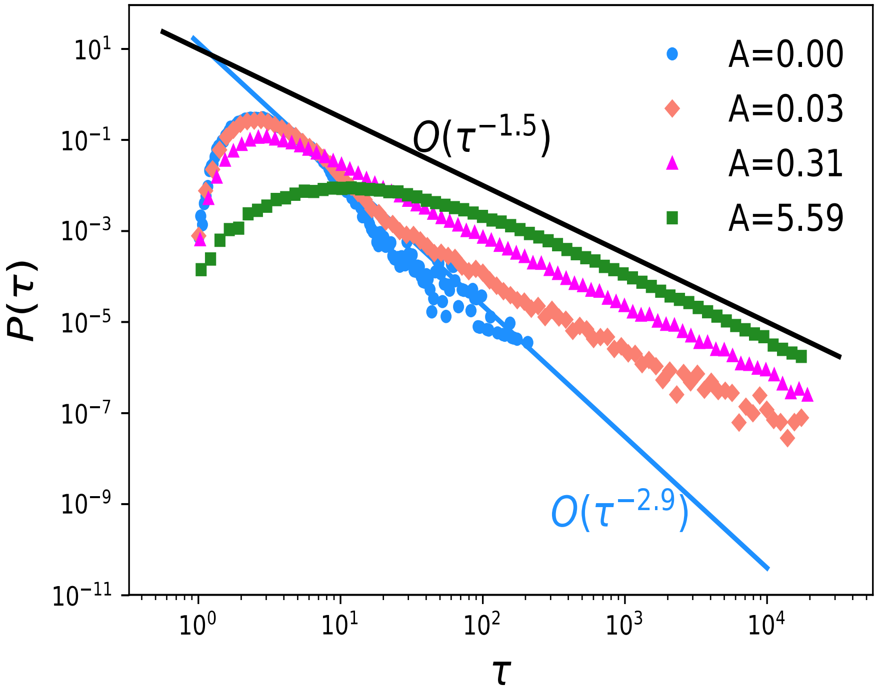
- Time Domain Random Walk
- Interaction with the rock matrix surrounding the network is currently not considered in dfnWorks

- We've including matrix diffusion into dfnWorks simulations using a Lagrangian approach

- Can also be included into graph transport using the same approach

- Verification of matrix diffusion -> recover classic -3/2 slope

- Will be compared with DFM models



Matrix Diffusion in Fractured Media: New Insights into Power-Law Scaling of Breakthrough Curves, JD Hyman, H Rajaram, S Srinivasan, N Makedonska, S Karra, H Viswanathan, G Srinivasan. In prep for Geophysical Research Letters

Matrix diffusion included in dfnWorks for fracture-matrix interactions

Benefits of Participation

- International program has provided comprehensive field tests for detailed validation of fracture networks models in different types of geologic media
- International collaborations have pushed the need to develop new capabilities (e.g. dfnWorks, fracture continuum model) that utilize high performance computing, multi-physics and multi-scale methods
- International programs have many world leaders in flow and transport in fractured systems
- DOE is an important contributor in areas of physics-based, HPC simulation methods, uncertainty quantification and reduced order models

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Questions?

Clean. Reliable. Nuclear.