SAND2017-10605C

Task C: GREET

Hydro-mechanical-chemical-biological processes during groundwater recovery in crystalline rock

Step 1 Preliminary Results:

Part I. Fracture Model Development

Part II. Flow and Transport Simulation

Part III. Chemical Analysis

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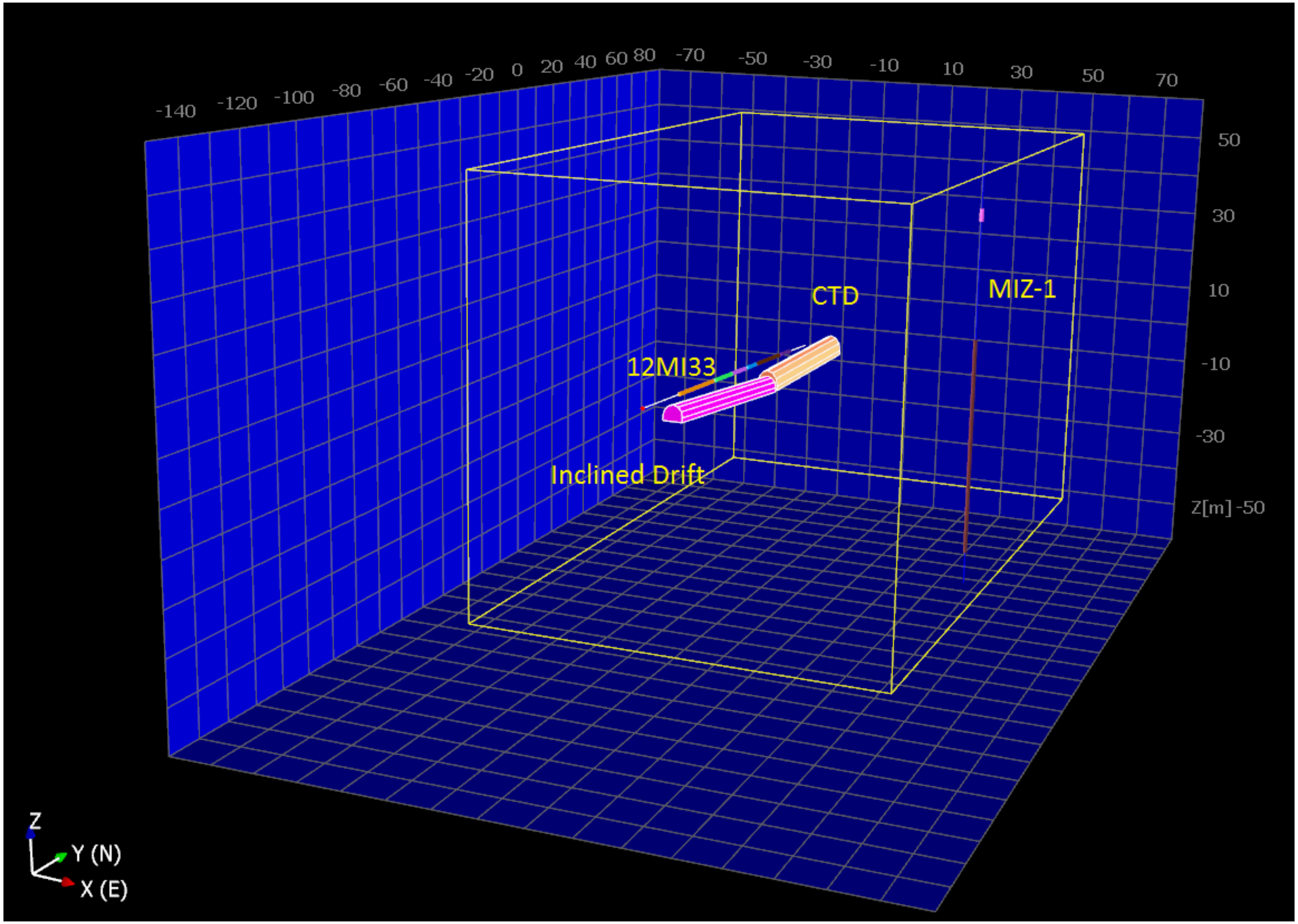
Part I. Fracture Model Development

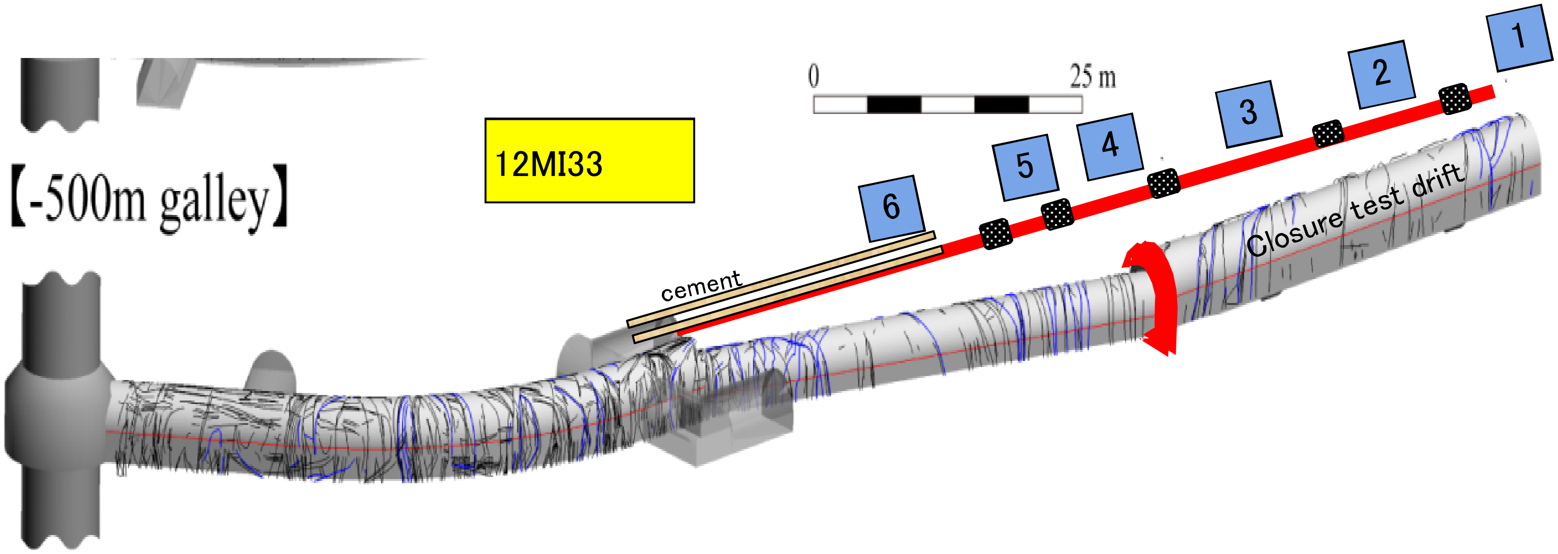
- Data:
  - Fracture traces on the walls of CTD, Inclined Drift, and Access Drift
  - Fractures observed in borehole 12MI33
  - Borehole packer test data in 6 test intervals of 12MI33 and 2 test intervals of MIZ-1
  - Measured total inflow into the research drift.

- Modeling Approach:
  - Develop DFN assuming
    - Fractures in the tunnel and borehole 12MI33 have deterministic locations and stochastic sizes and properties.
    - Fractures outside the tunnel and borehole are stochastic fractures with regard to both, location and properties.
  - Upscale DFN to ECM using Oda's method for flow and transport simulations.

Modeling Domain and Data Location

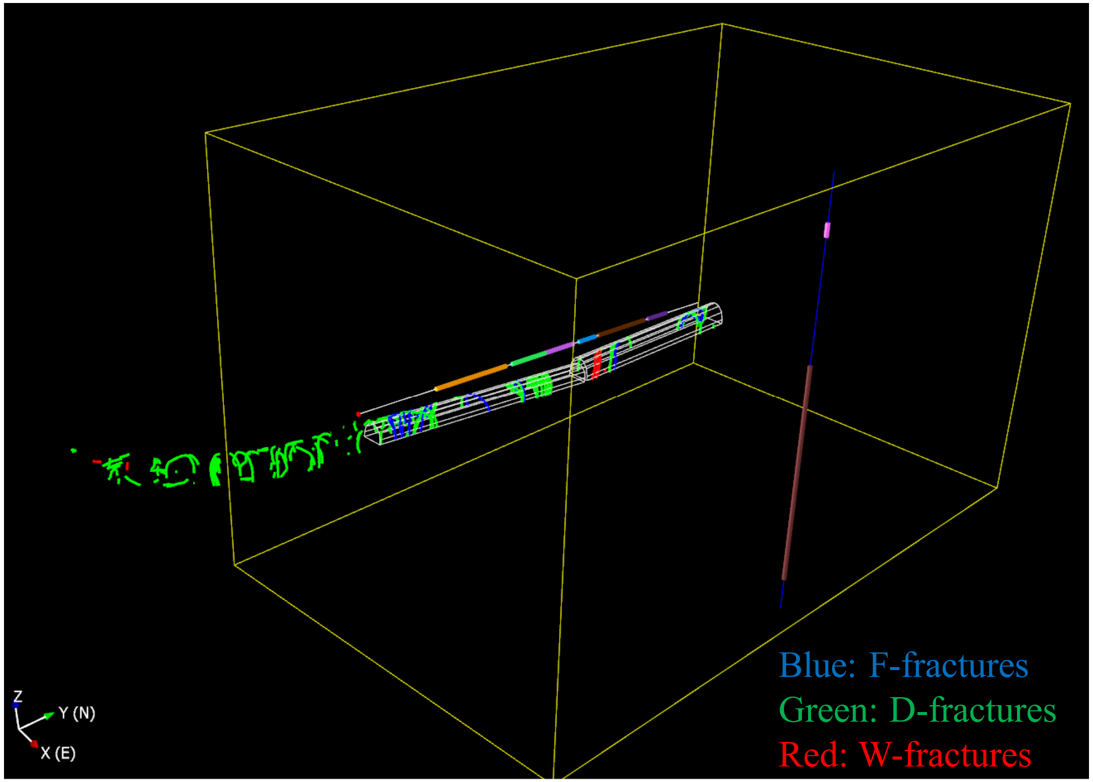


Generating Fractures in the Tunnel from Fracture Trace Data



- 2,023 fractures on the walls of Access Drift, Inclined Drift, and CTD
- Trace data: trace location, length, dip, strike, alteration, and flow range
- Aperture: not measured

Fractures Selected for Analysis



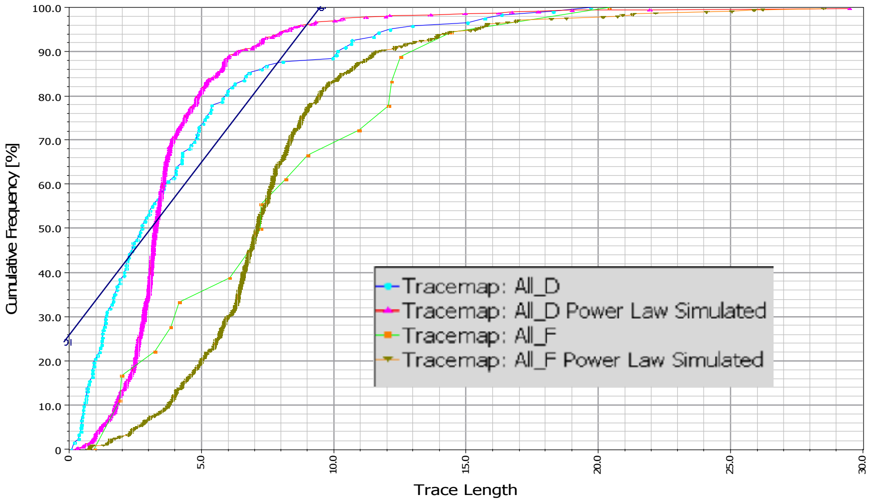
- Only the tunnel fractures with observed flow are included in DFN.
- Other fractures are assumed to be closed or small fractures not connected to the fracture network.

Number of Fractures with Observed Flow

Type	F (>1.0 L/min)	D (>0.1 L/min)	W (<0.1 L/min)
CTD	4	15	3
Inclined Drift	14	42	-
Access Drift	-	65	3
Total	18	122	6

Fracture Size Analysis

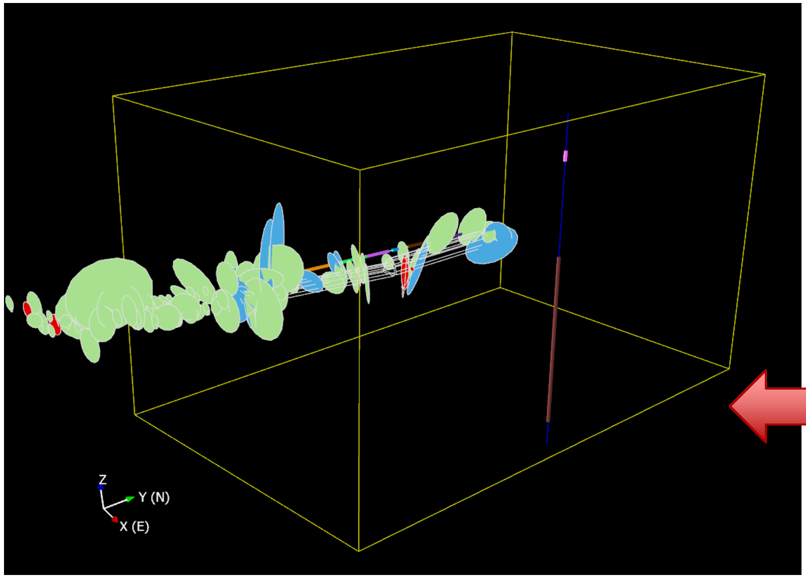
Power-Law Fit



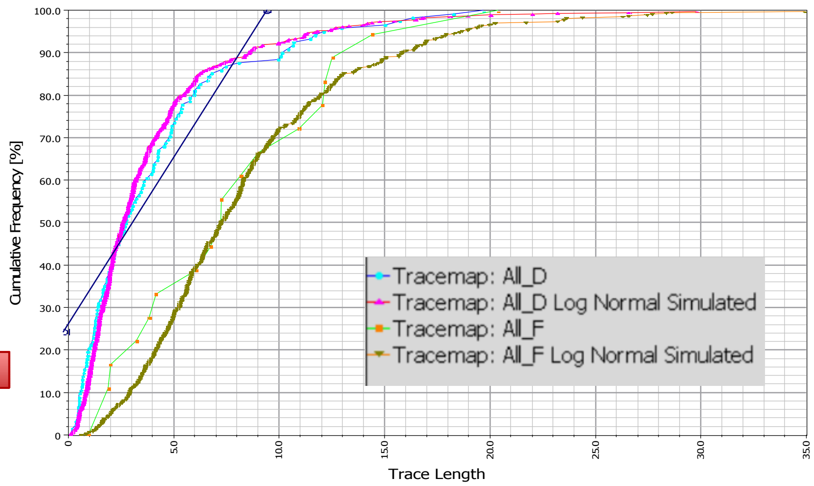
Results of Trace Length Analysis

Fracture Set	Distribution Type	Mean/min Radius (m)	St. Dev./Exp
D and W	Lognormal	1.42	1.29
F	Lognormal	3.88	2.15
D and W	Power-Law	1.5	3.4
F	Power-Law	3.3	3.9

D and W fractures were combined

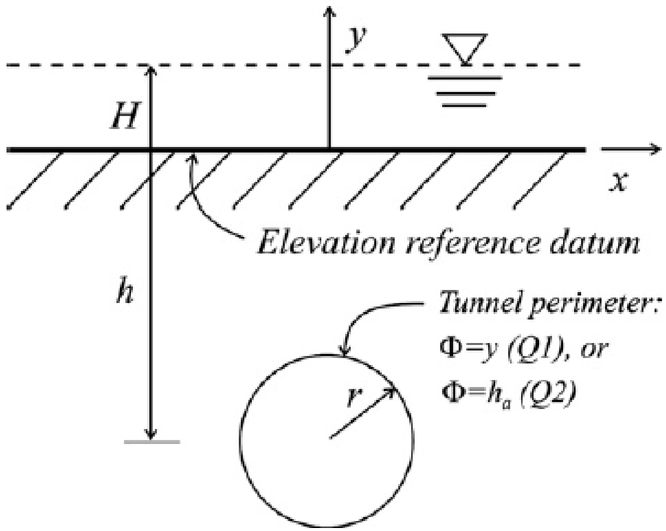


Lognormal Fit - Selected



Fracture Transmissivity Evaluation

Analytical Solution for Unit Inflow (Q) into Circular Tunnel Butscher (2012)



Inflow into the fracture (Q_{fr}) with aperture b:

$$Q_{fr} = Q \cdot b = \frac{2\pi T(A+H)}{\ln\left(\frac{h}{r}+\sqrt{\frac{h^2}{r^2}-1}\right)} \qquad \text{(Eq. 1)}$$

$$A = h(1-\alpha^2)/(1+\alpha^2)$$

$$\alpha = \frac{1}{r}\left(h - \sqrt{h^2 - r^2}\right)$$

$$T = k \cdot b$$

Q_{fr} >1 L/min (F fractures) -> T >3.2x10^{-8} m^2/s
Q_{fr} >0.1 L/min (D fractures) -> T >3.2x10^{-9} m^2/s
Q_{fr} <0.1 L/min (W fractures) -> T <3.2x10^{-9} m^3/s

Using Measured Inflow into the Tunnel to Adjust T

Research Tunnel Area	Measured Tunnel Inflow (L/min)	Number of Fractures			Calculated Inflow, Eq.1 (L/min)			
		F	D	W	F	D	W	Total
CTD	13	4	15	3	9.2	3.45	0.3	12.95
Inclined Drift	43	14	42	0	32.2	9.66	0	41.86

Adjusted Transmissivity

F: T =7.3x10^{-8} m^2/s
D: T= 7.3x10^{-9} m^2/s
W: T =3.2x10^{-9} m^2/s

Fracture Permeability and Aperture

Fracture aperture (*b*) and permeability (*k*) can be evaluated from fracture transmissivity (*T*):

$$T = \frac{b^3}{12}\frac{\rho g}{\mu} \qquad k = \frac{b^2}{12}\frac{\rho g}{\mu}$$

ρ - water density
g - gravity acceleration
μ - water viscosity

- Fracture transmissivity (T): $3.2\text{x}10^{-9} – 7.3\text{x}10^{-8}$ m^2/s.
- Fracture aperture (b): 16 – 45 micron
- Fracture permeability (k): $3.5\text{x}10^{-12} – 1.7\text{x}10^{-10}$ m^2

Developing Correlation between Fracture Radius (*R*) and Fracture Properties

$$k = \gamma_1 \cdot R^{\omega}$$

$$b = \gamma_2 \cdot R$$

<u>Calculated Coefficients:</u>
γ_1=1.55x10^{-12}
γ_2=1.16xE^{-5}
ω=2.3

Results for Fractures with *k* and *b* Correlated to *R*

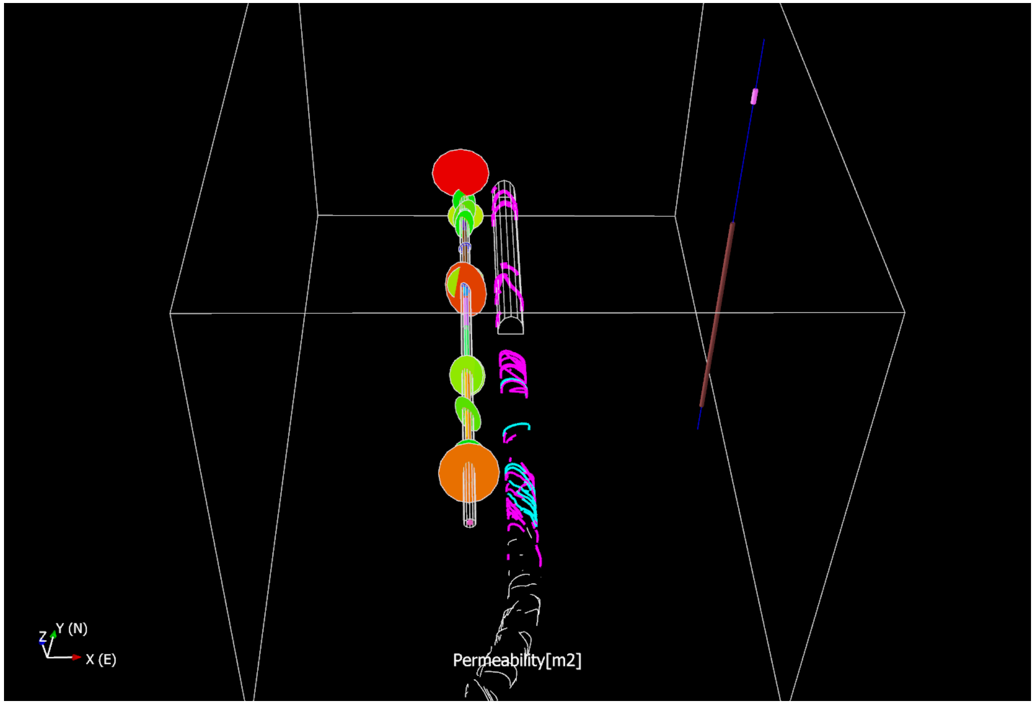
Fracture Type	Transmissivity (m^2/s)	Calculated Inflow (L/min)
D	1.94E-06	61.03
F	1.58E-06	49.78
W	9.71E-08	3.06
Total	3.62E-06	113.87
Measured Inflow (L/min): 104		

Average fracture transmissivity is $2.5\text{x}10^{-8}$ m^2/s

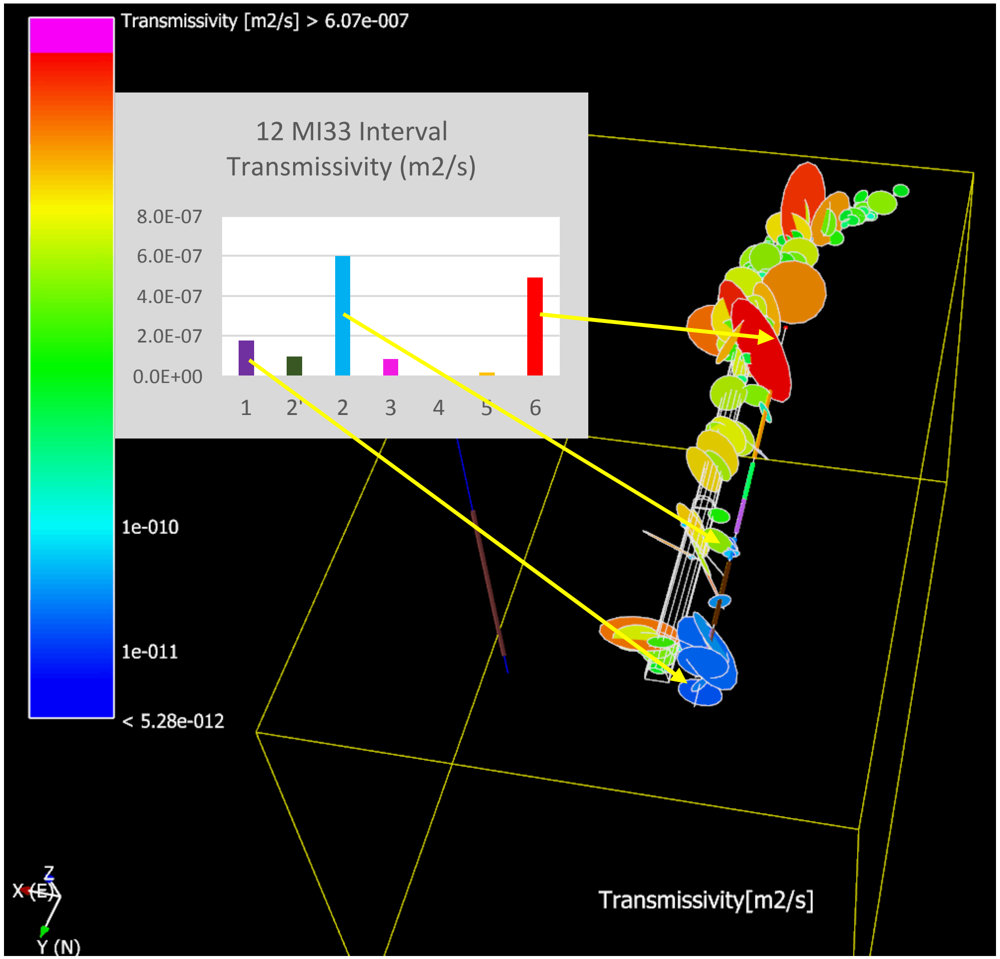
Analysis of Fractures in Borehole 12MI33

- 297 fractures were observed.
- The fractures were classified as
  - Crack
  - Hair crack
  - Discontinuity crack
  - Mineral vein
- The cracks with recorded apertures were considered to be permeable fractures similar to F, D, or W fractures in the tunnel.
- 17 such fractures were identified.
- Well log provides the fracture location and orientation. The fracture size is not known.
- The fractures were generated using the fracture size distributions and parameters derived for the tunnel.

Fractures Generated in Borehole 12MI33



Transmissivity from Packer Tests and Generated Fractures in 12MI33



Transmissivity of Generated Fractures	
Fracture	**T, m2/s**
1	1.14E-08
2	2.71E-09
3	1.74E-08
4	7.26E-09
5	1.39E-08
6	2.94E-09
7	6.28E-08
8	5.01E-08
9	2.30E-08
10	8.30E-09
11	5.36E-09
12	2.62E-09
13	1.60E-08
14	2.34E-08
15	4.27E-07
16	6.59E-08
17	1.82E-08
Total	**7.58E-07**

Transmissivity from Packer Tests	
Interval	**T, m2/s**
1	1.78E-07
2'	9.78E-08
2	6.01E-07
3	8.65E-08
4	4.96E-09
5	1.93E-08
6	4.91E-07
Total	**9.88E-07**

Stochastic Fracture Generation

Additional Information Required to Generate Stochastic Fractures

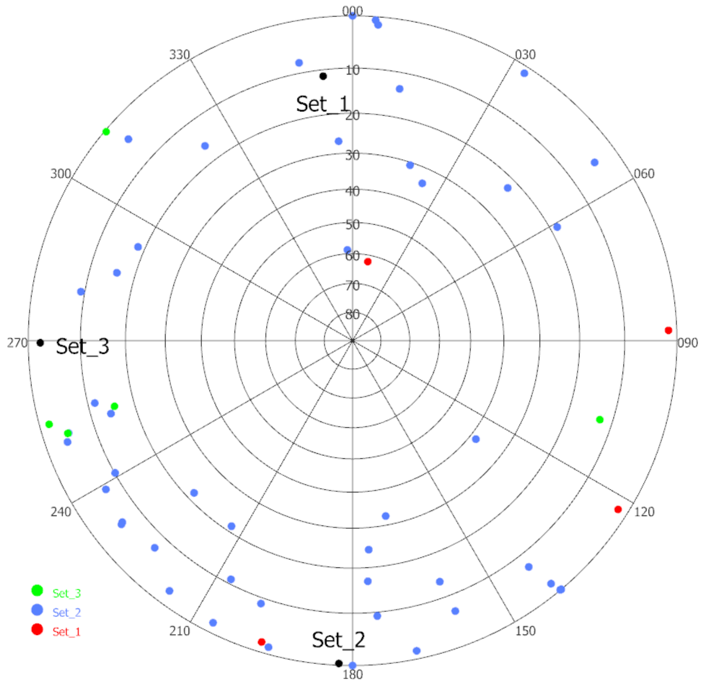
- How many fracture sets are present?
- Orientation distribution for each fracture set.
- Fracture intensity for each set.

This information can be obtained from the analysis of the fractures generated in the tunnel using Fracman tool **Interactive Set Identification System** (**ISIS**).

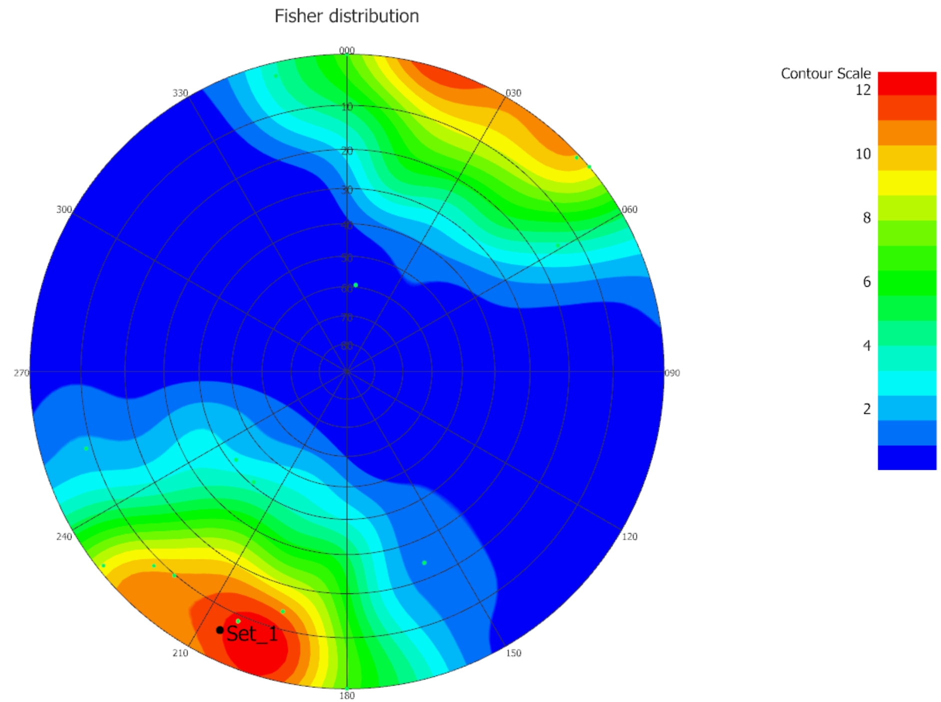
- ISIS defines fracture sets from field data using an adaptive probabilistic pattern recognition algorithm.
- ISIS calculates the distribution of orientations for the fractures assigned to each set, and then reassigns fractures to sets according to probabilistic weights proportional to their similarity to other fractures in the set.
- The orientations of the sets are then recalculated and the process is repeated until the set assignment is optimized.

Fracture Orientation Analysis Results

ISIS Set Assignment Results for the Tunnel Fractures



Calculated Fisher Distribution for the Main Fracture Set



<u>Main Fracture Set</u>

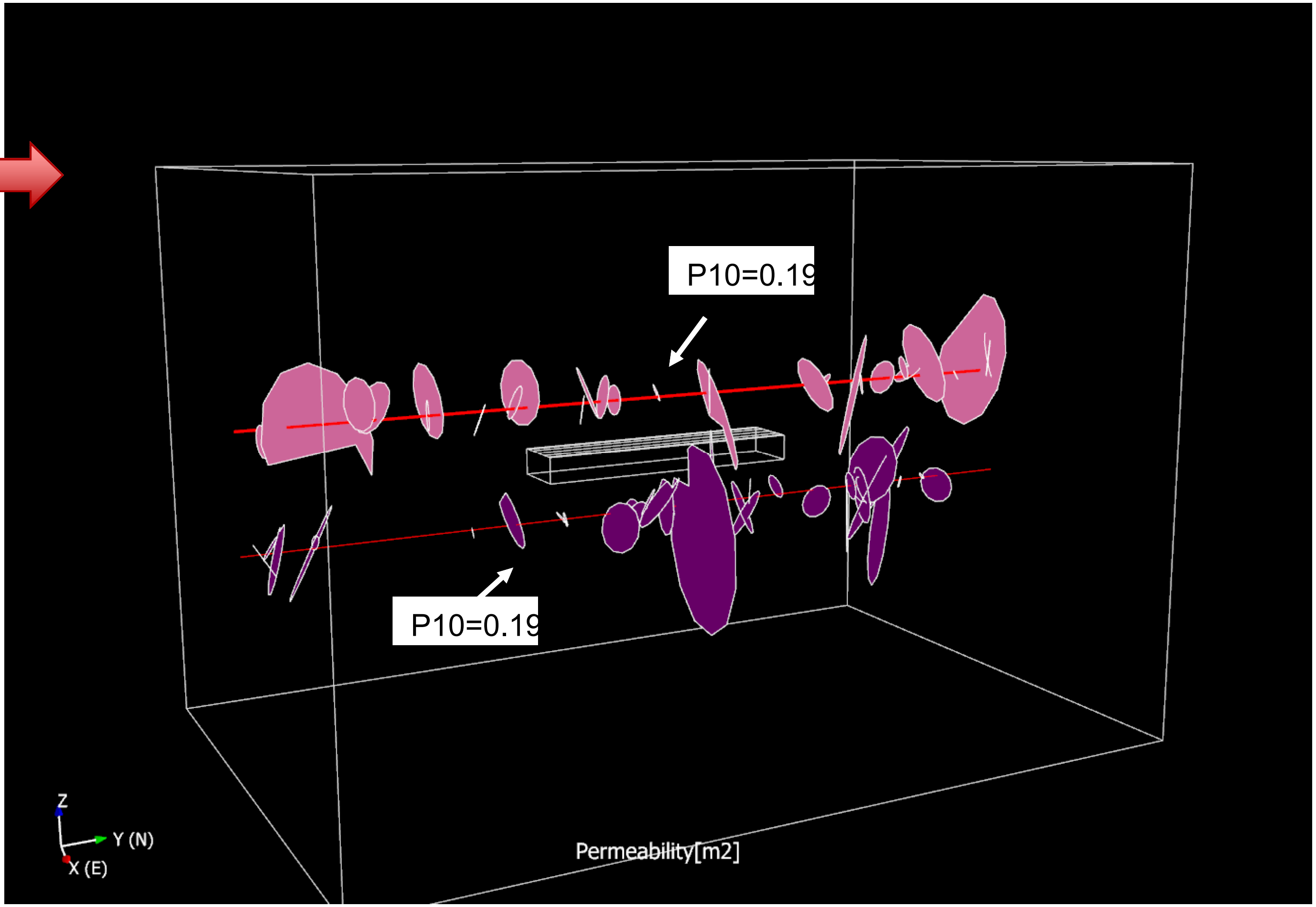
- North trending fractures
- mean plunge 80
- concentration parameter ķ equal to 7

Fracture Intensity Analysis Results

Calculated D fractures P_{10} matches the observed P_{10}

Calculated Fracture Intensity	
P_{10} (fr/m)	P_{32} (1/m)
0.19	0.22
0.08	0.086

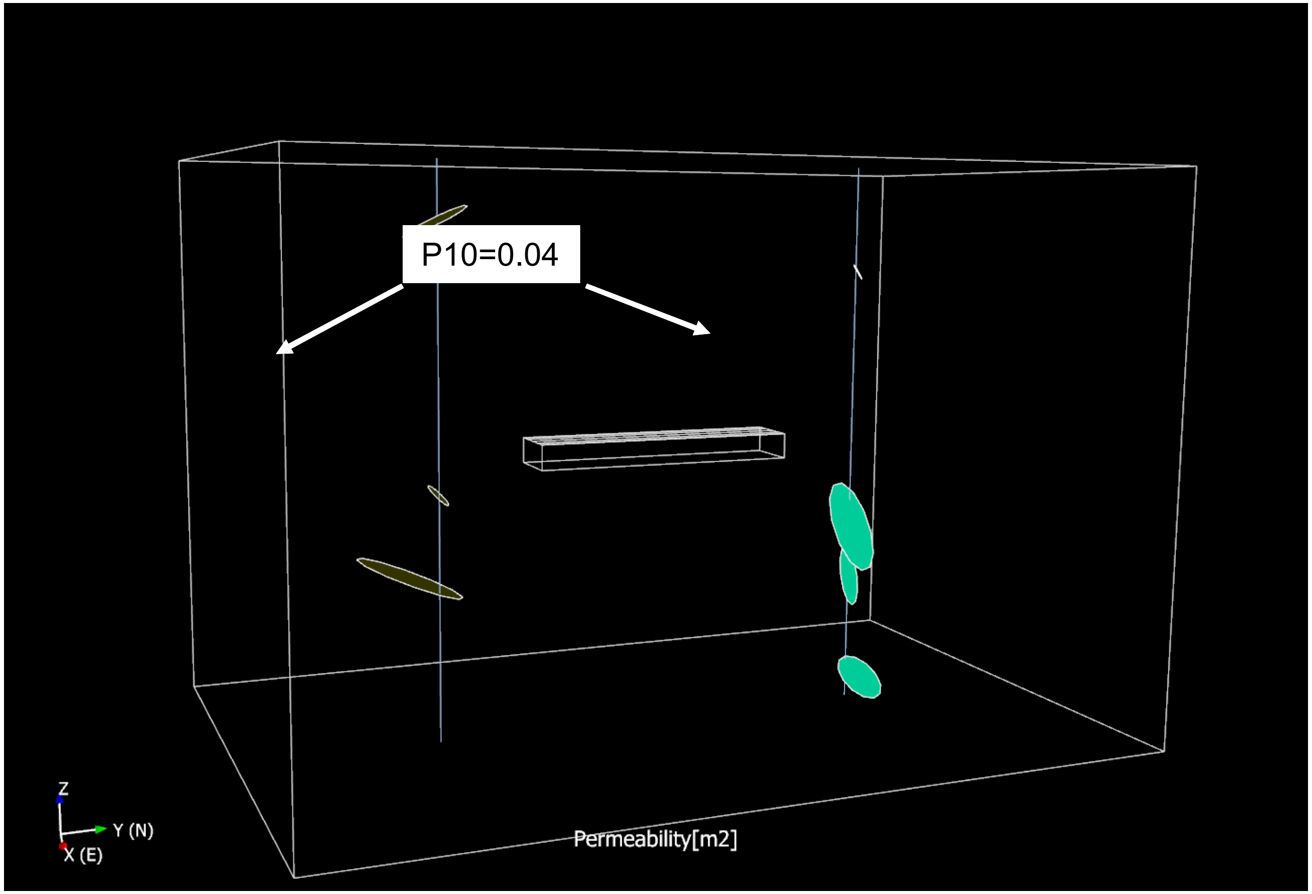
Stochastic Fractures Intersecting Arbitrary Horizontal Boreholes



Fracture Intensity Analysis Results (cont)

- Vertical borehole has smaller probability of intersecting sub-vertical fractures.
- Calculated P_{10} is lower than in horizontal boreholes.

Stochastic Fractures Intersecting Arbitrary Vertical Boreholes



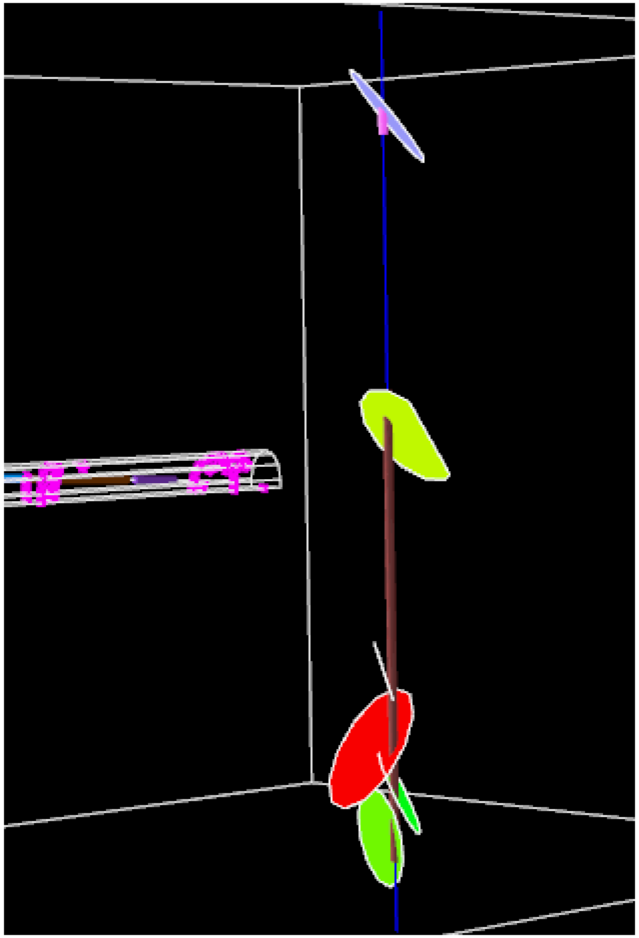
Transmissivity from Packer Tests and Stochastic Fractures in MIZ-1

Transmissivity from Packer Tests

Interval		T, m2/s
Top, m	**Bottom, m**	
-260.4	-263.3	3.69-08
-290.9	-342.4	5.16-09
Total		**4.20-08**

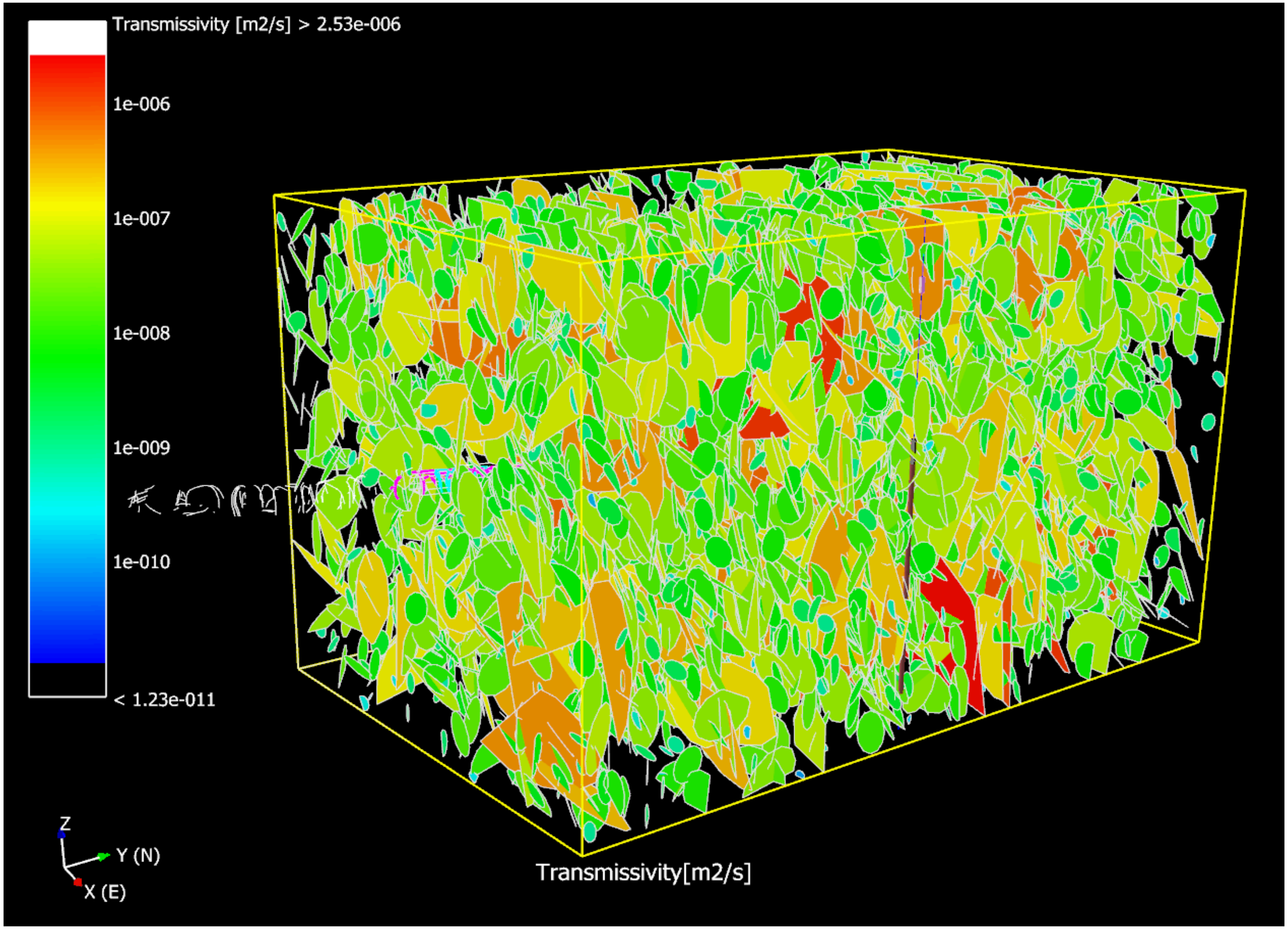
Transmissivity of Stochastic Fractures Intersecting MIZ-1

Fracture	T, m2/s
1	9.54E-08
2	3.54E-08
3	7.34E-09
4	2.52E-08
5	4.38E-08
Total	**2.07E-07**

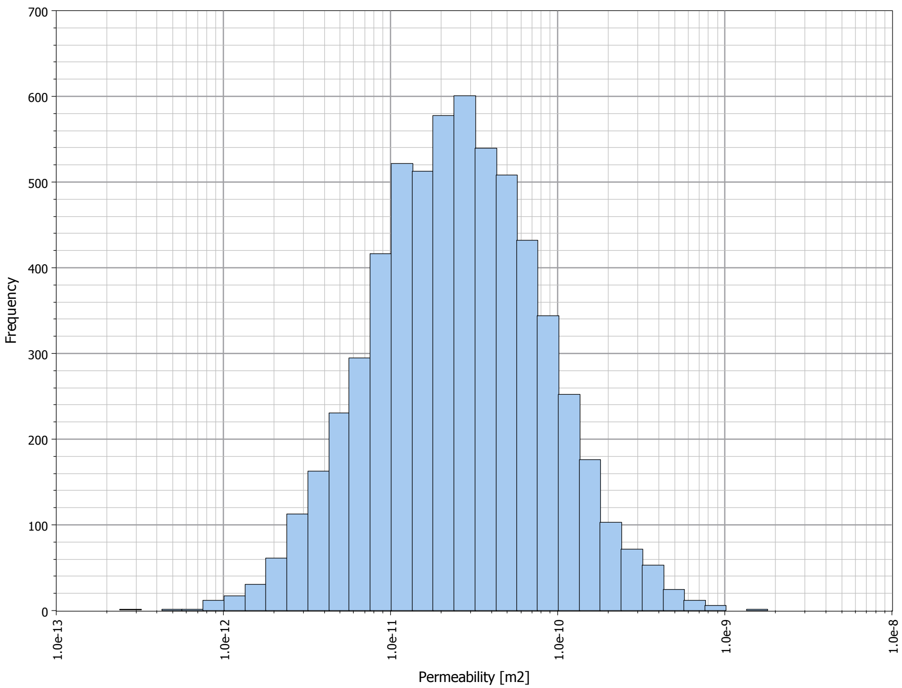


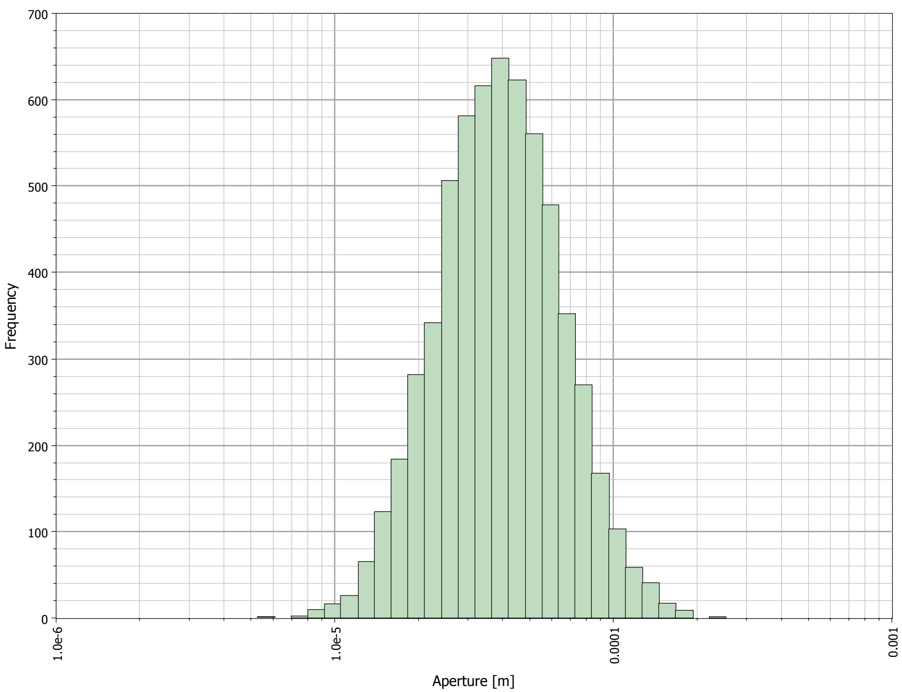
Possible reason for deviation: the packer test is influenced by the horizontal permeability that is lower than vertical permeability.

One Realization of Stochastic Fractures



Sampled Stochastic Fracture Properties





Converting DFN to Continuum Model with Oda Method

- Oda calculates permeability tensors in three dimensions for each cell.
- Oda tensor is a simplification of Darcy's Law for flow through an isotropic porous medium.
- The fracture permeability (k) is projected onto the plane of the fracture and scaled by the ratio between the fracture volume (porosity) and the volume of the grid cell.

$$F_{ij} = \frac{1}{V} \sum_{k=1}^{N} A_k T_k n_{ik} n_{jk}$$

Fij = fracture tensor
V = grid cell volume
N = total number of fractures in grid cell
Ak = area of fracture k
Tk = transmissivity of fracture k
nik, njk = the components of a unit normal to the fracture k

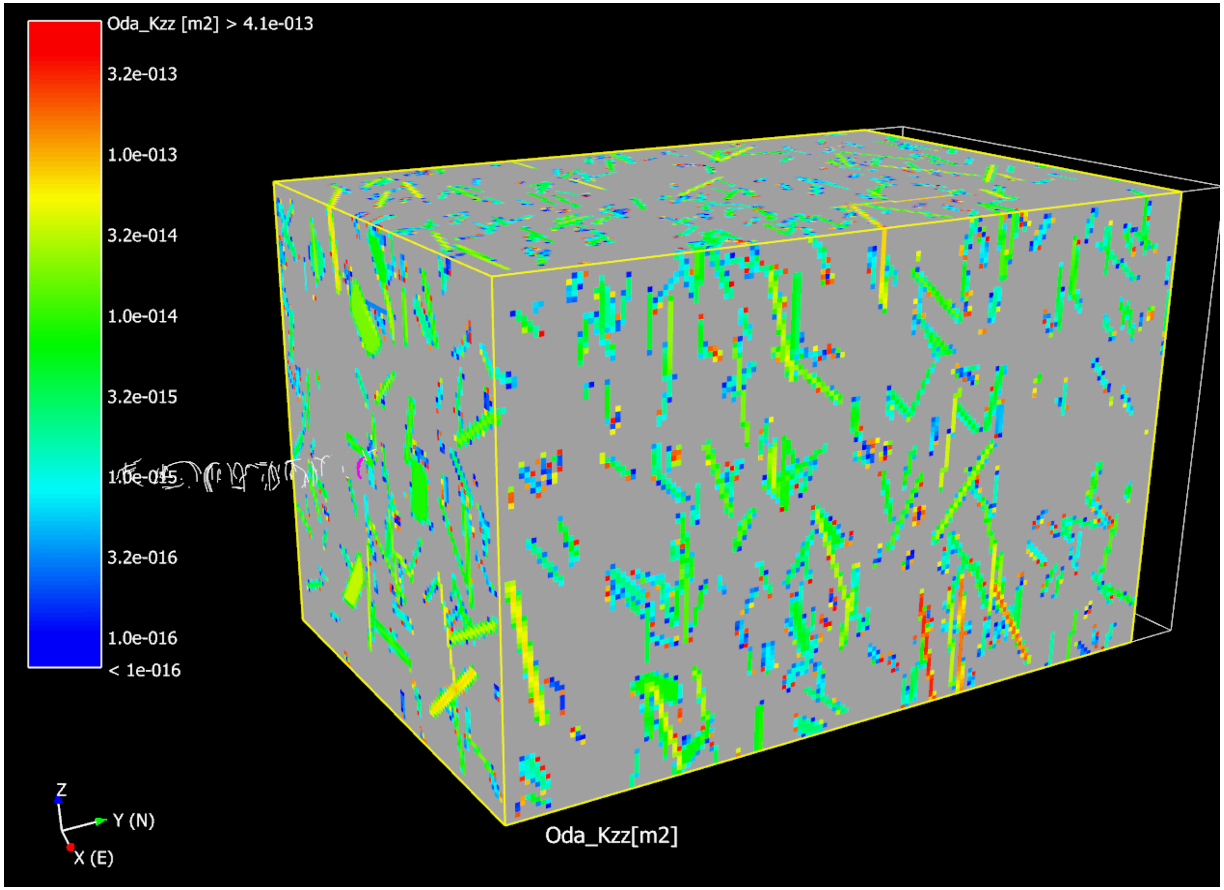
$$k_{ij} = \frac{1}{12} \left(F_{kk} \delta_{ij} - F_{ij} \right)$$

kij = permeability tensor
Fij = fracture tensor
δij = Kroenecker's delta

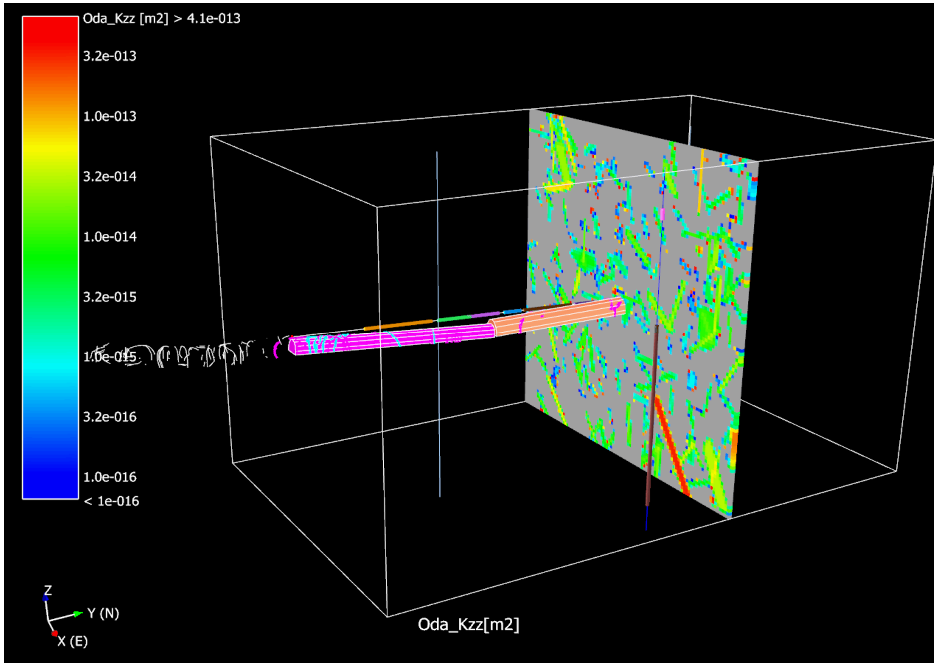
Continuum Model Permeability

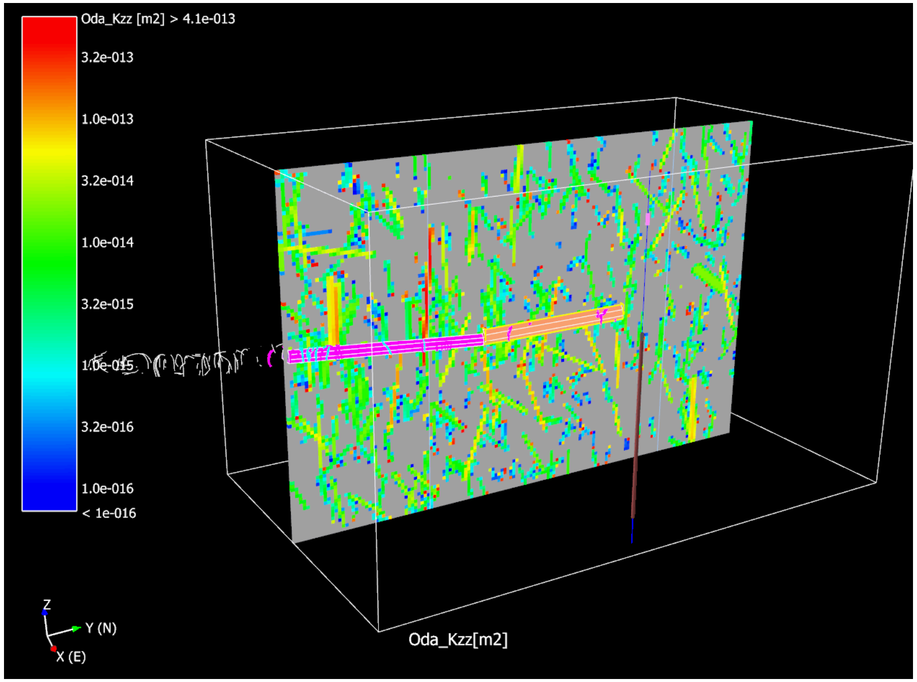
<u>Mean Grid Properties:</u>
K_{xx}=3.0E-15 m2
K_{yy}=1.3E-15 m2
K_{zz}=3.5E-15 m2
K_{xx}/K_{zz}=0.87
K_{yy}/K_{zz}=0.37
K_{yy}/K_{xx}=0.43
Porosity: 1.64E-05
Number of cells with fractures: 40%

Reference Permeability:
$K_{xx}=K_{yy}=K_{zz}$=1E-15 m2

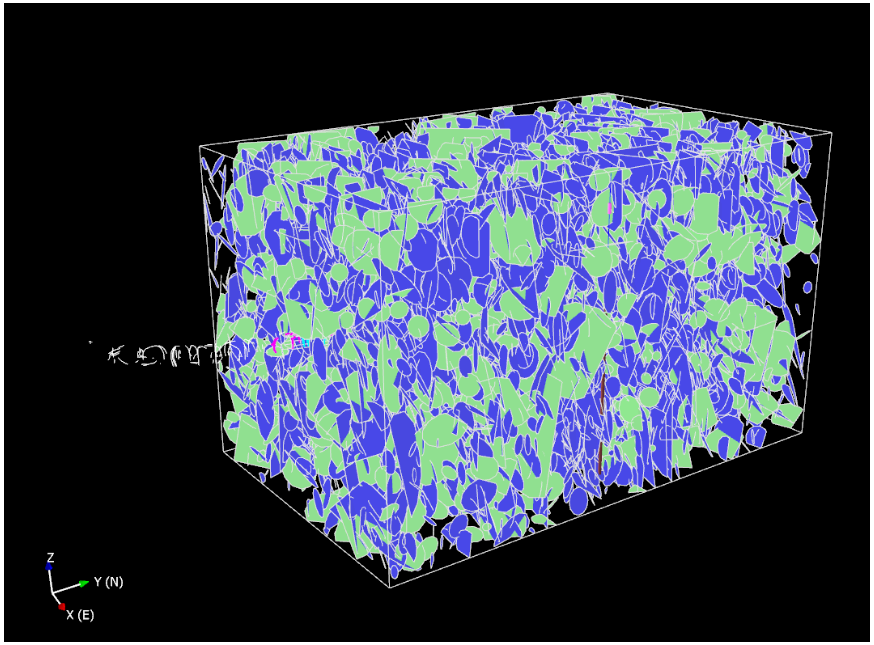


Vertical Slices of Vertical Grid Cell Permeability

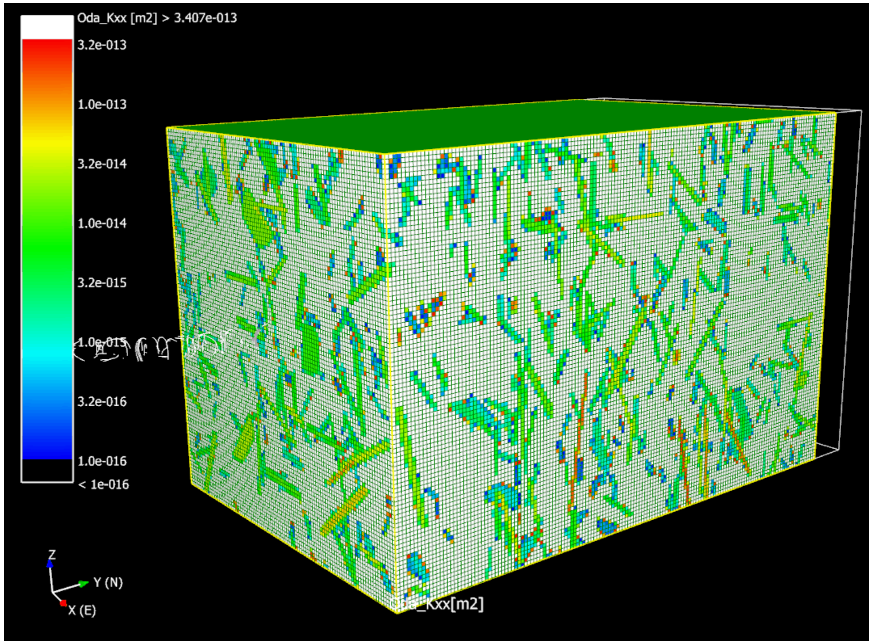




Continuum Model Permeability with 2 Fracture Sets



Mean Grid Properties:
K_{xx}=3.5E-15 m2
K_{yy}=1.84E-15 m2
K_{zz}=4.15E-15 m2
K_{xx}/K_{zz}=0.84
K_{yy}/K_{zz}=0.44
K_{yy}/K_{xx}=0.52
Porosity: 2.1E-05



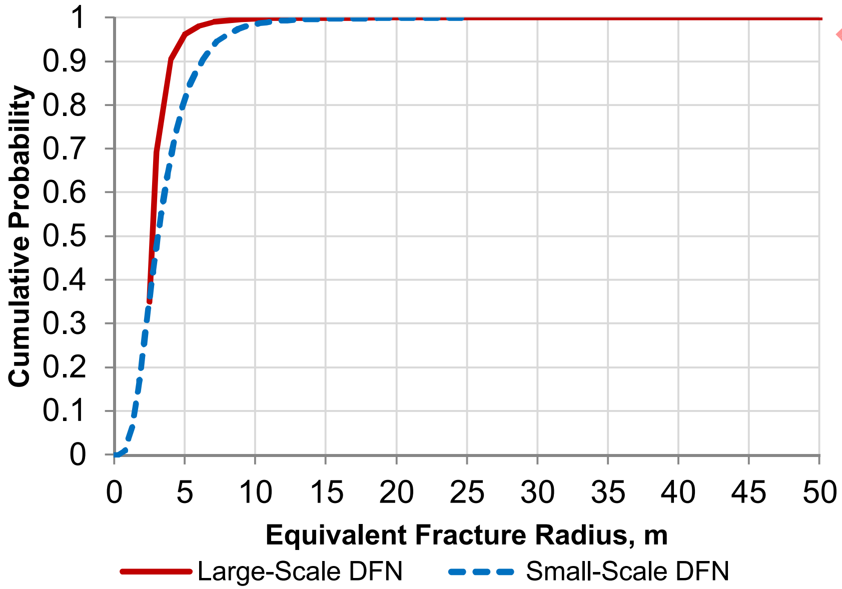
Second Fracture Set Parameters

- North-west trending fractures
- mean plunge 1.30
- concentration parameter ķ equal to 3.6

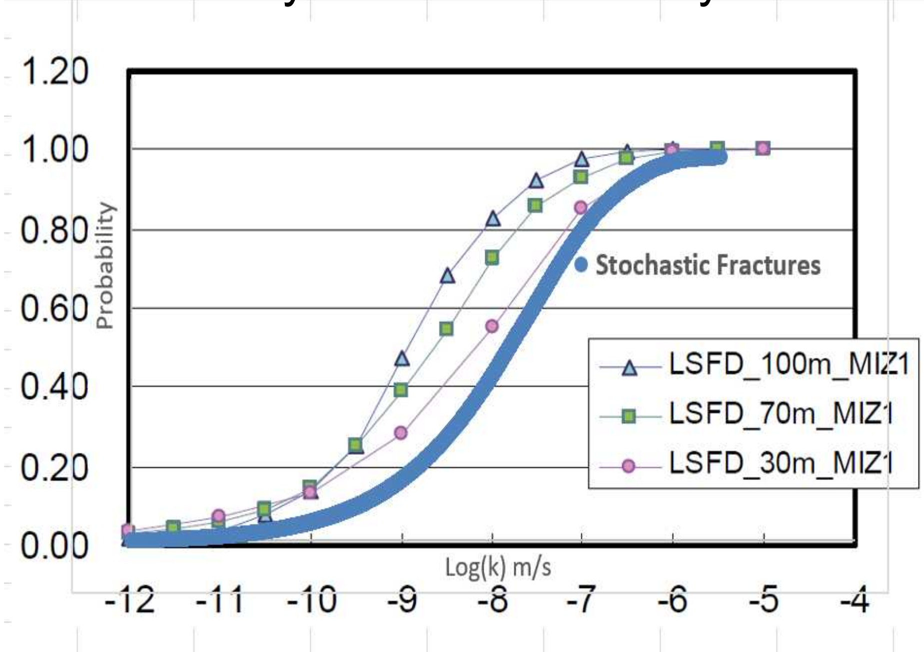
Corroboration with Other Studies of the Tono Area

Parameters of the small-scale model are consistent with the parameters of the large-scale models (Ando, 2012).

Equivalent Fracture Radius



Effective Hydraulic Conductivity in LSFD



Part I Summary

- **The DFN model includes**
  - Conductive fractures in CTD, Inclined Drift, and borehole 12MI33. These fractures have deterministic locations based on observations and stochastic properties (developed).
  - Stochastic fractures - locations and properties (developed) change from realization to realization.

- **Data Used to Develop Fracture Properties:**
  - Fractures traces on the walls of CTD, Inclined Drift, and Access Drift.
  - Fractures observed in borehole 12MI33.
  - Packer test data in 6 test intervals of 12MI33 and 2 test intervals of MIZ-1.
  - Measured total inflow into the research tunnel.

- **Developed Fracture Properties:**
  - Fracture size distributions
  - Relationship between the fracture aperture and permeability and the fracture radius.
  - Fracture orientation – one and two fracture sets were considered.
  - Fracture volumetric intensity

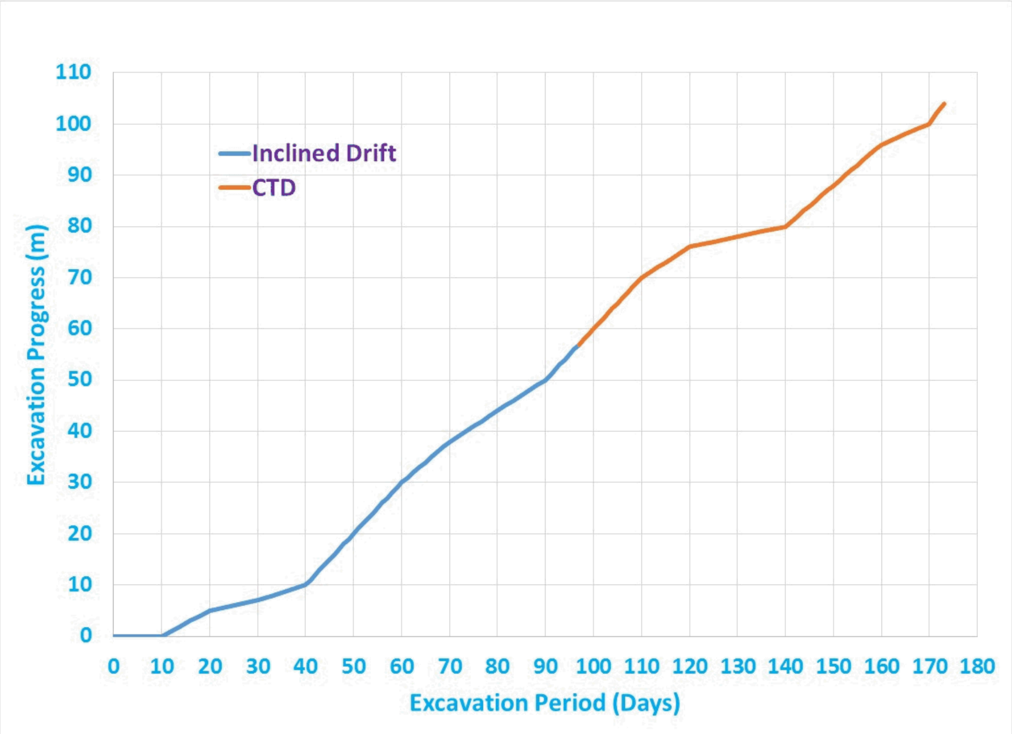
- **Fracture properties are consistent with the other studies in Tono area.**
- **DFN was upscaled to 1x1x1m resolution effective continuum model.**

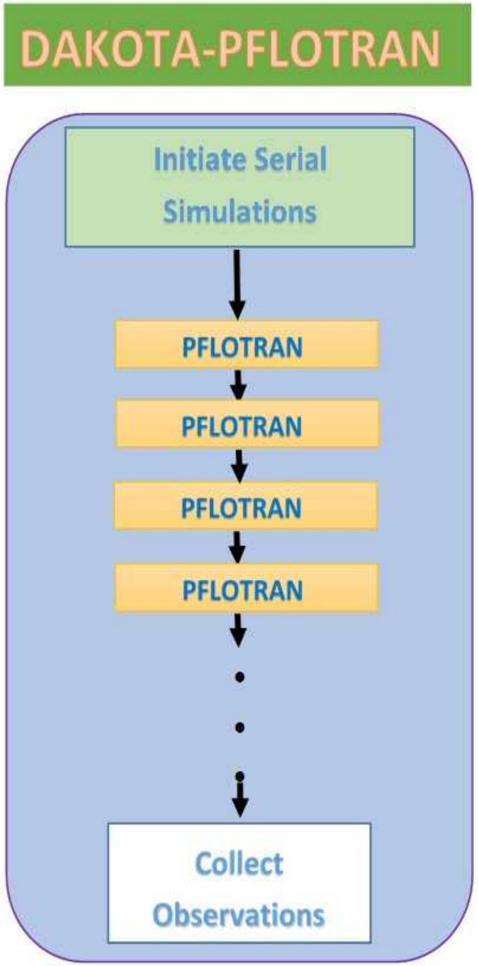
Part II: Flow and Transport Modeling Work

- Homogenous CTD-Scale model (Visualization Area domain)
- Homogenous large domain model
- Fracture model with a single fracture set
- Fracture model with two fracture sets
- Pressure and chloride concentration prediction at observation points
- Inflow rate prediction

Simulation Approach

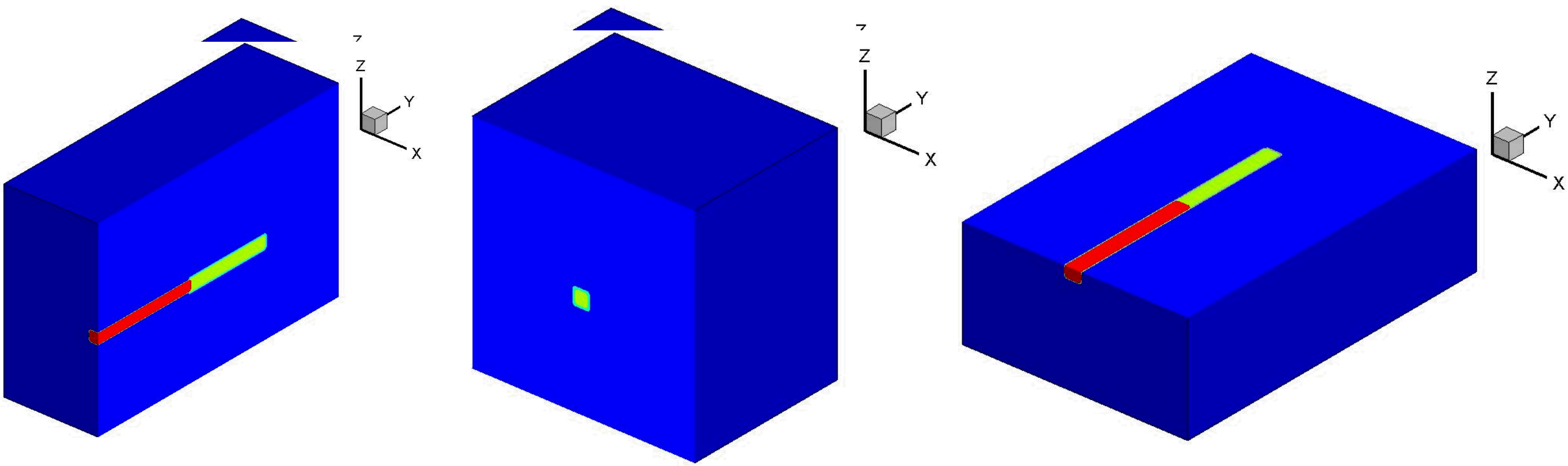
- Progressively removing material
  - 1m at a time for a total of 103 m
- DAKOTA : Optimization Code - Driver
- PFLOTRAN: Massively parallel Numerical Code
- Time zero: 4/6/2013 and 173 days: 9/25/2013





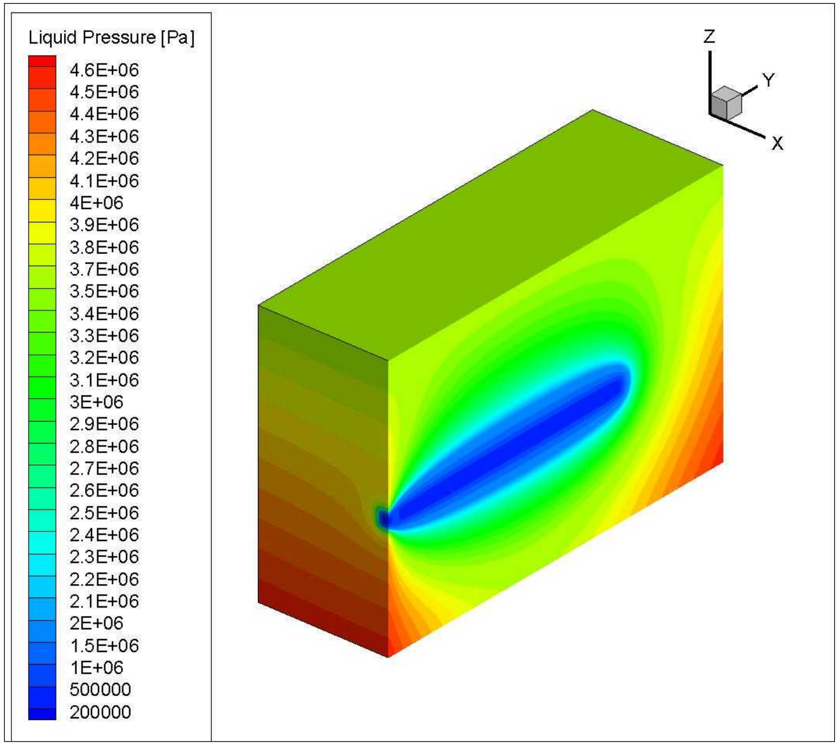
Homogenous Model: CTD-Scale Domain

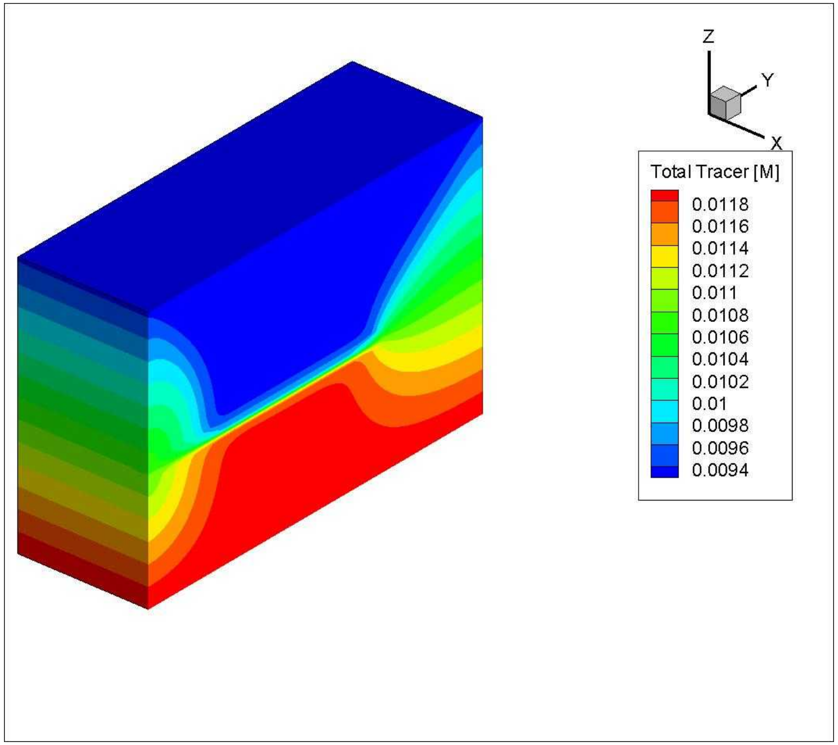
- Domain: 150 m x 100 m x 100 m
  - with cell size of: 1 m x 1 m x 1 m (1,500,000 elements)
- Porosity: 0.001
- Permeability: 10-15 m2 (Hydraulic conductivity: 10-8 m/s)
- Initial Conditions: Hydrostatic pressure and chloride conc. gradient
- Boundary Conditions: Specified pressure and chloride conc.



Distributions of Pressure and Chloride Conc. Homogenous CTD-Scale Model

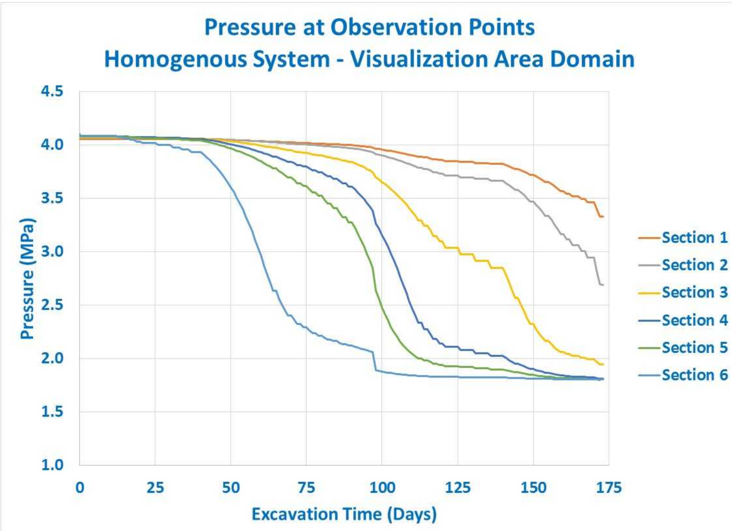
- Initial conditions run provides steady state condition
- Pressure and chloride concentration distributions at simulation time of 173 days (slice along tunnel axis)



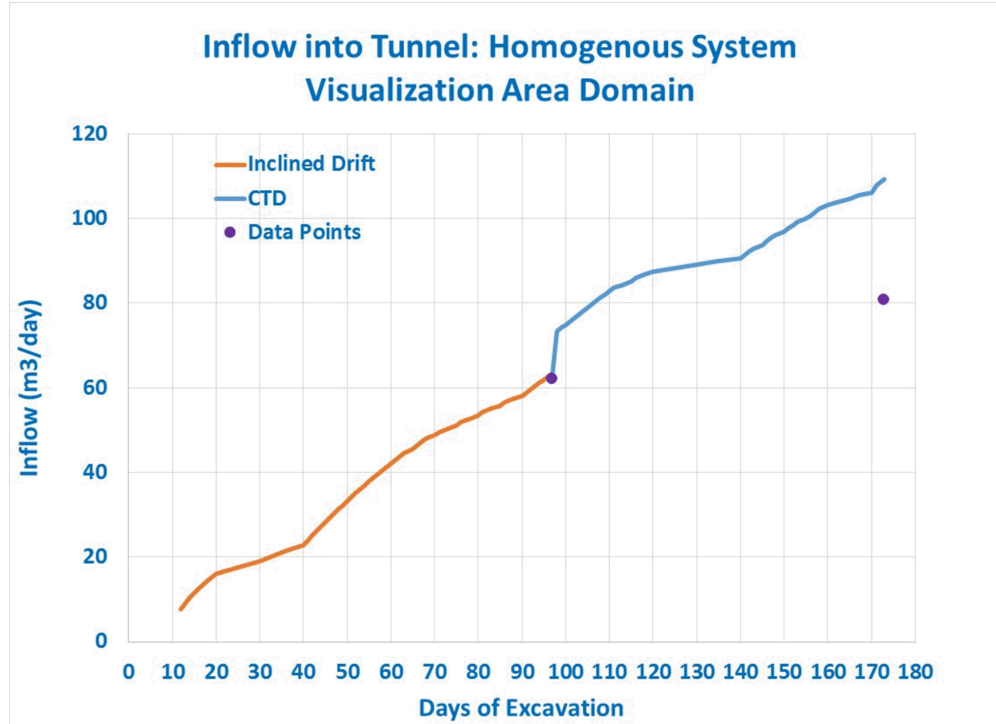


Homogenous CTD-Scale Model Predictions

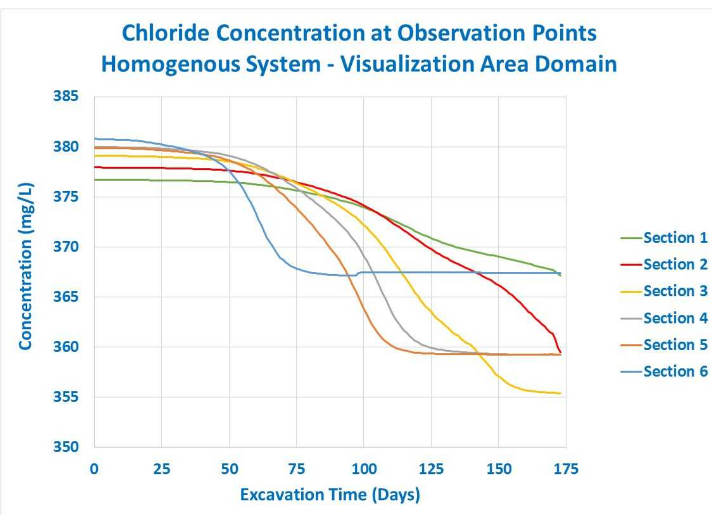
Pressure

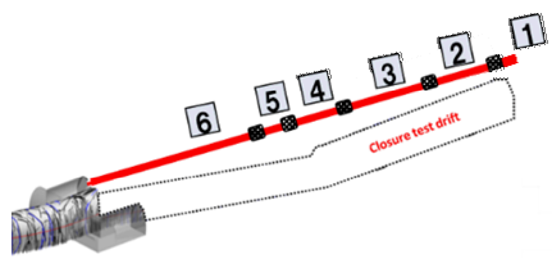


Inflow



Chloride Concentration

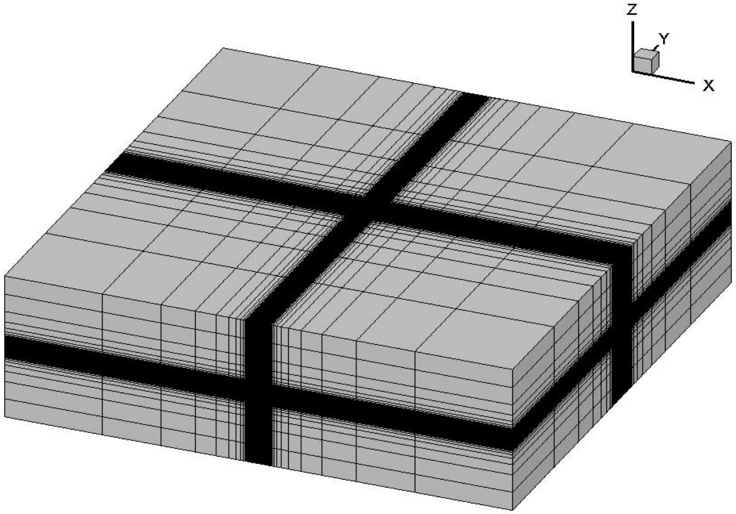




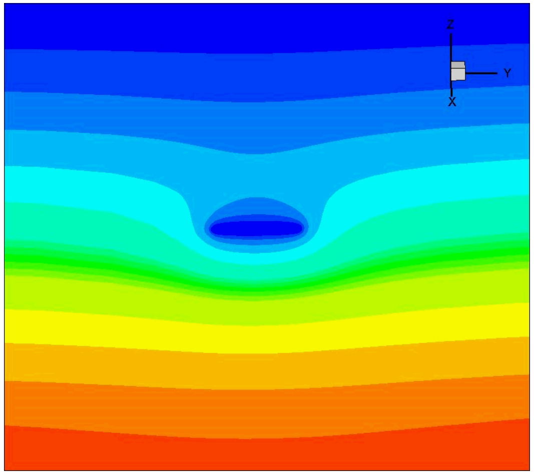
Homogenous Model: Use of Large Domain

Domain: 2080 x 2130 x 700 m^3

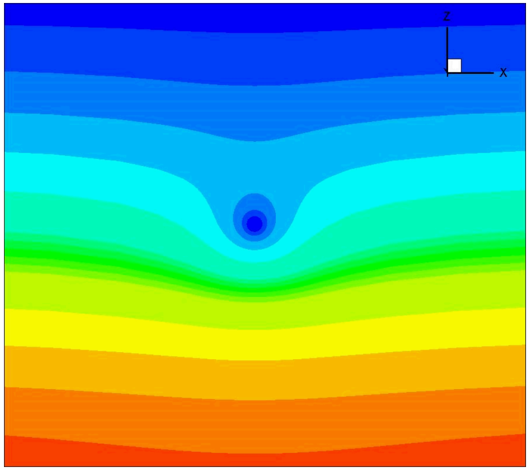
Mesh size: 122 x 122 x 117
= 1,741,428 elements



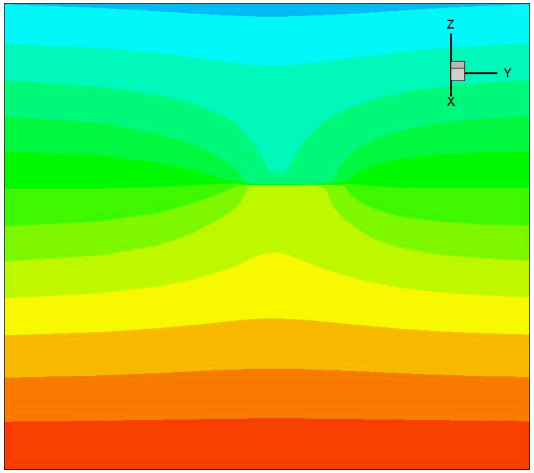
Pressure Distributions at Tunnel

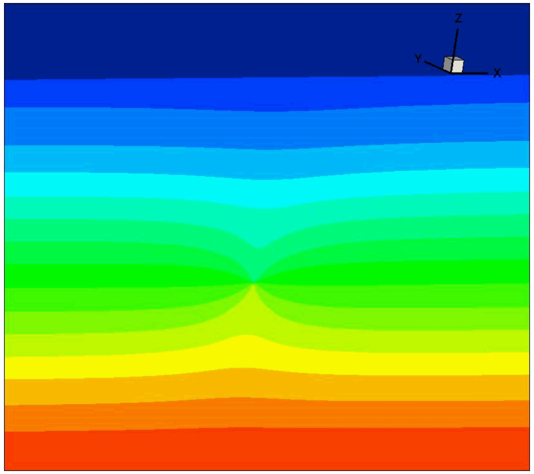


Along Tunnel Axis



Perpendicular to Tunnel Axis

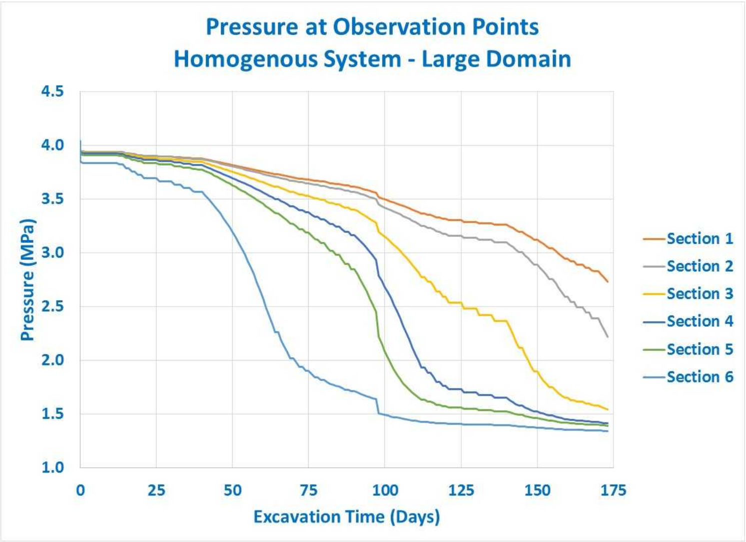




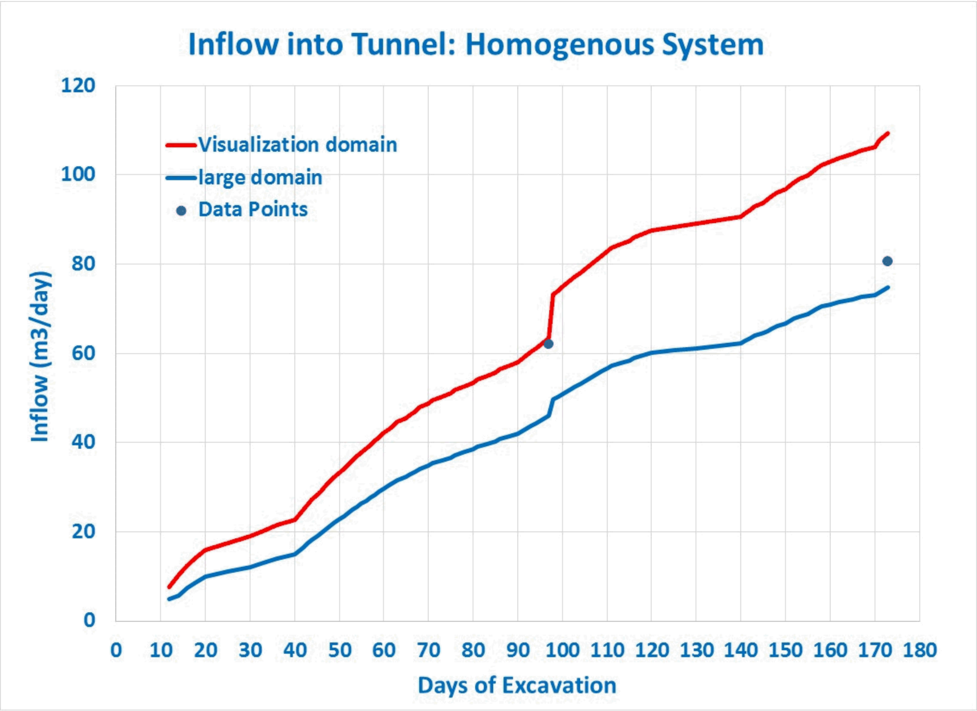
Chloride Concentration Distributions at Tunnel

Homogenous Large Domain Predictions

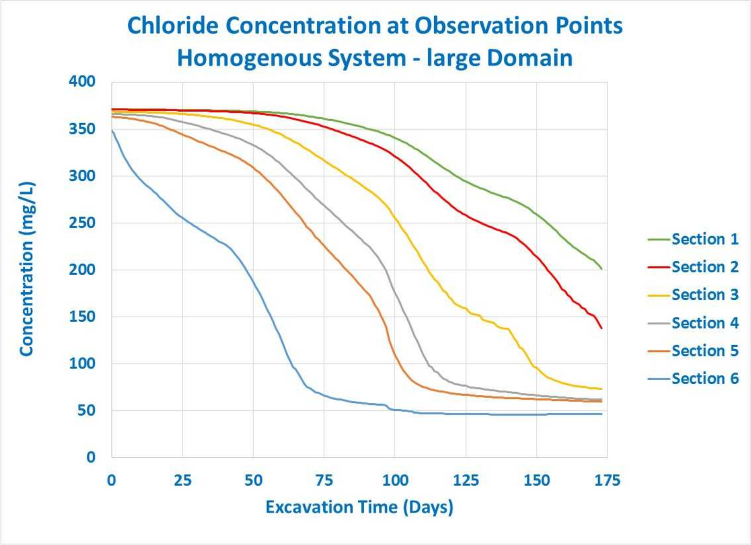
Pressure

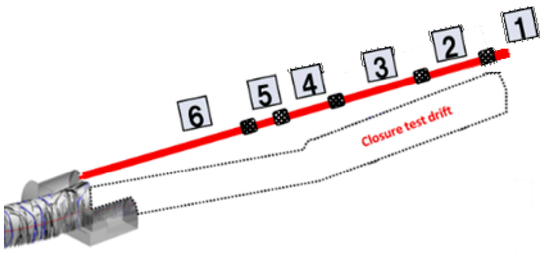


Inflow



Chloride Concentration





Flow and Transport Simulation in Fractured Rock: CTD-Scale Domain

- Fracture model used to generate permeability and porosity fields
- Domain represented by isotropic permeability and porosity
- Two realizations representing a single set and two sets
- Applied west-east pressure gradient
- Darcy's law and east face flux used to calculate effective permeability:

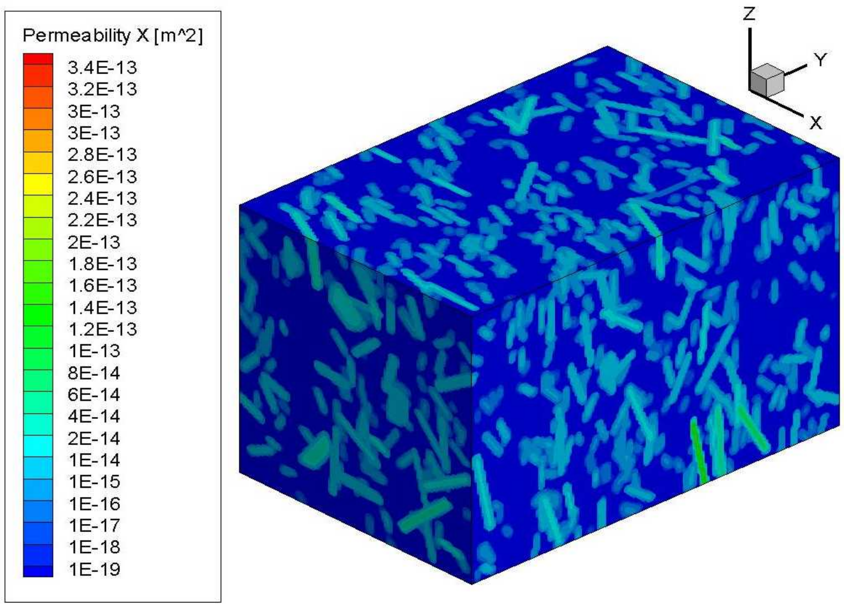
$$q = \frac{-k_{eff}\Delta P}{\mu L}$$

q = flux, k_{eff} = effective permeability, ΔP = pressure difference,
μ = dynamic viscosity, L = distance between west and east faces

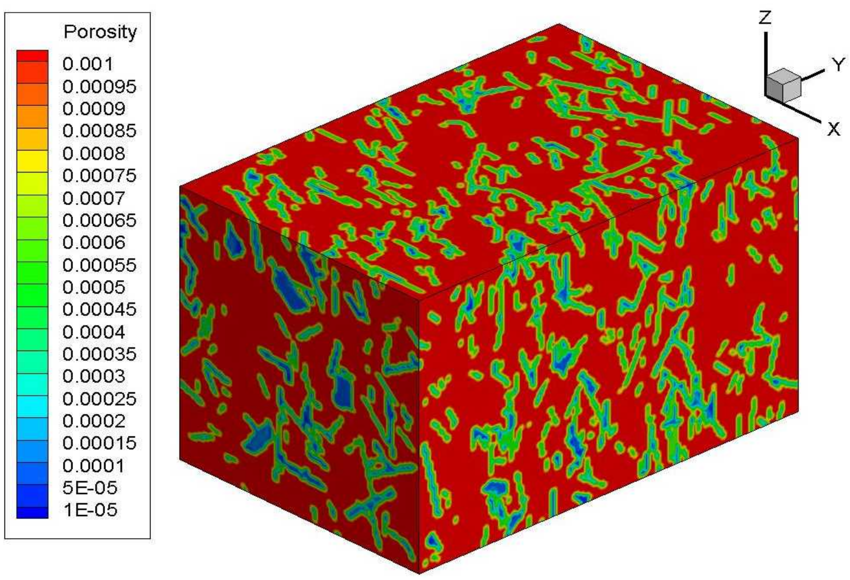
- Effective permeability values: single set (**1.62×10^{-16} m^2**), two sets (**3.27×10^{-16} m^2**)

Permeability and Porosity Fields Fracture System with Single Set

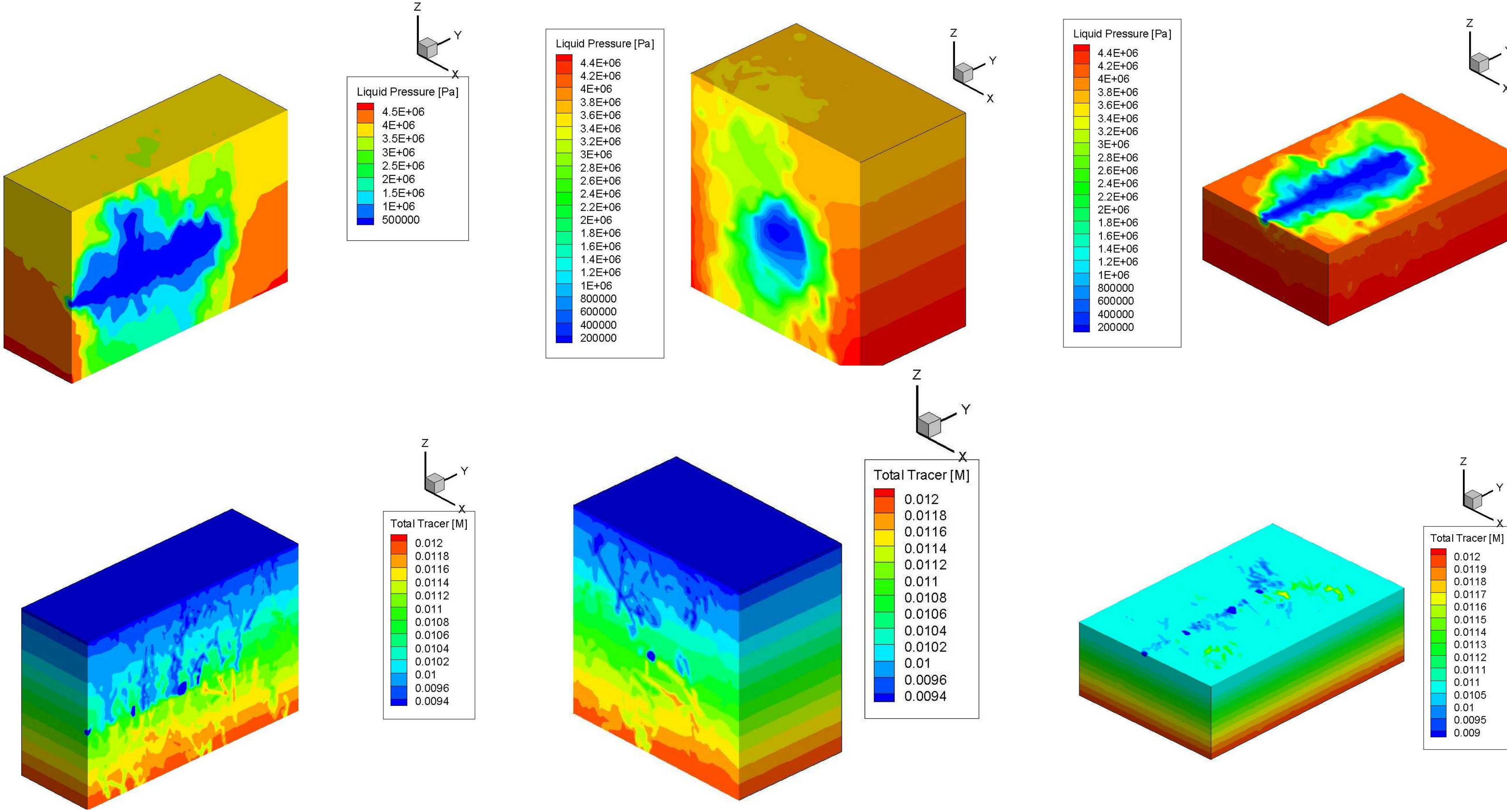
Permeability



Porosity



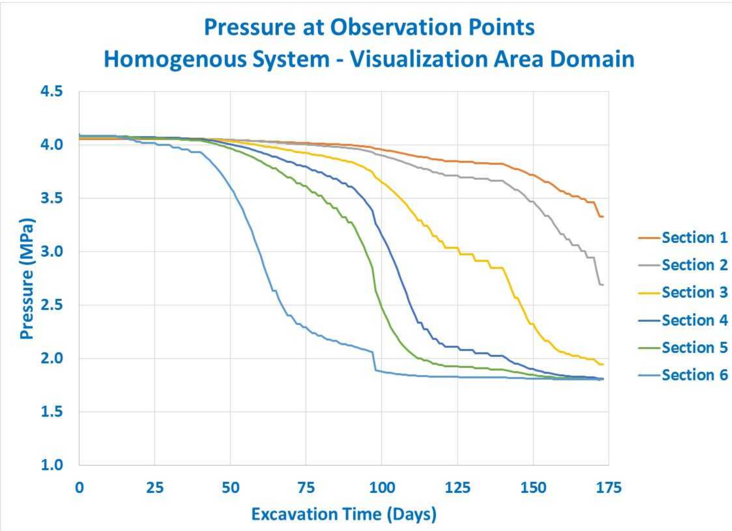
Distributions of Pressure and Chloride Conc.
Fractured System with a Single Fracture Set



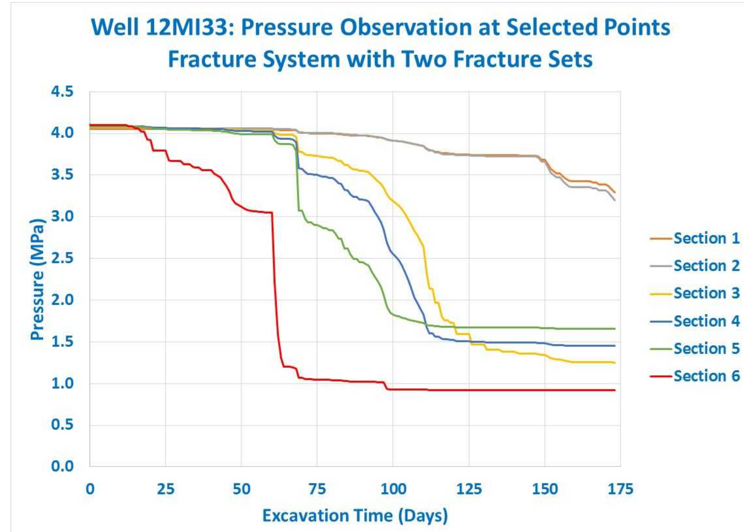
Along Tunnel Axis **Perpendicular to Tunnel Axis** **Horizontal Slice**

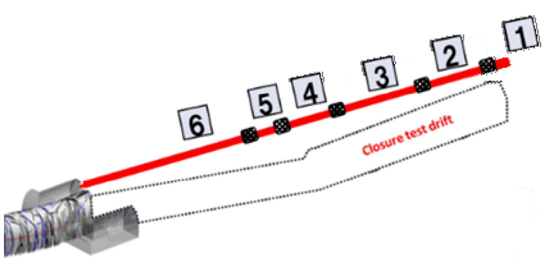
Pressure Predictions at Observation Points

Homogenous Model

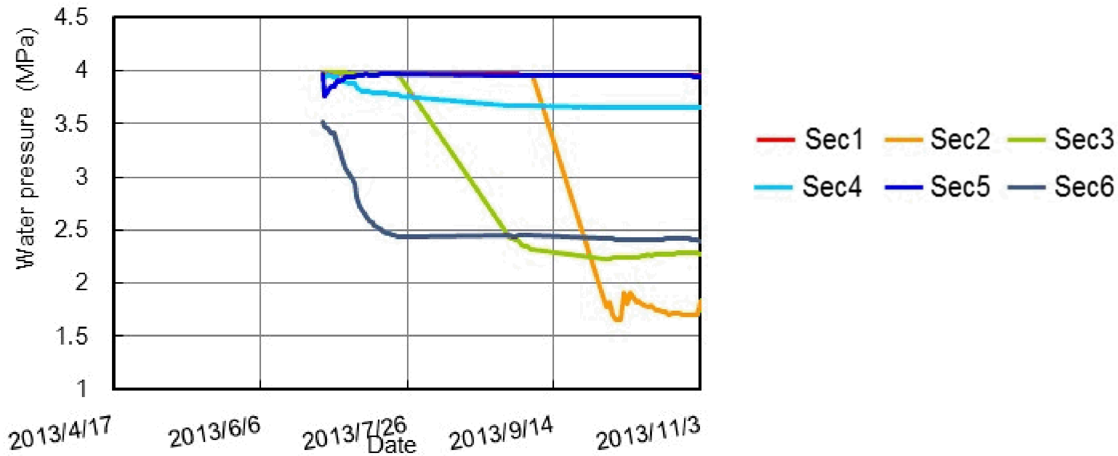


Fracture Model



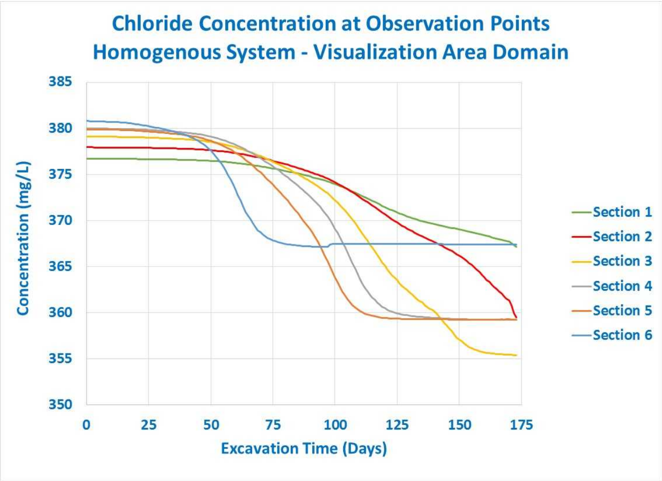


Observation Data

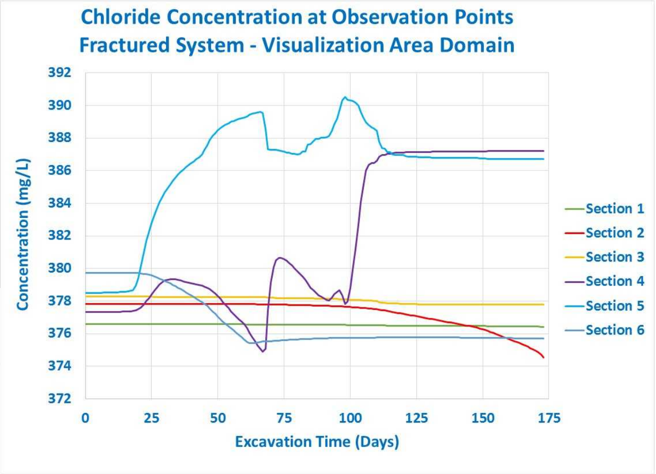


Chloride Predictions at Observations Points

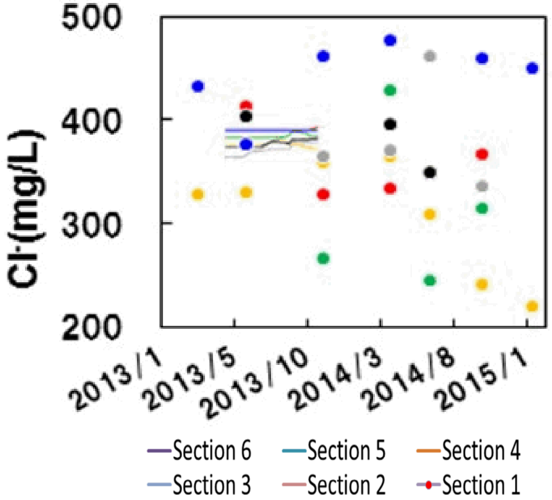
Homogenous CTD-Scale



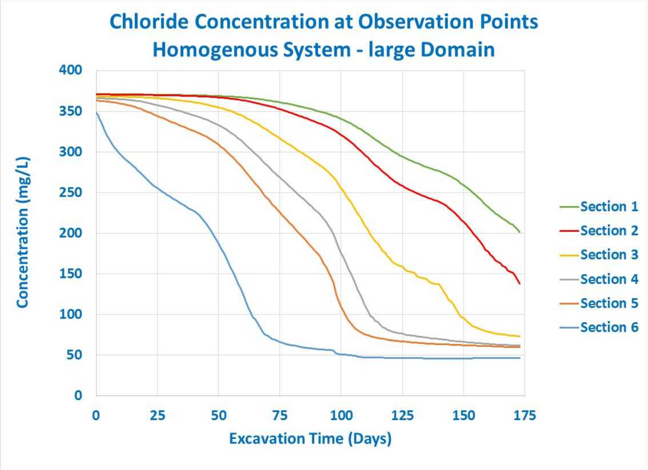
Fractured Single Set



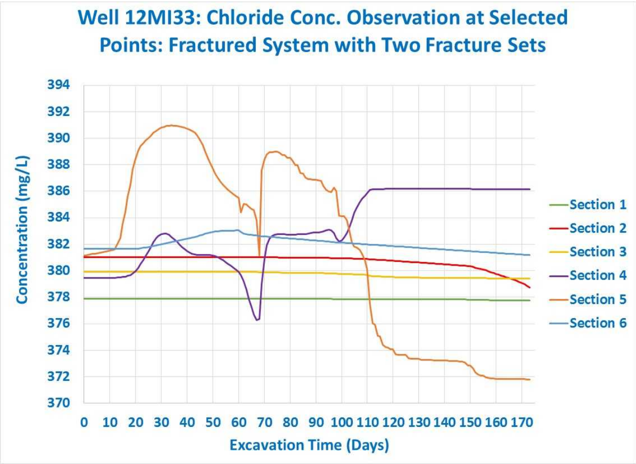
Observation Data



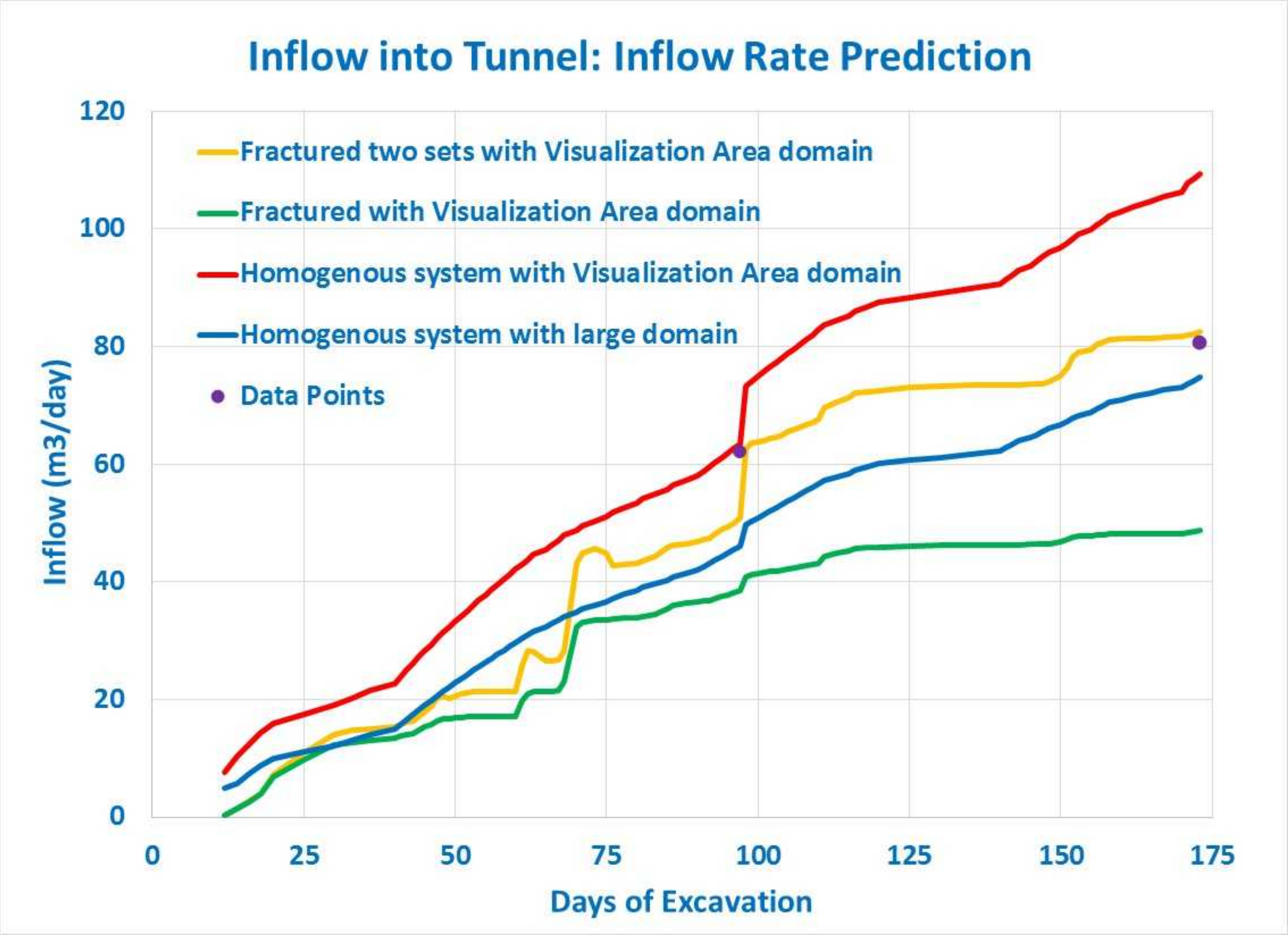
Homogenous Large Domain



Fractured Two Sets



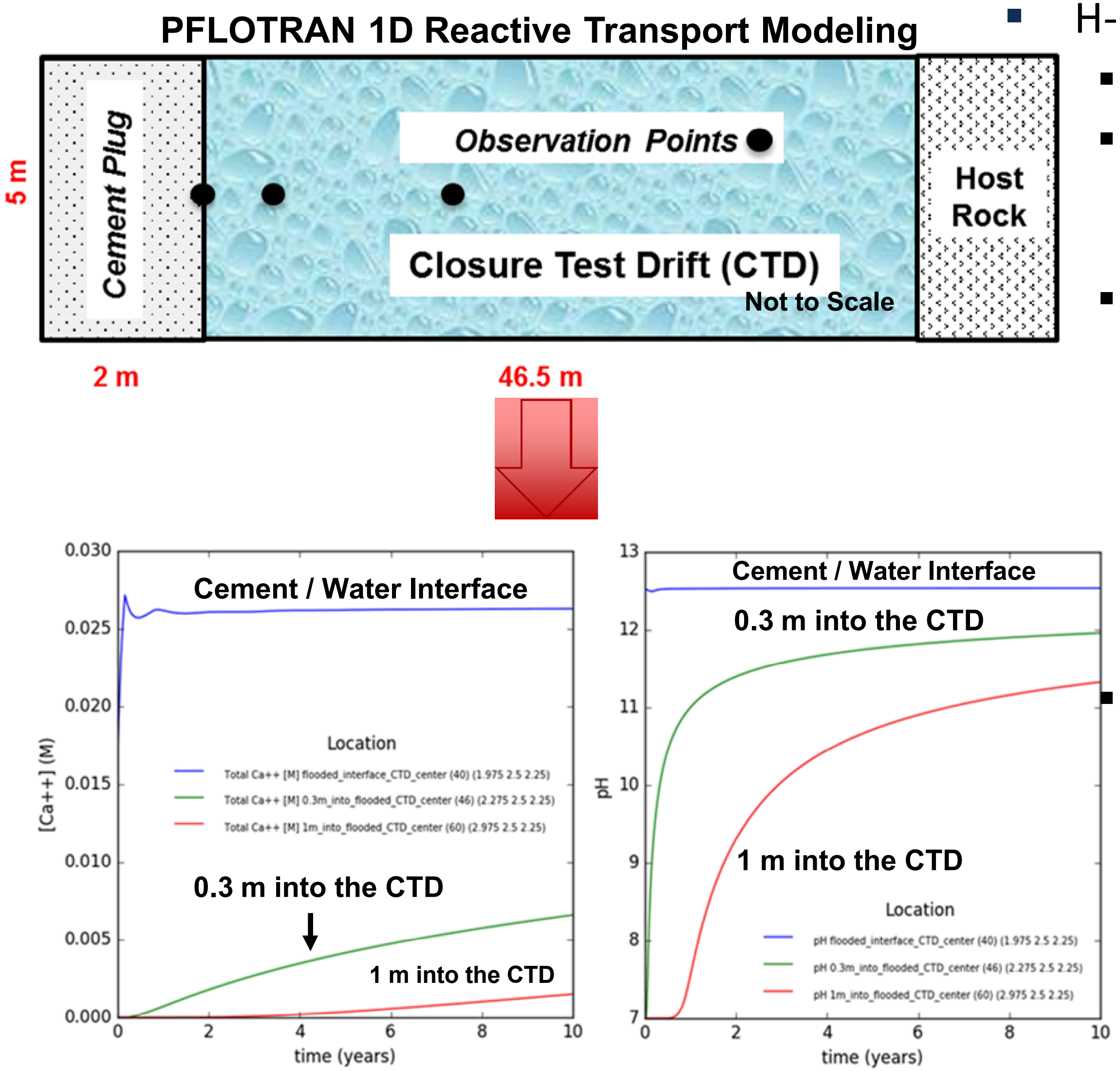
Inflow Prediction for All Models



Part II Summary and Conclusions

- Preliminary flow and transport modeling was conducted to
  - predict inflow into the Inclined Drift and the CTD
  - Predict pressure and chloride concentration at observation points
- Simulations for a homogenous system with reference parameters
  - CTD-Scale (Visualization Area) domain
  - large domain
- Simulations for a fractured system based on fracture model
- Initial and boundary conditions based on project data
- Obtained reasonable predictions of inflow, pressure and chloride concentration profiles

Part III: CTD H-C Model



- H-C (Reactive-transport - RT) modeling
  - **PFLOTRAN** RT simulation tool
  - **GOAL:** Simple 1D RT model to evaluate high pH effects with distance from the cement barrier interface
  - 1D reactive-transport model
    - Sensitivity analyses on transport parameters, reaction rates, aqueous species profiles (ongoing)
    - OPC Cement plug / CTD region
    - Diffusion only (10^{-9} m^2/s)
    - THERMODDEM thermodynamic database including cement phases
  - Effects on water chemistry
    - As expected, rapid pH and [Ca] increases in pore & bulk fluid composition at or near the cement-water interface – need further testing on diffusivities
    - **Next:** incorporate RT into 3D hydrological model with cement liner effects and comparison with borehole 12MI33 observations