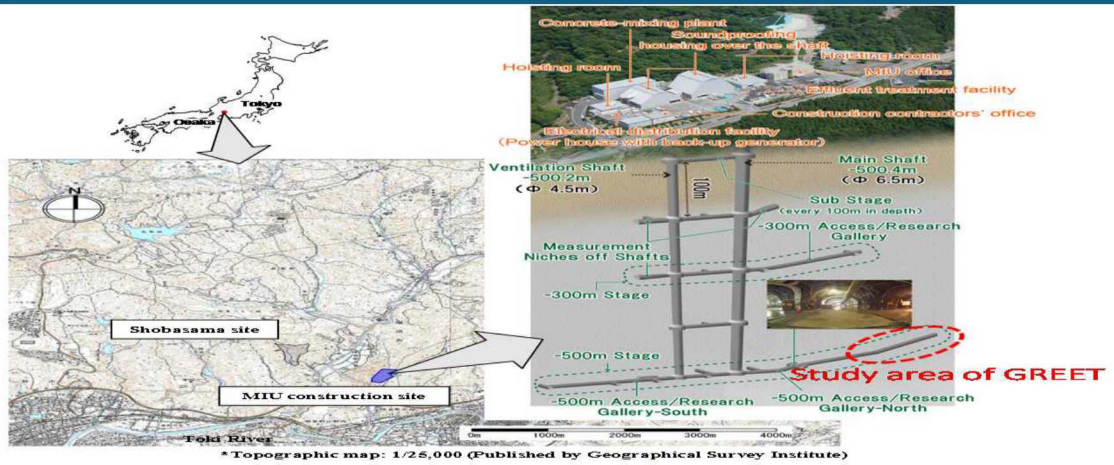
SAND2019-3724C

DECOVALEX19 TASK C: GREET Step 3 Hydrology and Geochemical Analysis Update of SNL Team

DECOVALEX19
WORKSHOP 7
Prague, Czech Republic
April 9-12, 2019



PRESENTED BY

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SAND2019-XXXX

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Step 3: Hydrology and Geochemical Analysis Update of SNL Team

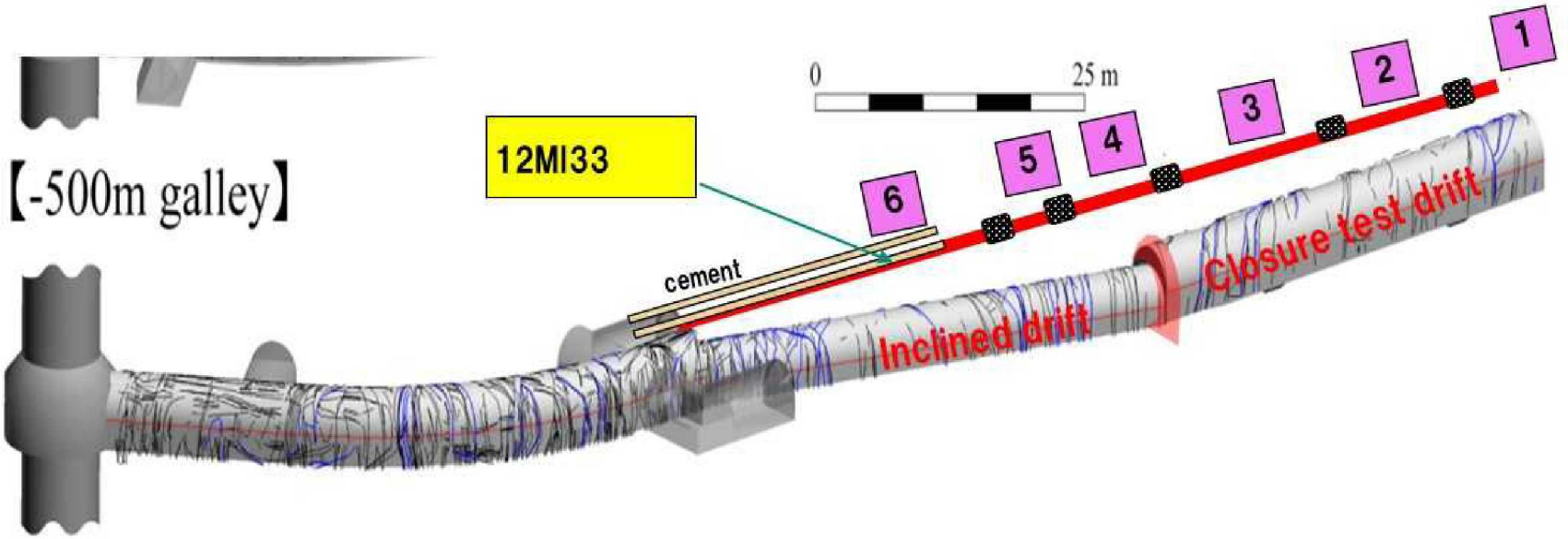
- Part I: Step 3 – Update on hydrology analysis
- Part II: Closure Test Drift (CTD) Geochemistry

Task C: Part I - Update on Hydrology Analysis

- Step 3 – Updated flow modeling of CTD filling and recovery.
- Used previously generated modeling tools.
- Used experimental pressure history data in CTD.
  - Predict flow and leakage at CTD.
  - Predict pressure history at observation points in borehole 12MI33.
- Used fracture model of ten realizations
- Studied effect of boundary condition by comparing results of the base case domain and a larger domain

Study Area: Tunnel and an Observation Borehole

- Tunnel sections: Inclined Drift and Closure Test Drift
- Monitoring Sections in Observation Borehole 12MI33



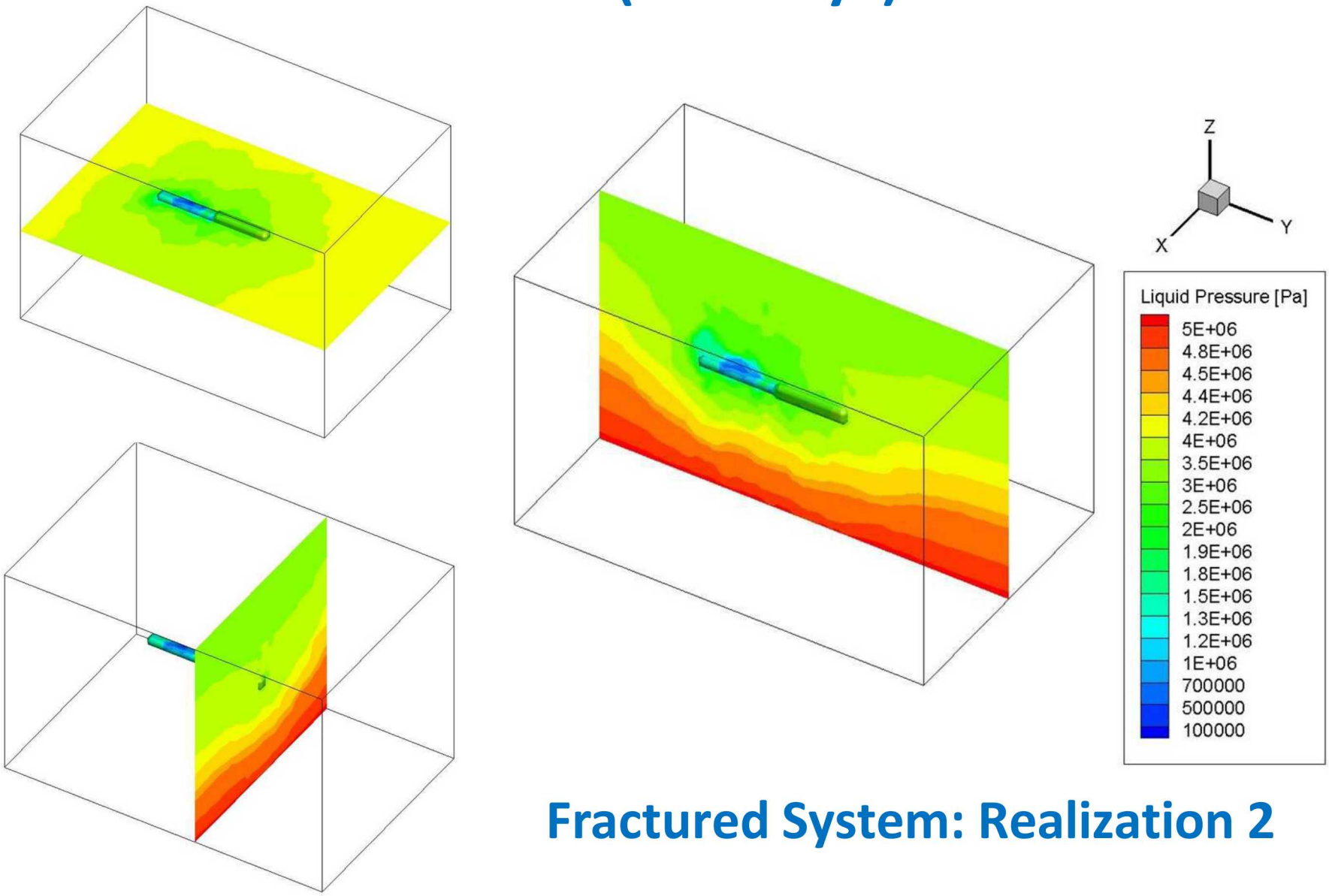
Step3 Pressure Recovery Model Setup

- Base Case Domain: 200 m x 300 m x 200 m.
  - Grid block size: 2 m x 2 m x 2m.
  - Mesh Size: 1,500,000 grid blocks.
- Utilized fracture model with two fracture sets.
  - 10 realizations selected.
  - Permeability and porosity upscaled to continuum grid.
- PFLOTRAN numerical code was used for flow and transport simulations.

Step 3 Recovery: Updated Flow Modeling

- Updated predictions of CTD filling and post-filling period.
- Ran model to steady state with CTD and P1 to P6 pressure values set:
  - CTD = 1 atm.
  - Inclined Drift = 1 atm.
  - P1 = 3.822 MPa
  - P2 = 1.286 MPa
  - P3 = 1.76 MPa
  - P4 = 3.48 MPa
  - P5 = 3.79 MPa
  - P6 = 3.357 MPa
- Ran flow model to one year (Starting Jan. 7/2016) using steady state as initial condition.
  - Applied experimental pressure vs time boundary condition at all CTD walls. Maintained 1 atm. at inclined drift walls.
  - Simulated injection and leakage at CTD.
  - Simulated pressure history at observation points in Well 12 MI33.

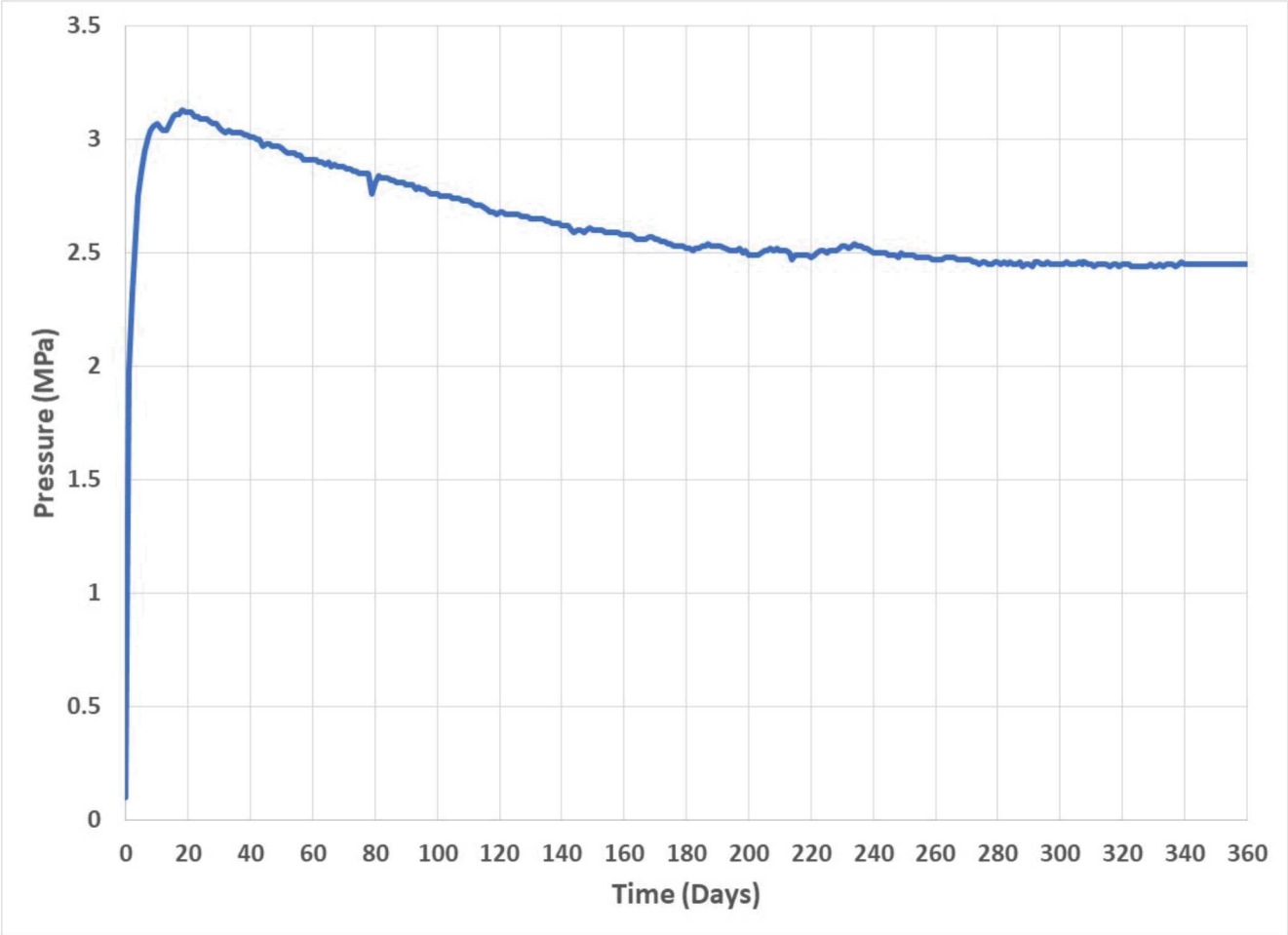
Step3 Recovery: Pressure Distribution at End of Simulation Time (360 days)



Fractured System: Realization 2

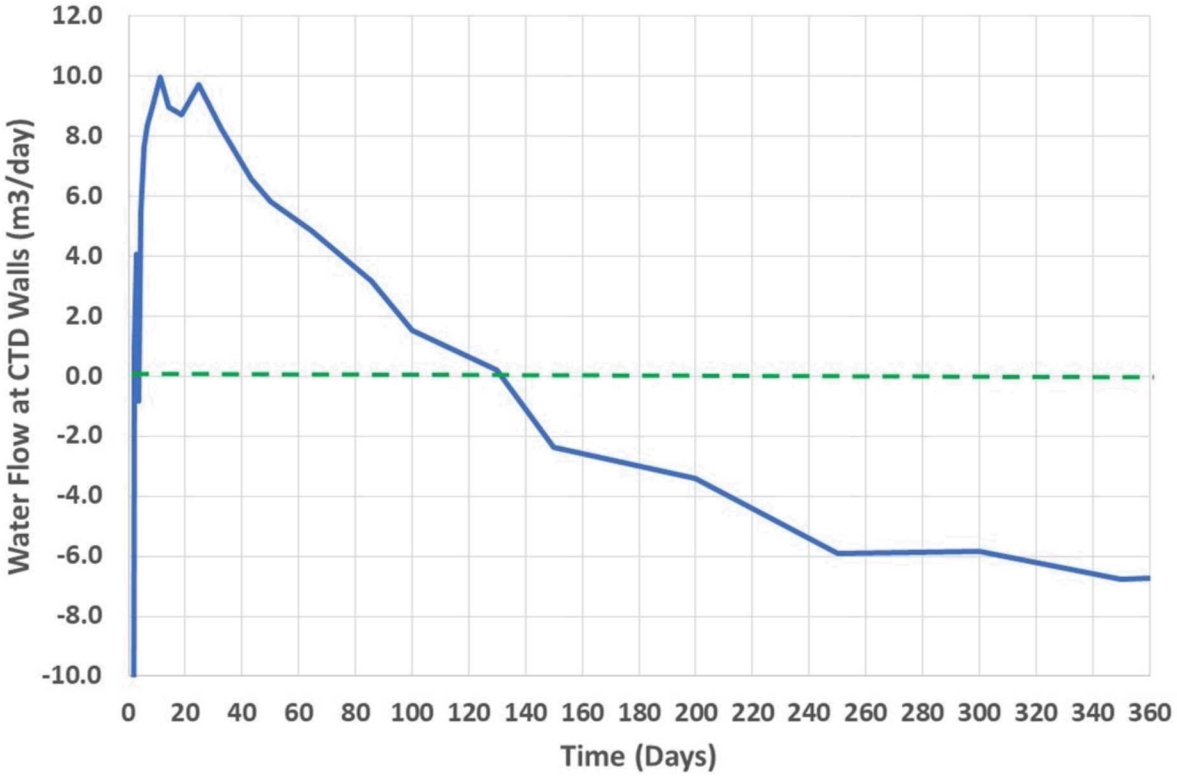
Experimental CTD Pressure During Recovery Experiment

- Used the experimental CTD pressure history as boundary condition at CTD walls.

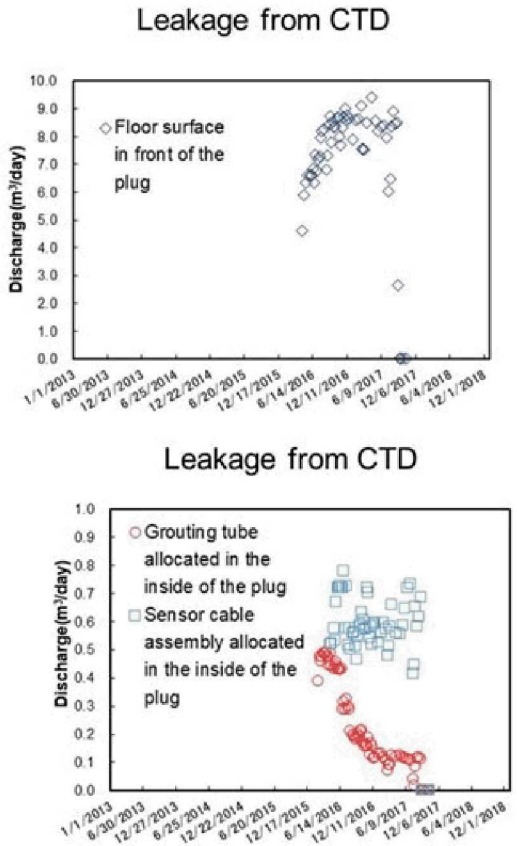


Step3 Recovery: Predicted Flow History at CTD (Injection and Leakage)

- Flow simulations were conducted to predict the flow of water to the CTD.
- Results for fracture Realization 2 are shown.

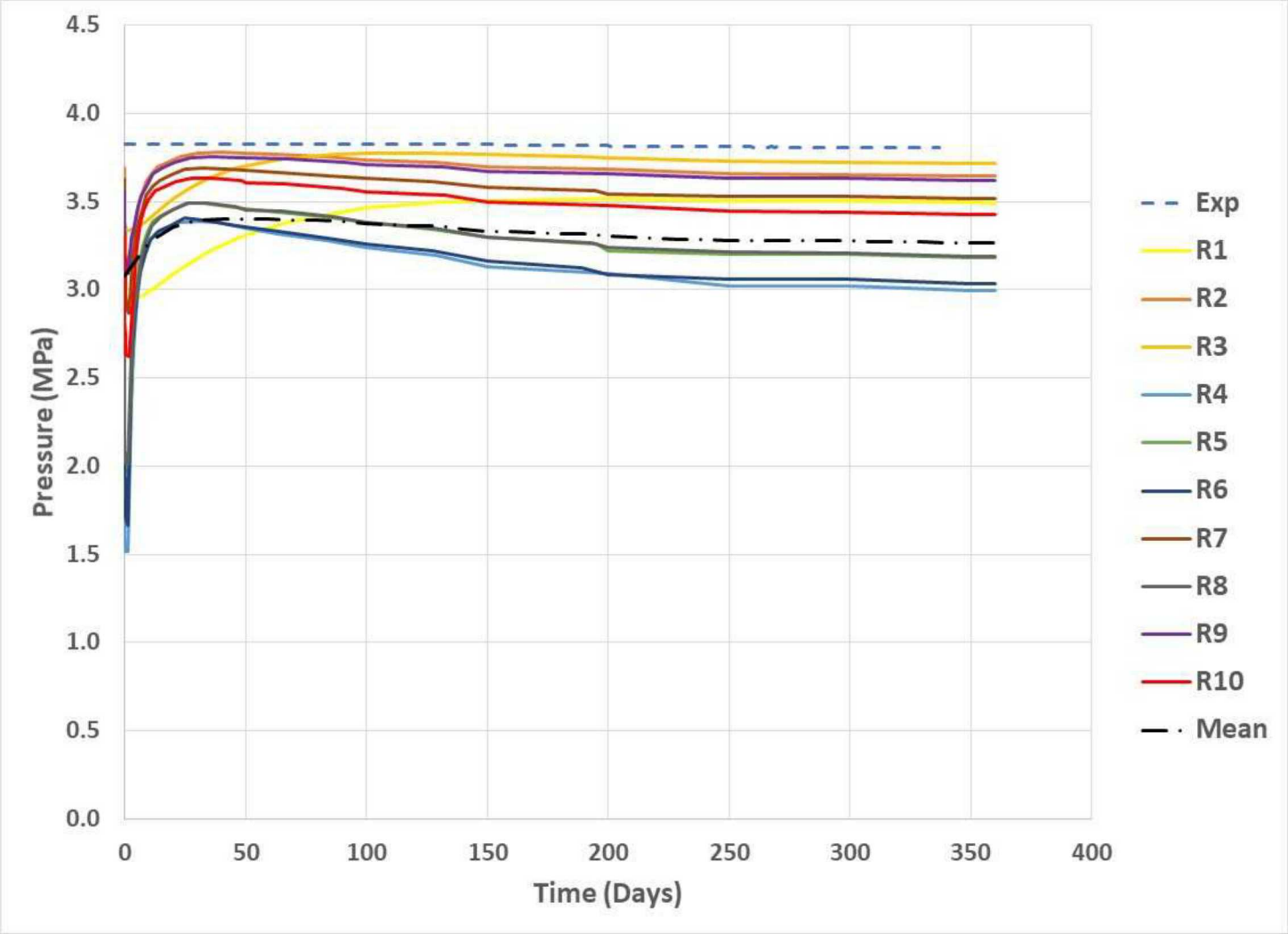


Predicted water flow at CTD

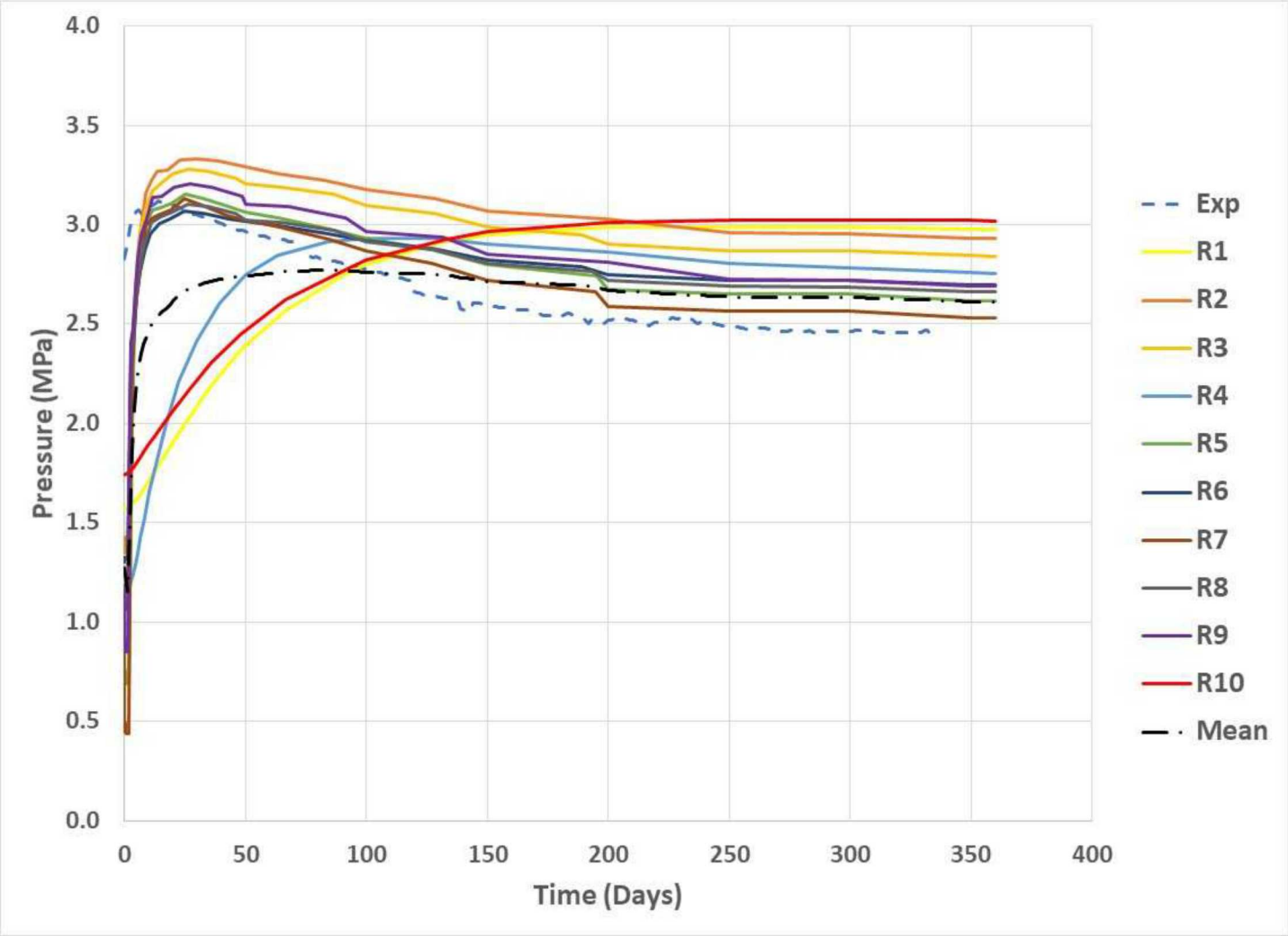


Experimental leakage

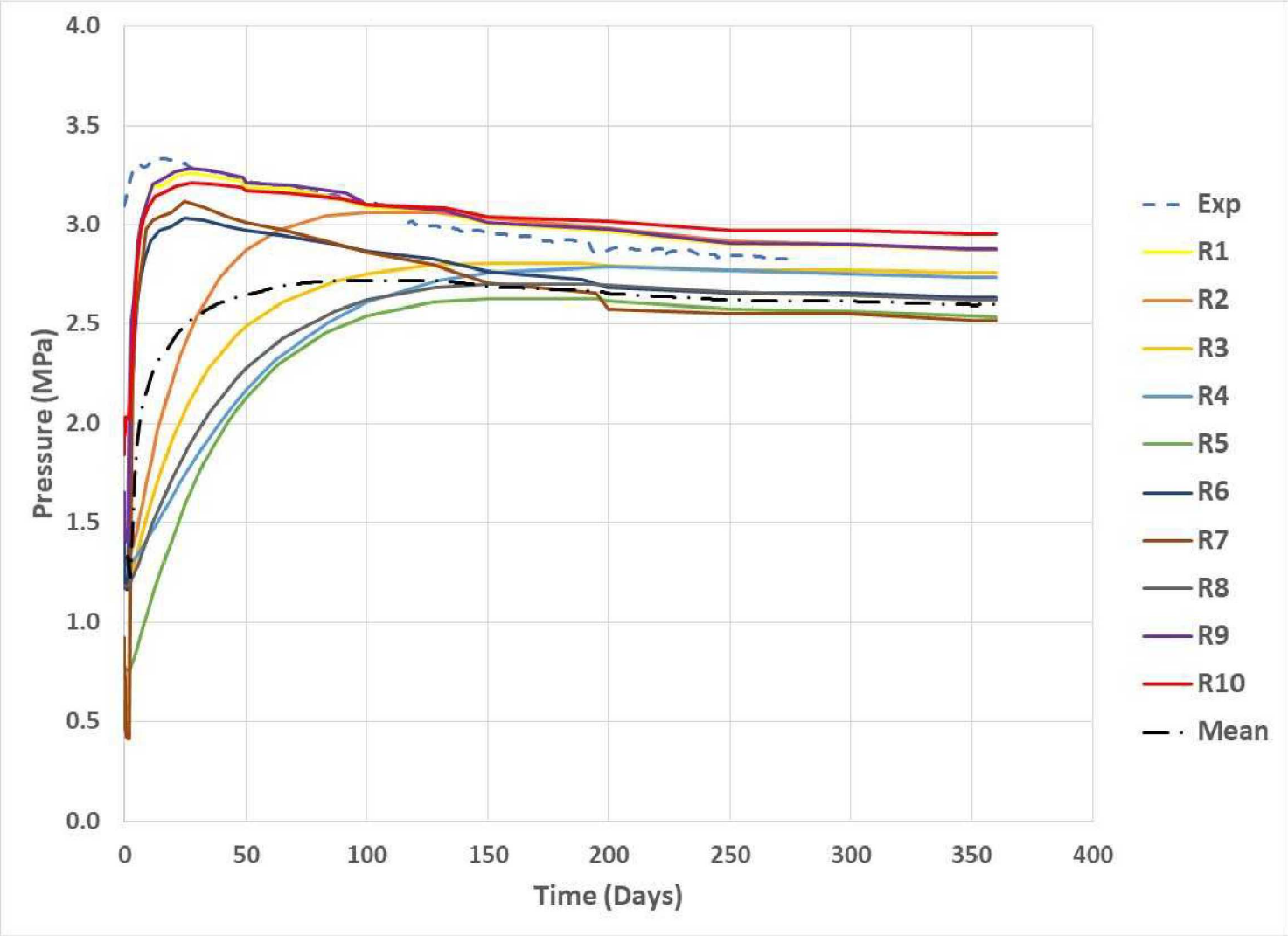
Step3 Recovery: Predicted Pressure History at Observation Point P1 in Well 12MI33 (Ten Fracture Realizations and Mean)



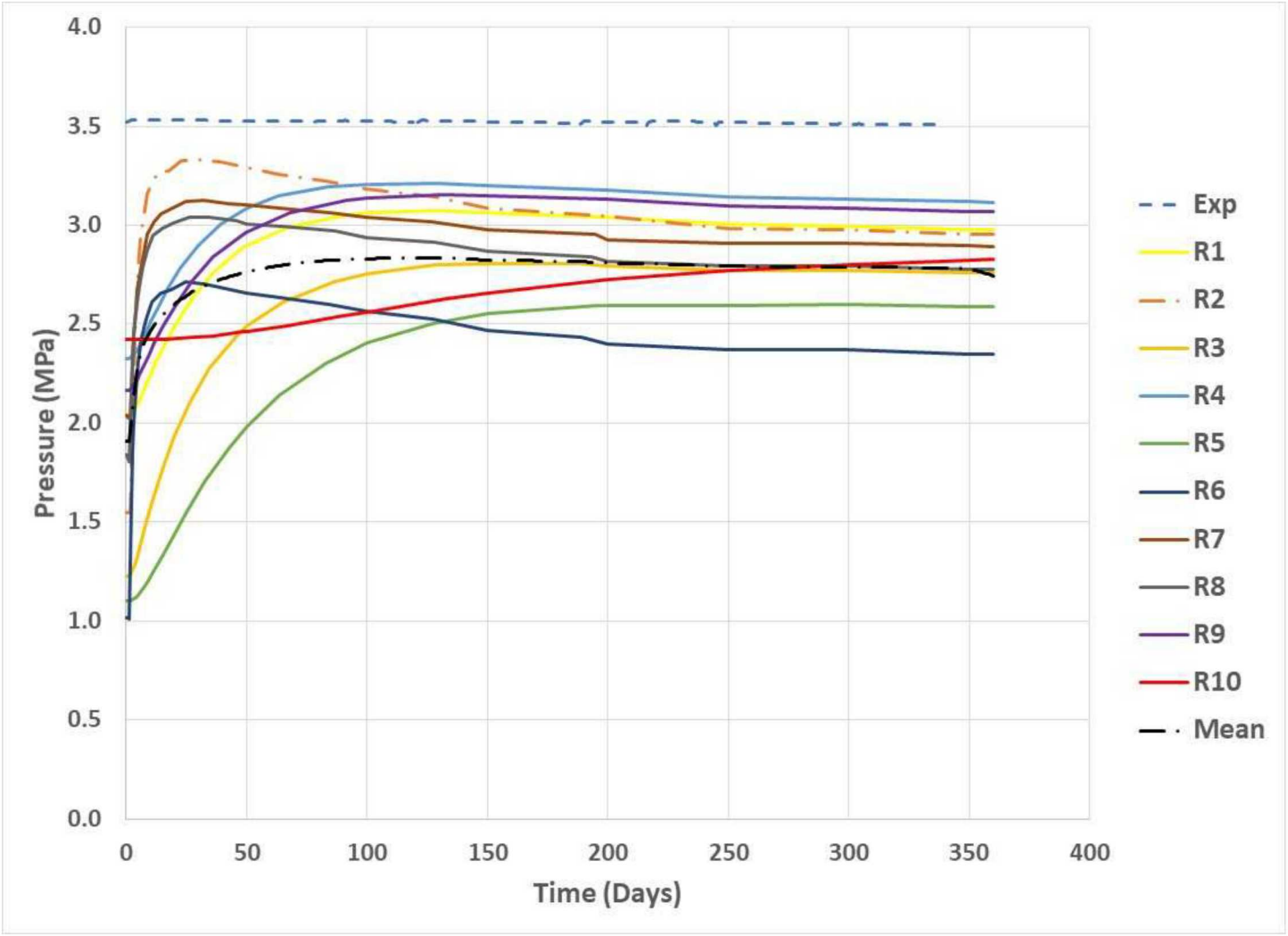
Step3 Recovery : Predicted Pressure History at Observation Point P2 in Well 12MI33 (Ten Fracture Realizations and Mean)



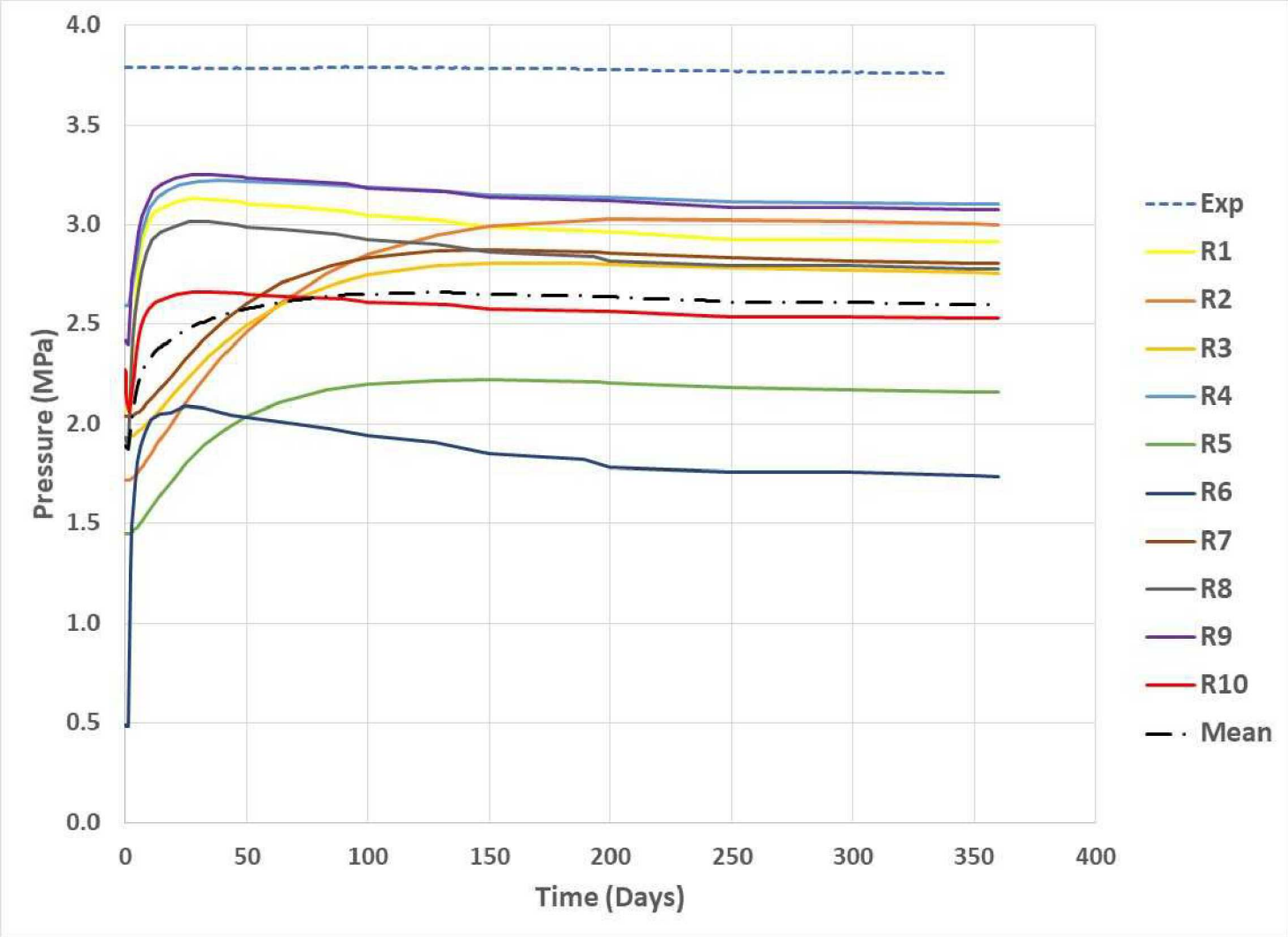
Step3 Recovery: Predicted Pressure History at Observation Point P3 in Well 12MI33 (Ten Fracture Realizations and Mean)



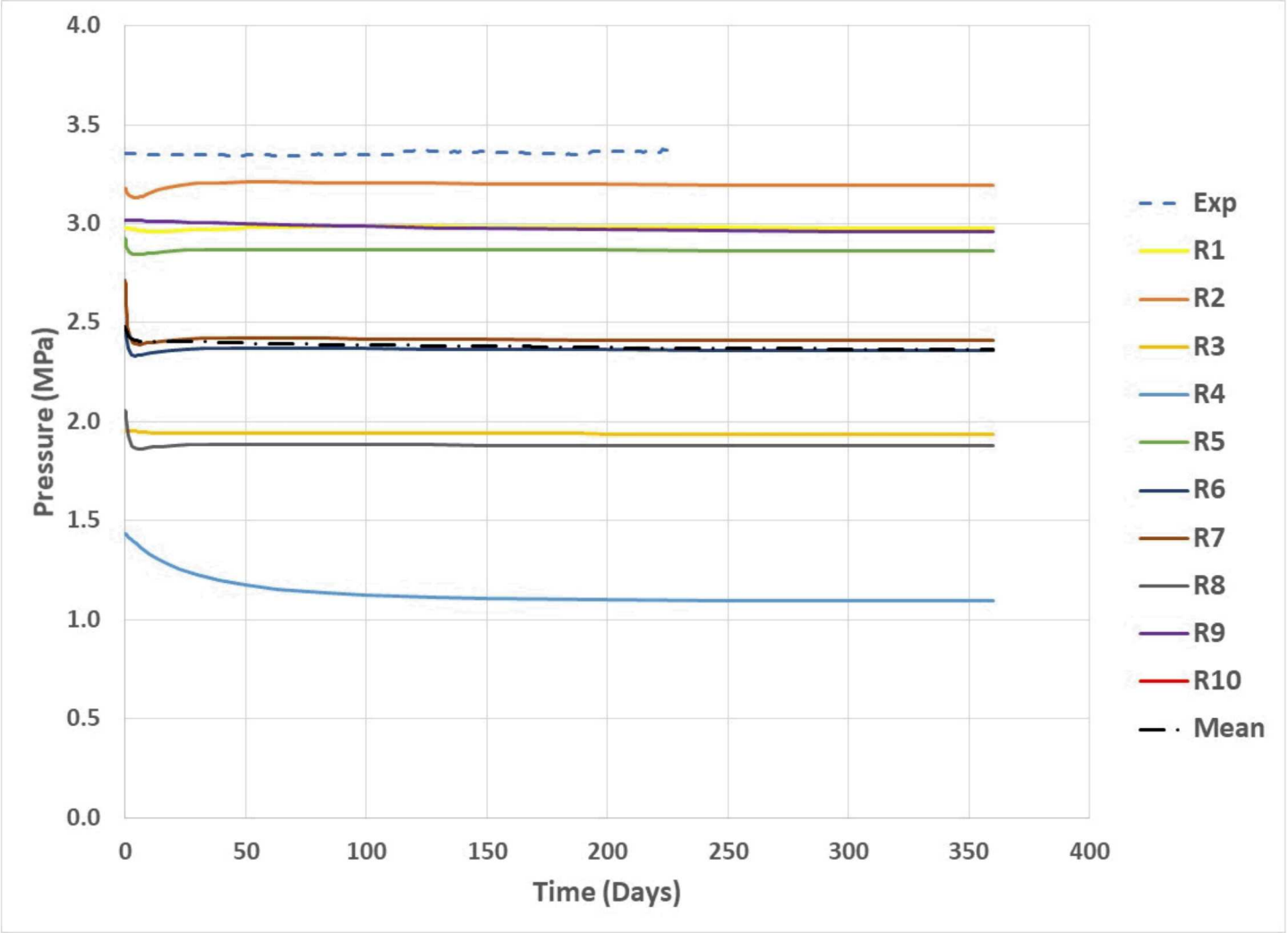
Step3 Recovery: Predicted Pressure History at Observation Point P4 in Well 12MI33 (Ten Fracture Realizations and Mean)



Step3 Recovery: Predicted Pressure History at Observation Point P5 in Well 12MI33 (Ten Fracture Realizations and Mean)



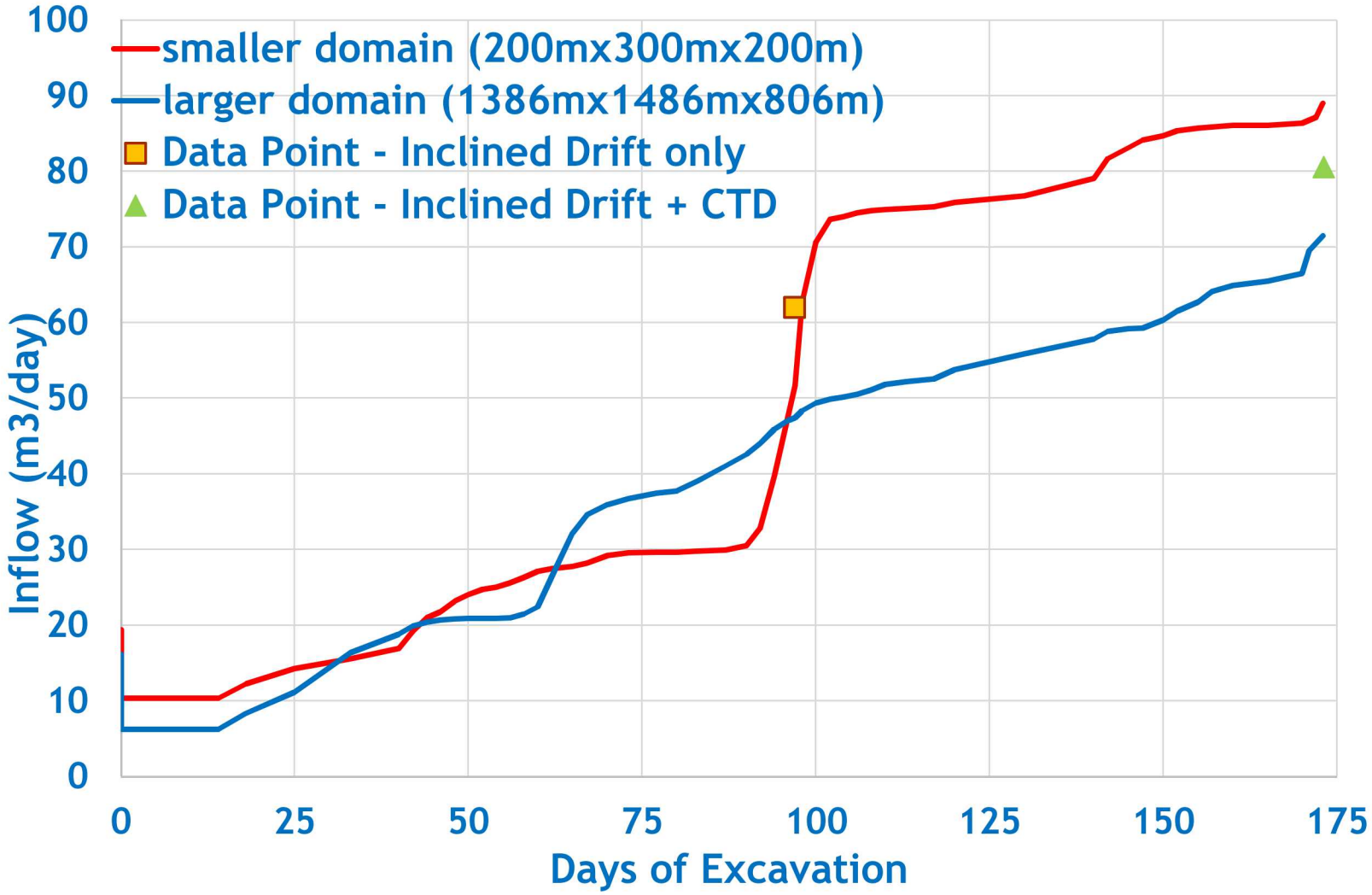
Step3 Recovery: Predicted Pressure History at Observation Point P6 in Well 12MI33 (Ten Fracture Realizations and Mean)



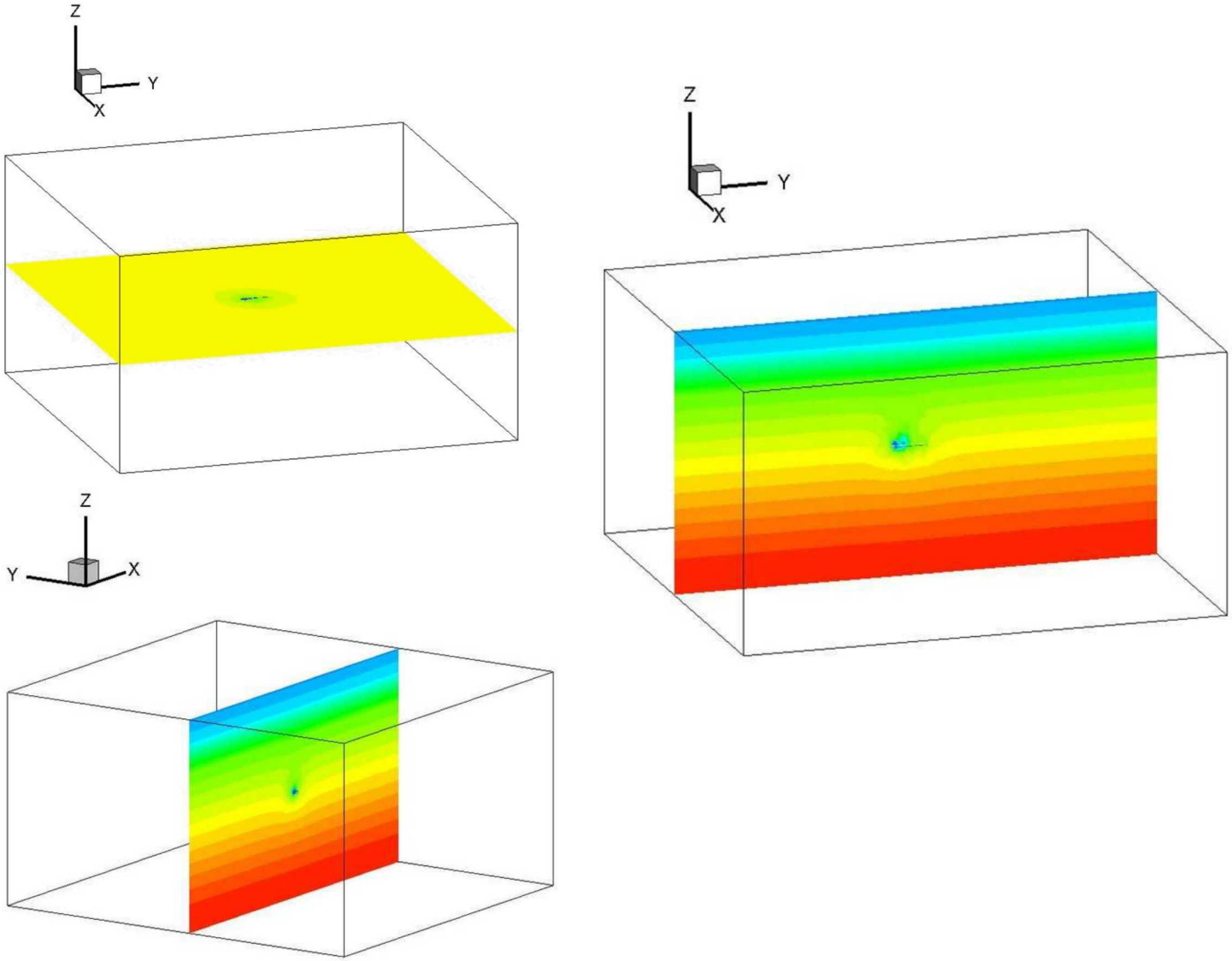
Effect of Boundary Condition

- Use of boundary condition on the sides of the modeling domain may cause boundary effects if the boundary is too close to the tunnel.
- To quantify any boundary effect, the inflow and recovery experiments were modeled using a larger domain.
- Use of the larger domain does not account for additional site features that may exist such as a fault.
- Larger domain dimensions: 1386 m x 1486 m x 806 m.
  - unstructured mesh added to the original mesh
  - Mesh Size: 2,352,987 grid blocks.
- Fracture model was developed for the larger domain using Realization 2 data. Future simulations will include 10 realizations.
  - Permeability and porosity upscaled to continuum grid.
- PFLOTRAN numerical code was used for flow simulations.
- Results were compared with those of the base case domain.

Comparison of Prediction of Inflow During Tunnel Excavation (Fracture Realization 2)

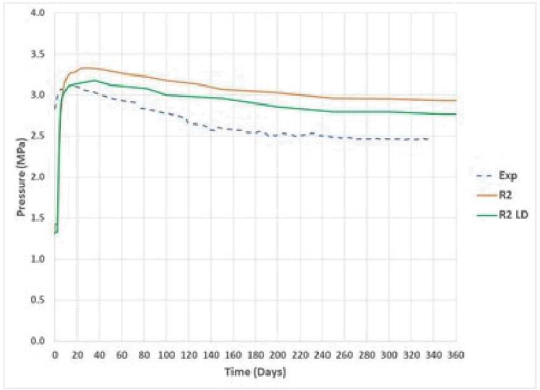


Larger Domain Recovery: Pressure Distribution at End of Simulation Time (360 days) (Fracture Realization 2)

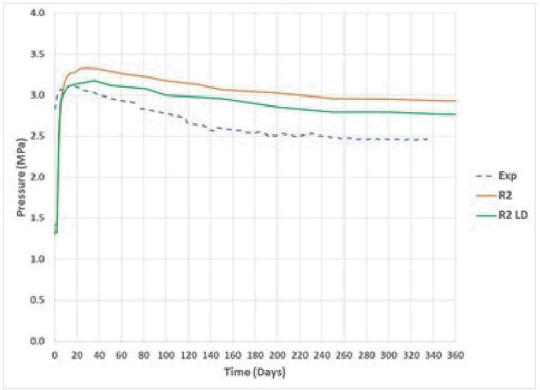


Effect of Boundary Condition1: Large Domain Predicted Pressure History at Observation Points in Well 12MI33 (Fracture Realization 2)

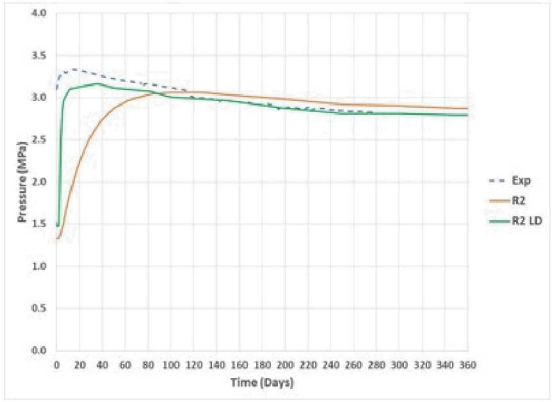
P1



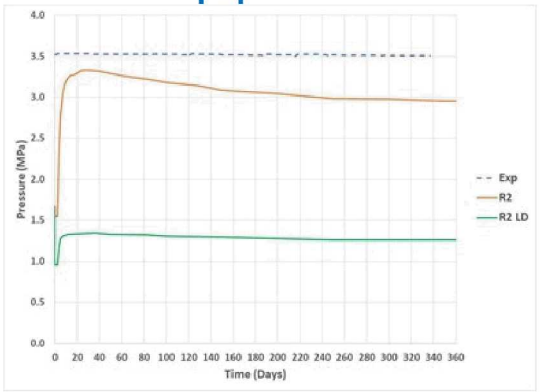
P2



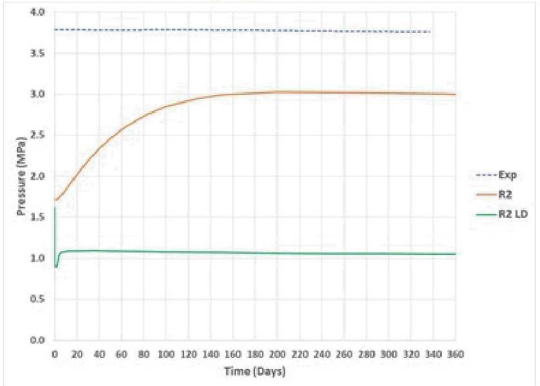
P3



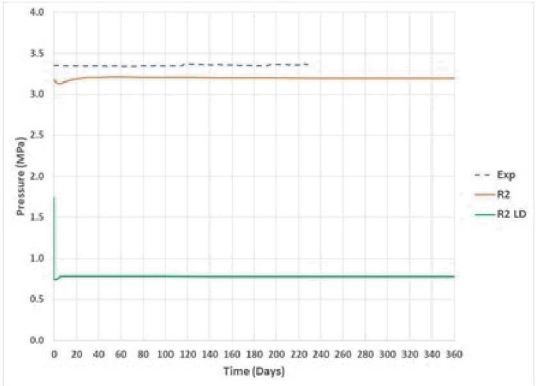
P4



P5



P6



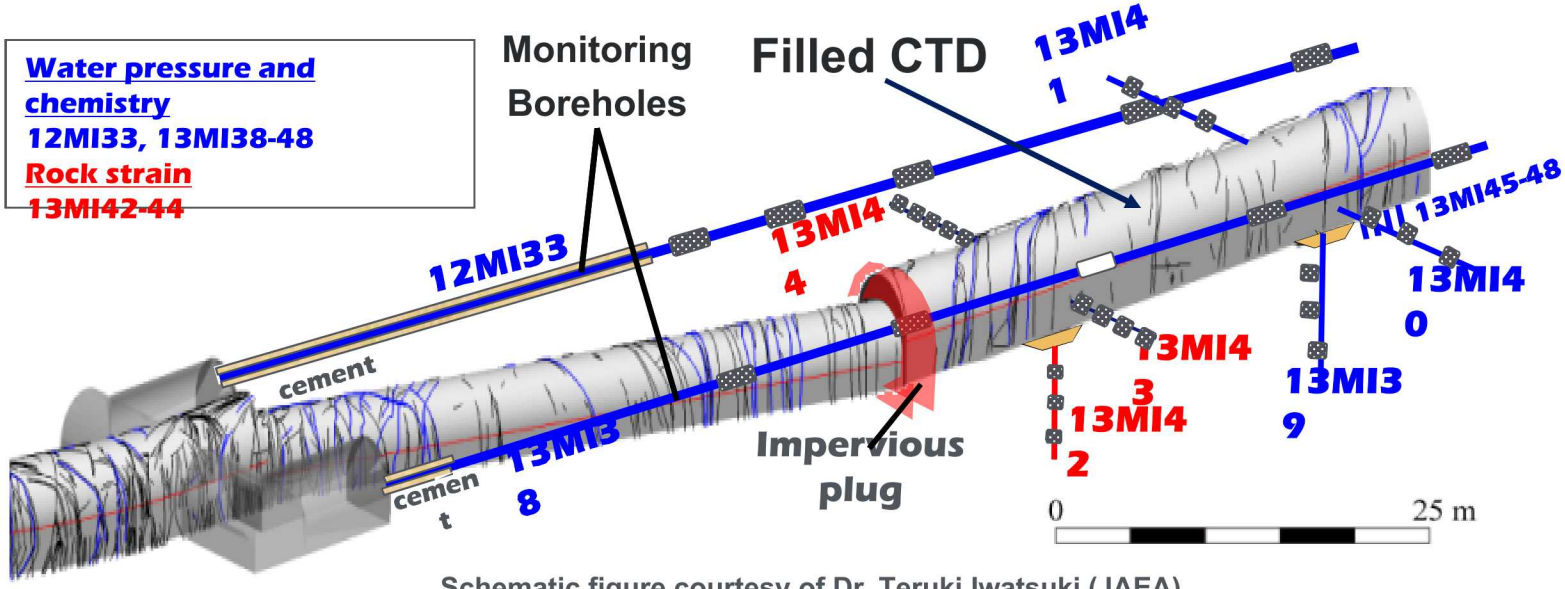
Summary of Hydrology Analysis

- Updated flow modeling was conducted for Task C, Step3.
- The same domain and mesh as previous simulations were used for the base case.
- Flow simulations were conducted for 10 fracture realizations and upscaled permeability and porosity fields.
- Modeled CTD filling and post-filling using experimental pressure history at CTD as boundary condition.
  - Predicted injection and leakage amount. Reasonable predictions were obtained for leakage.
  - Predicted pressure history in observation points in Well 12MI33. Predictions were reasonable for all except P5 and P6. Further study is needed on P5 and P6, and possibly P4 which are closer to the Inclined Drift.
- Use of a larger model domain shows that smaller domain sizes that are close to the tunnel exhibit boundary effects. A reasonably sized model domain is needed for better matching of experimental data. This may require incorporating additional features that are within the enlarged domain.

Task C: Part II – Closure Test Drift (CTD) Geochemistry

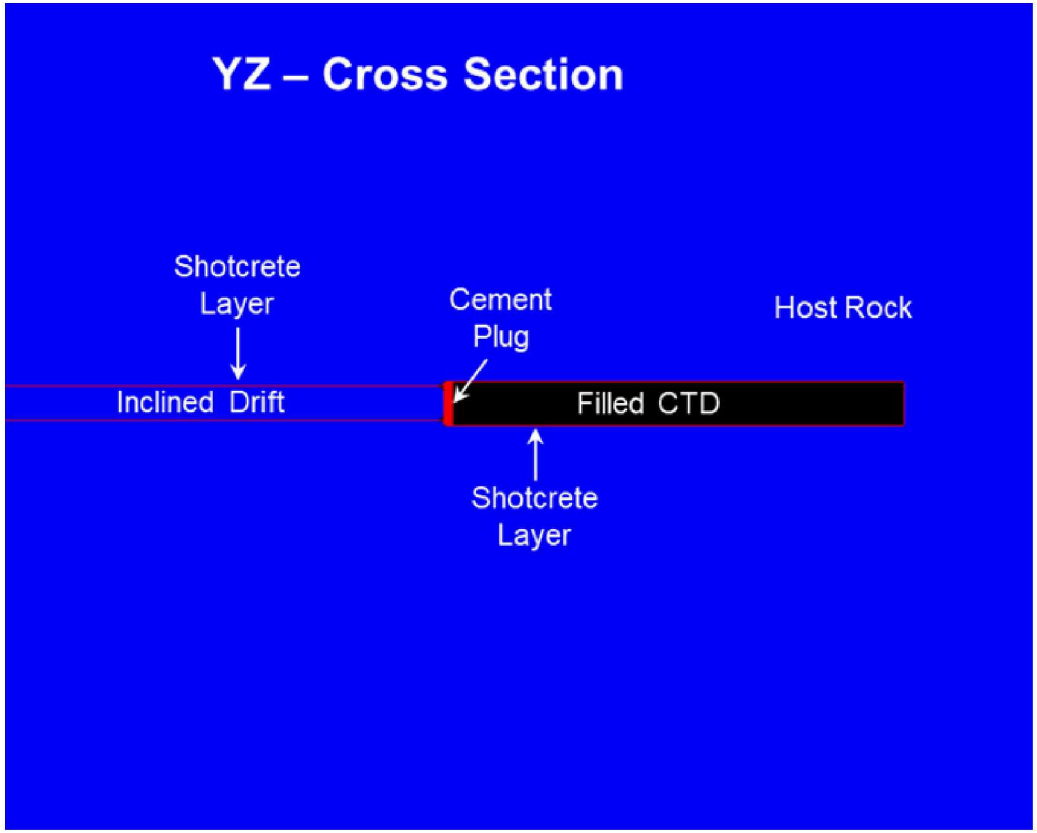
– Step 3 Preliminary Reactive Transport Simulations

- **GOAL**: Prediction 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 & brucite



Schematic figure courtesy of Dr. Teruki Iwatsuki (JAEA)

Task C: Part II – PFLOTRAN Reactive Transport (RT) Model Domain

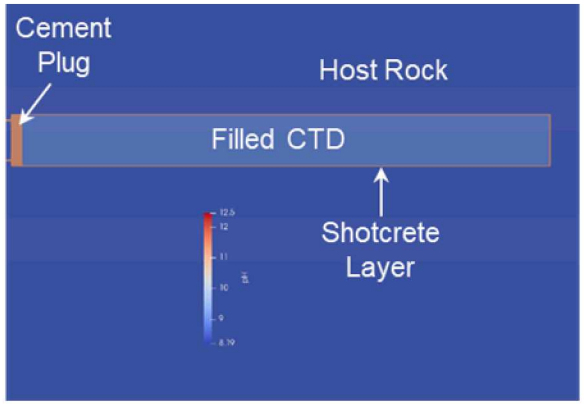


PFLOTRAN Reacting Transport (RT) Simulation

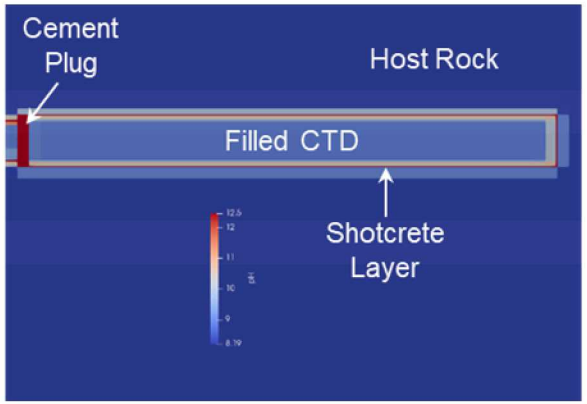
- 3D structured mesh
- Filled CTD with dilute groundwater
- Starting pH 8.9
- Shotcrete: generic OPC (with added brucite & Friedel salt)
- Diffusion only problem
- 400-600 days simulation

Task C: Part II – PFLOTRAN 3D Reactive Transport (RT) Simulation

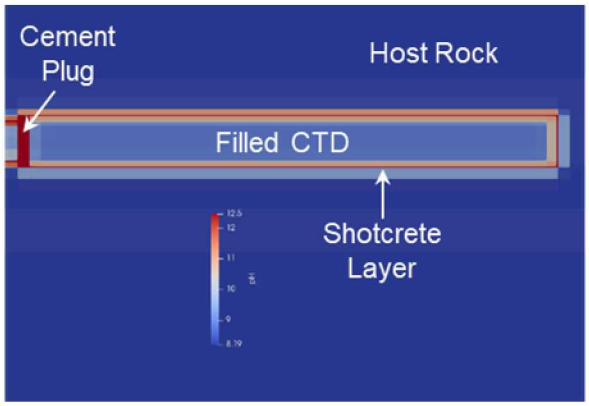
Filled CTD → pH Mapping (similar results as in previous meeting)



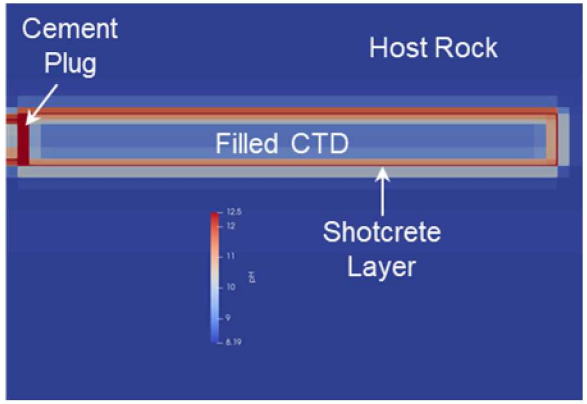
0 days



60 days



150 days



300 days

WORK IN PROGRESS!!!

❑Reaction Front Simulation

pH increase with time within CTD

Diffusion front migration towards inner CTD center

[Na, Cl,] decreases with time

❑Observations

Deviations from measured data – both pH, [Ca], and [Cl]

Diffusive transport effects? – Not likely

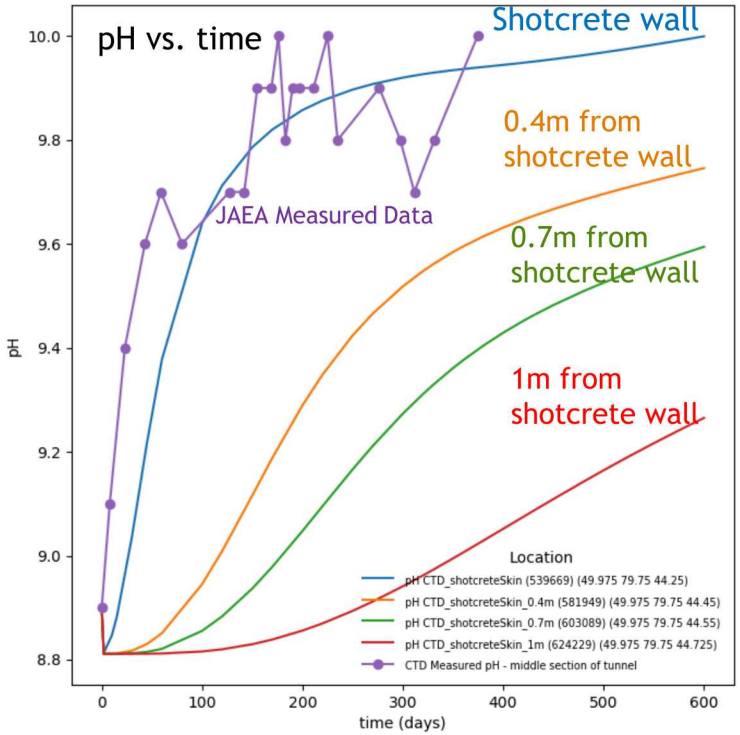
Kinetic rate treatment (upcoming):

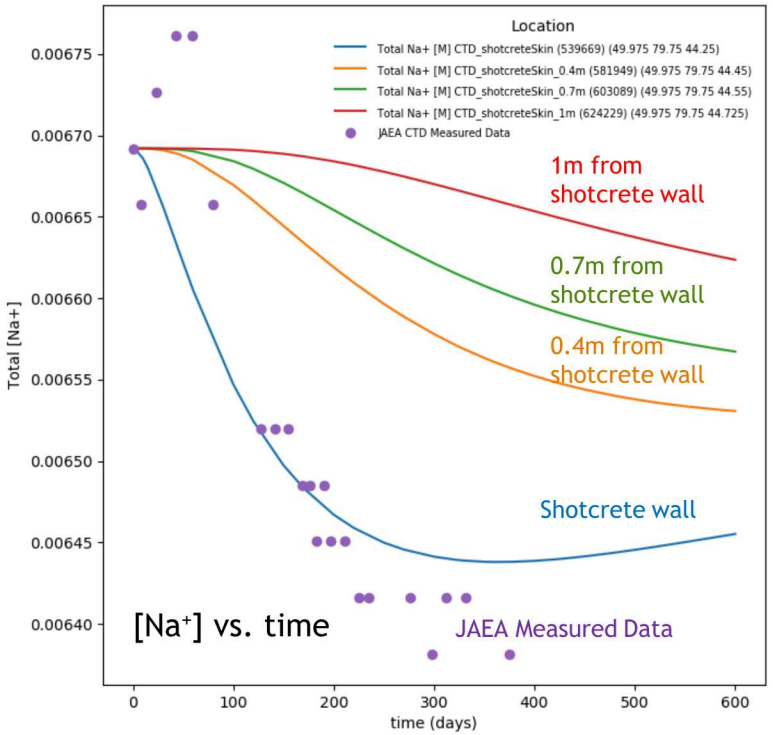
- TST rate law for portlandite & brucite with [Ca], pH, and [Mg] dependencies

Consideration of cement phases:

- Cl-bearing phase (Friedel salt)
- Mg-bearing (Brucite)

Task C: Part II – (Step3) PFLOTRAN 3D Reactive Transport (RT) Model



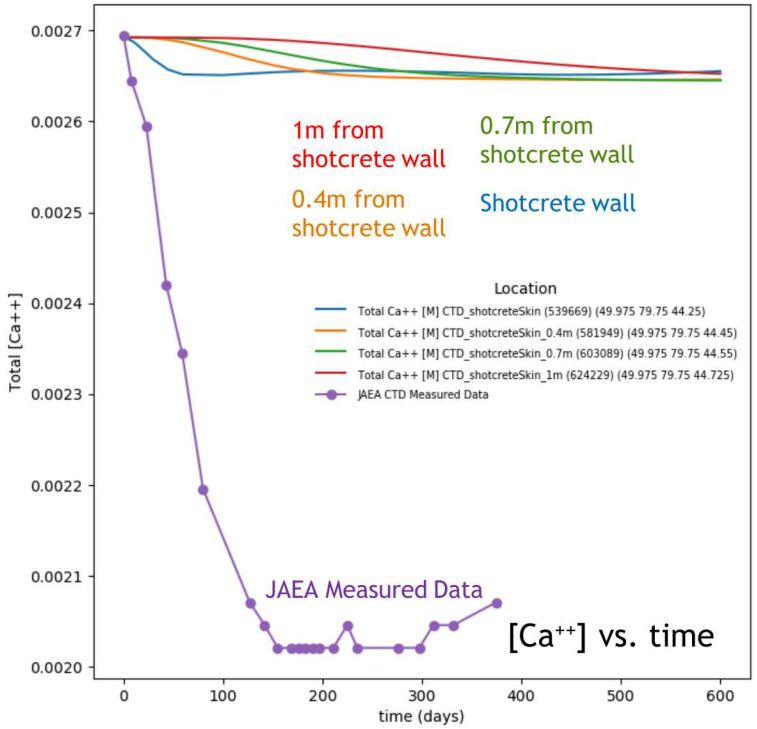


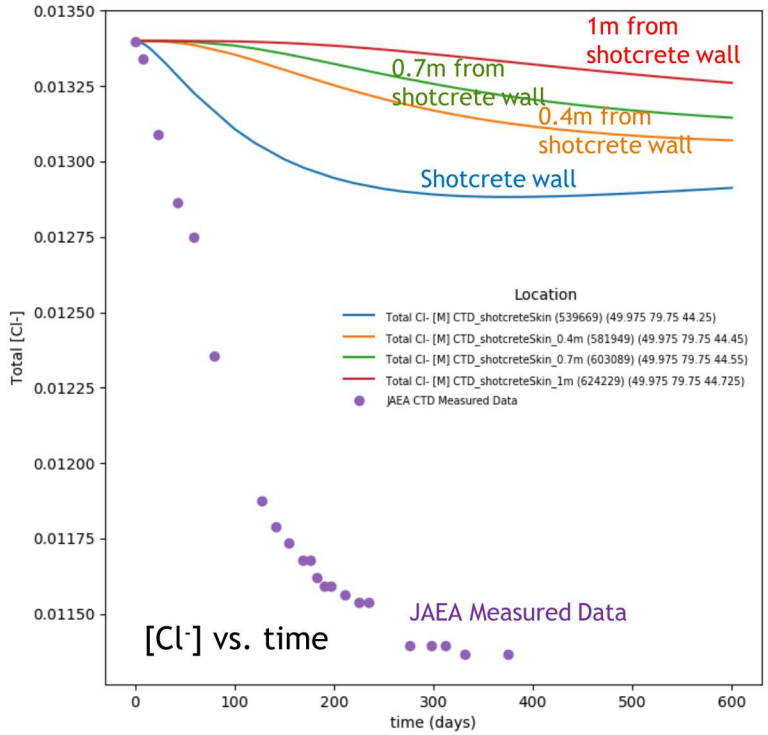
WORK IN PROGRESS!!!

Summary & Results

- Added brucite ($Mg(OH)_2$) and Friedel salt ($Ca_4Al_2Cl_2O_6{:}10H_2O$) to the cement phase assemblage – based on CTD shotcrete cement chemistry data
- Sensitivity analyses (SA) on TST rate law parameters for portlandite & brucite
- Some improvements on representing pH and [Na^+]. Still work to do on other solutes.

Task C: Part II – (Step3) PFLOTRAN 3D Reactive Transport (RT) Model





Summary & Results (Cont.)

WORK IN PROGRESS!!!

- The simulation of [Ca] vs. time profile still can't represent the large drop in concentration.
- Some improvement on representing the measured [Cl^-] drop with time but still not as large

Next Step

- ❑ Coupling heterogeneous permeability fields from the hydrology part with HC simulations – Evaluate these effects on HC
- ❑ Expand SA evaluation of TST rate parameters of solids, documentation of current findings