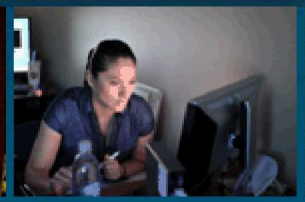
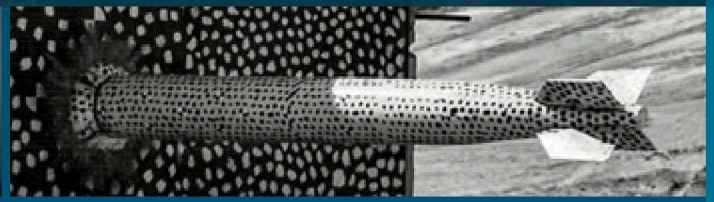
SAND2018-9281PE

Reactive Transport Modeling of Cement Interactions Using PFLOTRAN





PRESENTED BY

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Nuclear Waste Disposal Research & Analysis Dept.

SAND2018-??????

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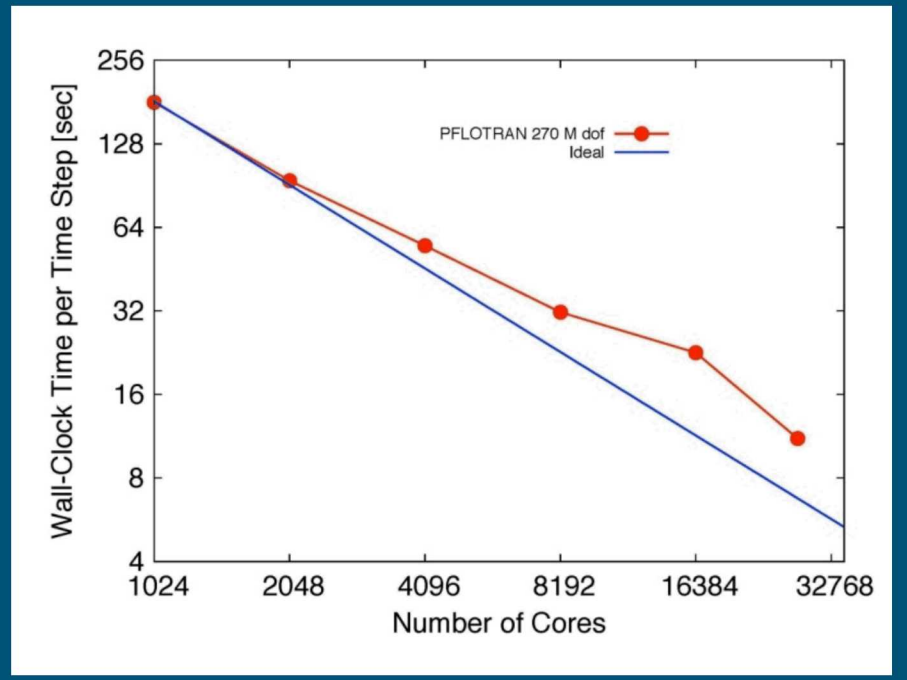
PFLOTRAN Simulation Code (http://www.pflotran.org)

PFLOTRAN

- **Massively parallel** subsurface flow and reactive transport code
- **Open source**, founded upon well-known open source libraries including MPI, PETSc, and HDF5
- Written in object-oriented **Fortran 2003/2008**
- Scales well to over 10K cores
- Varied applications including:
  - Nuclear waste disposal
  - Biogeochemical transport modeling
  - CO_2 sequestration
  - Radioisotope tracers
  - Colloid-facilitated transport
  - Fracture flow modeling



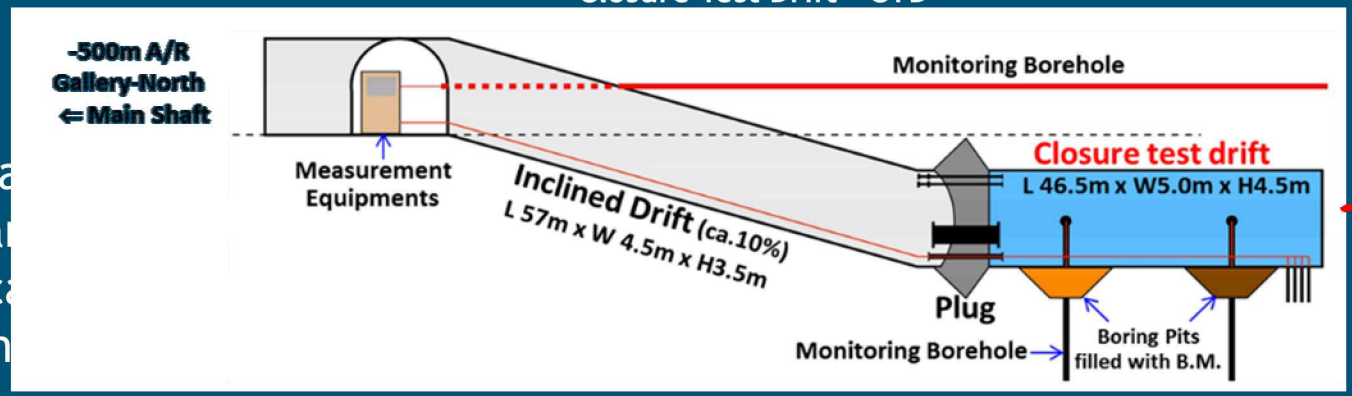
Slide courtesy of Glenn Hammond, SNL

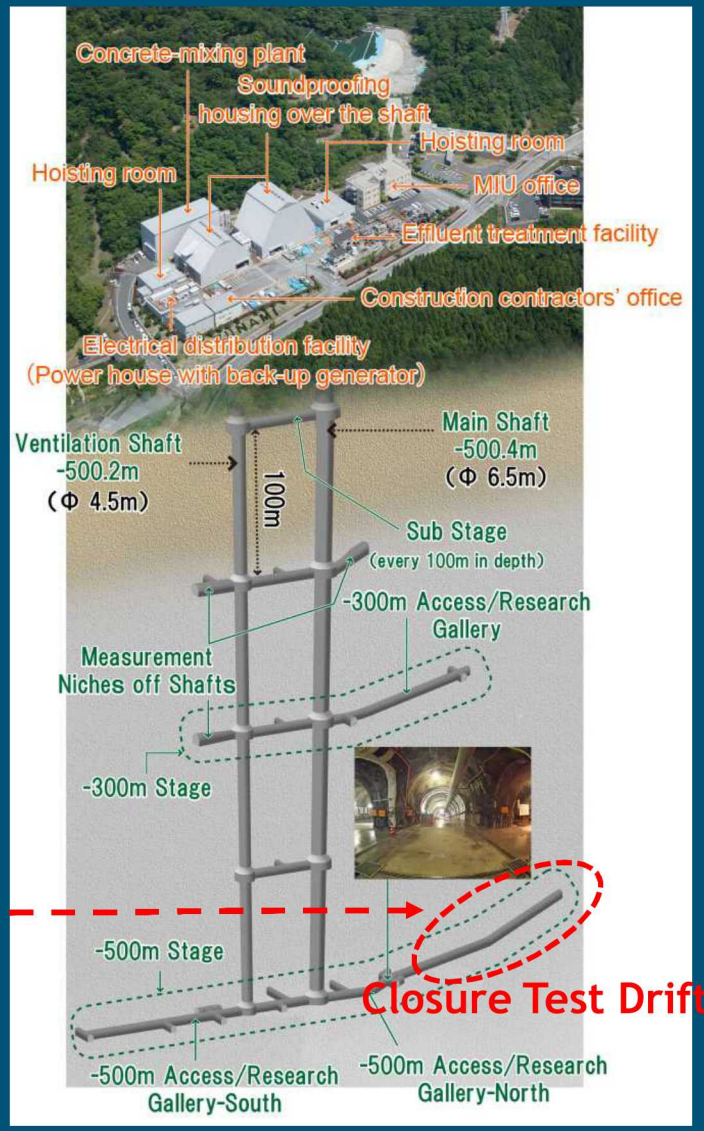
Motivation: GREET (Groundwater REcovery Experiment in Tunnel), Mizunami URL, Japan

- GREET (Groundwater REcovery Experiment in Tunnel)
  - Conduct drift closure and (ground)water-filling to estimate recovery process in granitic rock
  - Geochemical evaluation of groundwater site data
  - Verify Hydrological-Mechanical-Chemical-Biological process models in granite
- DECOVALEX-19 Task C:
  - Evaluation of monitoring hydrological and geochemical site data (Closure Test Drift - CTD)
  - Study interactions with host-rock and barrier materials
  - Develop simulation procedure to estimate post closure environments in fractured media

Goal: Develop a
1D reactive tra
problem applic
cement leachin
scenarios

Closure Test Drift - CTD





Figures courtesy of
Dr. Teruki Iwatzuki (JAEA)

PFLOTRAN 1D Model Setup

Three Regions:

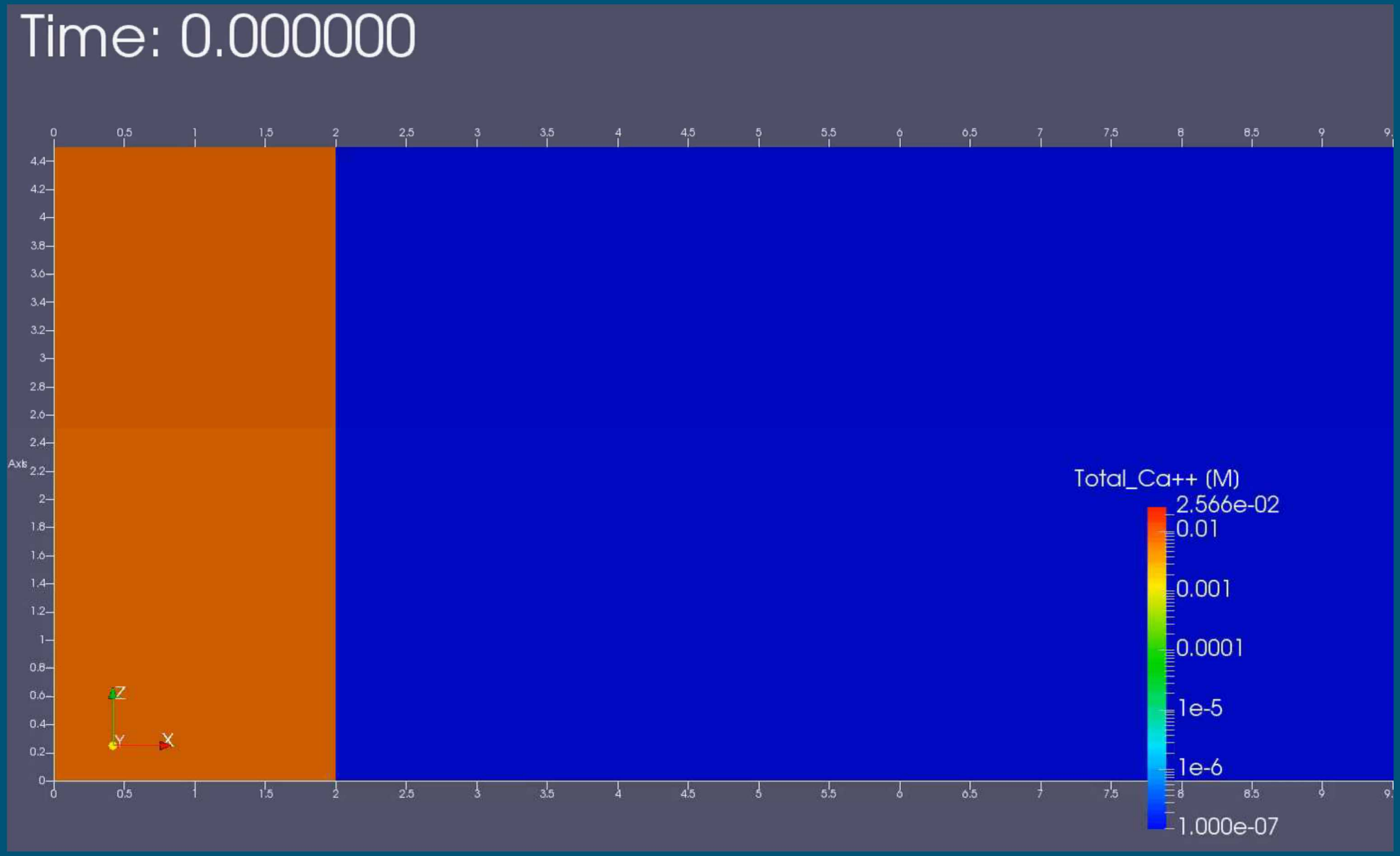
- OPC Cement Plug (light blue; x = 0 – 2 m)
- Flooded Tunnel (red; x = 2 – 46.2 m)
- Granite (dark blue; x = 46.2 m – 48.5 m)

Three Observation Points (dots – left to right):

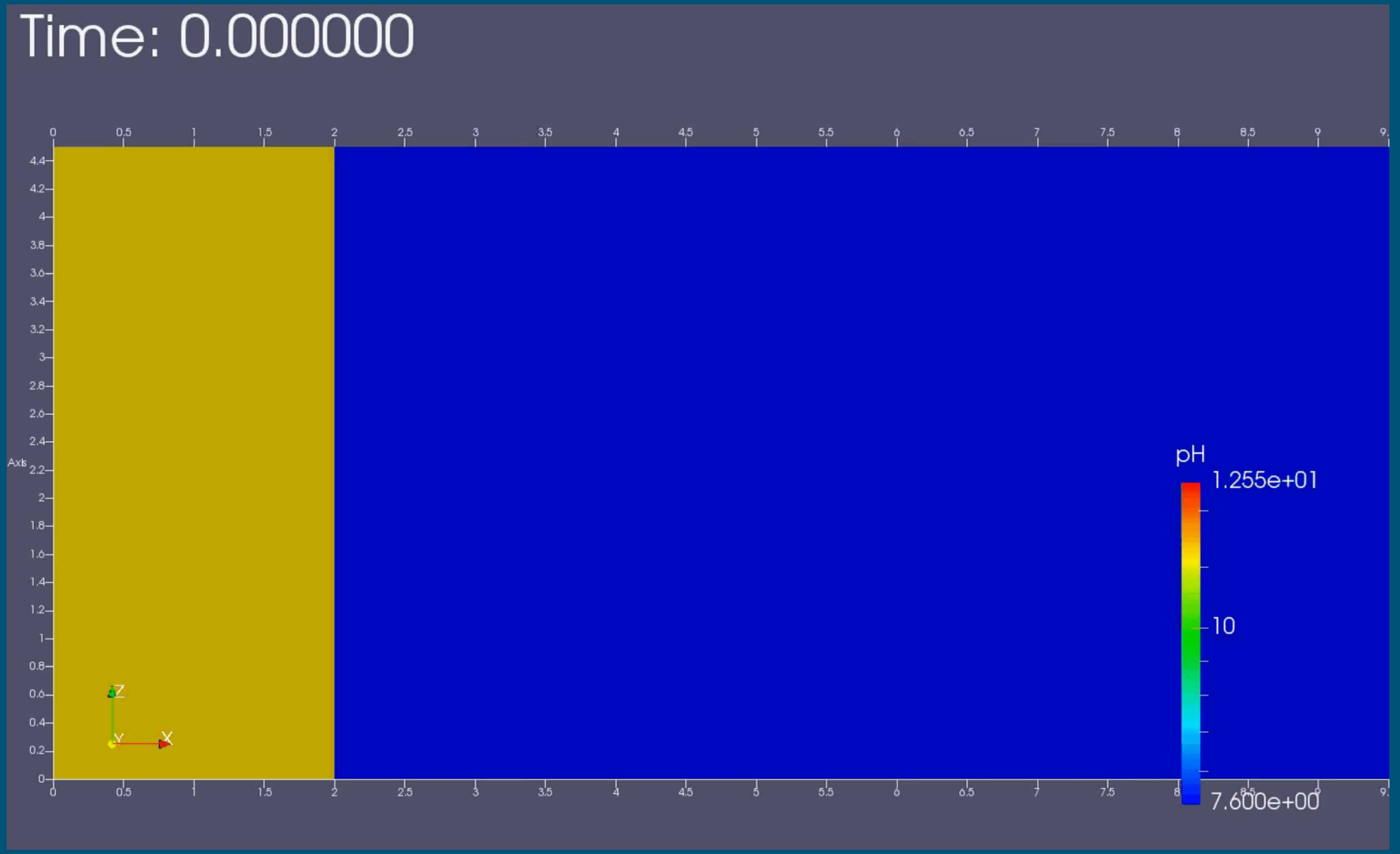
- Cement center
- 0.2 m from cement-flooded region interface
- Cement-flooded region interface

Thermodynamic Database: THERMODDEM (BRGM)

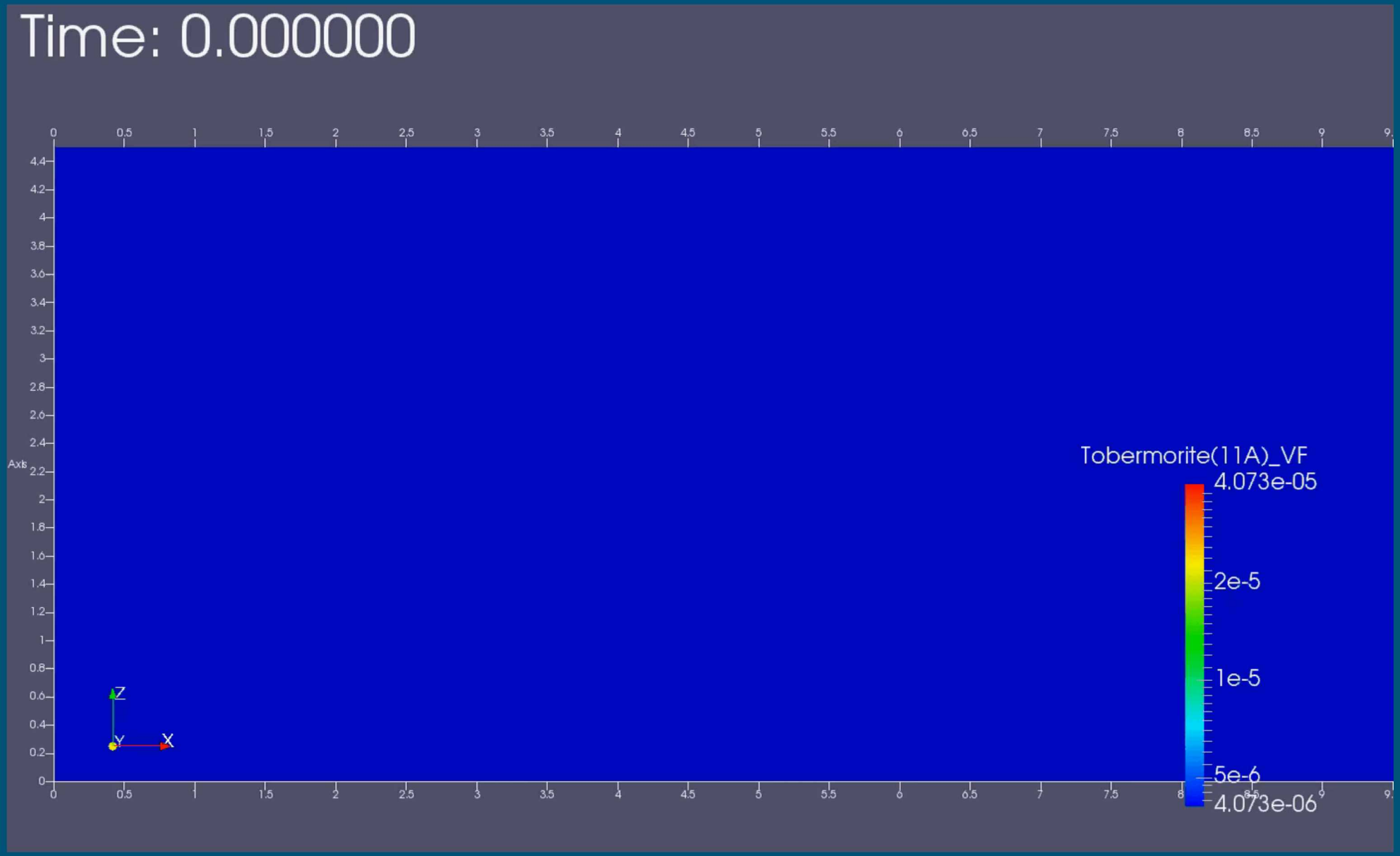
1D Model Results: [Ca^{++}]



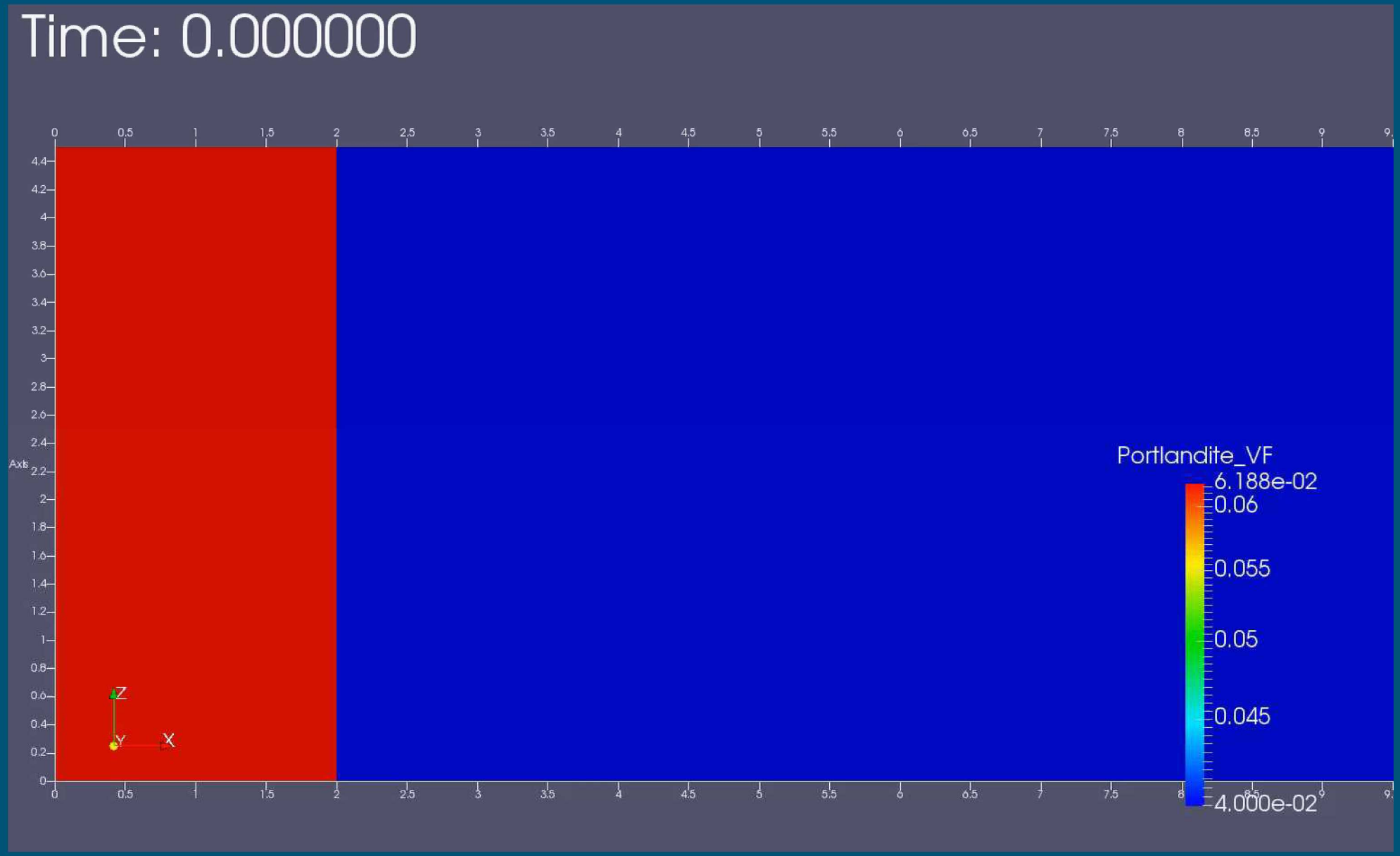
1D Model Results: pH



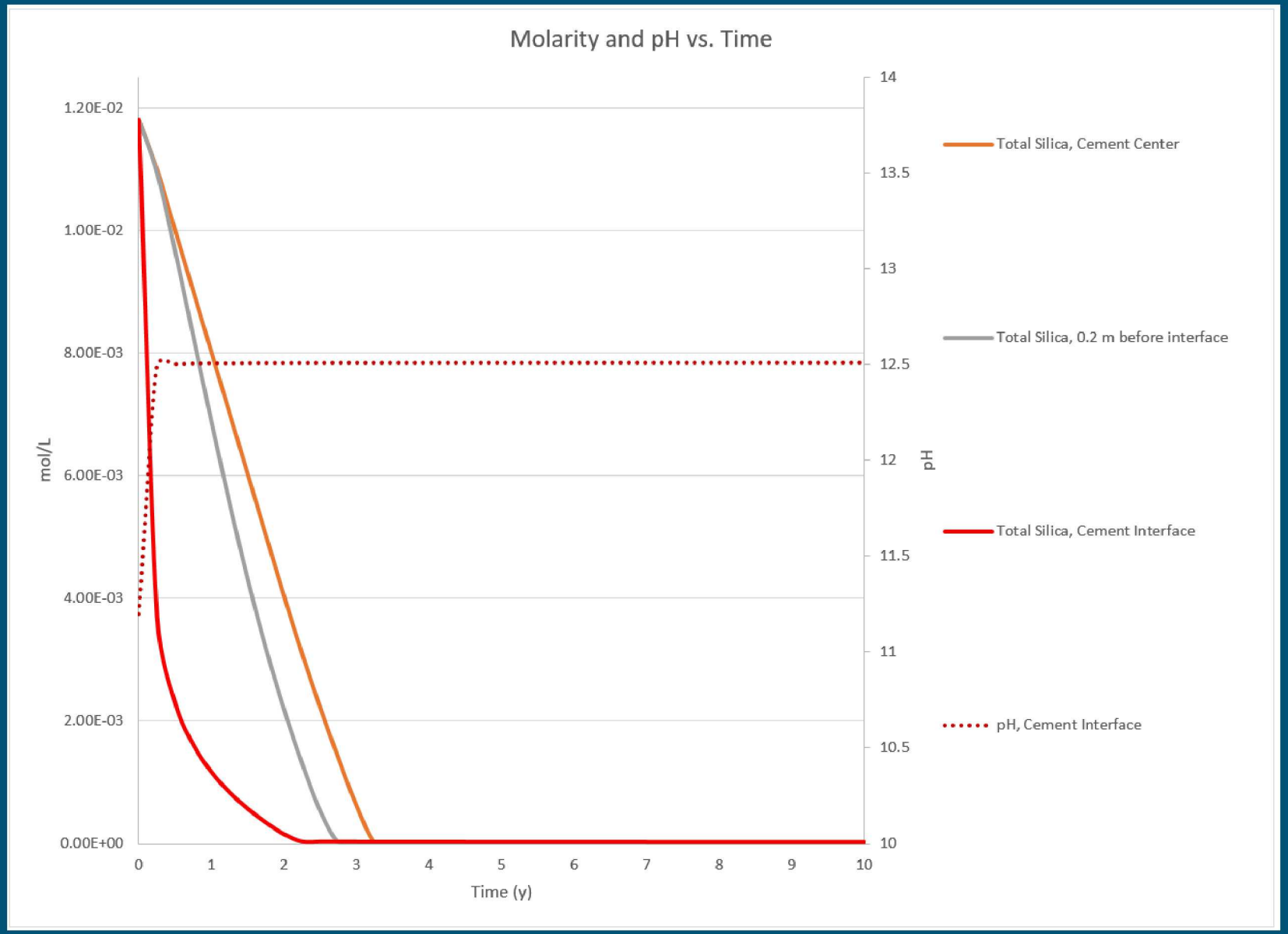
1D Model Results: Tobermorite ($Ca_5Si_6O_{16}(OH)_2 \cdot 4H_2O$)



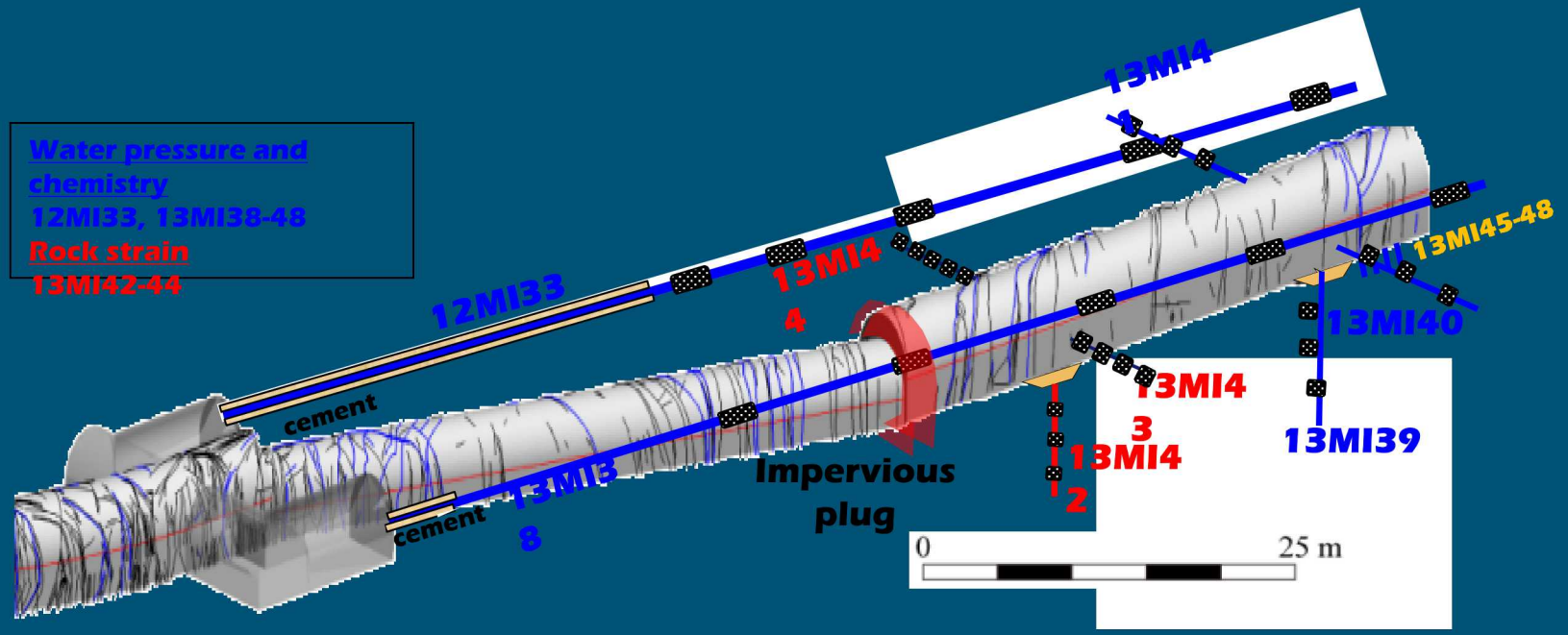
1D Model Results: Portlandite ($Ca(OH)_2$)



1D Model Results: Total Dissolved Silica



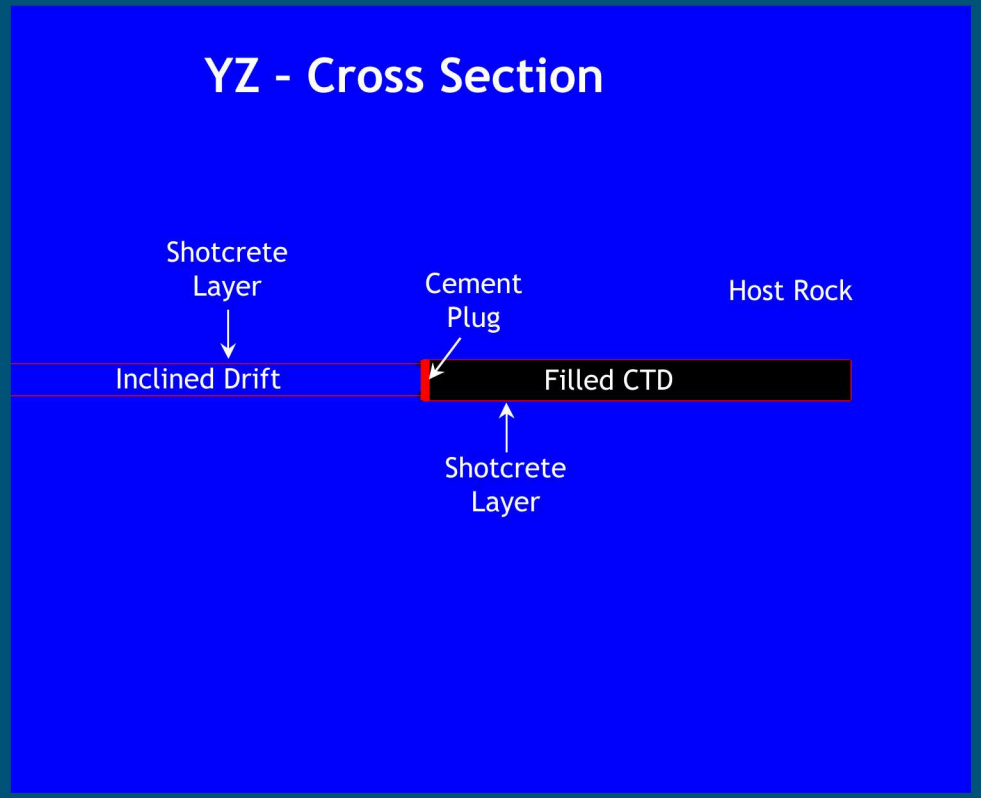
3D CTD: Closure Test Drift (CTD) Experiment



Schematic figure courtesy of Dr. Teruki Iwatsuki (JAEA)

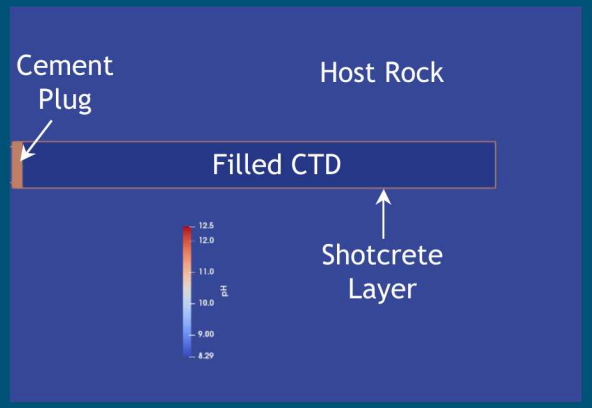
- Preliminary geochemical predictions at 12MI33 monitoring zones
- PFLOTRAN simulation code with THERMODDEM TDB
- Current mesh doesn't capture rock fracture effects
- Assuming shotcrete layer (0.1 m thick) covering CTD walls

3D CTD: PFLOTRAN Reactive Transport (RT) Model Domain

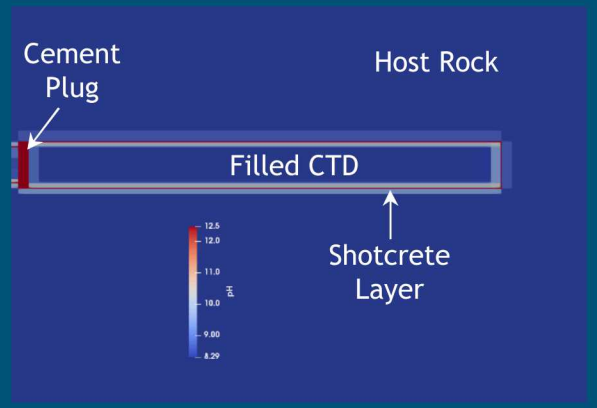


- **PFLOTRAN Reacting Transport Simulation**
  - **3D structured mesh**
  - **Filled CTD with dilute groundwater**
  - **Starting pH 8.3**
  - **Shotcrete: generic OPC (no brucite)**
  - **Diffusion only problem**
  - **400 days simulation**

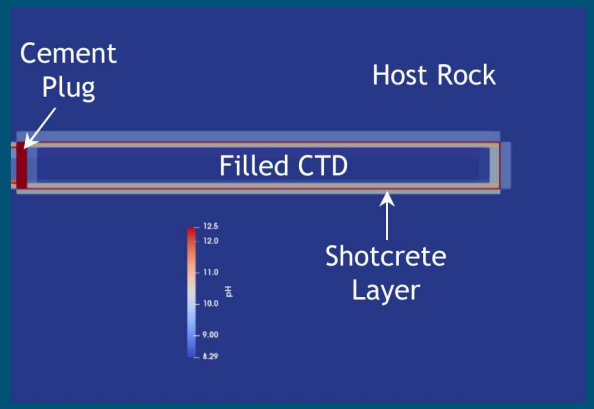
3D CTD: PFLOTRAN 3D Reactive Transport (RT) Model (I)



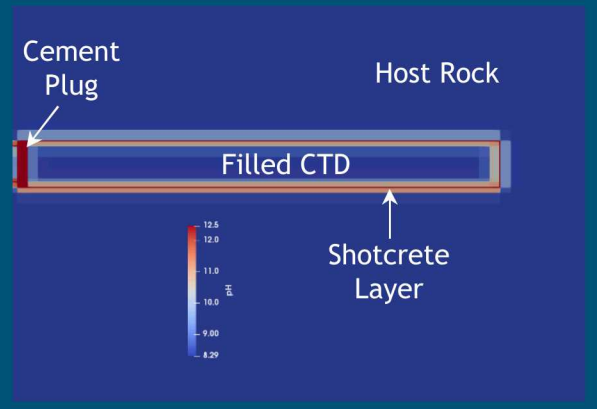
0 days



70 days



150 days

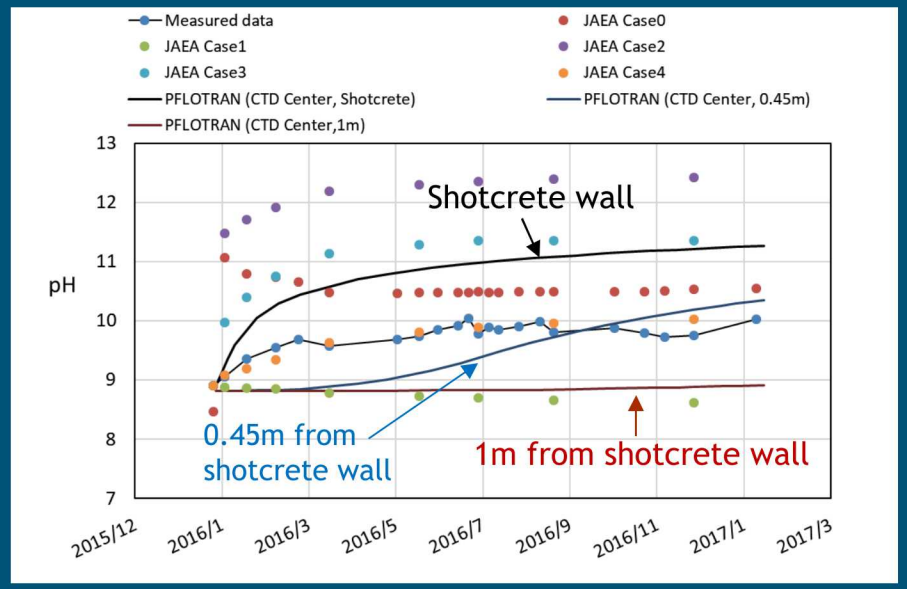


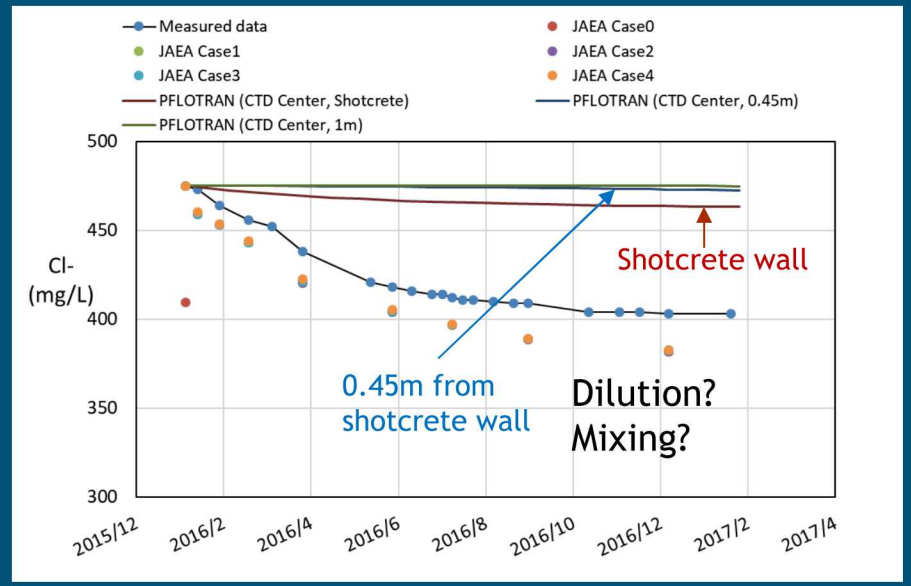
310 days

- Reaction Front Simulation
  - Focus on filled CTD domain
  - pH increase with time within CTD and around the shotcrete lining
  - pH remains relatively unchanged around tunnel central region
- Questions?
  - pH deviations from measured
  - Kinetic rate law parameters?
  - Hydrologic flow through fractures?

WORK IN PROGRESS!!!

3D CTD: PFLOTRAN 3D Reactive Transport (RT) Model (II)



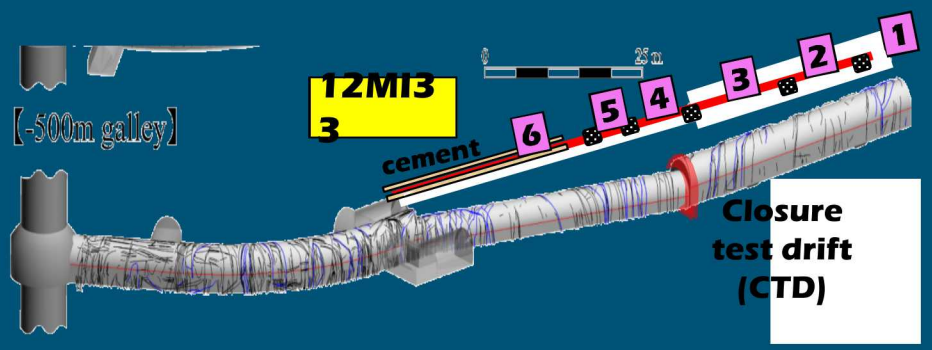


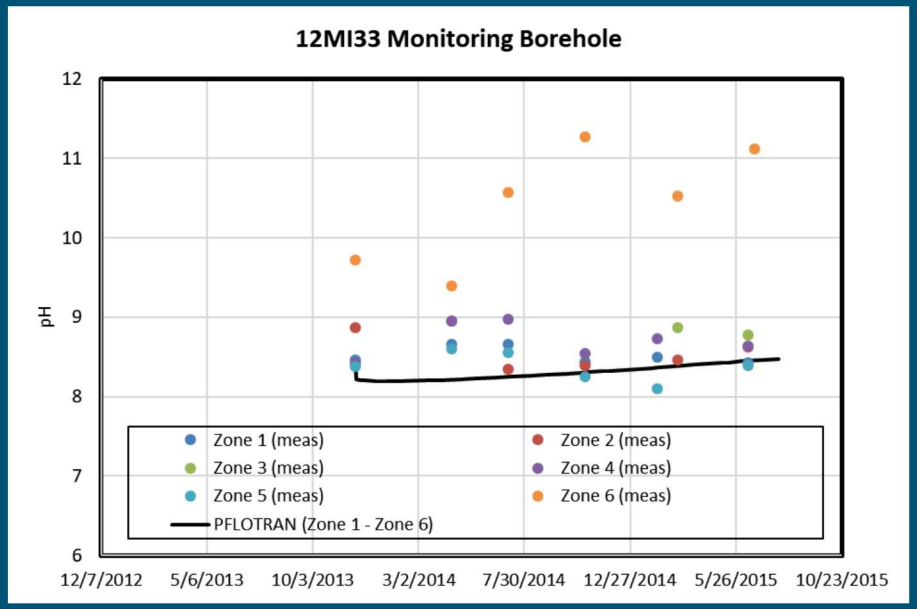
Filled CTD → Preliminary Results

- **Filled CTD RT Simulation Summary**
  - Increase in pH with time → still far from measured pH data at 1m within the CTD
  - Small decrease in [Cl-] concentration → much smaller than that of measured data
  - **Next step:** Resolve discrepancies with measured data
    - Evaluation of transport and kinetic rate law parameters
    - Update shotcrete composition → include Mg-bearing phases
    - Eh (ORP) predictions → PFLOTRAN comparisons with measured data

WORK IN PROGRESS!!!

PFLOTRAN 3D Reactive Transport (RT) Model (III) – 12MI33 Borehole Zones





WORK IN PROGRESS!!!

12MI33 Borehole Zones → Predictions & Comparisons To Measured Data

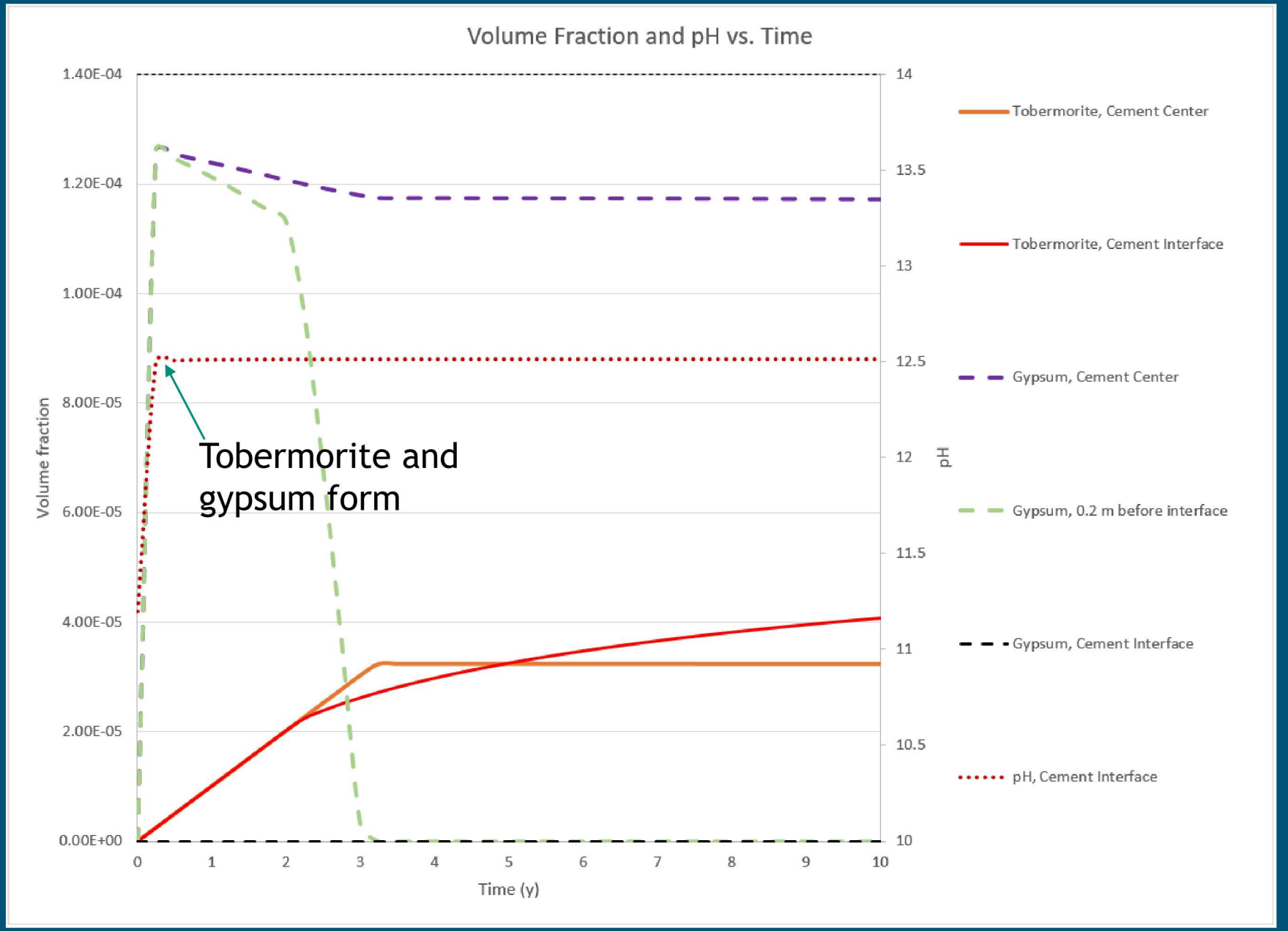
- PFLOTRAN RT Simulations 12MI33 Borehole Zones Summary:
  - Overall, PFLOTRAN RT model predictions for pH are within the band of measurements (except Zone 6)
  - Marked Deviations from measurements in **Zone 6:**
    - **Close proximity to cement - expected higher pH's**
    - **Need to explore hydrologic effects in this zone:**
      - **Fractures?**
      - **Water mixing effects?**

Concluding Remarks

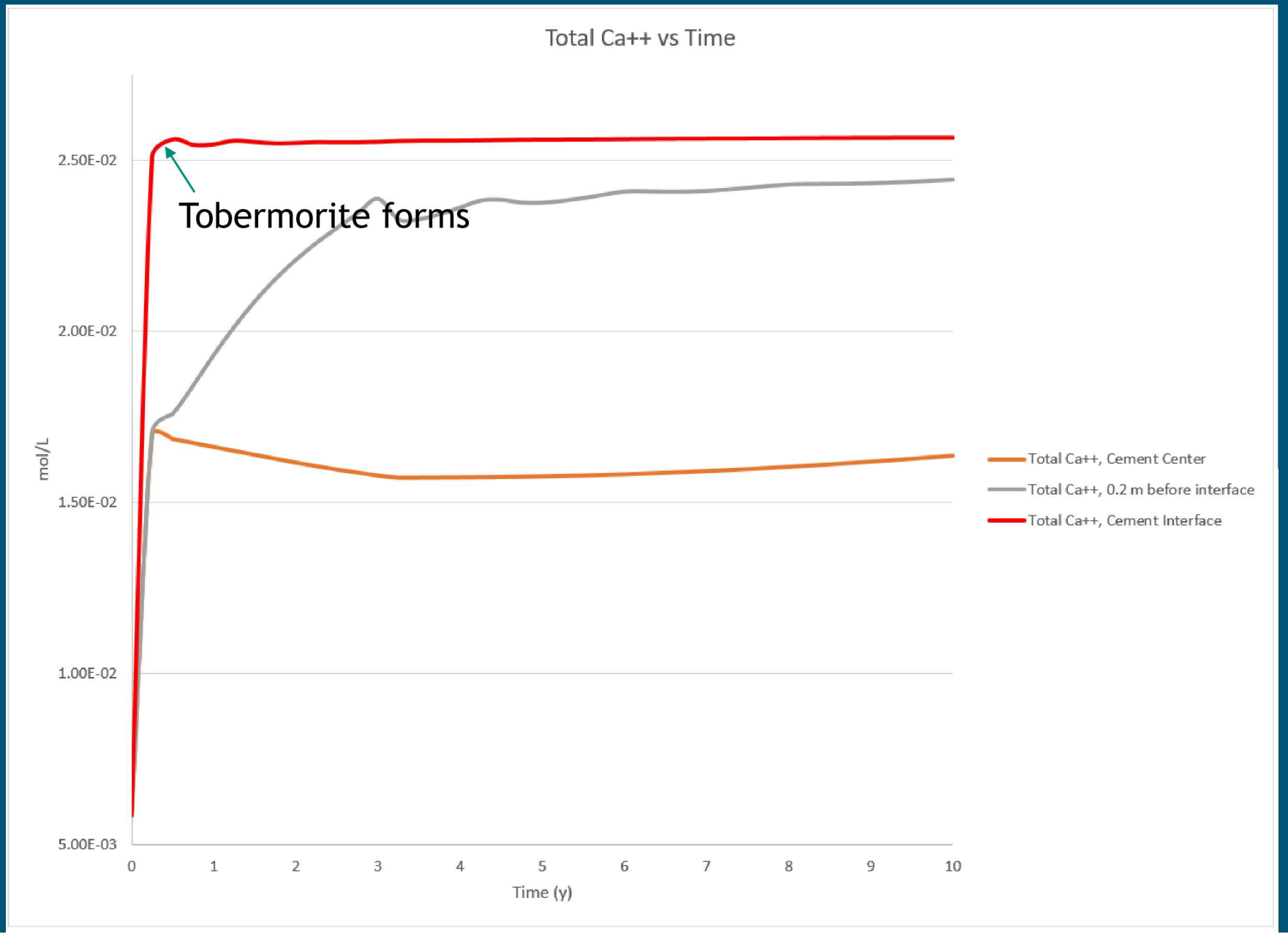
- Simple 1D reactive-transport problem of cement (OPC) plug – groundwater interactions in PFLOTRAN
  - Model can be expanded to various cement leaching scenarios
  - Suitable for benchmarking problems: code-to-code comparisons
- 3D CTD model of shotcrete liner interactions on groundwater chemistry within flooded tunnel
  - Preliminary results – Spatio-temporal effects of shotcrete reaction on water chemistry within flooded tunnel
  - **Still work to do!!!!** – Evaluate deviations between model predictions and measured data (e.g., pH)
- Predictions of spatio-temporal changes on cement pore solution chemistry, focusing on leaching trends at the interface
  - Tobermorite formation affects dissolved silica distribution
  - Prediction of localized portlandite depletion at the interface

BACKUP SLIDES

Results: Tobermorite, Gypsum, pH



Results: [Ca^{++}]


Total Ca++ vs Time
Tobermorite forms
2.50E-02
2.00E-02
1.50E-02
1.00E-02
5.00E-03
mol/L
0
1
2
3
4
5
6
7
8
9
10
Time (y)
Total Ca++, Cement Center
Total Ca++, 0.2 m before interface
Total Ca++, Cement Interface