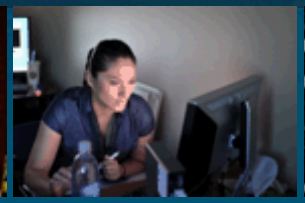
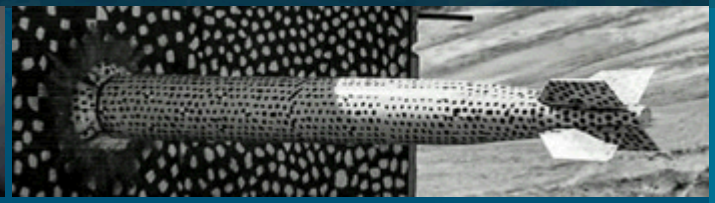
SAND2018-7855PE

One-Dimensional Reactive Transport Cement Interaction Problem





PRESENTED BY

Carlos M. Lopez and Carlos Jové Colón

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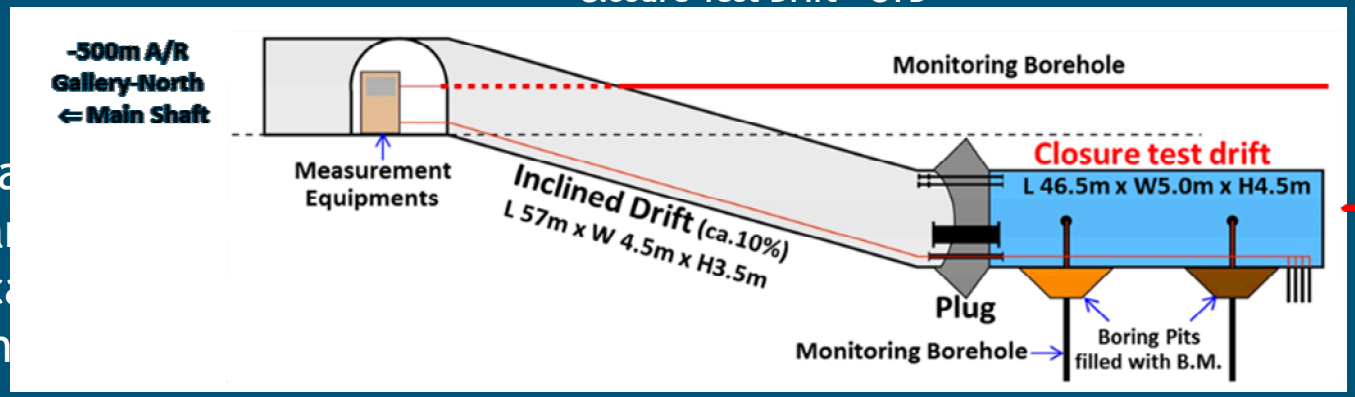
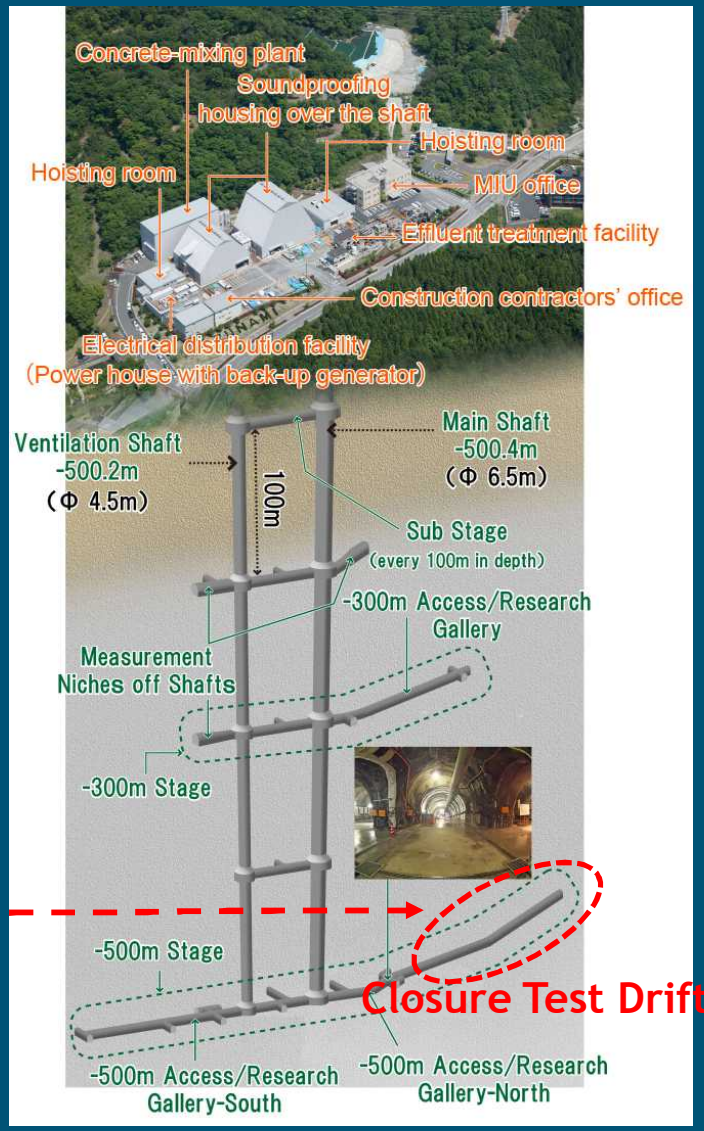
Motivation: GREET (Groundwater REcovery Experiment in Tunnel), Mizunami URL, Japan

- 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



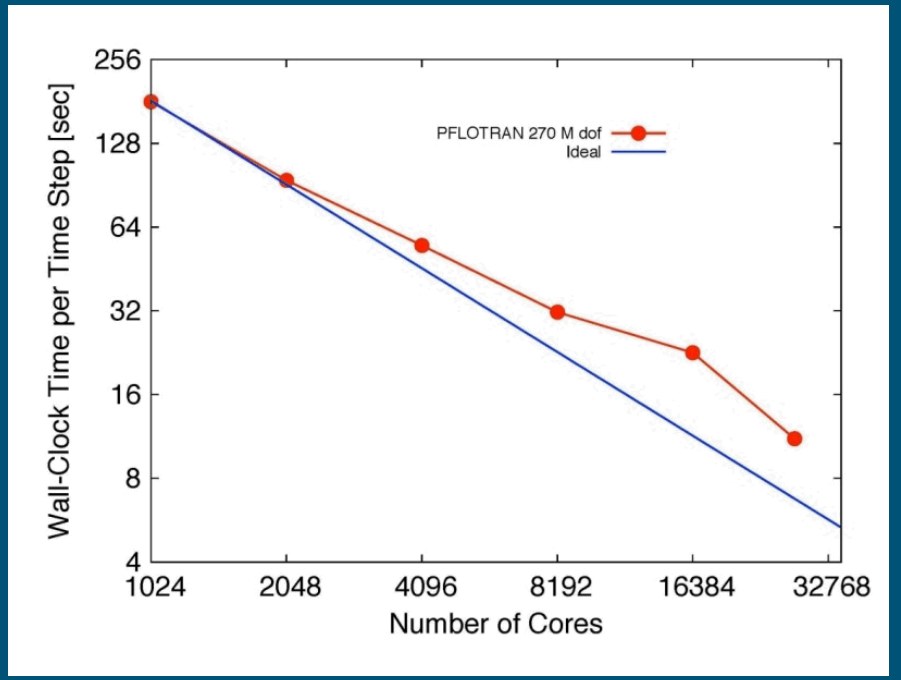


Figures courtesy of
Dr. Teruki Iwatzuki (JAEA)

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

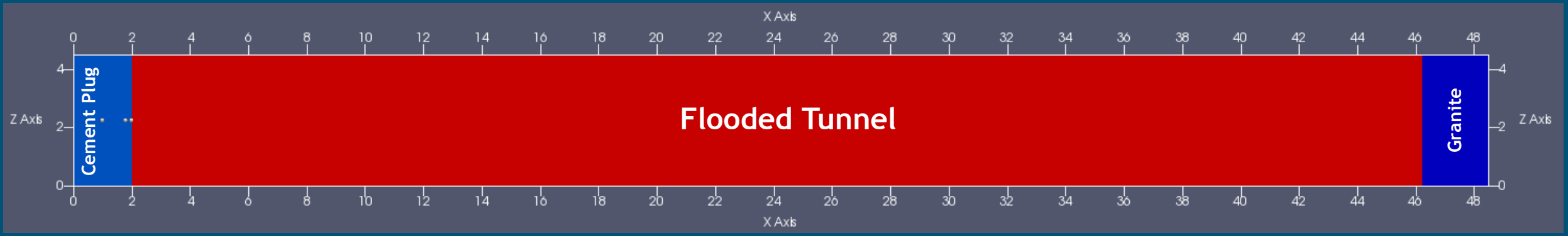
PFLOTRAN

- 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-fascilitated transport
  - Fracture flow modeling



Slide courtesy of Glenn Hammond, SNL

1D Model Setup



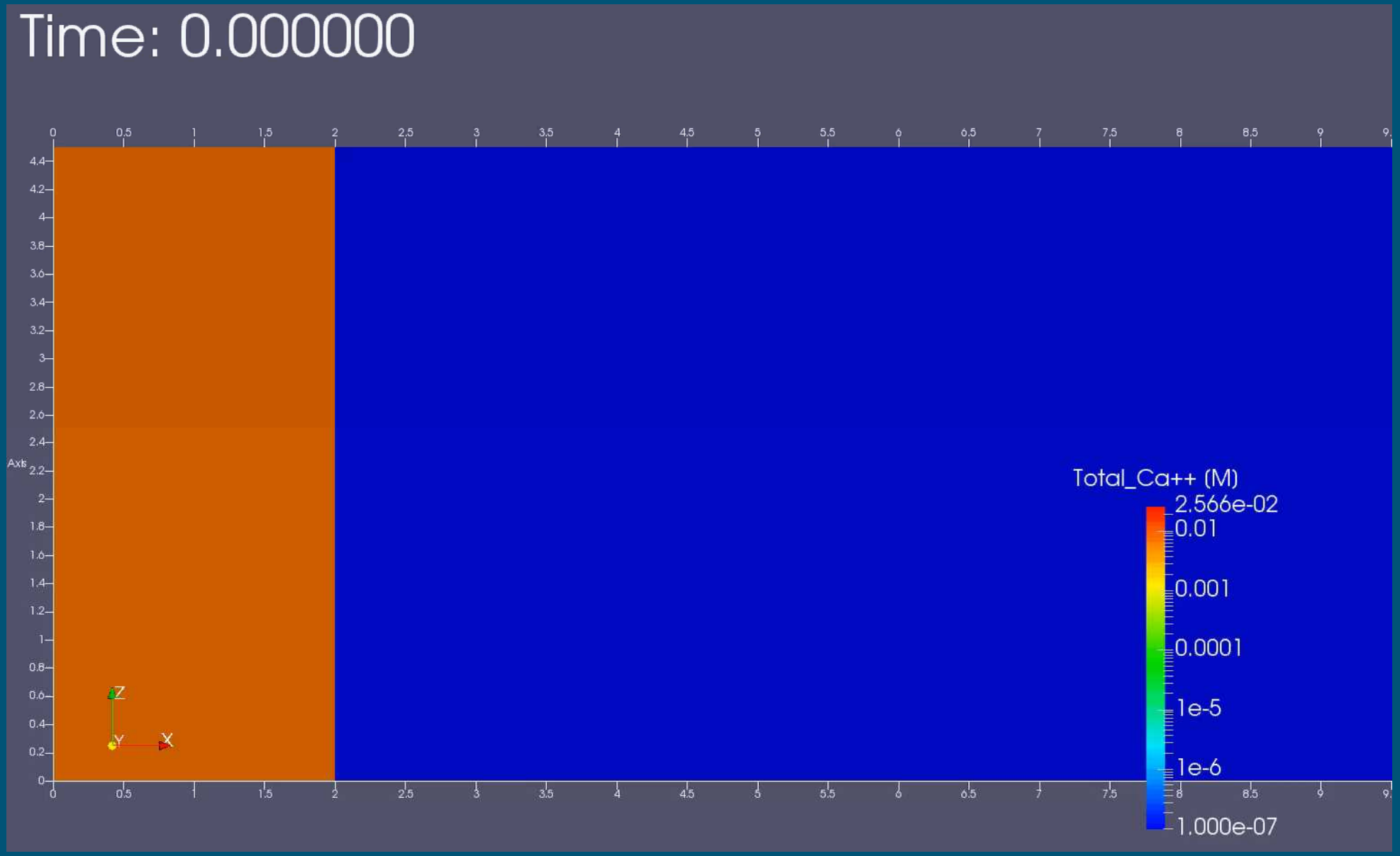
Three Regions:

- 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)

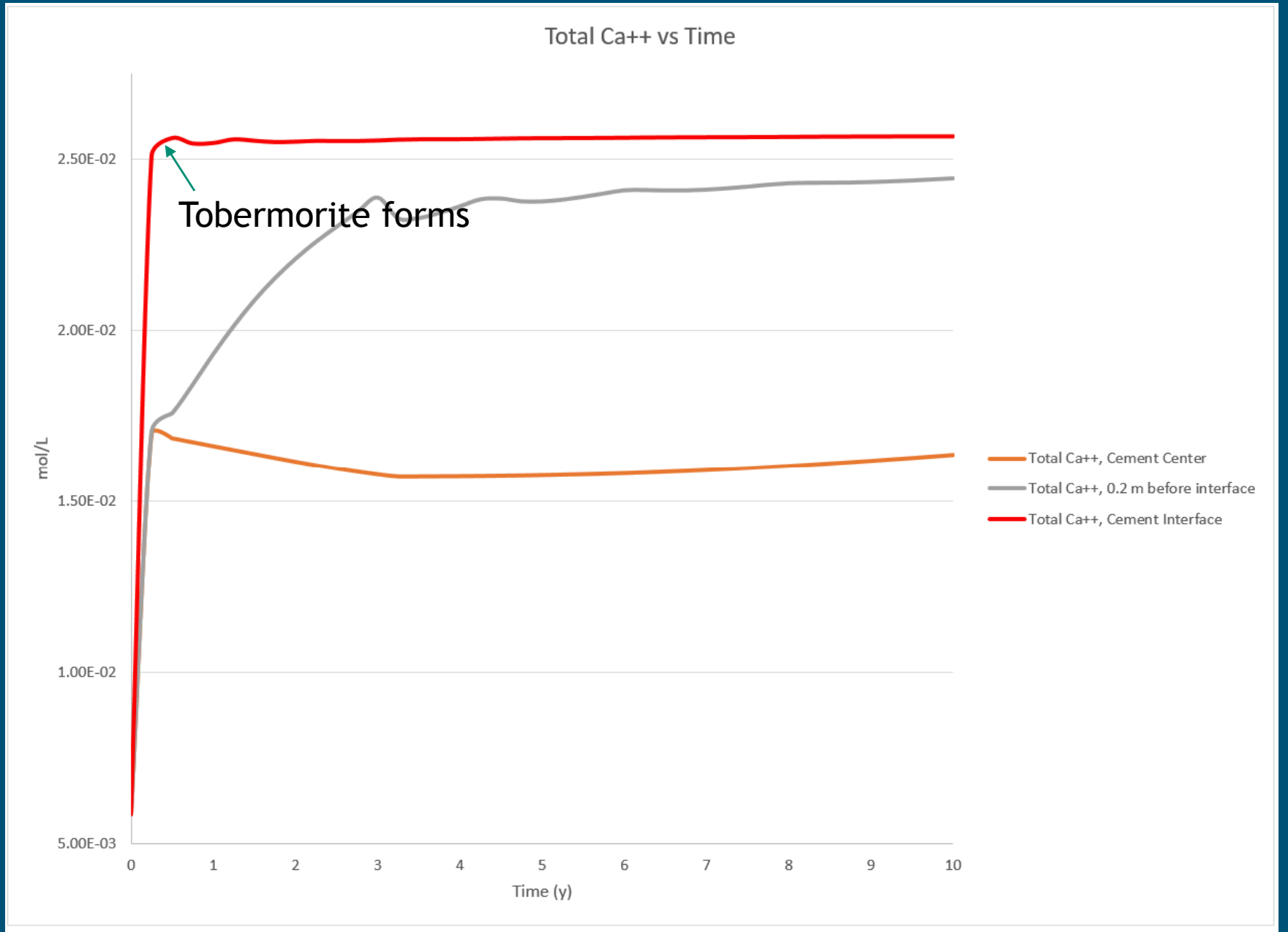
Three Observation Points (dots – left to right):

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

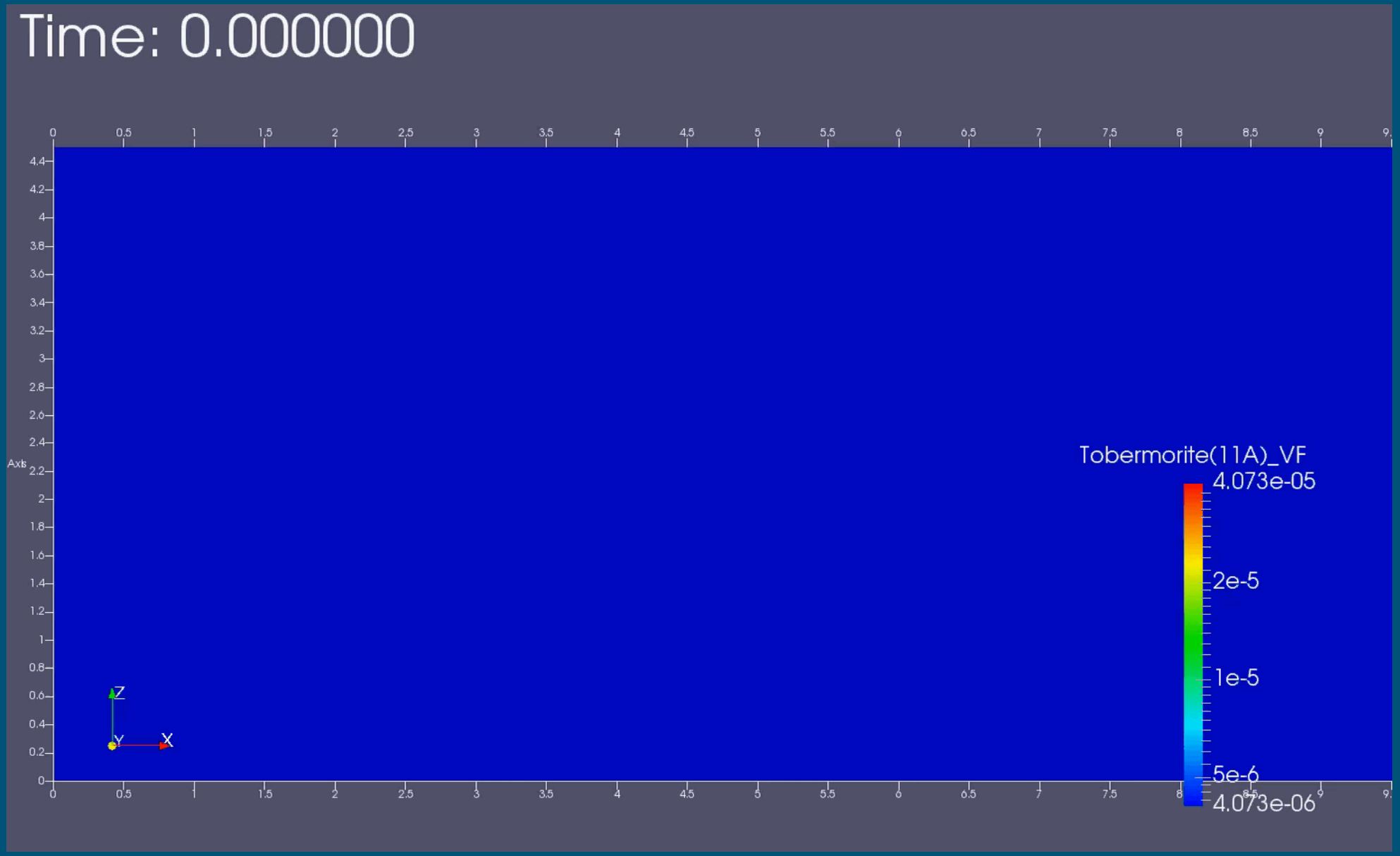
Results: [Ca^{++}]


Time: 0.000000
Total_Ca++ (M)
2.566e-02
0.01
0.001
0.0001
1e-5
1e-6
1.000e-07
Axis
Z
Y
X

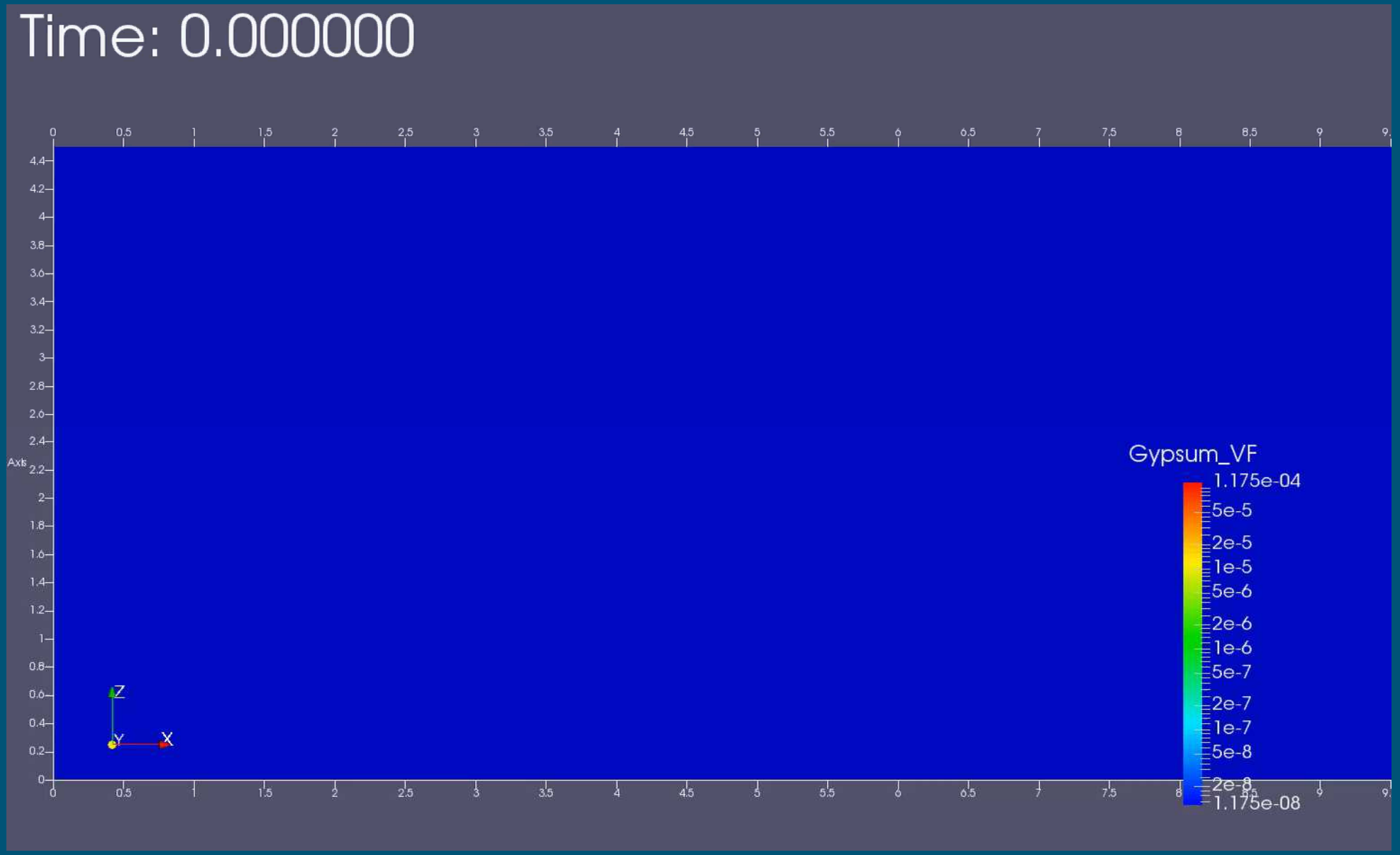
Results: [Ca^{++}]


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

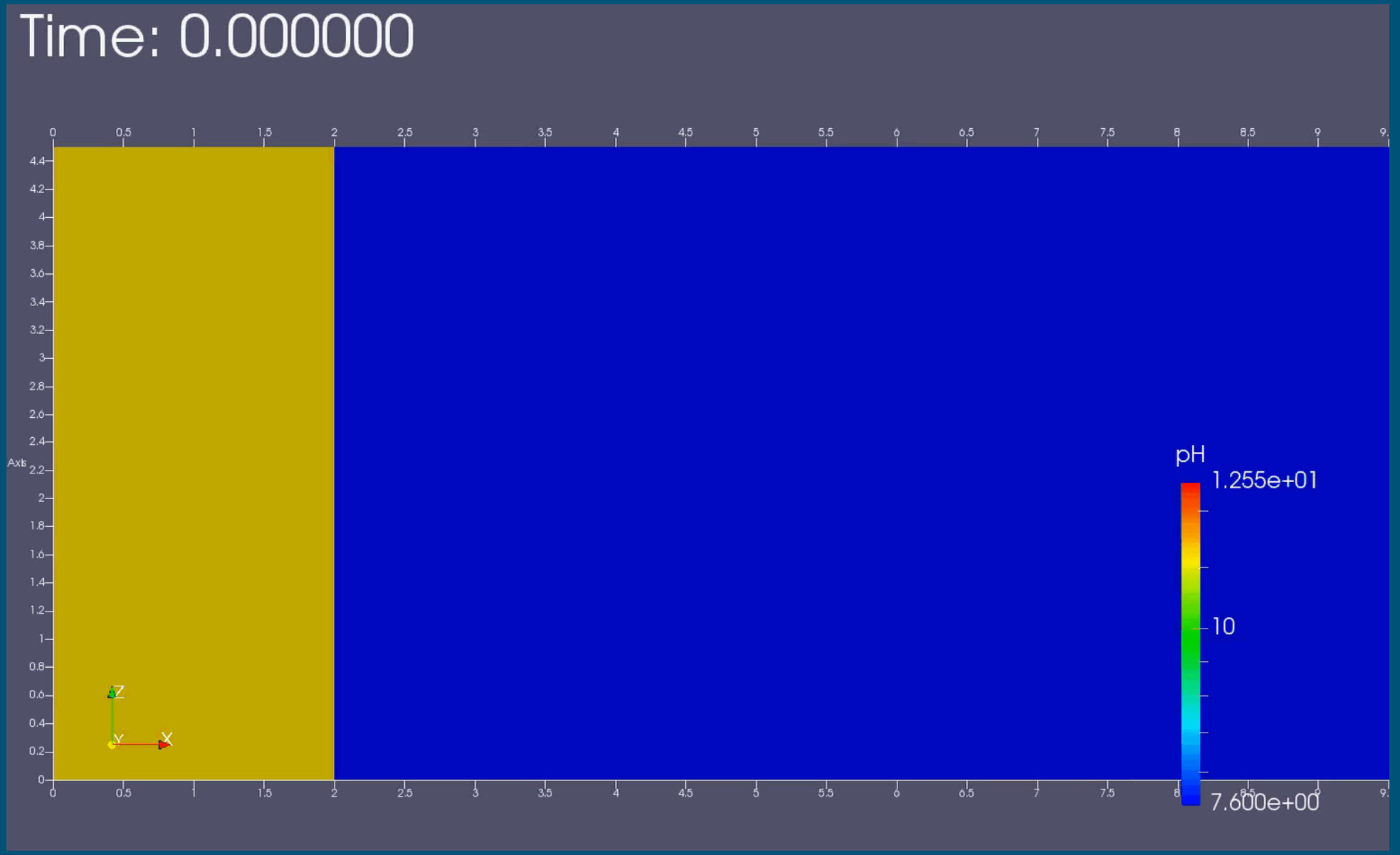
Results: Tobermorite ($Ca_5Si_6O_{16}(OH)_2 \cdot 4H_2O$)



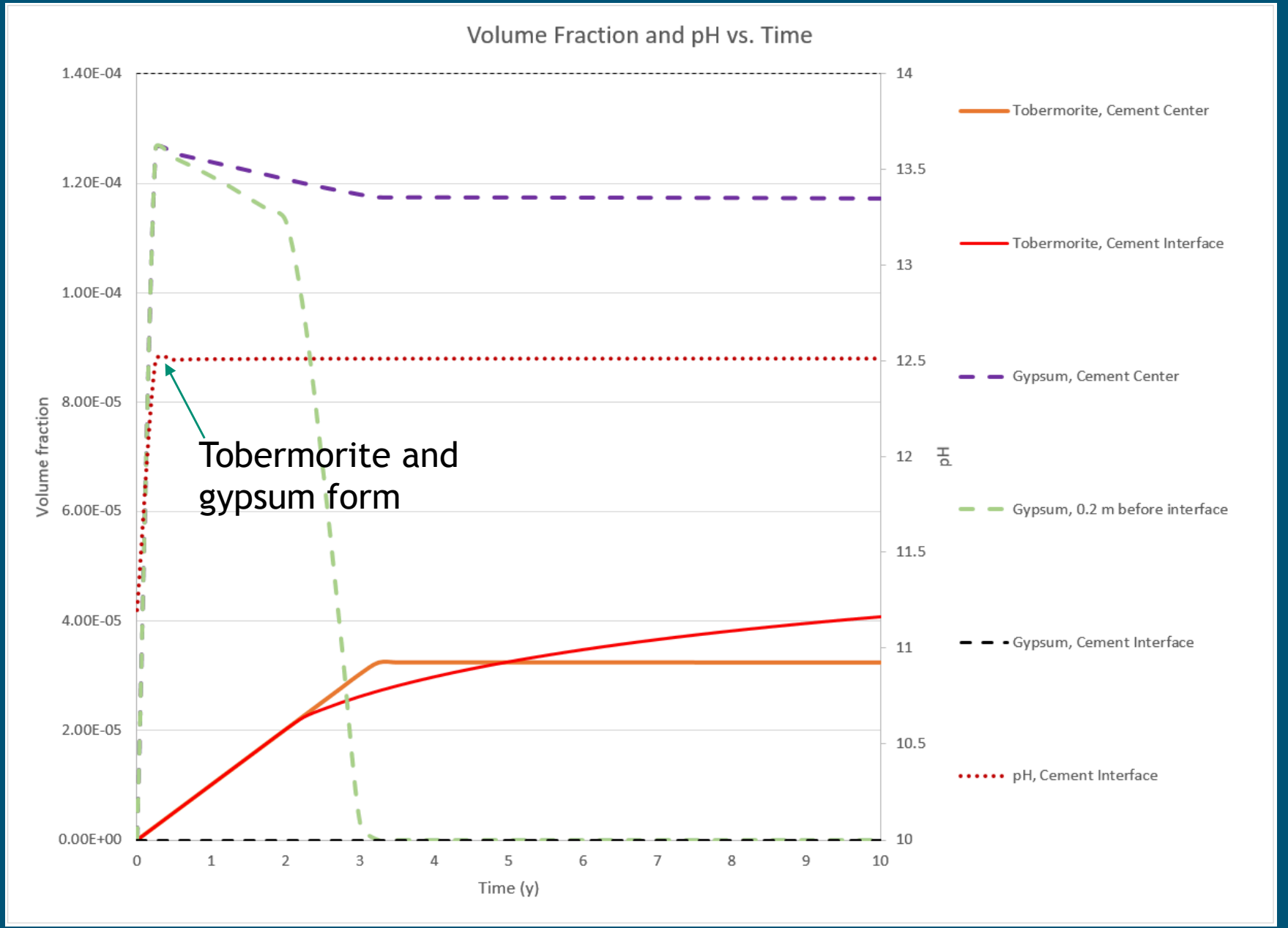
Results: Gypsum ($CaSO_4 \cdot 2H_2O$)



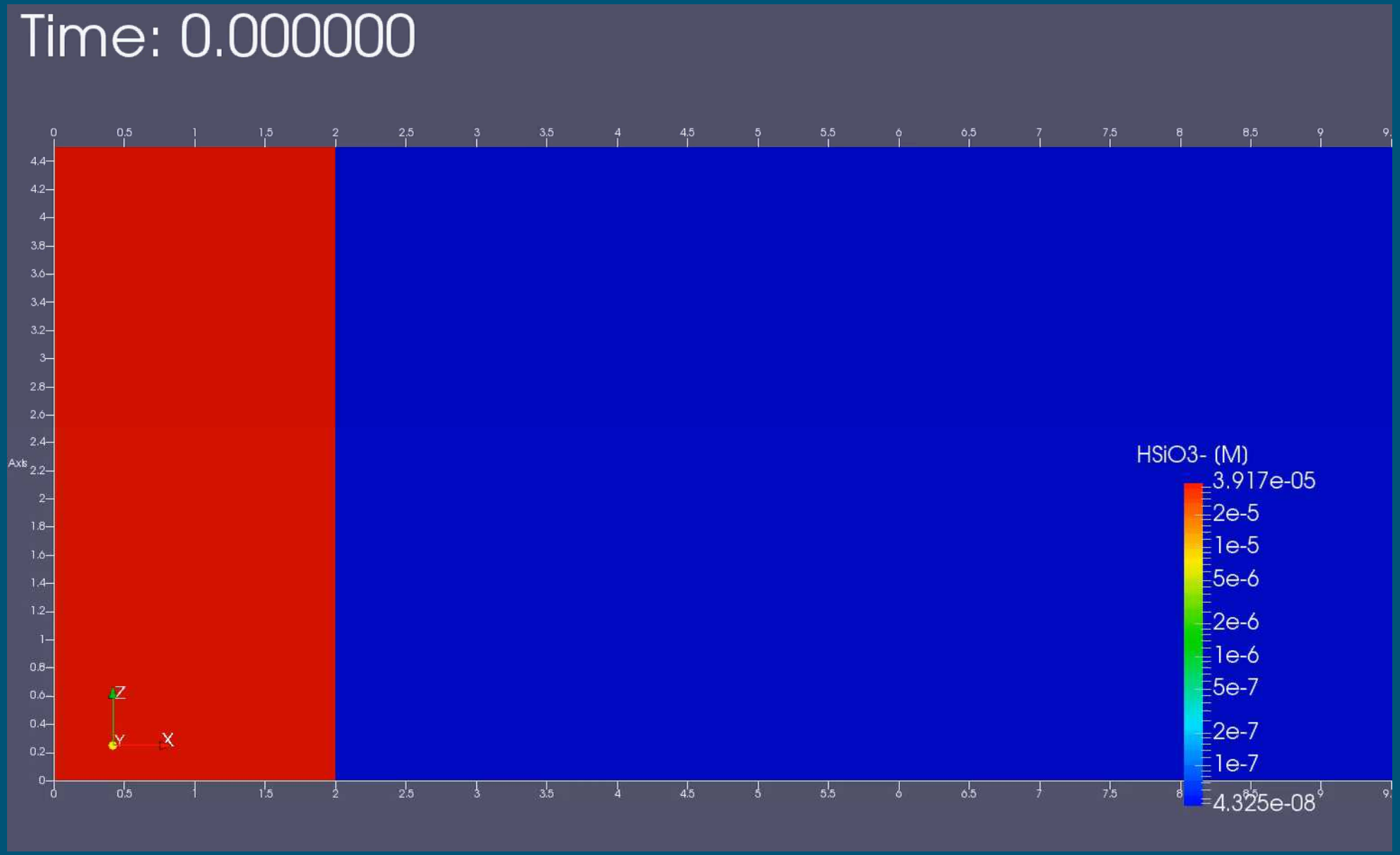
Results: pH



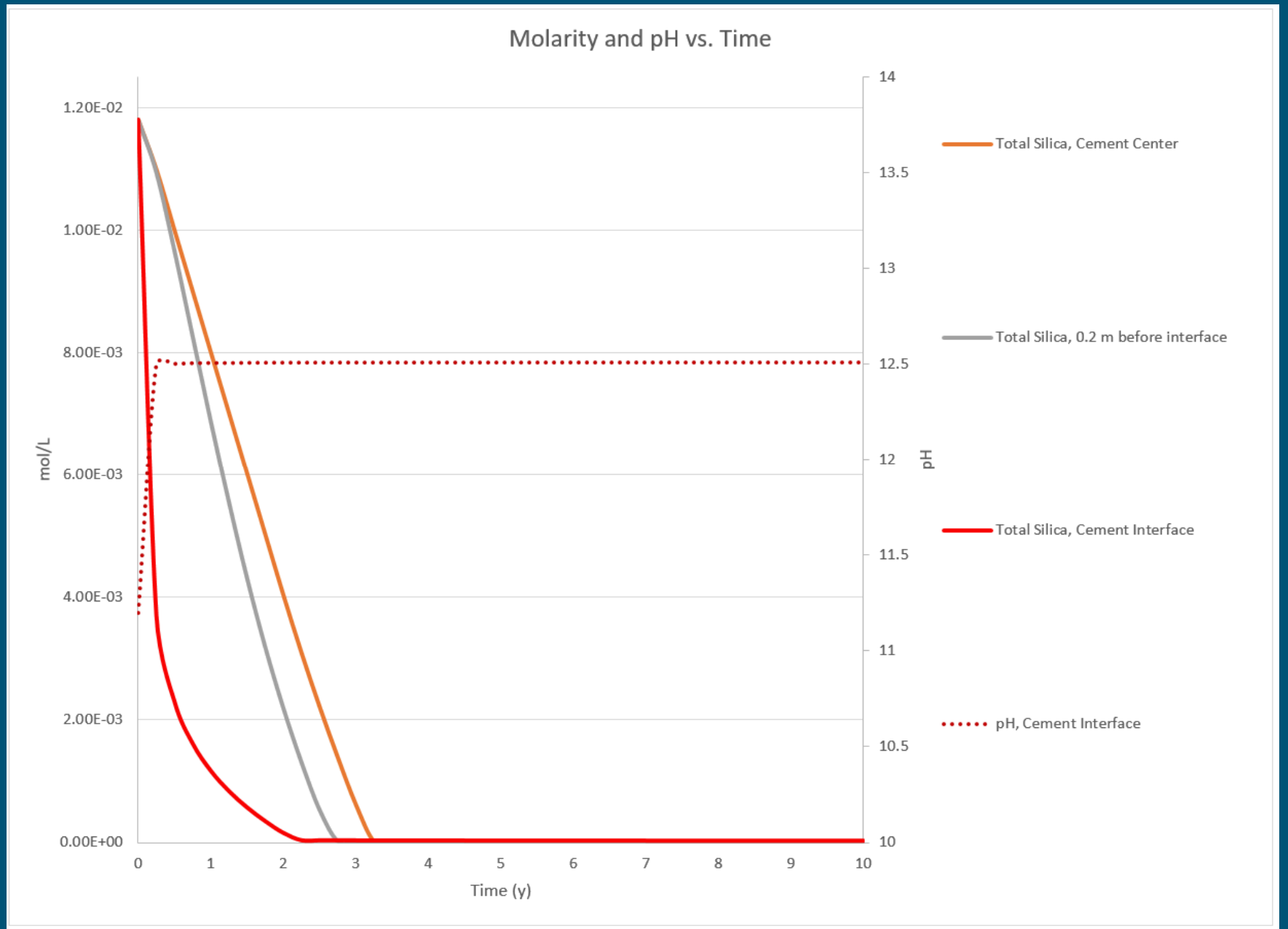
Results: Tobermorite, Gypsum, pH



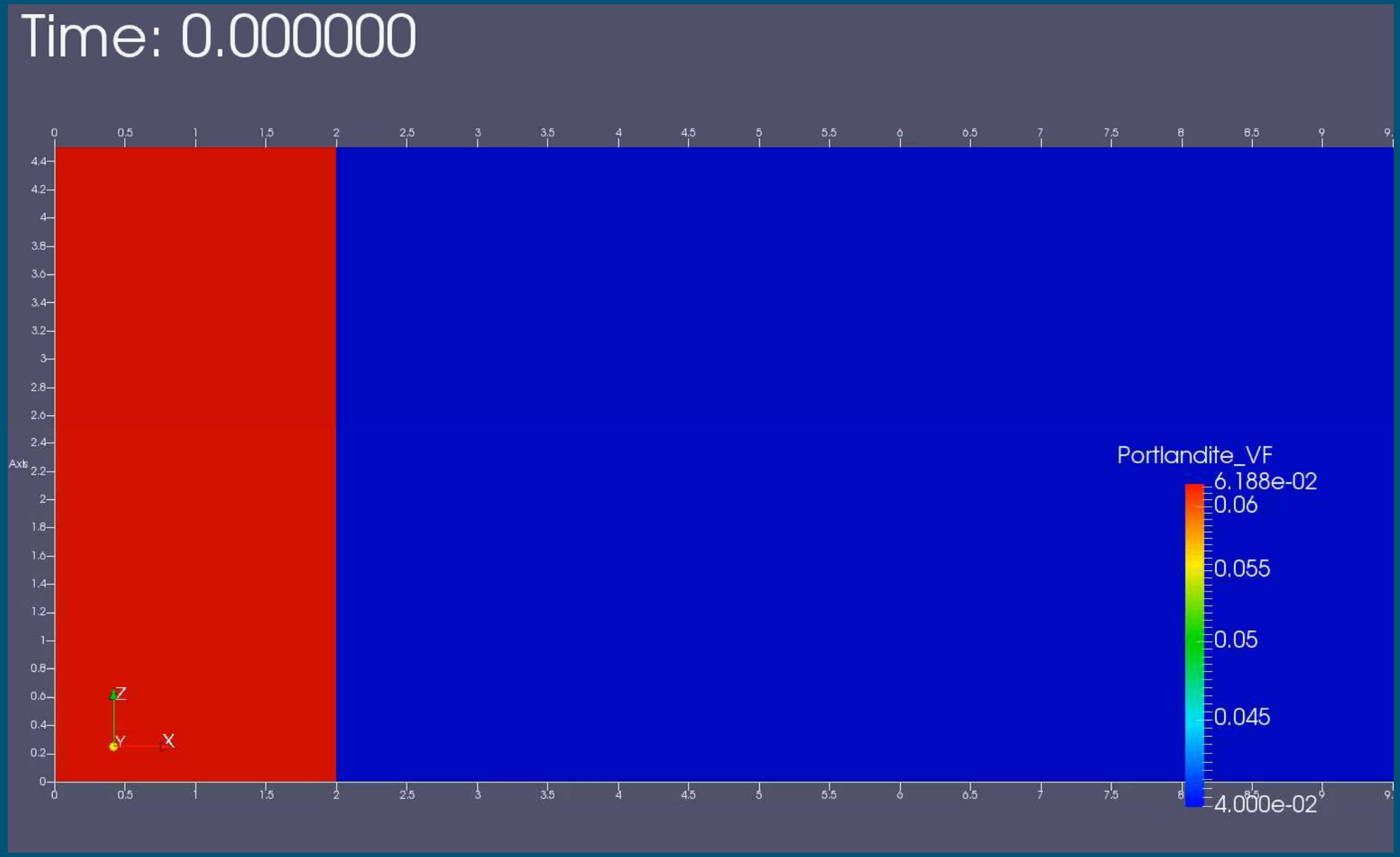
Results: $HSiO_3^-$



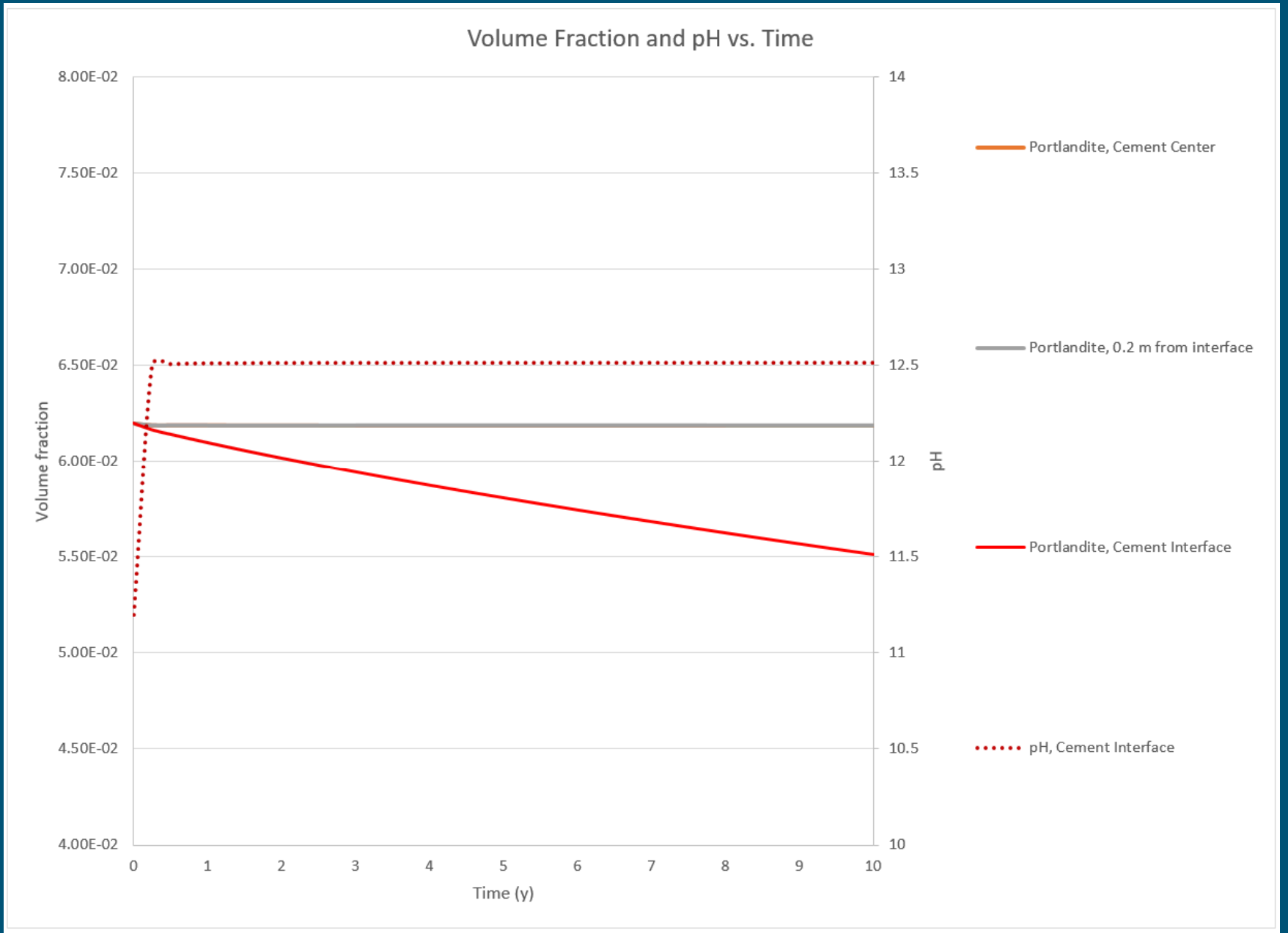
Results: Total Silica (H_4SiO_4 + $HSiO_3^-$)



Results: Portlandite ($Ca(OH)_2$)



Results: Portlandite



Concluding Remarks

- Developed simple 1D reactive-transport problem of cement (OPC) plug – groundwater interactions in PFLOTRAN
  - Model can be expanded to various cement leaching scenarios in subsurface disposal environments
  - NEXT: Modeling the effect of shotcrete liner interactions on groundwater chemistry within flooded tunnel
- 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
  - Gypsum depletion does not exert strong controls on [Ca^{++}]