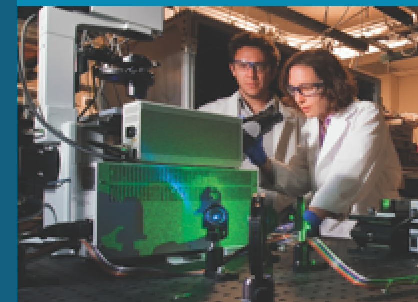
SAND2021-14285C

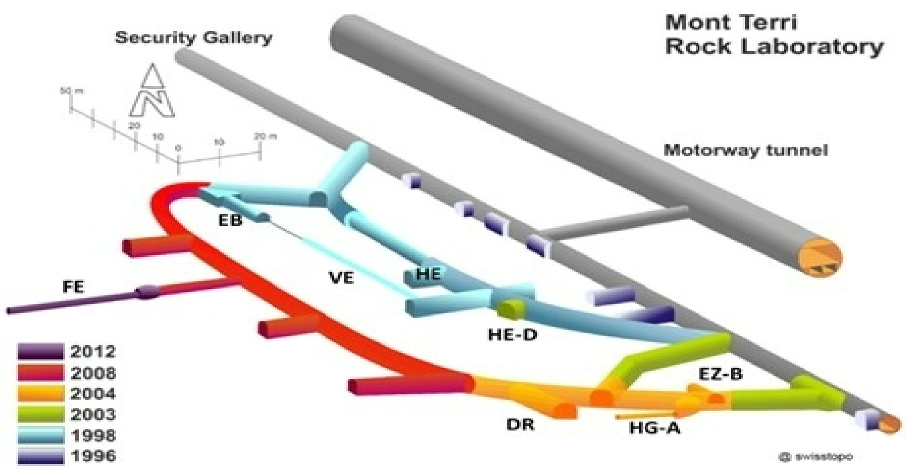
Sandia National Laboratories

DECOVALEX23: Task C, Step 0 SNL Updated Thermal Hydrologic Modeling of Full-Scale Heater Experiment



DECOVALEX23
4th Workshop

Nov. 11, 2021



PRESENTED BY

Teklu Hadgu, Thomas Dewers and Edward Matteo

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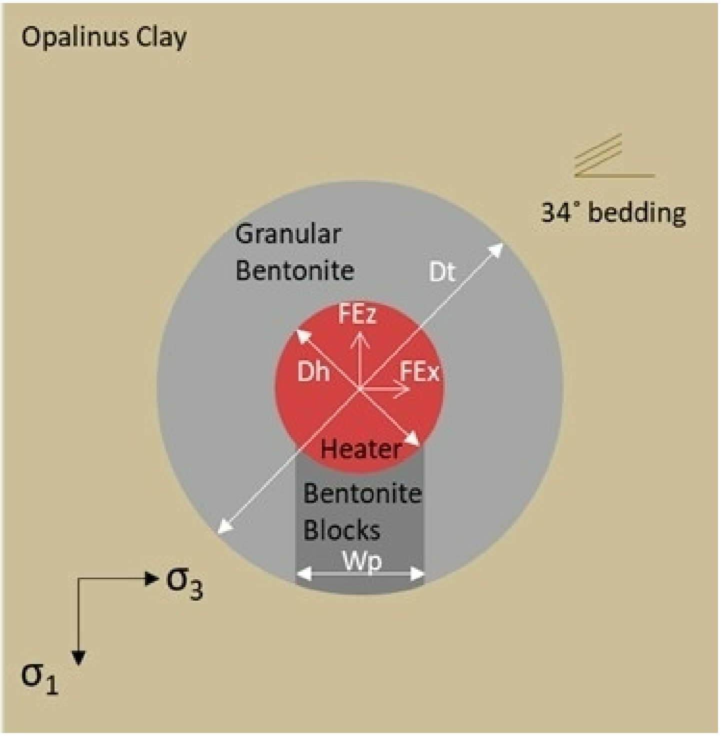
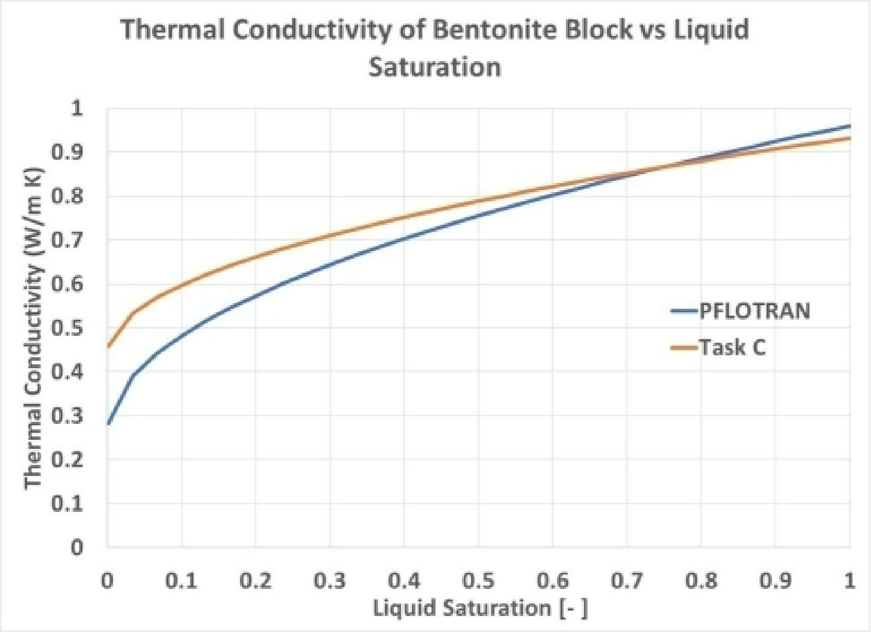
Outline

- Updated TH simulations of Step 0
- Code changes in PFLOTRAN
- Effect of fluid properties
- Summary of modeling results and future work



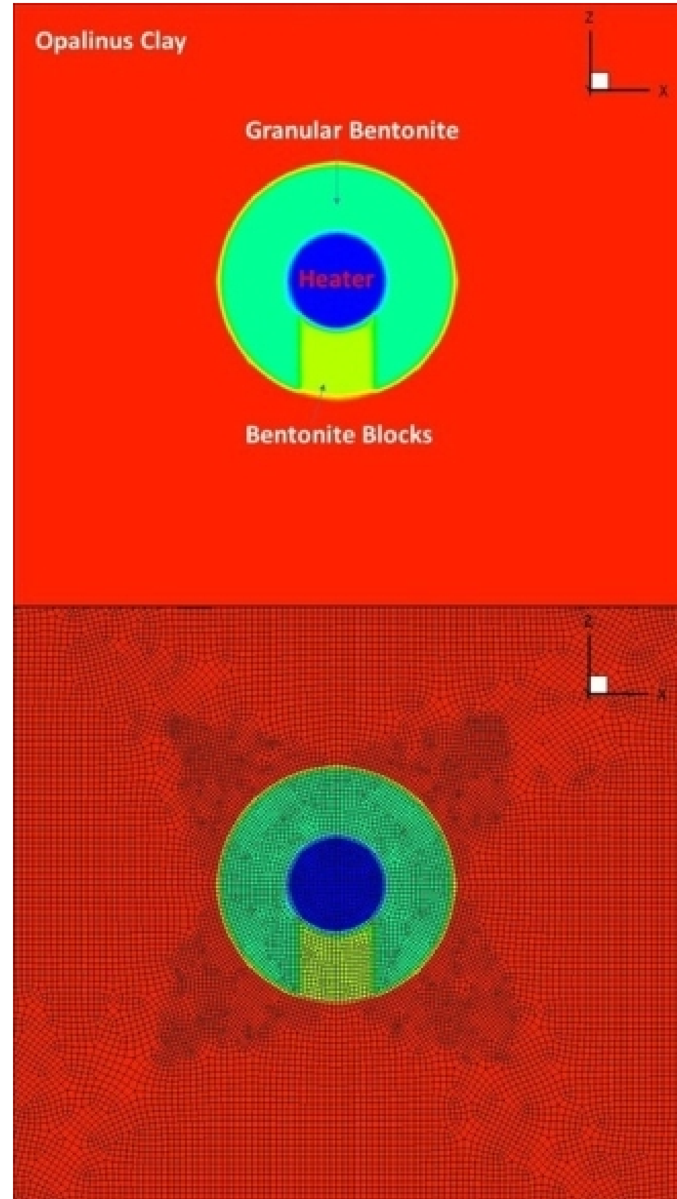
I. Step 0: TH Modeling using PFLOTRAN

- Updated thermal and thermal-hydrology modeling of Step 0 for the full-scale in-situ heater test
- Used Task C specified material properties:
  - Thermal conductivity vs saturation equation
  - Density of water equation with constant thermal expansion
  - Porosity and pore compressibility equation
- Conducted simulations to show the effect of using constant thermal expansion

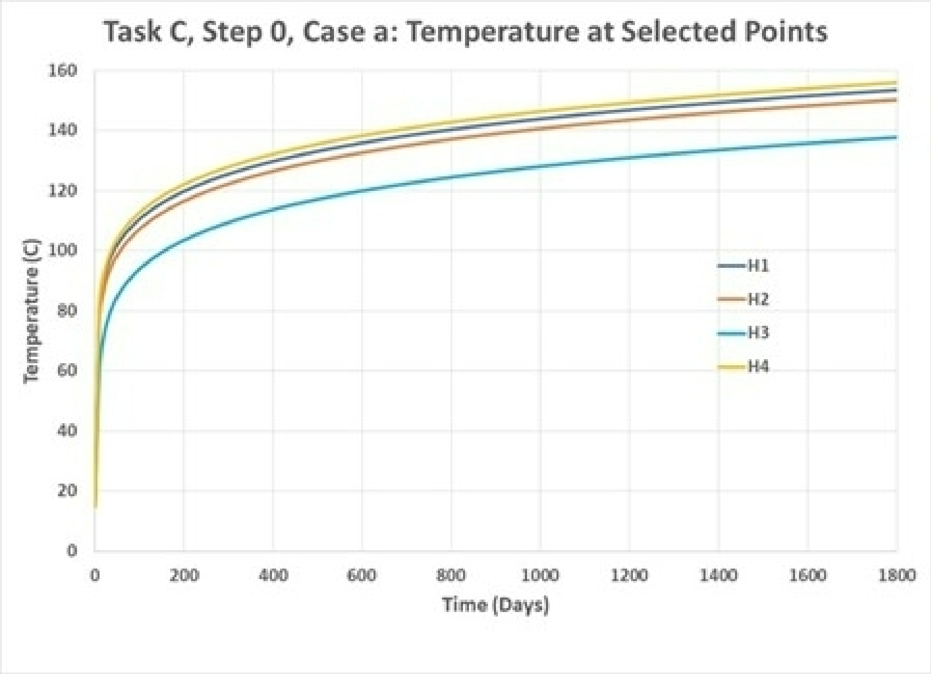


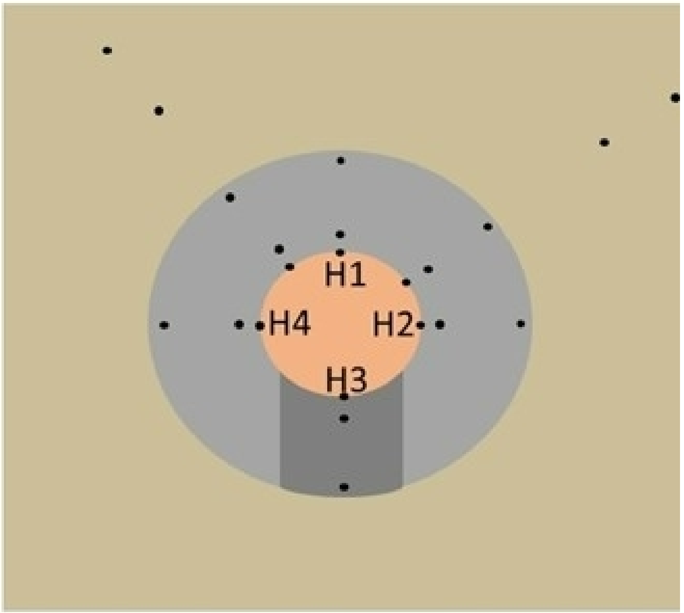
PFLOTRAN TH Model Setup

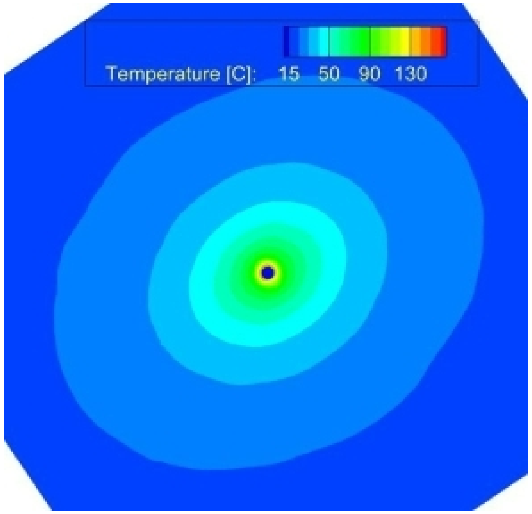
- Initial condition:
  - T = 15 °C everywhere
  - Hydrostatic pressure at opalinus clay
  - Bentonite blocks initial condition:
  - Calculated liquid saturation = 0.919
  - Granular bentonite initial condition:
    - calculated liquid saturation = 0.227
- Diffusion Coefficient:
  - Liquid phase: $2.0 \times 10^{-9}\ m^2/s$
  - Gas phase: $2.0 \times 10^{-5}\ m^2/s$
- Boundary Condition:
  - Column outer boundary at 2.0 MPa and 15 °C
  - Specified heat applied at heater boundary
- Opalinus Clay:
  - Anisotropy in permeability and thermal conductivity



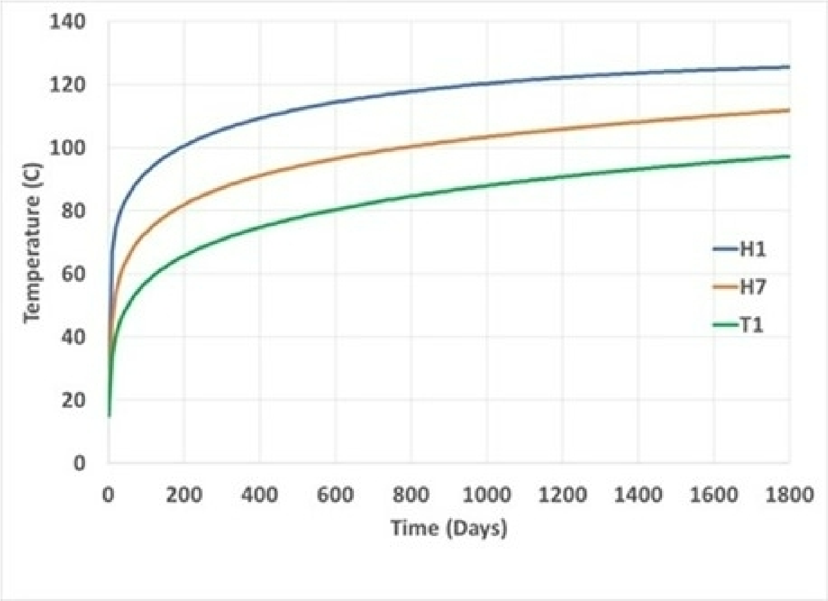
Step 0a Results: PFLOTRAN Predicted Temperature Distribution at 1800 Days (with anisotropy)

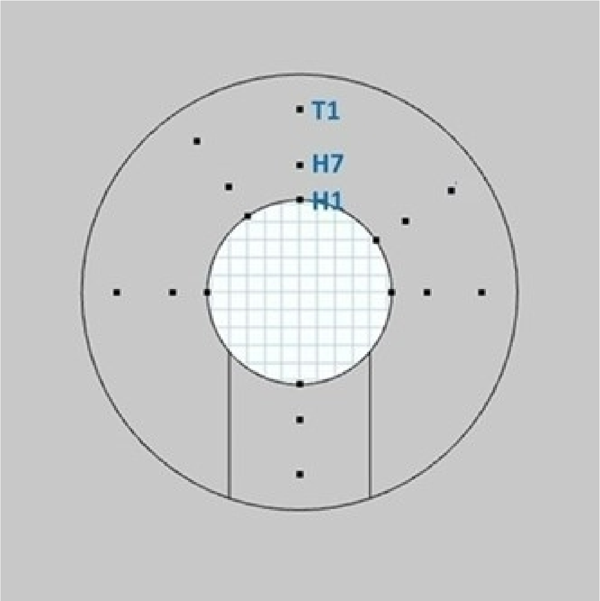


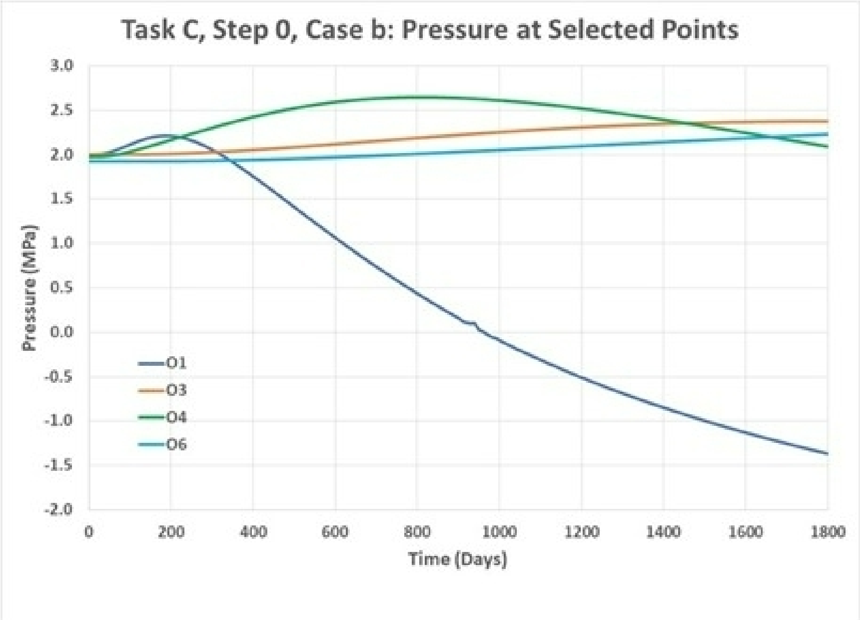


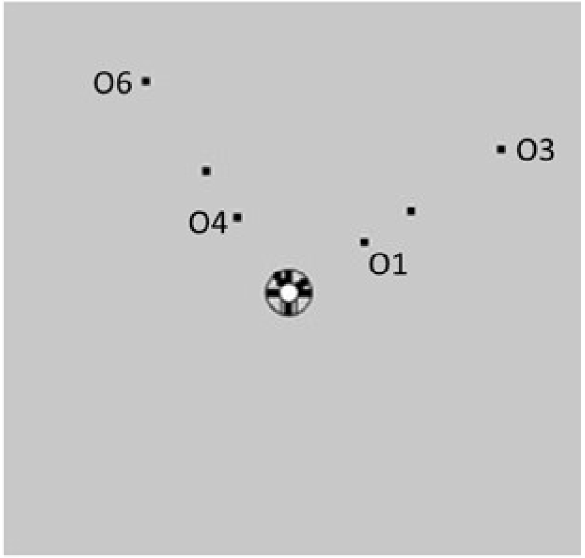


Step 0b: PFLOTRAN Predicted Evolution of Temperature at Specified Locations



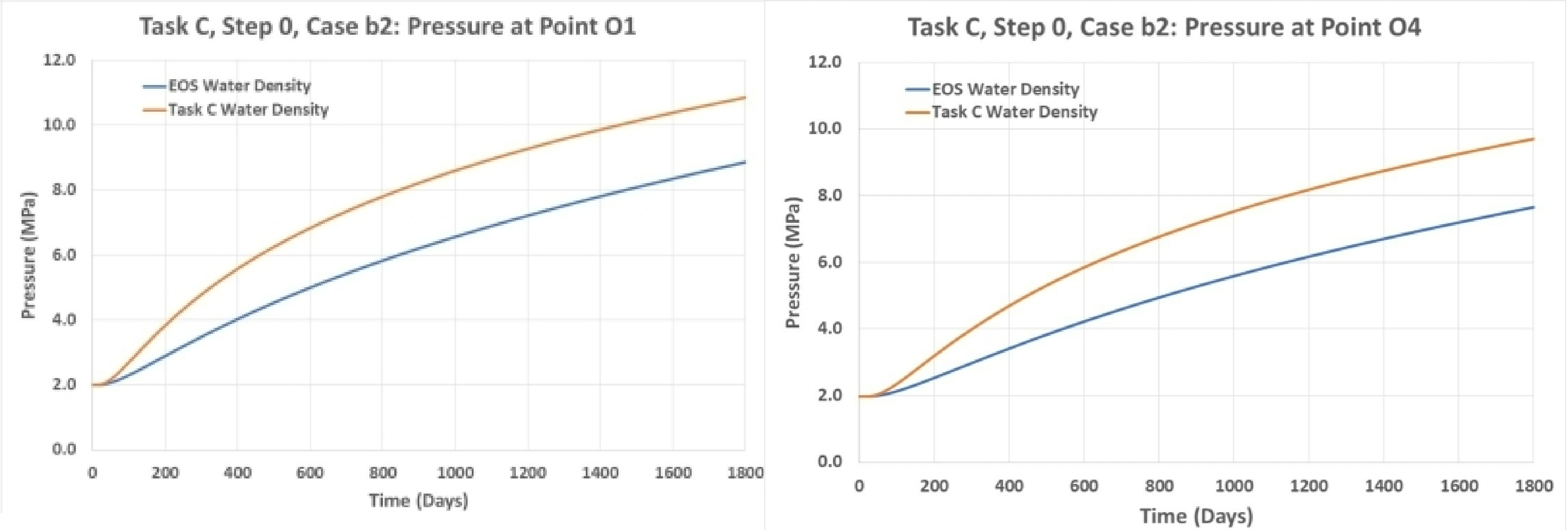




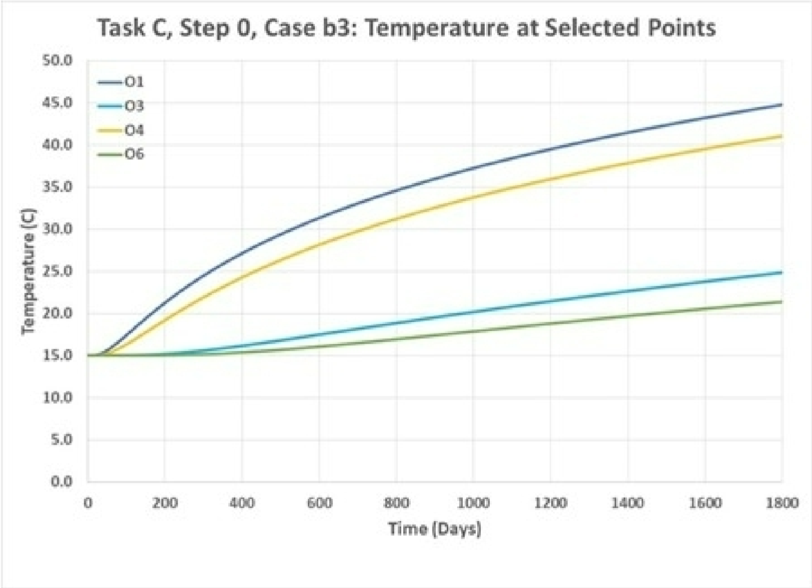


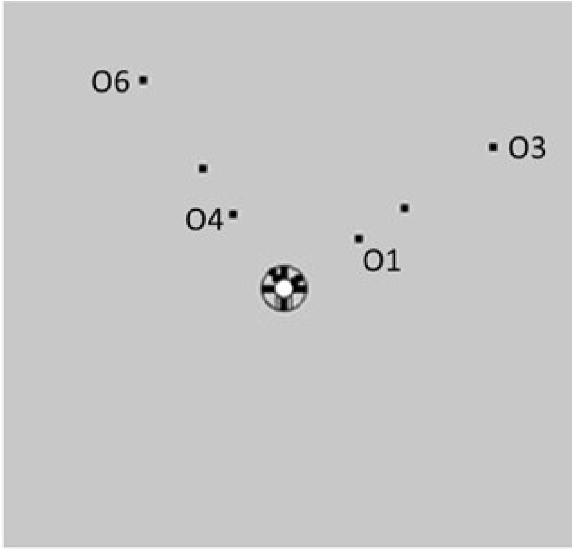
Step 0b2: PFLOTRAN Predicted Evolution of Pressure at Specified Locations – Effect of Water Density Equation

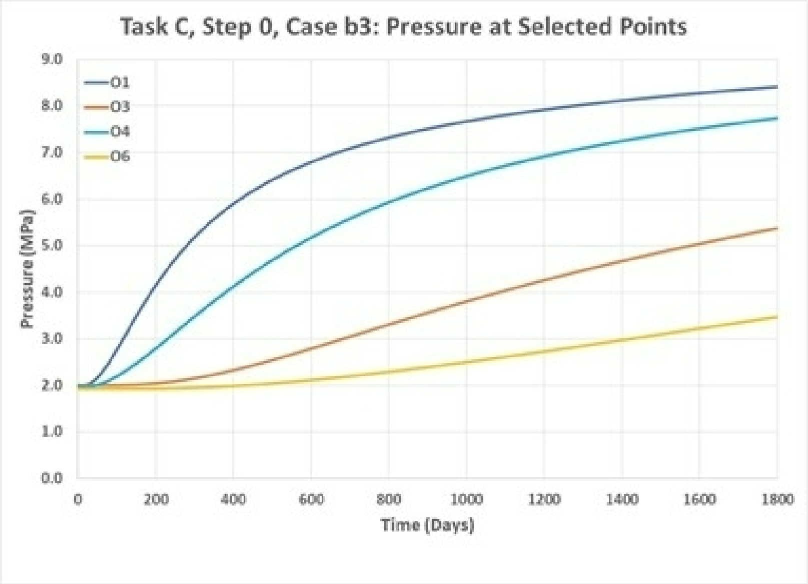
- Task C: Specified water density equation uses constant thermal expansion
- PFLOTRAN: Water Density: EOS based on International Formulation Committee (1967, 1997). Thermal expansion a function of temperature.
- Predicted pressure affected by the differences in thermal expansion

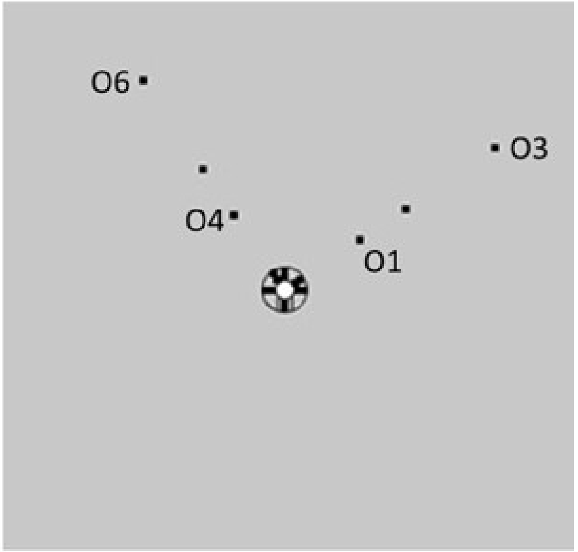


Step 0b3: PFLOTRAN Predicted Evolution of Temperature and Pressure at Specified Locations



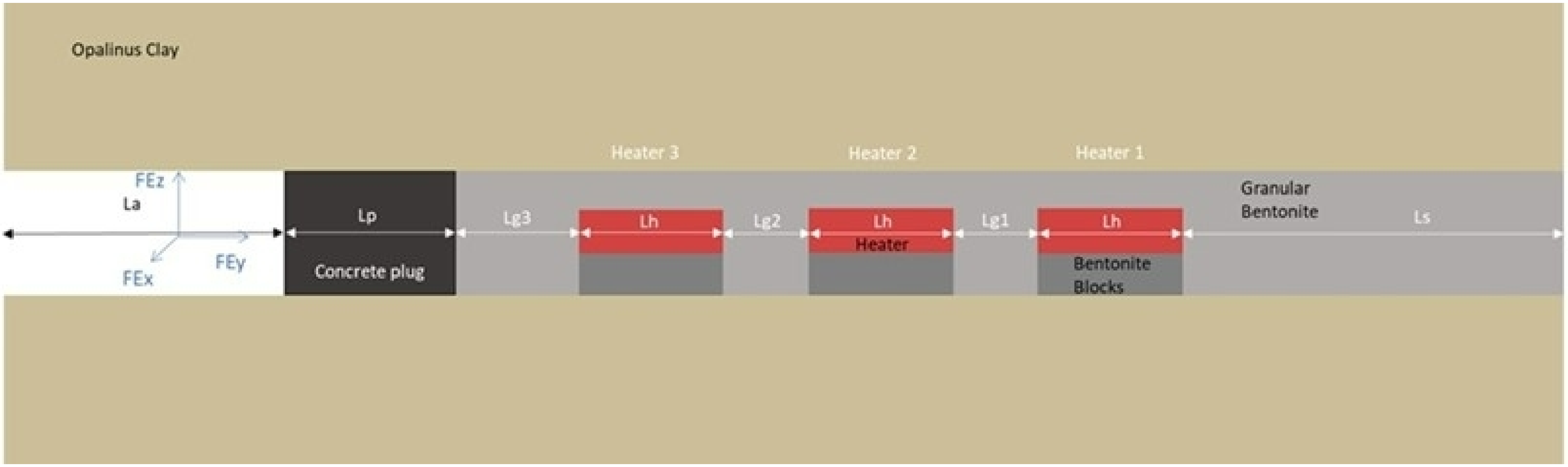






Summary

- Updated Task C, Step 0a, Step 0b, Case b2 and Case b3 PFLOTRAN simulations using Task C specified material properties
- Focusing on two-phase transport and wetting/drying
- Next Steps:
  - Code comparison between COMSOL & PFLOTRAN for two phase transport
  - Step 1 modeling



Meshing for Step 1