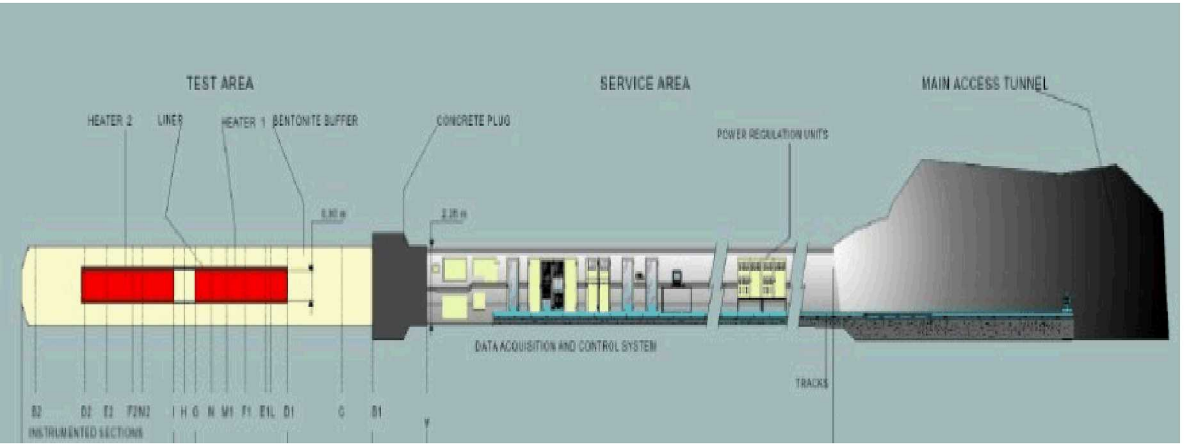
SAND2019-12683C

EBS Task Force: Task 9

SNL Updates on TH and THM Modeling of FEBEX In-Situ Test

EBS Task Force Meeting
Baden, Switzerland
Oct. 21-23, 2019



PRESENTED BY

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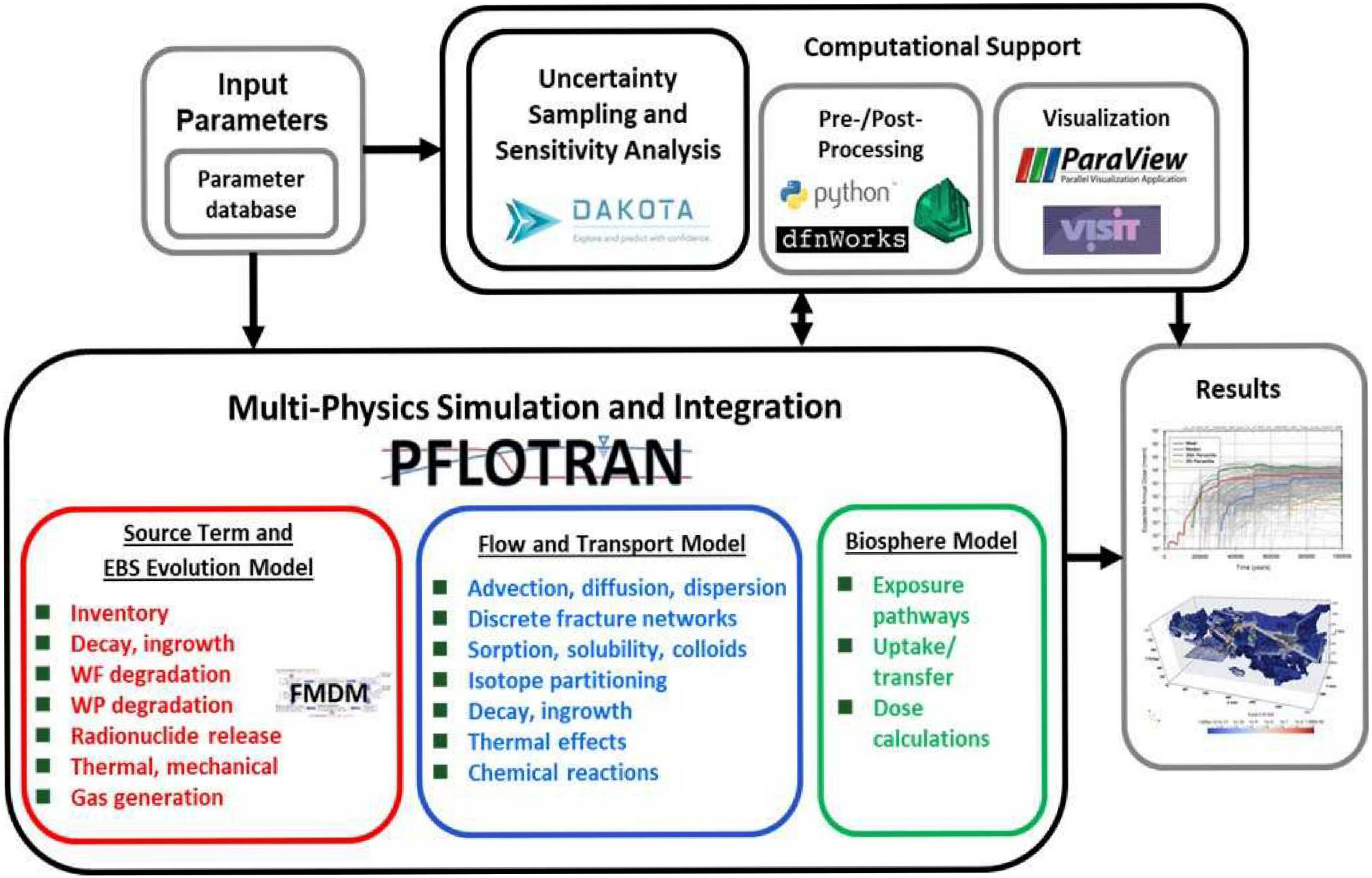
Outline

- Part I: TH Modeling of Stage 1 FEBEX in-situ test using PFLOTRAN
    - Model development
    - TH modeling results
- Part II: THM Modeling of Stage 1 FEBEX in-situ test using COMSOL (In Progress)
    - Model development
    - Future work

Sandia Geologic Disposal Safety Assessment (GDSA) Framework



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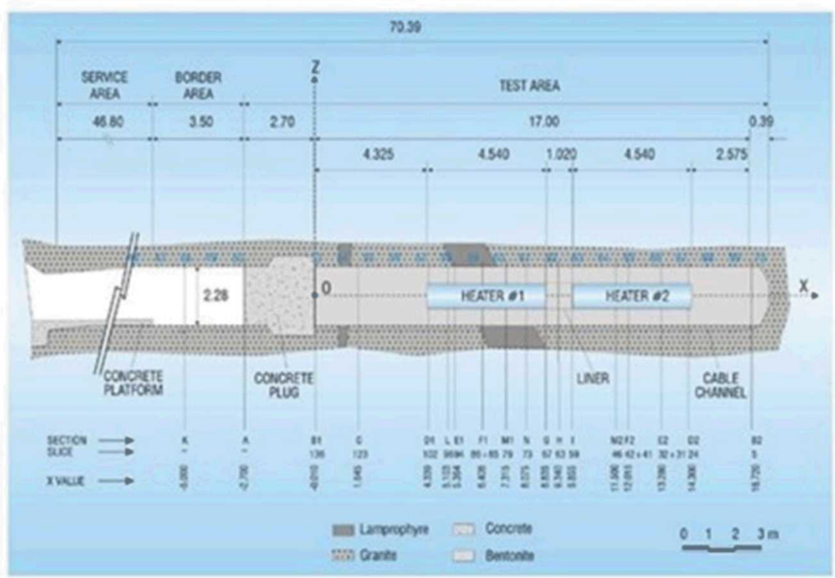
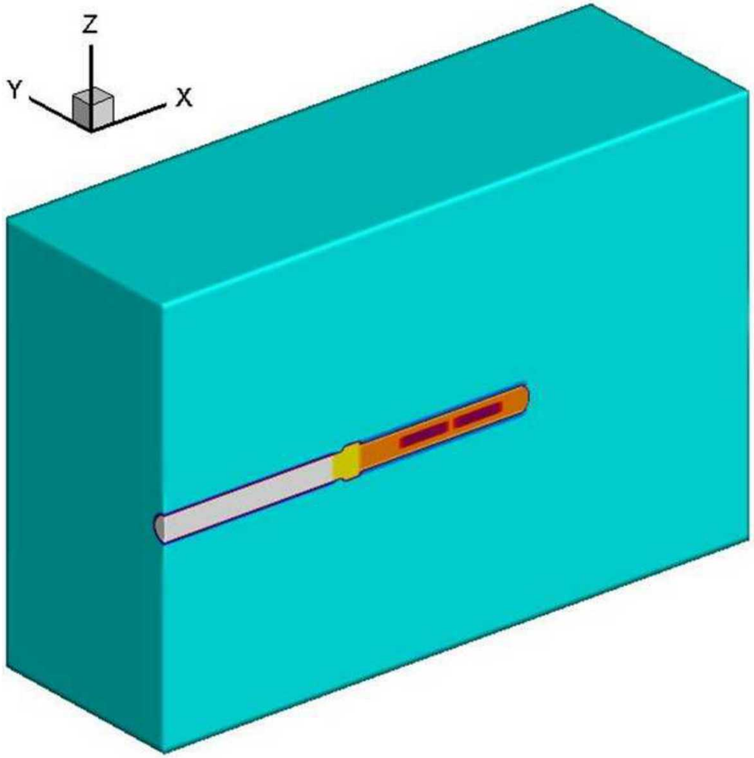
Part I: TH Modeling of Stage 1 FEBEX In-Situ Test using PFLOTRAN

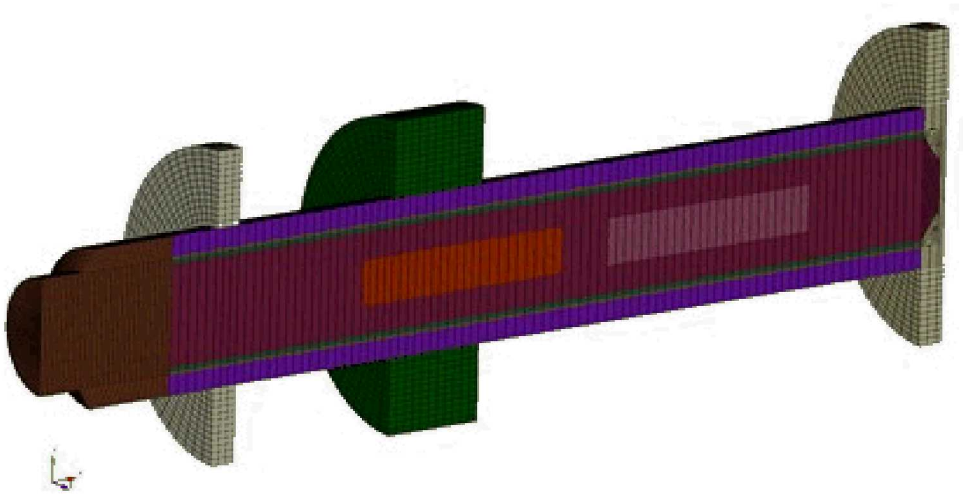
- Conducted thermal-hydrology modeling of the FEBEX in-situ test up to first dismantlement (5 years)
- Developed 3-D modeling domain and meshing based on project specifications
- Assumed low permeability concrete plug isolates the open tunnel from the test area



TH 3-D Modeling Domain

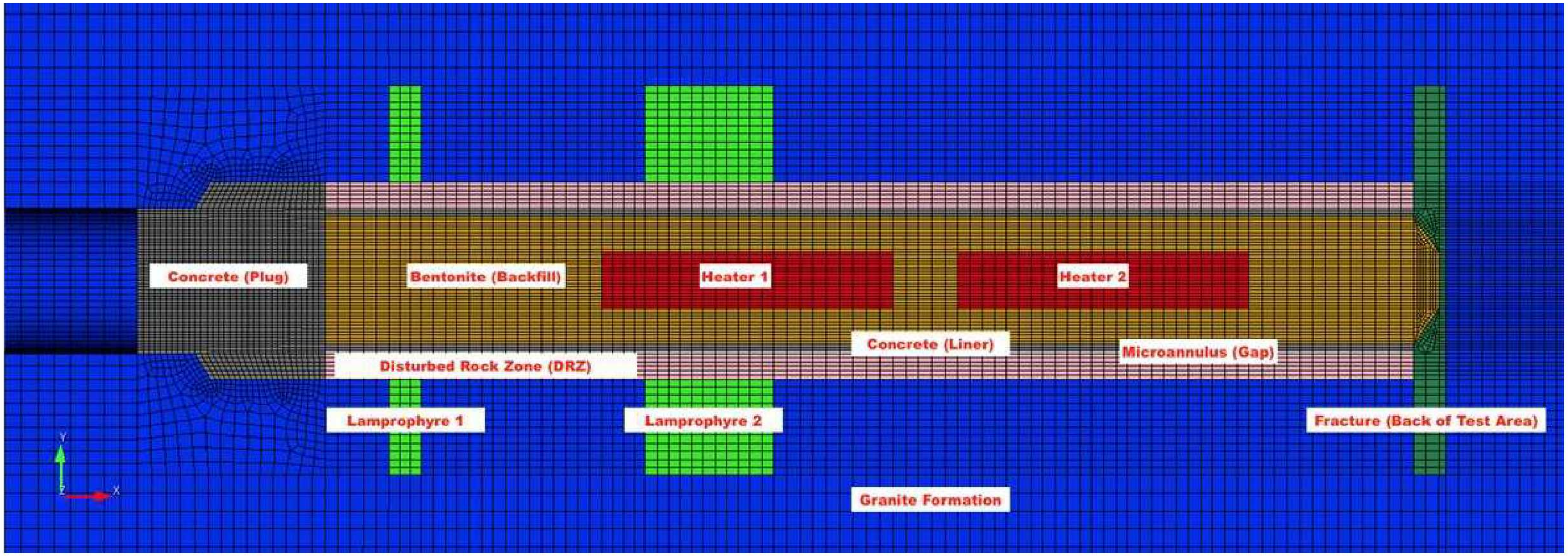


- Domain Size: 60 m x 20 m x 40 m (x, y, z)
- Mesh size: 467,992 grid blocks
- Axisymmetric: Symmetry boundary condition assumed



Meshing of TH Modeling Domain

- Simulation domain includes details of various regions representing different materials:
  - Granite, disturbed rock zone (DRZ), bentonite buffer, heaters, plug, liner, microannulus, lamprophyre and fracture at back of test area



Material Properties

	Units	Granite	Buffer	Plug
Permeability	m^2	1.23×10^{-20}	5.0×10^{-20}	1.0×10^{-20}
Porosity	-	0.01	0.365	0.01
Density	Kg/m^3	2700	1600	2600
Specific Heat	kJ/kg	793	1091	1000
Thermal Conductivity Dry/sat	W/m K	3.2/3.3	0.5/1.0	3.0/3.0

Thermal conductivity equation (Somerton et al.,1974):

$$k_{th} = k_{dry} + \sqrt{s_l}\left(k_{sat} - k_{dry}\right)$$

k_{th} = thermal conductivity
k_{dry} = dry thermal conductivity
k_{sat} = fully saturated thermal conductivity

Retention Curves

van Genuchten capillary pressure function:

$$Se = [1 + \left[\left(\frac{s}{P_o}\right)^{\frac{1}{1-\lambda}}\right]^{-\lambda}$$

$$Se = \frac{S_l - S_{lr}}{S_{ls} - S_{lr}}$$

S_l = liquid saturation
S_{lr} = residual liquid saturation
S_{ls} = maximum saturation
λ = van Genuchten parameter
s = suction (capillary pressure)
P_o = air entry pressure

Retention Curves (Contd.)

Mualem relative permeability functions based on van Genuchten saturation function:

$$k_{rl} = \sqrt{S_{el}}\left\{1 - \left(1 - S_{el}^{1/\lambda}\right)^{\lambda}\right\}^2$$

$$k_{rg} = \sqrt{1 - S_{eg}}\left\{1 - S_{eg}^{1/\lambda}\right\}^{2\lambda}$$

$$Sel = \frac{S_l - S_{lr}}{S_{ls} - S_{lr}} \qquad Seg = 1 - \frac{S_l - S_{lr}}{1 - S_{lr} - S_{gr}}$$

k_{rl} = liquid relative permeability
k_{rg} = gas relative permeability
S_{gr} = residual gas saturation

Retention Curve Parameters

	Units	Granite	Buffer	Plug
P_o	MPa	21.01	20.0	21.01
λ	-	0.7	0.2	0.7
S_{lr}	-	0.0	0.0	0.0
S_{gr}	-	0.0	0.0	0.0
S_{ls}	-	1.0	1.0	1.0

Relative Humidity Calculation

To calculate relative humidity Kelvin's law was used:

$$RH\,\% = 100exp\left(\frac{-s \cdot V_w}{10^{-6}R \cdot T}\right)$$

RH = relative humidity

s = suction (MPa)

V_w=molar volume of water (1.8 x 10^{-5} m^3/mol)

R = universal gas constant (8.3143 J/mol K)

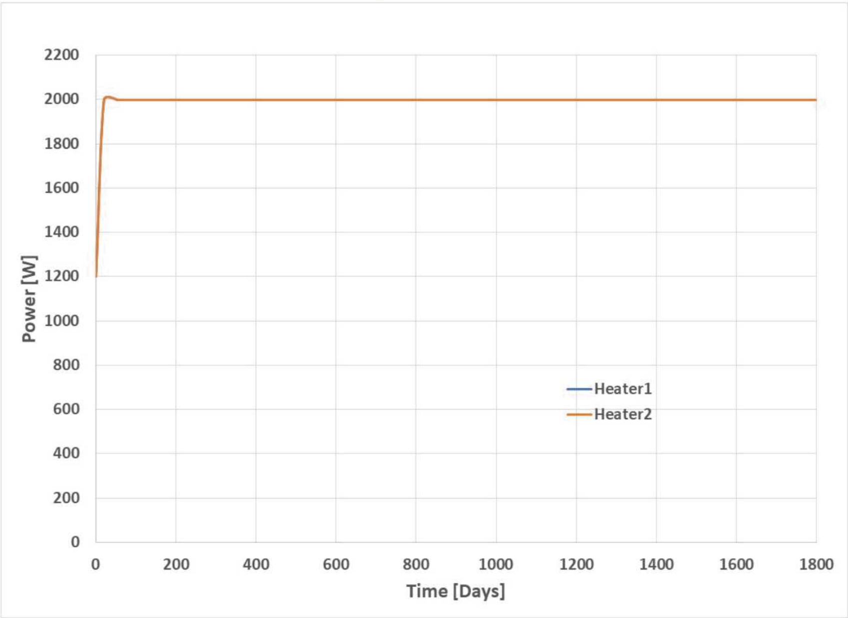
T = temperature in Kelvin

TH Model Setup

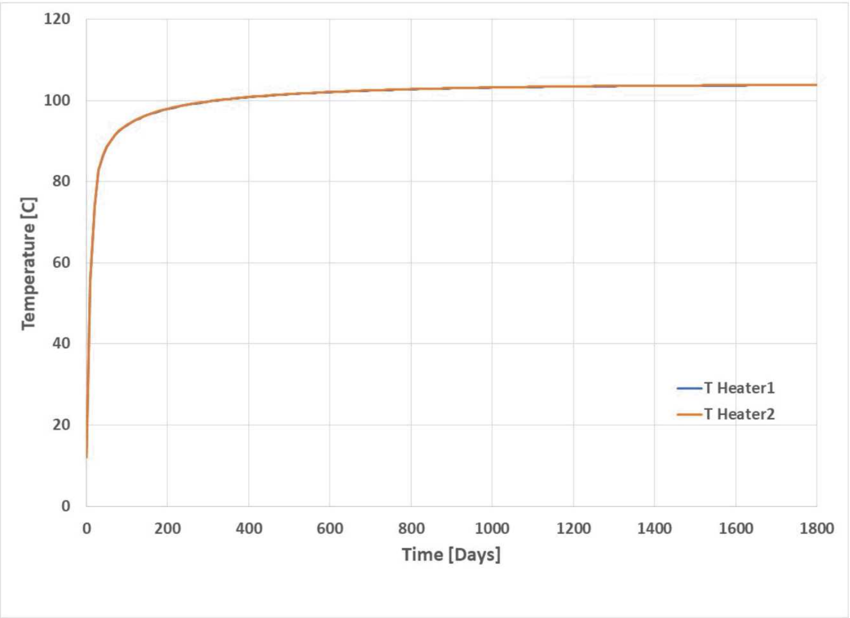
- Initial condition:
  - T = 12 °C everywhere
  - Hydrostatic pressure everywhere except in buffer
  - Buffer initial condition
    - liquid saturation = 0.36 at time zero
    - liquid saturation = 0.7 at time = 135 days (at the start of heating)
- Boundary Condition:
  - Top boundary at P = 4.5 MPa and T = 12 °C
  - Domain sides at hydrostatic pressure and T = 12 °C
  - Time varying heat applied at heaters
- PFLOTRAN numerical code was used for simulations
  - Solved variables for single liquid phase: liquid pressure, temperature and mole fraction of air
  - Solved variables for two-phase: gas pressure, temperature and gas saturation

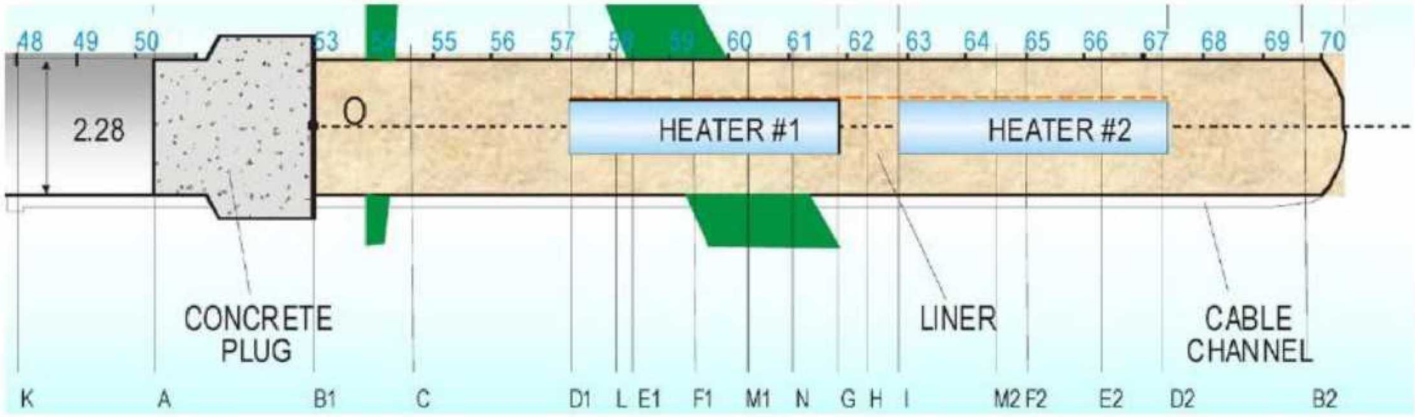
Evolution of Heater Power

Power input at heaters

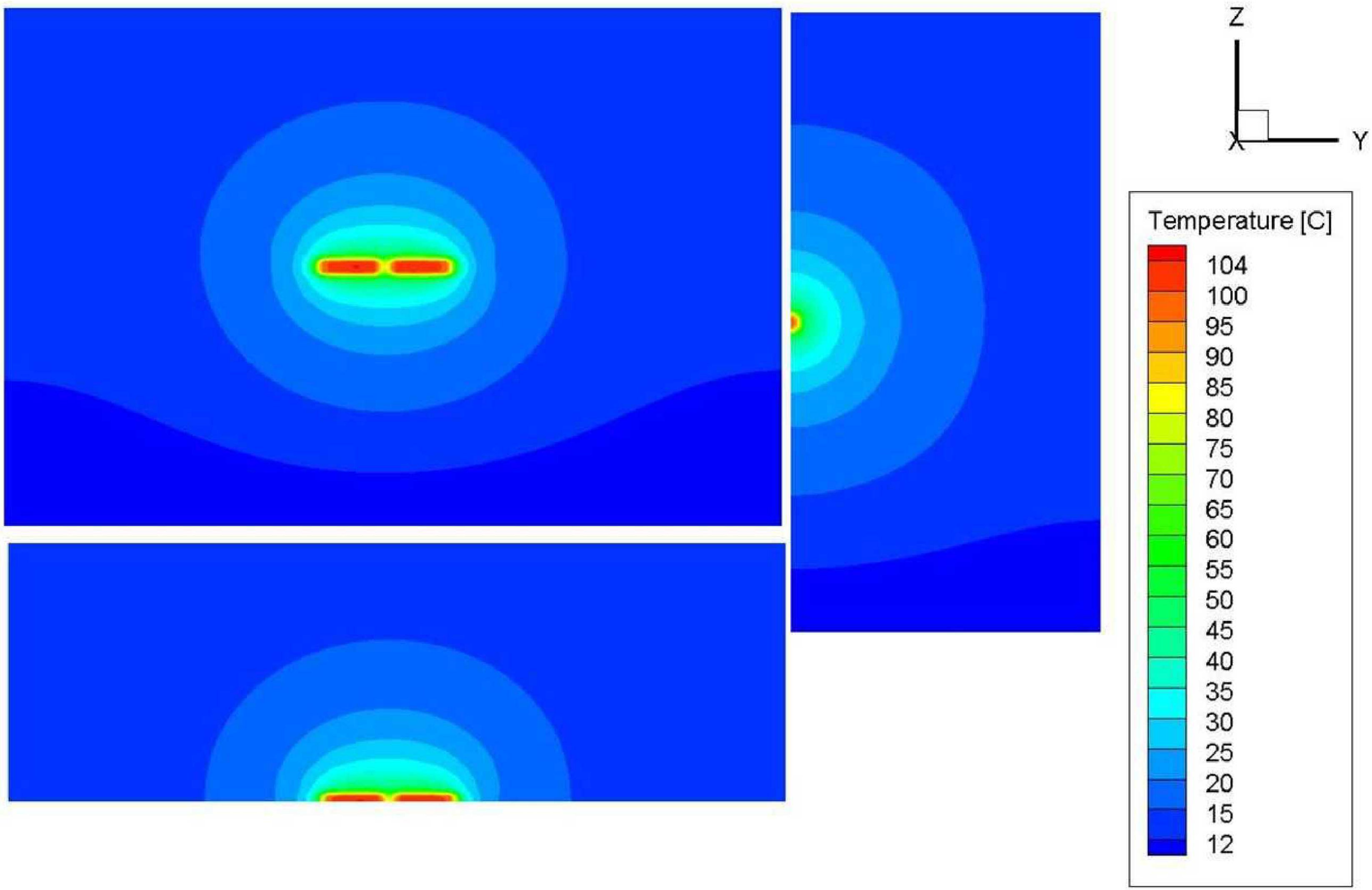


Evolution of temperature at heater surfaces

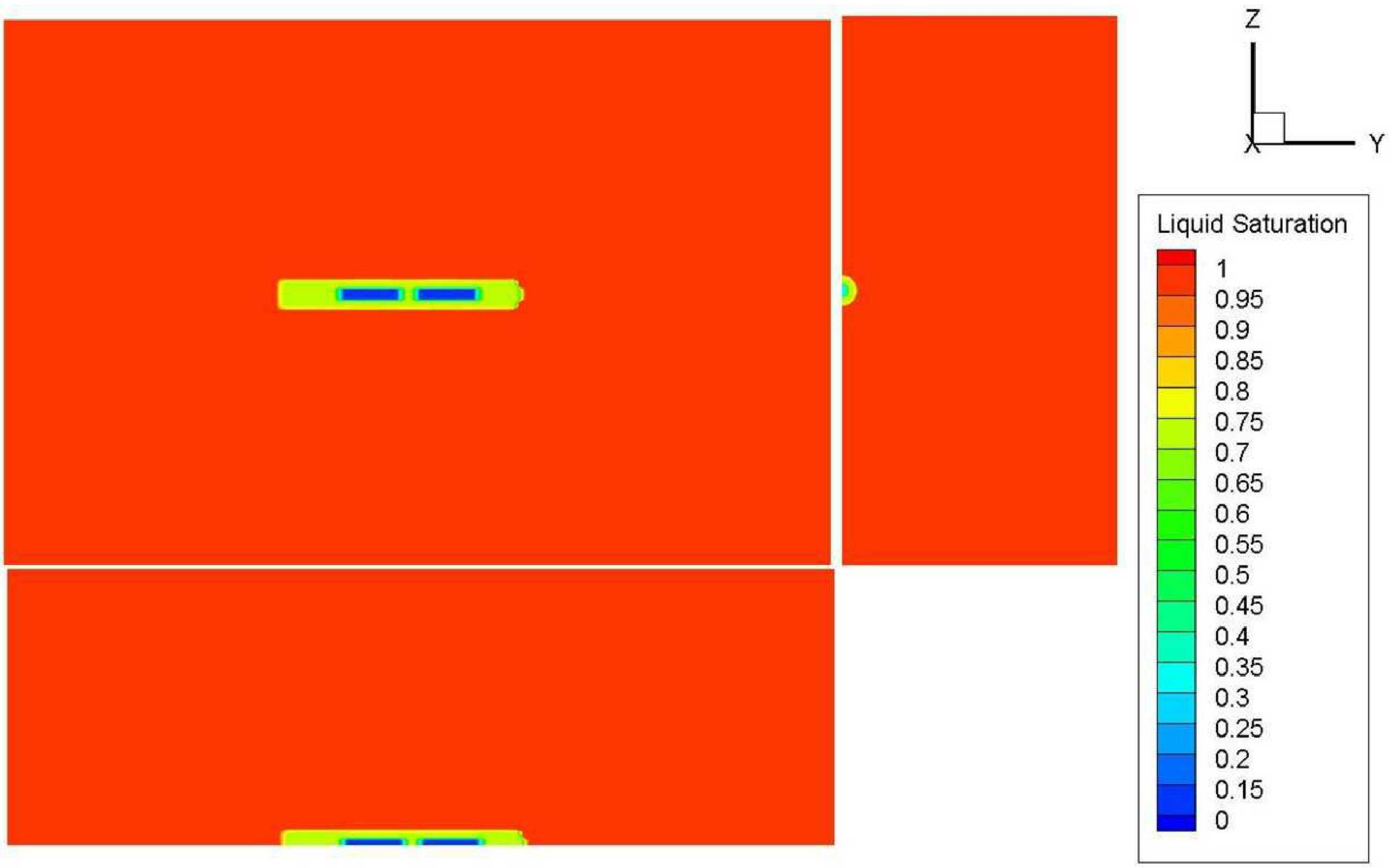




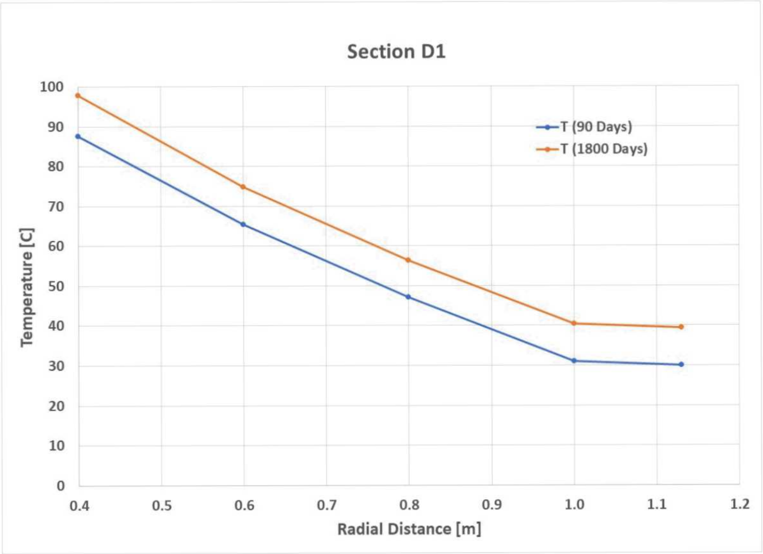
Temperature Distribution at 1800 Days

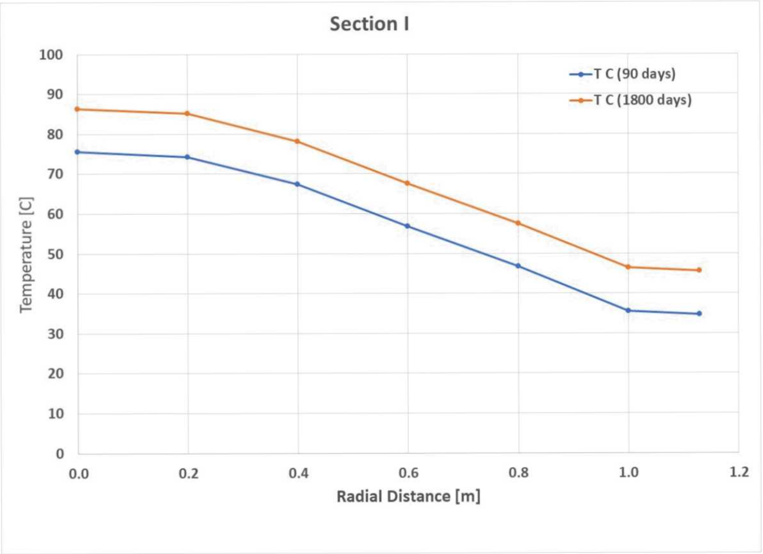


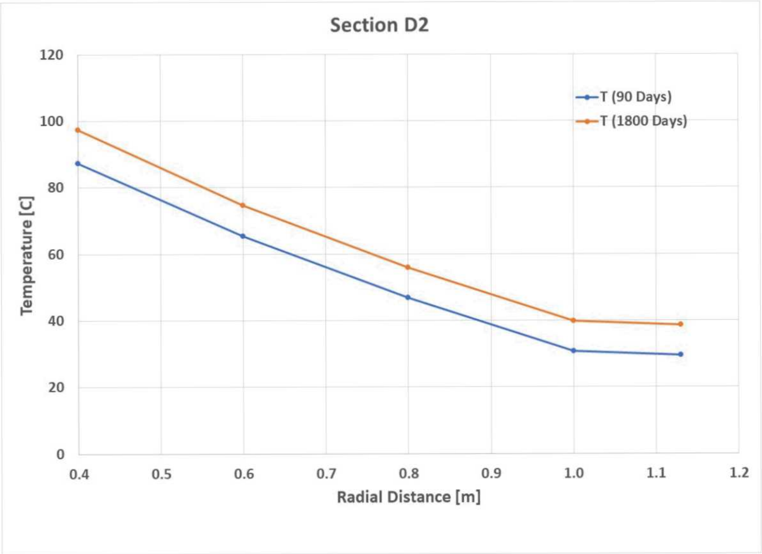
Liquid Saturation Distribution at 1800 Days

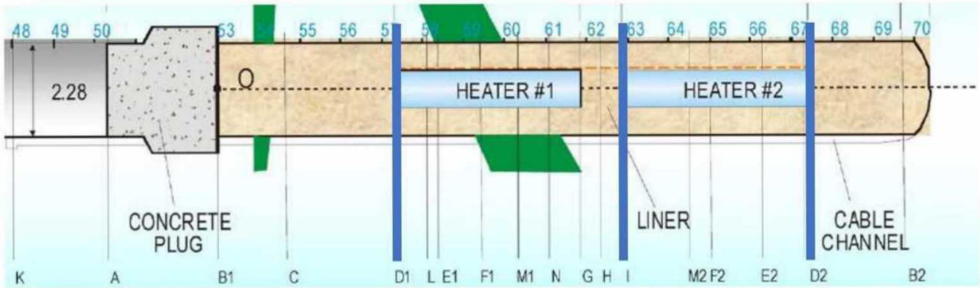


Distribution of Temperature: Radial Sections

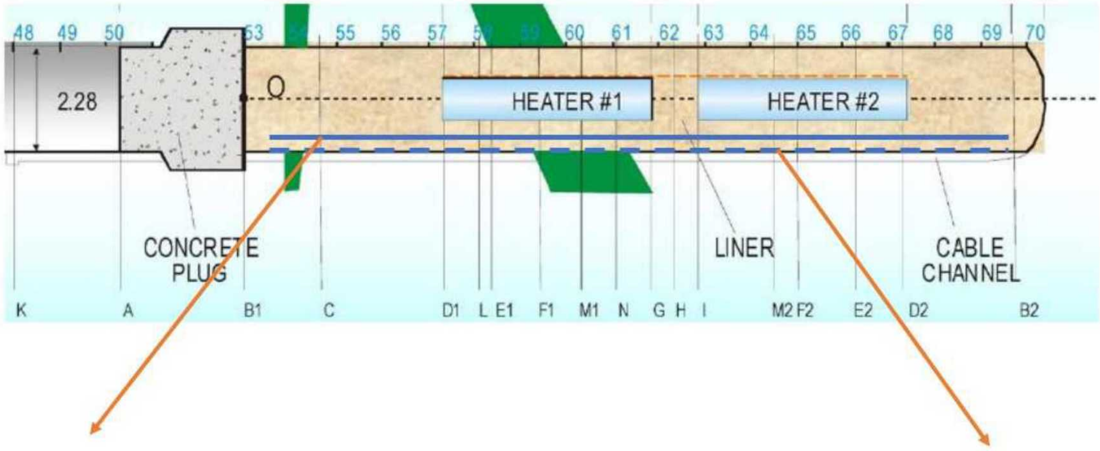


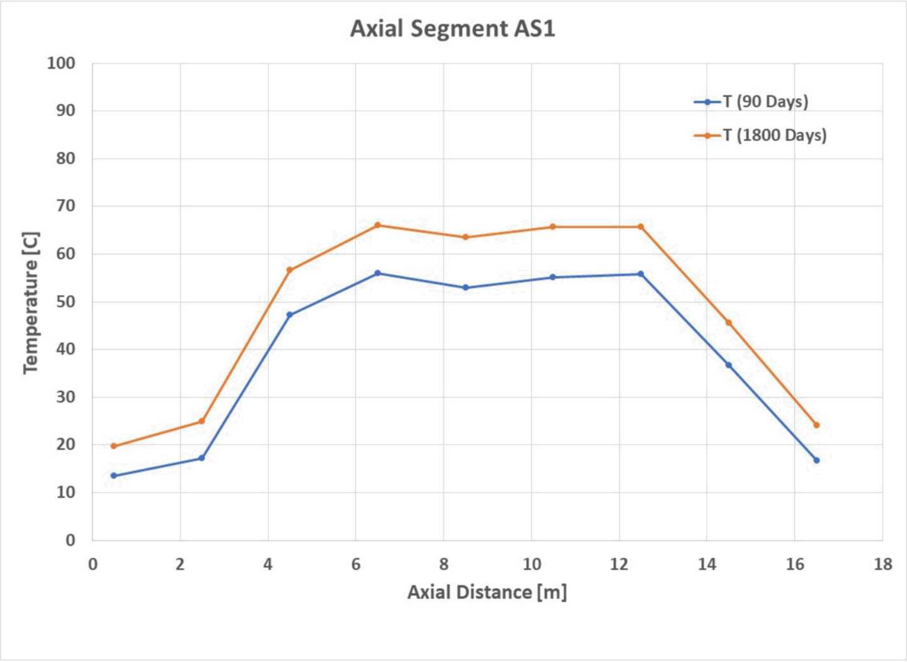


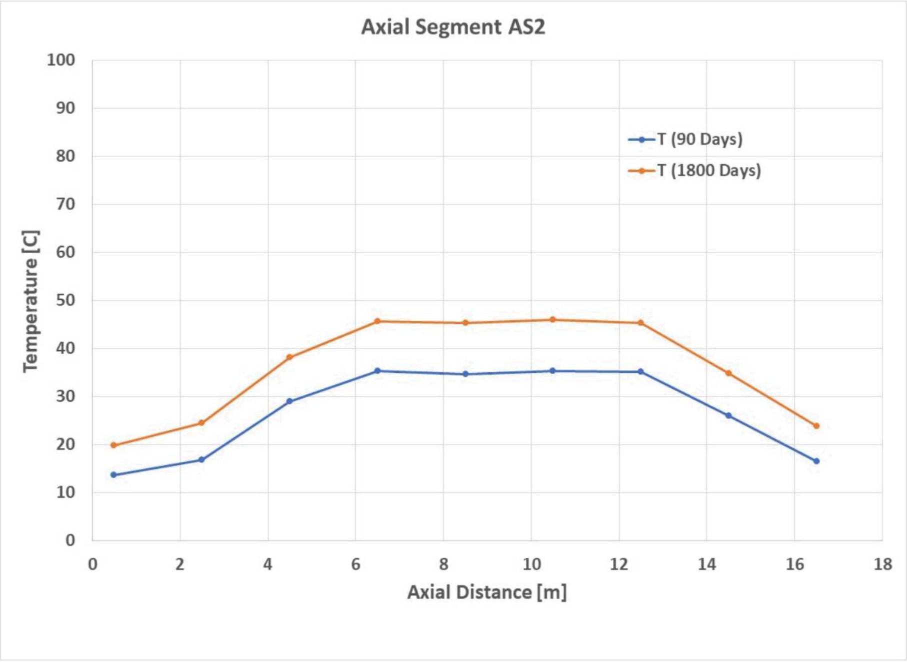




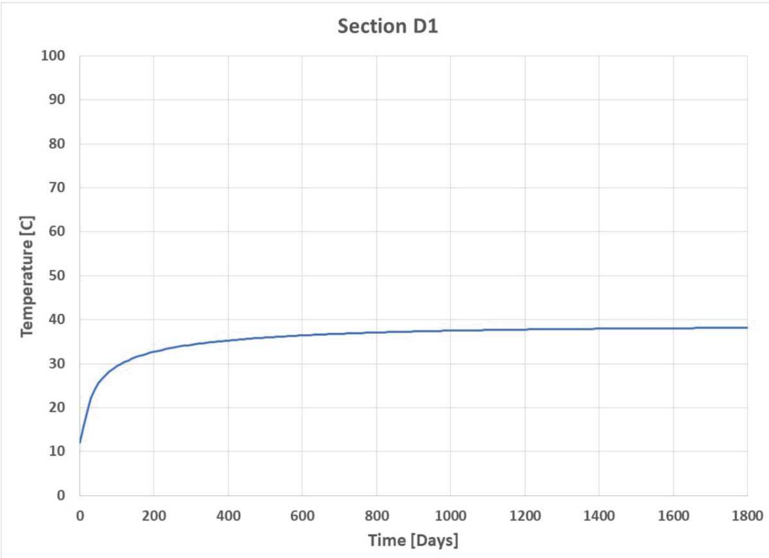
Distribution of Temperature: Axial Sections

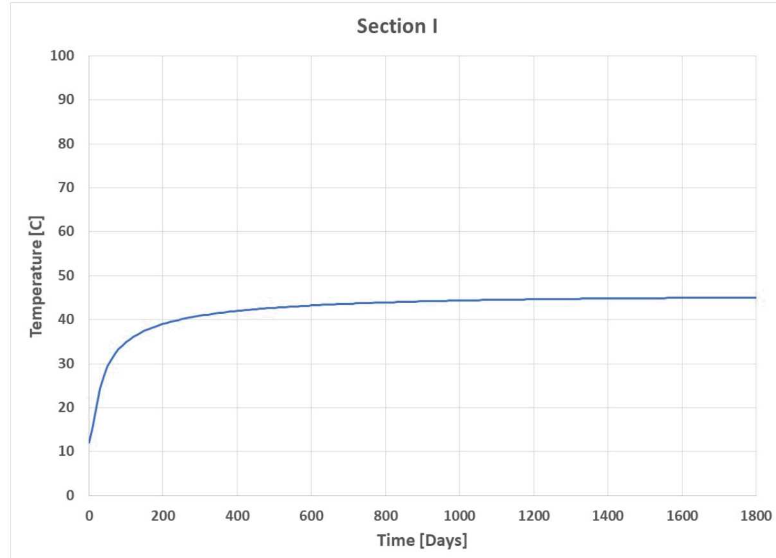


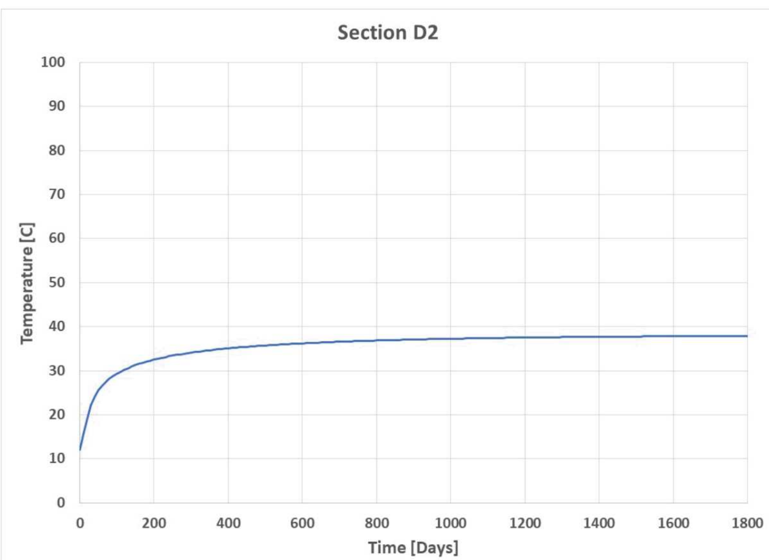


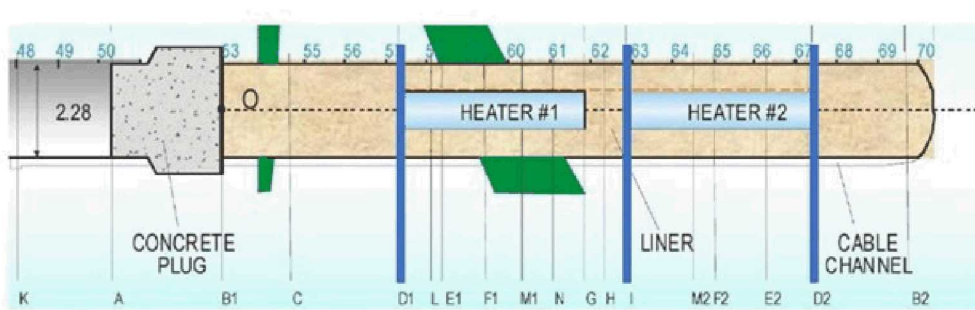


Evolution of Temperature

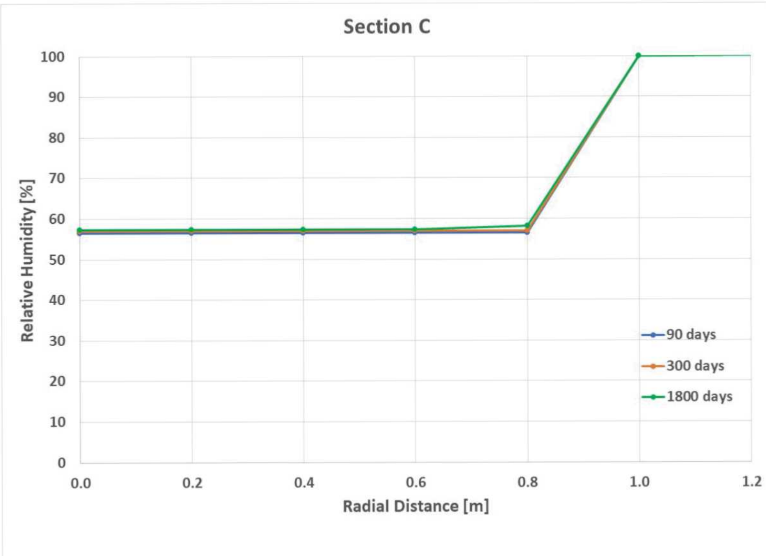


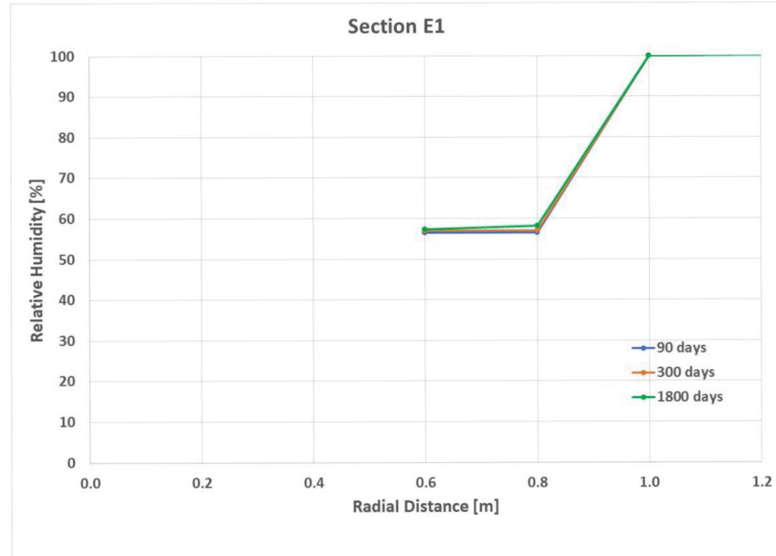


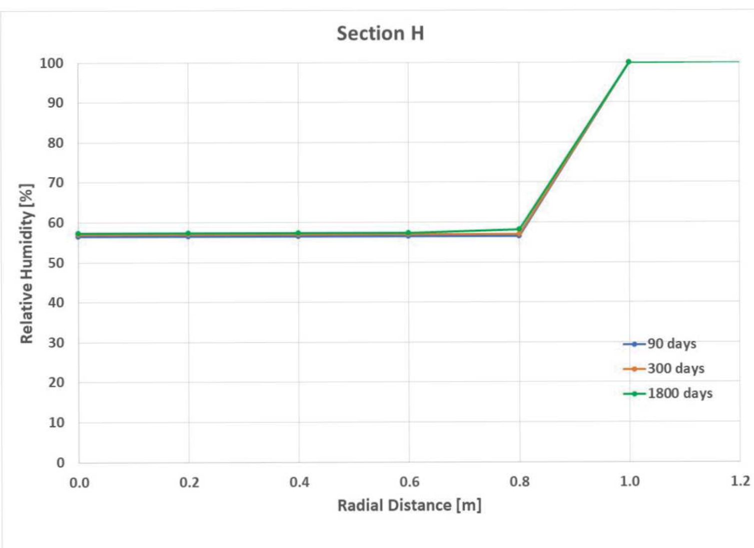


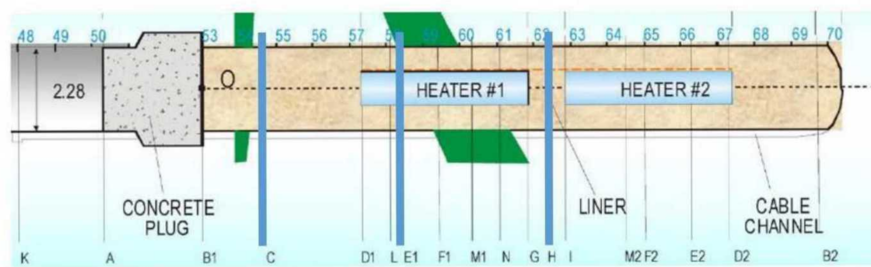


Distribution of Relative Humidity: Radial Sections

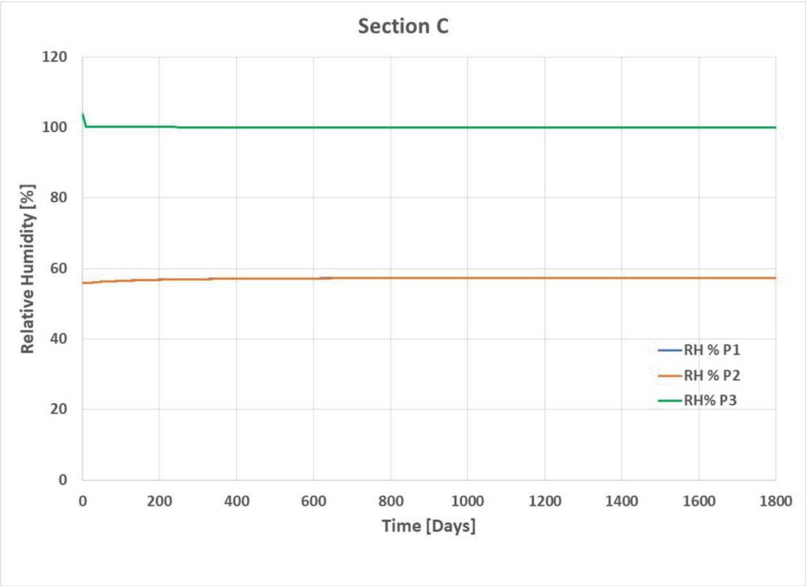


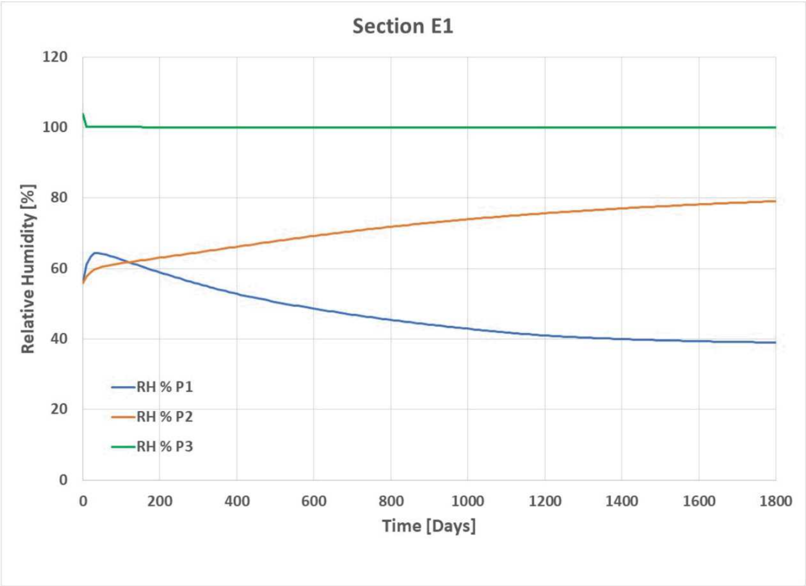


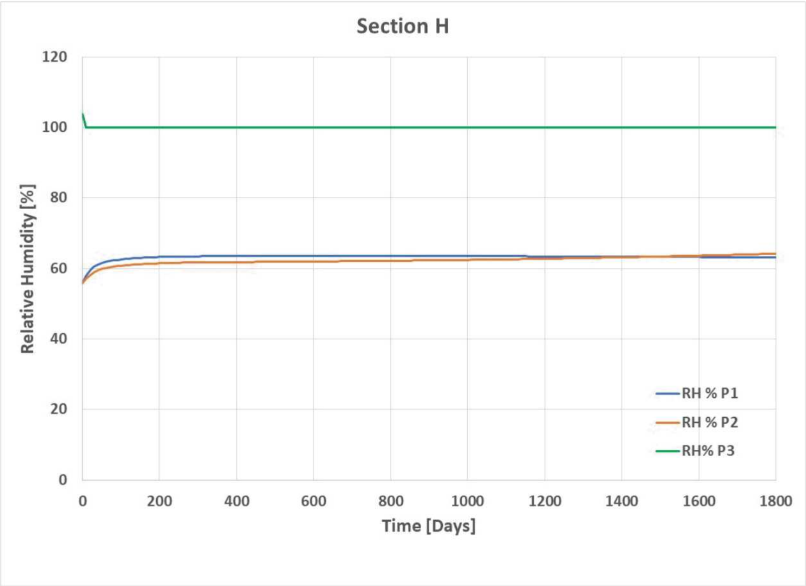


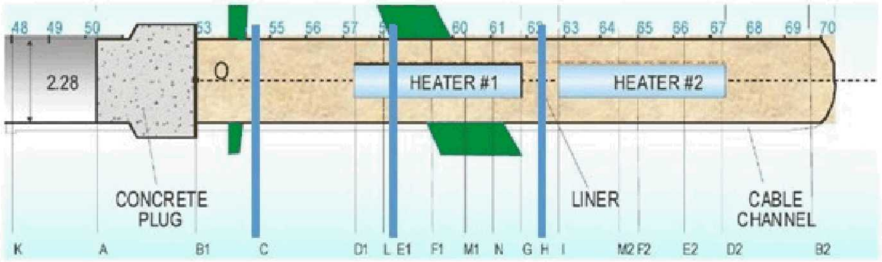


Evolutions of Relative Humidity







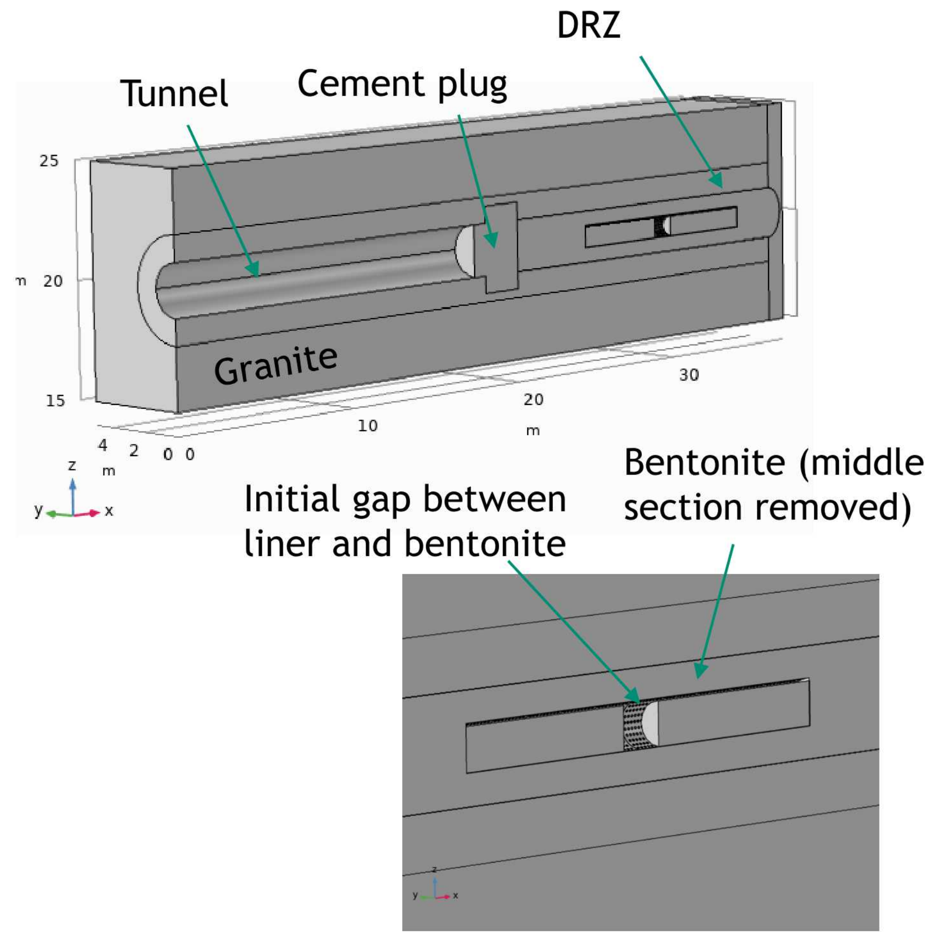


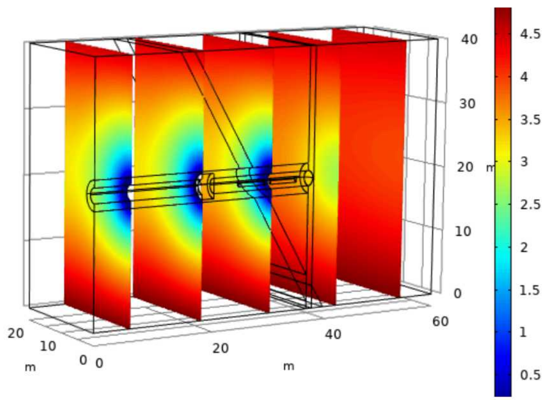
Summary of Stage 1 Simulations

- Results of heater outputs are about the same for Heater 1 but slightly lower for Heater 2.
- Temperature at heater surfaces are less than 100 C at early time and slightly over predicted at later time.
- Results of temperature in the bentonite buffer are fairly close to the experimental.
- Relative humidity is sensitive to various input parameters.

PART II: THM Model Exploring Effects of Gaps and Wetting Heterogeneity (in progress)

- Model gas transport and gap closure associated with swelling
- Computational Fluid Dynamics coupled with heat and compositional mass transport
- Explicit modeling of gaps, disturbed rock zone, and bentonite heterogeneity
- COMSOL Multiphysics™, attempting parameter estimation w/ cluster computing
- Biot poroelasticity in fractured granite and cement plug, extended Barcelona model in bentonite





COMSOL^{TM} Model Details

In tunnel, cement, bentonite, gaps:

- Variables in EBS are (T, P_{gas}, r_w)
- r_w is molar density of water component, used as "persistent variable"
- Ignore air dissolved in liquid phase

$$\frac{\partial \varphi \rho_w}{\partial t} = -\nabla \cdot \left(f_l^w + f_g^w\right) + Q^w$$

$$\rho_w = S_l \rho_l + (1 - S_l)\rho_v$$

$$\frac{\partial}{\partial t}\left(\varphi \rho_a S_g\right) = -\nabla \cdot f_g^a + Q^a$$

Gas flux modeled as Forscheimer flow (Navier-Stokes plus Brinkman equations):

In porous domains (with Forscheimer corrections):

$$\frac{1}{\varepsilon_p}\rho_g \frac{\partial \boldsymbol{u}}{\partial t} + \frac{1}{\varepsilon_p}\rho_g (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} \frac{1}{\varepsilon_p} = \nabla \cdot \left(-p_g \boldsymbol{I} + \boldsymbol{K}\right) - \left(\mu_g k^{-1} + \beta_F |\boldsymbol{u}| + \frac{Q_m}{\varepsilon_p^2}\right)\boldsymbol{u} + \boldsymbol{F} + \rho_{ag}\boldsymbol{g}$$

$$\boldsymbol{K} = \mu_g \frac{1}{\varepsilon_p}\left(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T\right) - \frac{2}{3}\mu_g \frac{1}{\varepsilon_p}(\nabla \cdot \boldsymbol{u})\boldsymbol{I} \qquad \varepsilon_p = \varphi S_g$$

In tunnel and initial barrier gaps (NS keeping inertial terms):

$$\rho_g \frac{\partial \boldsymbol{u}}{\partial t} + \rho_g (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = \nabla \cdot \left(-p_g \boldsymbol{I} + \boldsymbol{K}\right) + \boldsymbol{F} + \rho_g \boldsymbol{g}$$

$$\boldsymbol{K} = \mu_g\left(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T\right)$$

CONCLUSIONS

- Presented results of PFLOTRAN TH Modeling
- In progress: Coupling PFLOTRAN with DAKOTA for parameter estimation and uncertainty quantification
- CFD and FE THM modeling of FEBEX heater test examining effects of DRZs, gas flux in gaps, and effects of heterogeneous wetting and drying (in progress)