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Spent Fuel and Waste Science and Technology (SFWST)

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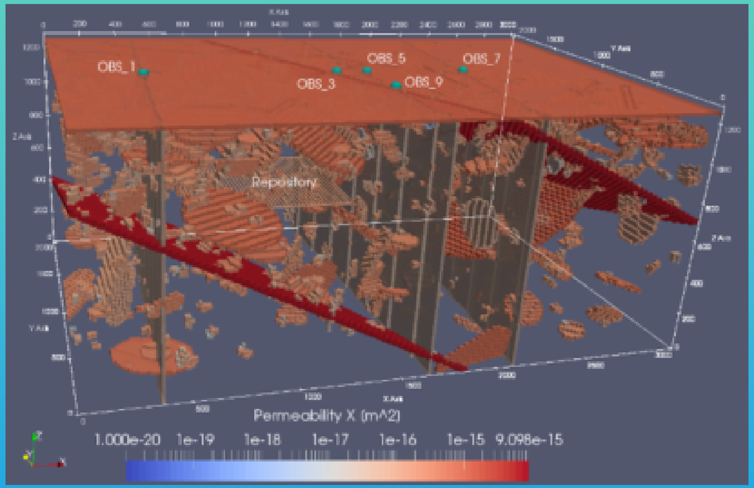

Analyzing Field Data from the Brine Availability Test in Salt (BATS): A High-resolution 3D Numerical Comparison between Voronoi and Cartesian Meshing

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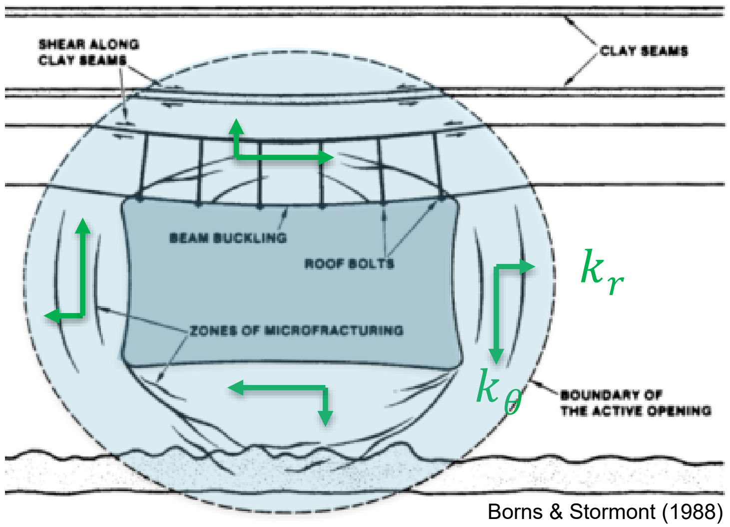
Why Salt for Radioactive Waste Disposal?

Alpine miner at WIPP

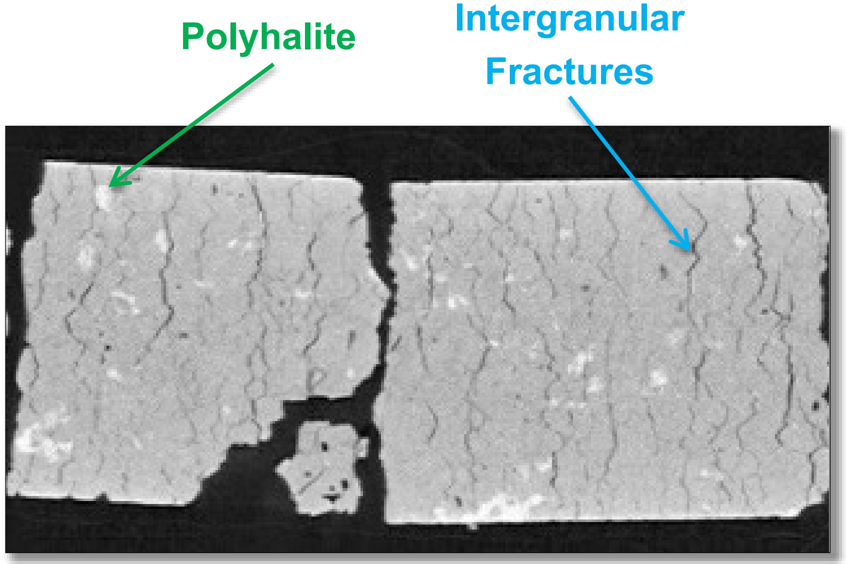
Cross-section view of Excavation Damaged Zone (EDZ) around drifts



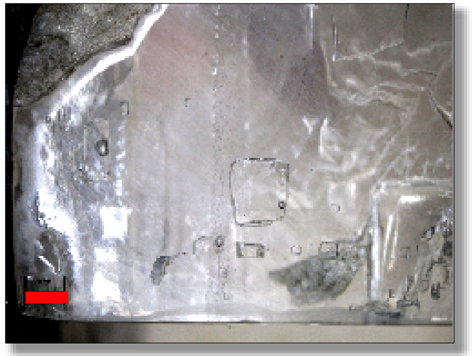
Borns & Stormont (1988)

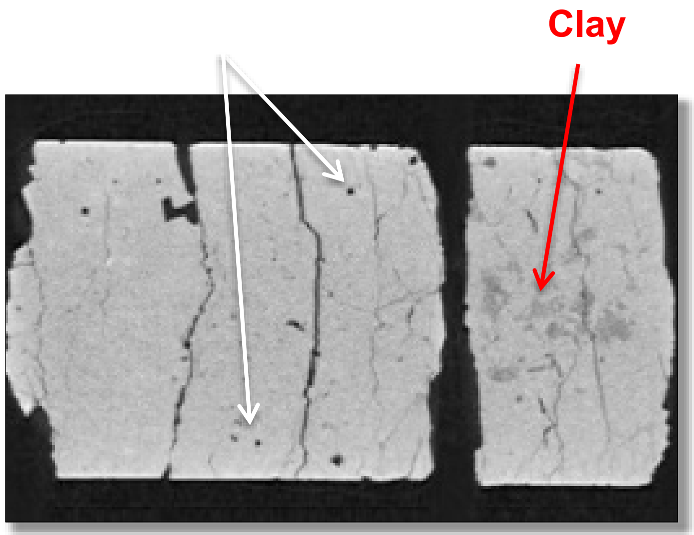
BACKGROUND ON BRINE IN SALT

- Water types in bedded salt
  1. Disseminated clay (< 5 vol-% total; ~25 vol-% brine)
  2. Intragranular brine (fluid inclusions; 1 – 2 vol-%)
  3. Hydrous minerals (e.g., polyhalite, bischofite, epsomite)
  4. Intergranular brine (between salt crystals; << 1 vol-%)



- These water types:
  - respond differently to heat & pressure
  - have varying chemical composition
  - differ in stable water isotope makeup



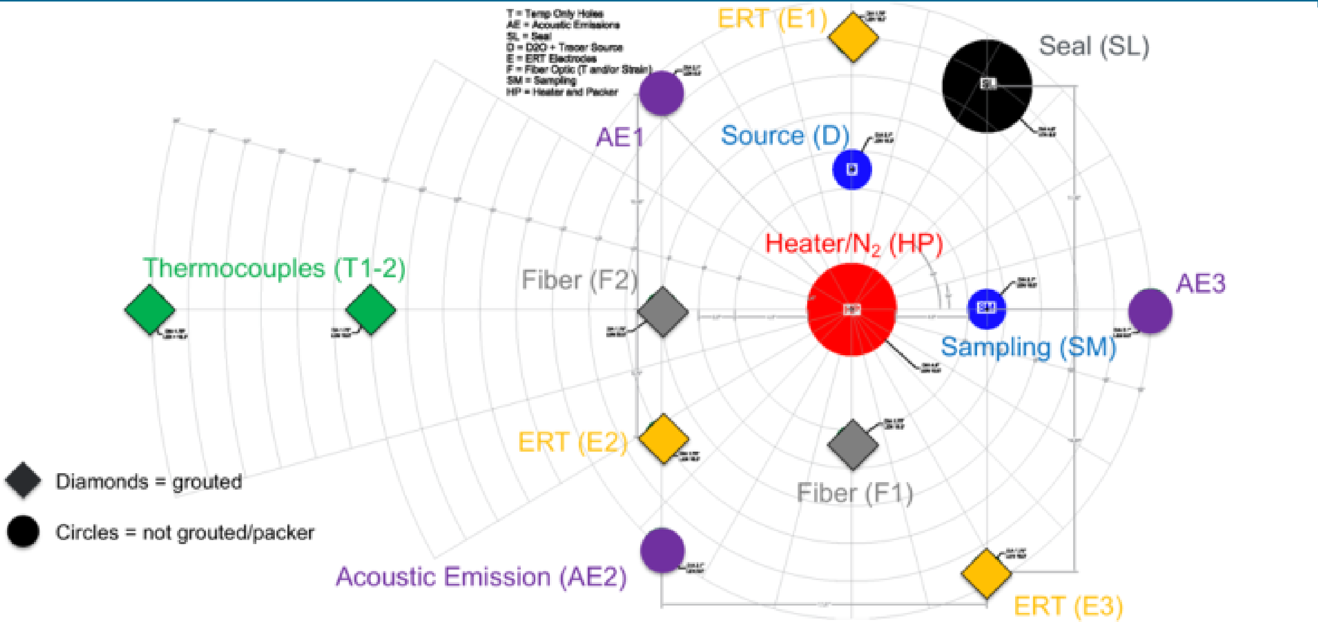


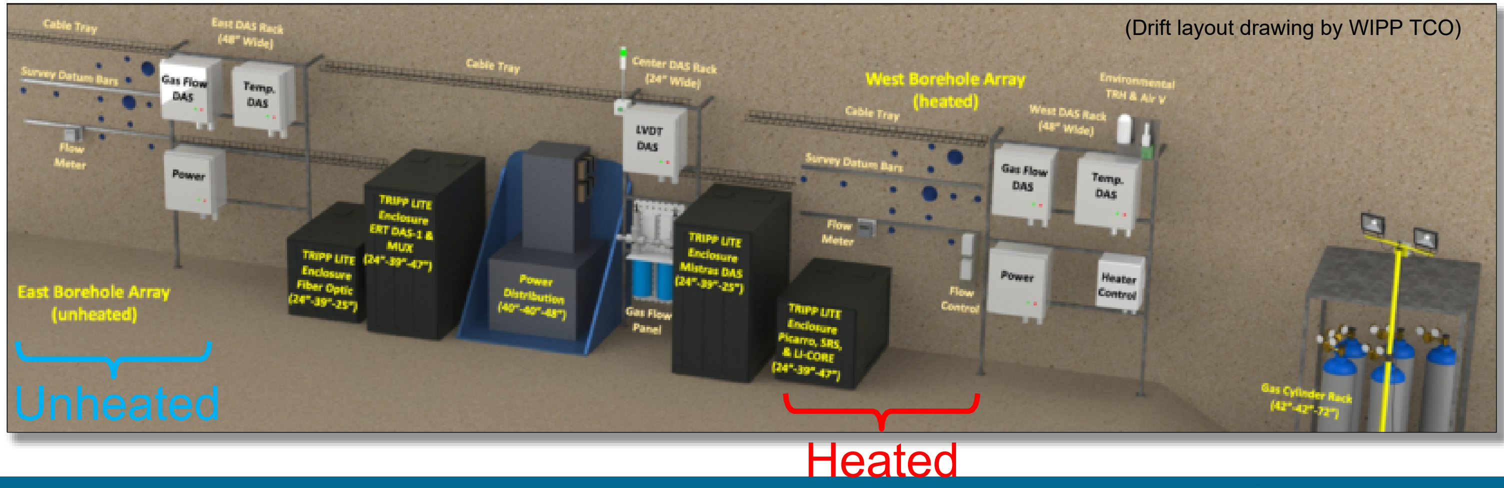
- EDZ increases intergranular $\phi \rightarrow$ primary flow path

Q: How do water types contribute to *Brine Availability?*

What is BATS?

- Brine Availability Test in Salt (BATS)
- Task E of DECOVALEX
- Salt heater experiment being conducted at the Waste Isolation Pilot Plant (WIPP)
- Investigating generic disposal concepts for heat-generating radioactive waste
- Focused on brine migration in salt

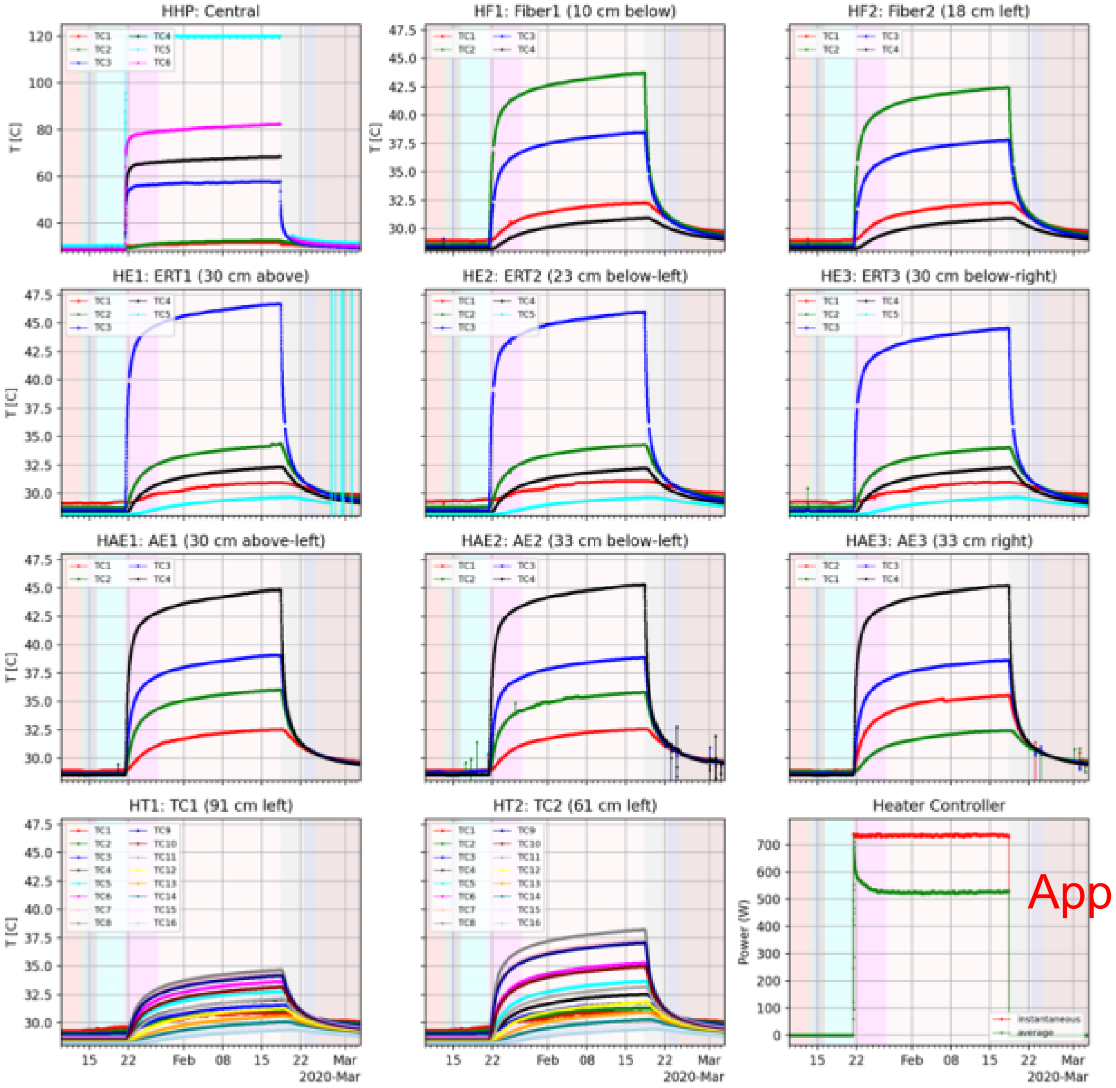




(Drift layout drawing by WIPP TCO)

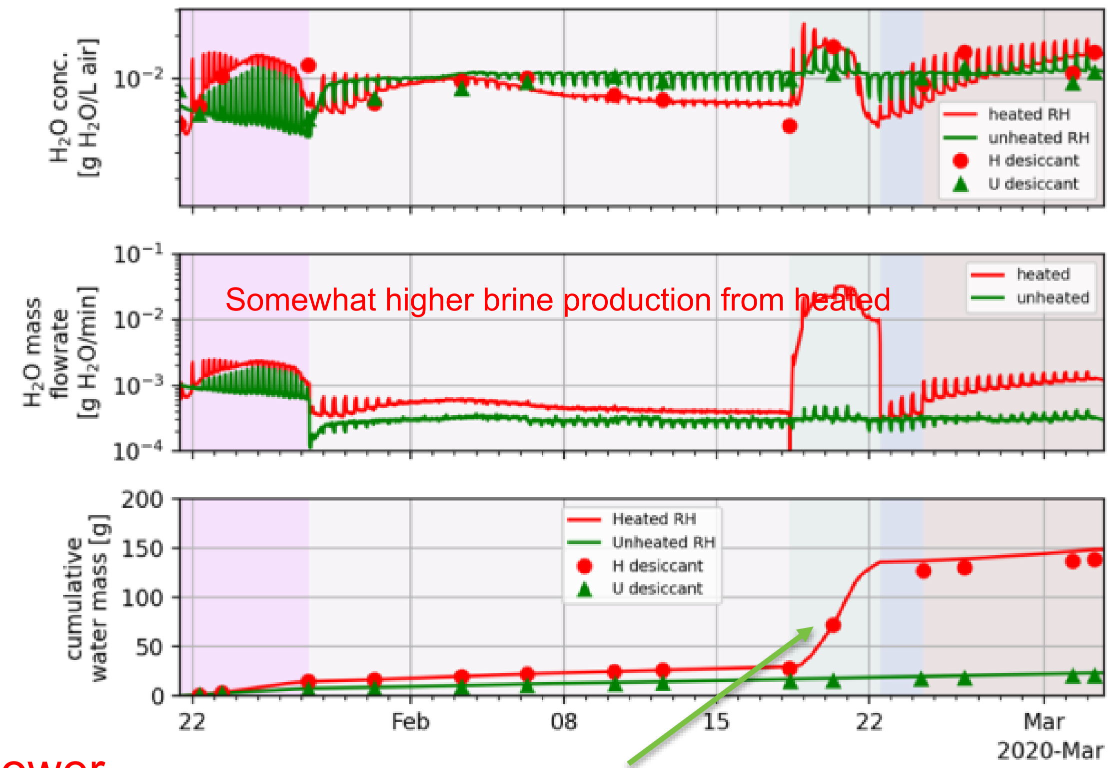
JANUARY-MARCH 2020 BATS 1A TEST DATA

Temperature data during BATS 1a



Applied power

Brine production data during BATS 1a

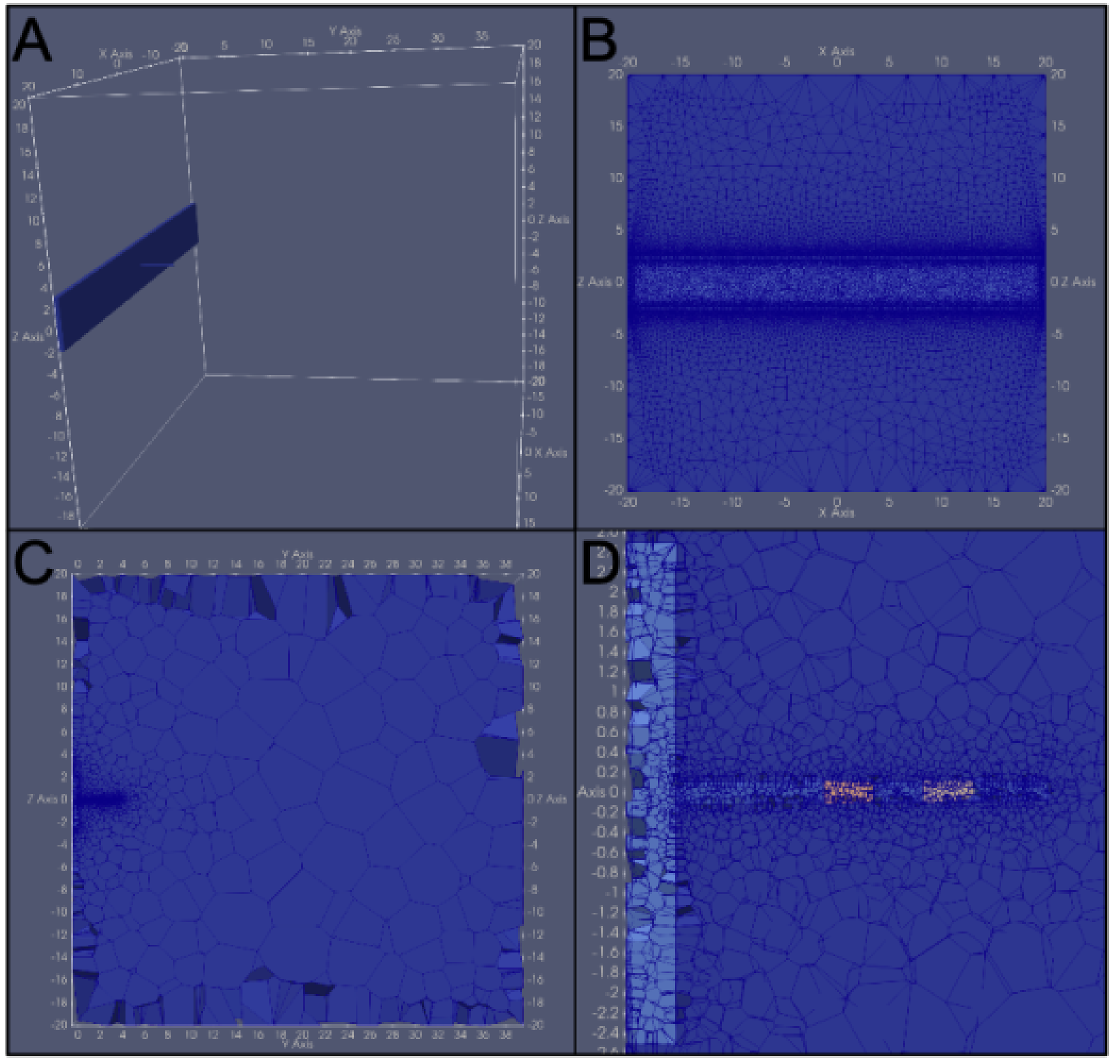


Brine inflow at heater shutdown

BATS 1a test and data summarized in Kuhlman et al. (2020)

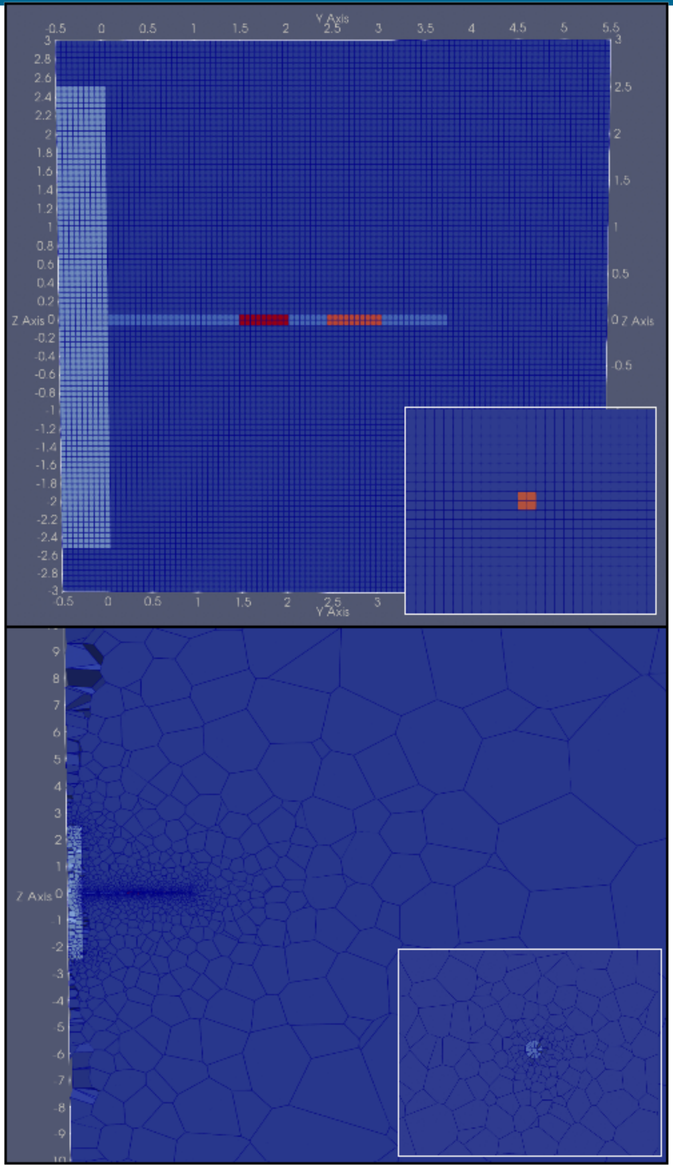
Modeling Approach - Meshing

- Voronoi vs. Cartesian
  - Vorocrust + LaGriT
  - High resolution near areas of interest
- Simplified geometry
  - Single heater borehole
- PFLOTRAN
- Excavation Damage Zone (EDZ)
  - Permeability and porosity decay away from excavations
- Model BATS 1a heating/cooling



Modeling Approach - Meshing

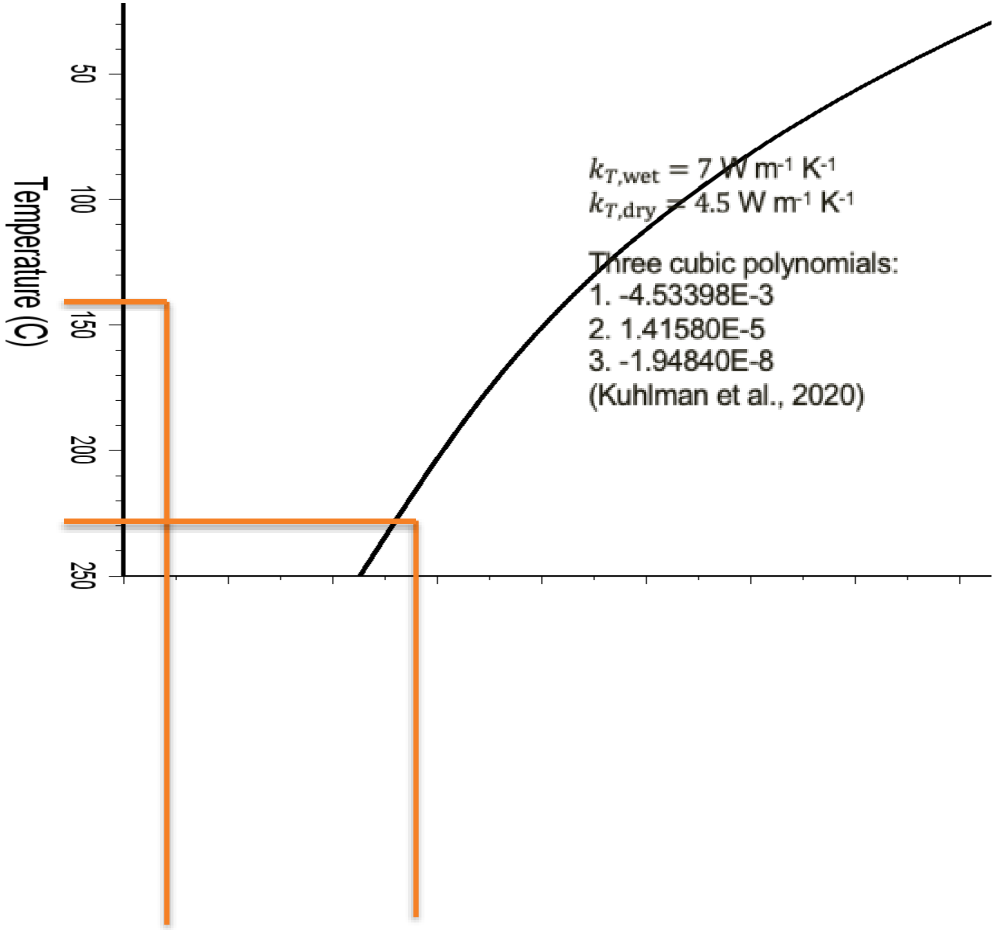
- Cartesian
  - 6m x 6m x 6m
    - 3cm x 3cm x 3cm
  - 1,000,000 grid cells
  - Computationally less complex
  - Potential grid orientation or geometric errors
- Voronoi
  - 40m x 40m x 40m
  - ~150,000 grid cells
  - Computationally difficult
    - Some grid cells have up to 36 connections
    - 869,761 total connections
    - Poorly conditioned residual matrix



Modeling Approach – Model Parameters

$$k_T(T,S_l) = k_{T,\text{dry}} + \sqrt{S_l}\left(k_{T,\text{wet}} - k_{T,\text{dry}}\right)[1 + \beta_0 T + \beta_1 T^2 + \beta_3 T^3]$$

Reservoir Parameters		Mualem – Van Genuchten Relative Permeability		Van Genuchten Capillary pressure	
Initial Temperature (°C)	29.5	λ	0.6	λ	0.6
Permeability (m^2)	Varies	S_{lr}	0.2	S_{lr}	0.2
Porosity (-)	Varies	S_{ls}	1	α (Pa^{-1})	10^{-6}
Thermal Conductivity W/m°C	Varies	S_{gr}	0.2	S_{ls}	0.999
Heat Capacity J/kg°C	620				



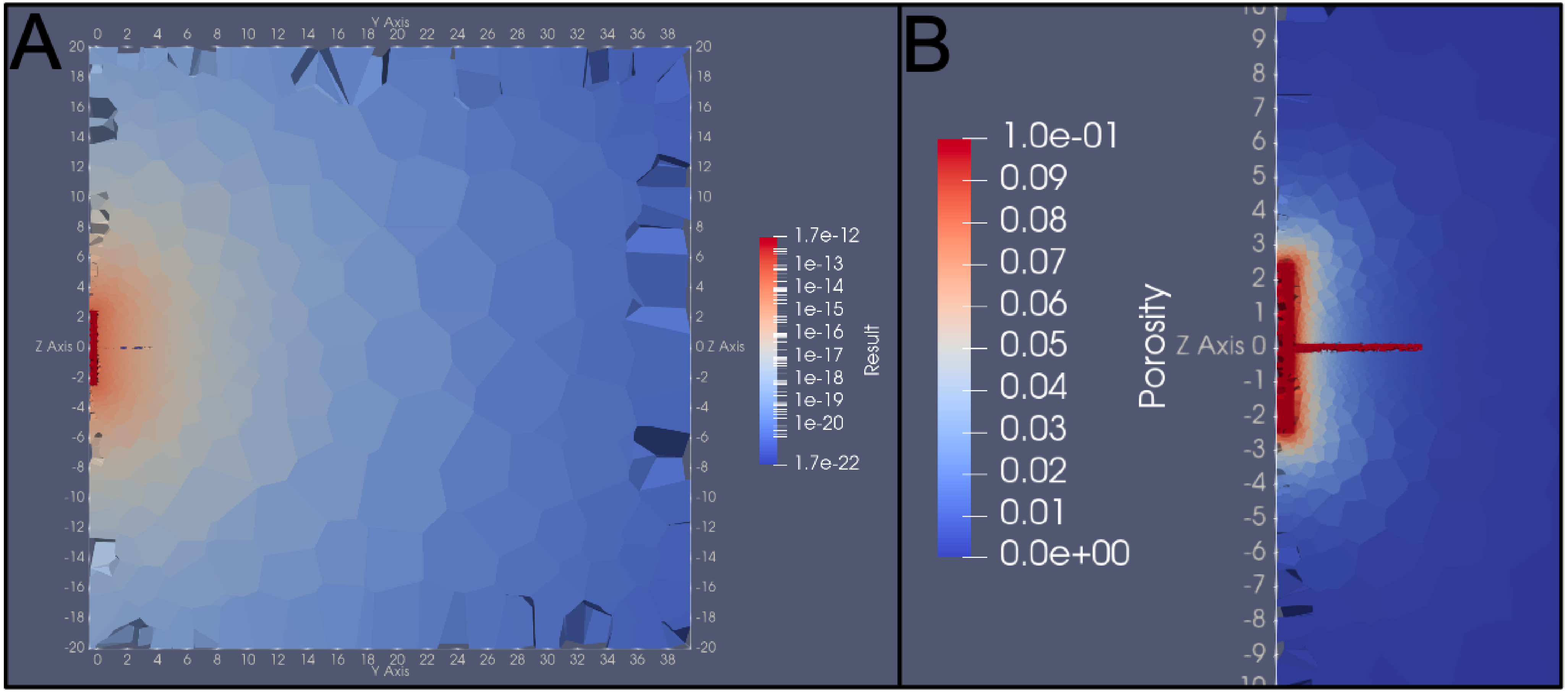
Modeling Approach – Permeability/Porosity Decay - Voronoi

Permeability Decay

$$k = k_0 \left[\frac{r}{r_0}\right]^{-5.5}$$

Porosity Decay

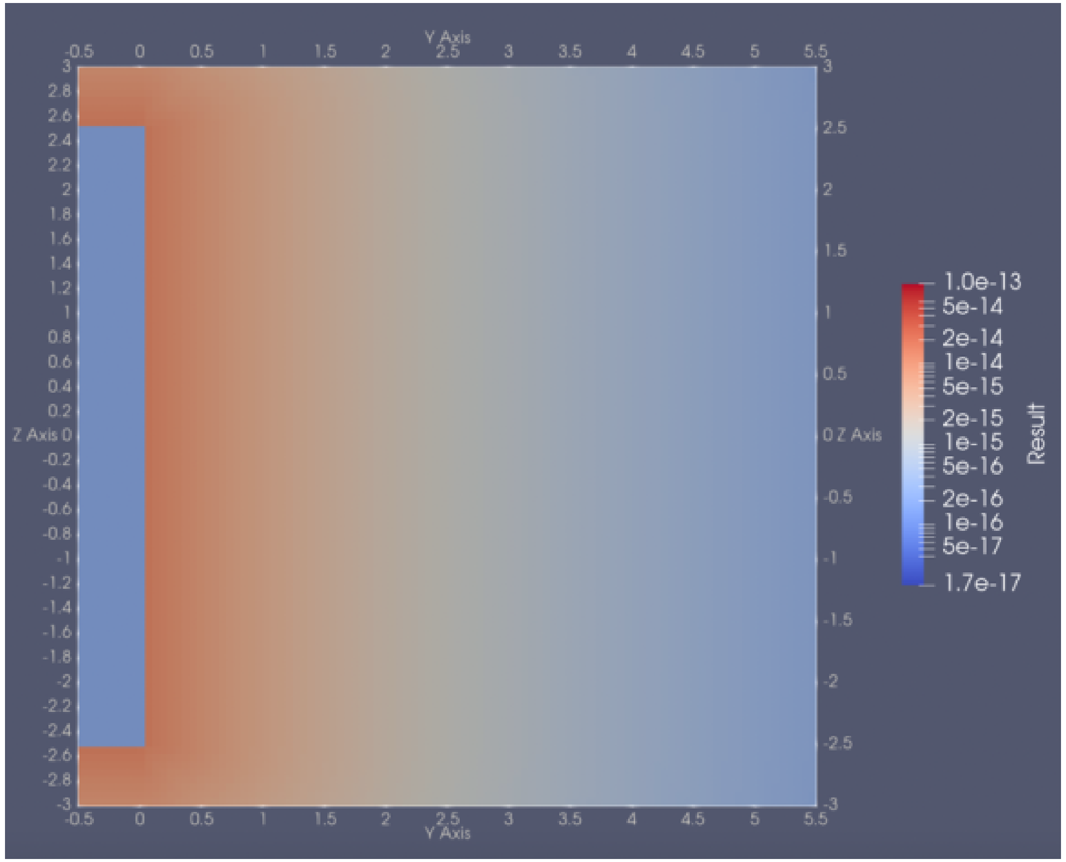
$$\theta = \theta_0 \left[\frac{r}{r_0}\right]^{-3.5}$$



Modeling Approach – Permeability/Porosity Decay - Cartesian

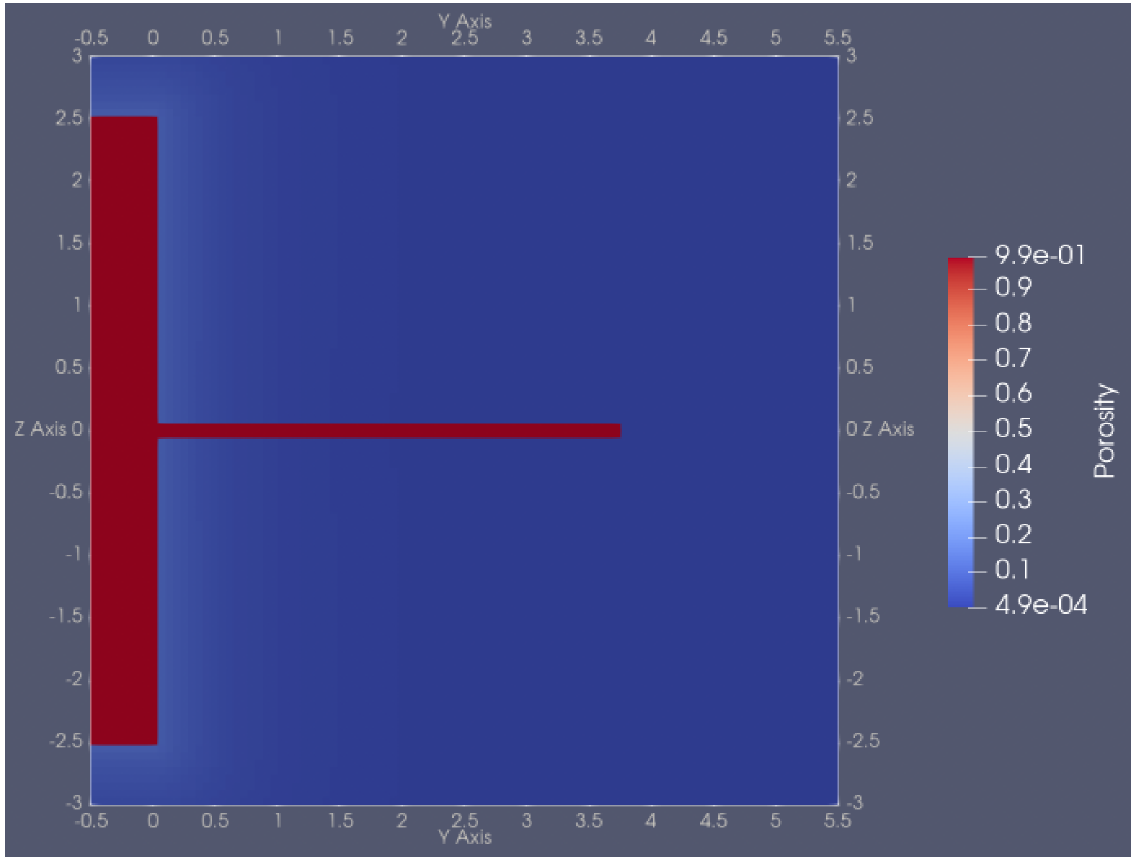
Permeability Decay

$$k = k_0 \left[\frac{r}{r_0}\right]^{-5.5}$$



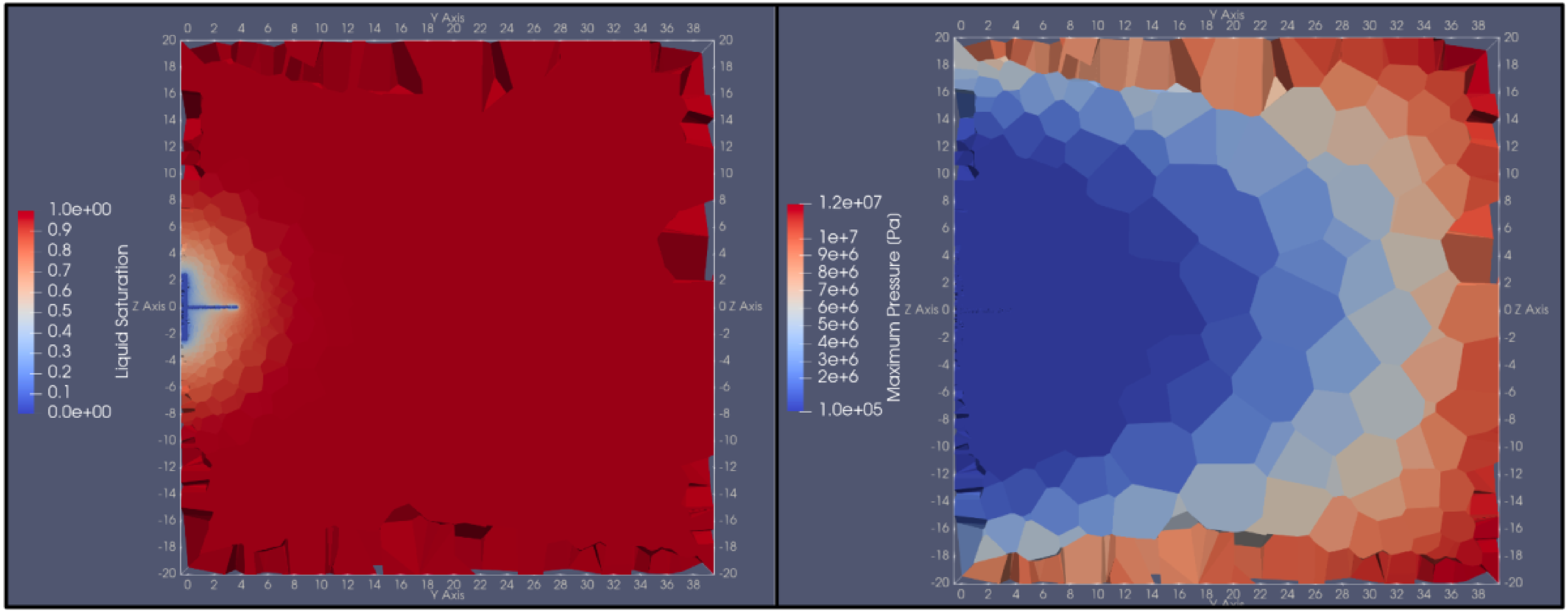
Porosity Decay

$$\theta = \theta_0 \left[\frac{r}{r_0}\right]^{-3.5}$$



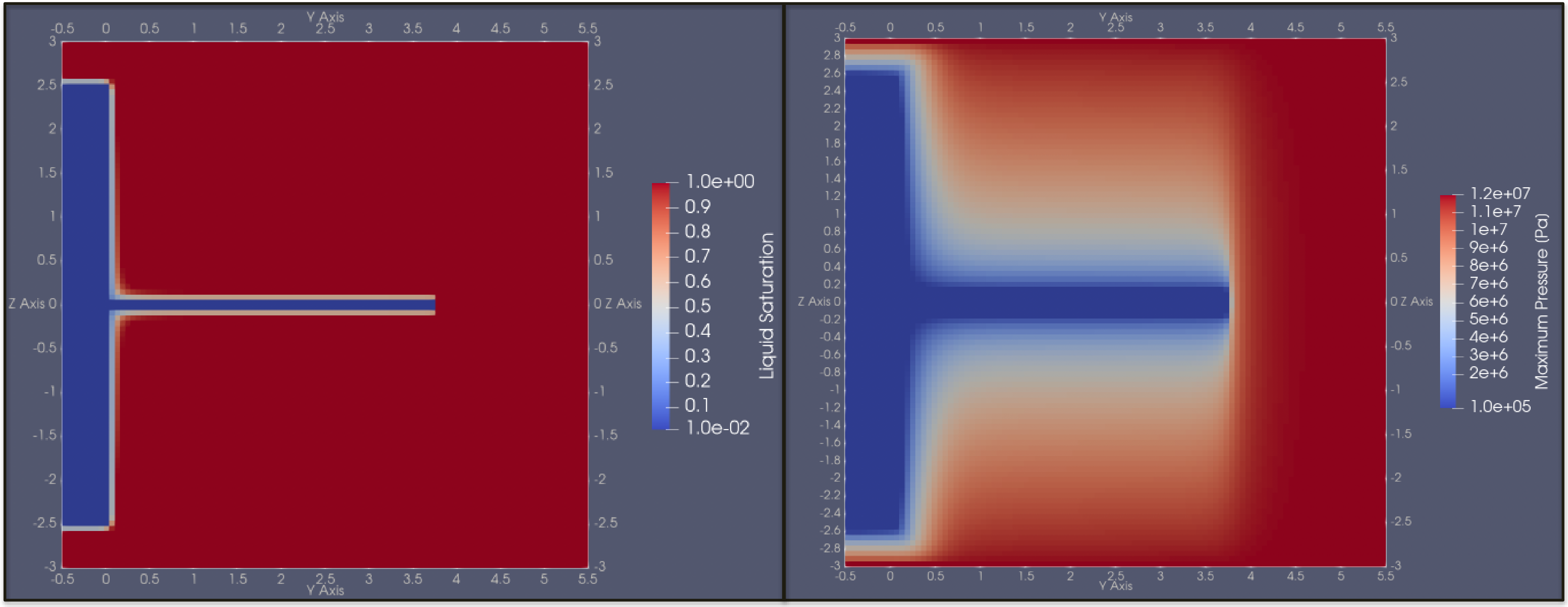
INITIAL CONDITIONS - VORONOI

- Pressure and saturation equilibrated for ~180 days before heating/cooling cycle



Initial Conditions - Cartesian

- Pressure and saturation equilibrated for ~180 days before heating/cooling cycle

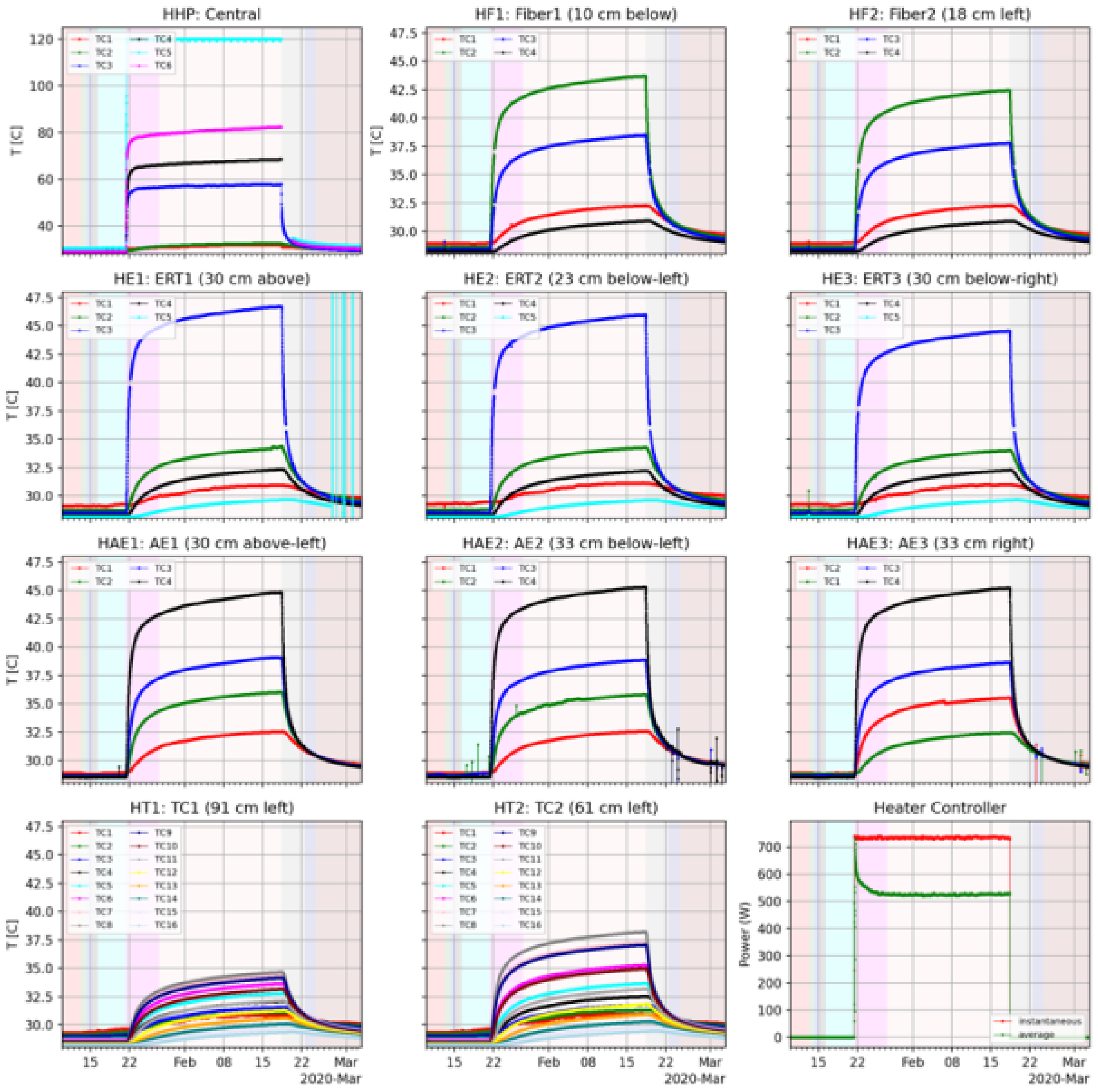


BATS 1A TEST – SIMULATION COMPARISON

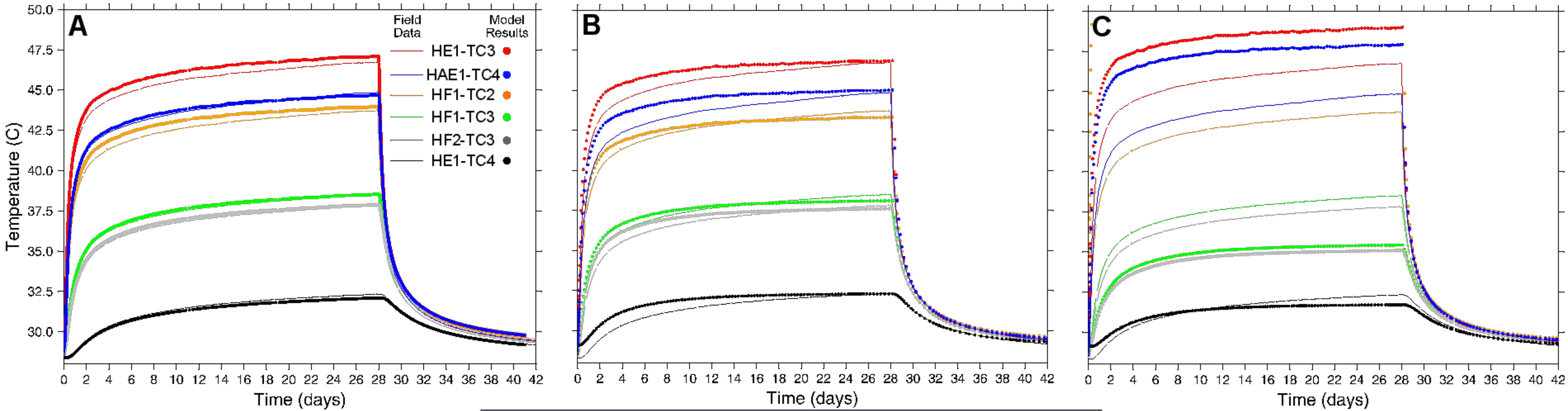
- 41 total days
  - 28 days of heating
  - 13 days of cooling
- Matching heater power from field test
- 6 thermocouples are chosen for comparison

How closely can each mesh match the measured temperature from the field experiment?

Temperature data during BATS 1a



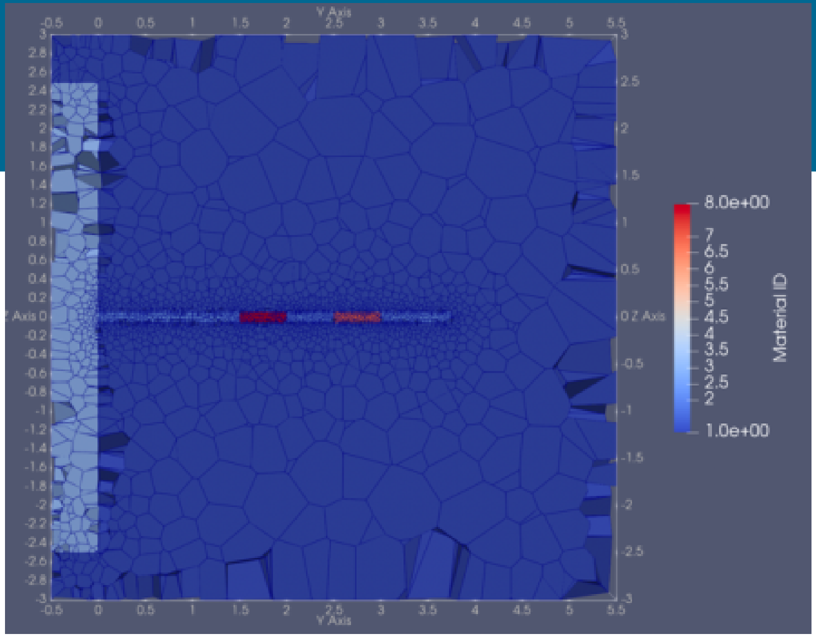
Temperature Results Comparison

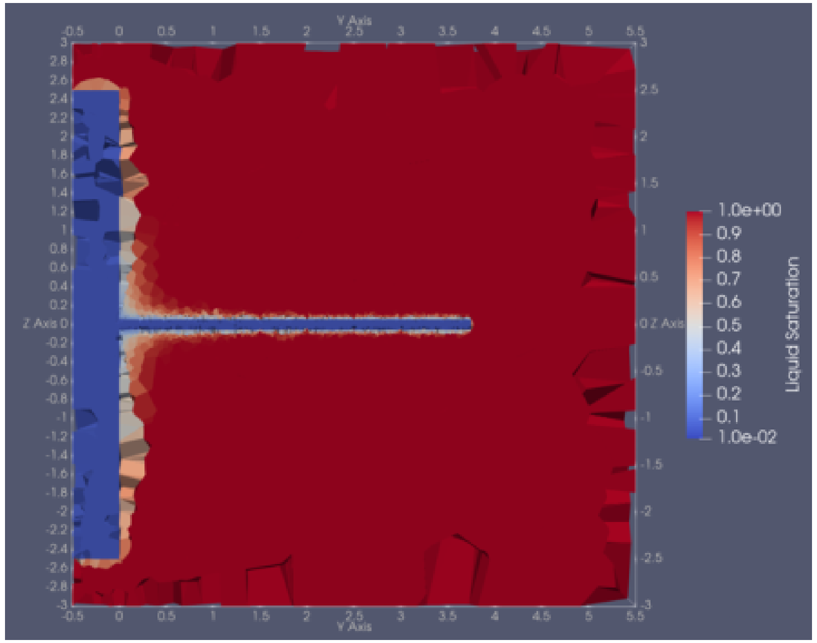


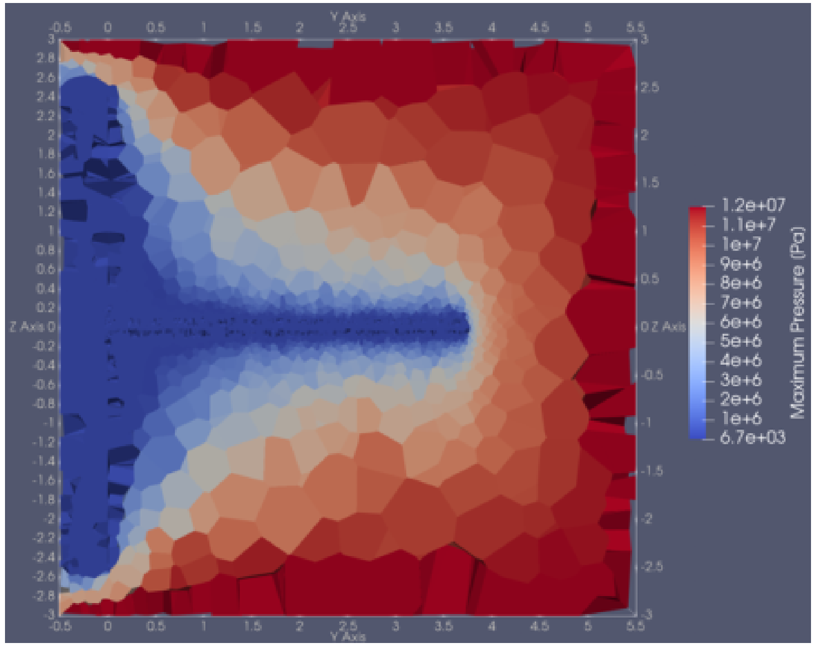
	Distance from measured location (m)		
	Voronoi	Cartesian	Cartesian Temperature Matching
HF1-2	0.00	0.03	0.07
HF1-3	0.00	0.03	0.07
HF2-3	0.01	0.02	0.08
HE1-3	0.00	0.02	0.15
HE1-4	0.00	0.11	0.11
HAE1-4	0.00	0.04	0.16

Simplified Comparison

- Fully liquid-saturated
- Straight borehole
- Same size domain
- No temperature dependent thermal conductivity
- No graded permeability/porosity
- Varied Voronoi mesh resolution
  - 20,000 – 80,000 grid cells
- Stepped heater test

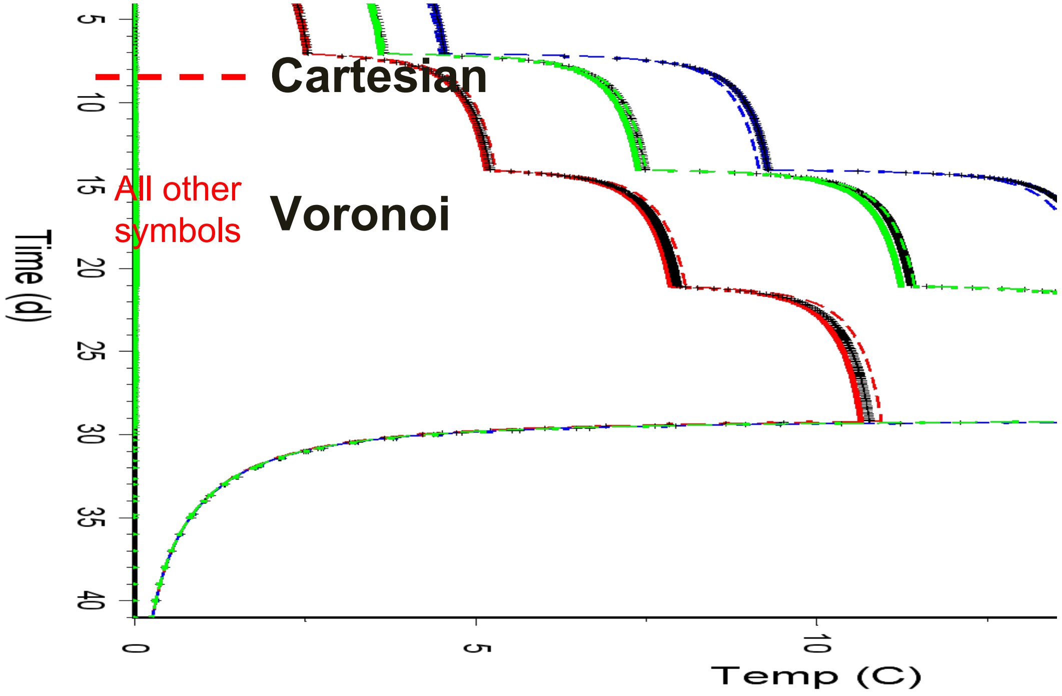






Simplified Comparison

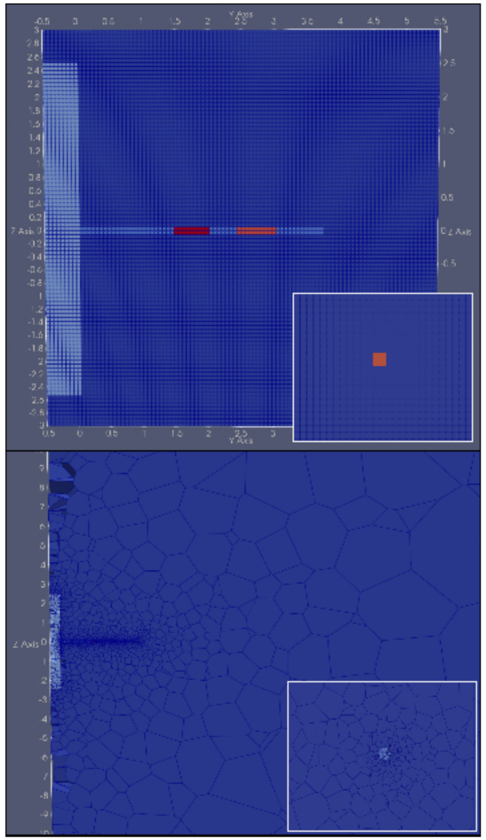
- Fully liquid-saturated
- Straight borehole
- Same size domain
- No temperature dependent thermal conductivity
- No graded permeability/porosity
- Varied Voronoi mesh resolution
  - 20,000 – 60,000 grid cells
- Stepped heater test
- 3 monitoring locations
  - X – 0.15m
  - Y – 0.45m
  - Z – 0.3m



Conclusions & Future Work

- Voronoi mesh provides a better match to temperature measured in the field
  - Fairly complex geometry and heterogeneity
- Errors in geometry lead to errors in temperature matching for cartesian mesh
- Voronoi meshes are challenging to create and work with
  - Voronoi meshes aren't always the correct choice
  - better solvers and pre-conditioners?

	Grid Cells	Required Time Steps	Simulation Time (min)
Voronoi	143,463	6586	30.7
Cartesian	1,000,000	277	15.2



Future Work

- Additional comparisons need to be made
  - How does brine inflow compare between the meshes?
  - Increase cartesian domain size
    - 10,000,000 grid cells?
- How would a flexed hexahedral mesh compare?

Thank you!