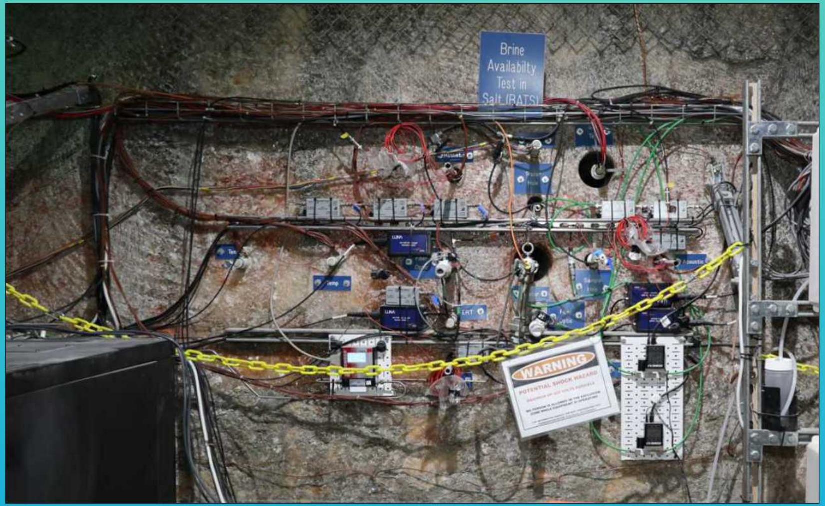
U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

Spent Fuel and Waste Science and Technology (SFWST)

SAND2020-5775PE



DECOVALEX-2023 Task E (BATS) Kickoff

DECOVALEX-2023 Task E Virtual Kickoff Meeting

Wednesday June 10, 2020

Kristopher L. Kuhlman

Sandia National Laboratories

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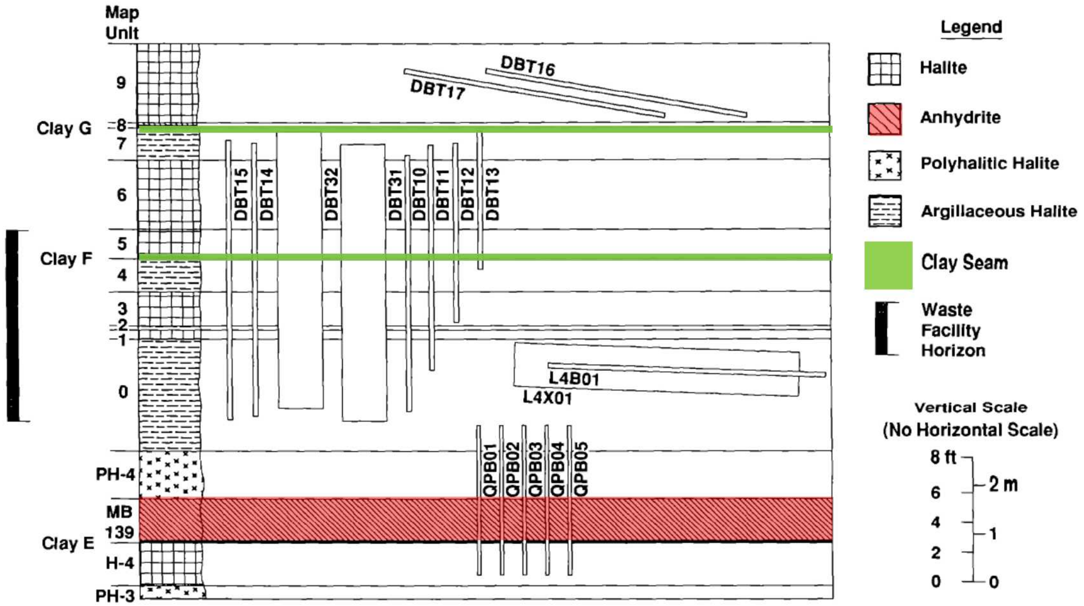
Task E Kickoff Meeting Outline

- First step (Step 0) of Task E
  1. Small-Scale Brine Inflow Test (unheated brine migration)
  2. Brine Availability Test in Salt temperature response (heat conduction)
  3. Sensitivity analysis
  4. Uncertainty quantification
- High-level review of all steps
- Introduction of teams
  - Who is participating / background & interests
  - Which modeling tools
  - Experience / knowledge about salt & WIPP
  - Thoughts on good/bad aspects of Task E

BATS heated array

1. WIPP Small-Scale Brine Inflow Test (1987-1992)

- Monitored brine inflow to 17 unheated boreholes
- Immediately after drilling (~new drifts)
- Weekly brine inflow mass
- Used in INTRAVAL comparison
- Effects of stratigraphy

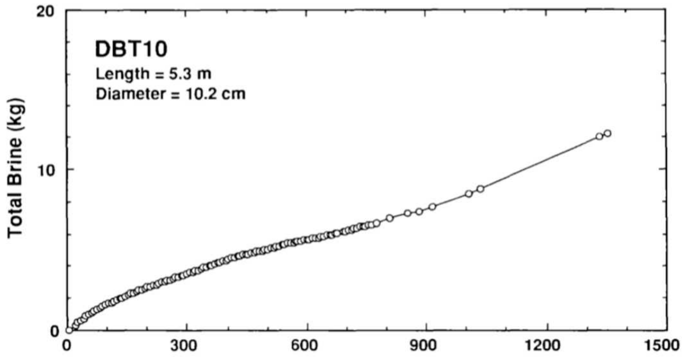


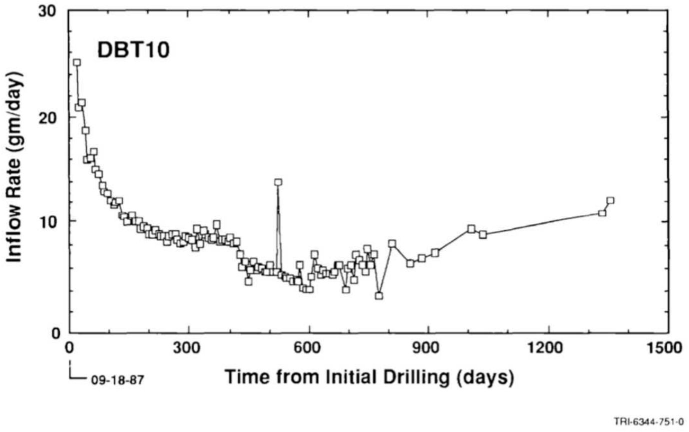
MB = marker bed

PH = polyhalite

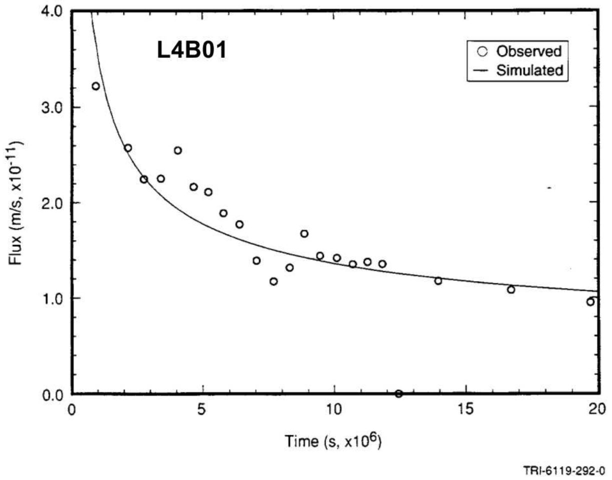
Finley et al. (1992)

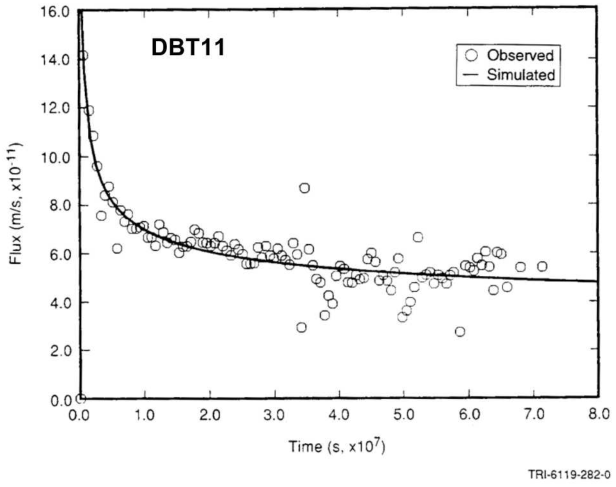
Finley et al. (1992)





(Beauheim et al., 1997)



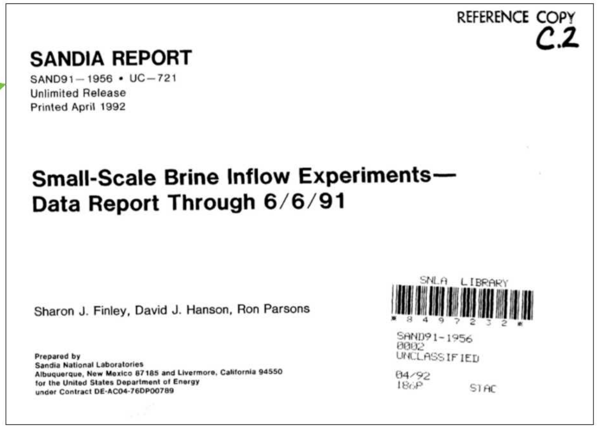


1. WIPP Small-Scale Brine Inflow Test (SSBIT)

- .pdf reports and .xlsx spreadsheets in D2023 fileshare

  `D2023 Team > Task E > Data > Finley-etal-1992`

- Data details presented in *Finley et al. (1992)*
  - Data from Appendix E copied into spreadsheets
  - <u>*Only simulate early monotonically decreasing brine production*</u>
- INTRAVAL project, Phase 2 (1990-1997)
  - Reported in *Beauheim et al. (1997)*
    - Dutch, French & US teams analyzed SSBIT data
    - ***Q:*** *Can Darcy's Law be used to predict brine flow?*
  - McTigue (1993) "Permeability and Hydraulic Diffusivity …"
    - Analytical solutions (unheated) fit to SSBIT
    - Details SSBIT "data cleanup" efforts (§ 6.2.1)
  - Webb (1992) "Brine Inflow Sensitivity Study …"
    - 1D simulations using TOUGH2
    - Single-phase vs. two-phase flow & uniform vs. intact + DRZ



SANDIA REPORT
SAND91—1956 • UC—721
Unlimited Release
Printed April 1992

Small-Scale Brine Inflow Experiments—Data Report Through 6/6/91

Sharon J. Finley, David J. Hanson, Ron Parsons

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550
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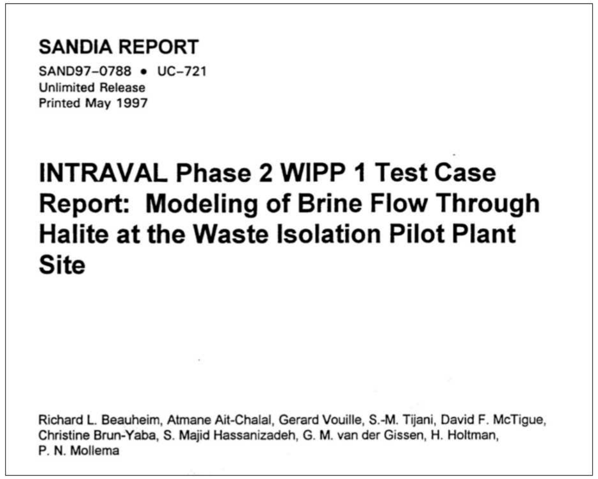
under Contract DE-AC04-76DP00789


SANDIA REPORT
SAND97–0788 • UC–721
Unlimited Release
Printed May 1997

INTRAVAL Phase 2 WIPP 1 Test Case Report: Modeling of Brine Flow Through Halite at the Waste Isolation Pilot Plant Site

Richard L. Beauheim, Atmane Ait-Chalal, Gerard Vouille, S.-M. Tijani, David F. McTigue, Christine Brun-Yaba, S. Majid Hassanizadeh, G. M. van der Gissen, H. Holtman, P. N. Mollema

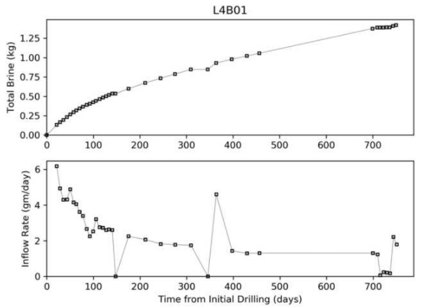
1. WIPP Small-Scale Brine Inflow Test (SSBIT)

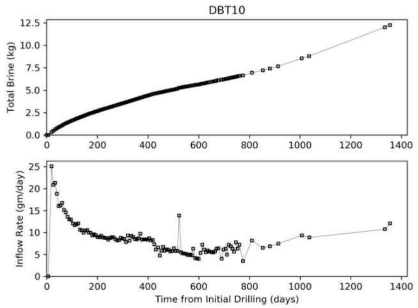
- <u>Comparison:</u> Simulate inflow rate to boreholes
  - *Only fit to monotonically decreasing brine production*
  - *Include boreholes L4B01, DBT10 & DBT11* (+ others if you want)

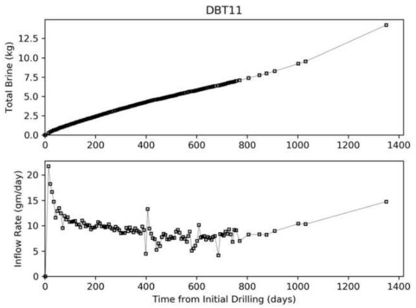
- Predictive H[1] models:
  - Simple or include geometrical (borehole extent + room DRZ) complexity
  - Uniform parameters or include geological complexity

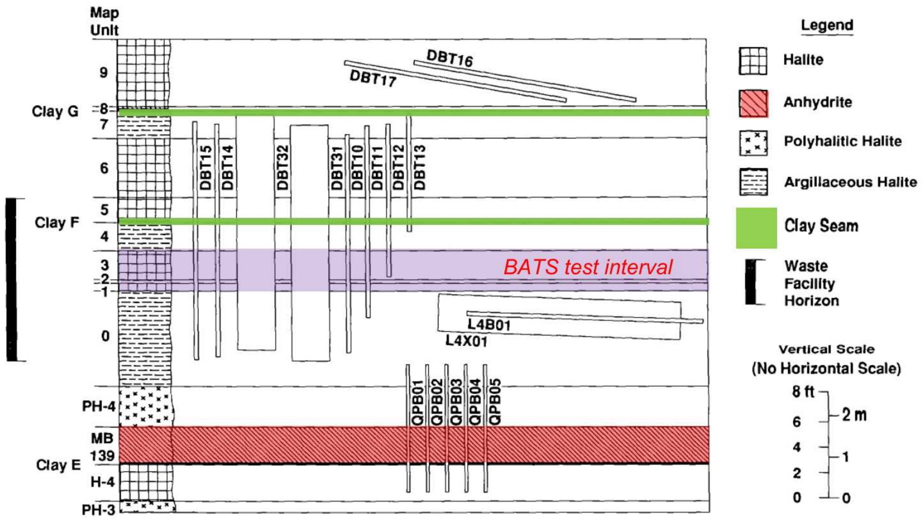
Horizontal borehole in Map Unit 0

Vertical boreholes that cross Clay F

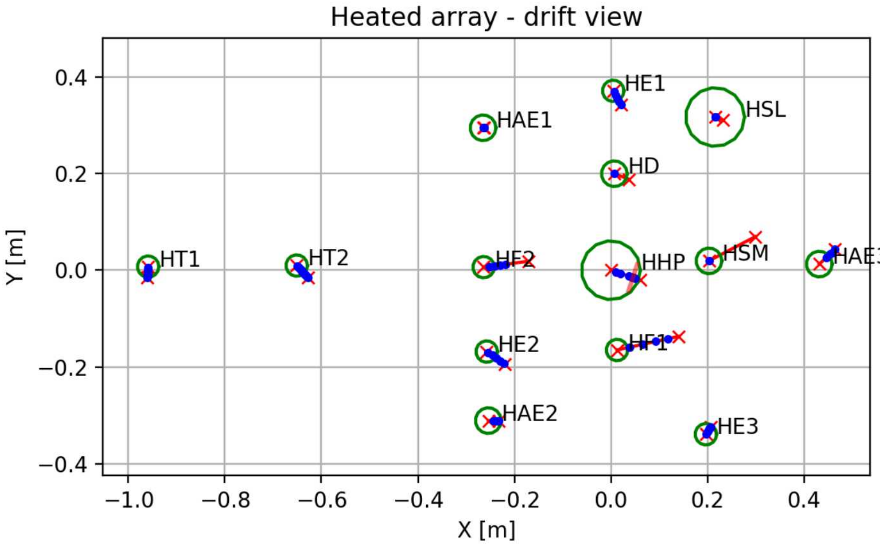


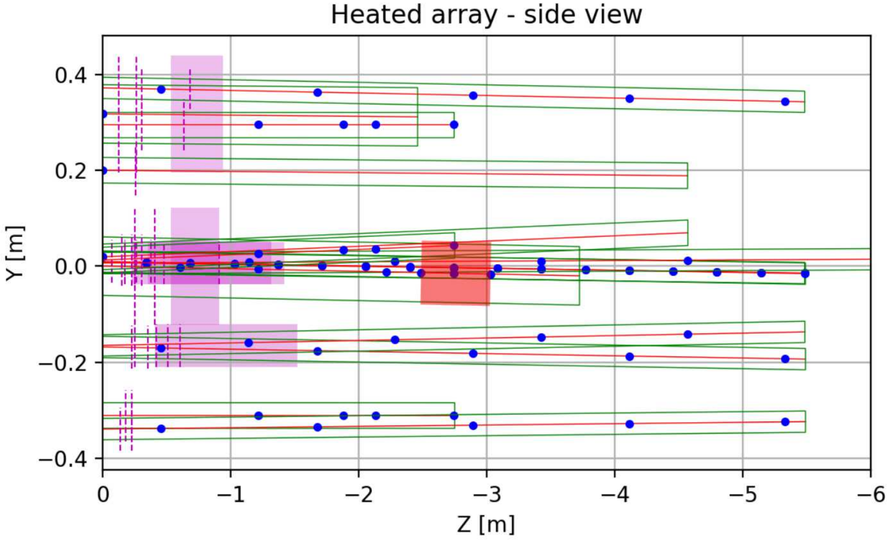


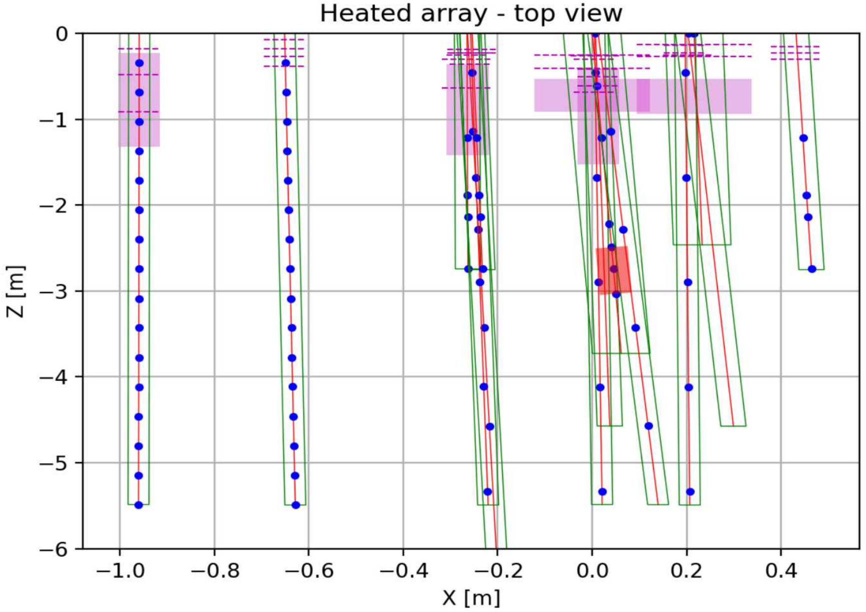




2. Brine Availability Test in Salt (BATS) As-Built





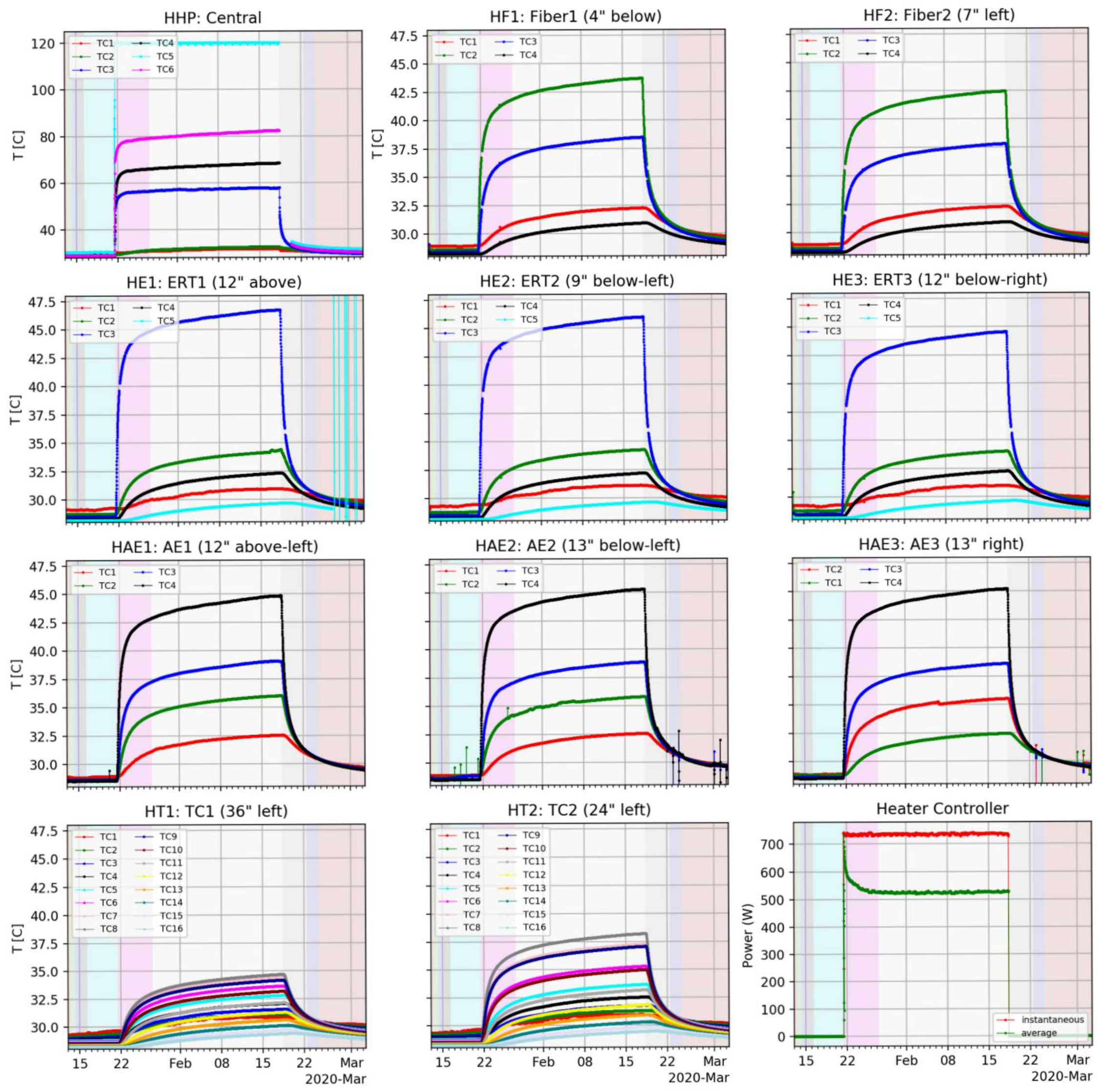


- Heated array as-built
- Drilled Feb-Apr 2019
- Side & top views show
  - thermocouples (blue dots)
  - Heated interval (red box)
  - Fractures/damaged zone (purple)

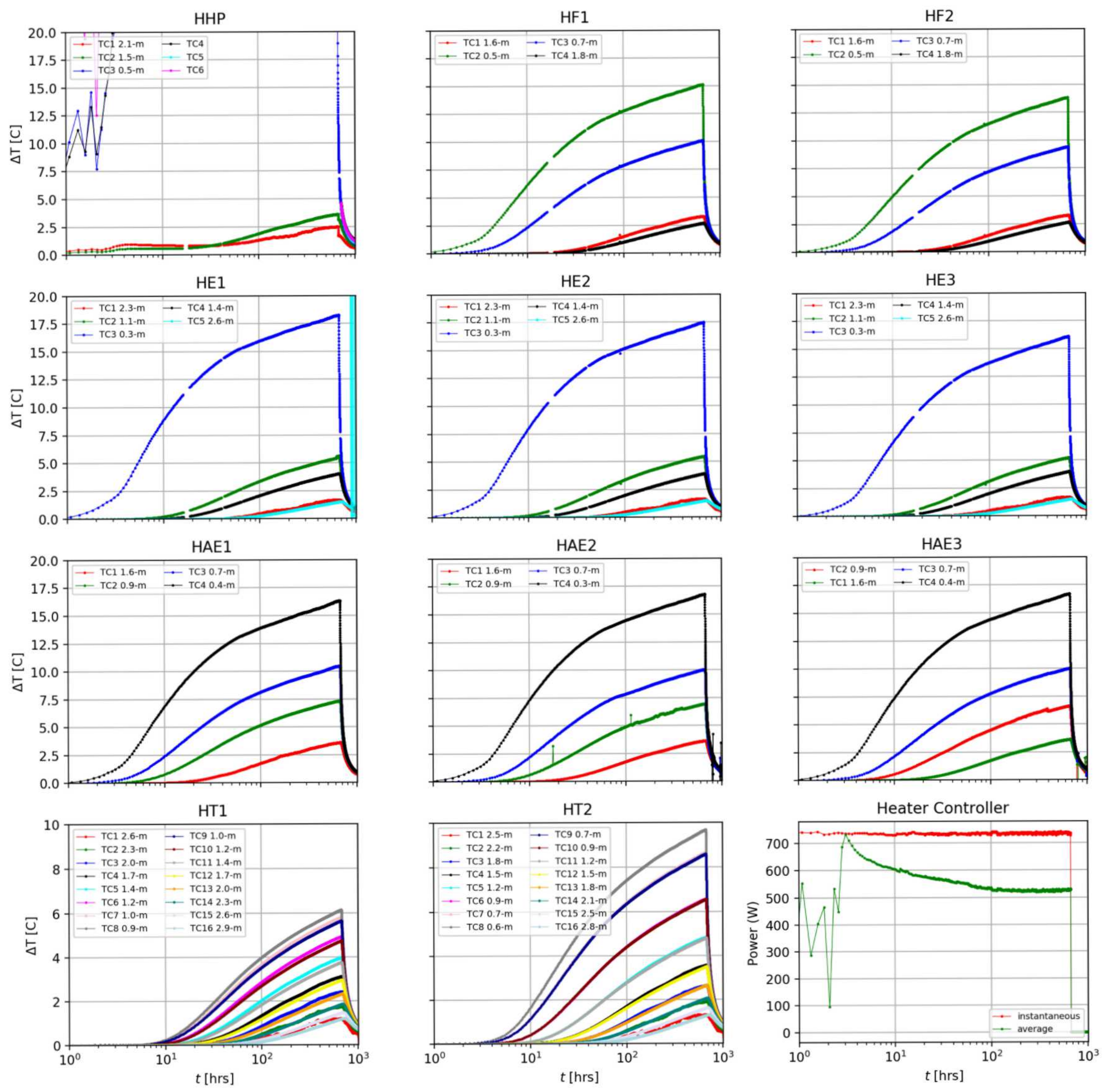
Discrete fractures in BATS near-drift EDZ

2. Jan-Mar 2020 BATS Temperature Response

Linear-linear scales (dates and T)

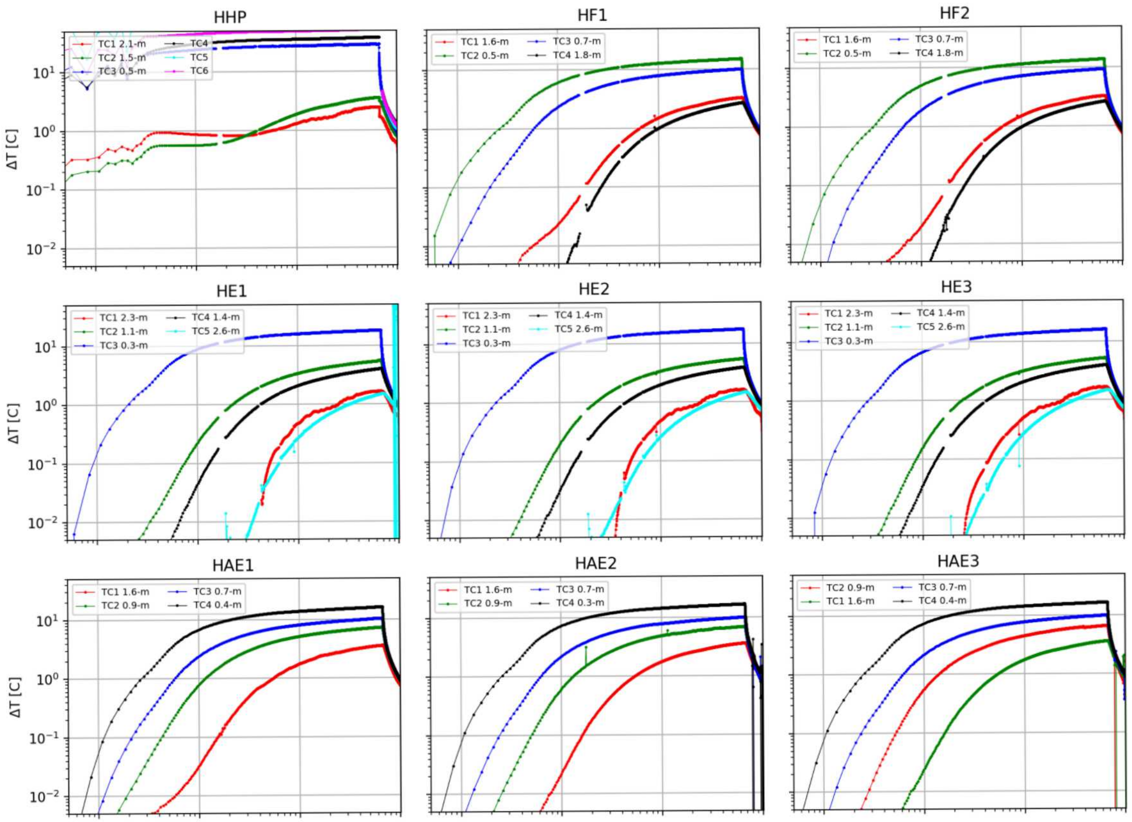


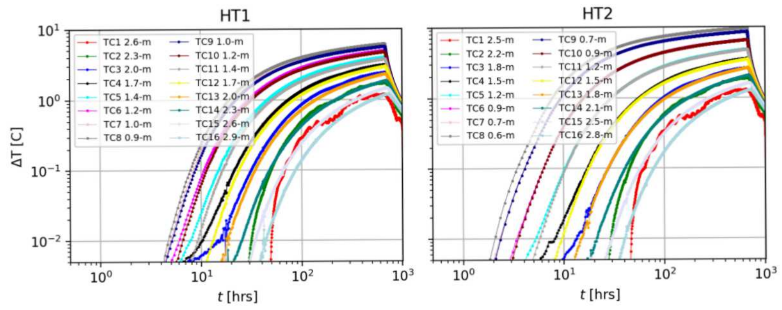
Semilog scale (elapsed time and ΔT)



2. Jan-Mar 2020 BATS Temperature Response

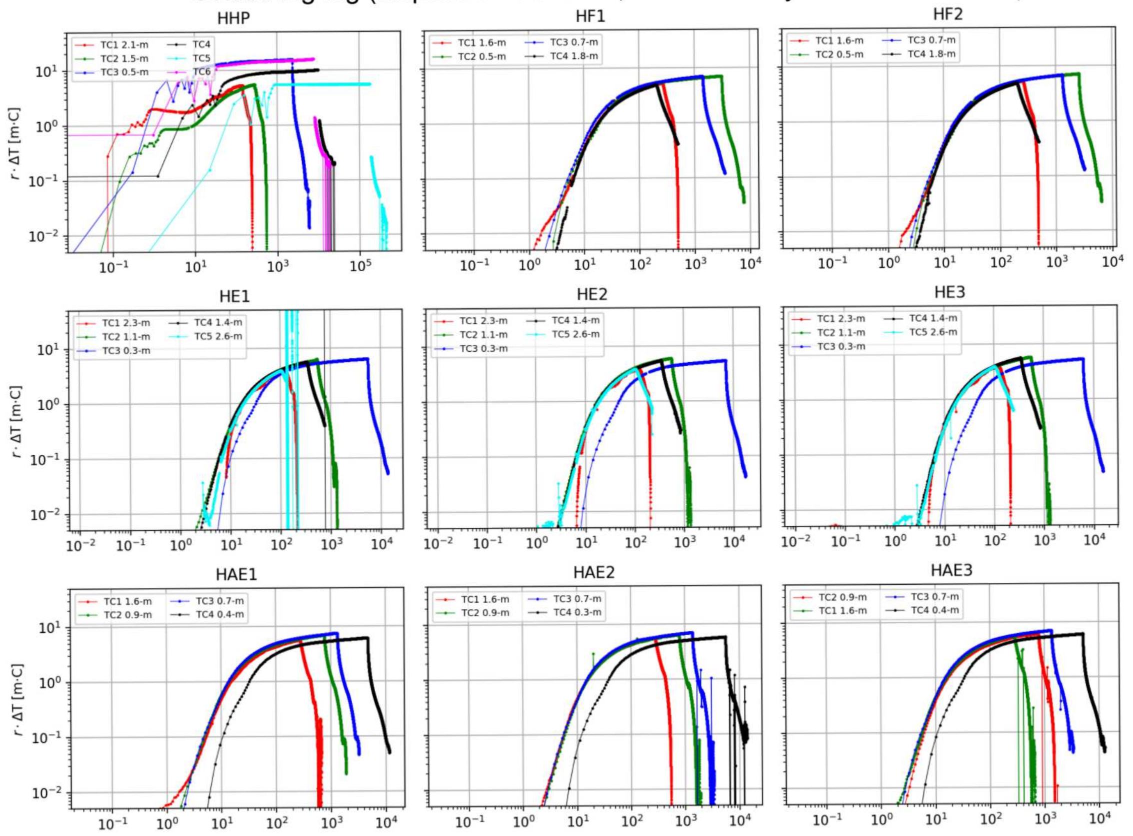
Log-log scales (elapsed time and ΔT)

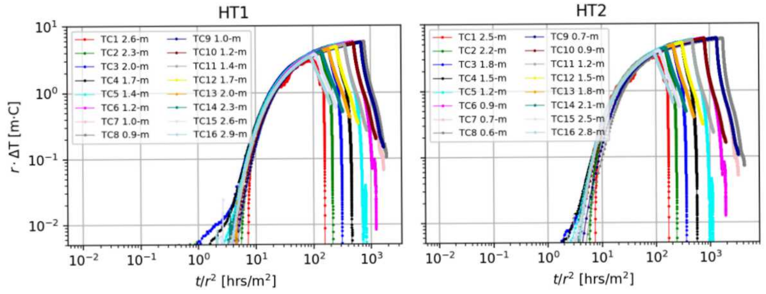




Distances in figure legends are sensor to midpoint of heater

Scaled log-log (elapsed time and ΔT, normalized by distance to heater)

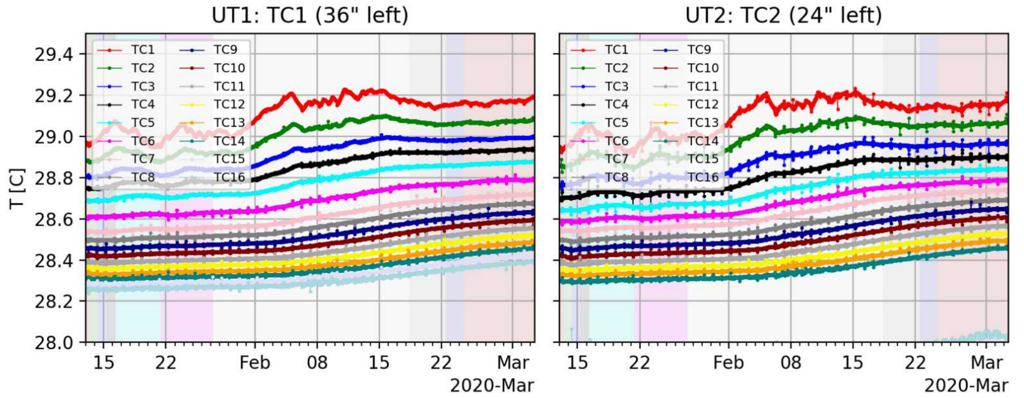




Scaling shows strong similarity to spherically symmetric solution (except at short distances)

2. Jan-Mar 2020 BATS Temperature Response

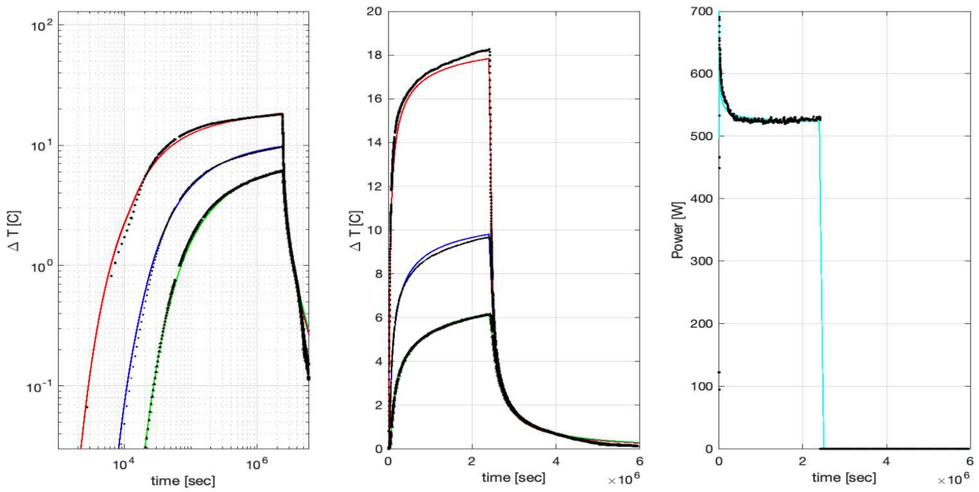
- Data:
  - Measured temperature at ~62 locations through time (15-minute averages)
  - Estimated x, y, z locations of thermocouples [TC] (assuming on borehole axis)
  - Power delivered to heater (15-minute averages)



- Possible complications:
  - Ambient 0.8 C ΔT over 6 m (hotter drift)
  - Near-drift temperatures fluctuate ~0.1 C (ventilation)
  - Heater controller had issues in first ~2 hrs (on-off 3x)
  - ERT nightly: applied current → crazy TC readings (deleted)
  - Salt thermal conductivity is a function of temperature (Acton, 1977; BATS lab data)
  - Most TC are grouted into boreholes (grout properties being characterized)
  - Constant-temperature heater controller
    - setpoint = 120 C (HHP-TC5), but actual borehole wall temperature may be less (96 to 120 C)
    - Possibly due to effect of lamp shining directly on controller thermocouple
    - Possibly due to poor contact between controller TC and borehole wall

2. Jan-Mar 2020 BATS Temperature Response

- <u>Comparison:</u>
  - Change in temperature through time at least 5 locations (heating + recovery)
    - HT1-TC8, HT2-TC8, HE1-TC3 are ~same depth as the heater (0.3, 0.6, 0.9 m radially from heater)
    - HF2-TC4, TC1-TC16 are deeper into the salt (1.8, 2.8 m radially from heater)
  - Power and temperature at HHP borehole wall through time (one is specified)
- Early-time recovery data don't have on-off issues in early-time heating data
- BATS data are "preliminary" and cannot yet be released beyond the group
  - SNL/LANL/LBNL to coordinate release of data
- Predictive T (conduction) models:
  - Include material properties variability? (DRZ, grout)
  - Include effects of drift and air-filled boreholes?
  - Include temp-dependent thermal conductivity?



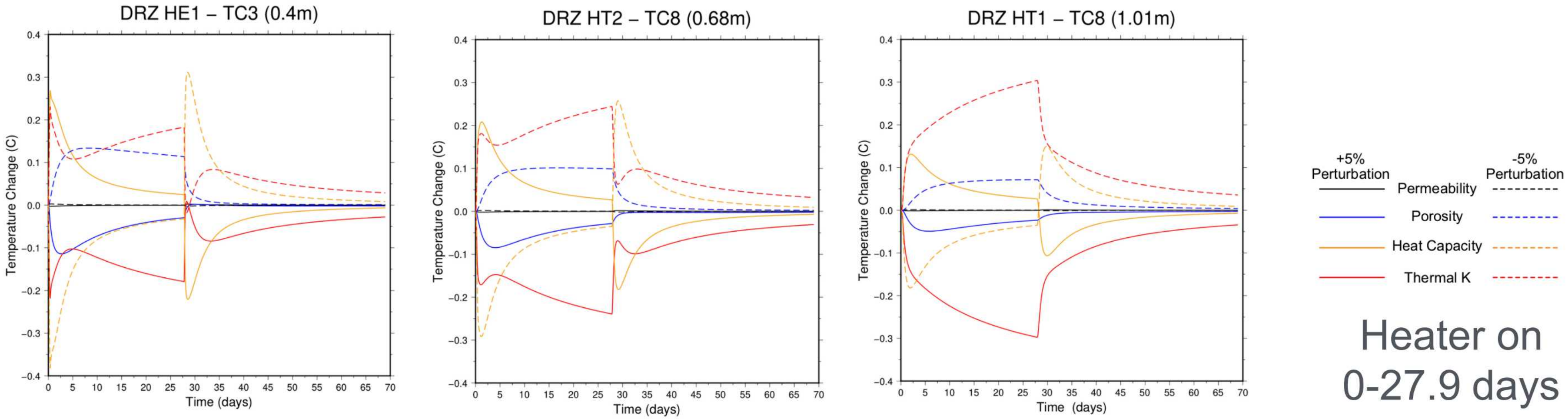
3. Sensitivity Analysis

- <u>Comparison:</u>
  - *“Local” sensitivity analysis of models near a best-fit solution*
  - columns of Jacobian: finite-difference derivative of solution w/ respect to parameters

1. Choose key parameters:
   - SSBIT e.g., permeability and storage coefficient (possibly for different layers)
   - BATS e.g., thermal conductivity & heat capacity (possibly salt, grout, DRZ), source temp.?
2. Perturb each parameter independently (<5%)
3. Compute change in prediction (e.g., temperature, power, brine flux) through time/space

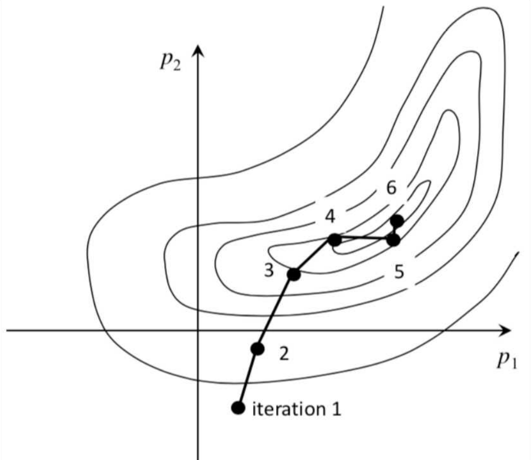
Example sensitivity of TOUGH2 temperature predictions through time from BATS heating and cooling

(by Rick Jayne, SNL)



4. Uncertainty Quantification (UQ)

- Automate fitting of models to observations
- General “parameter estimation” software provides
  - Illustration of parameter sensitivity (i.e., columns of Jacobian matrix)
  - Measure of uncertainty near optimum
- PEST: http://www.pesthomepage.org
  - Straightforward to use, free software (Doherty, 2015)
  - Mostly gradient-based least-squares method
- DAKOTA: https://dakota.sandia.gov
  - Large open-source suite with many capabilities (Adams et al., 2019a; 2019b)
  - wide range of included methods, GUI, and parallel execution on clusters
- Many existing libraries, toolkits to use
  - Use any tools you know, if they provide sensitivity/UQ

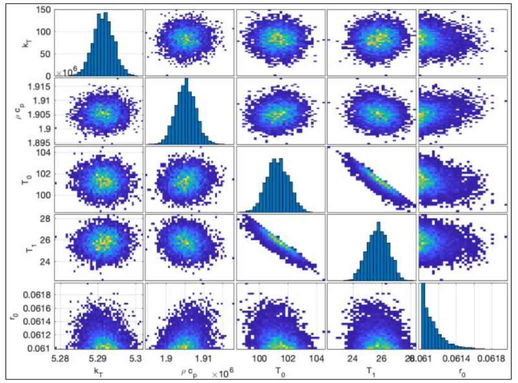


(Doherty, 2015)

4. Uncertainty Quantification (UQ)

What types of optimization methods or uncertainty quantification to use?

1. Least-squares methods (i.e., reduce sum of squared residuals)
   - Fast execution, needs estimate of derivatives (Jacobian)
   - *Efficiently find optimum*, give linearized uncertainty estimate "for free"
   - Works even for large, expensive-to-run models
2. Bayesian calibration methods
   - Estimate "prior distribution" of model parameters, conditioned on data
   - *Globally explore non-linear uncertainty*, give optimum solution "for free"
   - Typically only feasible for simple, fast-to-execute models



- <u>Comparison:</u>
  - Quantify some estimate of uncertainty bounds on parameters
    - 95% confidence interval, prior parameter distributions, or something else
  - Compare changes in uncertainty within each teams' models as complexity is added

Proposed Task E Steps

Step 0: Single-process H^1 and T benchmarks

Step 1: TH^1 benchmark & H^2M/H^2 unheated brine inflow test case

Step 2: TH^2M heated brine inflow test case

Step 3: Alternatives (ERT/AE joint inversion, seals, TH^2MC, creep)

Table 3. Proposed detailed Task E schedule of steps.

	Apr.	Nov.	Apr.	Nov.	Apr.	Nov.	Apr.	Nov.
	2020		2021		2022		2023	
Step 0								
Step 1								
Midterm Report → (Nov 2021)								
Step 2								
Step 3				?				
					Papers and Final Report → (Nov 2023)			

Infrared heater in BATS HP borehole

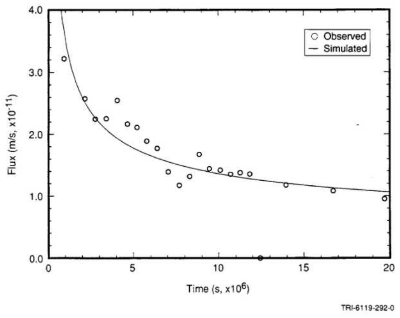
H^1= single-phase; H^2 = two-phase

Task E Step 0 (Jun. 2020 - Apr. 2021)

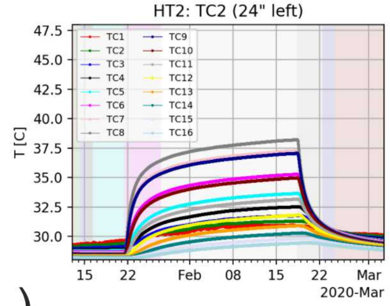
0. Single-process H[1] and T benchmarks

a) H[1] brine inflow to boreholes (small-scale brine inflow test)

(Beauheim et al., 1997)



- Simulate brine inflow to 3 (of 17) boreholes in Finley et al. (1992) dataset
- Data: weekly mass of brine produced from sealed boreholes
- INTRAVAL "WIPP 1" model comparison exercise, 3 international teams (Beauheim et al., 1997)
- Brine flow down p gradient (borehole @ 0.1 MPa, far-field @ hydrostatic ~6 MPa)



b) T due to conduction (BATS; Mills et al., 2019)

- Simulate T profile (heating and cooling) during heater test
- Data: 4 weeks heating, 2 weeks cooling: ΔT at 5 (of 67) remote locations (Δt 15 min.)
- Heat flux down T gradient: 60-cm interval of borehole wall is constant temperature (~96 ℃), heater midpoint is 2.75-m deep into 10-cm borehole,

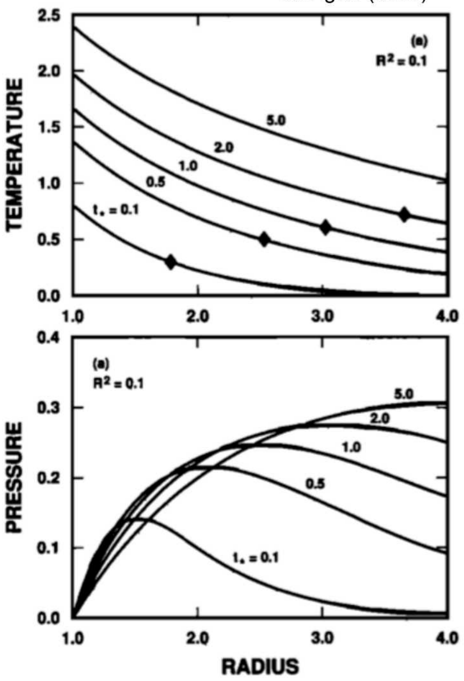
c) Estimate model parameter uncertainty and parameter sensitivity for both through time

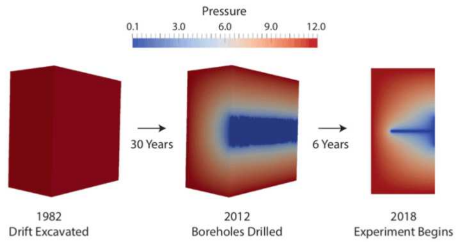
- *Quantify uncertainty* in prediction and measure Δ prediction with Δ input parameters (*sensitivity*)

Task E Step 1 (Nov. 2020 - Apr. 2022)

1. TH^1 benchmark & $\text{H}^2\text{M}/\text{H}^2$ unheated brine inflow test case
   a) Benchmark TH^1 brine production to analytical solution (McTigue, 1990)
      - Compare numerical models against coupled linear solution (space & time)
      - Halite properties from Table 1, McTigue (1986)
      - Compare with/without model non-linearities (e.g., fluid viscosity $f(T)$)
   b) Parameterize two-phase flow in salt EDZ (few data exist)
      - *Laboratory imbibition test*. Mass imbibed & wetting front w/ time $->$ estimate capillary pressure (p_c) & relative permeability (k_r) relationships
      - *CT core data*. Predict p_c & k_r from pore-network models
      - *Literature*. Granular salt: (Cinar et al., 2006; Olivella et al., 2011). Non-salt EDZ at WIPP (Davies, 1991; Howarth & Christian-Frear, 1997)
   c) H^2 brine inflow to boreholes (BATS) w/ H^2 characterization
      - H^2 or H^2M simulation of "initial conditions" for BATS heater test

McTigue (1990)



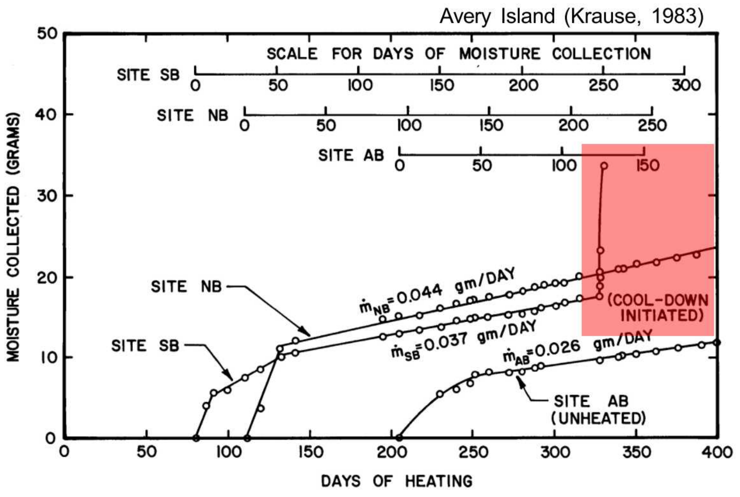


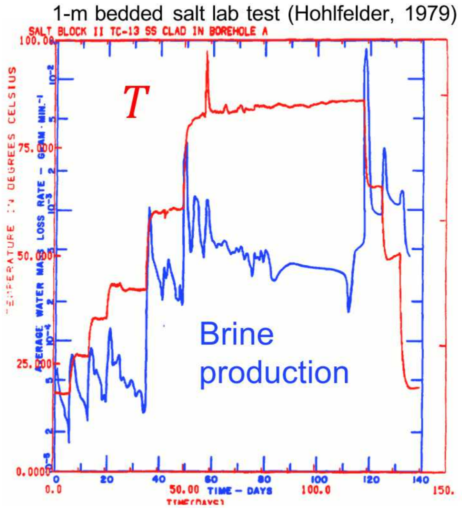
Guiltinan et al. (2020)

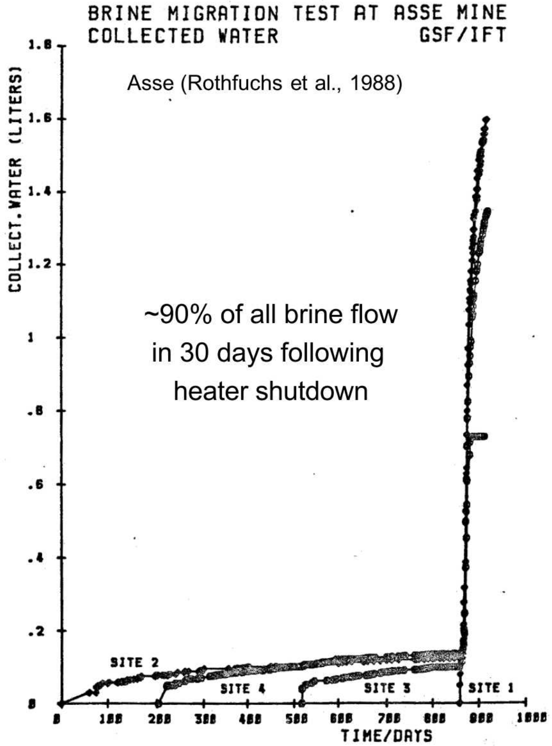
Task E Step 2 (Apr. 2021 - Apr. 2023)

2. TH^{2}M heated brine inflow test case

   a) Predict brine production during increases and decreases in T







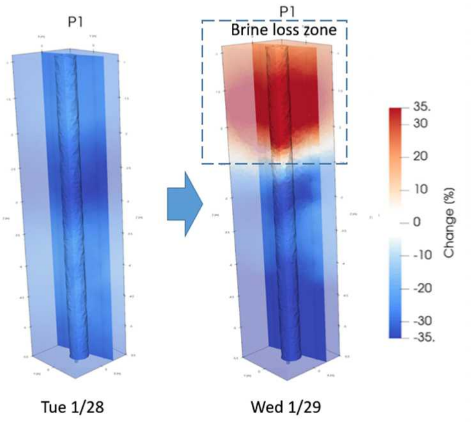
   b) *Optional:* predict breakthrough of gases/liquid tracers in BATS tracer tests

      a) Gas flow (N_2 + Kr, Ne, SF_6) breakthrough via quadrupole mass-spec (5 min. data)

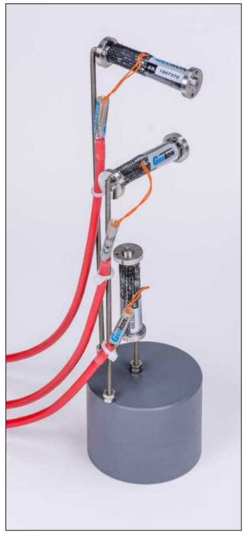
      b) Liquid flow (isotopically distinct water + fluorescein & perrhenate) via Picarro & liquid samples (~daily samples)

      c) Spatial distribution of liquid tracers in post-test cores

Task E Step 3 (Alternatives)



1. ERT/AE data to constrain brine inflow estimates
   - ERT sensitive to brine saturation, daily ERT tomograms
   - AE source locations to confirm changes in ϕ, k
2. Predict behavior of BATS seals / GRS lab tests
   - GRS laboratory experimental data (WIPP brine & salt)
   - BATS strain, T data in cement plugs (Sorel & salt concrete)



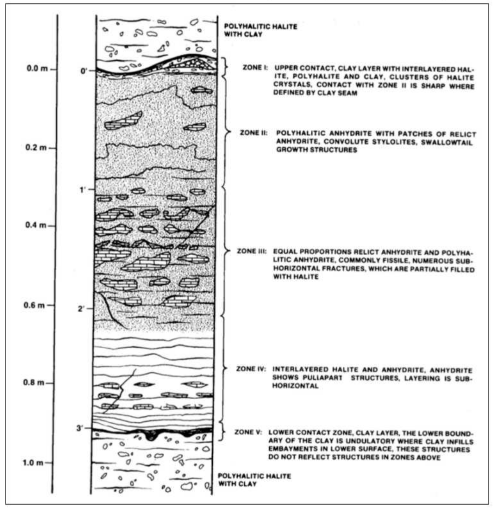
3. Additional C processes
   - Include 4 water sources explicitly in models (composition and stable water isotopes), impacts on ϕ, k from dissolution & precipitation of salt (condensation & boiling)
4. Effects of viscoplastic creep on brine production

Based on interest of teams: Choose one/two? Move to step 2?

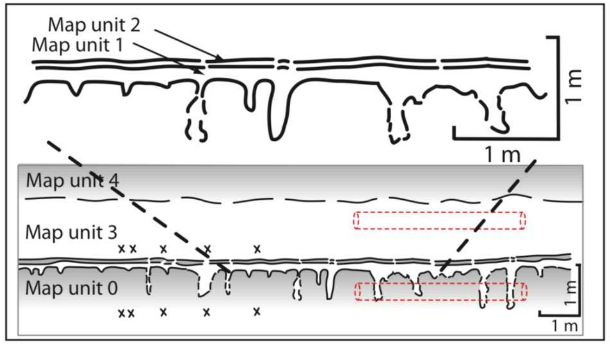
Appendix: WIPP Salt Geology

- Fileshare: `D2023 Team > Task E > References-WIPP-Geology`
- Regional & WIPP-specific geology
  - Salado comprised of repeating sequences
  - MB-139 is 1-m thick anhydrite/clay layer
  - BATS is in Map Units 1-3
  - *cm- to m-scale complexity and heterogeneity*

Idealized MB-139 description (Borns, 1985)



BATS area core description (Powers, 2017)



MU-4

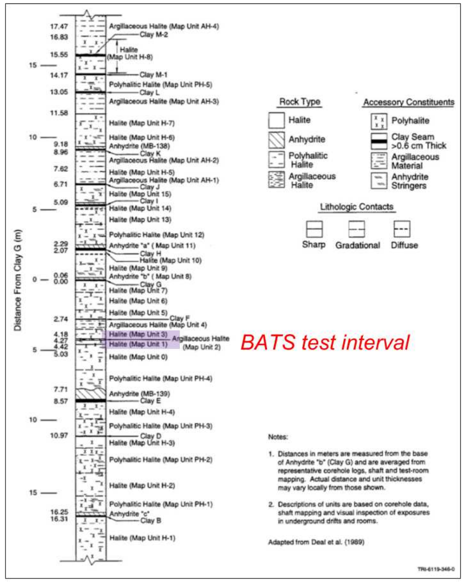
MU-3

MU-1 & MU-2

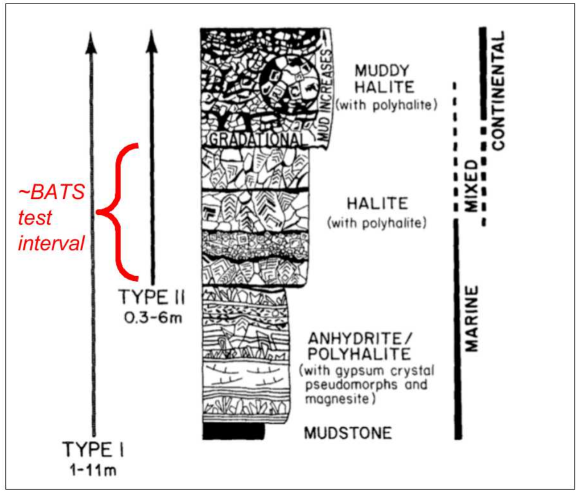
MU-0

Heated BATS array, photo by Brian Dozier (WIPP TCO)

(Beauheim et al., 1997)



Geology of Salado (Lowenstein, 1988)



Salado sequence (Holt, 1993)

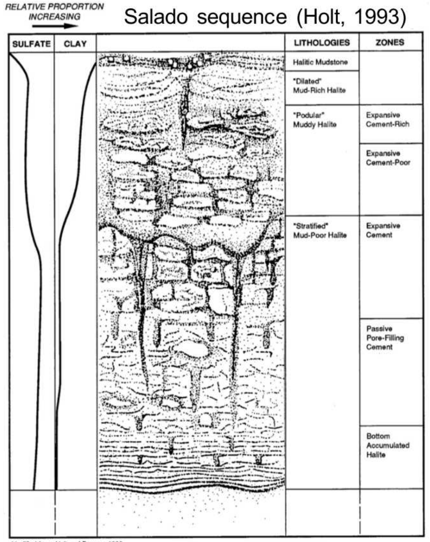
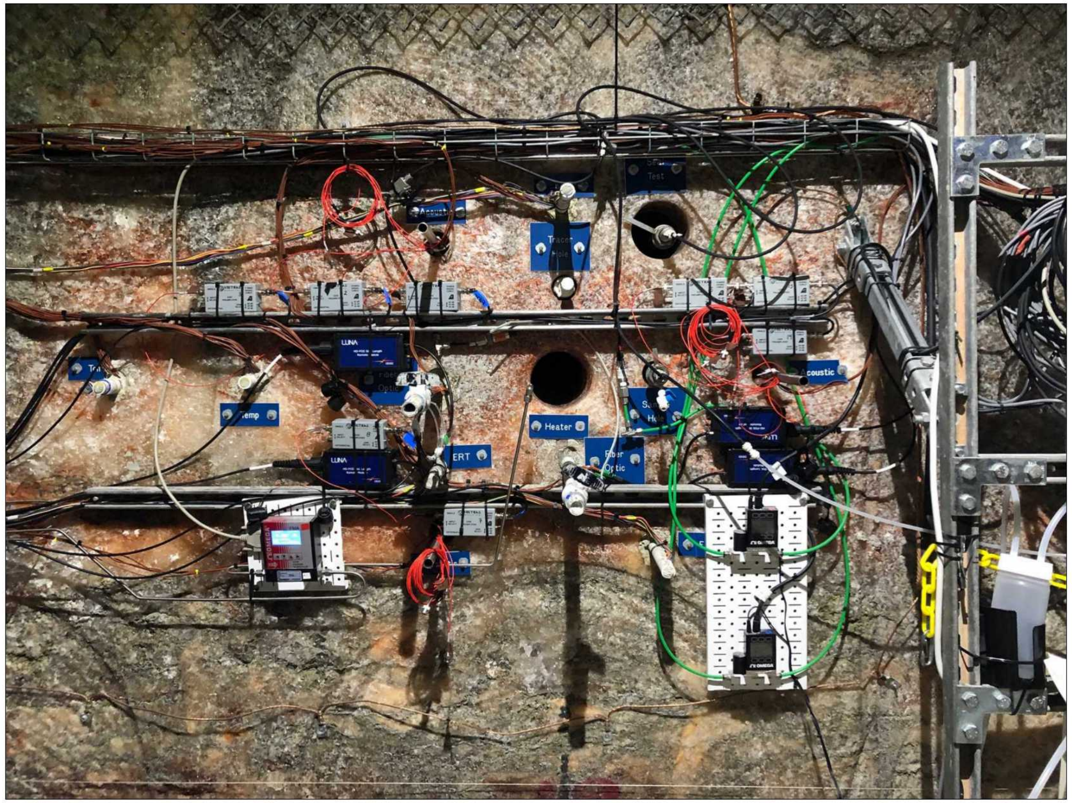


Figure 4-1
Idealized Salado Halite Sequence Lithofacies and Zones

Task E Kickoff Meeting Introductions

- Interested Teams
  - USA (SNL, LANL & LBNL)
  - UK (RWM & Quintessa)
  - Netherlands (COVRA)
  - Germany (BGR & GRS)



- Introductions
  - Who is participating / background & interests
  - Which modeling tools
  - Experience / knowledge about salt & WIPP
  - Thoughts on good/bad aspects of Task E

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These and further references can be downloaded as .pdf from DECOVALEX fileshare system https://team2023.decovalex.org

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Acronyms and Initialisms

AE	acoustic emissions
BATS	brine availability test in salt
CT	computed tomography
DECOVALEX	DEvelopment of COupled models and their VALidation against Experiments
DOE	Department of Energy
DOE-EM	DOE Office of Environmental Management (energy.gov/em)
DOE-NE	DOE Office of Nuclear Energy (energy.gov/ne)
DOPAS	full-scale Demonstration Of Plugs And Seals
DRZ	disturbed rock zone
DSS, DTS	distributed strain, temperature sensing
EDZ, EdZ	Excavation Damaged Zone, Excavation disturbed Zone
ERT	electrical resistivity tomography
GRS	Gesellschaft für Anlagen- und Reaktorsicherheit
LANL	Los Alamos National Laboratory
LBL	Lawrence Berkeley National Laboratory
NETL	National Energy Technology Laboratory
SFWST	Spent Fuel and Waste Science & Technology (DOE-NE program)
SNL	Sandia National Laboratories
TCO	WIPP Test Coordination Office (LANL)
TH^2MC	thermal, two-phase hydrological, mechanical, and chemical (also TH^1, TH^2M, TH^2C)
US	United States
WIPP	Waste Isolation Pilot Plant (DOE-EM site, wipp.energy.gov)