

## Modeling of the Long-Term Integrity of the Argillite Host Rock Barrier

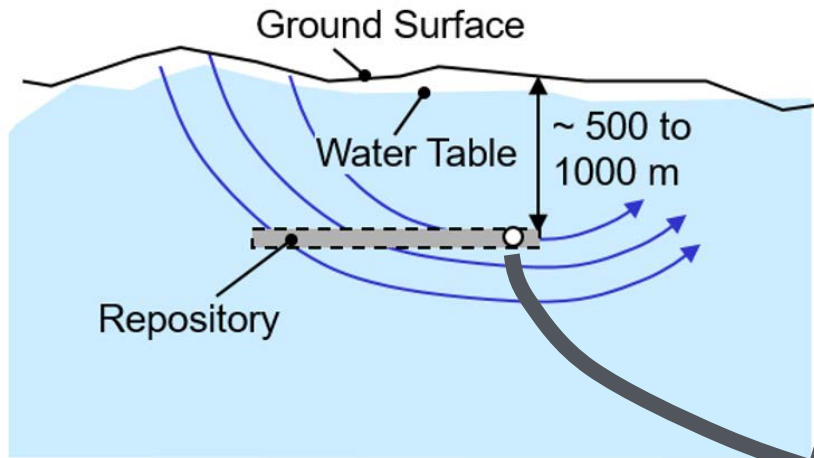
U.S. Nuclear Waste Technical Review Board  
Summer 2022 Board Meeting  
September 13–14, 2022

Jonny Rutqvist  
Lawrence Berkeley National Laboratory



Funding was provided by the Spent Fuel and Waste Science and Technology, Office of Nuclear Energy, of the U.S. Department of Energy under Contract Number DE-AC02-05CHI1231 with Lawrence Berkeley National Laboratory.

# Barriers and Functions



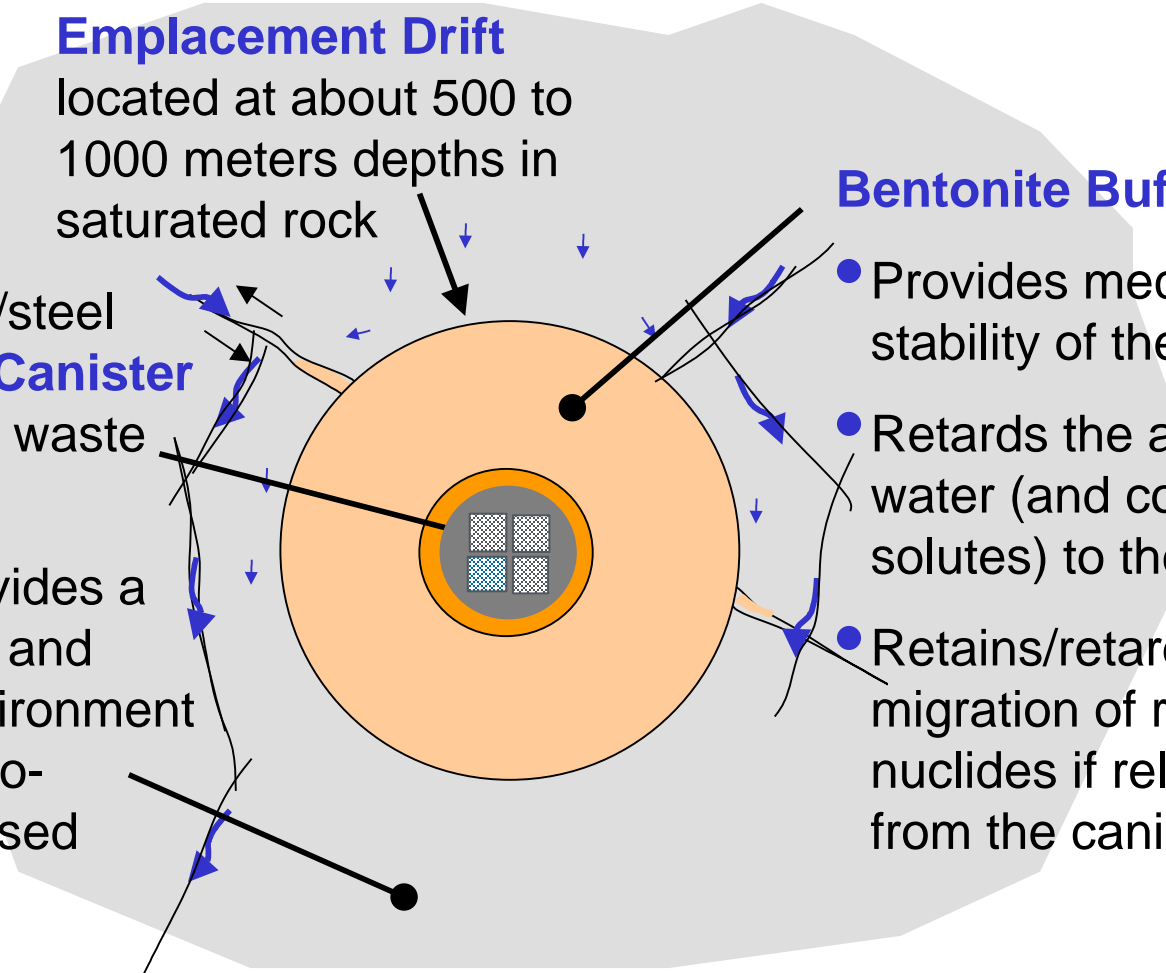
**Emplacement Drift**  
located at about 500 to 1000 meters depths in saturated rock

Copper/steel  
**Waste Canister**  
isolates waste

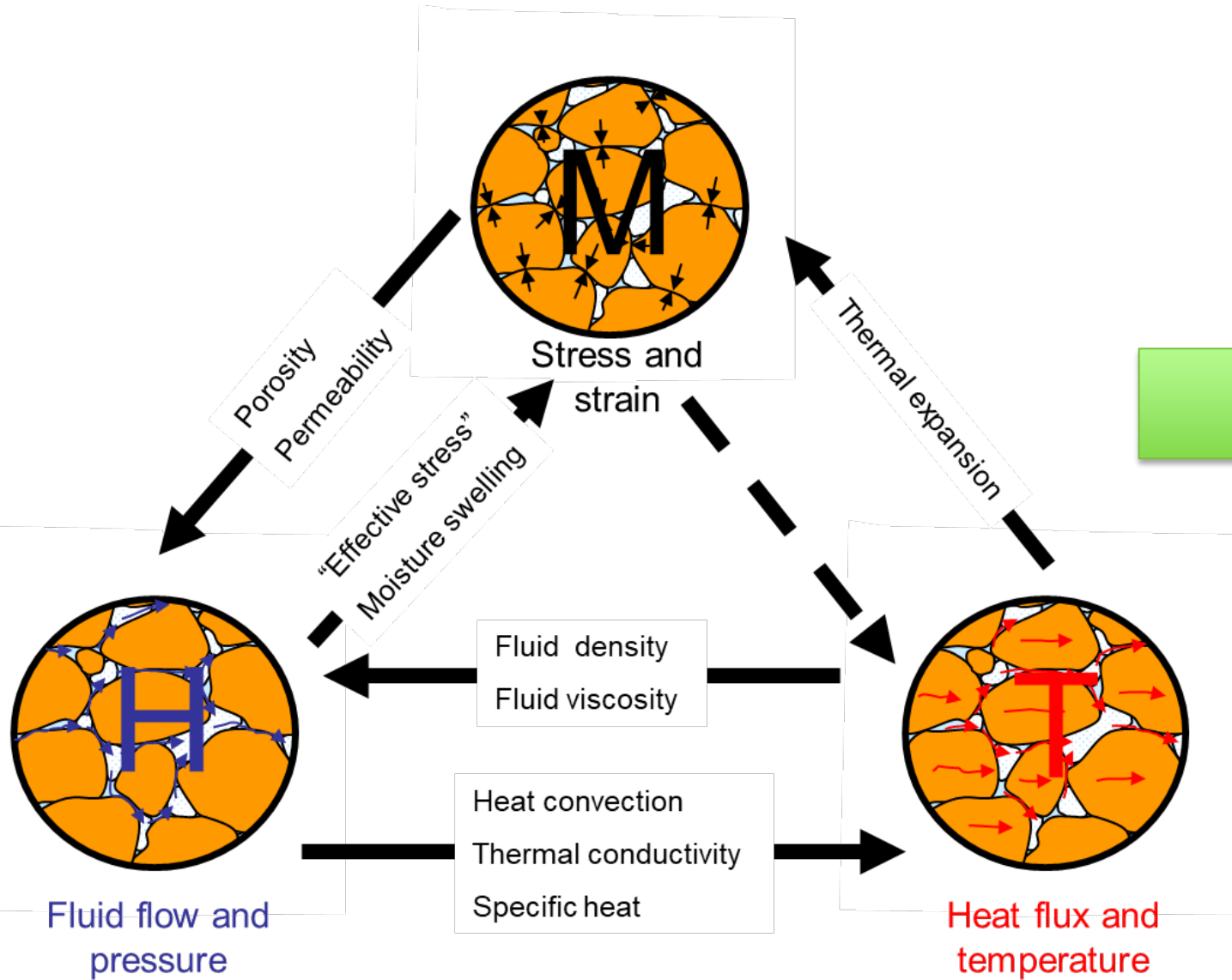
**Bedrock:** Provides a stable chemical and mechanical environment and retards radio-nuclides if released

**Bentonite Buffer:**

- Provides mechanical stability of the canister
- Retards the arrival of water (and corrosive solutes) to the canister
- Retains/retards migration of radio-nuclides if released from the canister

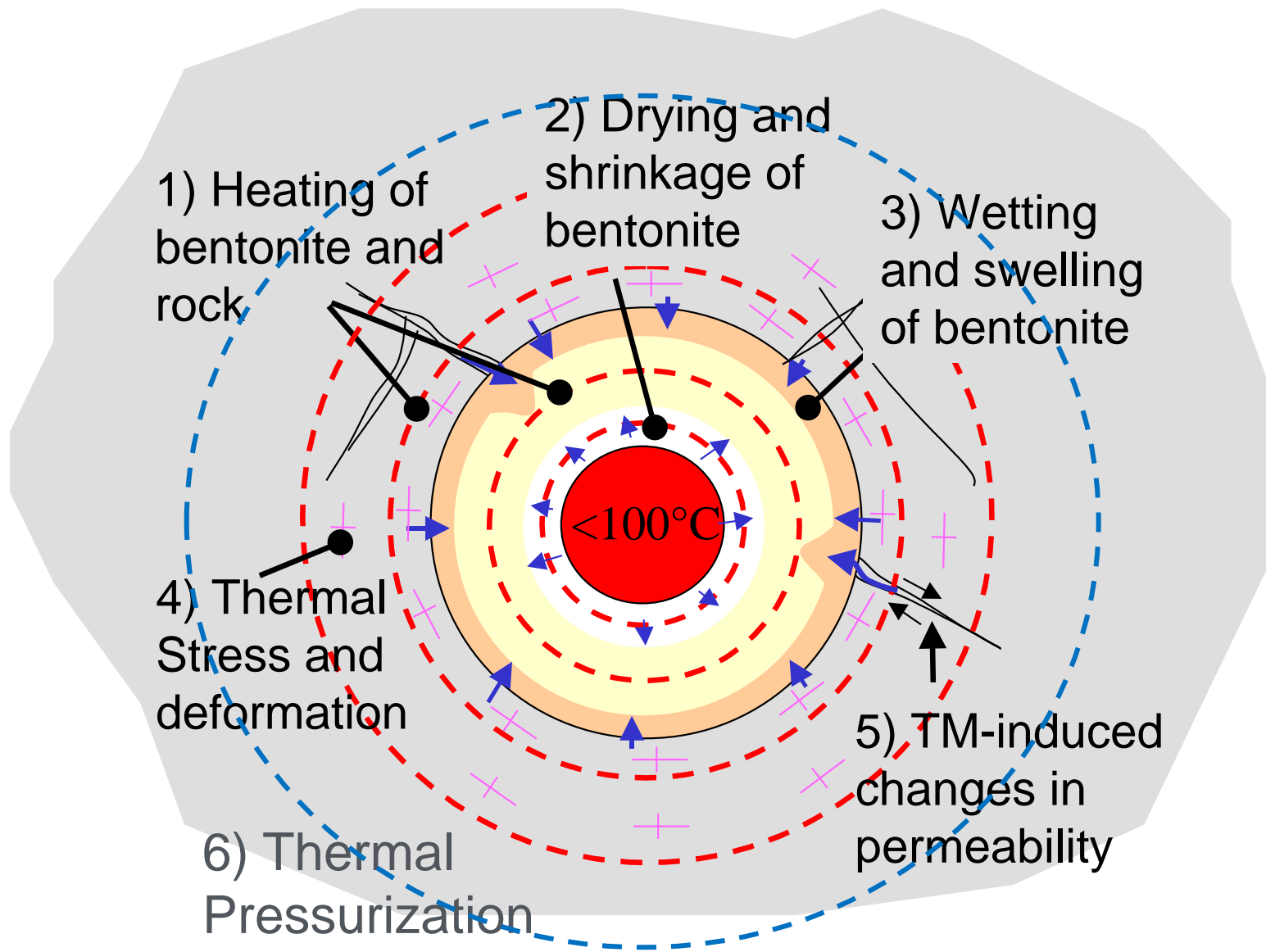


# Thermal-Hydraulic-Mechanical (THM) Couplings



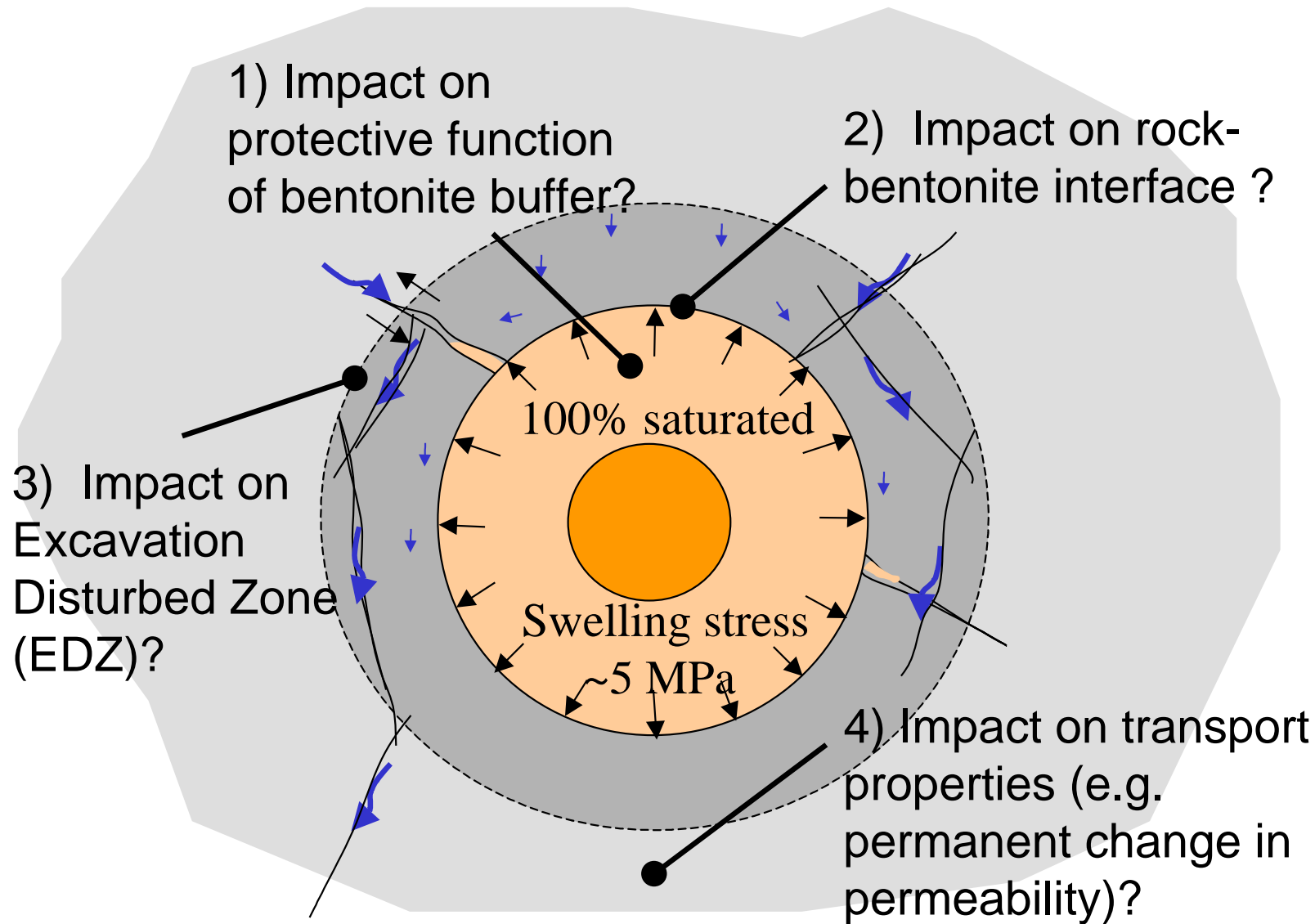
**Impact on barrier integrity and contaminant transport?**

# Short Term (0 to 1000 years) Thermally Driven Coupled THM Processes



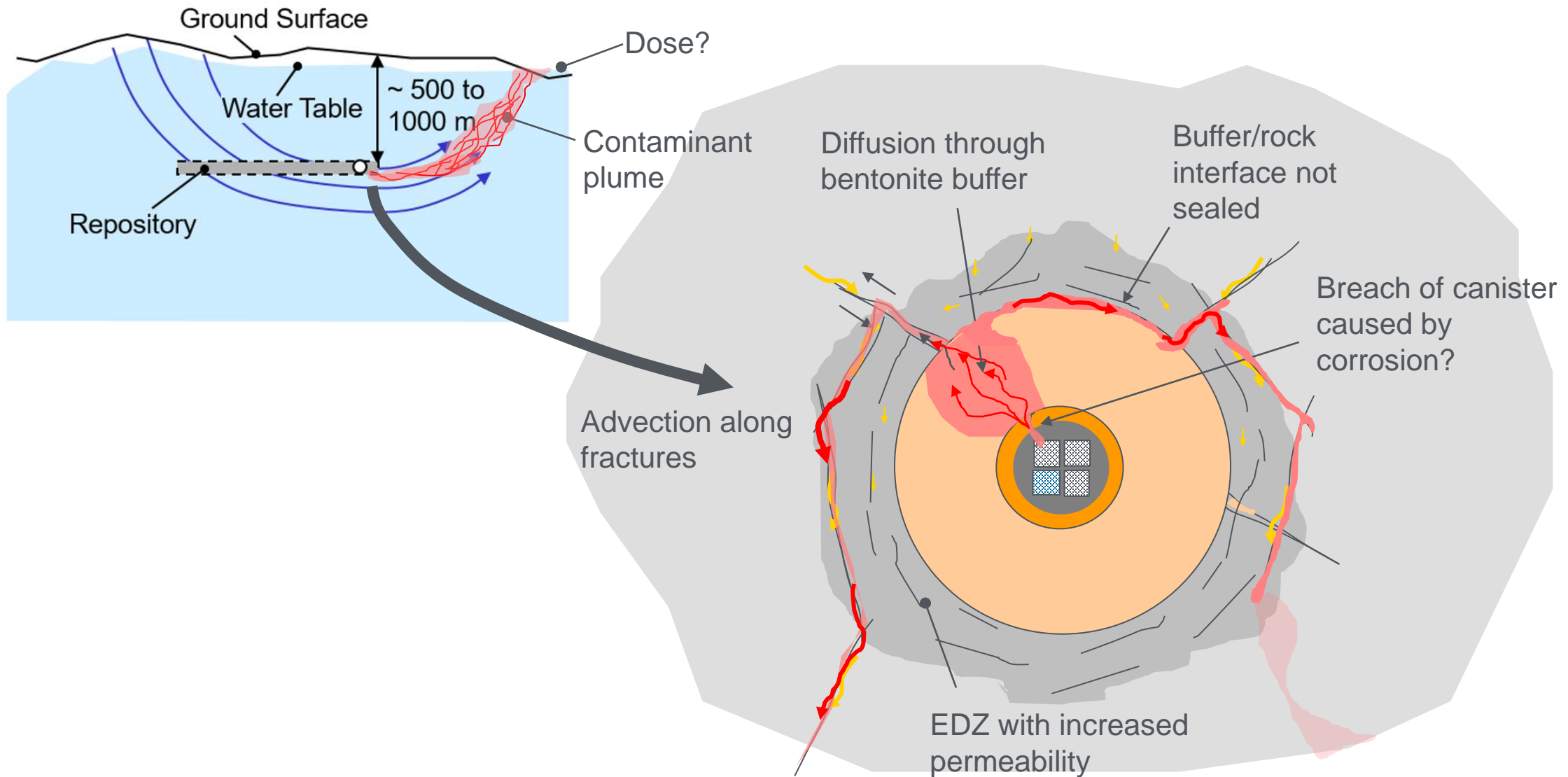
(Rutqvist, 2015)

# Long Term (1000 to 100,000 years) Impact of Coupled THM Processes



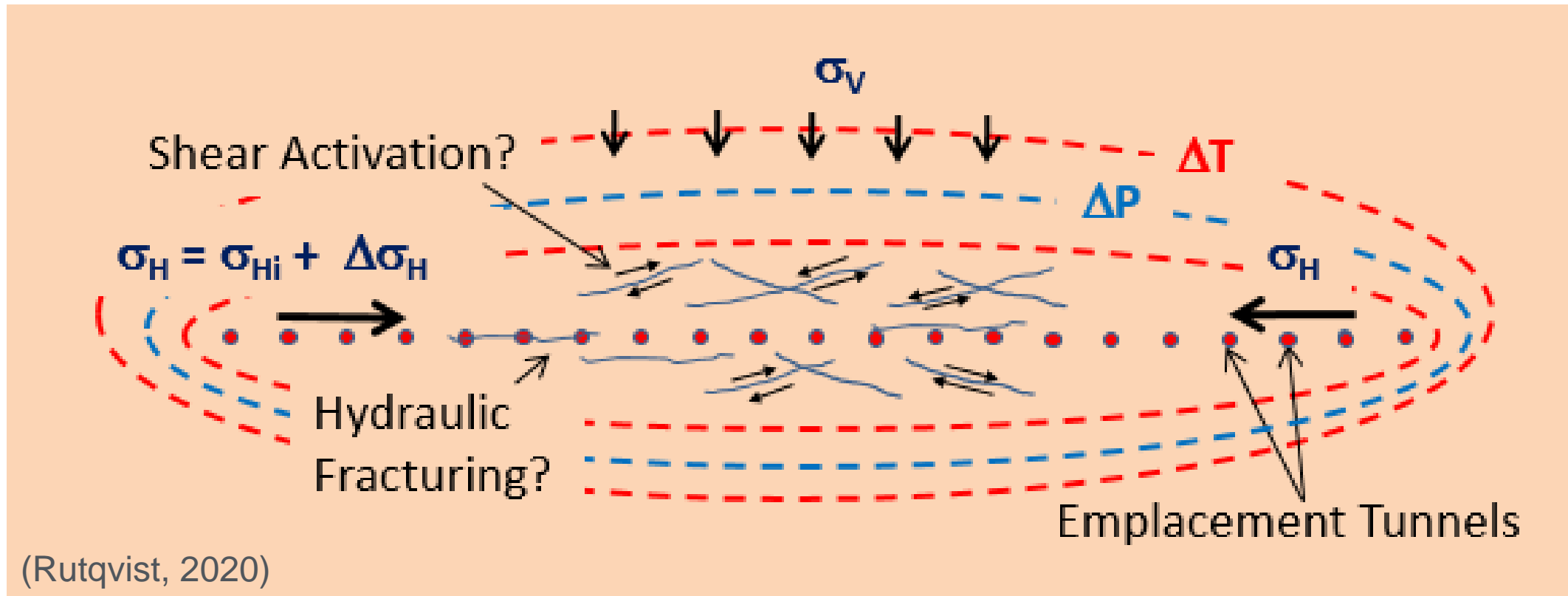
(Rutqvist, 2015)

# Breached Barriers (Illustrated)



(Rutqvist, 2015)

# Repository THM-Induced Stress Changes

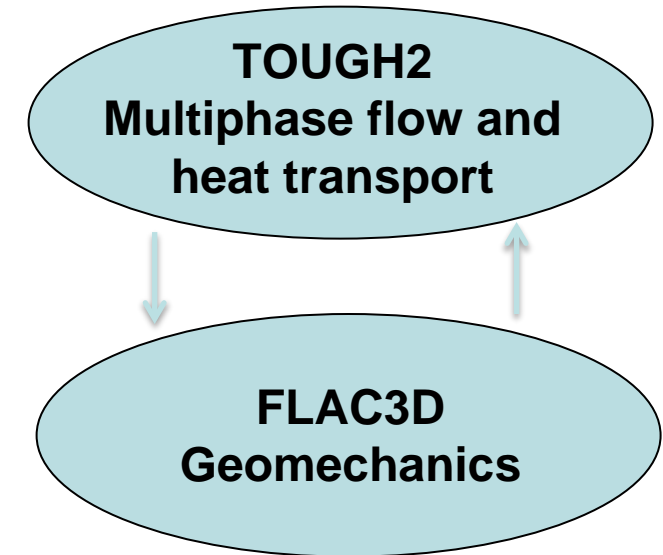


- Repository temperature change ( $\Delta T$ ) results in thermal pressurization ( $\Delta P$ )
- $\Delta T$  and  $\Delta P$  results in thermal stress and poro-elastic stress ( $\Delta\sigma_H$ )
- **Impact on host rock integrity? (Fracturing?, Shear?, Opening of flow paths?)**

# A Thermo-Hydro-Mechanical Model Framework

## TOUGH-FLAC Simulator:

- Linking two established codes (each thousands of users)
- Both codes continuously developed and applied in their respective fields
- Large number of fluid and mechanical constitutive material models

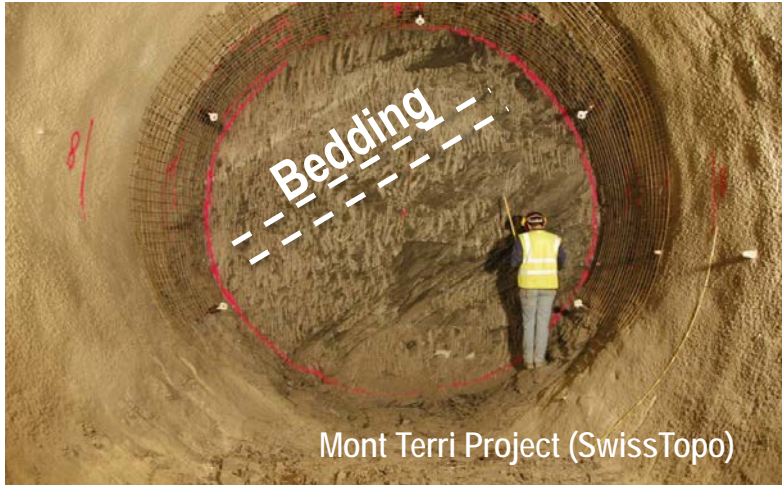


(Rutqvist et al., 2002; Rutqvist 2011; 2017)

- First developed and applied in the Yucca Mountain Project (2000-2008)
  - Bentonite and Argillite host rock (from 2011)
  - Salt host rock and backfill (from 2013)
- } **By adding to existing model capability**
- International TOUGH-FLAC users related to nuclear waste disposal in Germany, United Kingdom, Switzerland, and South Korea



# Argillite Host Rock Modeling



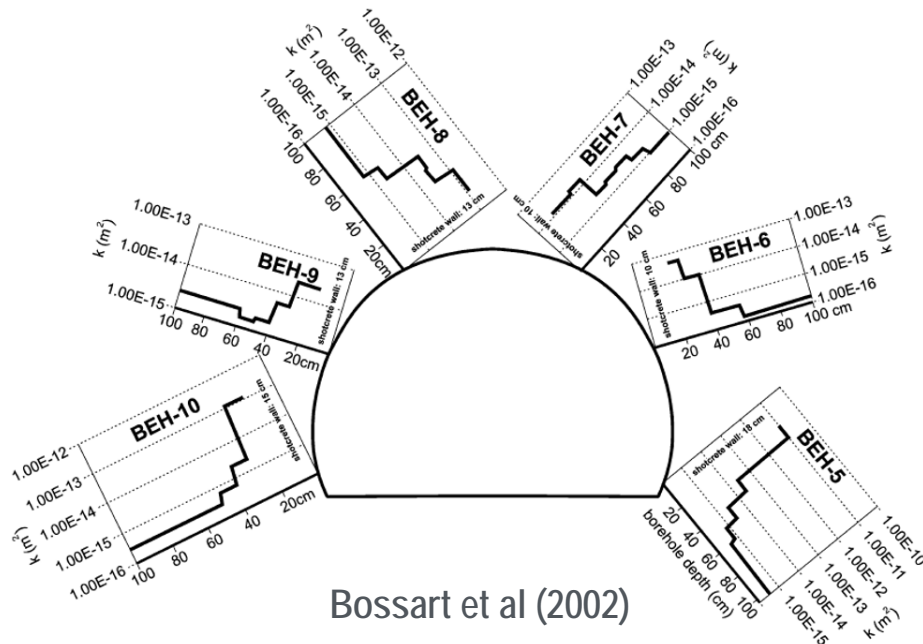
Mont Terri Project (SwissTopo)

## 1) Anisotropic THM properties

- Mechanical model considering weak planes along bedding (e.g. reduced shear strength)
- Higher thermal conductivity along bedding
- Higher permeability along bedding

## 2) Excavation Disturbed Zone (EDZ)

- Anisotropic stress-dependent permeability
- Brittle versus more ductile (sealing) argillite
- Models could be calibrated against field measurements (site specific)



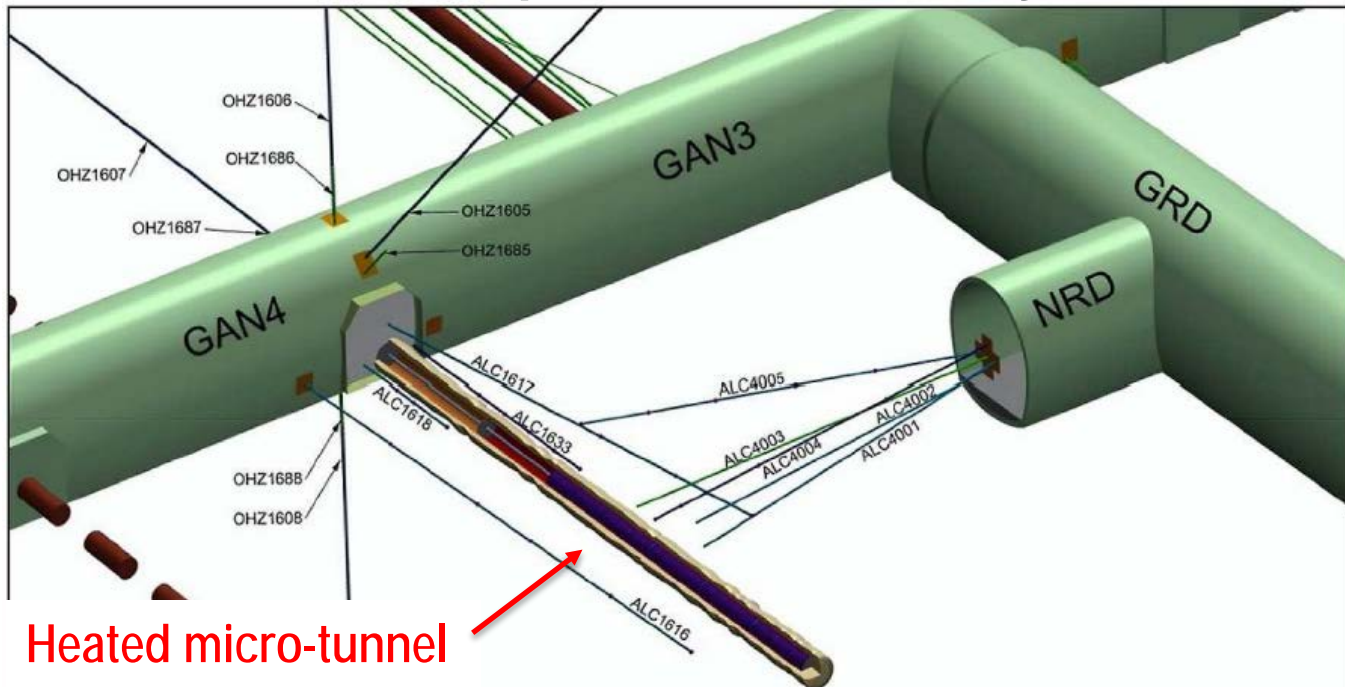
Bossart et al (2002)

# Model Verification and Validation in Argillite

1. Analytical solutions (thermo-poro-elasticity)
  2. Laboratory experiments (Argillite THM properties)
  3. Experiments at Mont Terri (Opalinus Clay)
    - HE-D thermal-pressurization (DECOVALEX-2015)
    - HE-E half-scale bentonite-argillite interaction (DECOVALEX-2015)
    - Fault slip experiment (DECOVALEX-2019)
    - FE-E Full-scale emplacement (DECOVALEX-2023)
  4. Experiments at Bure (Cox Claystone)
    - TED Borehole scale heater thermal-pressurization (DECOVALEX-2019)
    - ALC Micro-tunnel heater thermal-pressurization (DECOVALEX-2019)
    - Thermal and gas fracturing experiments (DECOVALEX-2023)
- TOUGH-FLAC code
  - Argillite THM model
  - Bentonite THM model
  - Compare with data
  - Compare with other codes in DECOVALEX
  - Compare with other models in DECOVALEX

# Modeling of Thermal Pressurization Experiment at Bure (DECOVALEX-2019)

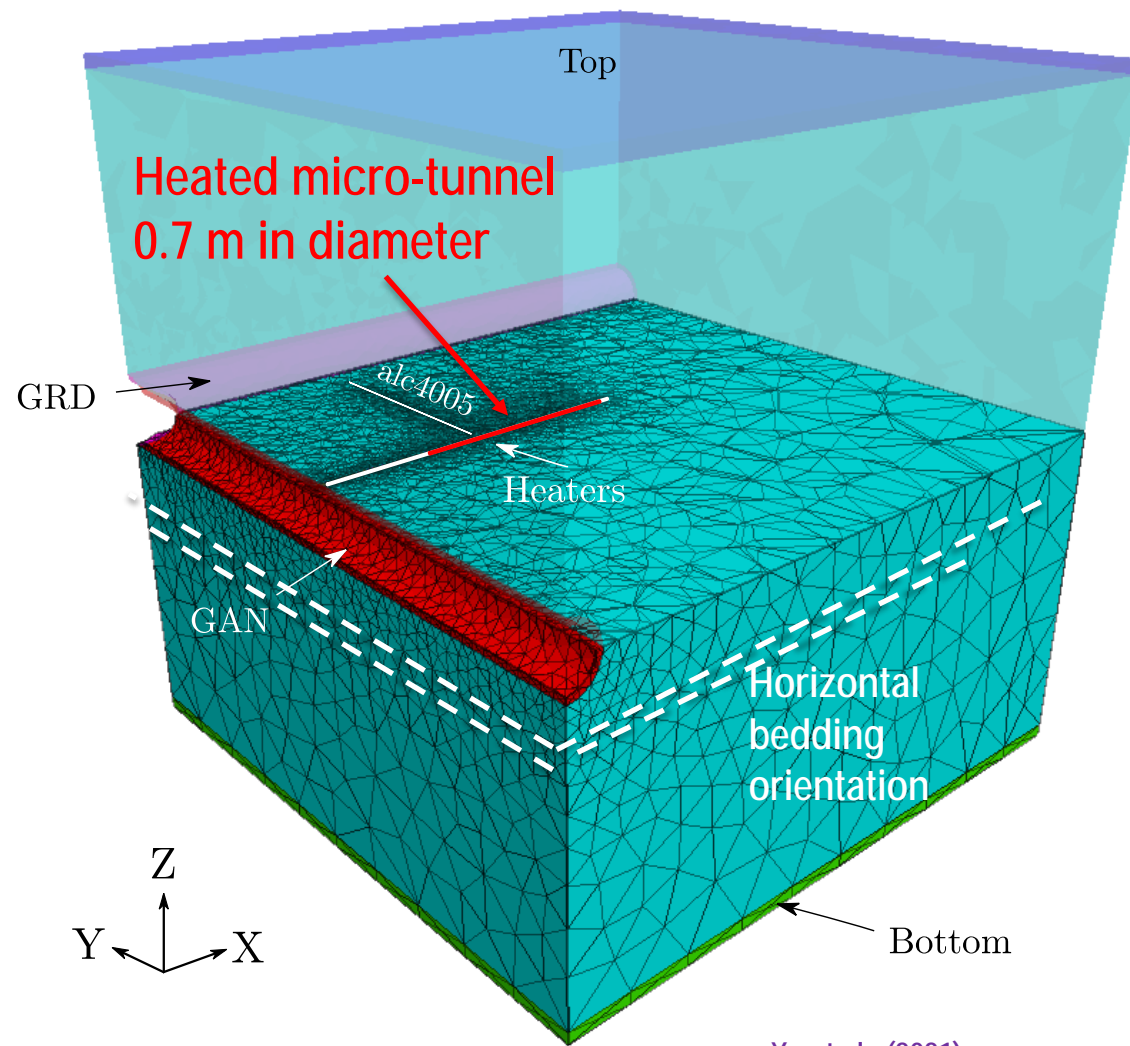
## The Micro-Tunnel Experiment in Cox Claystone at Bure



Heated micro-tunnel  
0.7 m in diameter  
25 m long

Sayed et al., (2021)

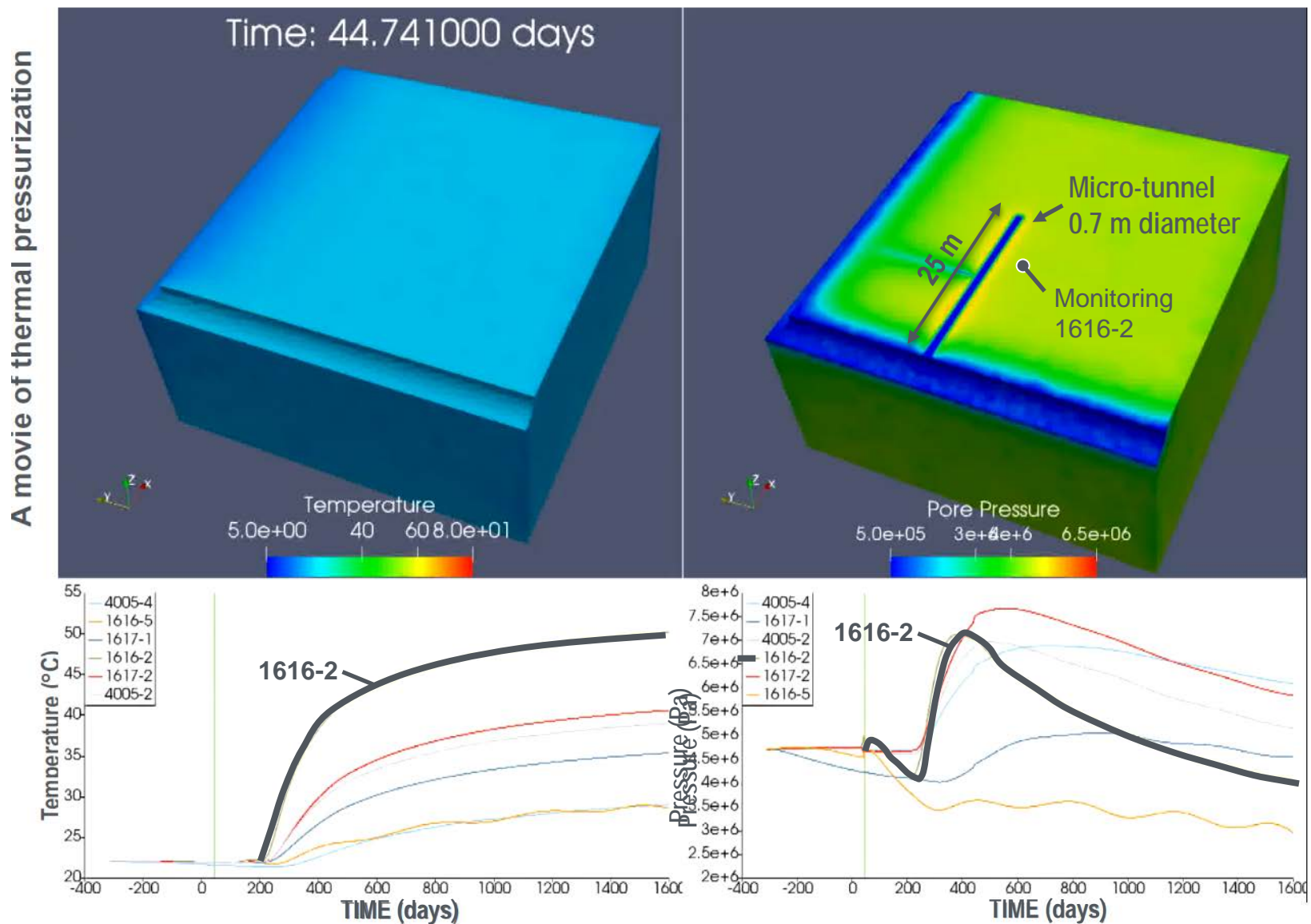
## Numerical Model



Xu et al., (2021)

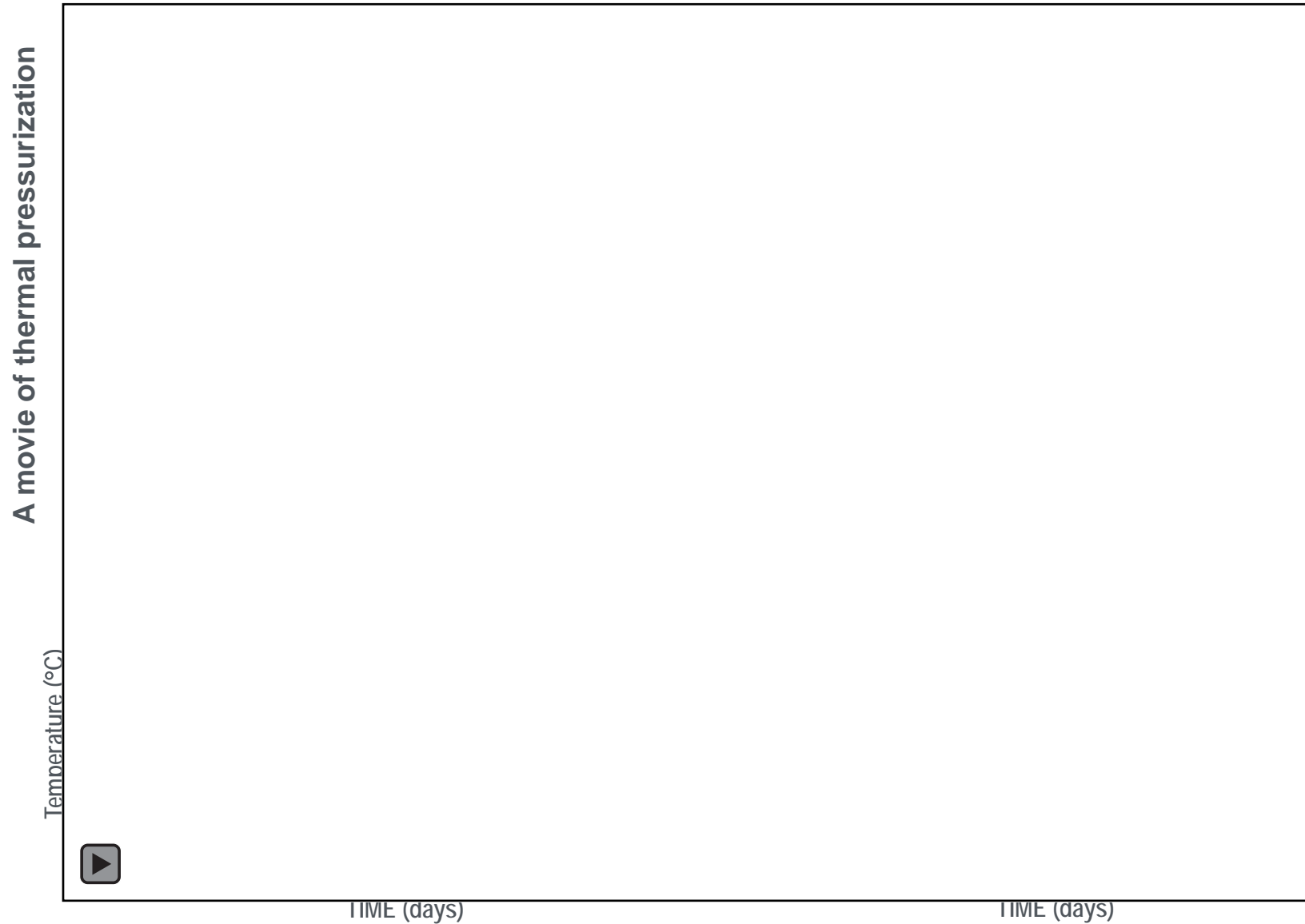
- Four years of heating up to about 50°C
- 5 DECOVALEX-2019 modeling teams and models
- Properties from modeling of previous experiment at Bure
- Compare predicted temperature and pressure responses

# Modeling of Thermal Pressurization Experiment at Bure (DECOVALEX-2019)



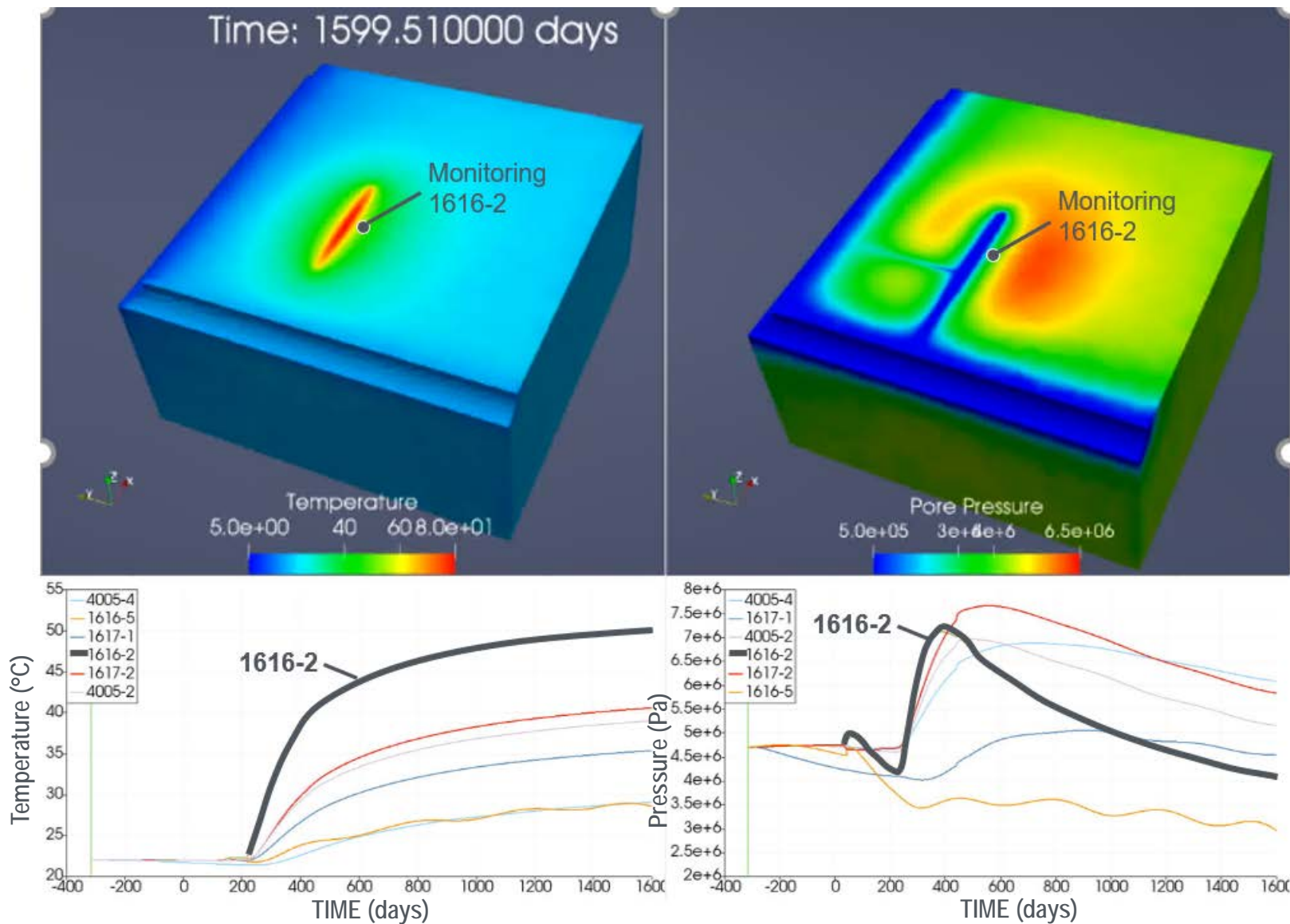
Xu et al., (2021)

# Modeling of Thermal Pressurization Experiment at Bure (DECOVALEX-2019)



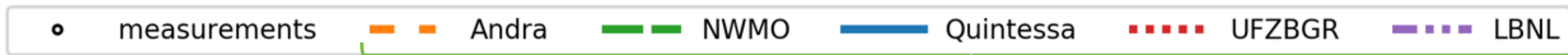
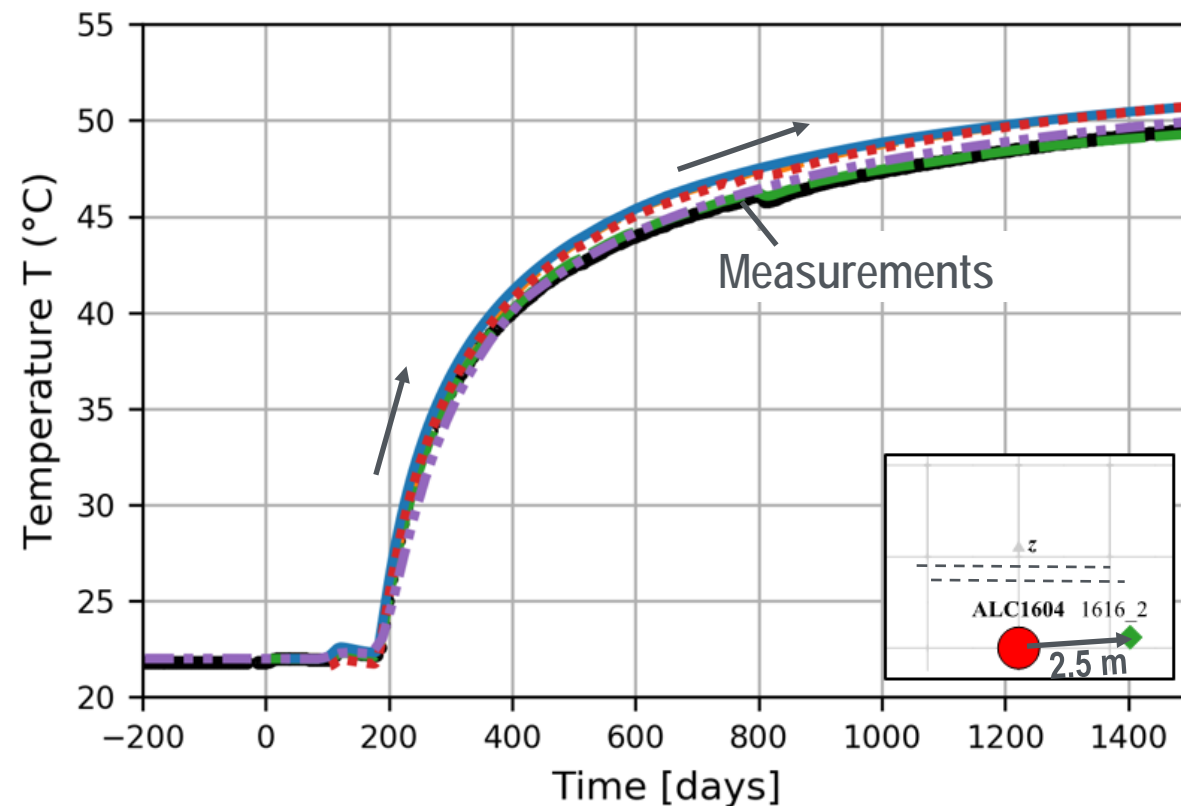
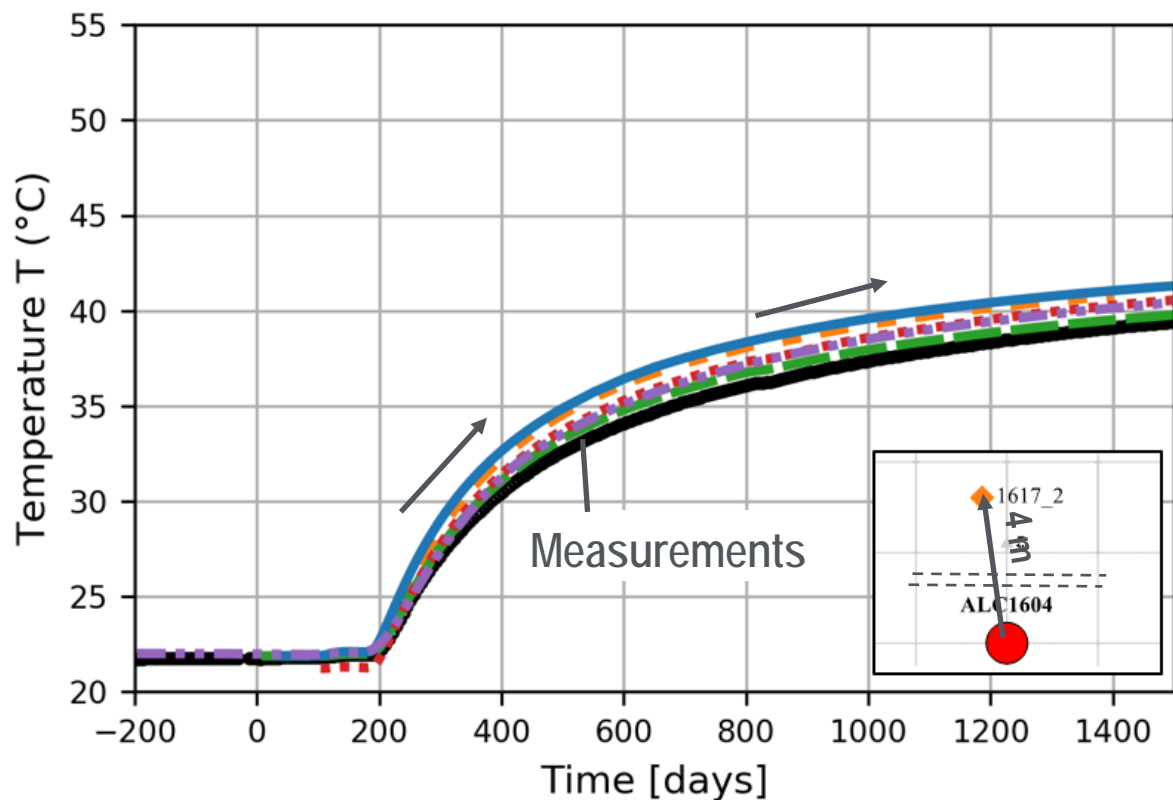
Xu et al., (2021)

# Modeling of Thermal Pressurization Experiment at Bure (DECOVALEX-2019)



Xu et al., (2021)

# Modeling of Thermal Pressurization Experiment at Bure (DECOVALEX-2019)

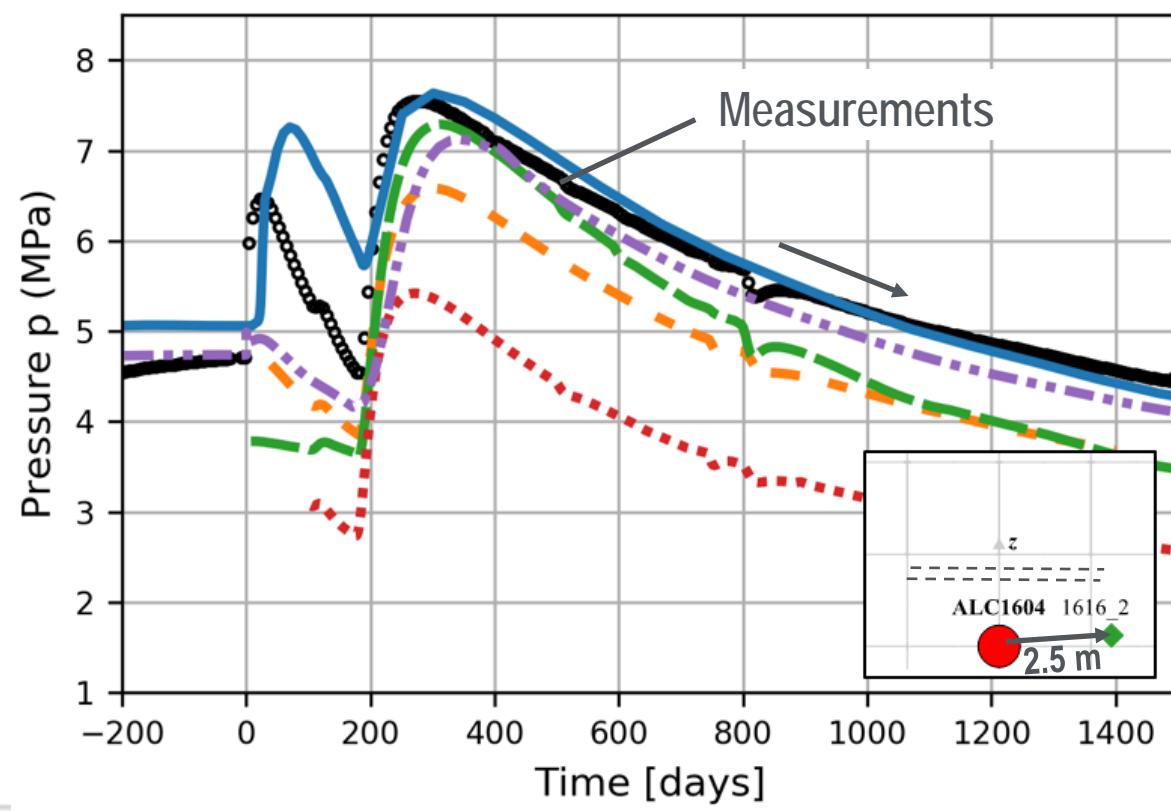
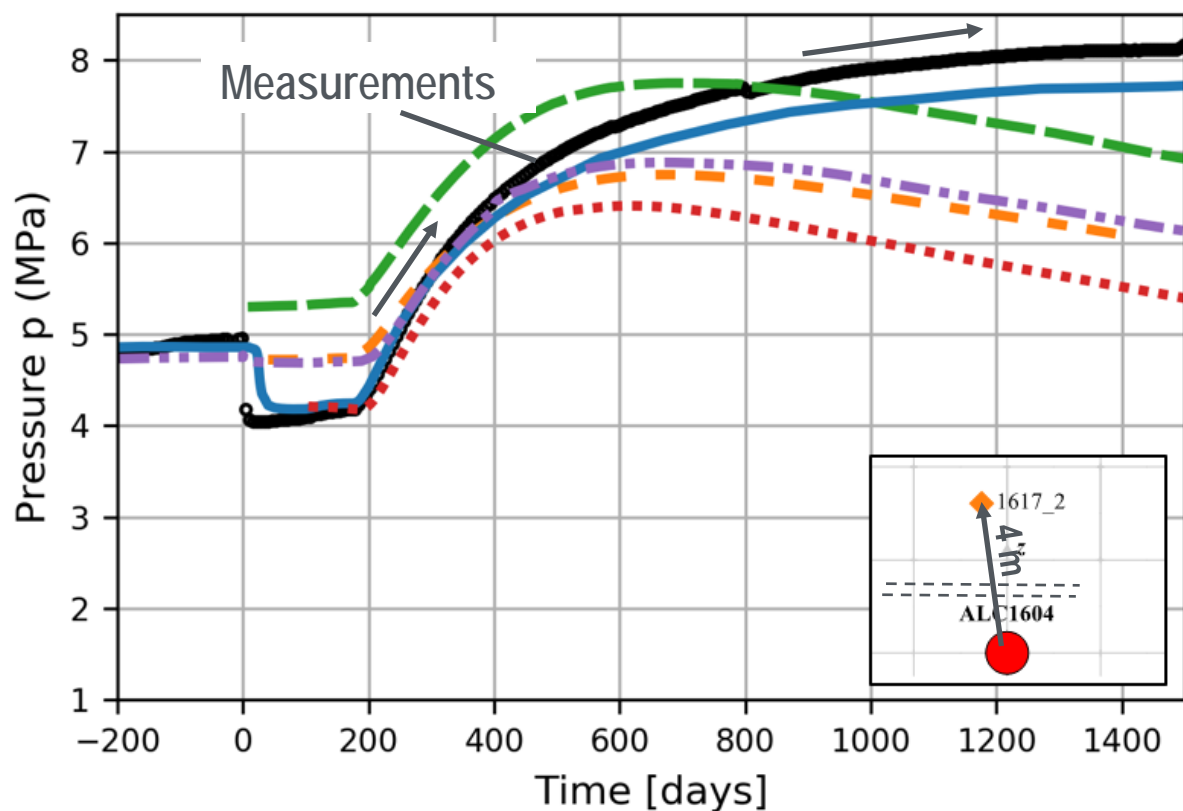


DECOVALEX Modeling Teams

- Anisotropic temperature evolution accurately predicted by all modeling teams

Sayed et al., (2021)

# Modeling of Thermal Pressurization Experiment at Bure (DECOVALEX-2019)



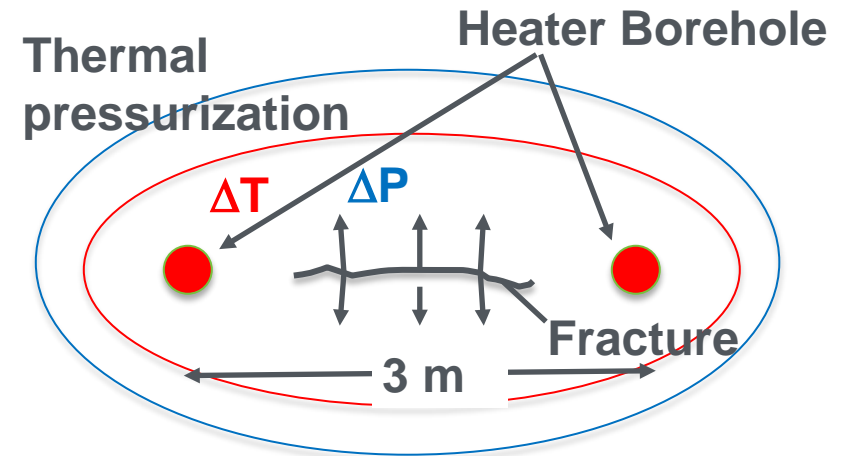
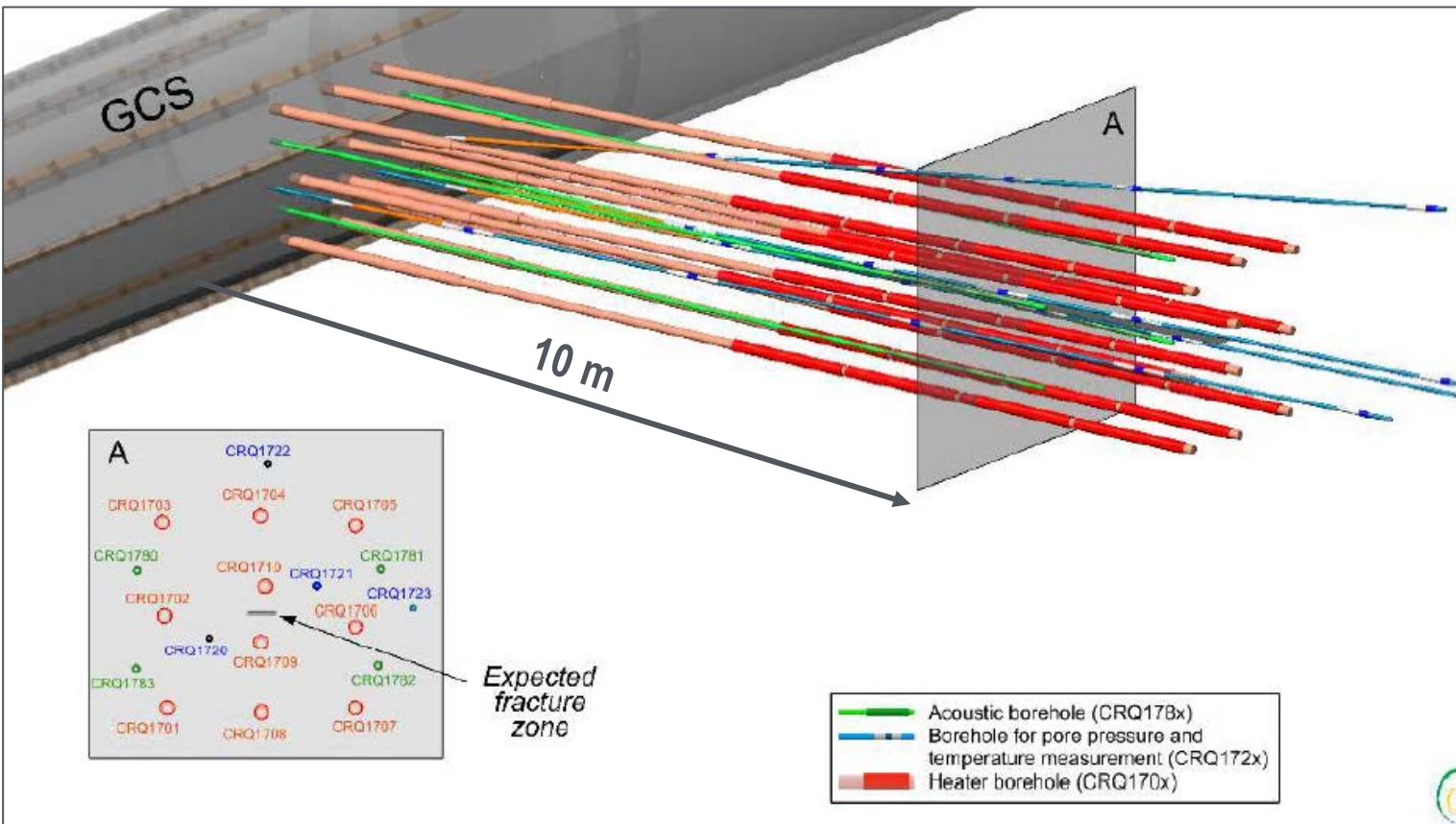
measurements    
  Andra    
  NWMO    
  Quintessa    
  UFZBGR    
  LBNL

- Some deviations between measured and modeled anisotropic pressure evolution
- Deviations attributed to complex excavation effects and spatial variability in permeability
- Quintessa (blue line) is calibrated model results

Sayed et al., (2021)



# Modeling Thermal-Pressurization Fracturing at Bure in COx claystone (Ongoing in DECOVALEX-2023)



Borehole array on tunnel wall



- Two years with heat pulses up to about 100°C
- 5 DECOVALEX-2023 modeling teams and models
- Compare temperature, pressure, stress, fracturing
- Fracturing and fracture sealing?

# Summary of Bure Argillite Modeling

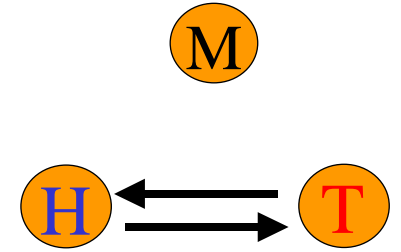
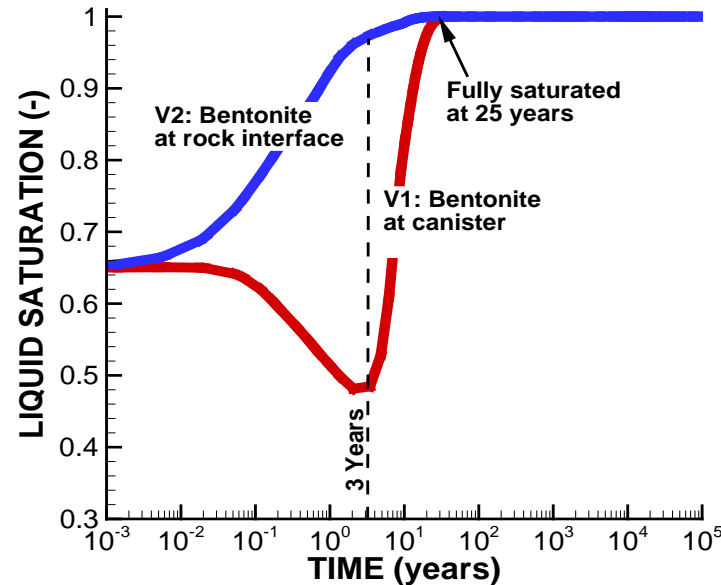
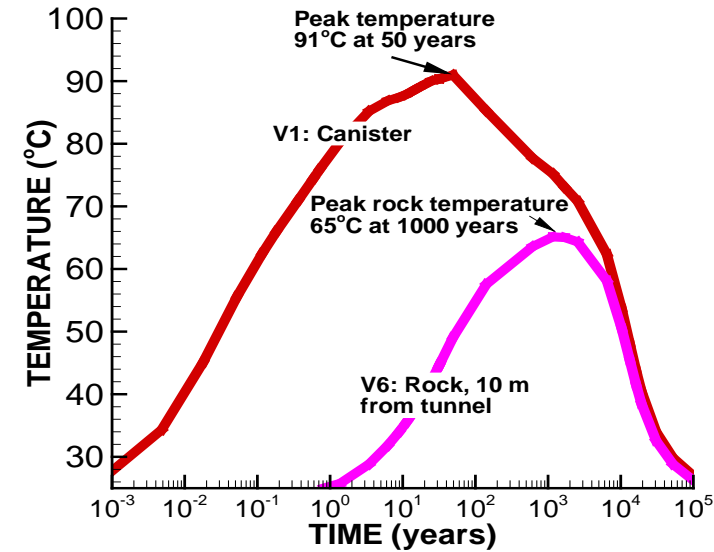
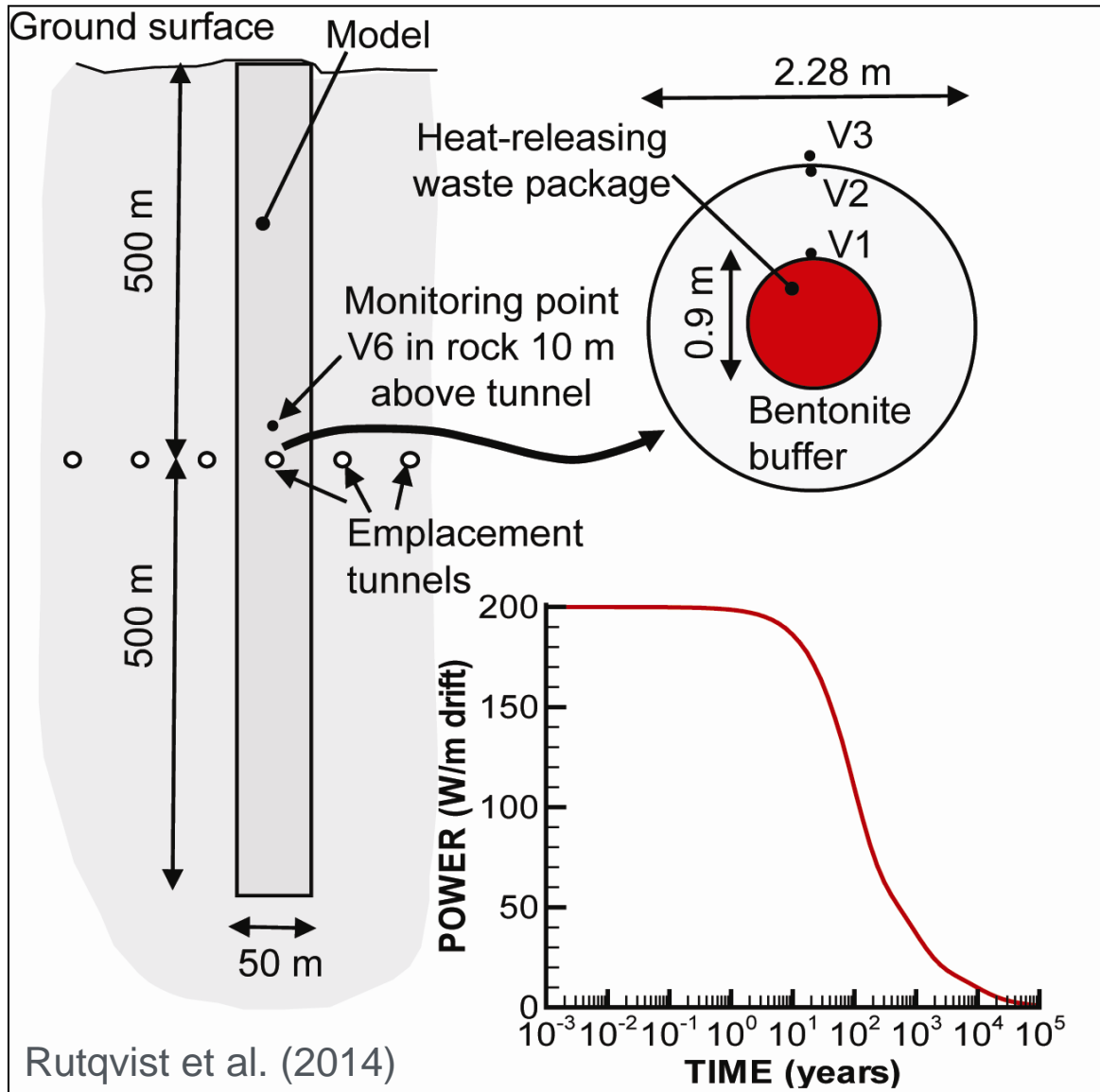
- Key parameters: anisotropic thermal conductivity and permeability, fluid and solid thermal expansion, solid-fluid storage, tensile strength
- Temperature and pressure can be predicted more confidently than mechanical responses
- Sensitivity study quantifies spatial variability in properties
- Such variability in properties can be applied for bounding predictions of the long-term repository response

# Modeling Long-term Repository Behavior

Three aspects:

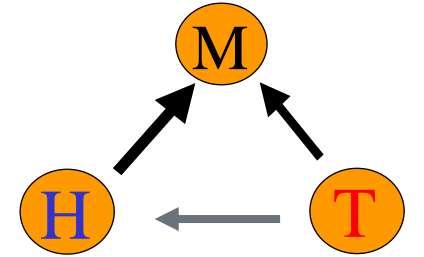
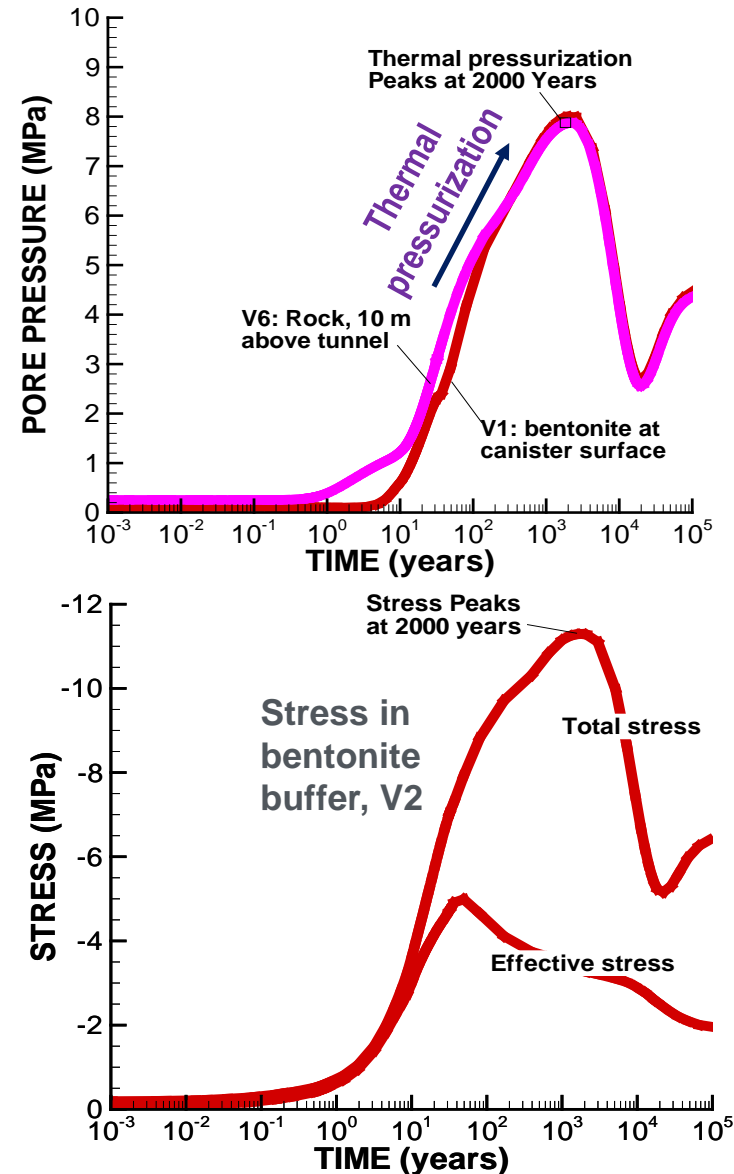
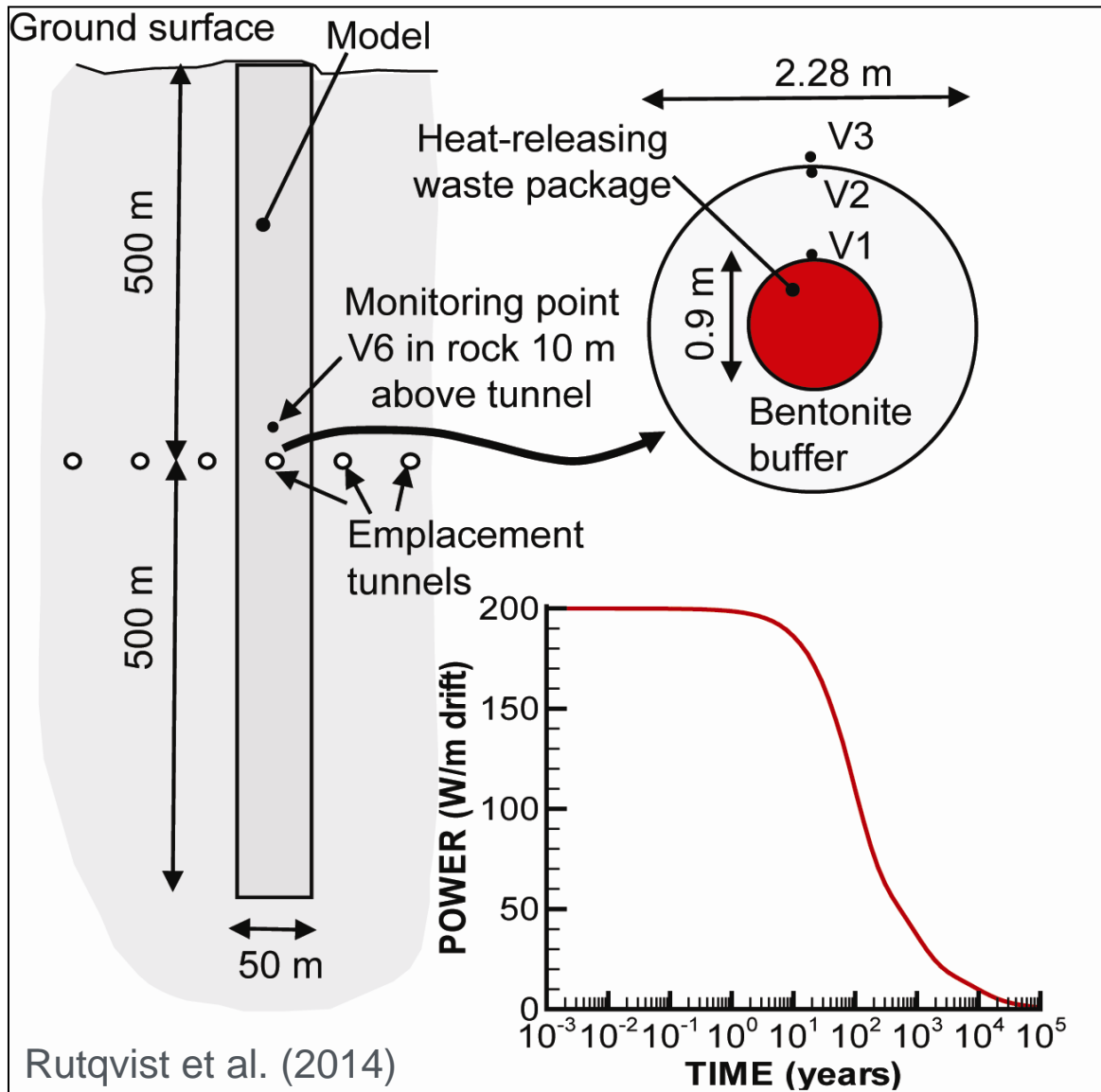
1. Repository THM responses of the argillite barrier
2. Near-field EDZ THM response
3. Impact of creep in the argillite barrier (ductile-brittle)

# Long-term Coupled Processes Simulation



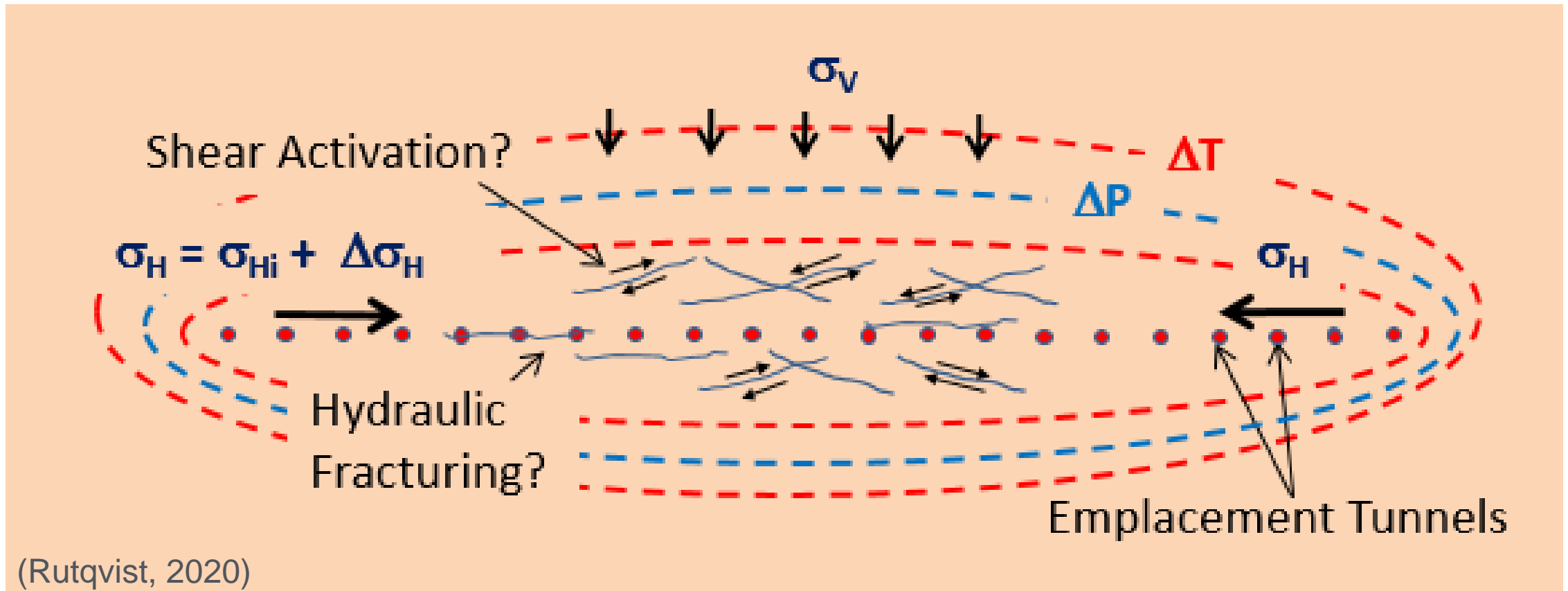
- Peak temperature?
- Time to peak temperature?
- Time to full saturation?

# Long-term Coupled Processes Simulation



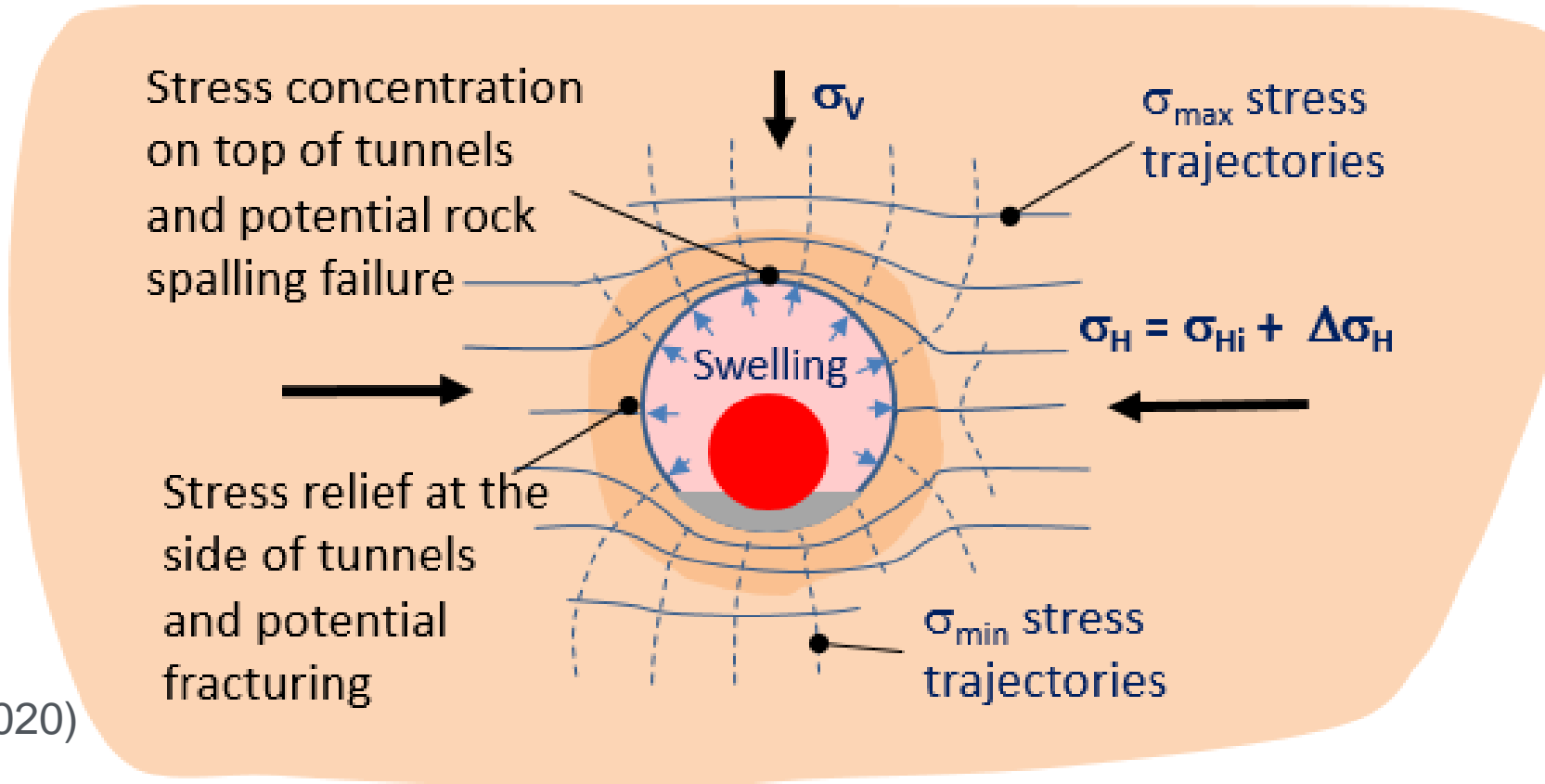
- Peak temperature?
- Time to peak temperature?
- Time to full saturation?
- Peak pressure?
- Time to peak thermal impact?
- Sufficient swelling stress?

# Repository Temperature-induced Stress Changes



- $\Delta T$  can result in high pressure, shear stress, and potential fracturing
- May become the limiting temperature for thermal management

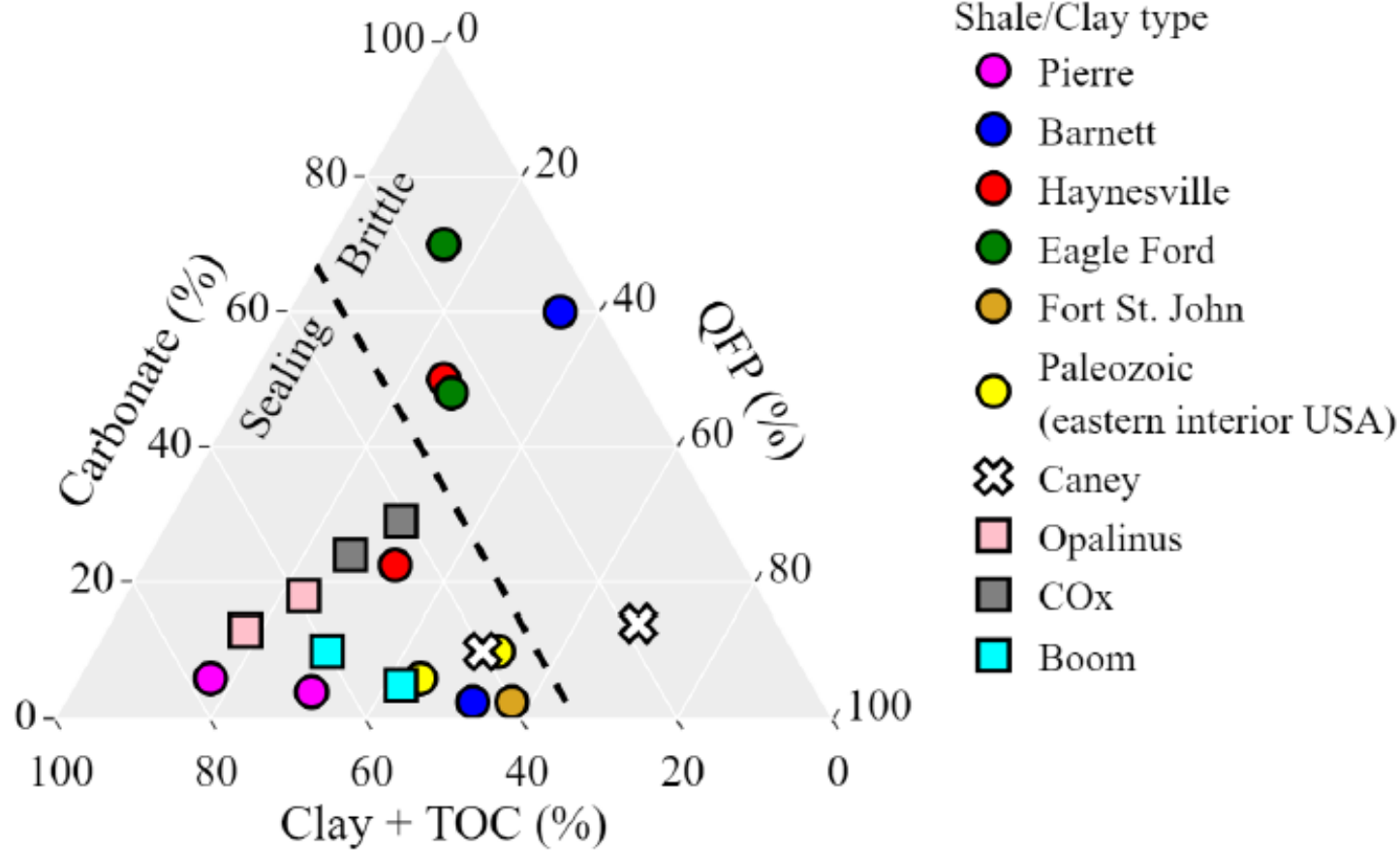
# Repository Temperature-induced Stress Changes



- Can impact EDZ thousands of years after repository closure (when repository temperature peaks)
- Important to have a supporting buffer stress at that time

# Simulating Impact of Long-Term Creep

## Sealing vs Brittle Argillite



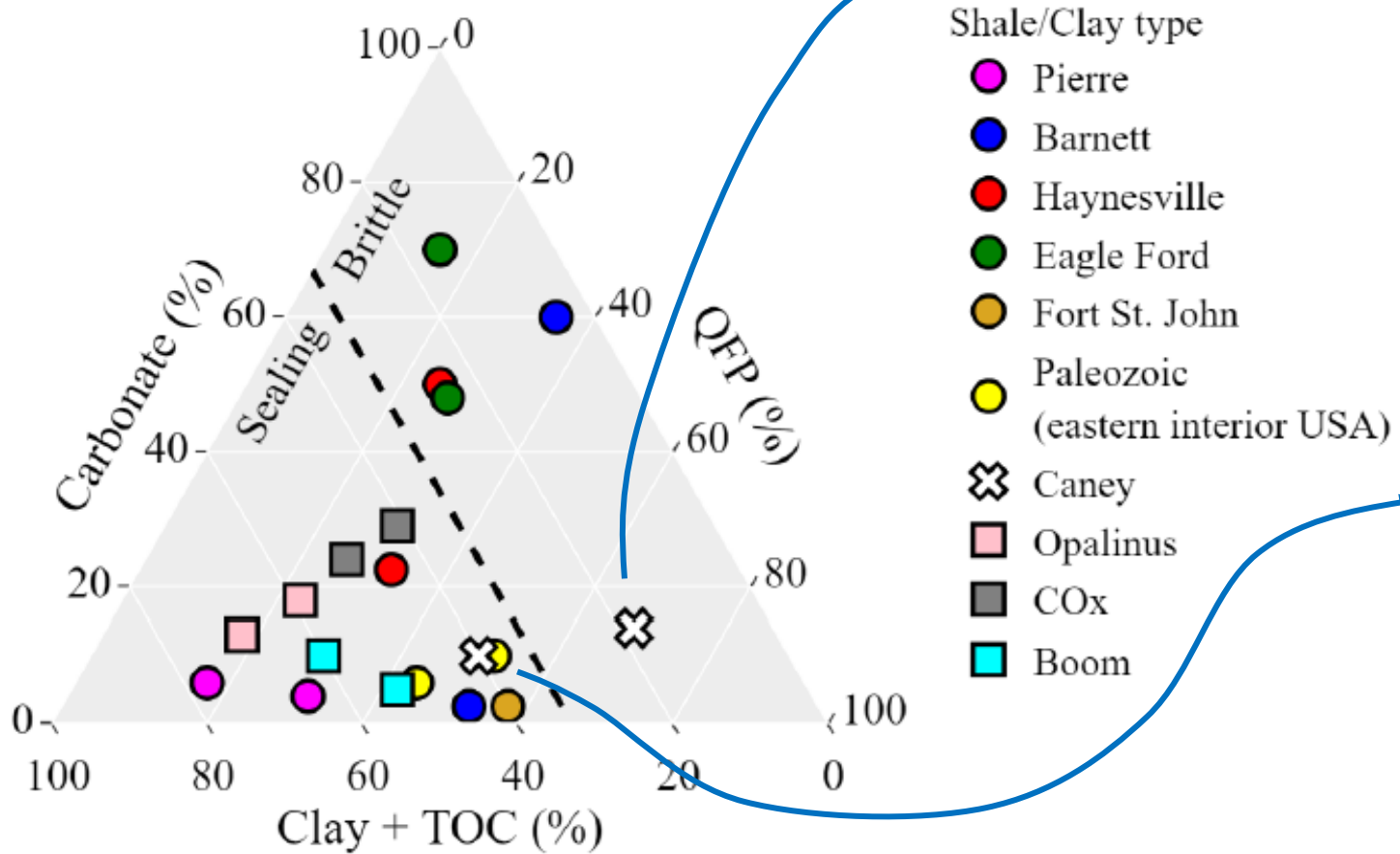
QFP = Quartz + Feldspar + Pyrite  
 TOC = Total Organic Carbon

Sasaki and Rutqvist (2022)

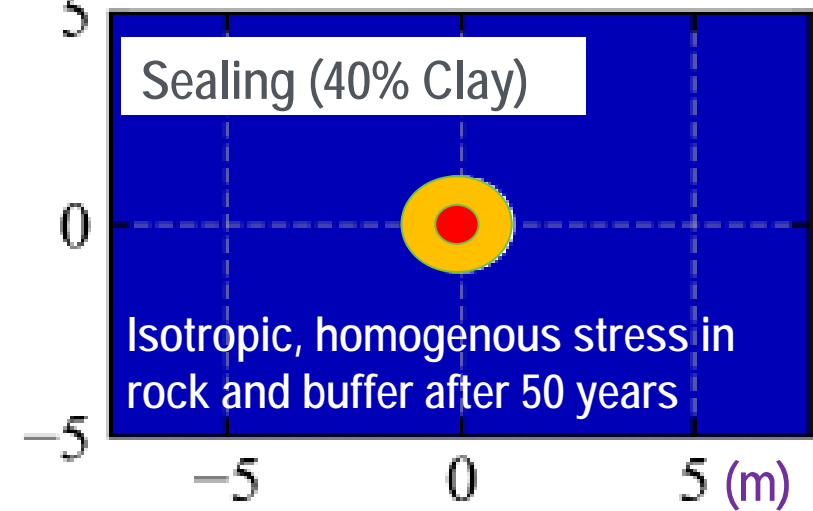
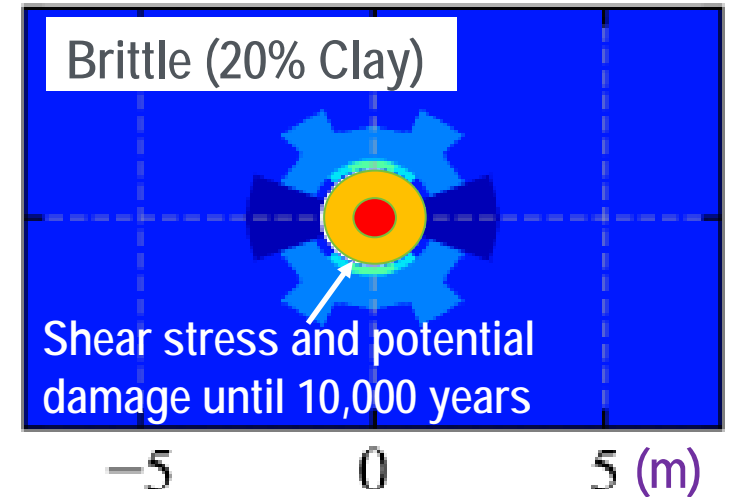


# Simulating Impact of Long-Term Creep

## Sealing vs Brittle Argillite



High clay content  $\Rightarrow$  Soft + high creep  $\Rightarrow$  self-sealing



Sasaki and Rutqvist (2022)

# Summary

- Repository coupled thermal-hydraulic-mechanical (THM) processes can have a significant impact on the argillite barrier integrity
- Field experiments at underground research laboratories have been designed to study phenomena such as thermal pressurization and fracturing
- Modeling of these experiments in DECOVALEX provides confidence in the models applied to predict these processes for a repository
- The type of argillite, whether more ductile or more brittle, could have a significant impact on the argillite barrier behavior
- High temperature would cause stronger thermal pressurization, but could also accelerate creep and sealing of clay-rich shale
- Coupled THM modeling can be applied in the thermal management and repository design to assure argillite barrier integrity

# References

- Bossart, P., Meier, P.M., Moeri, A., Trick, T., Mayor, J.C., Geological and hydraulic characterisation of the excavation disturbed zone in the Opalinus Clay of the Mont Terri Rock Laboratory. *Eng. Geol.* 66 (1–2), 19–38. [https://doi.org/10.1016/S0013-7952\(01\)00140-5](https://doi.org/10.1016/S0013-7952(01)00140-5) (2002).
- Rutqvist J. Thermal Management Associated with Geologic Disposal of Large Spent Nuclear Fuel Canisters in Tunnels with Thermally Engineered Backfill. *Tunnelling and Underground Space Technology*. Volume 102, August (2020), 103454. <https://doi.org/10.1016/j.tust.2020.103454>.
- Rutqvist J. An overview of TOUGH-based geomechanics models. *Computers & Geosciences*, 108, 56–63 (2017).
- Rutqvist J. Coupled Thermo-Hydro-Mechanical Behavior of Natural and Engineered Clay Barriers. In Tournassat, Steefel, Bourg and Bergaya editors. *Natural and Engineered Clay Barriers*. Elsevier. pp. 329-255 (2015).
- Rutqvist J. Status of the TOUGH-FLAC simulator and recent applications related to coupled fluid flow and crustal deformations. *Computers & Geosciences*, 37, 739–750 (2011).
- Rutqvist J., Zheng L., Chen F, Liu H.-H. and Birkholzer J. Modeling of Coupled Thermo-Hydro-Mechanical Processes with Links to Geochemistry Associated with Bentonite-Backfilled Repository Tunnels in Clay Formations. *Rock Mechanics and Rock Engineering*, 47, 167–186 (2014).
- Rutqvist J., Wu Y.-S., Tsang C.-F. and Bodvarsson G. A Modeling approach for analysis of coupled multiphase fluid flow, heat transfer, and deformation in fractured porous rock. *International Journal of Rock Mechanics and Mining Sciences*, 39, 429-442 (2002).
- Sasaki T. and Rutqvist J. Effects of time-dependent deformation of shale on the integrity of a geological nuclear waste repository. *International Journal of Rock Mechanics and Mining Sciences*, 158 (2022). <https://doi.org/10.1016/j.ijrmms.2022.105206>.
- Seiphoori A. Thermo-hydro-mechanical characterisation and modelling of Wyoming granular bentonite. NAGRA, Technical Report NTB 15-05 (2015).
- Seyedi D.M., Plúa C., Vitel M., Armand G., Rutqvist J., Birkholzer J., Xu H., Guo R., Thatcher K.E., Bond A.E., Wang W., Nagel T., Shao H., Kolditz O. Upscaling THM modelling from small-scale to full-scale in-situ experiments in the Callovo-Oxfordian claystone. *International Journal of Rock Mechanics and Mining Sciences* 144, 104582 (2021). <https://doi.org/10.1016/j.ijrmms.2020.104582>.
- Xu H., Rutqvist J., Plúa C., Armand G., Birkholzer J. Modeling of Thermal Pressurization in Tight Claystone using Sequential THM Coupling: Benchmarking and Validation against In-situ Heating Experiments in COx Claystone. *Tunnelling and Underground Space Technology*. 103, 103428. (2020) <https://doi.org/10.1016/j.tust.2020.103428>.

# Acronyms and Abbreviations

ALC	Micro-tunnel experiment at Bure
ANDRA	National Radioactive Waste Management Agency (France)
COx	Callovo-Oxfordian claystone
DECOVALEX	DEvelopment of COupled Models and their VALidation Against EXperiments
EBS	Engineered Barrier System
EDZ	Excavation Damage Zone (or Excavation Disturbed Zone)
FE	Full-scale Emplacement Experiment at Mont Terri
FLAC	Fast Lagrangian Analysis of Continua
LBNL	Lawrence Berkeley National Laboratory
NAGRA	Swiss waste management organization
NWMO	Nuclear Waste Management Organisation (Canada)
QFP	Quartz + feldspar + pyrite
Swisstopo	Federal Office of Topography (Switzerland)
THM	Thermo-hydro-mechanical
TOC	Total Organic Carbon
TOUGH	Transport Of Unsaturated Groundwater and Heat
UFCBGR	Federal Institute for Geosciences and Natural Resources and Helmholtz Centre for Environmental Research (Germany)