

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

U.S. Nuclear Waste Technical Review Board  
Fact Finding Meeting  
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# Argillite Coupled Processes Modeling Team

## Lawrence Berkeley National Laboratory

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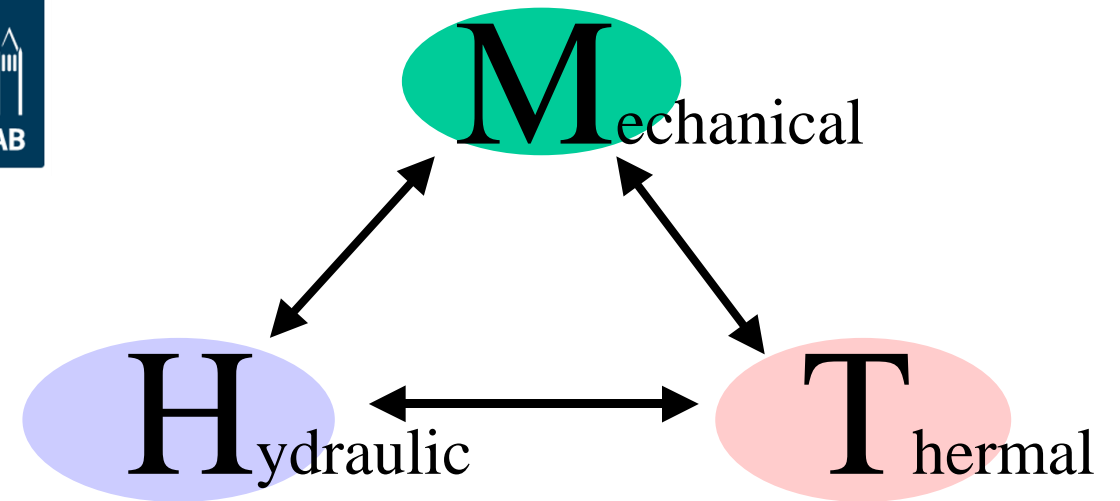


## International Collaboration

Task Leads from NAGRA and SwissTopo, Switzerland, for Mont Terri heater experiments, in Opalinus Clay.

Task Leads from ANDRA, France, for heater experiments at Bure underground research laboratory in COx Claystone.

DECOVALEX Research Teams (> 10 international teams)



T = Thermal

H = Hydraulic

M = Mechanical

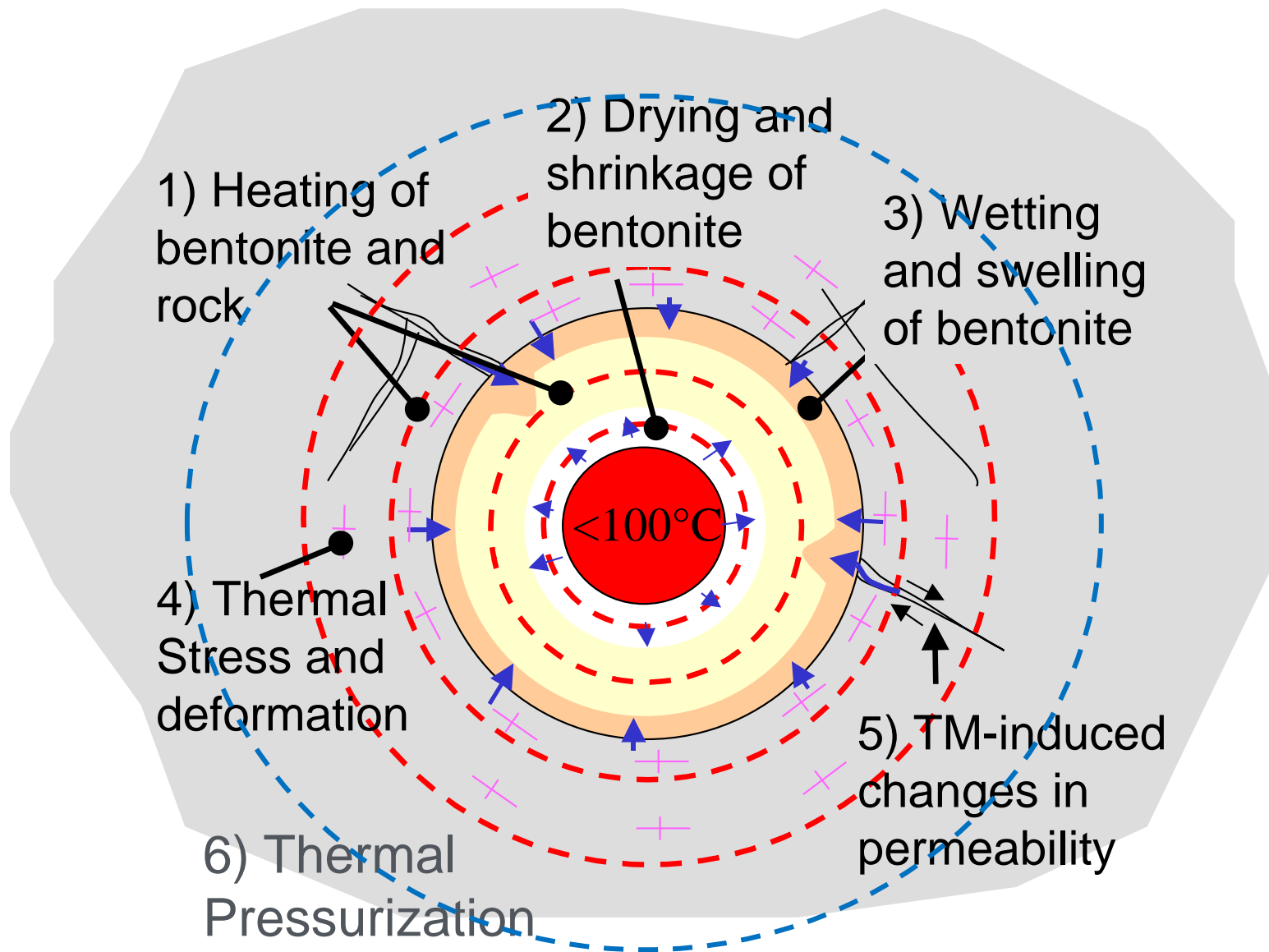
THM = Thermo-hydro-mechanical

P = Pressure

T = Temperature

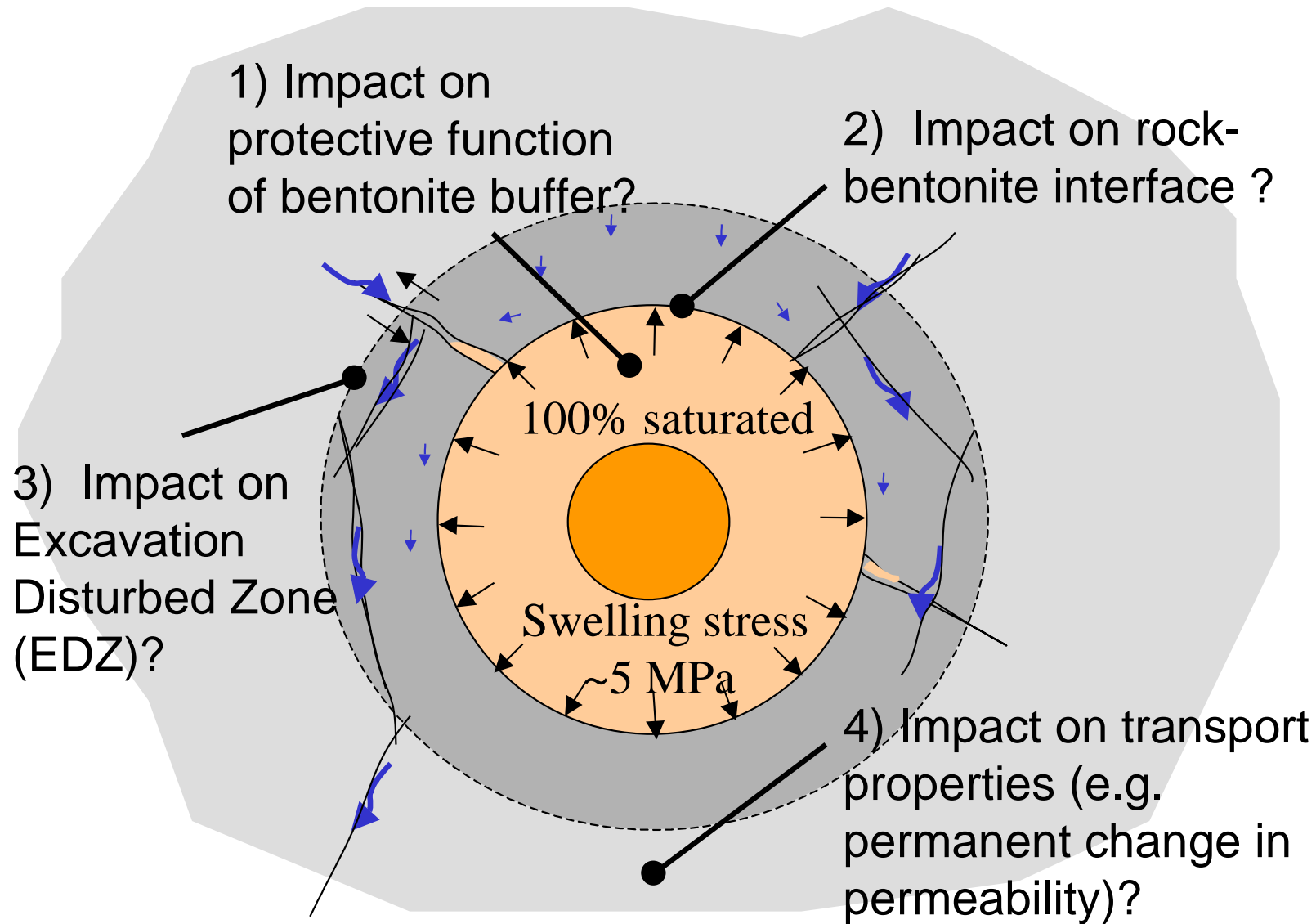
$\sigma$  = Stress

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



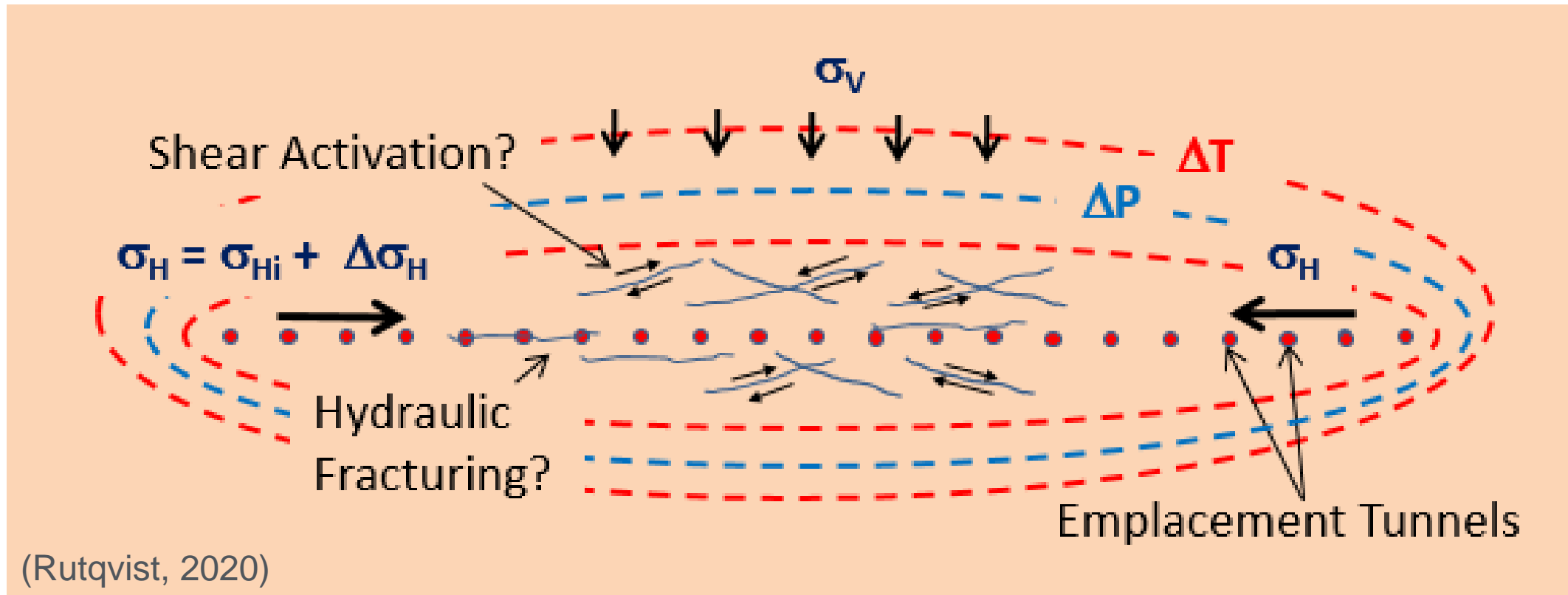
(Rutqvist, 2015)

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



(Rutqvist, 2015)

# Repository THM-Induced Stress Changes

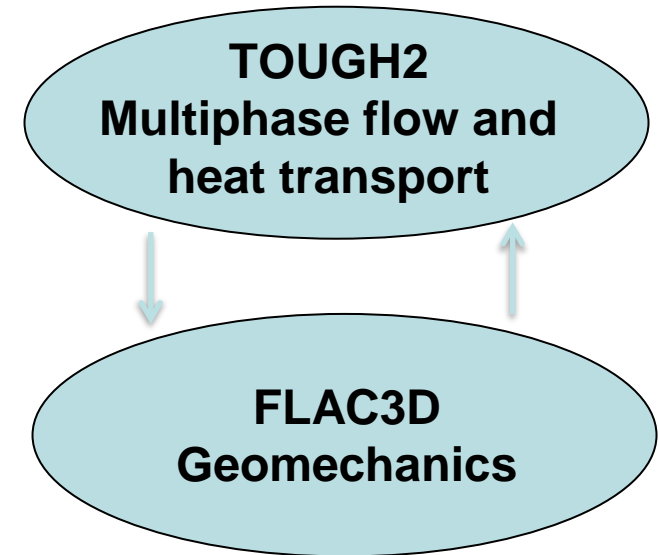


- Repository temperature change ( $\Delta T$ ) results in thermal pressurization ( $\Delta P$ )
- $\Delta T$  and  $\Delta P$  results in thermal stress and poro-elastic stress ( $\Delta\sigma_H$ )
- **Impact on host rock integrity? (Fracturing?, Shear?, Opening of flow paths?)**

# 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

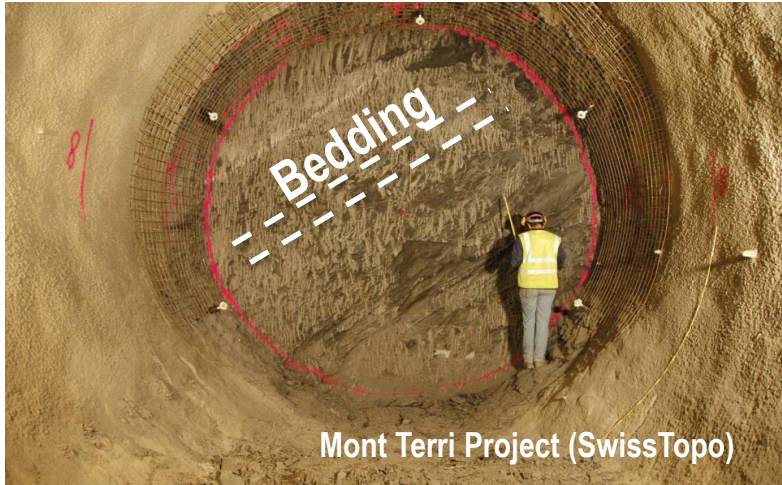


(Rutqvist et al., 2002; Rutqvist 2011; 2017)

- 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

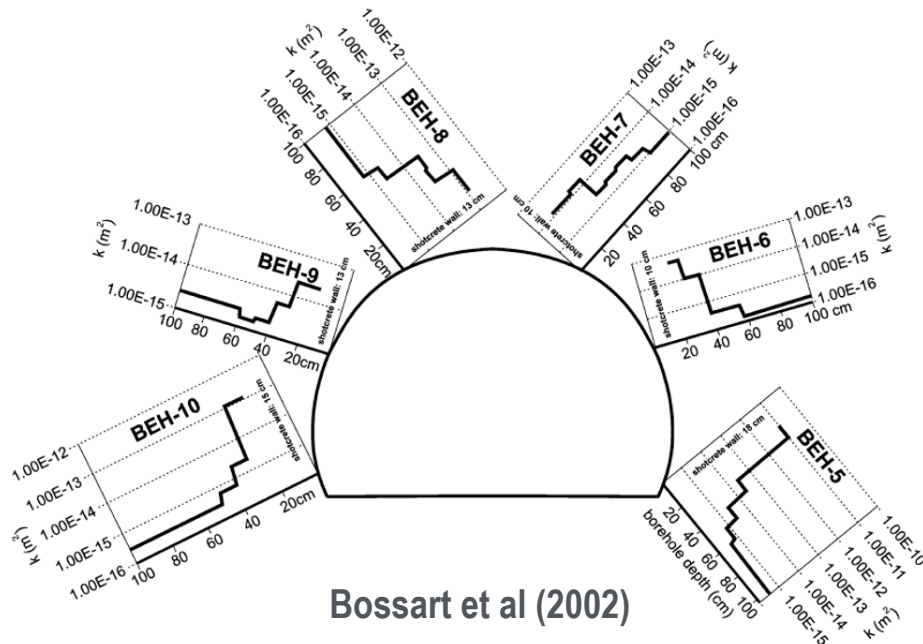


## 1) Anisotropic THM properties

- 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)



# Model Validation

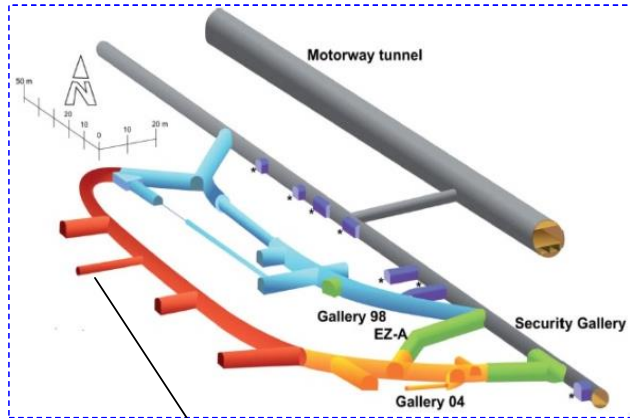
Three examples of modeling of field experiments:

1. **Full Scale Emplacement Experiment in Opalinus Clay at Mont Terri Laboratory, Switzerland**
2. **Heated micro-tunnel experiment in CO<sub>x</sub> Claystone at Bure, France**
3. **Thermal-pressurization fracturing experiment in Cox Claystone at Bure, France**



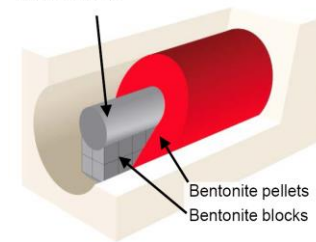
# Modeling Mont Terri Full-Scale Emplacement Experiment (DECOVALEX-2023)

## Site



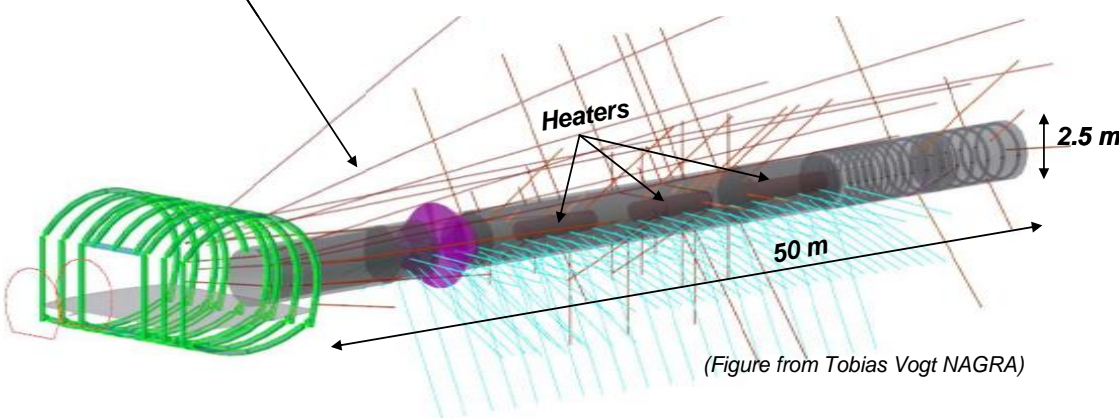
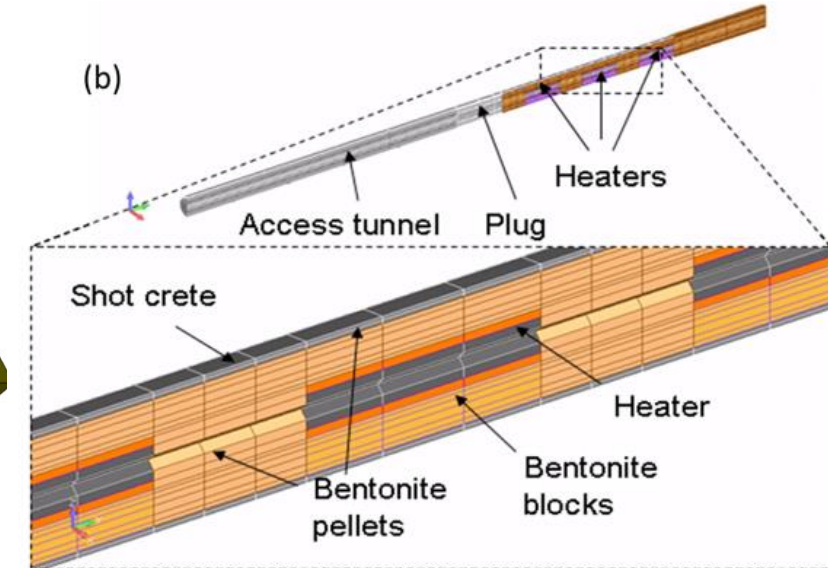
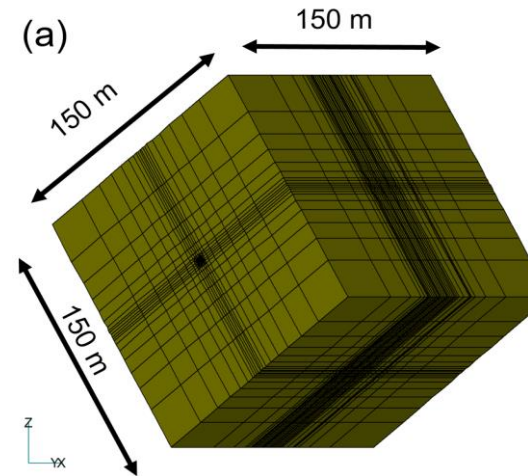
NAGRA's HLW emplacement concept

in 'reality': Canister  
for FE: Heater



Full-scale  
15-20 years of heating  
Granular bentonite emplacement

## Numerical Model

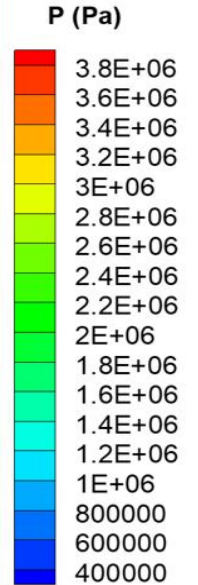
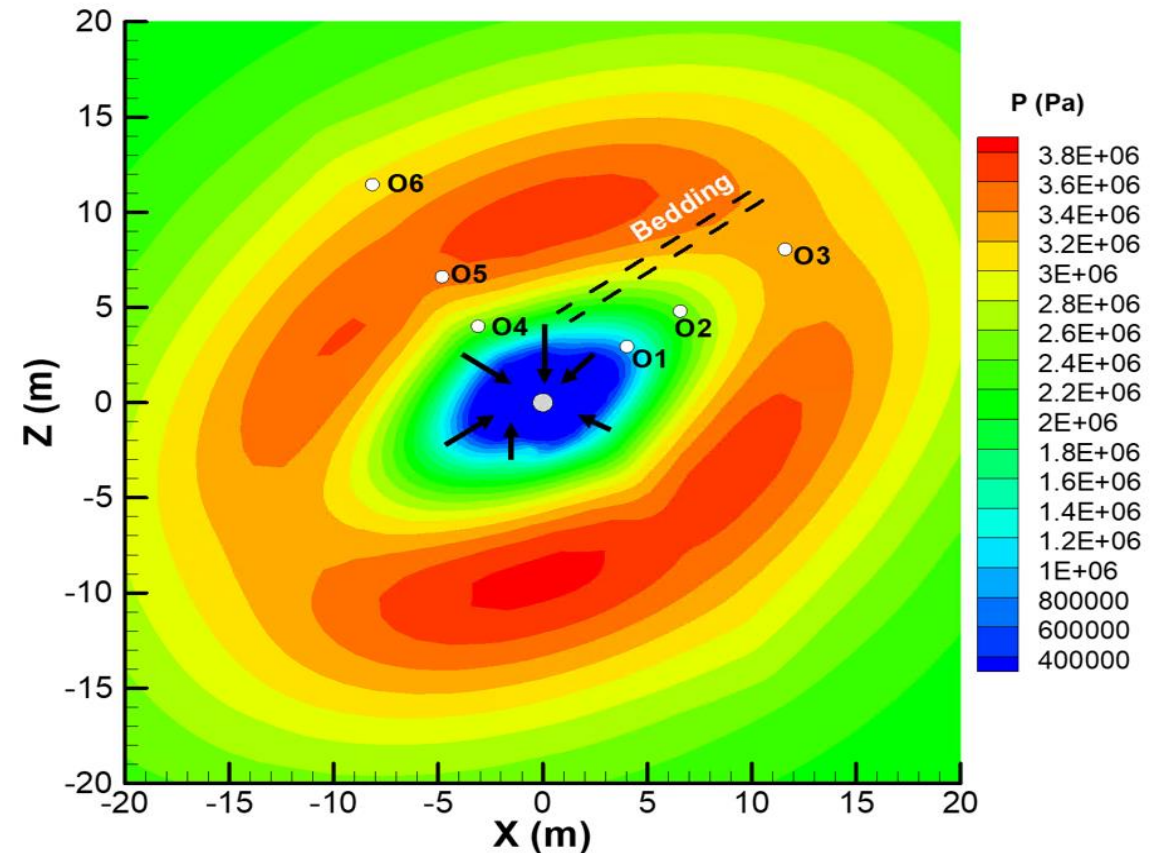
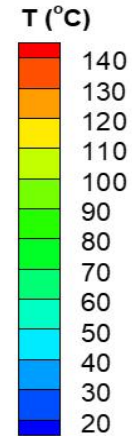
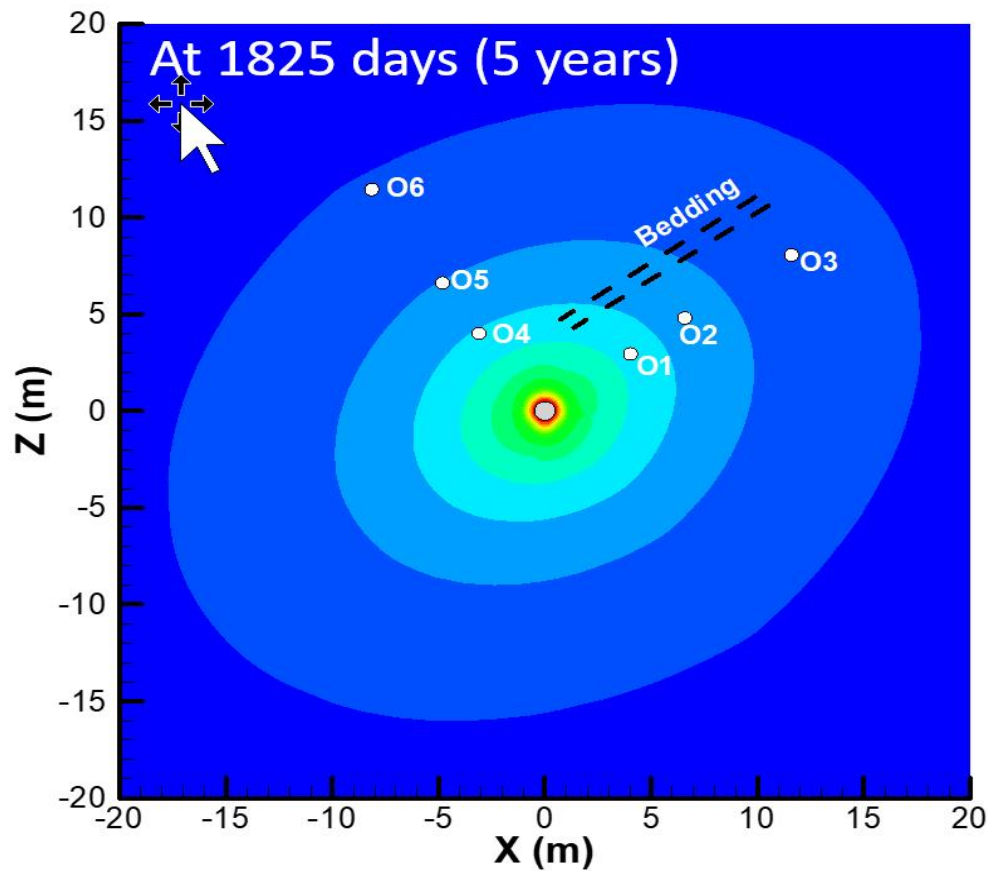


(Figure from Tobias Vogt NAGRA)

- 15-20 years of heating
- Temperature up to 140°C in bentonite

- 9 Modeling Teams in DECOVALEX-2023
- Comparison with five years of field data is ongoing
- Predict thermal pressurization and interaction with bentonite buffer

# Modeling Mont Terri Full-Scale Emplacement Experiment (DECOVALEX-2023)

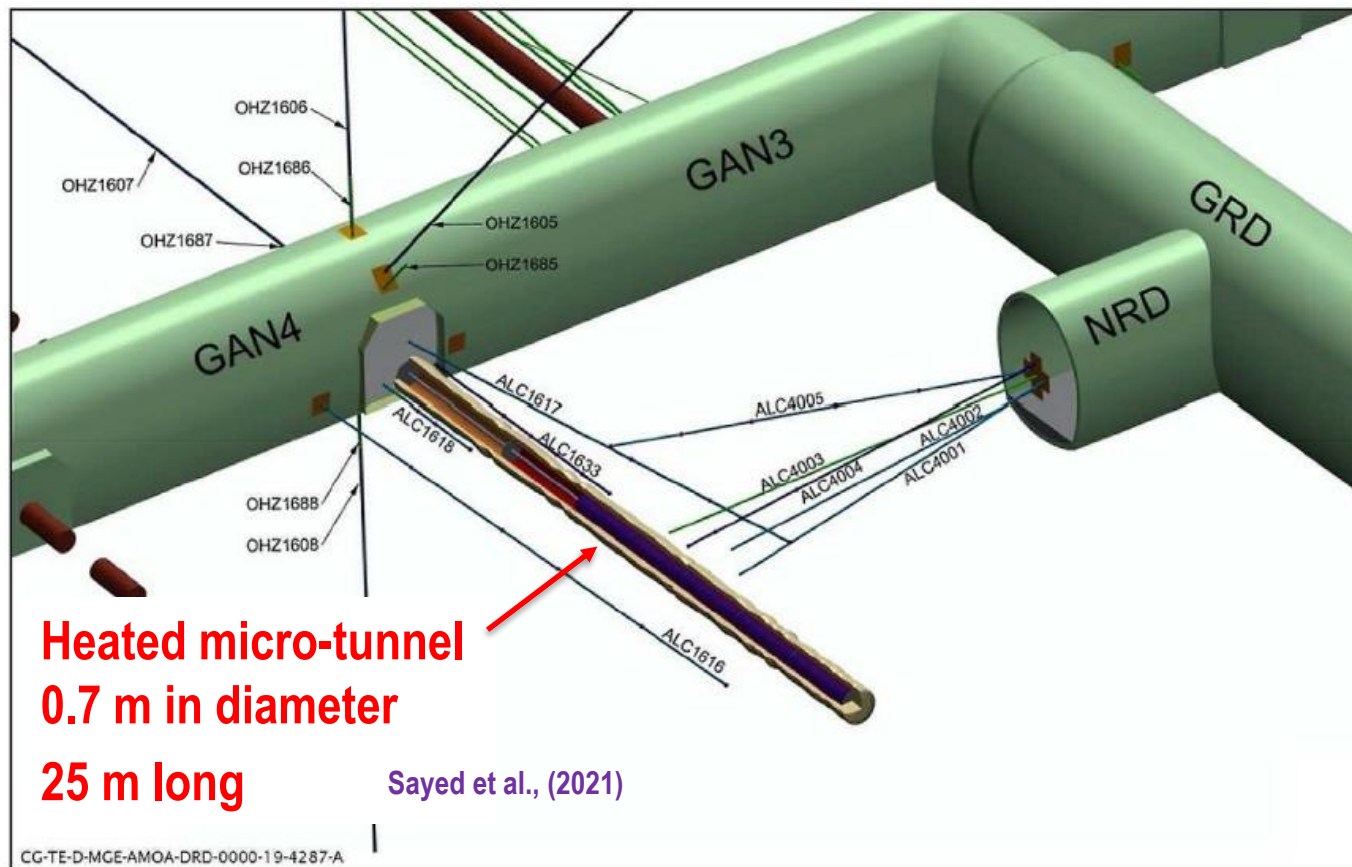


- Temperature and pressure responses are anisotropic
- Flow and suction into bentonite has a significant impact on pressure response near the tunnel
- Key parameters: permeability, fluid thermal expansion coefficient, porous media compressibility



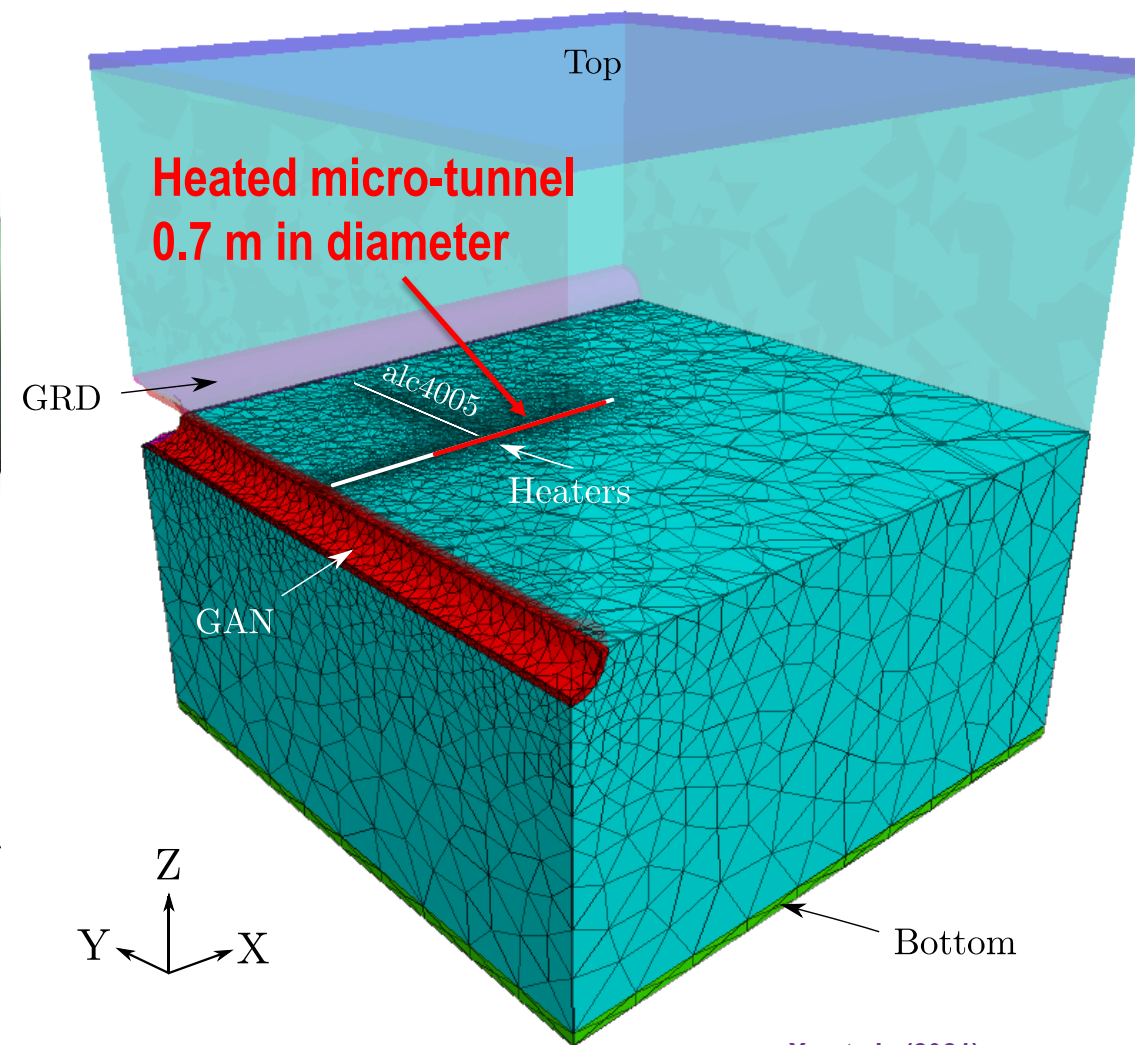
# Modeling of Thermal Pressurization Experiment at Bure (DECOVALEX-2019)

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



- Four years of heating up to about 50°C
- 5 DEOCOVALEX-2019 modeling teams and models
- Compare temperature and pressure responses

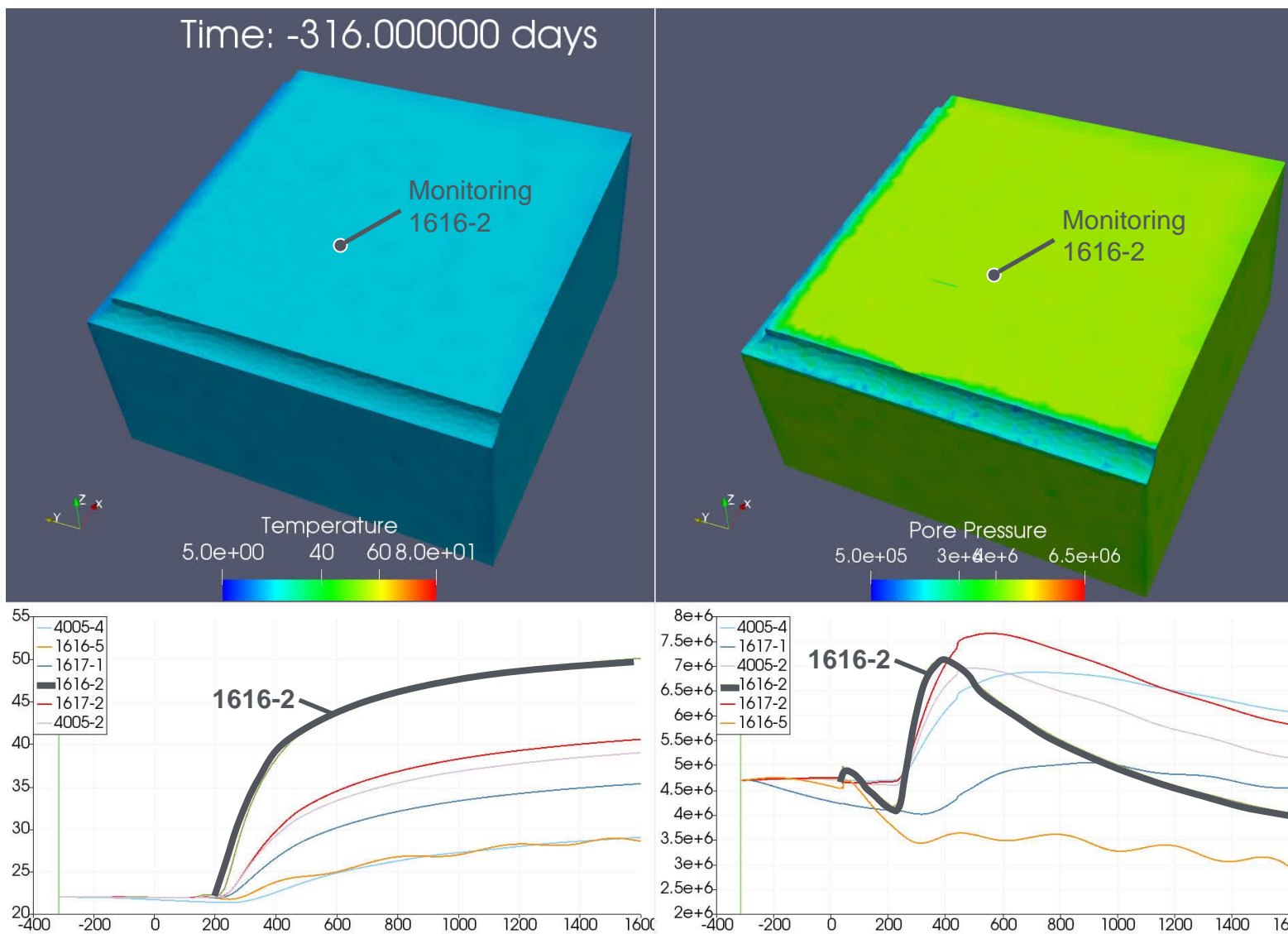
## Numerical Model



Xu et al., (2021)

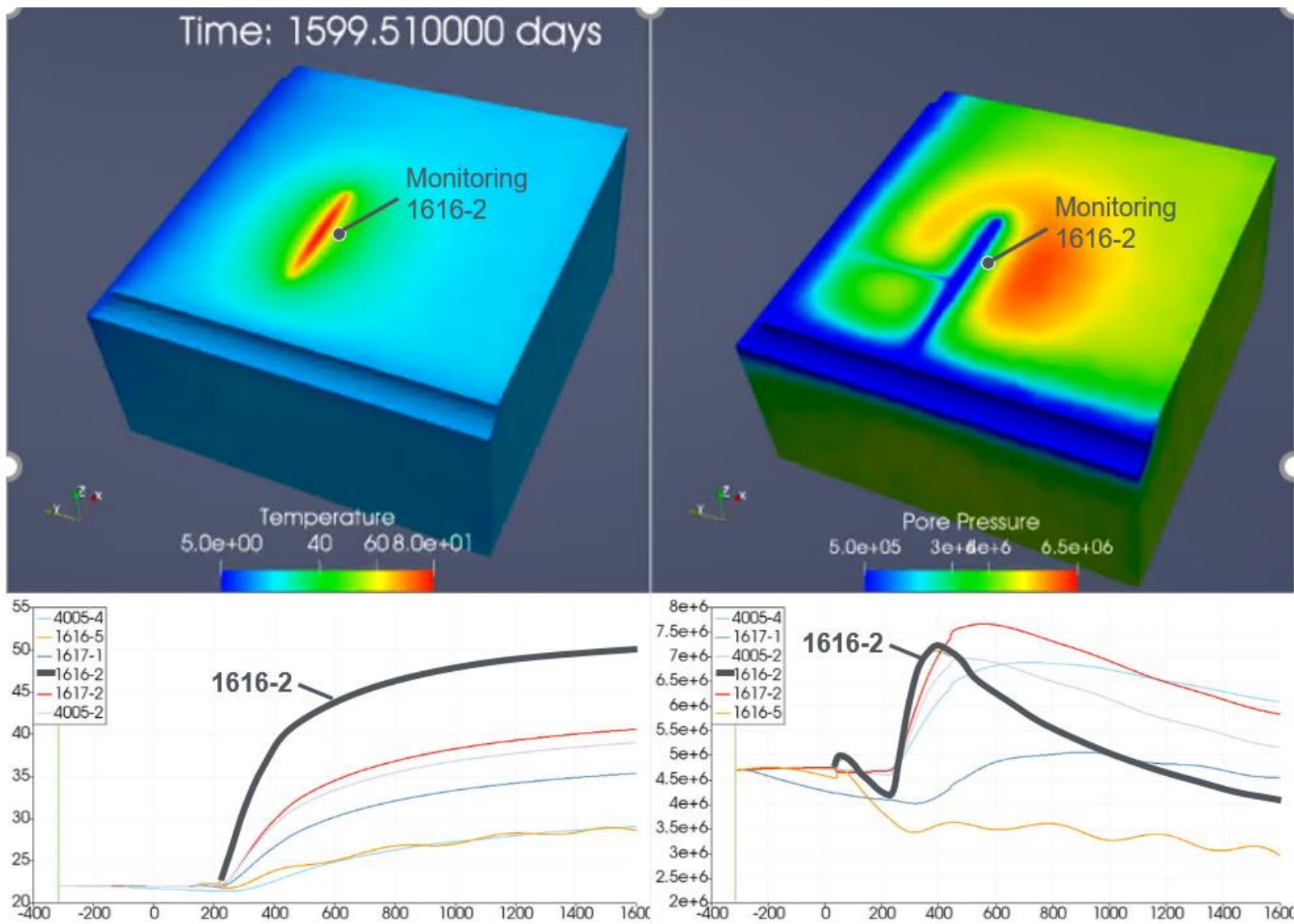
# Modeling of Thermal Pressurization Experiment at Bure (DECOVALEX-2019)

A movie of thermal pressurization



Xu et al., (2021)

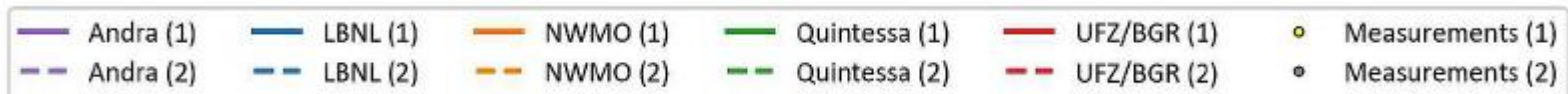
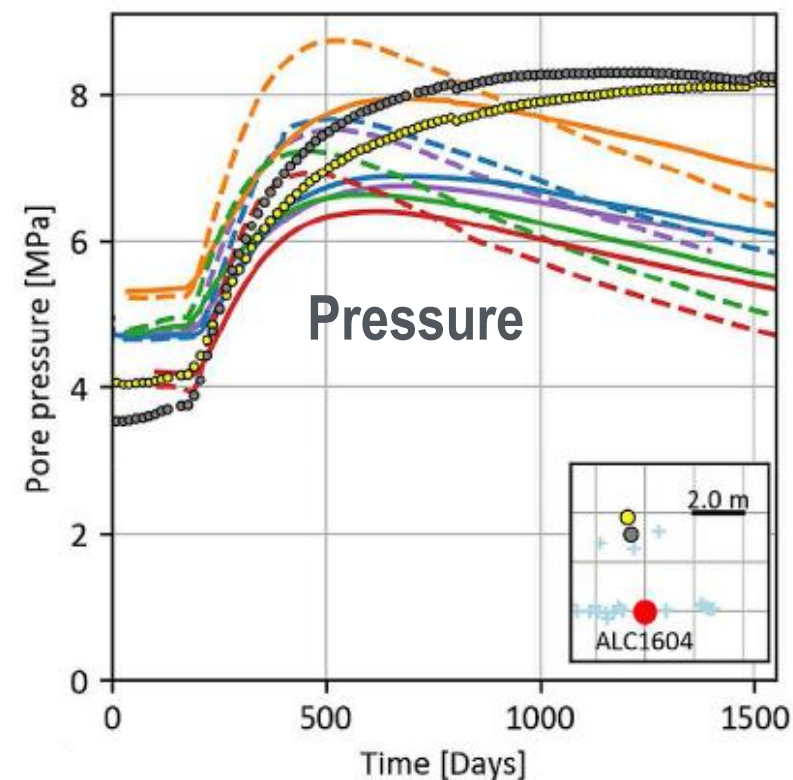
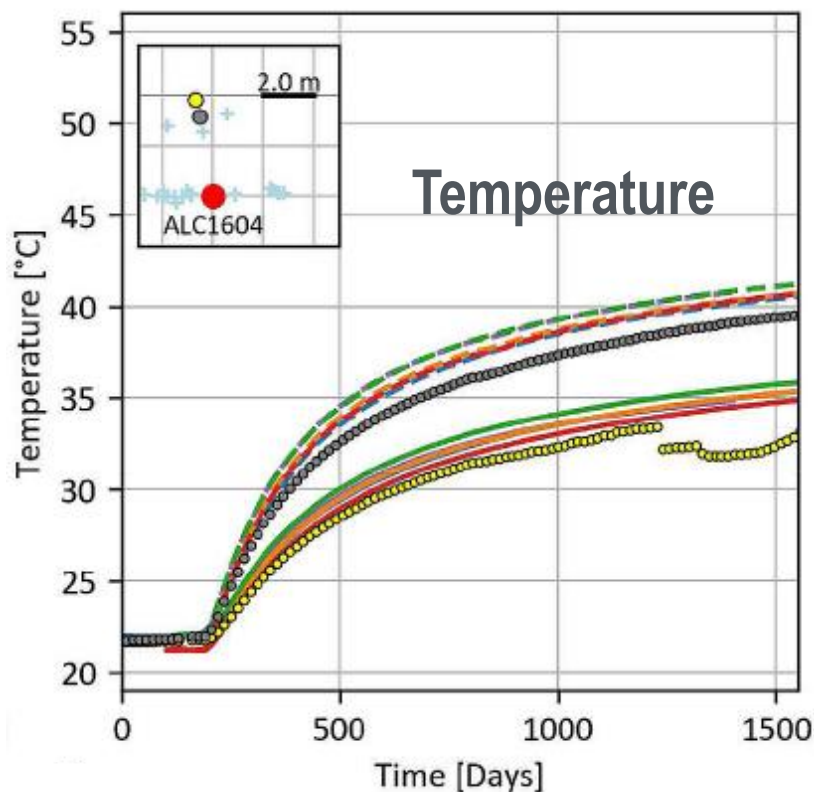
# Modeling of Thermal Pressurization Experiment at Bure (DECOVALEX-2019)



Xu et al., (2021)



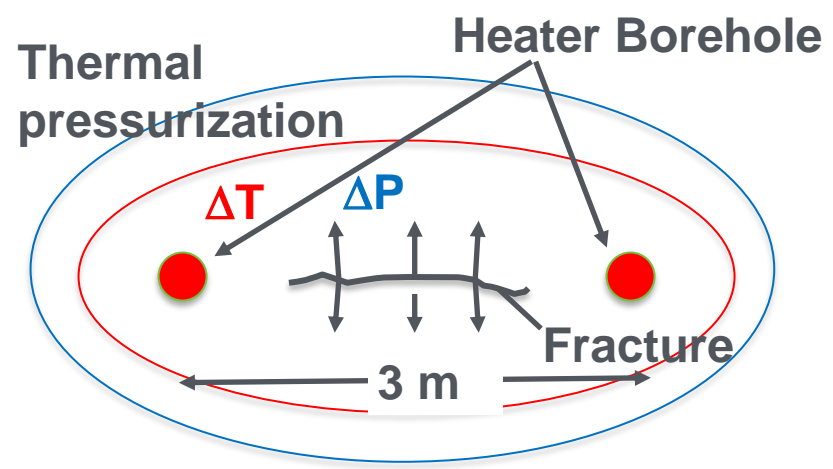
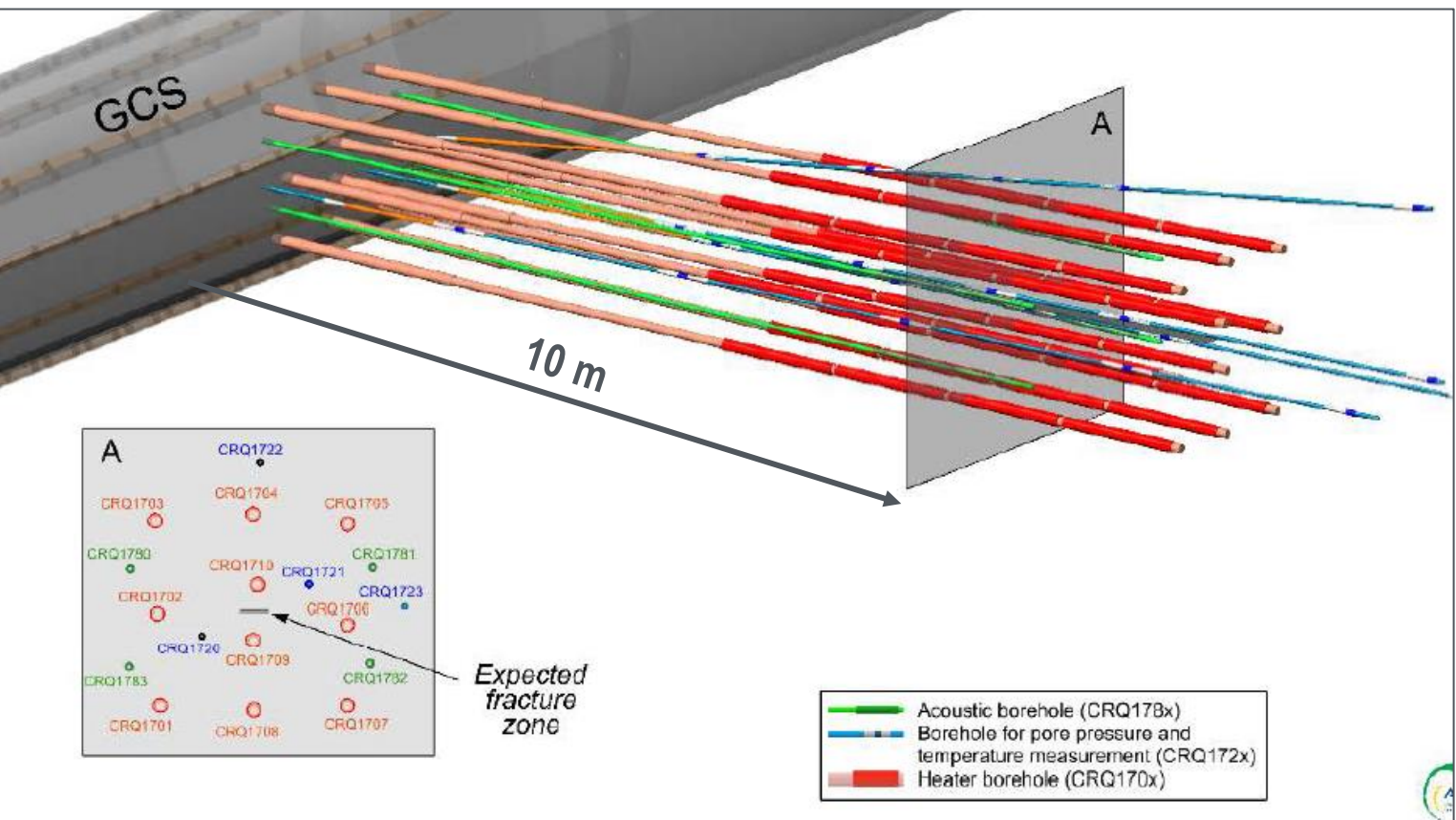
# Modeling of Thermal Pressurization Experiment at Bure (DECOVALEX-2019)



Sayed et al., (2021)

- Temperature accurately predicted while pressure response deviate at later times for monitoring points located away from the tunnel
- Pressure much less than the least principal stress magnitude (far from hydro-fracturing)

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



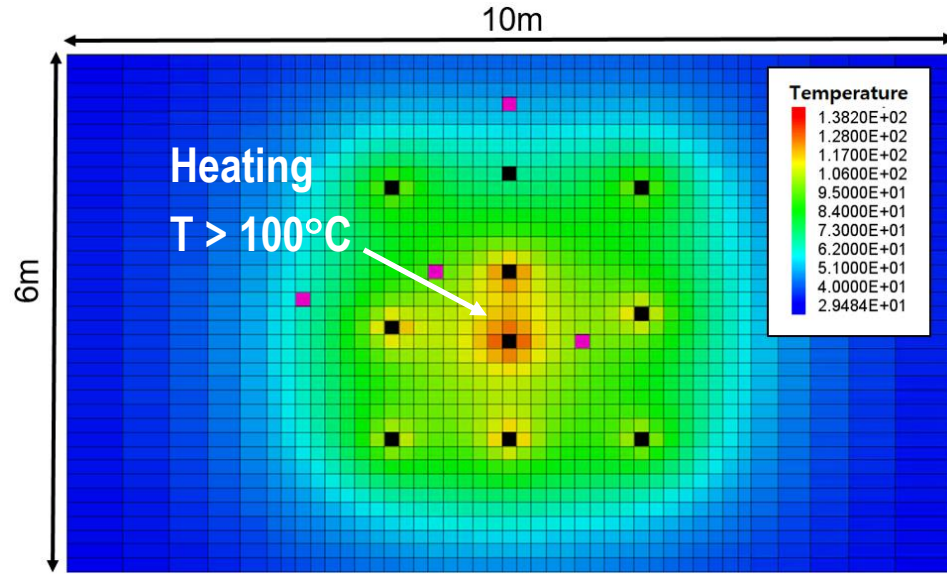
Borehole array on tunnel wall



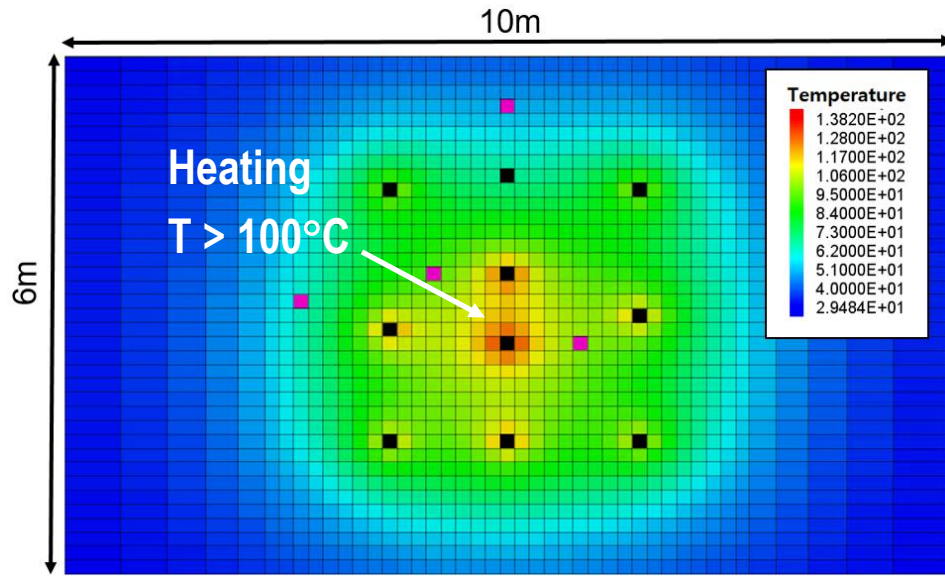
- Two years with heat pulses up to about 100°C
- 5 DEOCOVALEX-2023 modeling teams and models
- Compare temperature, pressure, stress, fracturing



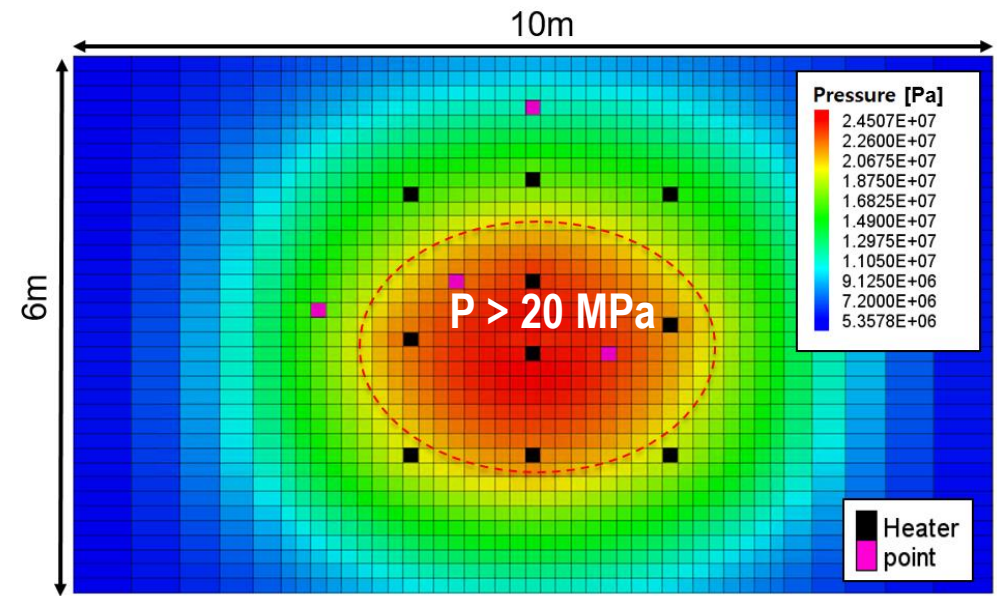
# Modeling Thermal-Pressurization Fracturing at Bure in CO<sub>x</sub> claystone (DECOVALEX 2023)



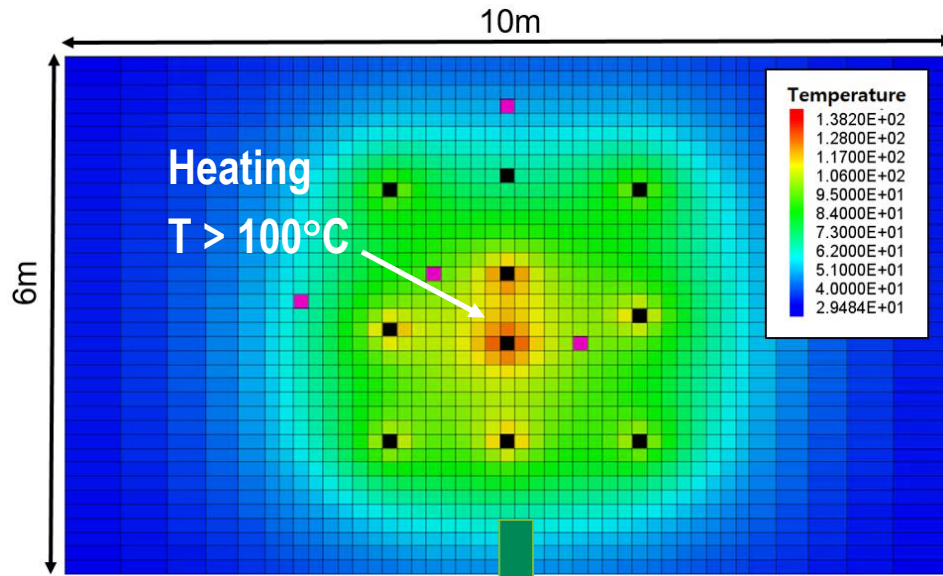
# Modeling Thermal-Pressurization Fracturing at Bure in CO<sub>x</sub> claystone (DECOVALEX 2023)



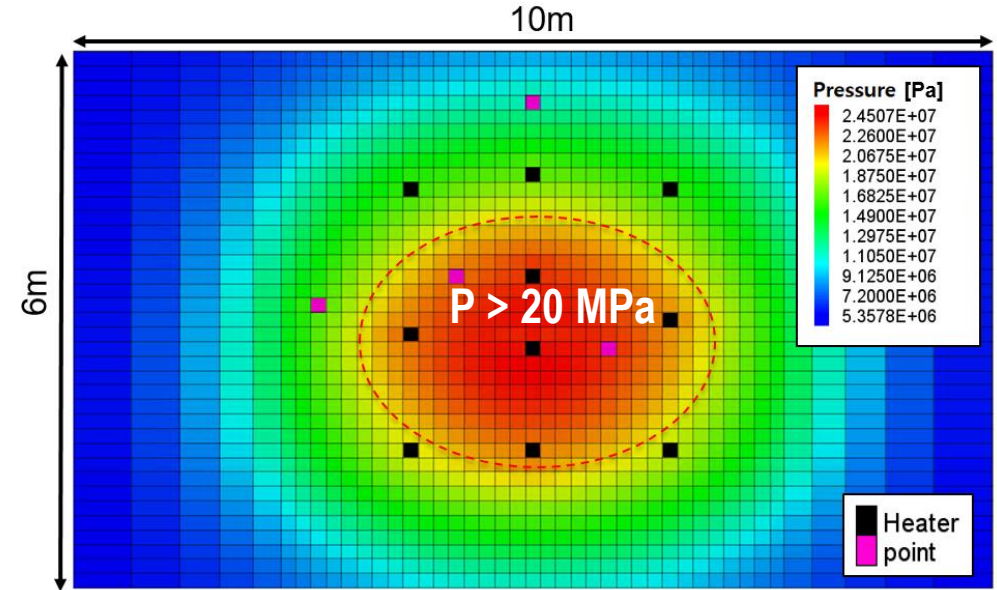
Thermal  
Pressurization



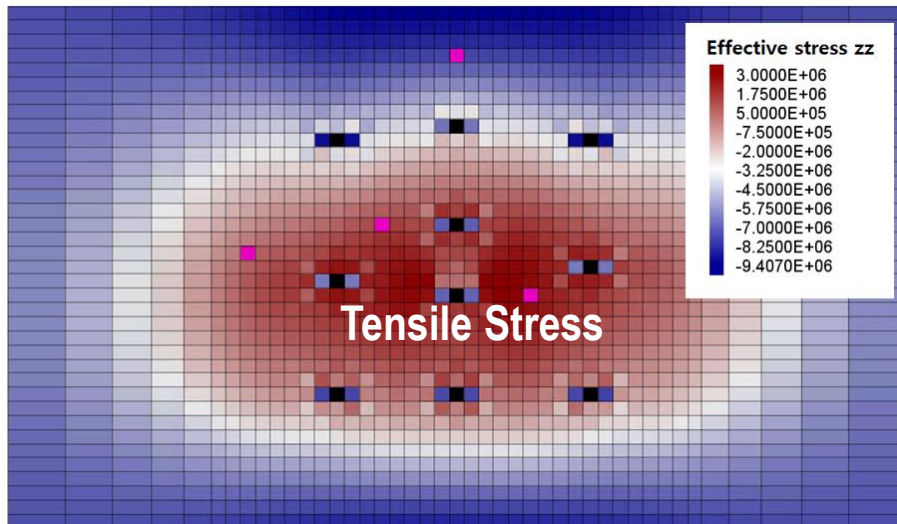
# Modeling Thermal-Pressurization Fracturing at Bure in CO<sub>x</sub> claystone (DECOVALEX 2023)



Thermal Pressurization

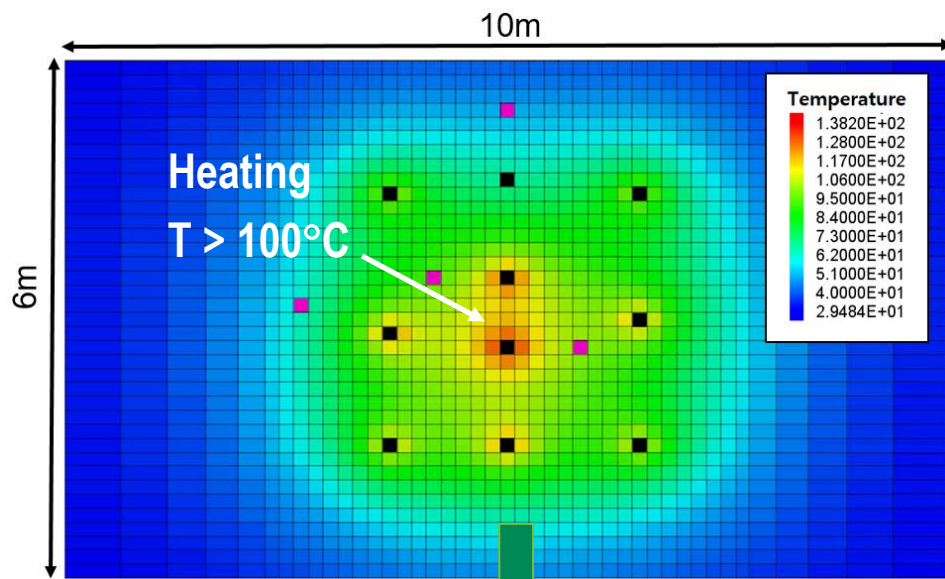


Effective stress

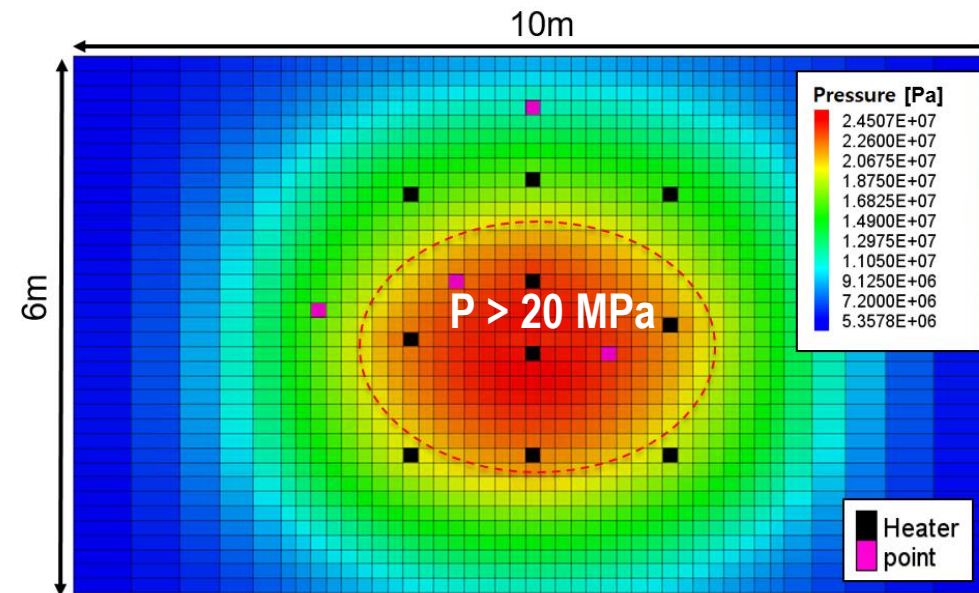




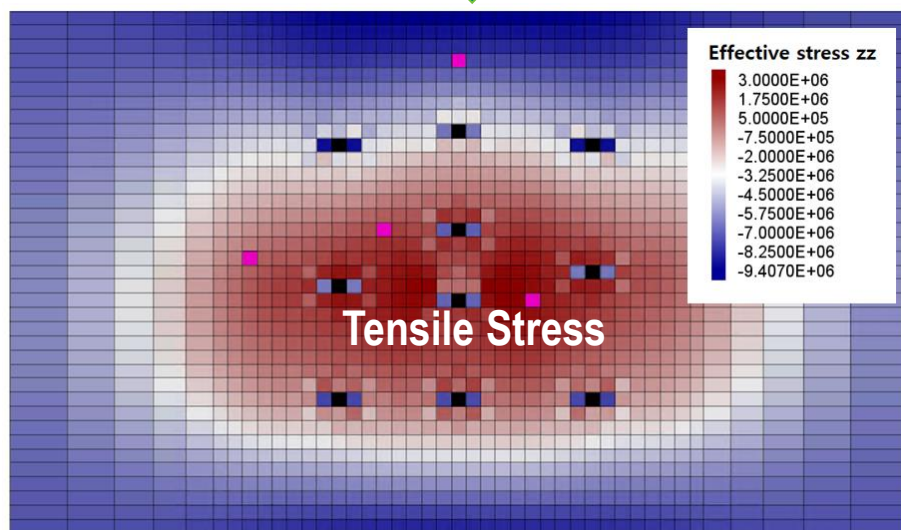
# Modeling Thermal-Pressurization Fracturing at Bure in CO<sub>x</sub> claystone (DECOVALEX 2023)



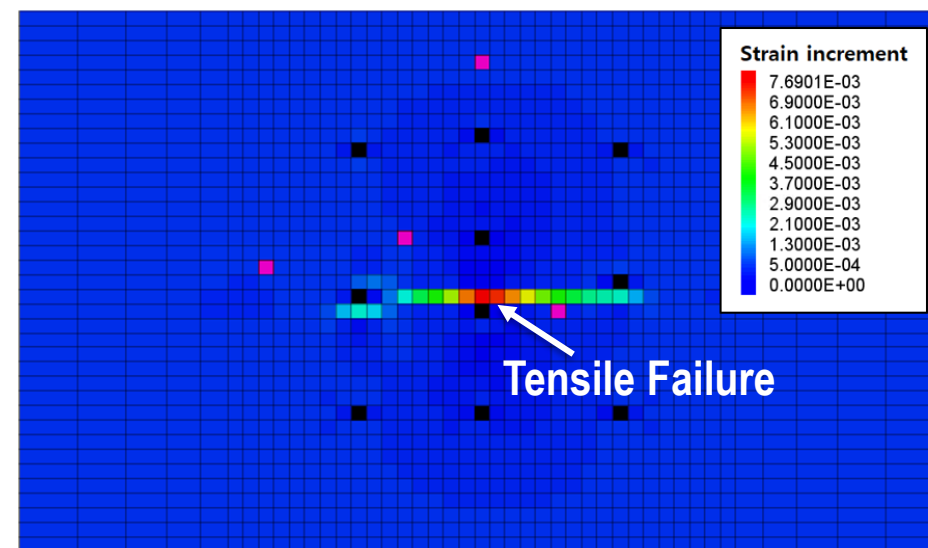
Thermal  
Pressurization



Effective stress



Fracturing

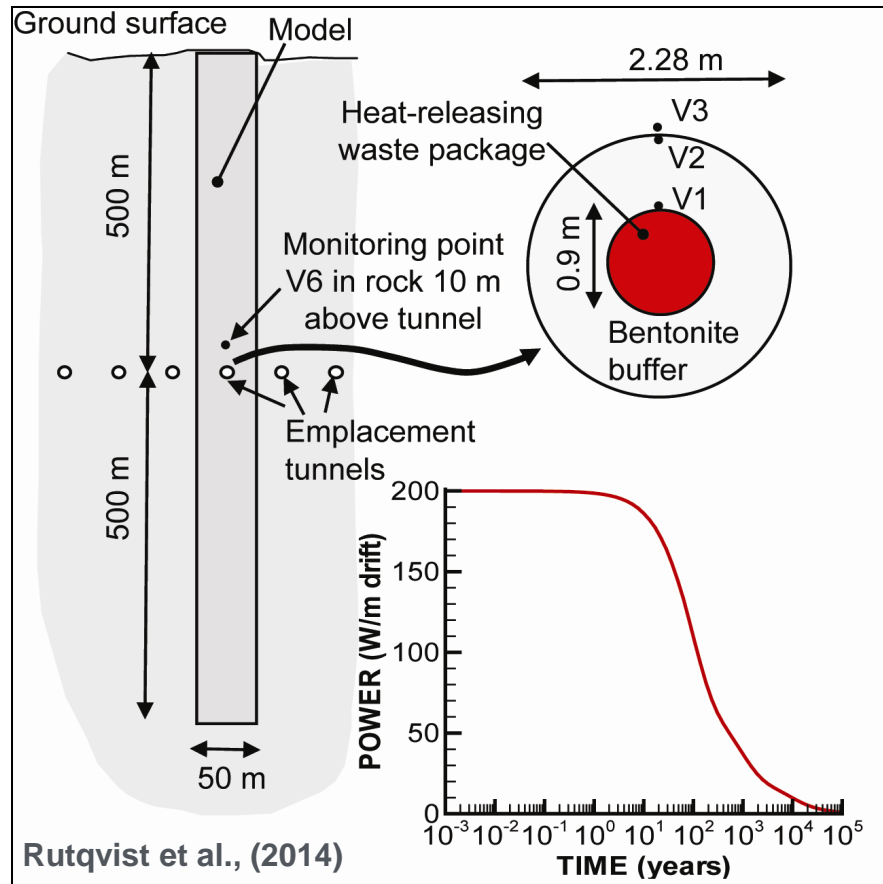


# Modeling Long Term Repository Behavior

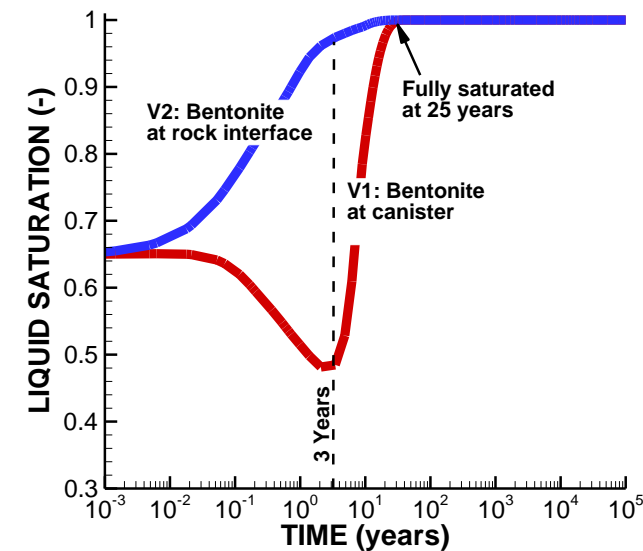
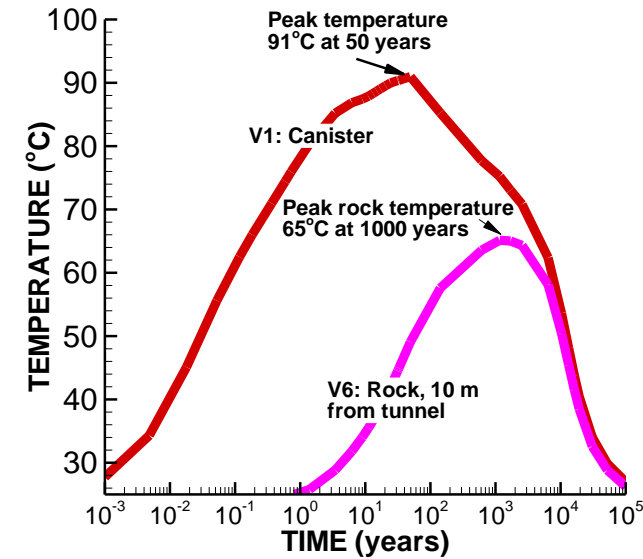
Three aspects:

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

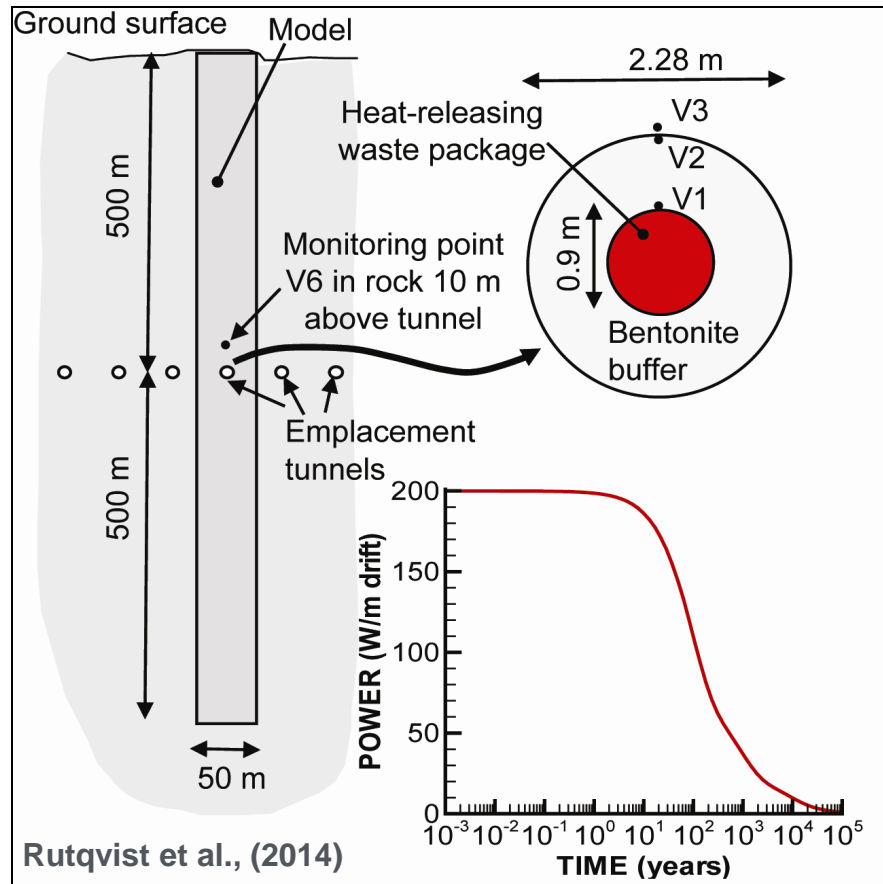
# Long-term Coupled Processes Simulation



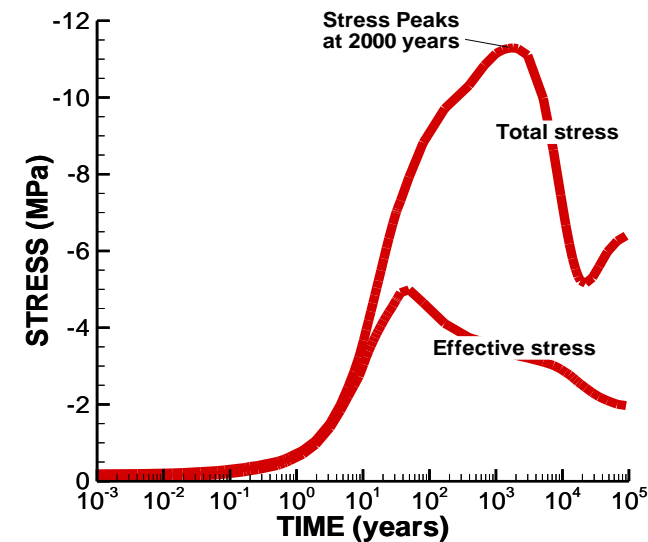
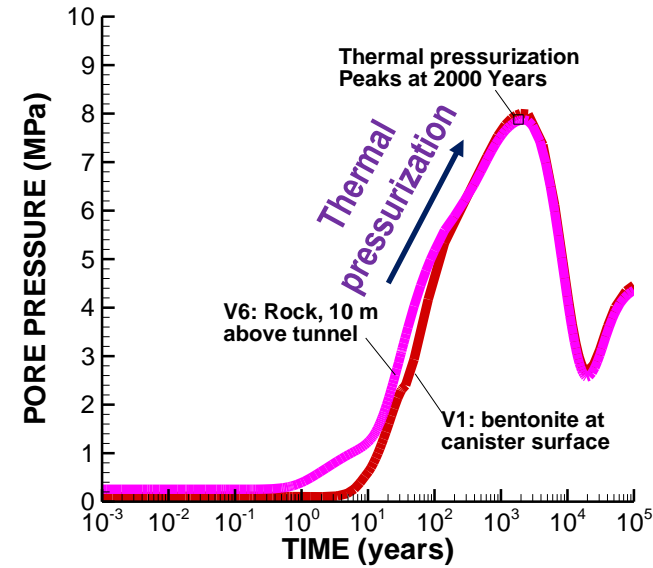
- Time to peak thermal impact?
- Time to full saturation and swelling?



# Long-term Coupled Processes Simulation

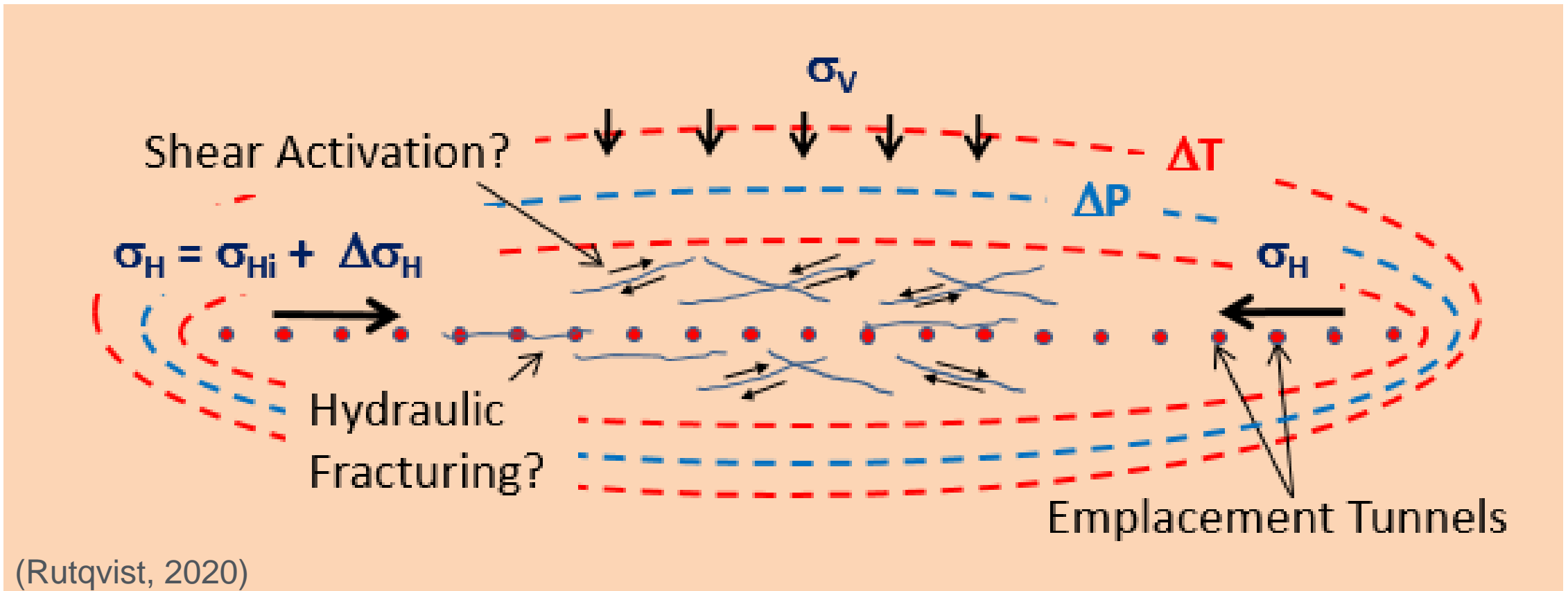


- Time to peak thermal impact?
- Time to full saturation and swelling?



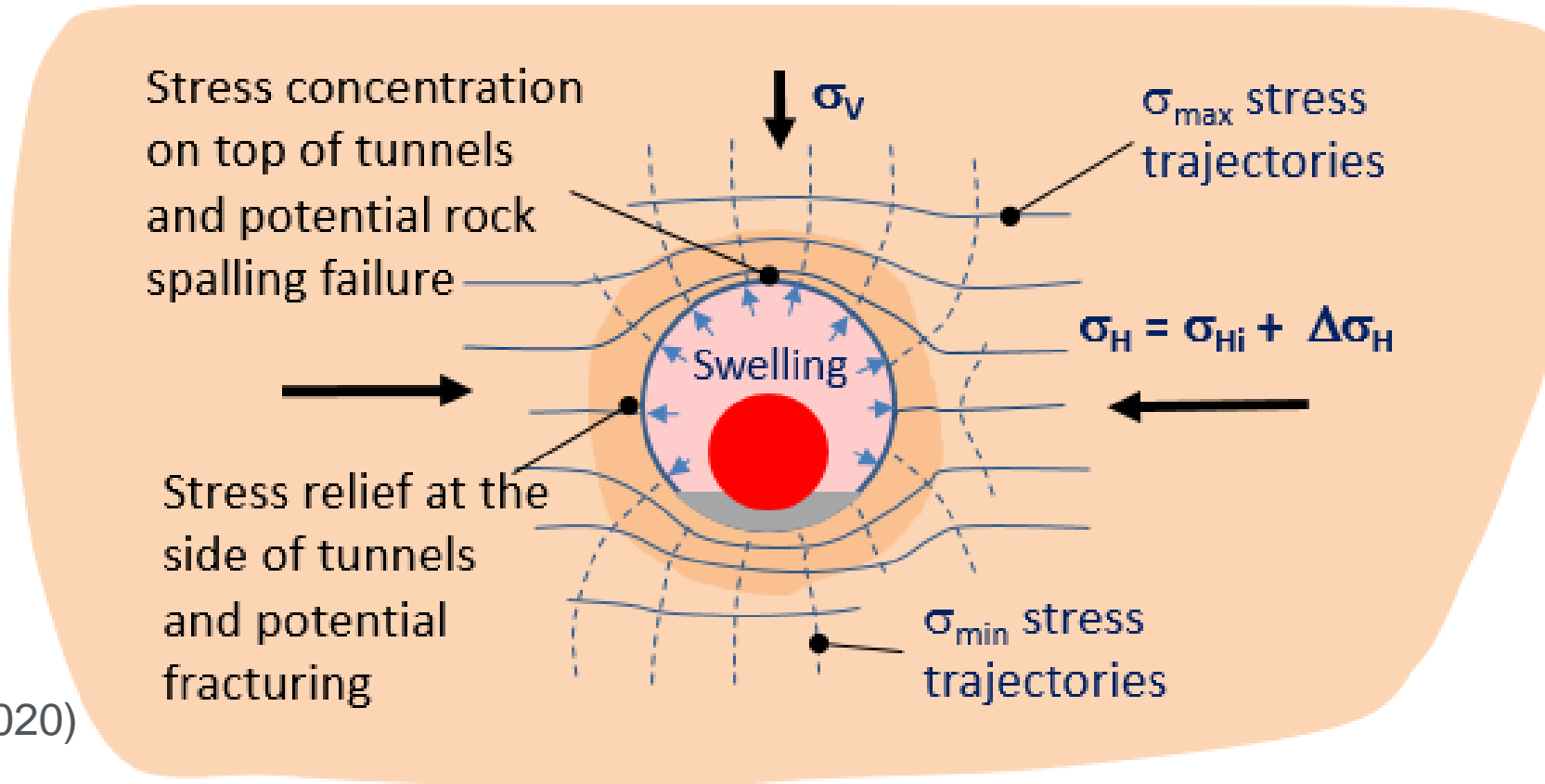


# Repository Temperature-induced Stress Changes



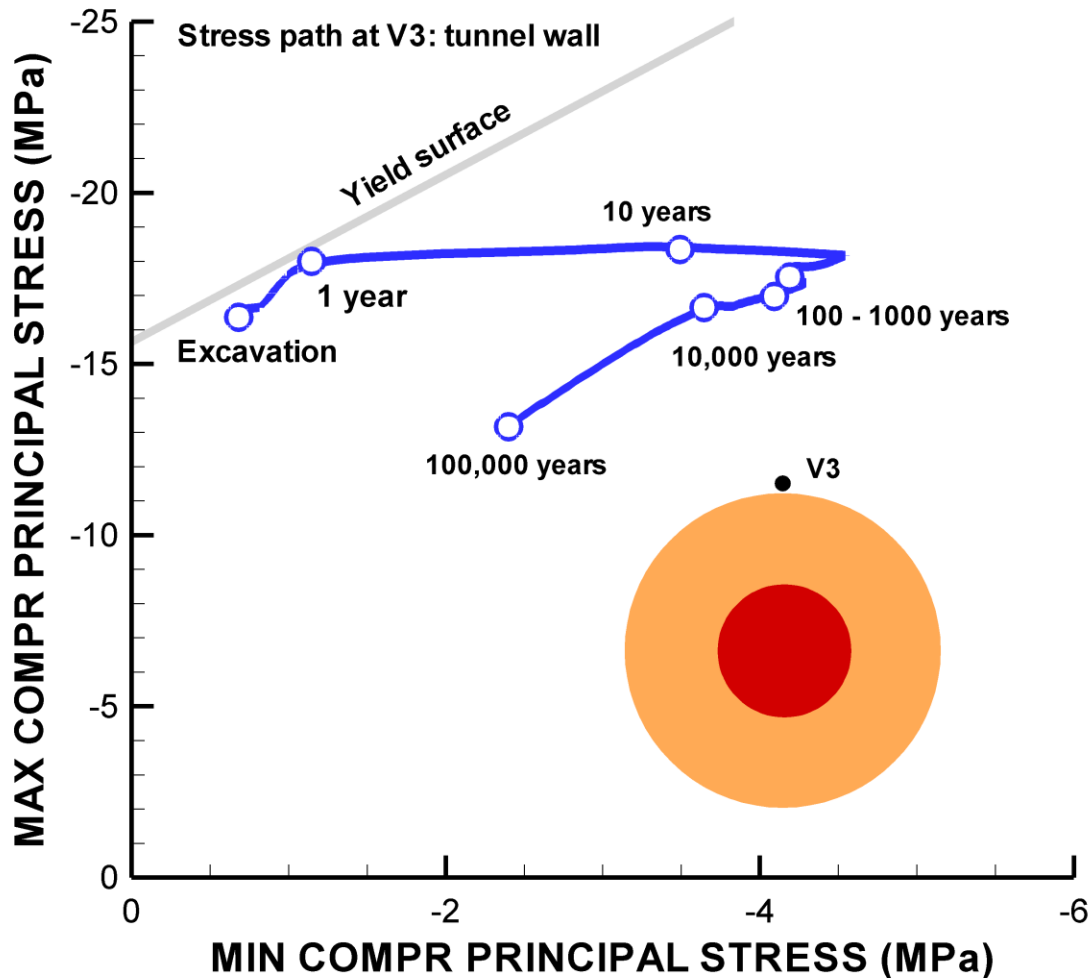
- $\Delta T$  can result in high pressure, shear stress, and potential fracturing
- May become the limiting temperature for thermal management

# Repository Temperature-induced Stress Changes



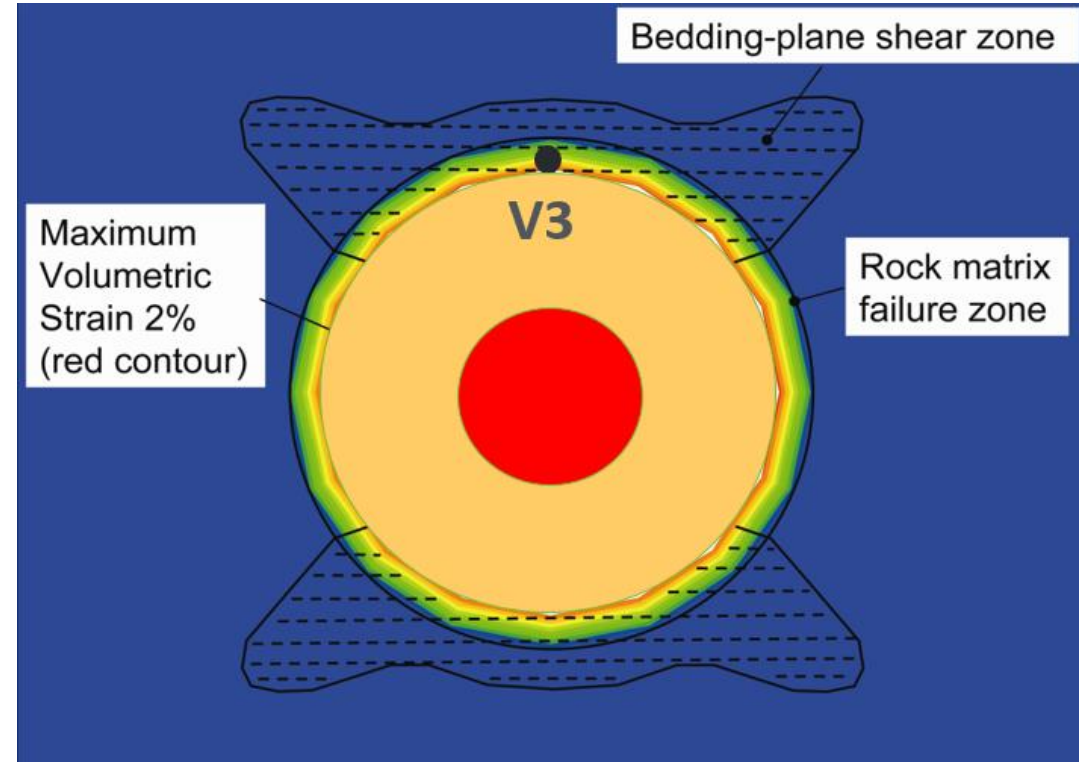
- Can impact EDZ thousands of years after repository closure (when repository temperature peaks)
- Important to have a supporting buffer stress at that time

# Long-term Coupled Processes Simulation



Rutqvist et al., (2014)

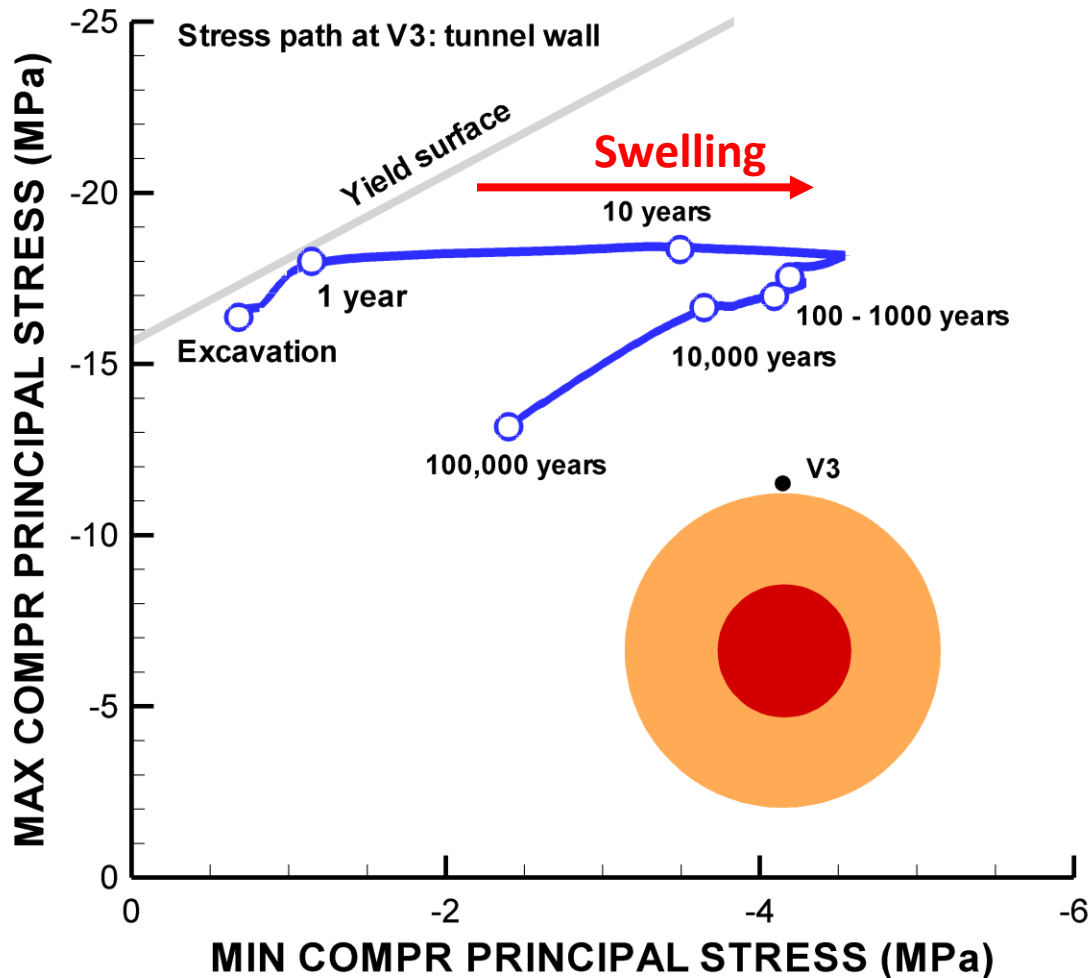
## Excavation Disturbed Zone (EDZ) Evolution



EDZ evolution impacted by:

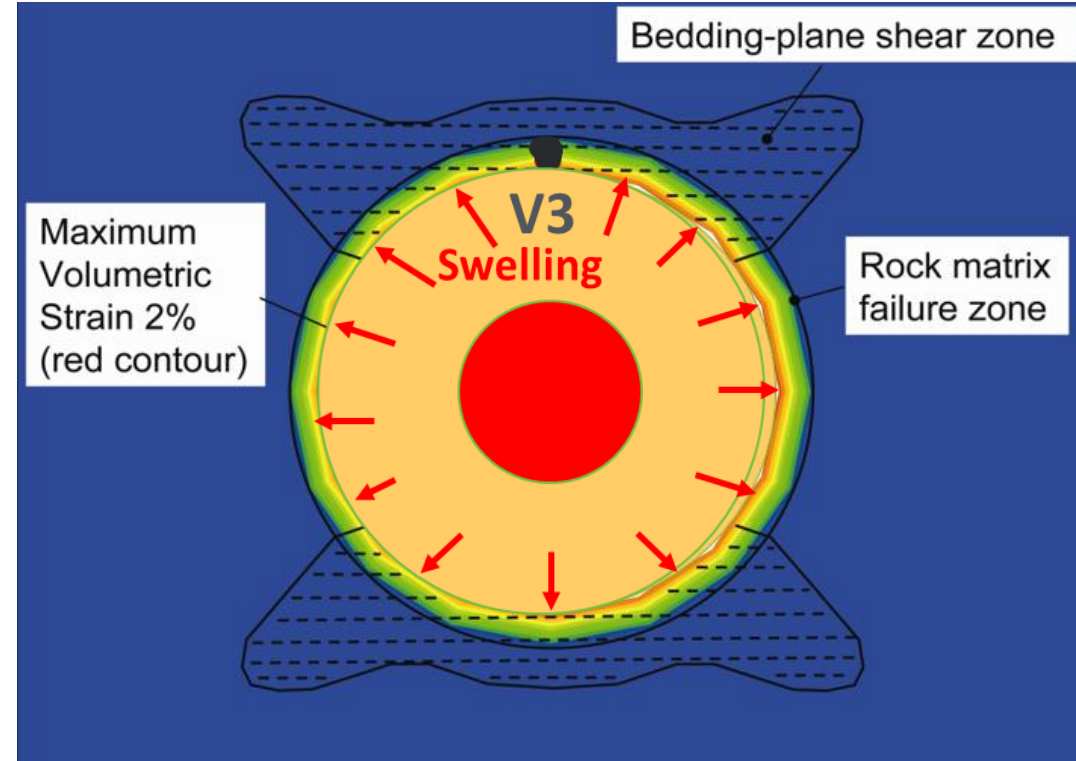
- 1) Thermal pressurization
- 2) Thermal stress
- 3) Wetting-induced bentonite swelling

# Long-term Coupled Processes Simulation



Rutqvist et al., (2014)

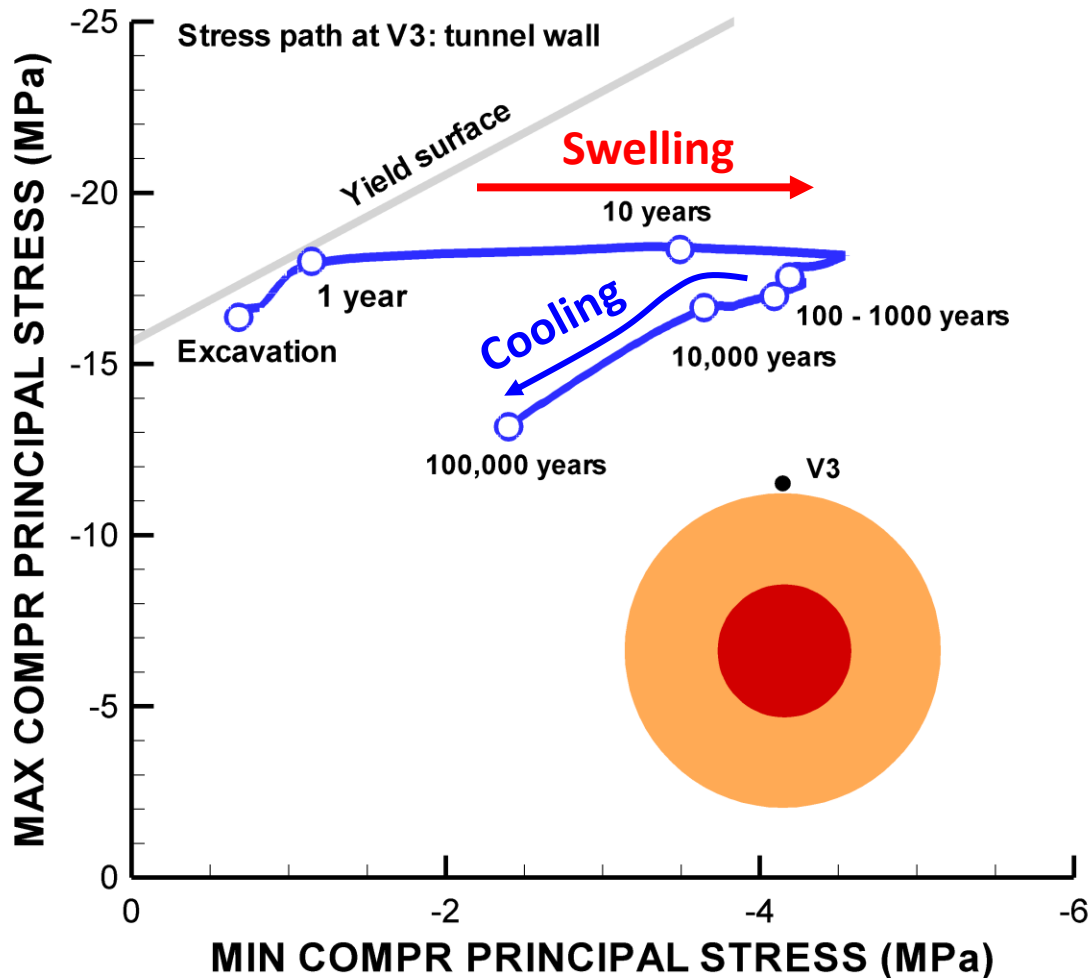
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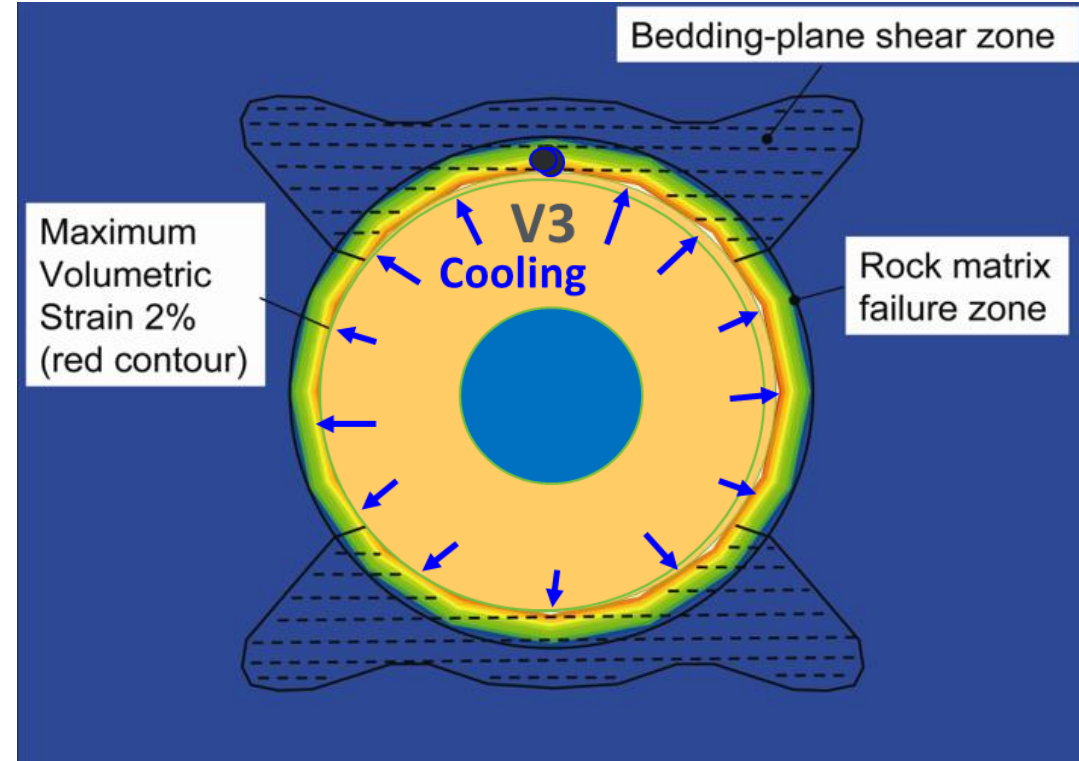
- 1) Thermal pressurization
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# Long-term Coupled Processes Simulation



Rutqvist et al., (2014)

## Excavation Disturbed Zone (EDZ) Evolution

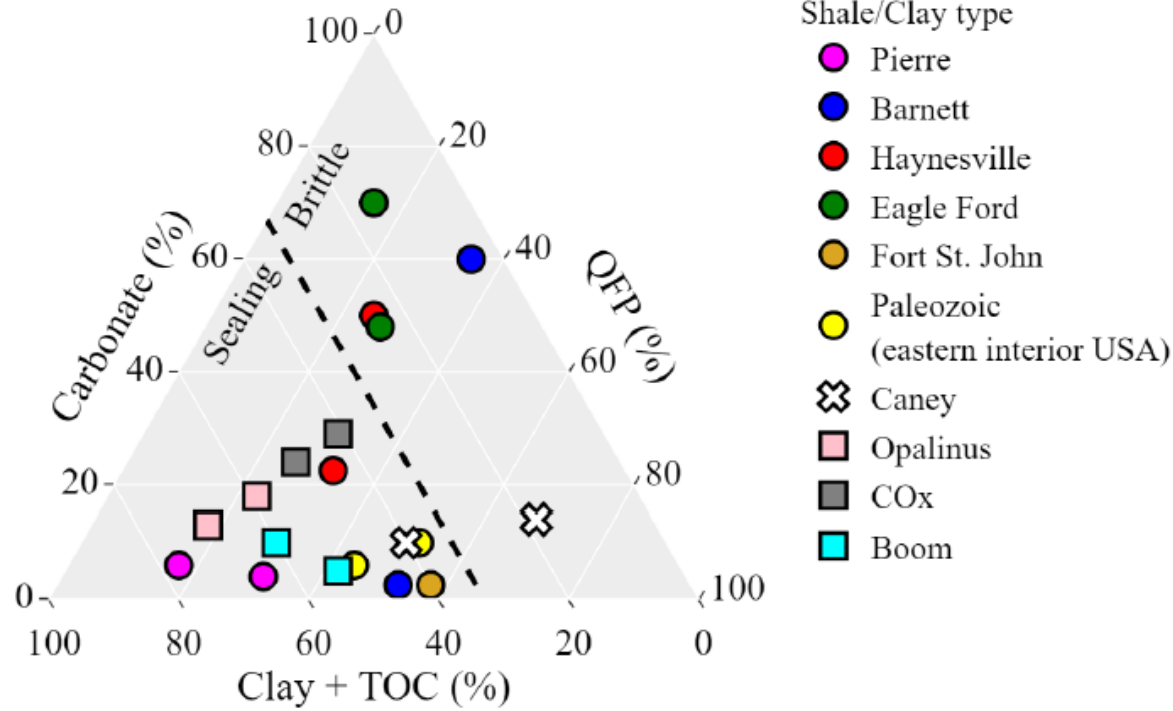


EDZ evolution impacted by:

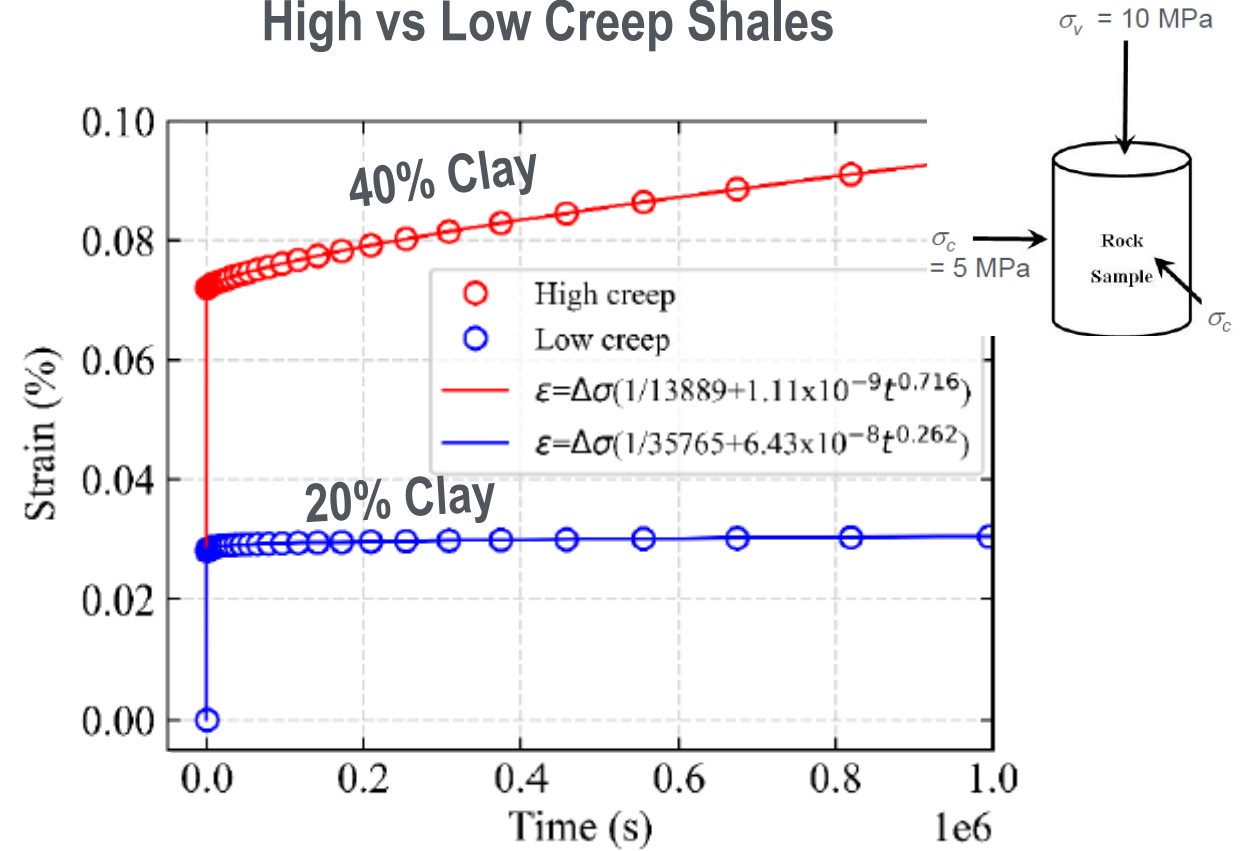
- 1) Thermal pressurization
- 2) Thermal stress
- 3) Wetting-induced bentonite swelling

# Impact of Long-Term Creep

## Sealing vs Brittle Shales



## High vs Low Creep Shales

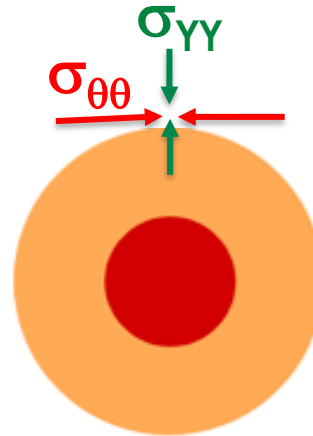
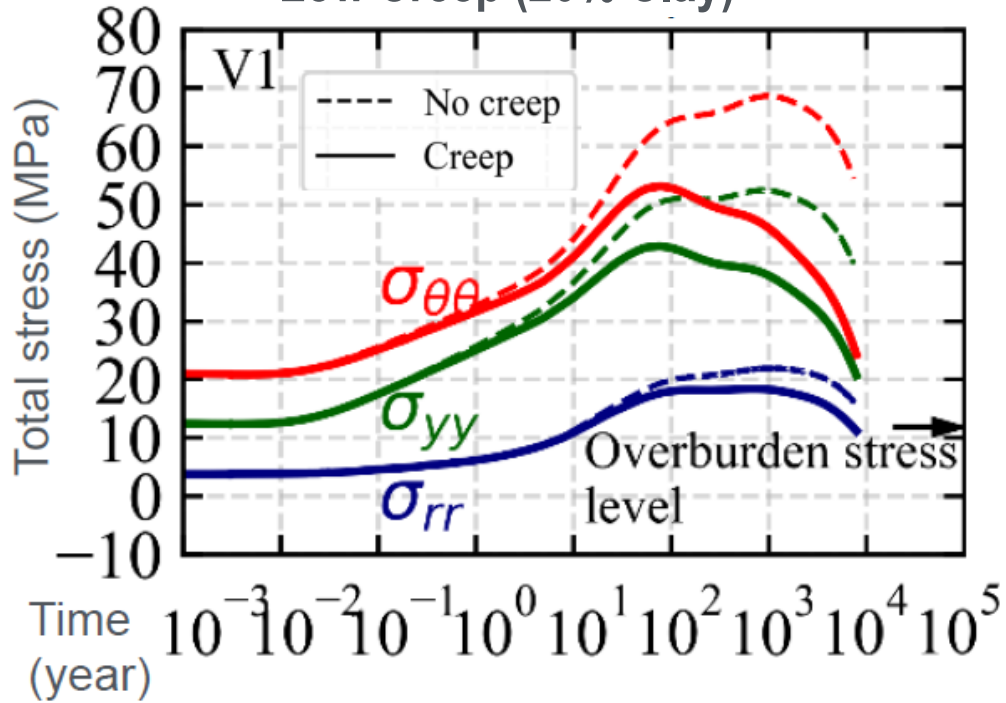


High clay content  $\Rightarrow$  Soft + high creep  $\Rightarrow$  self-sealing

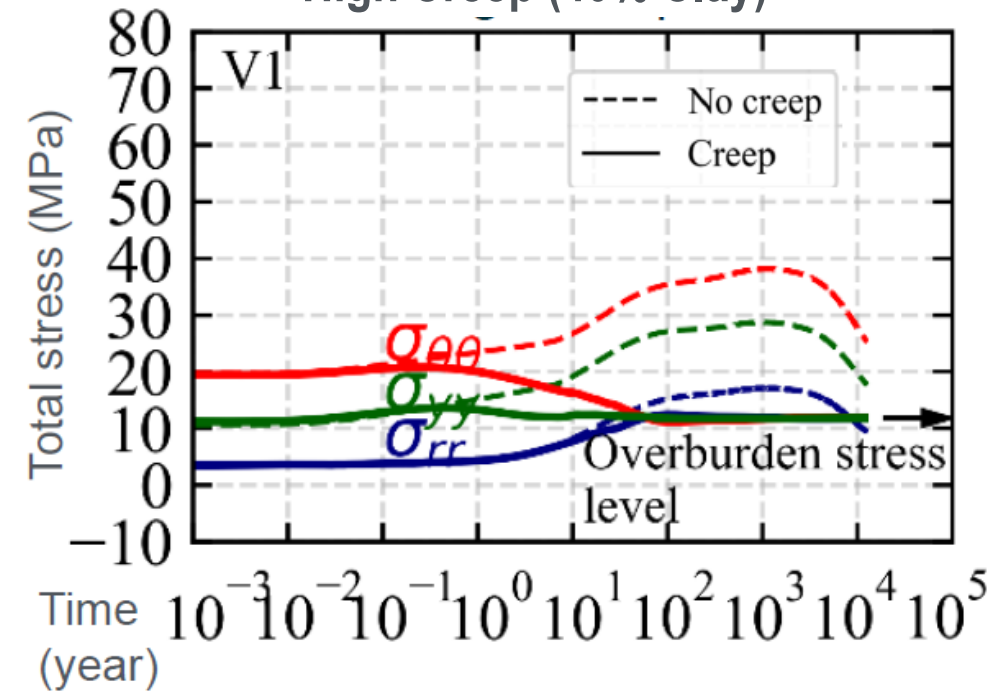
Sasaki and Rutqvist (2022)

# Impact of Long-Term Creep

Low Creep (20% Clay)



High Creep (40% Clay)



Stiffer rock and higher thermal stress  
 Shear stress remains elevated to 10,000 years  
 Risk of brittle damage in EDZ

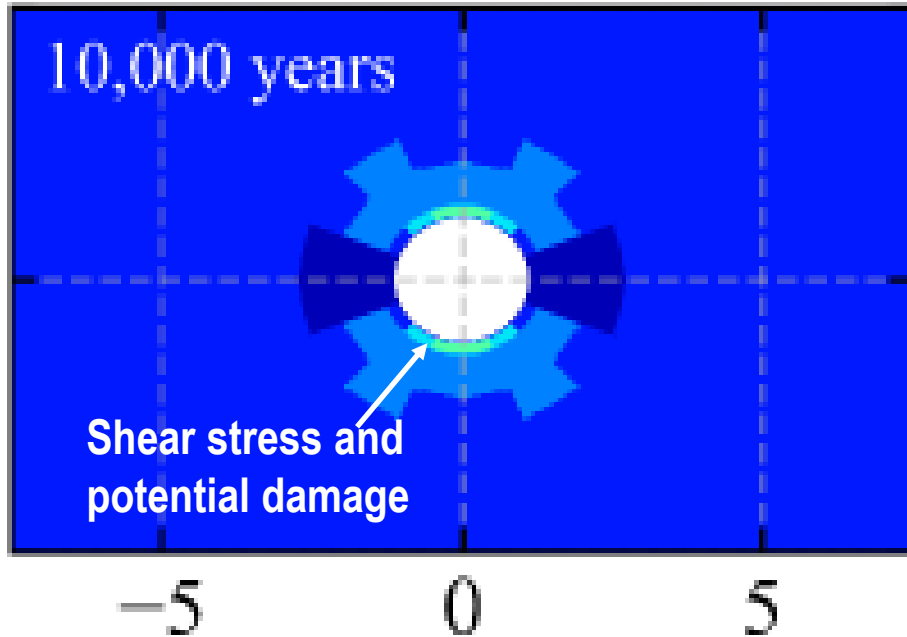
Softer rock and lower thermal stress  
 Shear stress released by creep in 50 years  
 Self-sealing EDZ

Sasaki and Rutqvist (2022)

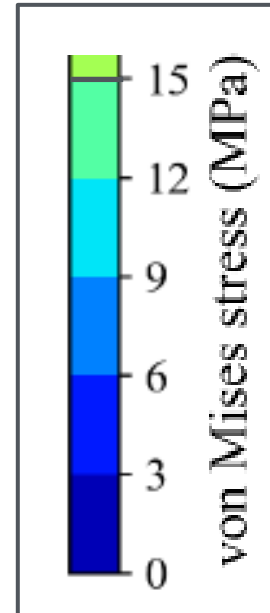


# Impact of Long-Term Creep

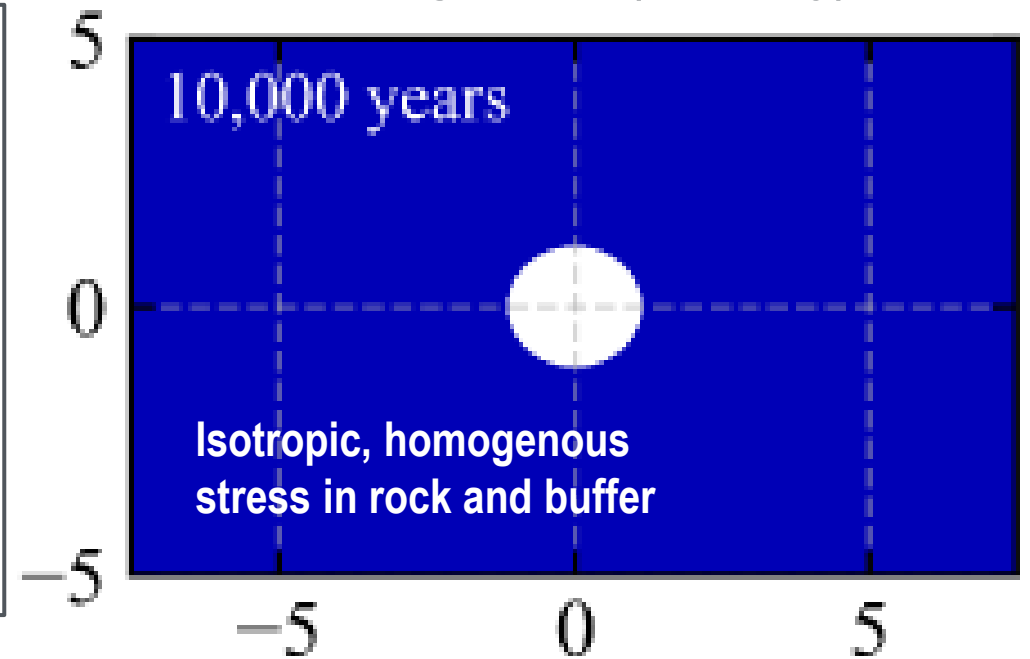
Low Creep (20% Clay)



Shear Stress



High Creep (40% Clay)



Stiffer rock and higher thermal stress  
Shear stress remains elevated to 10,000 years  
Risk of brittle damage in EDZ

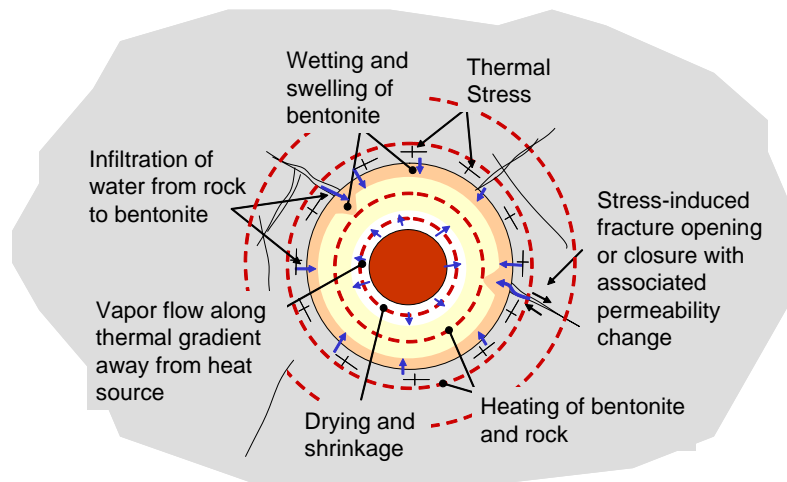
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Sasaki and Rutqvist (2022)

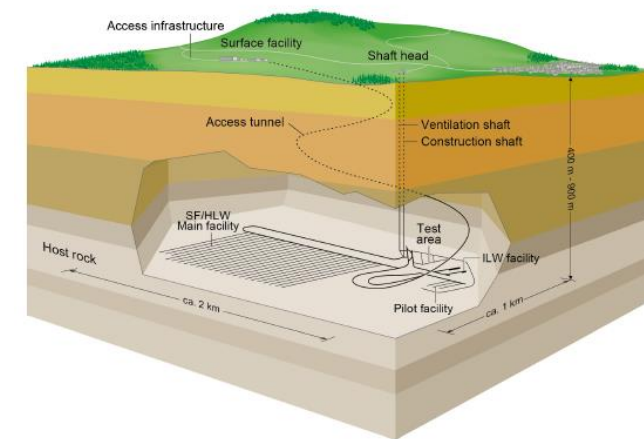
# Coupled Processes Model $\Leftrightarrow$ Performance Assessment (PA) Model

- Near field of emplacement tunnels in different parts of a repository, for different FEPs such as nominal case or cases of extensive gas generation.
- **Output** to the PA model: (1) **changes in flow properties** (e.g. permeability and porosity) in the near-field, including the buffer and Excavation Disturbed Zone (EDZ), (2) inform PA about local flow created by coupled processes.

## Coupled Processes Model of an Emplacement Tunnel



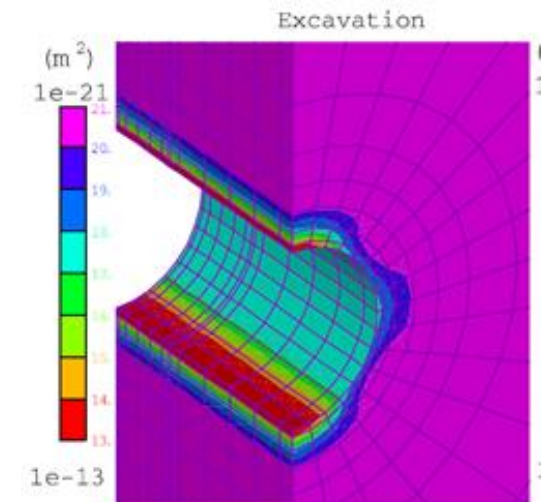
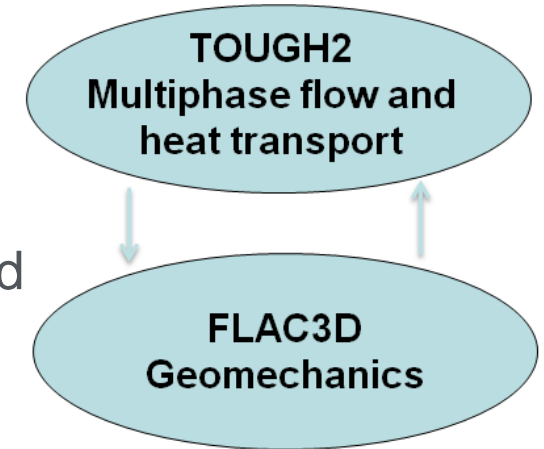
## PA Model of Entire Repository



Example layout from the Swiss Concept (Seiphoori, 2015)

# State of the Art and R&D Needs for Argillite THM Modeling

- **THM model framework established (TOUGH-FLAC)**
- **Constitutive THM models for argillite host rocks**
  - Anisotropic shale THM constitutive model validated
  - Thermal pressurization fracturing, fault shear and sealing being investigated
  - Need for creep parameters, such a low stress creep, anisotropic creep
- **Models for EDZ in argillite**
  - No established model for damage, sealing and healing
  - Site specific studies at Mont Terri and Bure URLs
- **Very active research in European Programs**
  - Switzerland, France, Belgium, Germany, UK.,.....
  - Can also learn from shale-gas research



# 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
- 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 (In revision, *International Journal of Rock Mechanics and Mining Sciences* (2022)).
- 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
FEPs	Features, Events, and Processes
FLAC	Fast Lagrangian Analysis of Continua
LBNL	Lawrence Berkeley National Laboratory
NAGRA	Swiss waste management organization
PA	Performance Assessment
Swisstopo	Federal Office of Topography, Switzerland
THM	Thermo-hydro-mechanical
TOUGH	Transport Of Unsaturated Groundwater and Heat