

# Reduced-order THMC coupled simulation of nuclear waste disposal in shale

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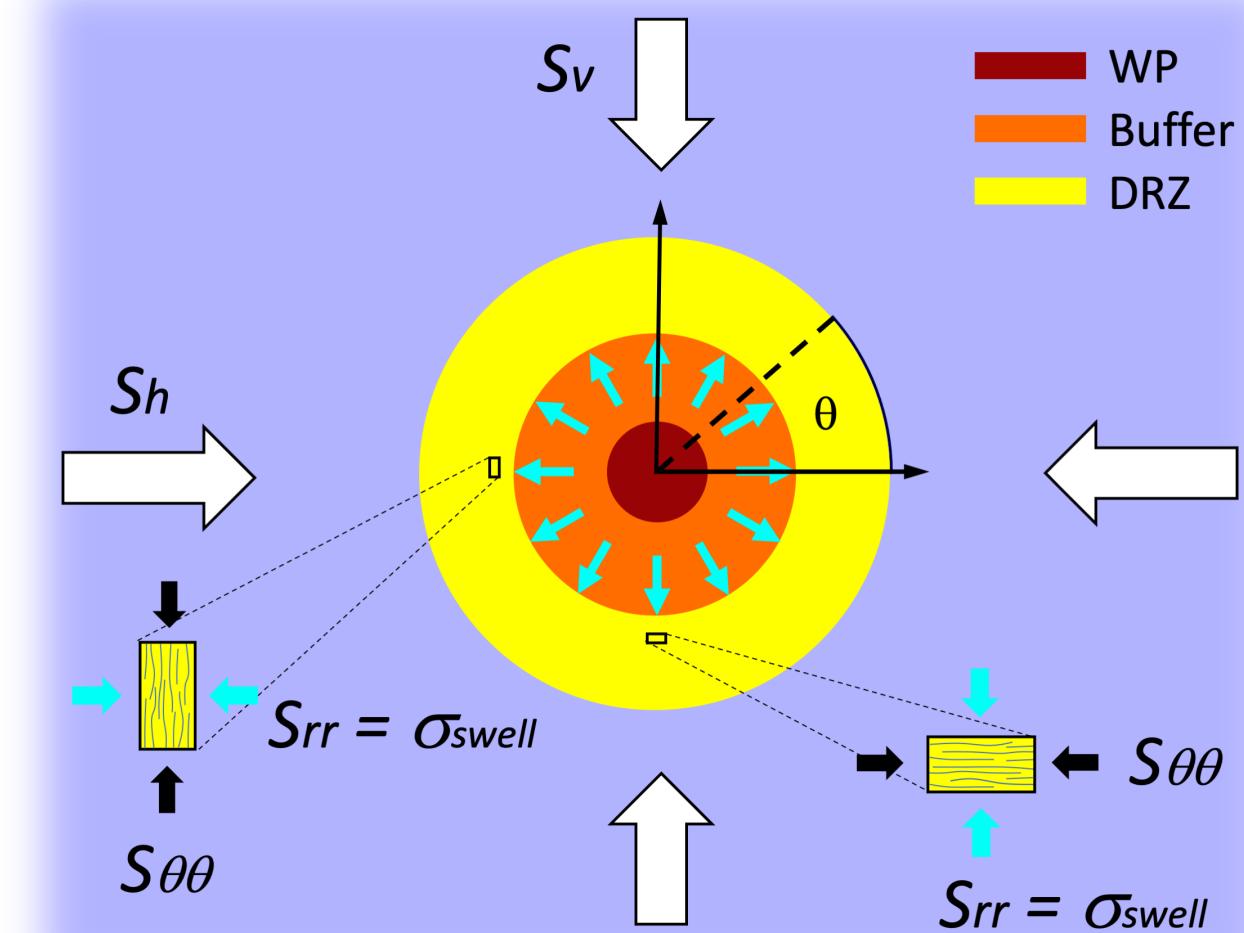
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## Motivation & Objective

Thermal and hydrological behaviors of multiphase pore fluids in the presence of heat cause the near-field thermo-hydro-mechanical-chemical (THMC) coupled processes that can influence performance of geologic radioactive waste repositories. This hydro-thermal impacts may perturb the geomechanical stability of the disturbed rock zone (DRZ) surrounding the drifts in a shale-hosted deep geological repository, which links heat/fluid flow and chemical/reactive transport between the engineered barrier system (EBS) and the host rock.

This work focuses on integrating the effects of a near-field hydro-thermal behaviors as well as swelling-driven geomechanical process into THMC simulations by implementing stress-dependent permeability and saturation-temperature-dependent thermal conductivity functions to reduce dimensionality and improve computational efficiency.



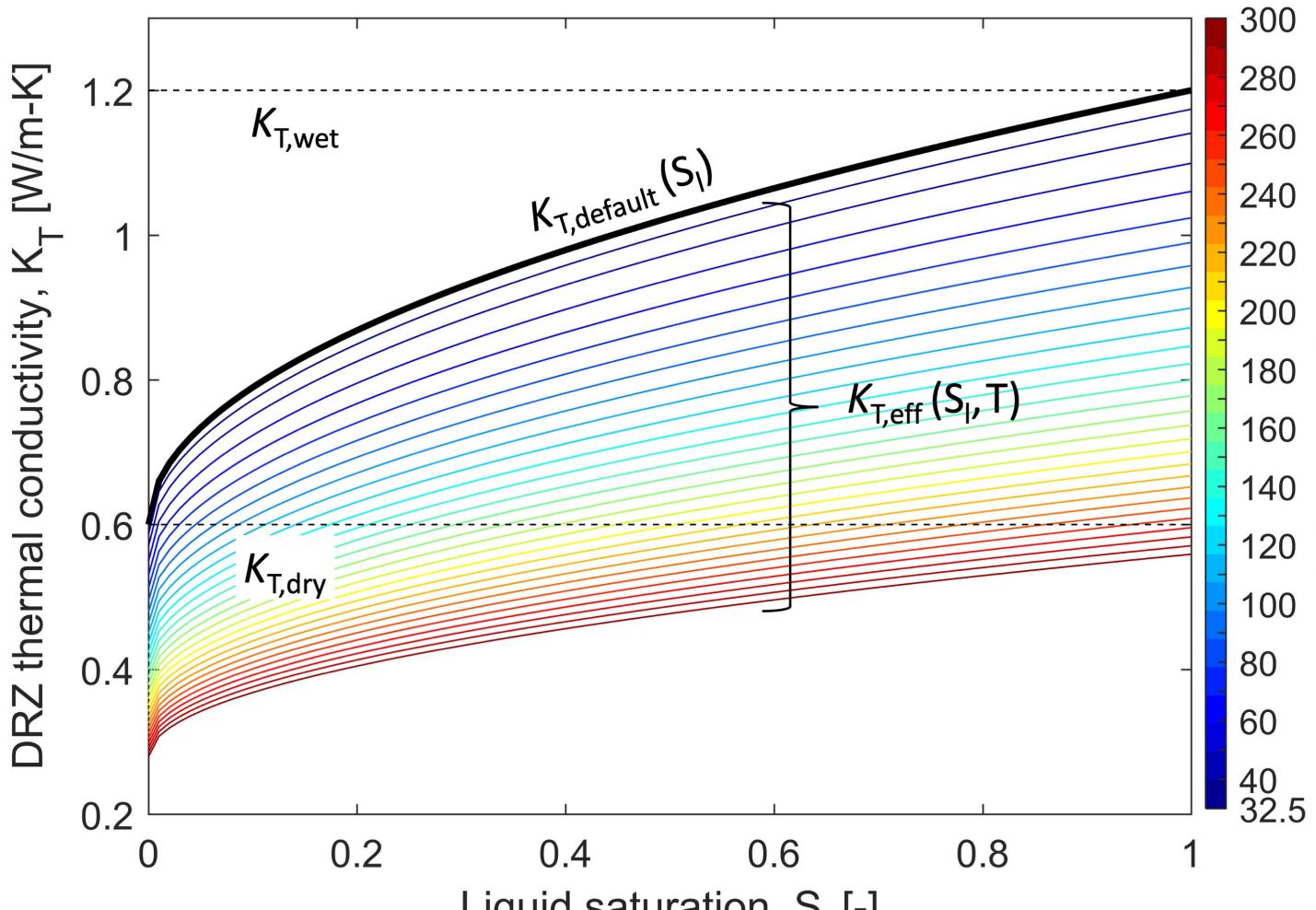
## Stress-dependent DRZ Permeability

As heat decays, re-saturation of the buffer generates swelling-driven compression to the DRZ, which may close fissures/fractures within the DRZ mechanically.

$$\Delta\sigma_{swell} = 3K\Delta S_l \beta_{sw}$$

This hydro-mechanical coupled process is represented by the reduction of DRZ permeability. This study implements Two-part Hooke's model (TPHM) for the DRZ permeability changes expressed as follows:

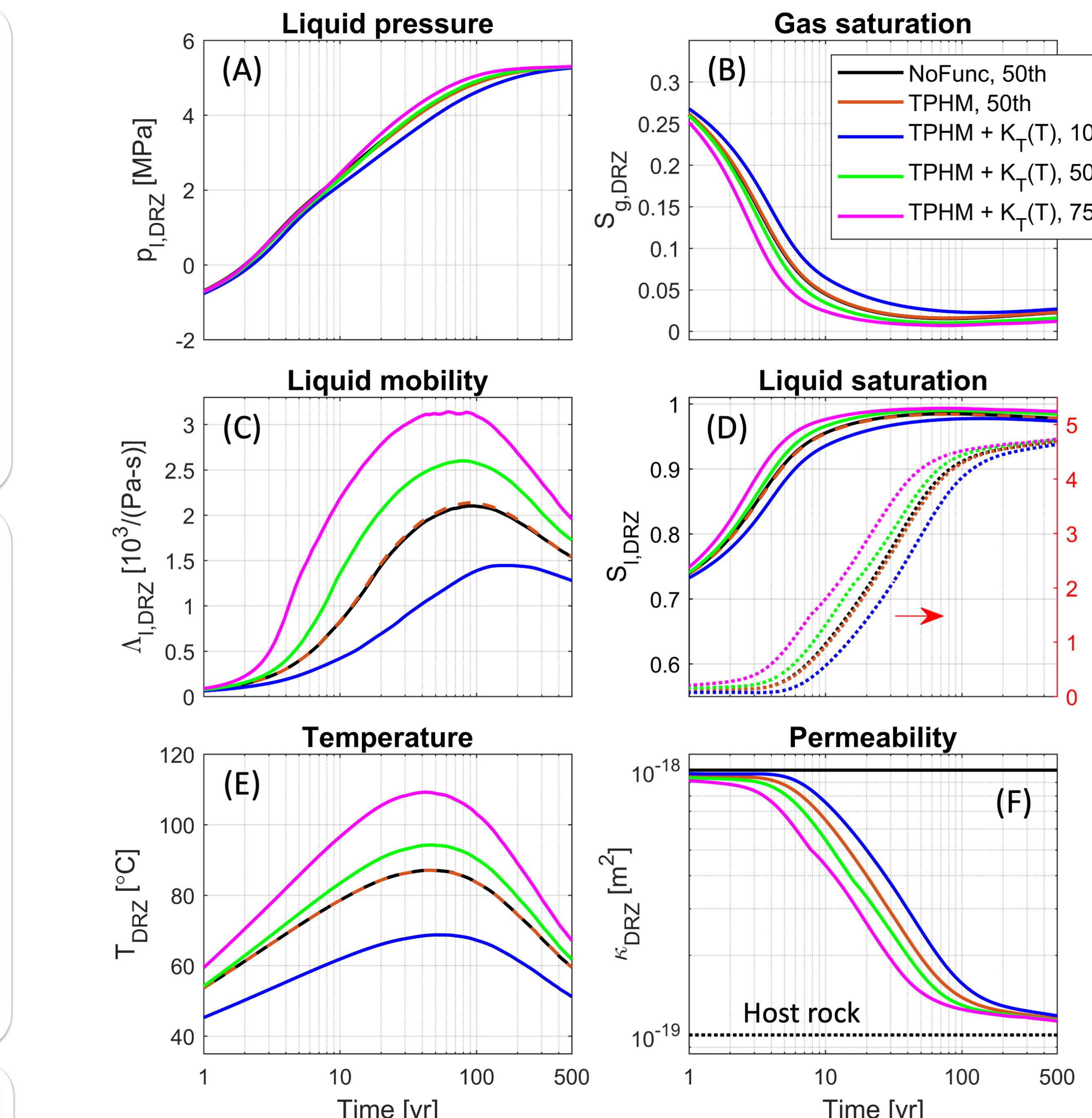
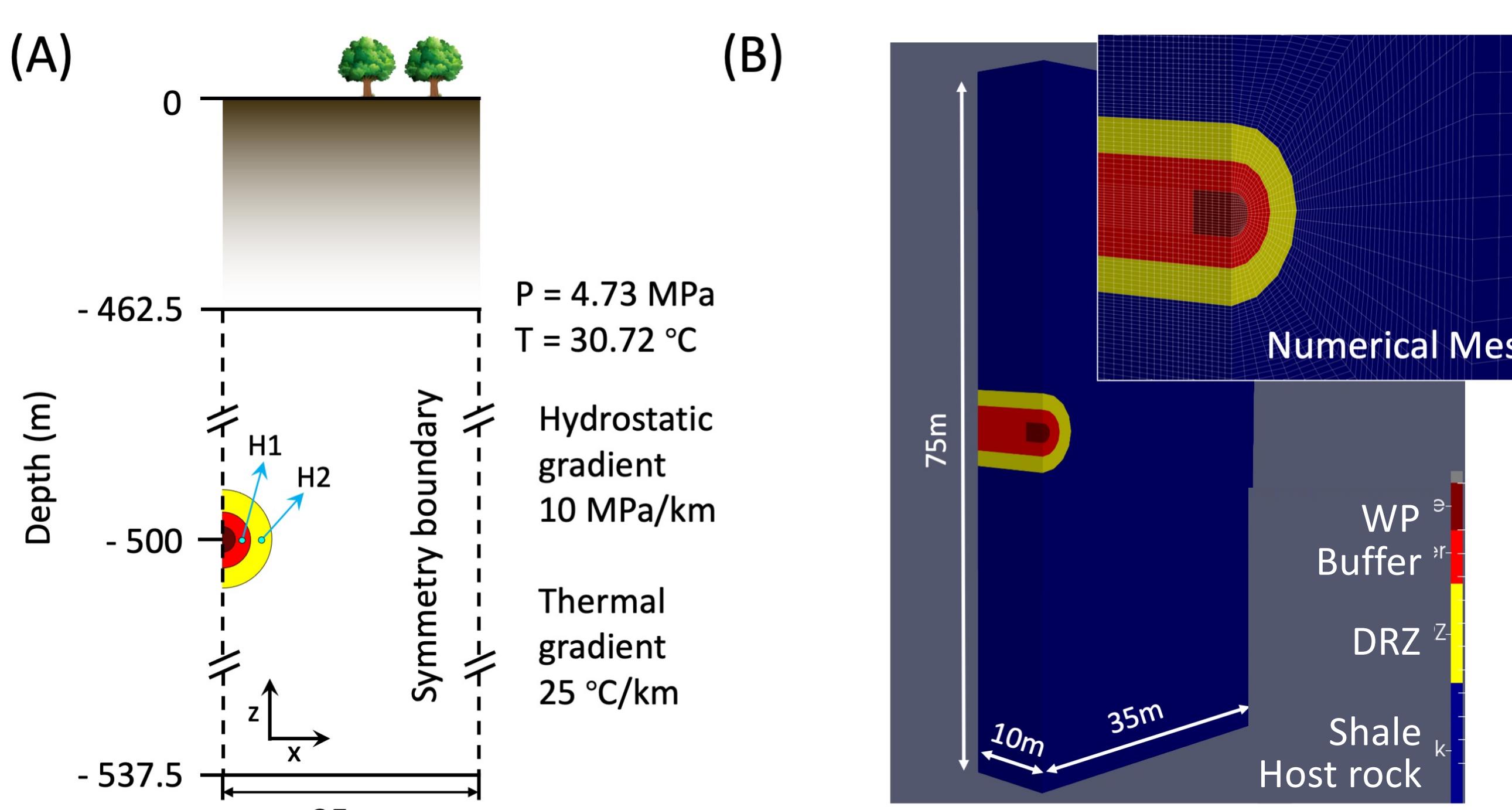
$$\kappa = \kappa_{e,0} e^{-\beta_{ce}\phi_{e,0}\Delta\sigma_{eff}} + \alpha \left[ \gamma_t \exp \left( -\frac{\Delta\sigma_{eff}}{K_t} \right) \right]^m$$



## Saturation-temperature-dependent Thermal Conductivity

This study implements the effective thermal conductivity with the power-law temperature function expressed as follows:

$$K_{T,eff}(S_l, T) = [K_{T,dry} + \sqrt{S_l}(K_{T,wet} - K_{T,dry})] \left( \frac{T - T_{ref}}{300} \right)^\gamma$$

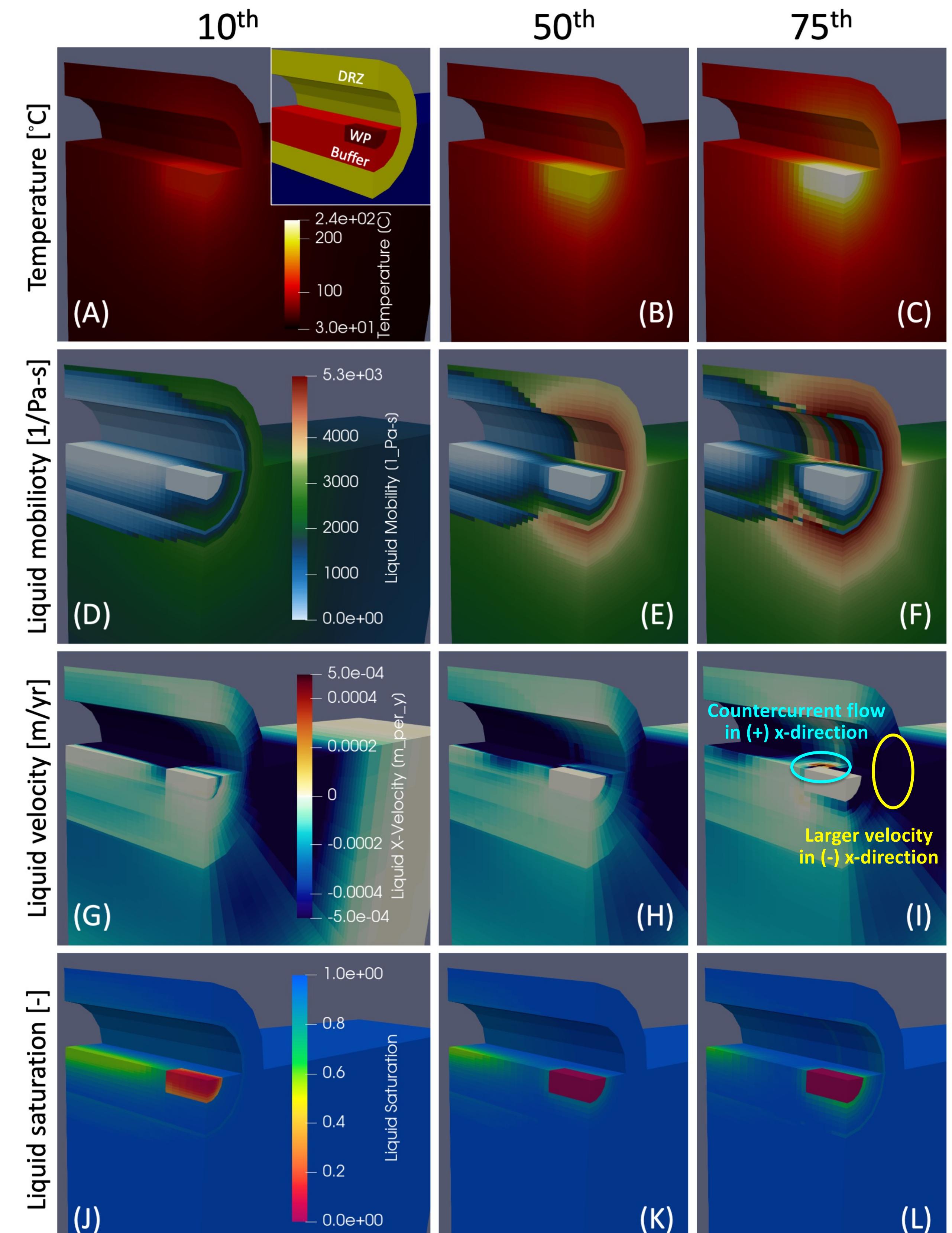


- Hotter heat source (magenta) causes
  - Higher temperature leading to larger mobility of liquid phase (Fig. C)
  - Faster re-saturation due to stronger inflow from the fully-saturated host rock (Fig. B or D)
  - Faster swelling causes faster increase of stress acting on DRZ (Fig. D; dash line), which results in faster reduction of DRZ permeability (Fig. F)
- The impact of stress-dependent permeability seems to be trivial even with reduction of DRZ permeability (brown vs. black lines of each Fig.)
- After 500 years, pressure, saturation, and permeability of DRZ converges for all cases.
- Hotter heat source (75<sup>th</sup>) causes
  - Higher temperature (Fig. C) leading to larger mobility of liquid phase (Fig. F) and velocity (Fig. I).
  - Thermal gradients outward from the waste package result in countercurrent flows locally (Fig. I).
  - Water inflow is still dominant at the region less affected by heat loading (buffer b/w WPs), causing faster re-saturation (Fig. L)

## Model Description & Setting

- Symmetric domain representing a quarter of single repository system, where the vertical heterogeneity (i.e. layering or interbedding) is neglected..
- Shale host rock is initially fully saturated, whereas the buffer and DRZ are unsaturated ( $S_{l,buffer} = S_{l,DRZ} = 0.65$ ).
- Hydrostatic pressure gradient and thermal gradient are implemented as initial conditions.
- Waste package is assumed as a porous medium with a porosity of 0.5 (equal to the fraction of void space) and a permeability three orders of magnitudes higher than shale host rock's.
- PFLOTTRAN GENERAL mode is used to solve heat and fluid flow problems.
- For the sensitivity test, three different heat sources are implemented.
  - 10<sup>th</sup>, 50<sup>th</sup> (reference), 75<sup>th</sup> percentiles of frequency distribution of heat outputs.

- Findings from this work
  - More heat will increase the near-field liquid mobility that leads to faster inflow into unsaturated zones from the fully-saturated host rock.
  - At the same time, thermal gradients outward from the waste package can generate countercurrent flow locally.
- Future work
  - Extended model domain in a vertical direction including layers to see thermal impacts on the surface.
  - Validating and generating site-specific relationship between buffer swelling pressure and deformation based on experimental data of swelling characteristics obtained from various compacted bentonites.
  - Implementing the evolution of the DRZ volume considering inelastic deformation and fracture dynamics as a function of swelling stress.



## Findings & Future Works