Coupled thermo-hydro-mechanical-chemical modeling by incorporating pressure solution for estimating the evolution of rock permeability

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Outline

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- Results
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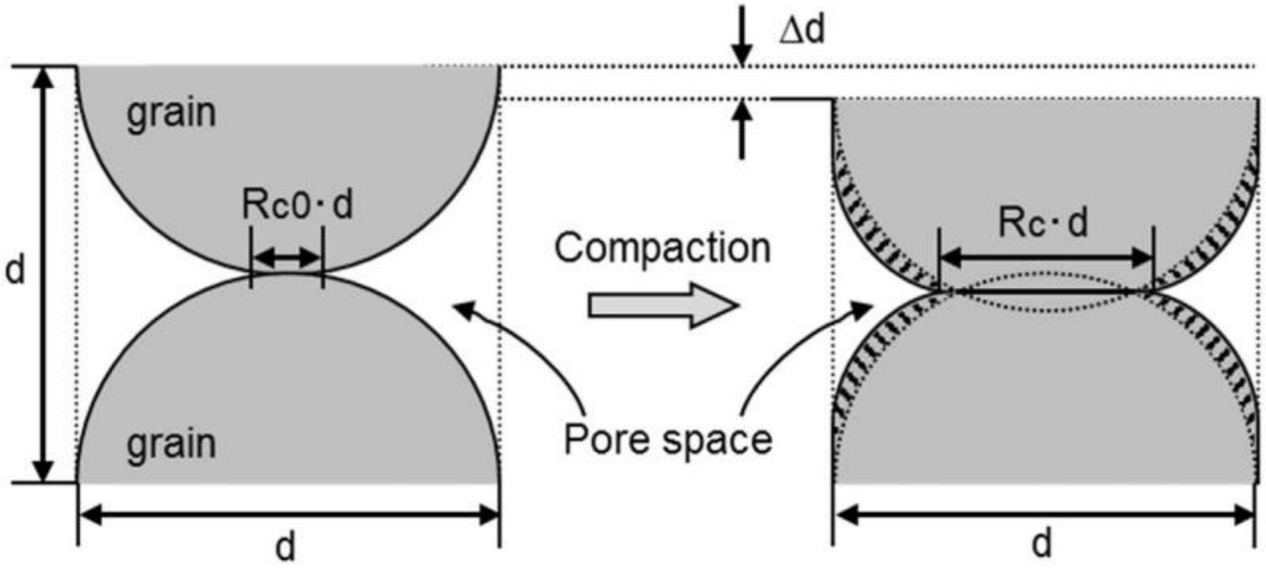
Introduction

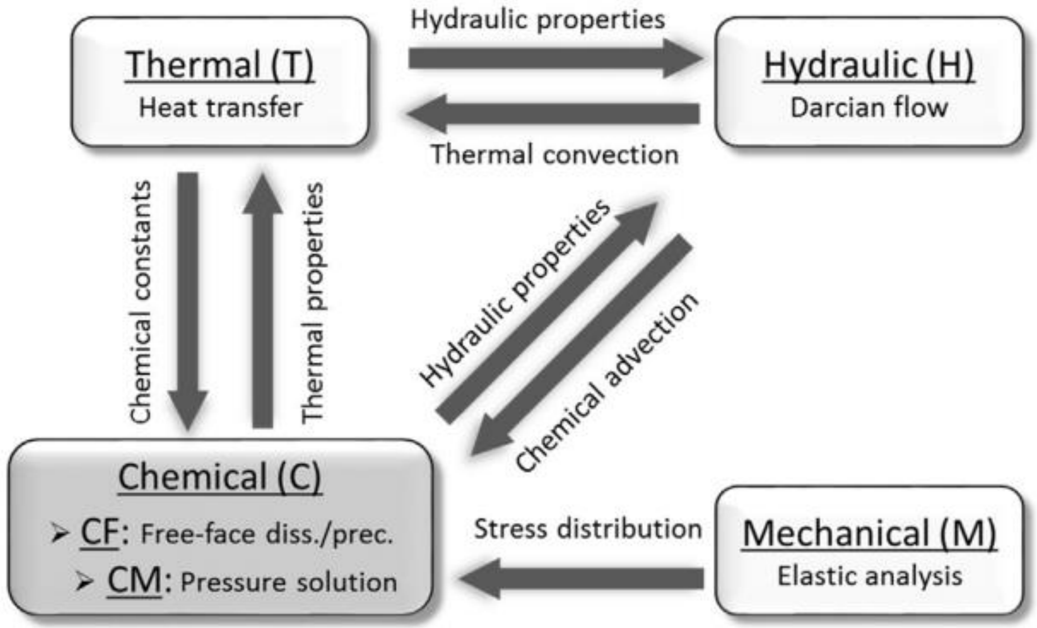
- When disposing high-level radioactive wastes in the deep subsurface, the influence of the disposal on the hydraulic property of the rocks must be examined in advance and should be estimated with a required precision.

- In order to predict the long-term evolution of hydraulic properties, a numerical model that can account for the thermo-hydro-mechano-chemical (THMC) coupling process is needed.

- In the geochemical calculations of the THMC model, mineral dissolution and precipitation occurring on the free surface of the rock are usually considered, but dissolution activities at particle contacts (pressure solution) are not considered. In order to assess the long-term hydraulic properties of rocks, this phenomenon must be incorporated into the modeling process.



Geometrical model of grain-to-grain contact.



Methodology

Groundwater flow

$$\frac{\partial(\rho_w \phi)}{\partial t} + \nabla\cdot(\rho_w \mathbf{u}) = f_m,$$

Heat-transport:

$$(\rho C_p)_{eq}\frac{\partial T}{\partial t} + \rho_w C_{p,w}\, \mathbf{u}\cdot\nabla T = \nabla\cdot(\mathbf{k_{eq}}\nabla T) + Q_h,$$

Mechanics:

$$-\nabla\cdot\boldsymbol{\sigma} = \mathbf{F_v},$$

Solute-transport:

$$\frac{\partial(c_i \phi)}{\partial t} + \mathbf{u}\cdot\nabla c_i = \nabla\cdot(\phi\tau\mathbf{D}_{b,i}\nabla c_i) + R_i,$$

The parameters Where:

ρ_w : *density of the fluid* $\left({}^{kg}/_{m^3}\right)$

ϕ : *porosity* $(-)$

u : *fluid velocity* $({}^{m}/_{s})$

f_m : *source term for the flow* $\left({}^{kg}/_{m^3 \cdot s}\right)$

$(\rho C_p)_{eq}$: *equilibrium volumetric heat capacity* $\left({}^{J}/_{K \cdot m^3}\right)$

T : *temperature* (K)

$C_{p,w}$: *heat capacity of the fluid* $\left({}^{J}/_{K \cdot kg}\right)$

k_{eq} : *equilibrium thermal conductivity* $\left({}^{W}/_{K \cdot m}\right)$

Q_h : *heat source* $\left({}^{W}/_{m^3}\right)$

σ : *stress* $\left({}^{N}/_{m^2}\right)$

F_v : *body force* $\left({}^{N}/_{m^3}\right)$

c_i : *concentration of solute i* $\left({}^{mol}/_{m^3}\right)$

τ : *coefficient related to tortuosity* $(-)$

$D_{b,i}$: *diffusion coefficient* $\left({}^{m^2}/_{s}\right)$

R_i : *source or sink of solute i* $\left({}^{mol}/_{m^3 \cdot s}\right)$

$$\frac{\partial(c_i\,\phi)}{\partial t} + \mathbf{u}\cdot\nabla c_i = \nabla\cdot(\phi\tau\mathbf{D}_{b,i}\nabla c_i) + R_i,$$

$$R_i = R_i^{FF} + R_{diss,i}^{PS},$$

$$R_i^{FF} = k_+ A(a_{H^+})^n(1 - Q/K),$$

$$R_{diss}^{PS} = \frac{3V_m k_+}{RTd}\left(\frac{\sigma_{VM}}{R_c} - \sigma_c\right).$$

R_i : *source or sink of solute i*

R_i^{FF} : *rates of free − face dissolution/precipitation*

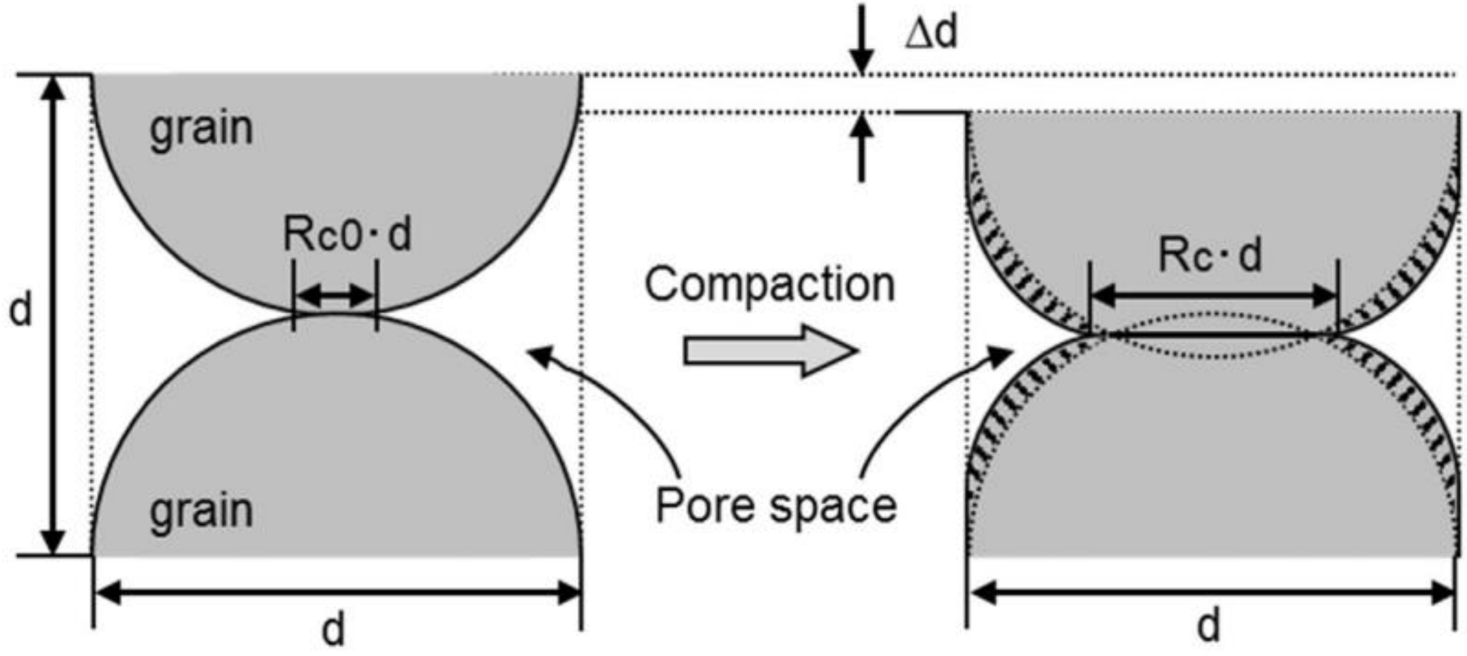
$R_{diss,i}^{PS}$: *rates of pressure dissolution*

$$\dot{\phi}^{FF} = V_m R^{FF},$$

$$\dot{\phi}_{diss}^{PS} = -V_m R_{diss}^{PS},$$

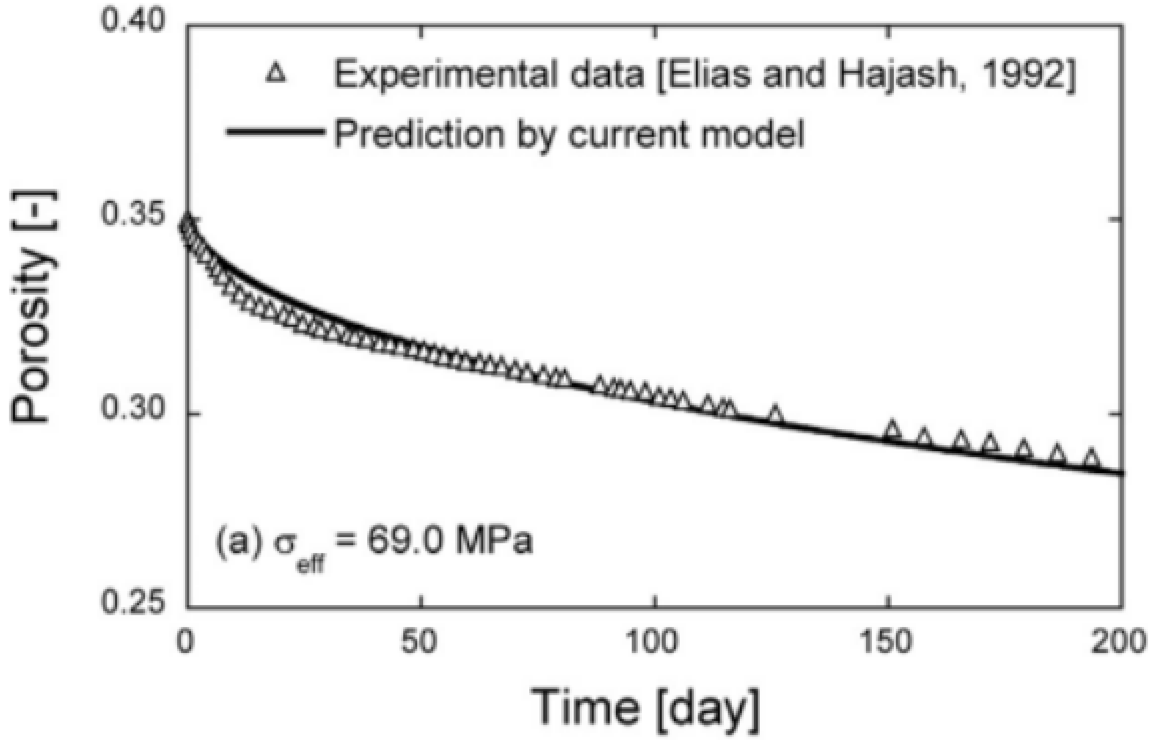
$$\phi = \phi_i + \int \dot{\phi}^{FF} dt + \int \dot{\phi}_{diss}^{PS} dt,$$

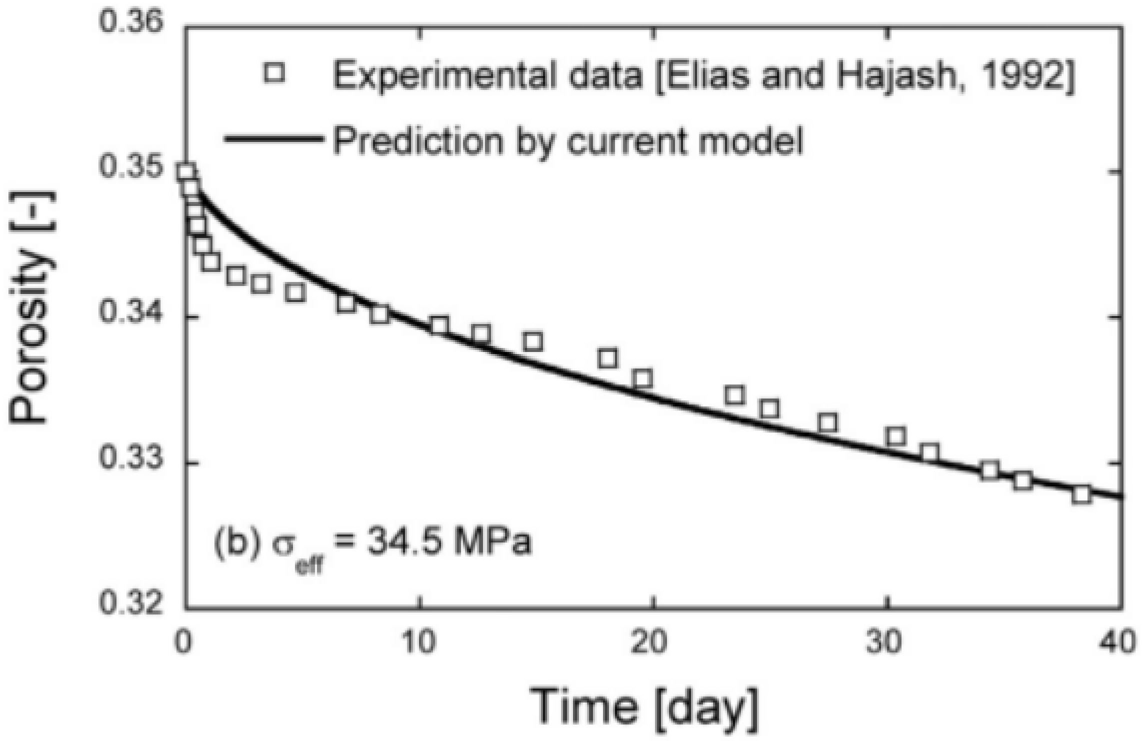
$$k = k_i \frac{(1-\phi_i)^2}{(1-\phi)^2}\left(\frac{\phi}{\phi_i}\right)^3,$$



Elias and Hajash (1992)

Diameter d [μm]	Temperature T [°C]	Effective stress σ_{eff} [MPa]	Critical stress σ_c [MPa]	Equilibrium constant K [mol m^{-3}]	Diffusion coefficient D_b [m^2 s^{-1}]	Dissolution rate constant k_+[mol m^{-2} s^{-1}]	Young's modulus E [GPa]	Poisson's ratio ν [–]
215	150	69.0, 34.5, 17.2	73.2	1.79	1.12×10^{-9}	2.51×10^{-9}	72.4	0.17





Domain size : 700 m vertical lengths
12.2 m horizontal lengths
2.22 m diameter of cavity

Heat source (radioactive wastes) :
laterally at a depth of 450 m

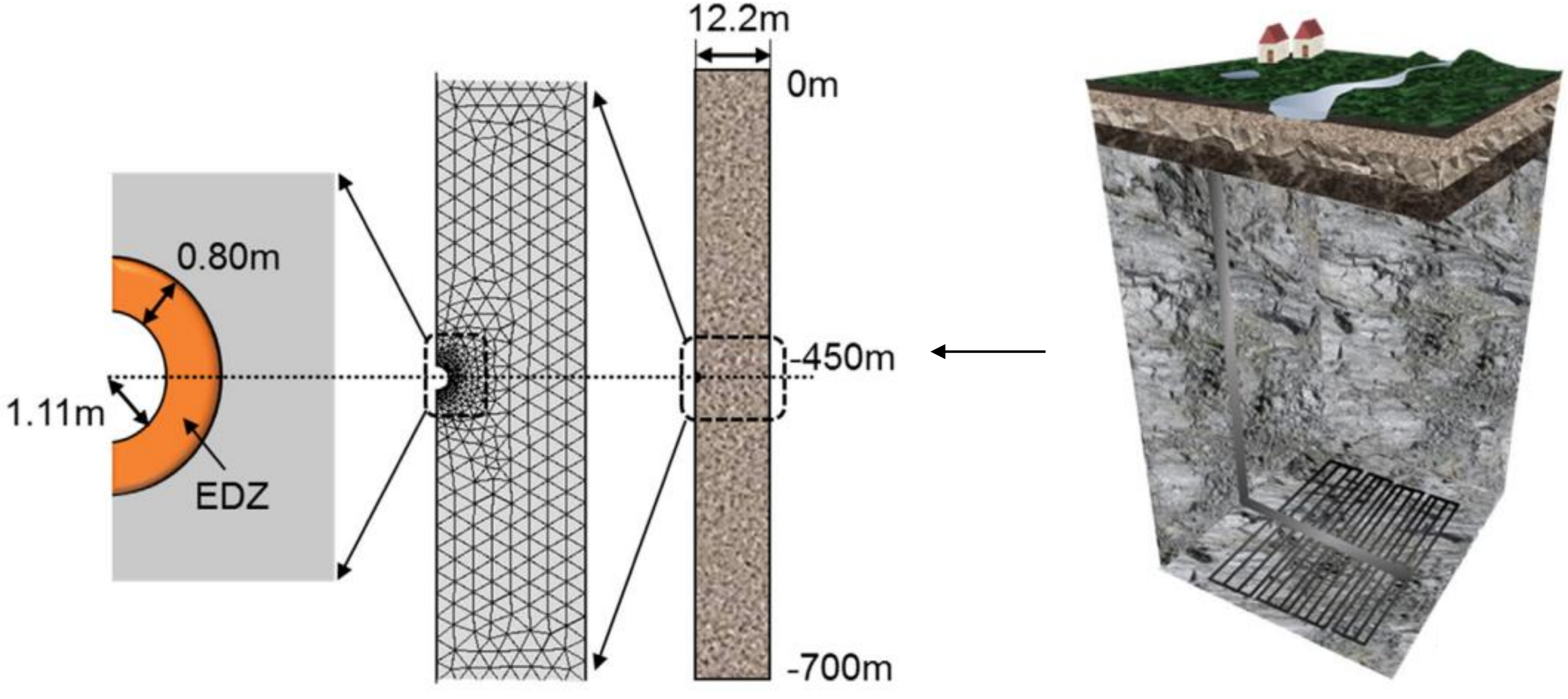
Hydraulic gradients : 1 m/1000 m

Thermal gradients : 5 °C/100 m

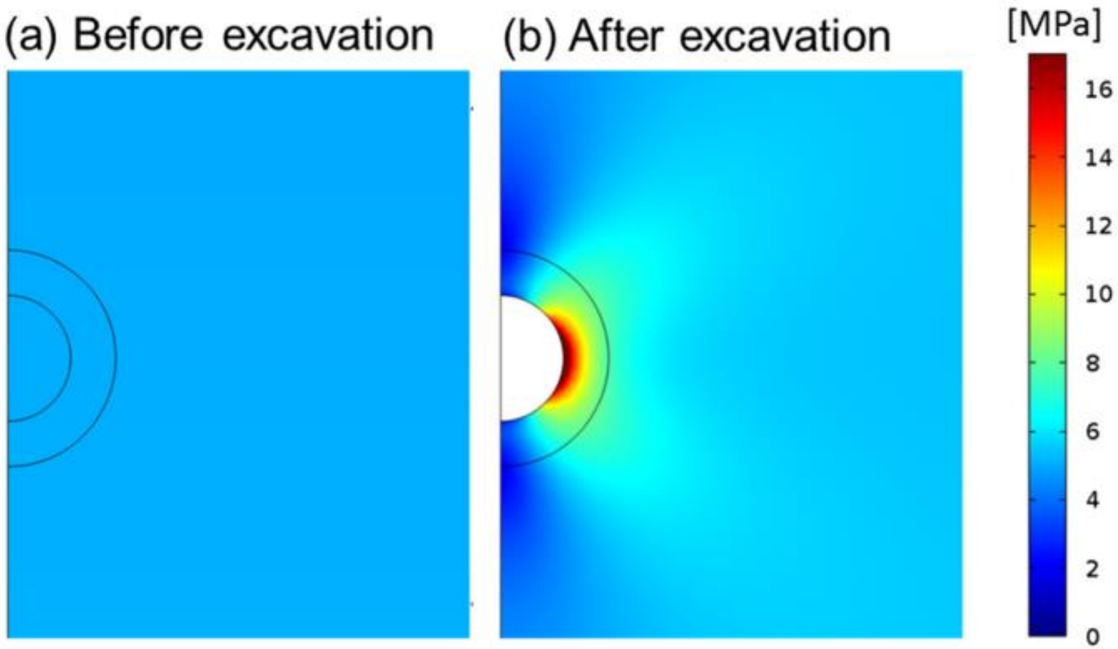
Surface temperature : 15 °C

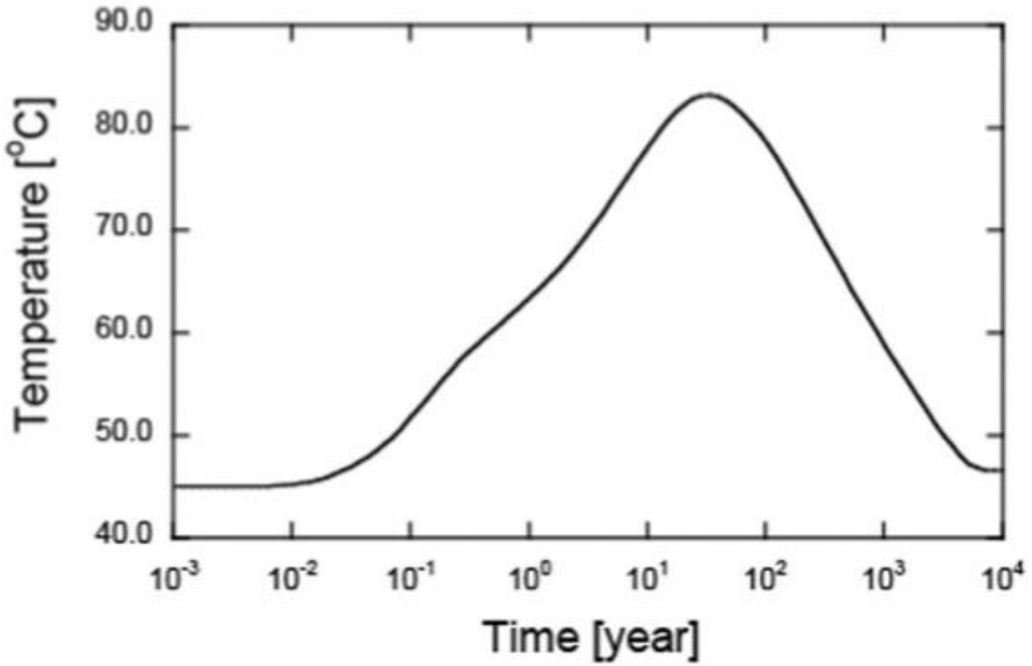
Boundaries : all the boundaries assumed to be thermally and hydraulically the outflow boundaries

EDZ : Excavation Distributed Zone



(Japan Nuclear Cycle Development Institute, JNC TN1410 2000-003)

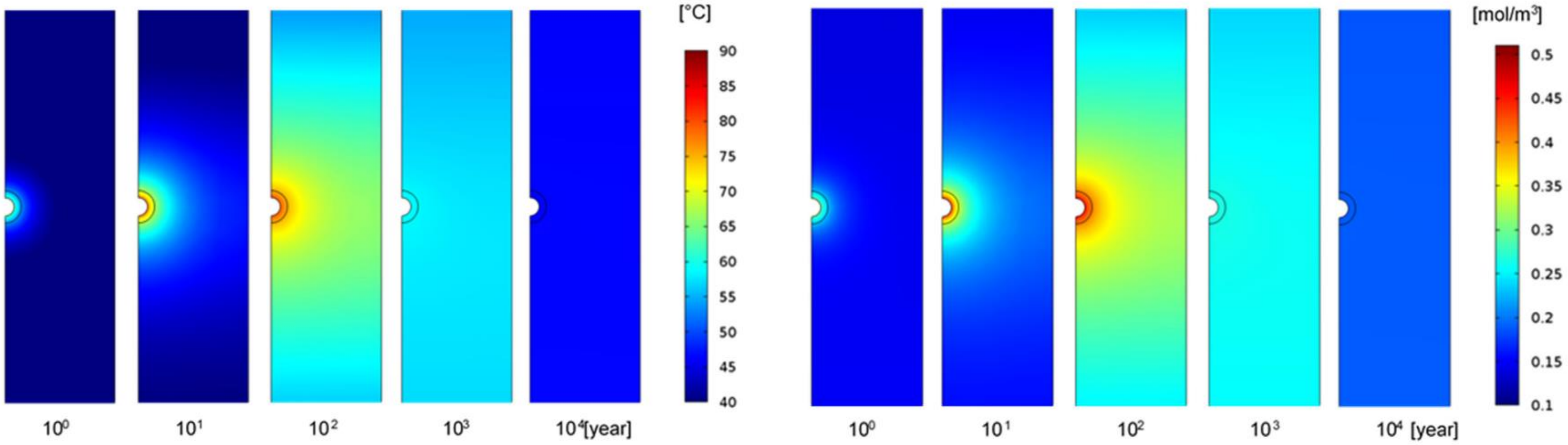

(a) Before excavation
(b) After excavation
[MPa]
16
14
12
10
8
6
4
2
0


Temperature [°C]
90.0
80.0
70.0
60.0
50.0
40.0
10-3
10-2
10-1
100
101
102
103
104
Time [year]

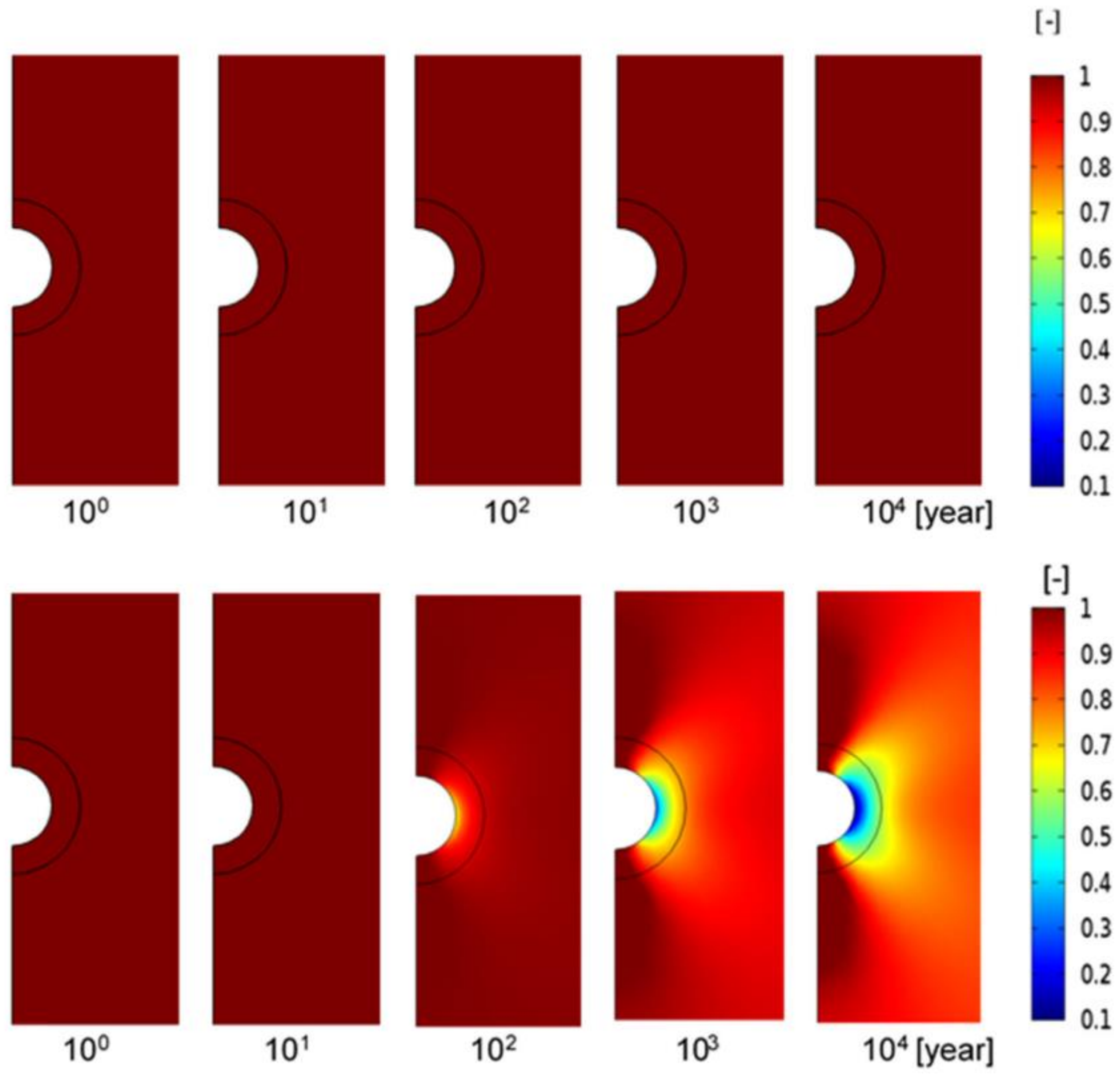
Results

Calculation parameters to simulate long-term permeability.

Rock type	Initial permeability k_i [m^2]	Young's modulus E [GPa]	Poisson's ratio ν [–]	Initial porosity ϕ_i [–]	Thermal conductivity k_{eq} [$W\ m^{-1}\ K^{-1}$]	Heat capacity C_p [$J\ kg^{-1}\ K^{-1}$]
EDZ	1.0×10^{-13}	2.5	0.30	0.40	1.60	1500
Sound	1.0×10^{-15}	2.5	0.30	0.40	1.60	1500



Change in temperature and Si concentration distribution with time in the range of $10^0 \sim 10^4$ years under the PS condition.

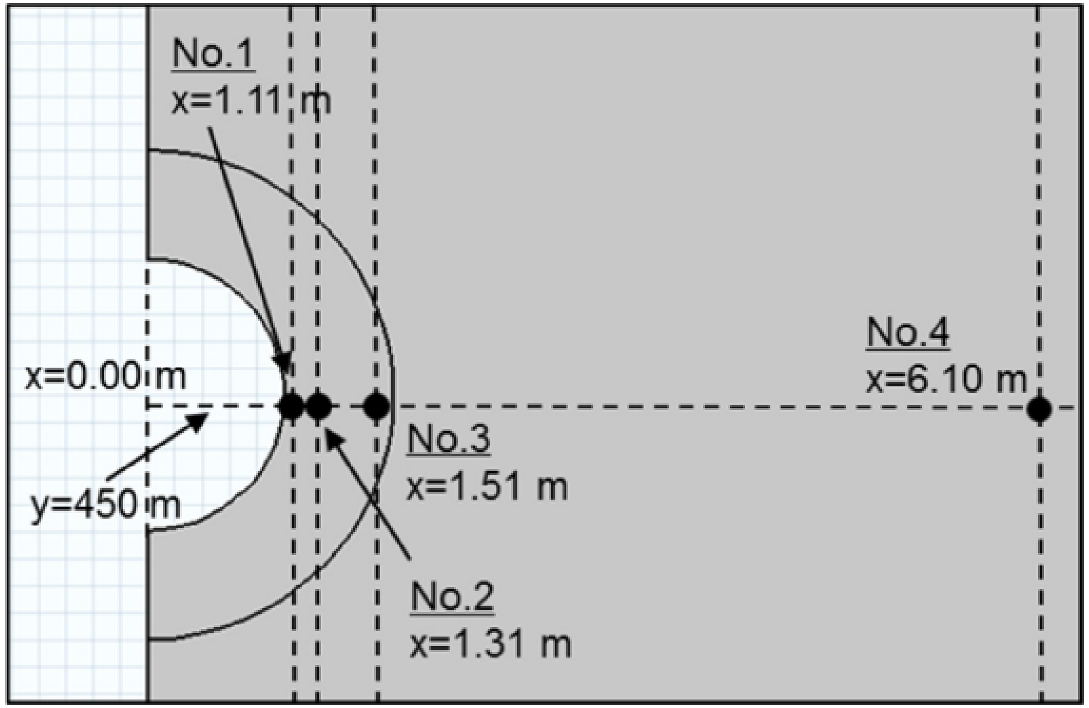


Change in normalized permeability with time in the range of $10^0 \sim 10^4$ years under :

no PS condition

PS condition

To further study the effect of pressure dissolution on permeability changes within the EDZ, the changes with time for the four specific. Three of these four points are located in the EDZ, and the fourth is 5 m from the cavity periphery.



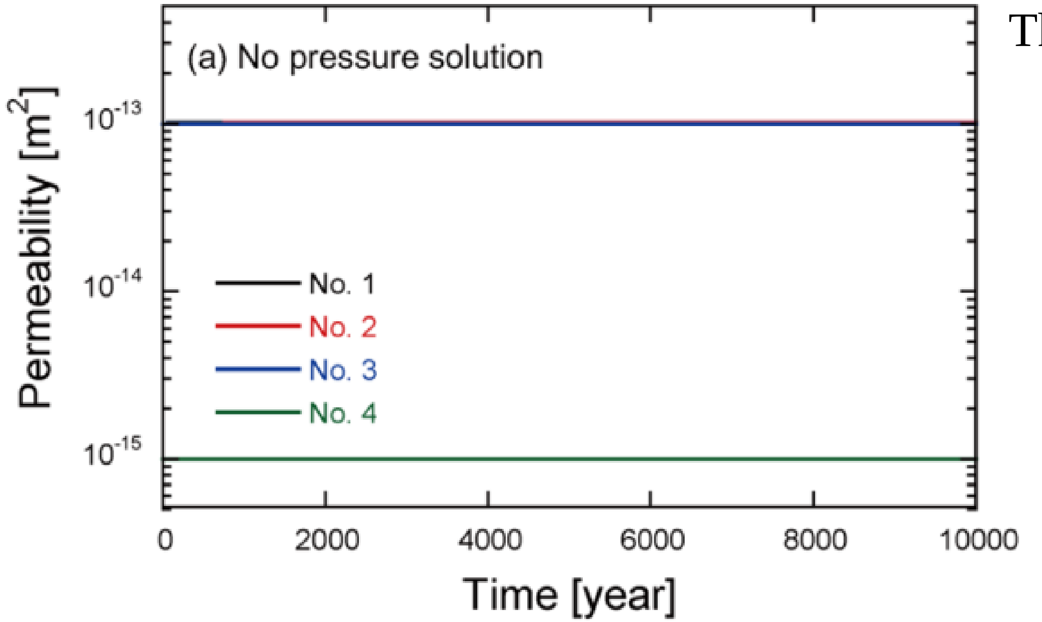
No. 1 : (1.11 m, 0 m)

No. 2 : (1.31 m, 0 m)

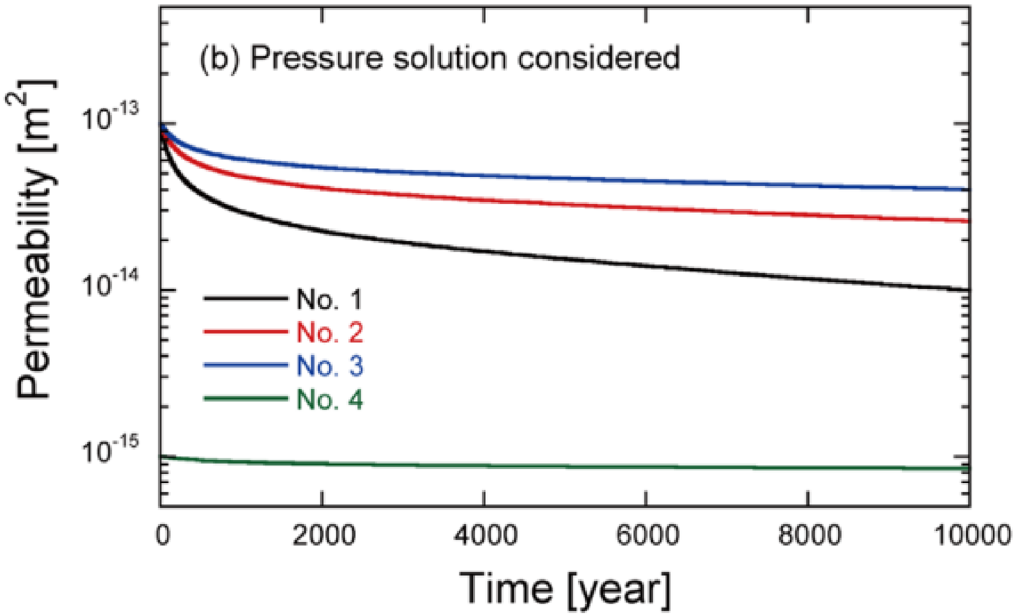
No. 3 : (1.51 m, 0 m)

No. 4 : (6.10 m, 0 m)

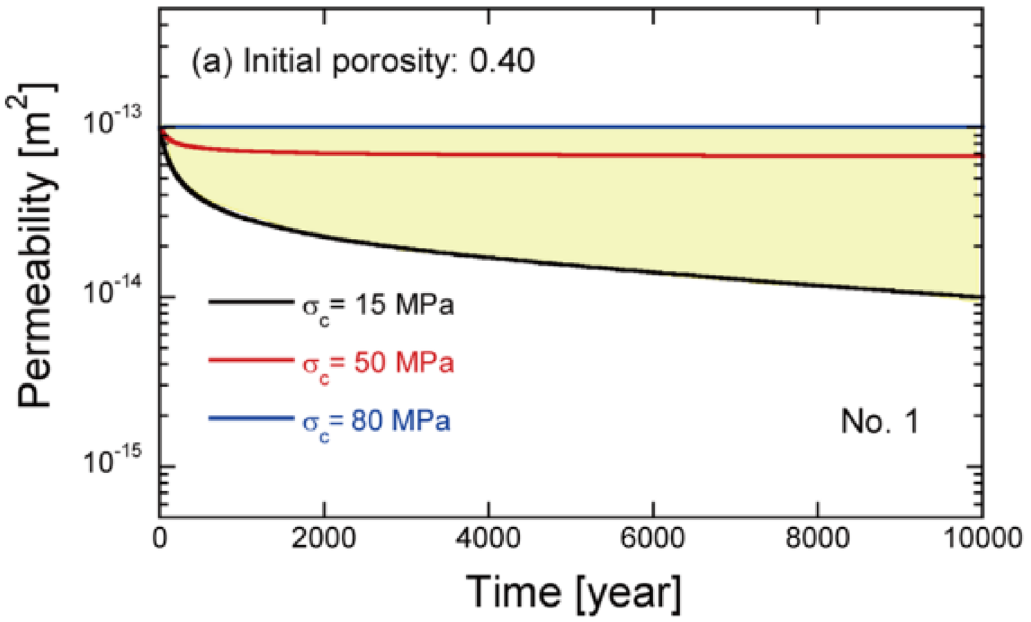
The permeability changes with time at specific locations indicated in :

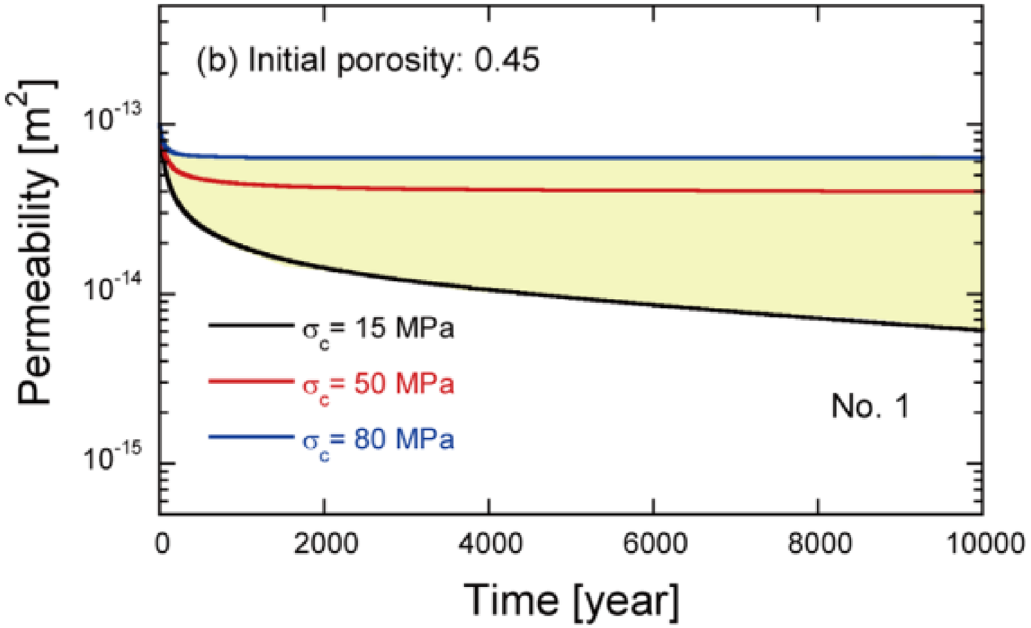


no PS condition



PS condition





The permeability changes with time under the PS condition at No. 1, indicated in:

initial porosity of 0.40

initial porosity of 0.45

- A coupled THMC model was developed to investigate the long-term evolution of the permeability in sedimentary rocks. The model solves the heat transfer, the groundwater flow, the variation in induced stresses, and the geochemical reactions.

- The predictions confirmed that the process of the pressure dissolution decreased the permeability especially close to the excavated cavity by one order of magnitude smaller than the initial value, which should delay the transportation of the radioactive materials.

Thank you for listening !