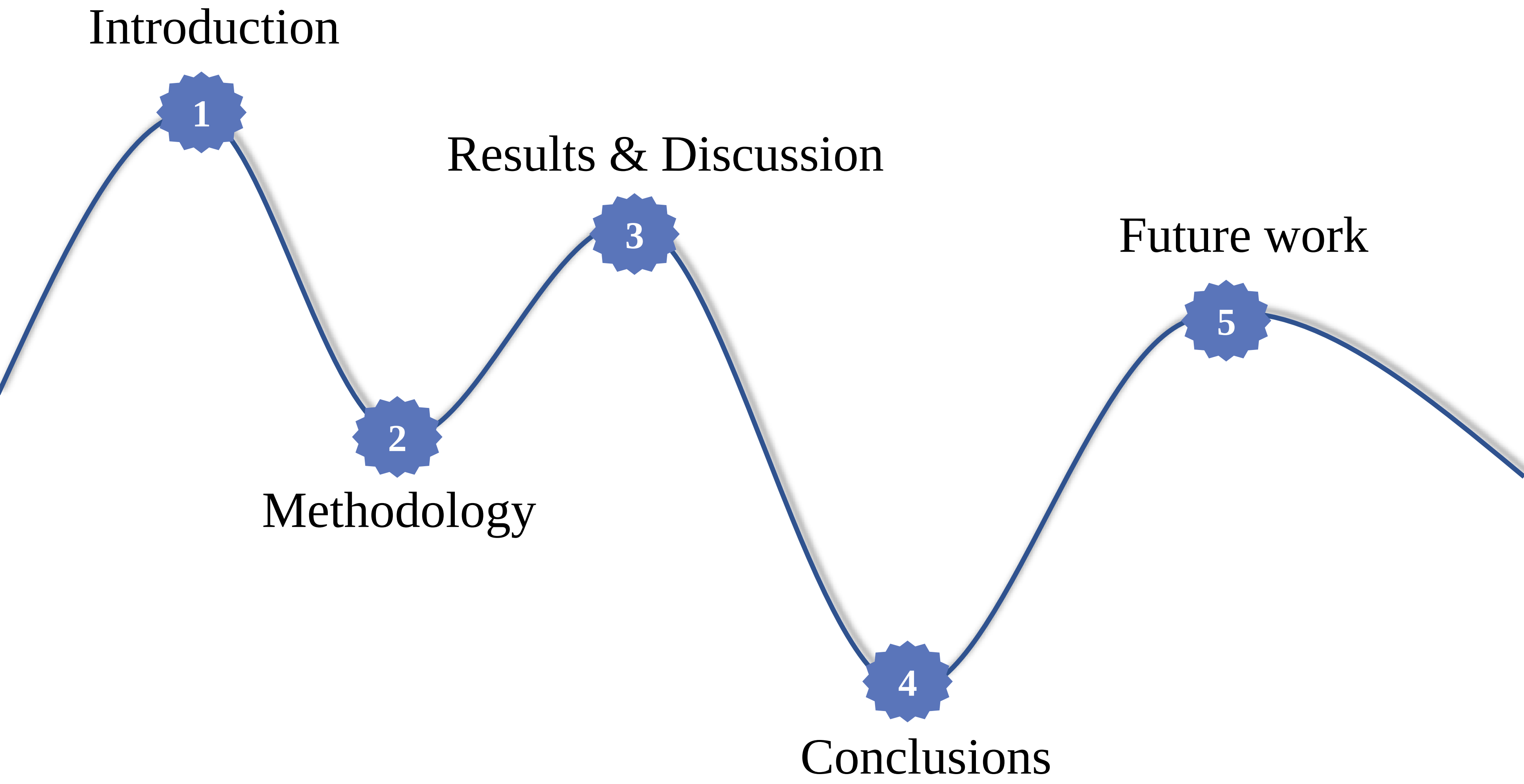
Numerical Simulation of the Evolution of Gas Migration in Bentonite

Presenter：Yu-Sheng Lin
Advisor：Prof. Jui-Sheng Chen
Date：2023/10/20

Outline


Introduction
1
Methodology
2
Results & Discussion
3
Conclusions
4
Future work
5

Introduction

Deep geological repository

- High-level waste has high level of radioactivity and a long half-life.
- After years of international research, it is considered that Deep Geological Disposal is the preferred option.
- Nuclear waste is buried in geological formations at depths greater than 300m. Canister and buffer materials are used to cover and place.
- By employing multiple barriers, the waste decays harmlessly, isolating it from the biosphere and protecting human health and environmental safety.

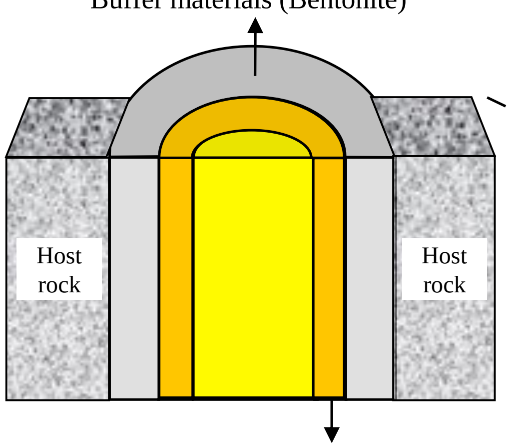


Fig.1. Schematic cross-section

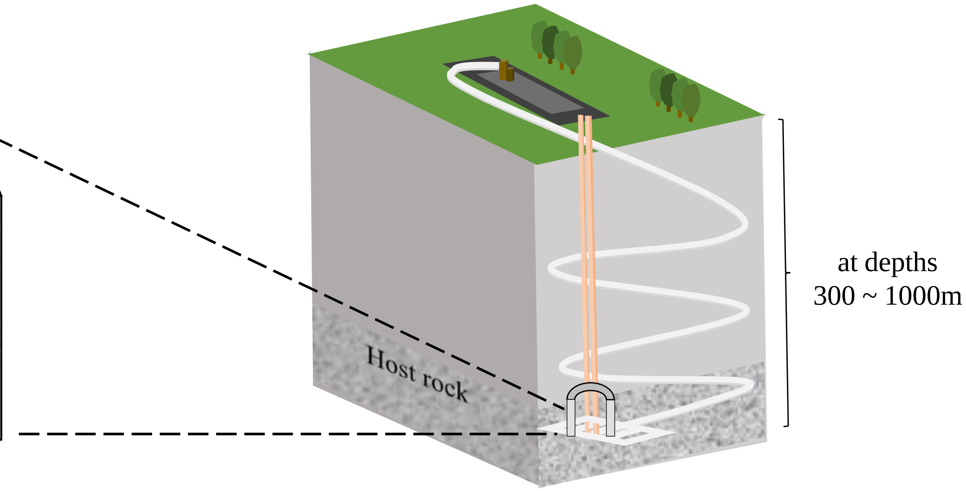
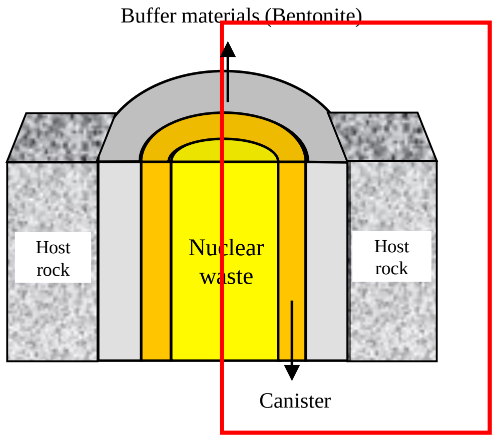


Fig.2. Design concept for the Deep Geological Repository

Coupled THMC processes (Thermal-hydraulic-mechanical-chemical)

- However, after hundreds of years of disposal, temperature will trigger hydrological, mechanical, and chemical processes that may impact the safety of the repository.
- This is because nuclear waste emits heat, thermal expansion induces fractures, groundwater then flows through fractures from host rock to buffer materials.



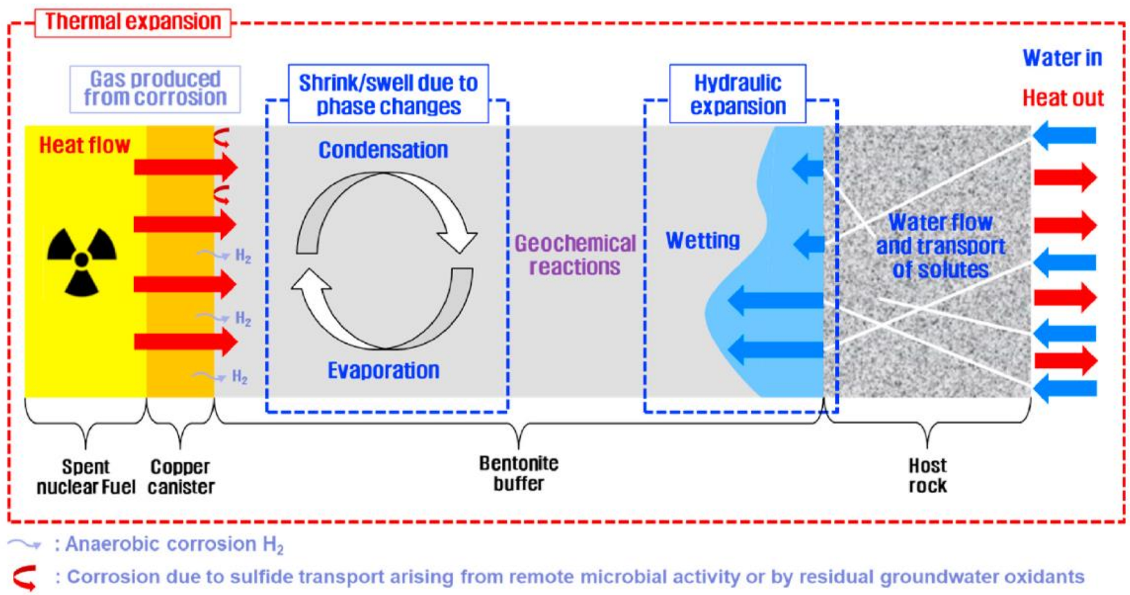
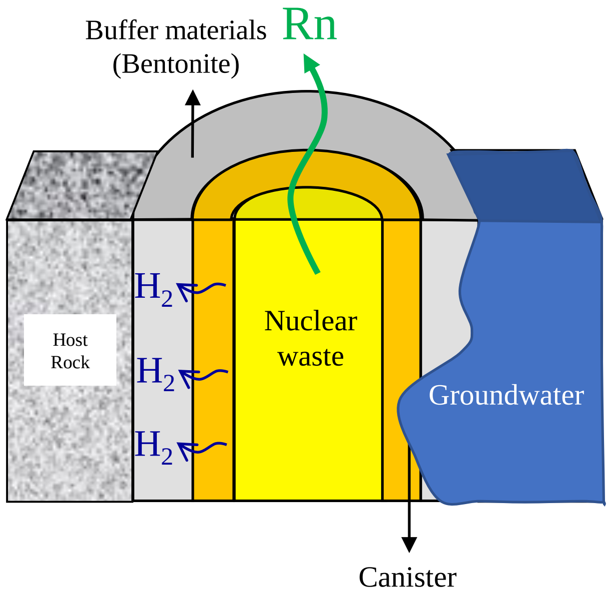


Fig.3. Schematic of the coupled THMC processes (Lee et al., 2021)

Gas generation in a deep geological repository

- In a deep geological repository, gas may be generated, which can degrade the capability of the barrier.
- Gas generation can occur due to the
  - A. corrosion of metallic materials under anoxic conditions (H_2)
  - B. the radioactive decay of waste (Rn)
  - C. the radiolysis of water (H_2)



- Gas may leak from canister, so buffer materials (bentonite) plays an important role.

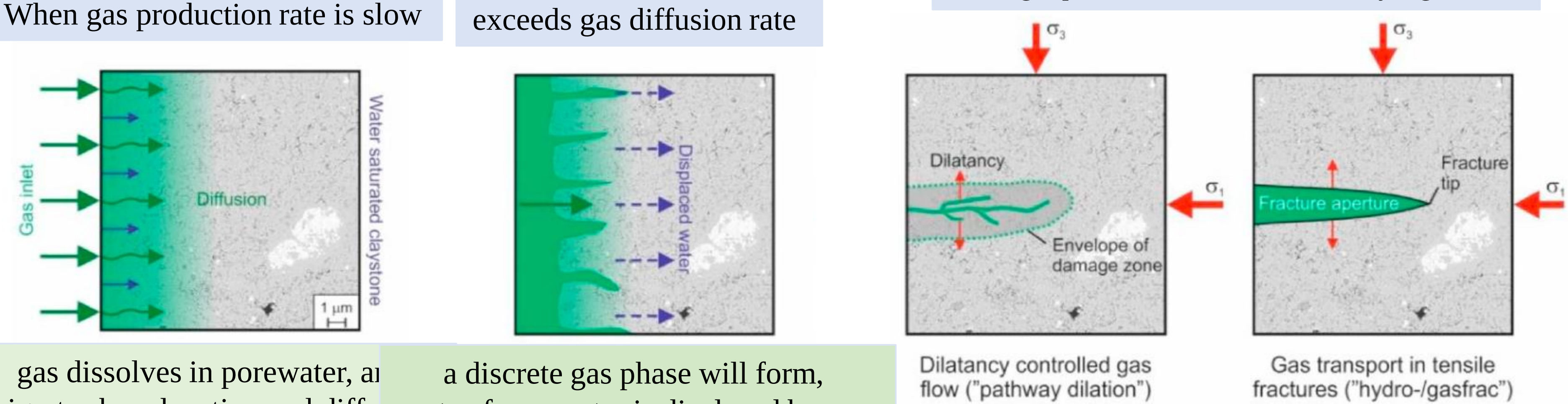
Gas migration in bentonite

What happened to gas migration in bentonite?

When gas production rate is slow

When gas production rate exceeds gas diffusion rate

When gas pressure accumulates to a very high value



gas dissolves in porewater, ar
migrates by advection and diffu

a discrete gas phase will form,
parts of porewater is displaced by gas.

Fig.4. The mechanisms of gas migration in clays. (Marschall et al., 2005)

- The stress acting on the bentonite cannot withstand gas pressure, leading to pathway dilation and tensile fractures, allowing gas to escape from bentonite.
- Therefore, gas migration in bentonite becomes a critical issue for the safety assessment of deep geological repository.

Literature reviews

- Several international projects aiming to understand the advective movement of gas through clay-rich materials have already been conducted. These include MEGAS, EVEGAS, PROGRESS, GAMBIT, NF-Pro and FORGE. (Tamayo-Mas el at., 2020)

- In a recent project, DECOVALEX-2019 developed four types of modeling approaches to study gas movement. The results were still unclear, like heterogeneity of materials, stochasticity of gas flow and upscaling challenges.

- Therefore, it is necessary to describe the full complexity of the processes for gas migration in clay-based repository systems.

Objective

Using the THMC7.1 numerical model to simulate gas migration in bentonite, and subsequently verifying the modeling results with experimental data.

- To explain the gas migration process in bentonite more clearly, including gas pressure accumulation and timing of gas breakthrough.
- To investigate the temporal distribution of intrinsic permeability, and analyze the effects of hydraulic-mechanical coupling.

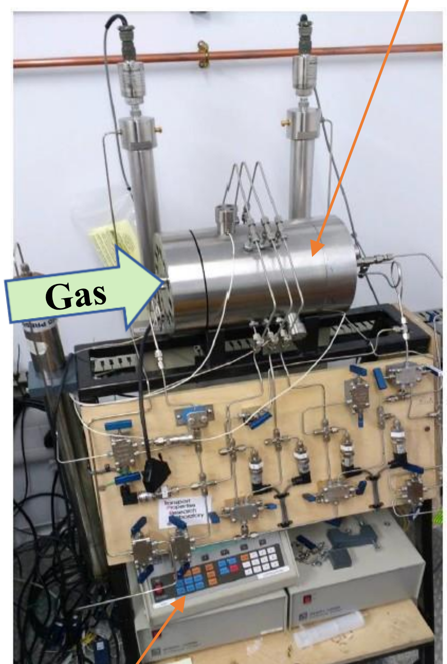
Experimental data

- Gas injection experiments were conducted in the laboratory by the British Geological Survey (BGS). (Daniels et al., 2017)

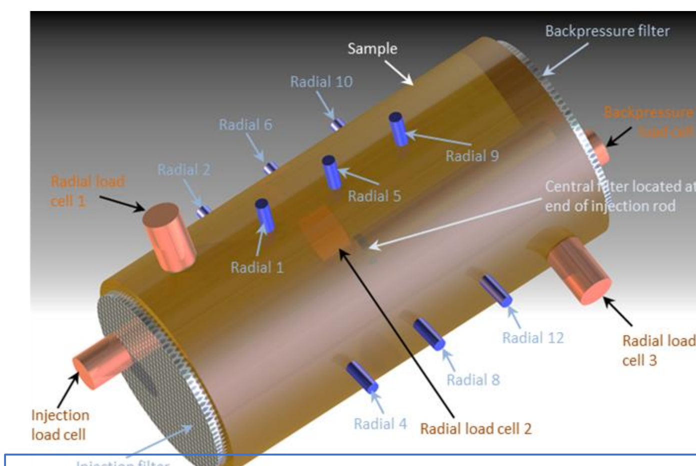
Table.1. The injection schedule

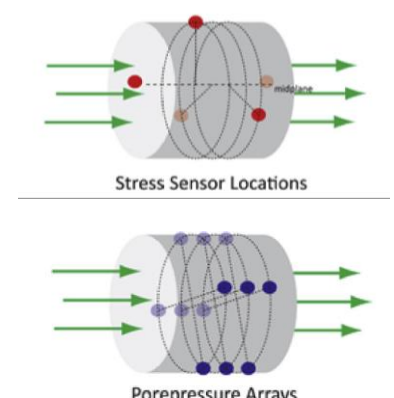
Start time	Injection pump rate ($\mu l/h$)	Comment
Day 39	0	Gas pressure: 3Mpa Gas volume: 235ml
Day 46	500	Start of injection pump
Day 54	375	Gas pressure: 5Mpa Gas volume: 139.7ml
Day 61		Gas refilled 59.95ml, pressure maintained
Day 71	0	Injection pump stopped

Pressure vessel contains a bentonite sample.
(in order to imitate the high pressure surrounding)



Pump controller

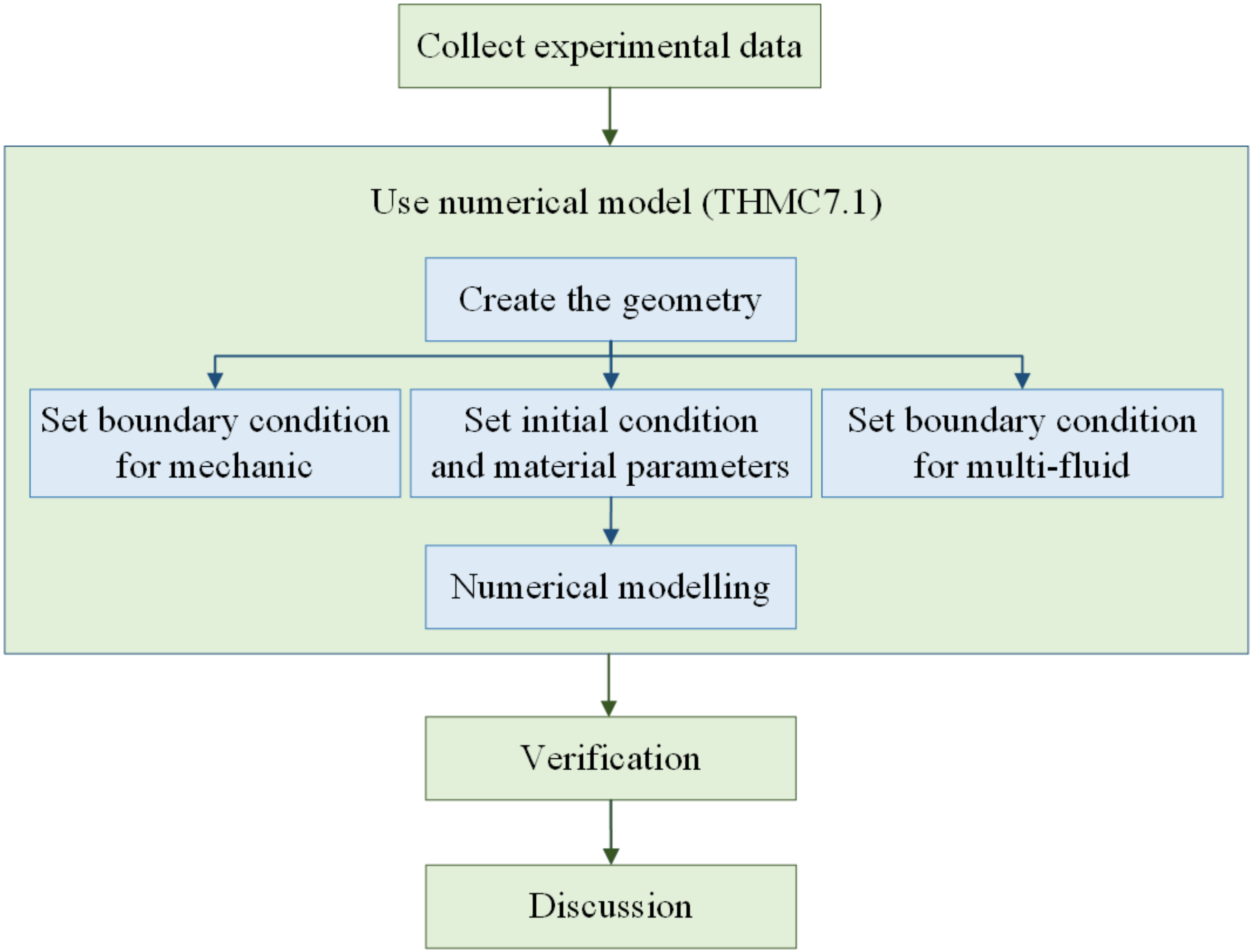




The outer surface of pressure vessel is equipped with sensors and filters

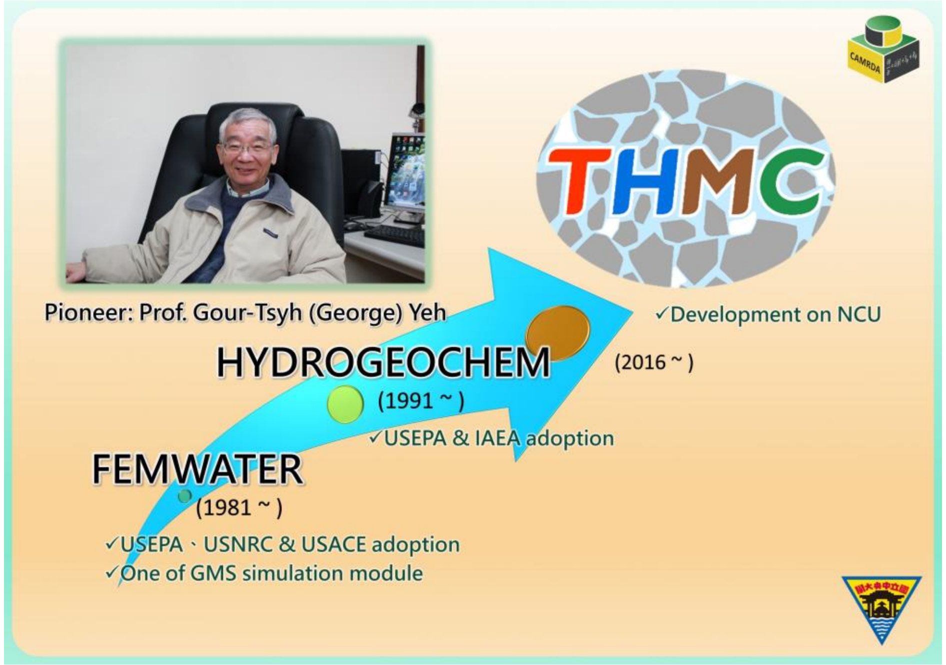
Methodology

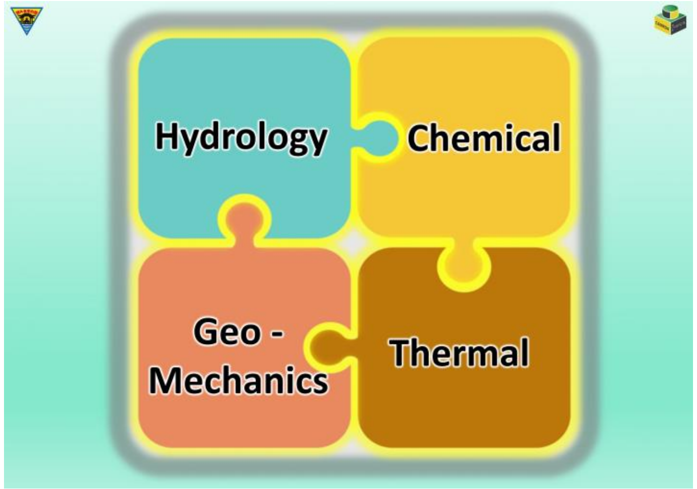
Flow chart


Collect experimental data
Use numerical model (THMC7.1)
Create the geometry
Set boundary condition for mechanic
Set initial condition and material parameters
Set boundary condition for multi-fluid
Numerical modelling
Verification
Discussion

Numerical model

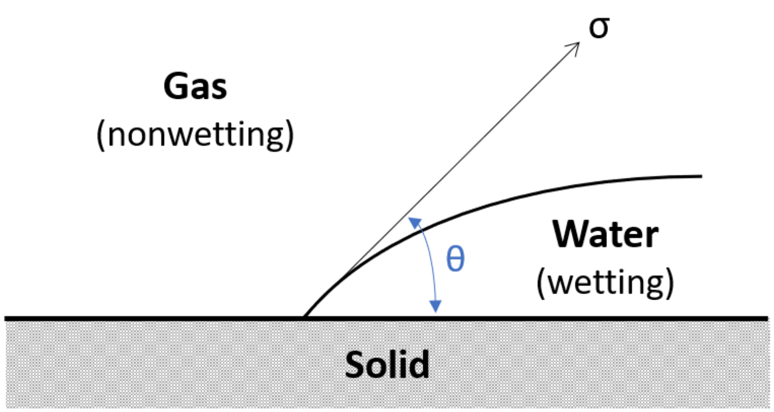
- THMC7.1 is a three-dimensional finite element model of coupled multiphase fluid flow (H), thermal transport (T), chemical transport (C), and geo-mechanics (M) modules.
- THMC7.1 is powerful and provides the design capability to simulate partially or completely coupled processes.





Concept of multiphase fluid

- Multiphase fluid includes water, gas, and NAPL(nonaqueous phase liquid).
- When two immiscible fluids contact, they form a curved surface at the interface. The tension on this surface is known as surface tension (σ).
- The angle between the surface and a solid is known as the contact angle (θ). It is a crucial parameter for determining the wetting degrees of fluid.



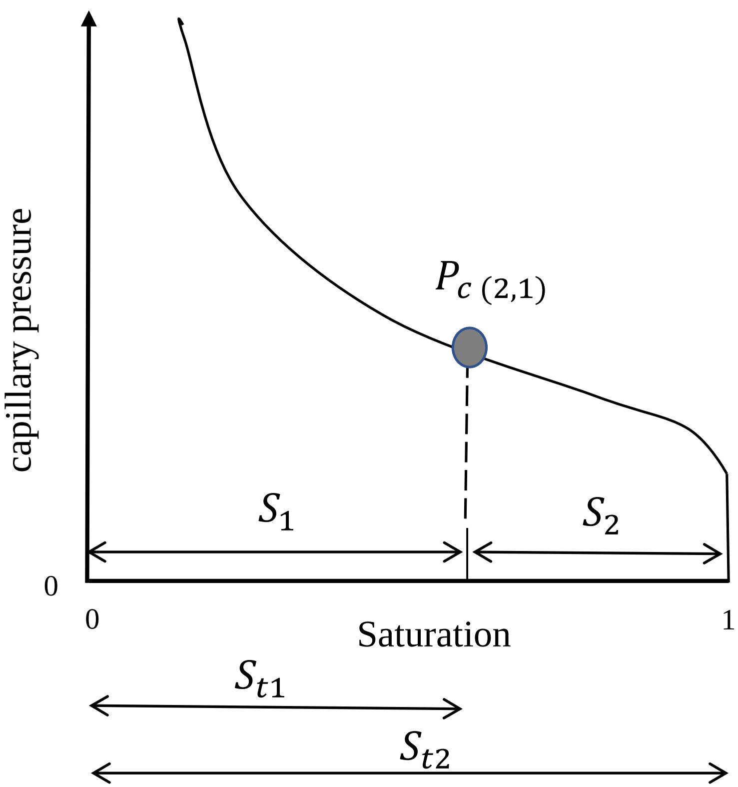
$\theta < 90°$: wetting phase
$\theta > 90°$: nonwetting phase

Concept of multiphase fluid

- In unsaturated zone, capillary pressure (Pc) is the main mechanism causing fluid flow. Pc changes with saturation, that is, Pc is a function of accumulated saturation (S_t).

$$Pc = Pn - Pw = f(S_t)$$

Pn: pressure of nonwetting phase
Pw: pressure of wetting phase



Parker et al.'s law (Parker et al., 1987)

$$P_{c\,(2,1)} = \frac{1}{\alpha}\left(s_{t1}^{-\frac{1}{M}} - 1\right)^{1/N}$$

α: scaling factor
N,M: curve shape parameter

Numerical model: Multiphase fluid flow (H) module

- Mass conservation equation:

Fluid phase

Suk and Yeh(2007,2008);
Tsai and Yeh(2012,2013)

$$\frac{\partial \rho_\alpha \phi S_\alpha}{\partial t} + \nabla \cdot (\rho_\alpha \boldsymbol{V}_\alpha) + \nabla \cdot (\rho_\alpha \phi S_\alpha \boldsymbol{V}_s) = M^\alpha, \alpha \in \{L\} \qquad \sum_{\alpha=1}^{L} S_\alpha = 1$$

ρ_α: the density of α-th fluid phase (kg/m^3)
ϕ: the volume fraction (-)
S_α: the normalized saturation of α-th fluid phase (-)
$\boldsymbol{V}_\alpha$: the Darcy velocity of α-th fluid phase (m/s)
$\boldsymbol{V}_s$: the velocity of the solid (m/s)
M^α: the sum of the artificial source/sink rate of all species in α-th fluid phase (kg·m^{-3}·s^{-1})

Numerical model: Geo-mechanics (M) module

- Momentum balance equation:

$$-\nabla \cdot \mathbf{T} + \sum_{\alpha\in\{L\}} \nabla\left(S_{\alpha} p_{\alpha}\right) - \left[\sum_{\alpha\in\{L\}} \rho_{\alpha}\phi\, S_{\alpha} + \rho_{s}\phi_{s}\right]\boldsymbol{g}\nabla\mathbf{z} = -\phi_{s}\rho_{s}\frac{d^{2}\boldsymbol{u}}{dt^{2}} \approx 0$$

T: the Cauchy stress tensor in the continuum mechanics (Pa)
p_α: the pressure of the α-th fluid phase (Pa)
$\boldsymbol{g}$: the gravitational acceleration (m/s^2)
z: the potential head (m)
$\boldsymbol{u}$: the displacement of the media (m)

Setting of geometry

- Using THMC7.1 to create a geometry with a diameter of 60 mm and a length of 120 mm, then generate quadrilateral prism mesh.

Table.2. Information of geometry

	Diameter (mm)	Length (mm)	Number of nodes	Number of elements
Quadrilateral prism	60	120	8425	7680

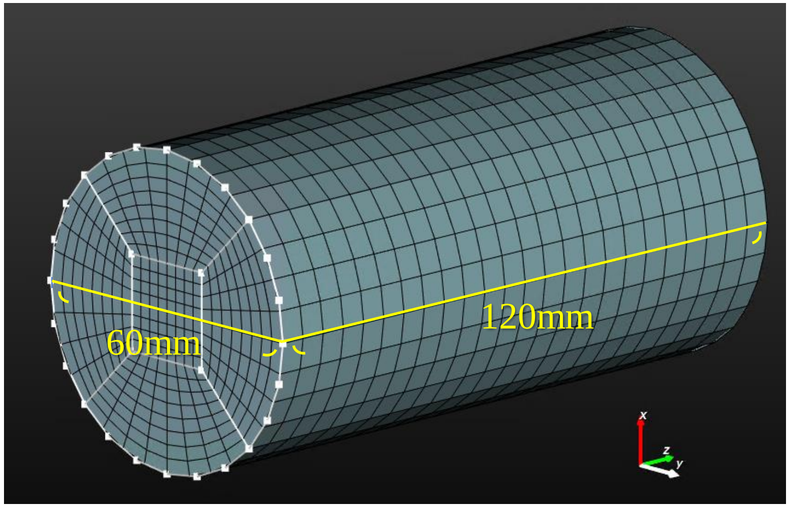


Fig.7. Quadrilateral prism mesh (bentonite sample)

Setting of boundary

Table.3. Information of initial condition

Initial condition	Parameter	Units	Value
Multiphase fluid flow (H)	Porewater pressure p_w	[MPa]	1
	Gas saturation S_g	[-]	0.01
Geo-mechanics (M)	Displacement $u_x.u_y.u_z$	[m]	0
	Stress tensor	[MPa]	0.0
	Porosity ϕ	[-]	0.43

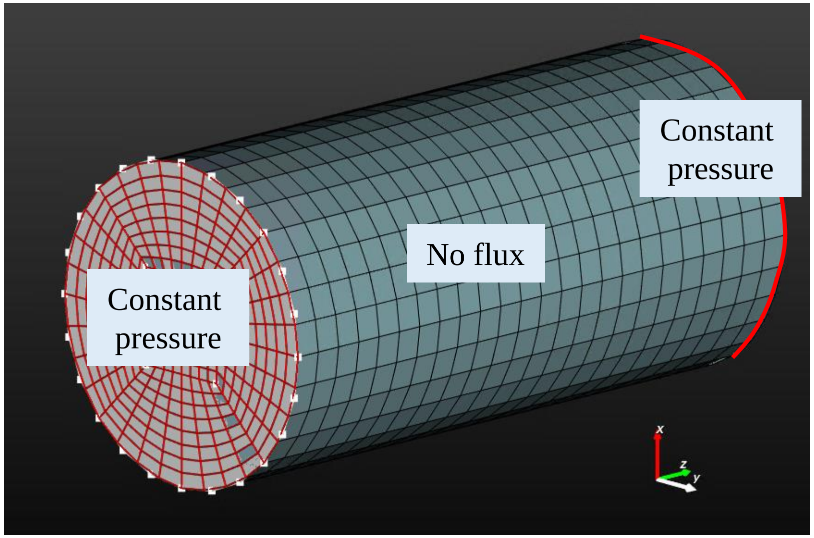


Fig.8. Localization of multi-fluid boundary

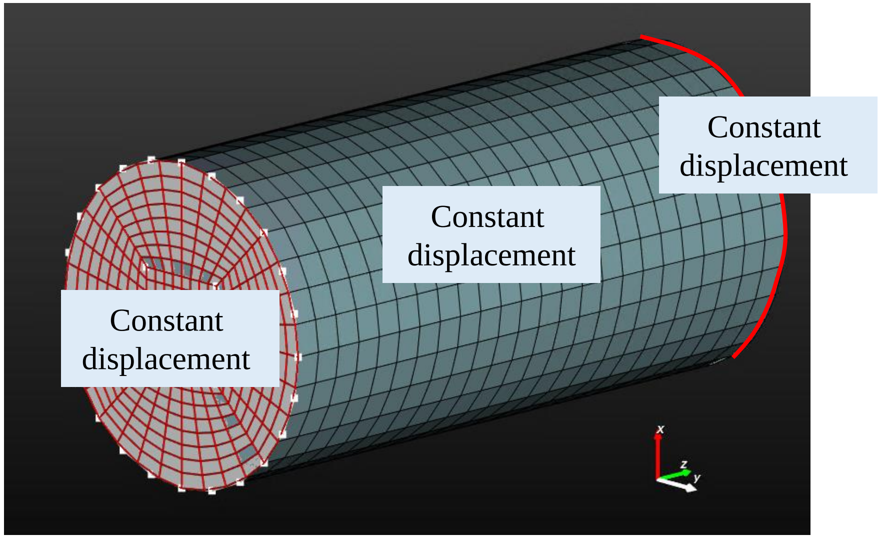


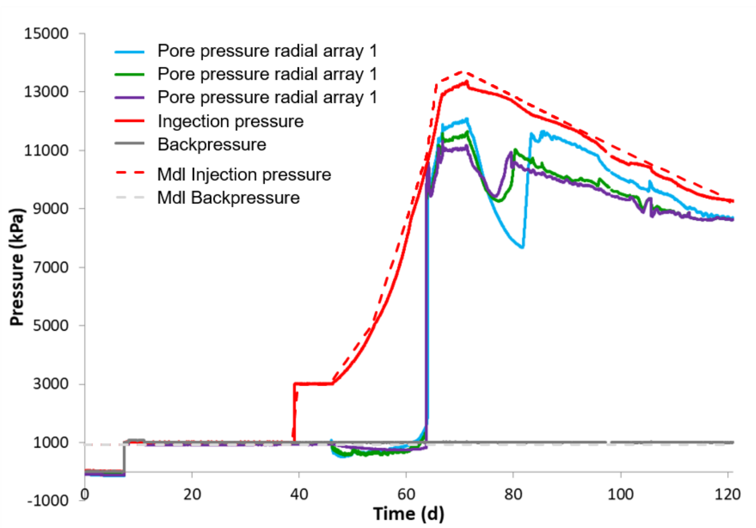
Fig.9. Localization of geo-mechanics boundary

Results& Discussion

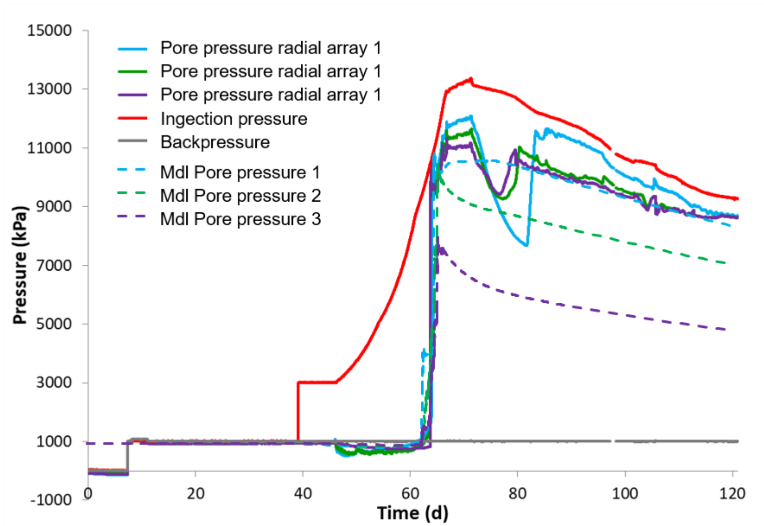
Verification

- Using the experimental data' gas pressure, pore pressure and total stress to verify the modeling results.

injection pressure & backpressure



pore pressure



The result is underestimated,
I will try to make it better.

Verification

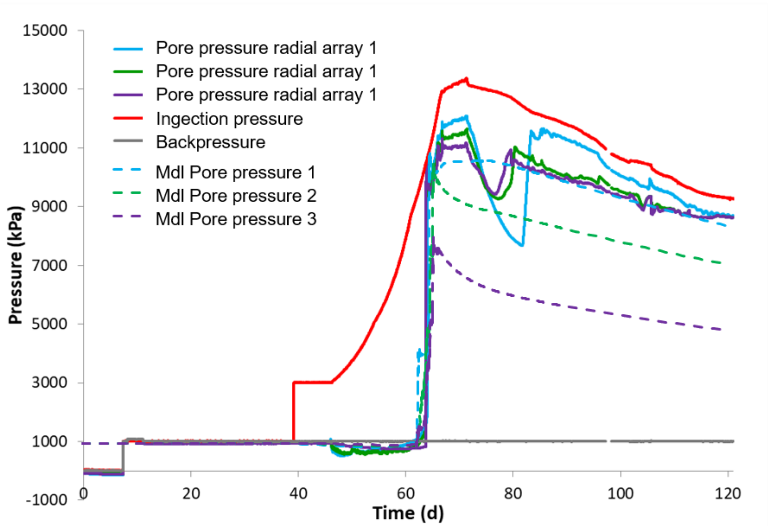
- Using the experimental data' gas pressure, pore pressure and total stress to verify the modeling results.

The trend can be roughly simulated.

✓ Gas breakthrough was captured at about Day64.

✓ After Day64, pore pressure gradually decrease because the stress acting on bentonite cannot withstand gas pressure, so porosity and permeability changes.

pore pressure



Results

- Gas entered into Bentonite at Day62.
- Gas breakthrough was captured at about Day64.

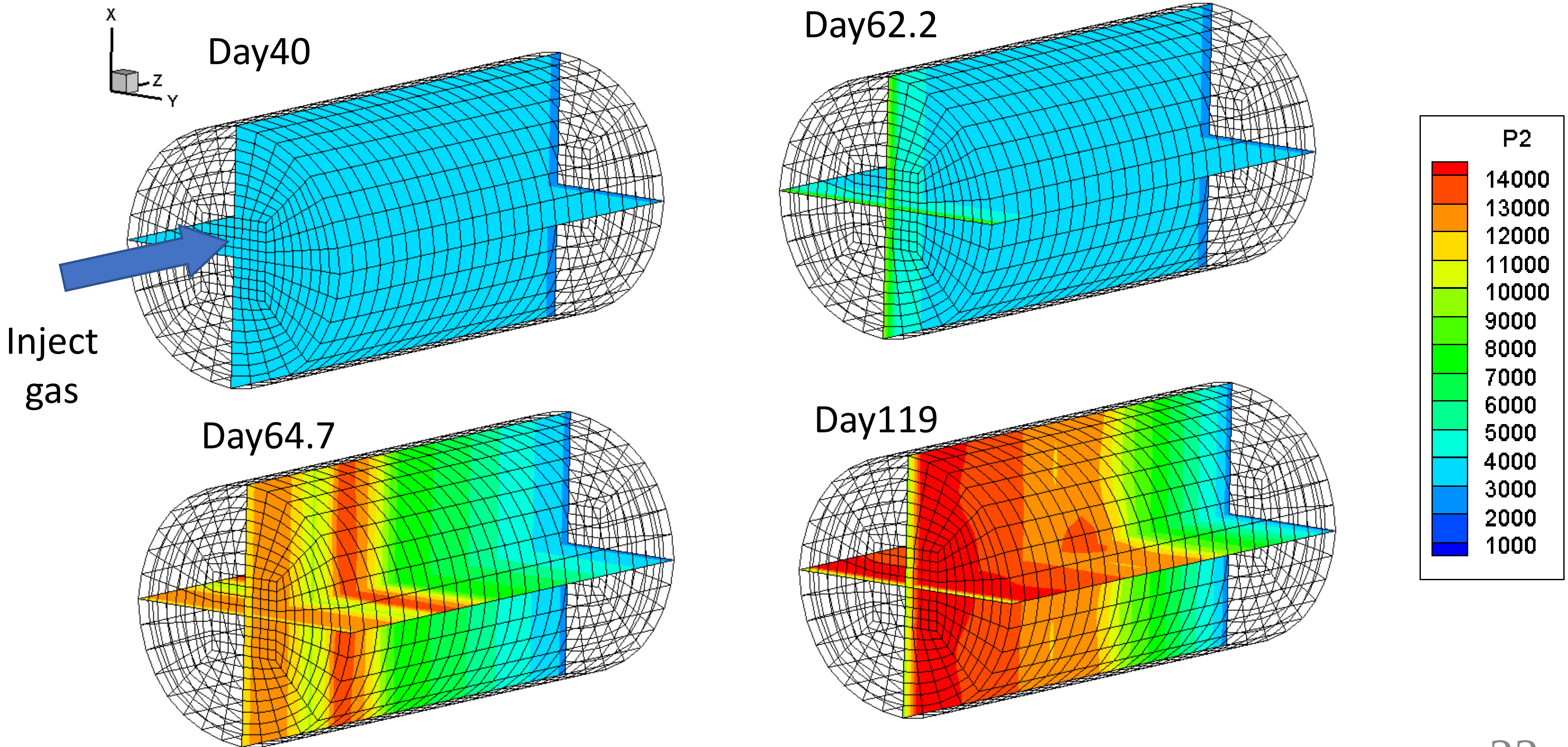


Fig.10. The modelling results of evolution of gas pressure.

Table of parameters

Table.4. Table of parameters

Parameter	Units	Value
Intrinsic permeability, k_x	m^2	3.4×10^{-21}
Intrinsic permeability, k_y	m^2	3.4×10^{-21}
Intrinsic permeability, k_z	m^2	6.0×10^{-21}
Dry density, ρ	kg/m^3	1560
Porosity, ϕ	-	0.43
Young's modulus, E	MPa	307
Poisson's ratio, υ	-	0.4
Ratio of elastic, s_2/s_1	-	0.75
Material compressibility, α	$m{\cdot}day^2/kg$	3.054×10^{-19}
Water compressibility	$m{\cdot}day^2/kg$	6.162×10^{-20}
Gas compressibility	$m{\cdot}day^2/kg$	1.8×10^{-17}

Conclusions

Conclusions

- This study can simulate the gas migration in bentonite and successfully capture the timing of gas entry and breakthrough.

- Pore pressure induced by the fluid flow also affects changes in the effective stress, leading to the displacement of the bentonite.

Future work

1. Continuing the verification the modelling results, using another boundary condition which mass flux to simulate.

2. Considering the heterogeneous materials with varying intrinsic permeability and porosity, which is used to compare with the homogeneous materials.

3. Investigating the temporal distribution of intrinsic permeability, analyzing the effects of hydraulic-mechanical coupling.

Thanks for your attention.