Numerical Simulation of Coupled Multiphase Fluid Flow and Mechanics for Gas Migration in Bentonite Considering Heterogeneous Distributions

Yu-Sheng Lin[1], Jui-Sheng Chen[1,2]

[1]Graduate Institute of Applied Geology, National Central University, Taoyuan, Taiwan

[2]Center for Advanced Model Research Development and Applications, National Central University , Taoyuan, Taiwan

Email : new095885@gmail.com

1. Introduction

The final disposal method for high-level waste is Deep Geological Disposal. By the principles of isolation and retardation, the waste decays harmlessly, isolating it from the biosphere and ensuring human health and environmental safety.

However, after hundreds of years of disposal, gas may be generated due to the corrosion of metallic materials under anoxic conditions, radioactive decay of waste, or the radiolysis of water. As gas degrades the barrier's capability, endangering the safety of the repository. Thus, buffer materials play a crucial role in the repository bentonite is commonly chosen as the buffer materials. In practical situations, bentonite exhibits different particle arrangements, porosity, and permeability, presenting heterogeneous distributions.

Therefore, this study utilized gas injection laboratory experiment data and applied the THMC7.1 numerical model to simulate gas migration, aiming to better understand gas pressure accumulation. Additionally, it investigated the impact of heterogeneous bentonite on gas flow.

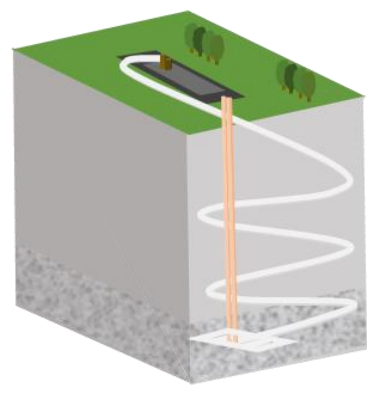


Fig. 1. Design concept for the Deep Geological Repository

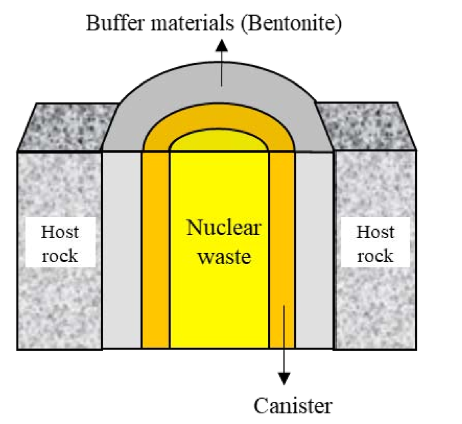
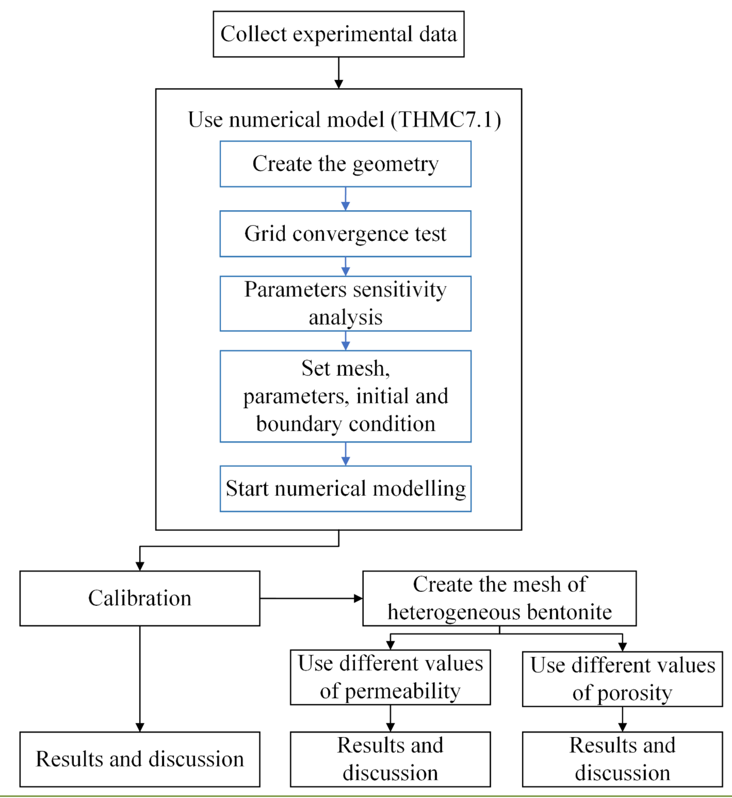


Fig. 2. Schematic cross-section of disposal system

2. Flow chart



3. Experimental data

Gas injection experiments were conducted in the laboratory by the British Geological Survey (Daniels et al., 2017). This experiment spanned 121 days and was divided into three phases: 1.Hydration (0-39d) 2.Gas injection (39-71d) 3.Gas turned-off (71-121d).

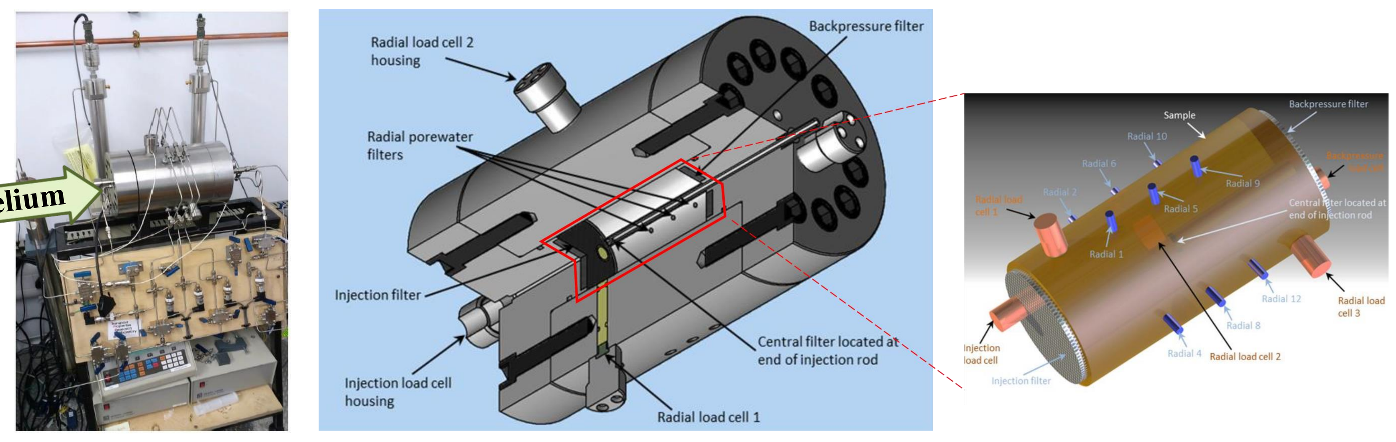


Fig. 3. The experimental apparatus and sample assembly

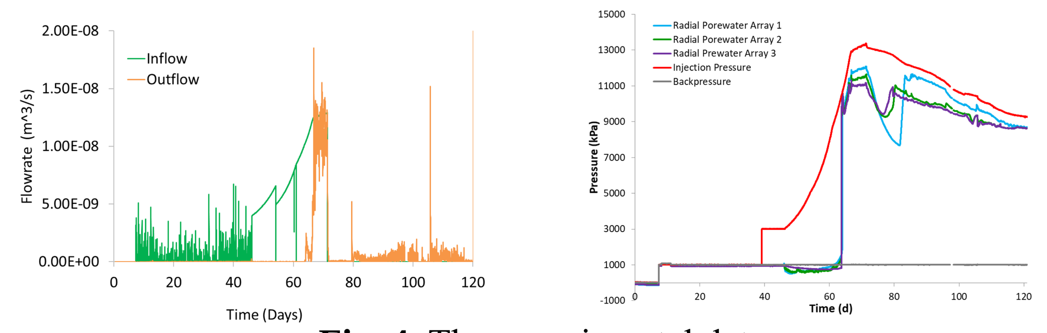


Fig. 4. The experimental data

4. Numerical model

THMC7.1 (Thermal-Hydrology-GeoMechanics-Reactive Chemical Transport Model) is a 3-D finite element model of fully coupled four processes.

Thermal Hydrology Geo-Mechanics Reactive Chemical Model

- ✓ Thermal transport (T)
- ✓ Multiphase fluid flow (H)
- ✓ Geo-mechanics (M)
- ✓ Chemical transport (C)

Multiphase fluid flow (H) module

- Mass conservation equation:

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

in which $\boldsymbol{V}_\alpha = -\frac{k_{r\alpha}\boldsymbol{k}}{\mu_\alpha}\cdot(\nabla P_\alpha + \rho_\alpha g \nabla z) \quad \boldsymbol{V}_s = \frac{d\boldsymbol{u}}{dt}$

t: the time (T)
ρ_α: the density of α-th fluid phase (ML^{-3})
ϕ: the porosity (-)
S_α: the normalized saturation of α-th fluid phase (-)
$\boldsymbol{V}_\alpha$: the Darcy velocity of α-th fluid phase (LT^{-1})
$\boldsymbol{V}_s$: the velocity of the solid (LT^{-1})
M^α: the sum of the artificial source/sink rate of all species in α-th fluid phase (ML^{-3}T^{-1})

$k_{r\alpha}$: the relative permeability of i-th fluid (-)
$\boldsymbol{k}$: the permeability of porous medium (L^2)
μ_α: the viscosity of α−th fluid (ML^{-1}T^{-1})
P_α: the pressure of the α-th fluid phase (ML^{-1}T^{-2})
$\boldsymbol{g}$: the gravitational acceleration (LT^{-2})
$\mathbf{z}$: the potential head (L)
$\boldsymbol{u}$: the displacement of the media (L)

- Capillary pressure / Relative permeability / Saturation law: (Parker et al., 1987)

$$\begin{cases} \tilde{S}_{t\alpha} = 1 & if \ \ P_{C\alpha+1,\alpha} \le 0 \\ \tilde{S}_{t\alpha} = \left[1 + \left(\bar{\alpha} P_{C\alpha+1,\alpha}\right)^N\right]^{-M} & if \ \ P_{C\alpha+1,\alpha} > 0 \end{cases} ,\alpha \in \{L-1\}\,;\ \tilde{S}_{tL} = 1$$

$\tilde{S}_{t\alpha}$: the accumulated saturation of α-th fluid phase (-)
P_C: the capillary pressure (ML^{-1}T^{-2})
$\bar{\alpha}$: the scaling factor related to the entry pressure (ML^{-1}T^{-2})
N and M: the curve shape parameter (-) M=1-1/ N

Geo-mechanics (M) module

- Mass conservation equation:

$$\frac{\partial \rho_s \phi_s}{\partial t} + \nabla\cdot(\rho_s \phi_s \boldsymbol{V}_s) = 0$$

ρ_s: the density of solid (ML^{-3})
ϕ_s: the porosity of solid (-)
$\mathbf{T}$: the Cauchy stress tensor (ML^{-1}T^{-2})

P_s: the pressure of solid (ML^{-1}T^{-2})
S_1, S_2 : the elastic parameters (ML^{-2}T^{-2})
$\lambda, \mu_1, \mu_2, \mu_3$: the viscous parameters (ML^{-1}T^{-1})

- Momentum balance equation:

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

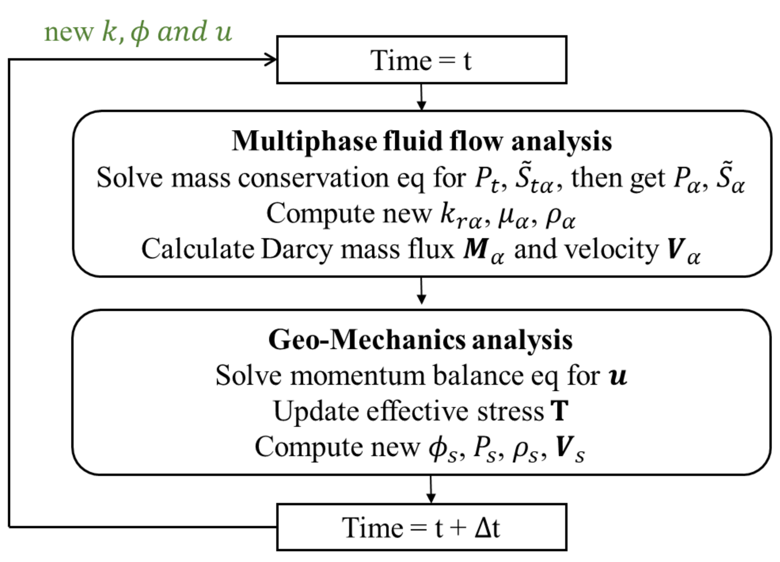
- Constitutive law for viscous-elastic material:

$$\mathbf{T} = -\phi_s P_s \mathbf{I} + S_1\mathbf{B} + S_2\mathbf{B}^{-1} + \lambda(tr\mathbf{D})\mathbf{I} + 2\mu_1\mathbf{D} + \mu_2(\mathbf{DB}+\mathbf{BD}) + \mu_3(\mathbf{DB}^{-1}+\mathbf{B}^{-1}\mathbf{D})$$

in which $\mathbf{B} = \mathbf{FF}^T, \mathbf{F} = \mathbf{I}+\mathbf{H}, \mathbf{H} = \nabla\mathbf{u}, \mathbf{D} = \frac{1}{2}(\dot{\mathbf{H}} + \dot{\mathbf{H}}^T), \dot{\mathbf{H}} = \nabla\dot{\mathbf{u}} = \nabla V_s$

Coupled H-M analysis

Pore pressure induced by fluid flow influences the formation of displacement and alterations in effective stress. Further affect the variation of porosity and intrinsic permeability.



$$P_{s1} = P_{s0} - \frac{1}{\alpha}\ln\left(\frac{1-\phi_{s1}}{1-\phi_{s0}}\right)$$

$$k_1 = k_0\left(\frac{1}{1+(\phi_0-\phi_1)}\right)^n$$

5. Geometry and parameters

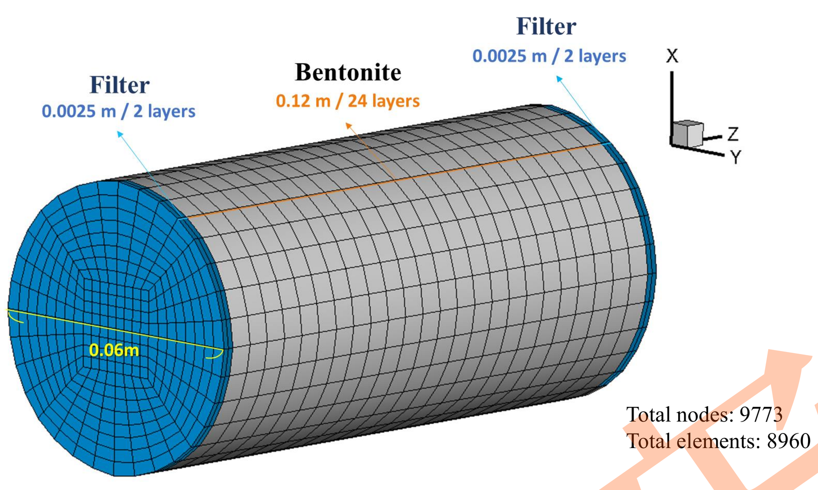


Fig. 5. The geometry and mesh

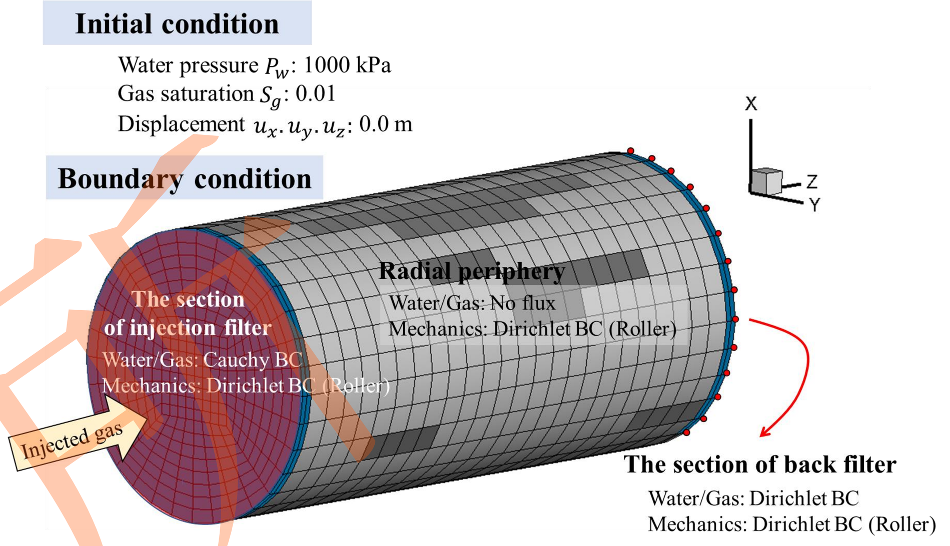


Fig. 6. The initial and boundary condition

Table.1. Table of parameters of multiphase fluid flow

Parameter	Units	Filter	Bentonite
Permeability, k	m^2	3.0 ×10^{-17}	5.0 ×10^{-19}
Porosity, ϕ	-	0.43	
Water compressibility, β_w	m·day^2/kg	6.162×10^{-20}	
Gas compressibility, β_g	m·day^2/kg	9.0 ×10^{-17}	
Water density, ρ_w	kg/m^3	1000	
Gas density, ρ_g	kg/m^3	0.1663	
Water viscosity, μ_w	kg/m/day	84.108	
Gas viscosity, μ_g	kg/m/day	1.6412	

Table.2. Table of parameters of geo-mechanics

Parameter	Units	Filter	Bentonite
Solid density, ρ_s	kg/m^3	1560	
Young's modulus, E	MPa	307	
Poisson's ratio, υ	-	0.4	
Solid compressibility, β_s	m·day^2/kg	3.054×10^{-19}	
Ratio of elastic, s_2/s_1	-	0.75	
Elastic parameter, s_1	kg/m/day	3.2739×10^{18}	
Elastic parameter, s_2	kg/m/day	2.4554×10^{18}	

6. Results& Discussion

Results

The initial gas saturation is 0.01. However, as gas is injected over time, the gas pressure increases, and the gas saturation gradually rises.

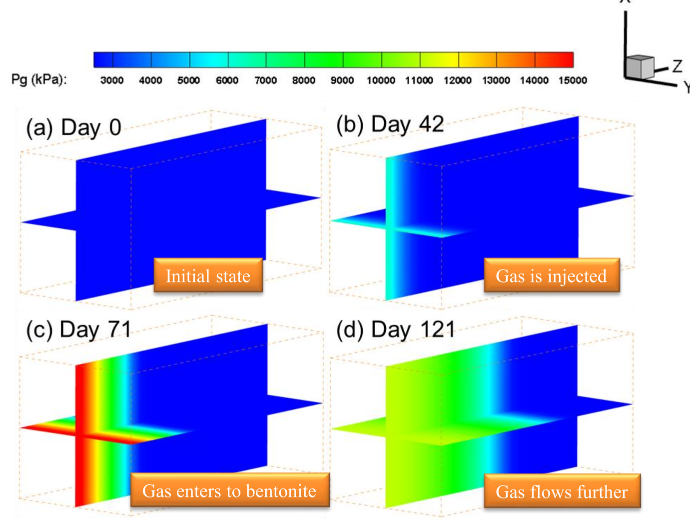


Fig. 7. The modelling result of gas pressure

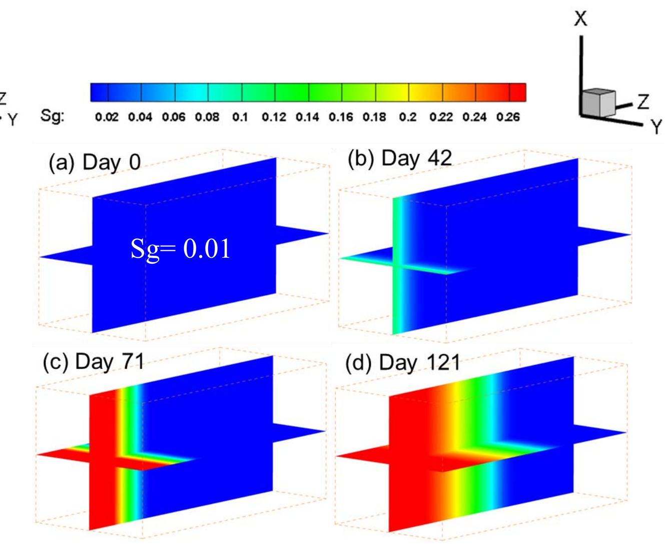


Fig. 8. The modelling result of gas saturation

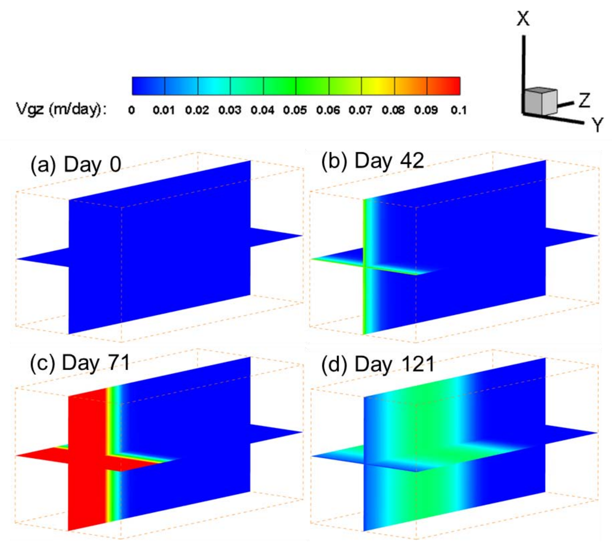


Fig. 9. The modelling result of gas velocity(z)

Results considering the heterogeneous distributions

Dividing into two distributions of bentonite.

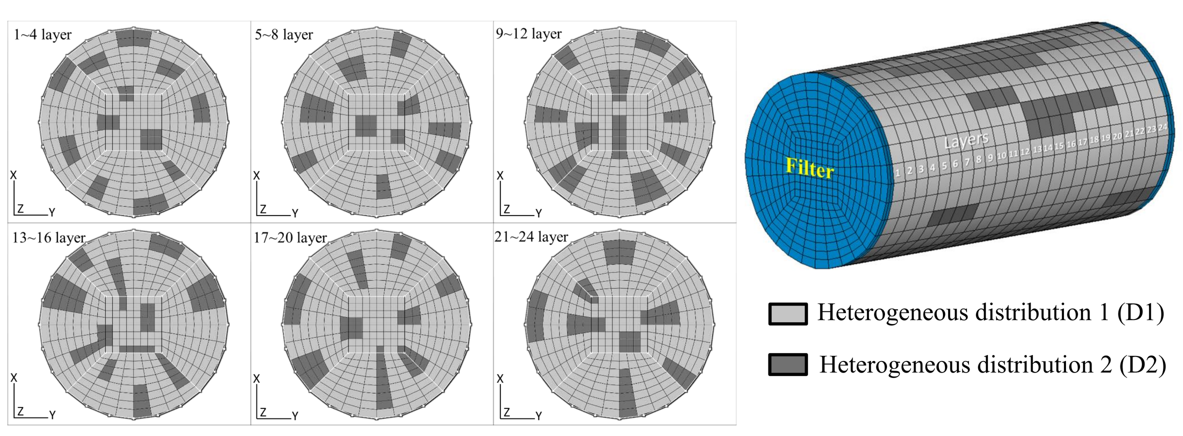


Fig. 11. The heterogeneous distributions of bentonite

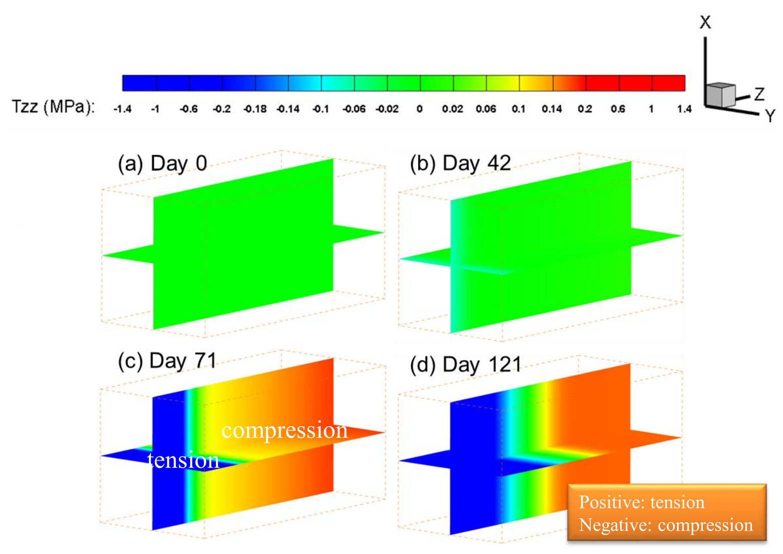


Fig. 10. The modelling result of effective stress

Using different values of permeability

D1: k=5.0 ×10^{-19}m^2
D2: k=9.0 ×10^{-19}m^2

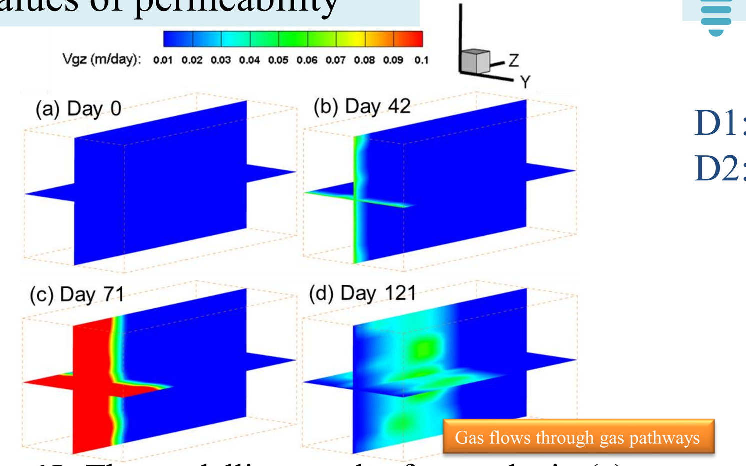


Fig. 12. The modelling result of gas velocity(z)

Using different values of porosity

D1: ϕ=0.43
D2: ϕ=0.44

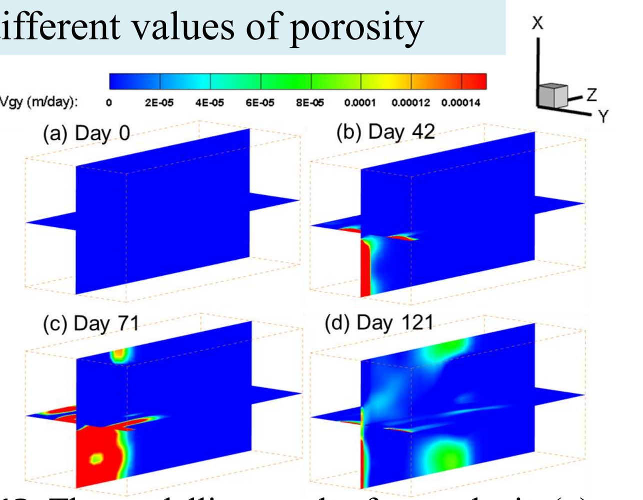


Fig. 13. The modelling result of gas velocity(y)

7. Conclusions

This study successfully simulated the migration behavior of water and gas two-phase fluids in bentonite using the THMC7.1 numerical model. Considering the heterogeneity of bentonite, the modelling results of gas velocity reveal that gas preferentially migrates to areas with high porosity and high permeability. This finding is significant for the design and safety assessment of deep geological disposal facilities.

8. References

1. Daniels, K.A., Harrington, J.F., "The Response of Compact Bentonite during a 1D Gas Flow Test" British Geological Survey Open Report, OR/17/067, 22pp, 2017.
2. Parker, J.C., Lenhard, R.J., Kuppusam, T.Y., "A parametric model for constitutive properties governing multiphase flow in porous media" Water Resoures., 23, 618-624, doi: 10.1029/WR023i004p00618, 1987.