Numerical simulation of CO_2 storage and CO_2 leakage along fault during CO_2 geo-sequestration in saline aquifer using THMC software

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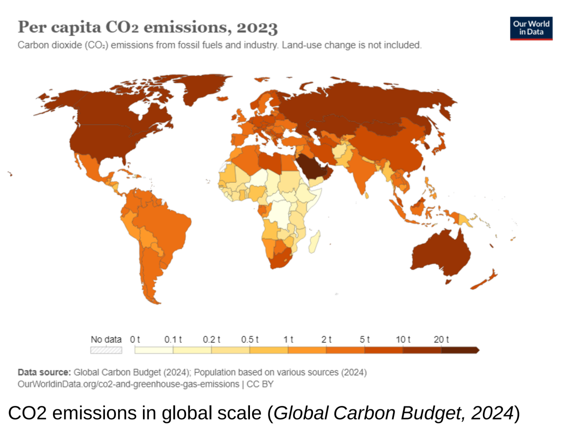
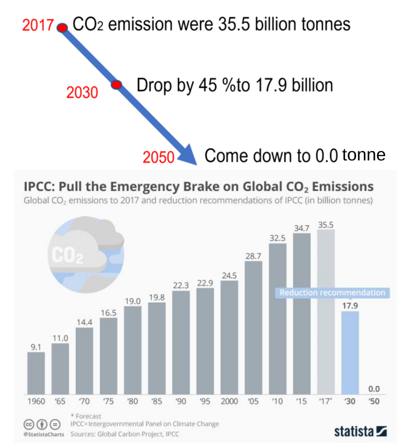
INTRODUCTION AND BACKGROUND

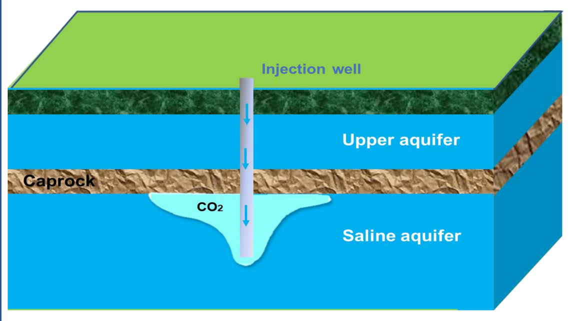


CO2 emissions in global scale (*Global Carbon Budget, 2024*)



Effective solutions:

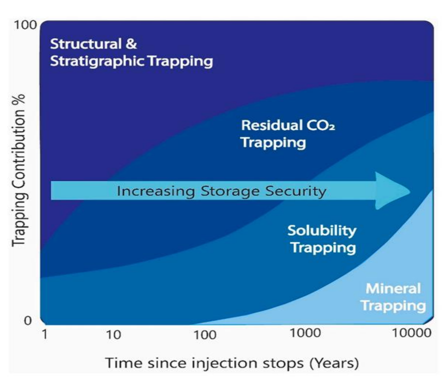
- ✓ **Carbon Capture and Storage (CCS)**
- ✓ Renewable Energy
- ✓ Afforestation & Reforestation
- ✓ Direct Air Capture (DAC)
- ✓ ...



Carbon Capture and Storage (CCS)

CO_2 geo-sequestration is process of **Capturing CO_2 emission** from large sources and **Storing** them at **the depth of thounsand feets** of geological formation beneath the groundsurface.

- One of the most effective solutions.
- Reducing greenhouse gas emissions and mitigating the effects of climate change.



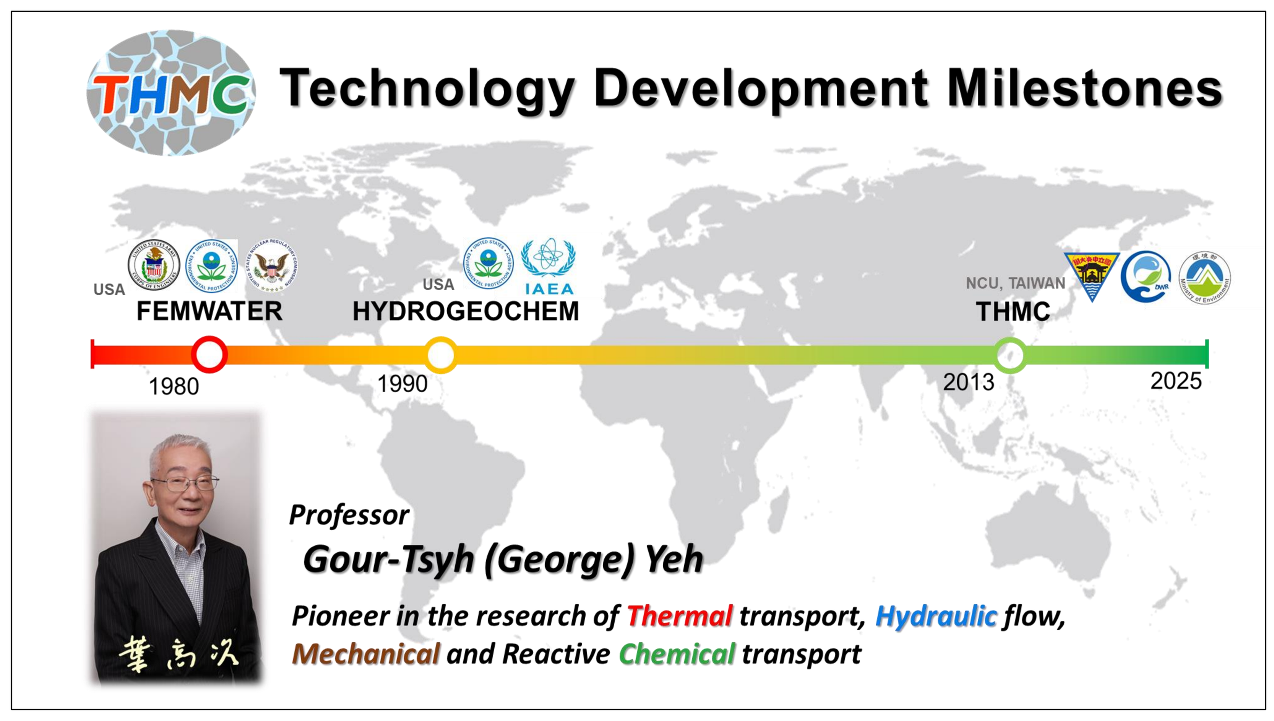
Contribution of trapping mechanisms in a CO_2 storage site at different time scales (IPCC, 2005).

Deep saline aquifers	Fault/ Reactivated fault
✓ Large storage capacity	✓ Seal integrity
✓ Depth of more than 800 m	✓ Natural Trapping Mechanisms
✓ Natural Trapping Mechanisms	✗ Potential risk

Deep saline aquifers are the suitable reservoir for long-term CO_2 storage. However, the faults/reactivated faults pose potential risks.

METHODOLOGY

THMC is a 3D finite element model of fully coupled simulation processes are developing by CAMRDA - Center for Advanced Model Research Development and Application at NCU.



➤ Mass conservation equation: (Parker *et al.*, 1987)

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

ρ_α: the density of α-th fluid phase (kg/dm³)
ϕ: the porosity (-)
S_α: the saturation of α-th fluid phase (-)
$\boldsymbol{V}_\alpha$: the Darcy velocity of α-th fluid phase (dm/day)
$\boldsymbol{V}_s$: the velocity of the solid (dm/day)
M^α, R^α : the sum of the artificial source/sink rate of all species in α-th fluid phase (kg·dm⁻³·day⁻¹)

➤ Darcy's law for multiphase:

$$\boldsymbol{V}_\alpha = -\frac{\boldsymbol{k}_{r,\alpha}\boldsymbol{k}}{\mu_\alpha}(\nabla P_\alpha + \rho_\alpha g \nabla z)$$

$$\boldsymbol{V}_s = -\frac{du}{dt}$$

$k_{r,\alpha}$: the relative permeability of α−th fluid (-)
k: the permeability of porous medium (dm²)
μ_α: the viscosity of α−th fluid (kg/dm/day)
P_α: the pressure of α−th fluid (kg/dm/day²)
ρ_α: the density of α-th fluid (kg/dm³)
g: the gravitational constant (dm/day²)
z: the elevation head (dm)

➤ Capillary pressure

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

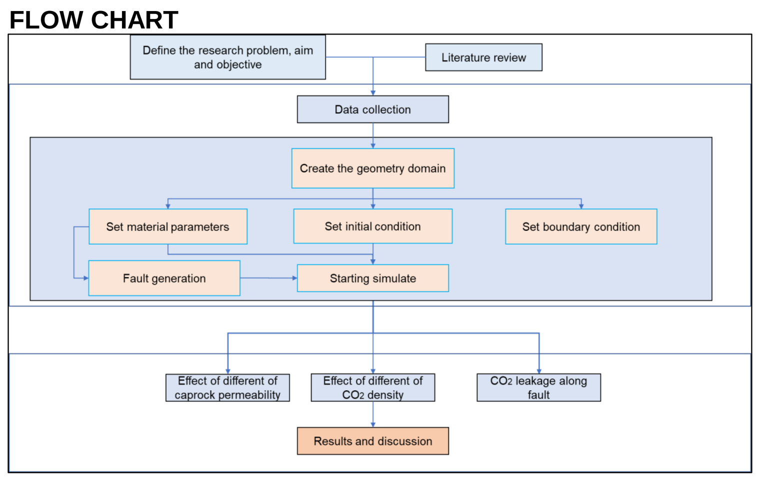
$$\alpha \in \{L-1\};\ \tilde{S}_{tL} = 1$$

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

OBJECTIVE

- ✓ This research will focus on **the movement and stabilization of CO_2** within the aquifer under **varying CO_2 density and caprock permeability** conditions.
- ✓ Conduct a preliminary assessment of the **potential for CO_2 leakage along faults** in the caprock layers using the THMC numerical model.

FLOW CHART



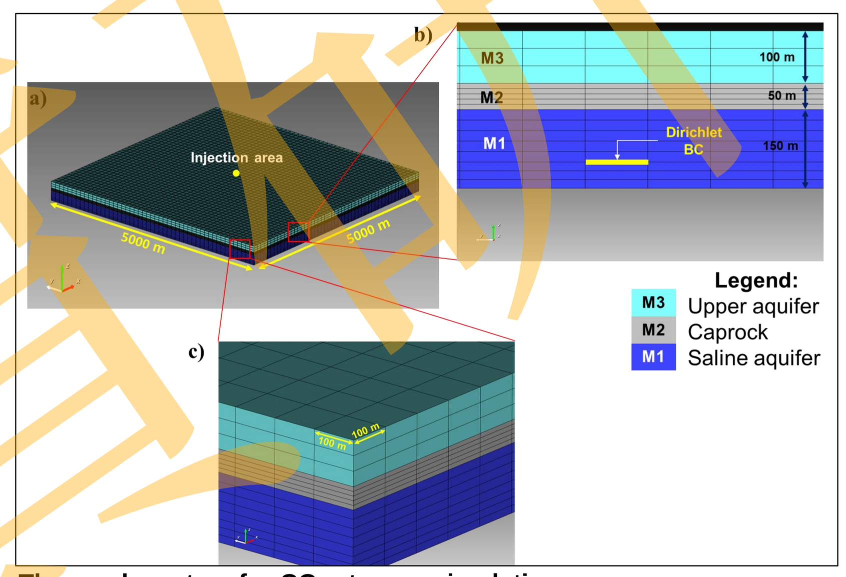
Initial condition for multiphase flow

Parameter	Initial value
Saline aquifer pressure (P_w) (MPa)	10
Salt mass fraction (%)	0.6
Gas saturation (S_g) (-)	0.05
Constant temperature (℃)	45

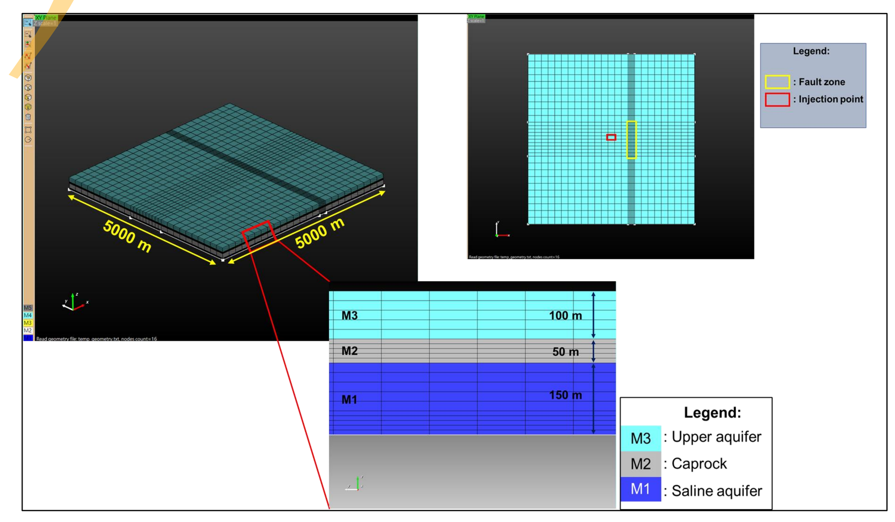
Parameters collection for CO_2 storage simulation

Parameters		Value	References
Intrinsic permeability (m²)	Saline aquifer, k_s Caprock, k_c	59×10^{-14} 59×10^{-20} 59×10^{-19}; 59×10^{-18};	(Khudaida & Das, 2014; Sung et al., 2014; Zhang et al., 2024; Zhang et al., 2018)
Compressibility (Pa^{-1})	Brine, β_s	5×10^{-10}	(Nordbotten & Celia, 2011)
	CO_2, β_{CO2}	5×10^{-7}	(Nordbotten & Celia, 2011)
	Caprock, β_c	4.5×10^{-10};	(Nordbotten & Celia, 2011; Zhang et al., 2018)
Porosity (-)	Saline aquifer, ϕ_s Caprock, ϕ_c	0.3 0.06	(Sung et al., 2014; Yu et al., 2017; Zhang et al., 2018)
Density (kg/m³)	Brine, ρ_s	1230	(Nordbotten & Celia, 2011)
	CO_2, ρ_{scCO2}	266; 500; 714	
	Caprock, ρ_c	2600	(Zhang et al., 2018)
Dynamic viscosity (mPa·s)	Brine, μ_s CO_2, μ_{CO2}	0.883 0.023	(Nordbotten & Celia, 2011)
Fracture pressure	($P_{fracture}$)	30.6 – 40.8	-
Overburnden pressure	σ_v	25.5	-
Parker empirical parameters (-)	$\bar{\alpha}$	9.524×10^{-4}	-
Parker empirical parameters (-)	N	2.0	-
Empirical parameter (-)	α	8.226×10^{-19}	-
Score index (-)	n	20.0	-

CO_2 storage model setting



The mesh system for CO_2 storage simulation



The mesh system in case of fault application in CO_2 storage simulation

Geometry mesh system parameters

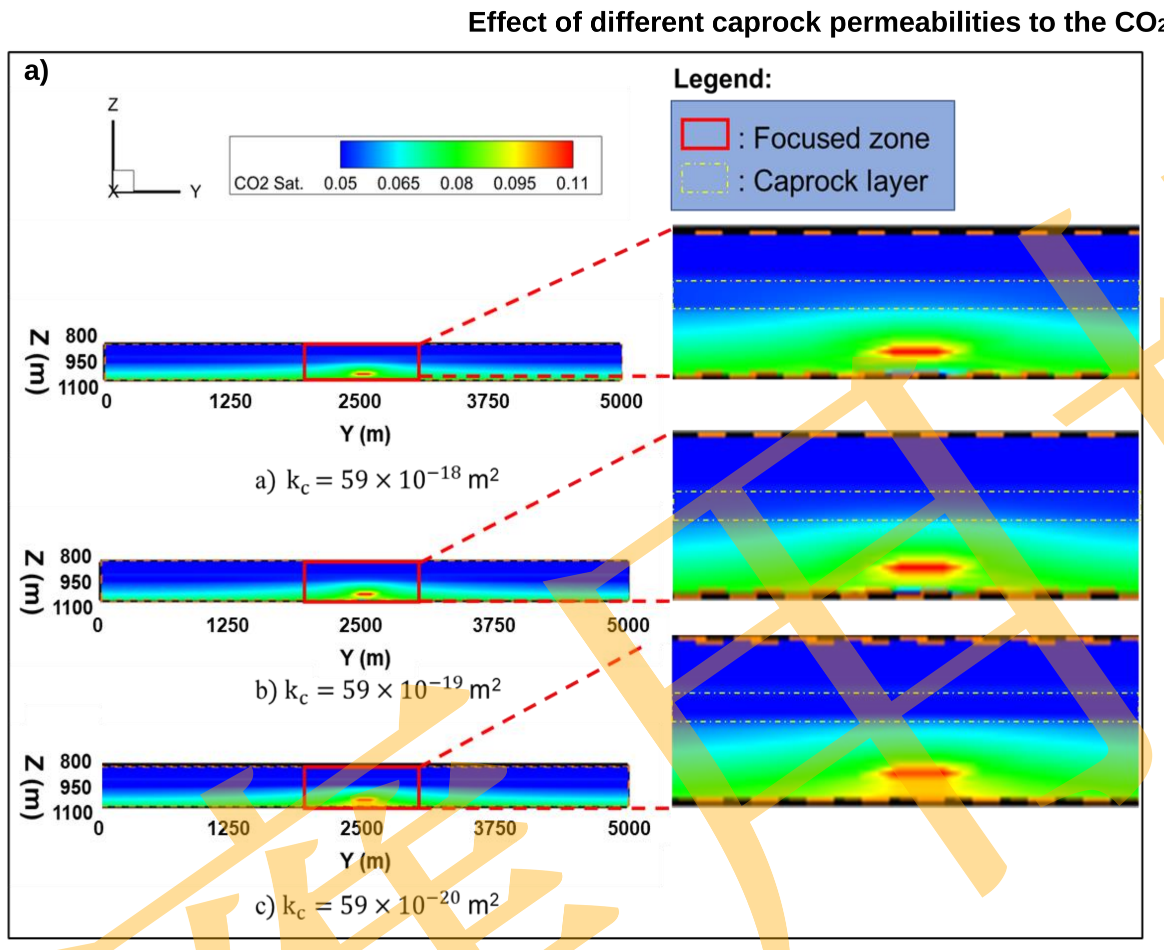
Parameters		Value
Total global nodes	42,500	50 * 50 * 17
Total global elements	38,416	49 * 49 * 16
Grid size (X:Y:Z)	Saline aquifer	100 : 100 : 18.75
	Caprock	100 : 100 : 10
	Upper aquifer	100 : 100 : 33.33

Geometry mesh system parameters

Parameters		Value
Total global nodes	21,483	31 * 33 * 21
Total global elements	19,200	30 * 32 * 20
Grid size (X:Y:Z) (m)	Saline aquifer	200 * 200 * 18.75
	Caprock	200 : 200 : 10
	Upper aquifer	200 : 200 : 33.33
	Fault zone	25 : 100 : 10
	Injection zone	200 : 100 : 20

RESULTS AND DISCUSSIONS

Effect of different caprock permeabilities to the CO_2 migration



a) $k_c = 59 \times 10^{-18}$ m²
b) $k_c = 59 \times 10^{-19}$ m²
c) $k_c = 59 \times 10^{-20}$ m²

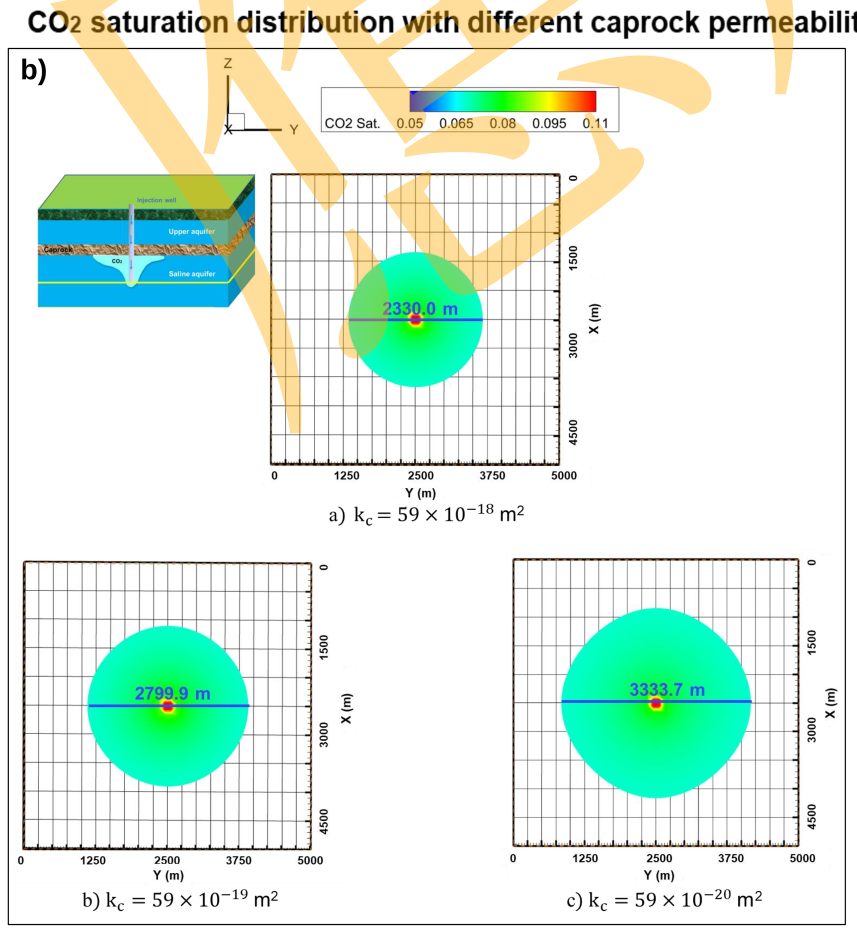
a) **CO_2 migration** into the caprock layer **is driven** by variations in **different permeabilities**.

b) **Significant of different permeability** induces the change of CO_2 migration in saline aquifer.

c) CO_2 migration into the caprock layer is driven by variations in different caprock permeabilities. Potential risk of creating the leakage path way.

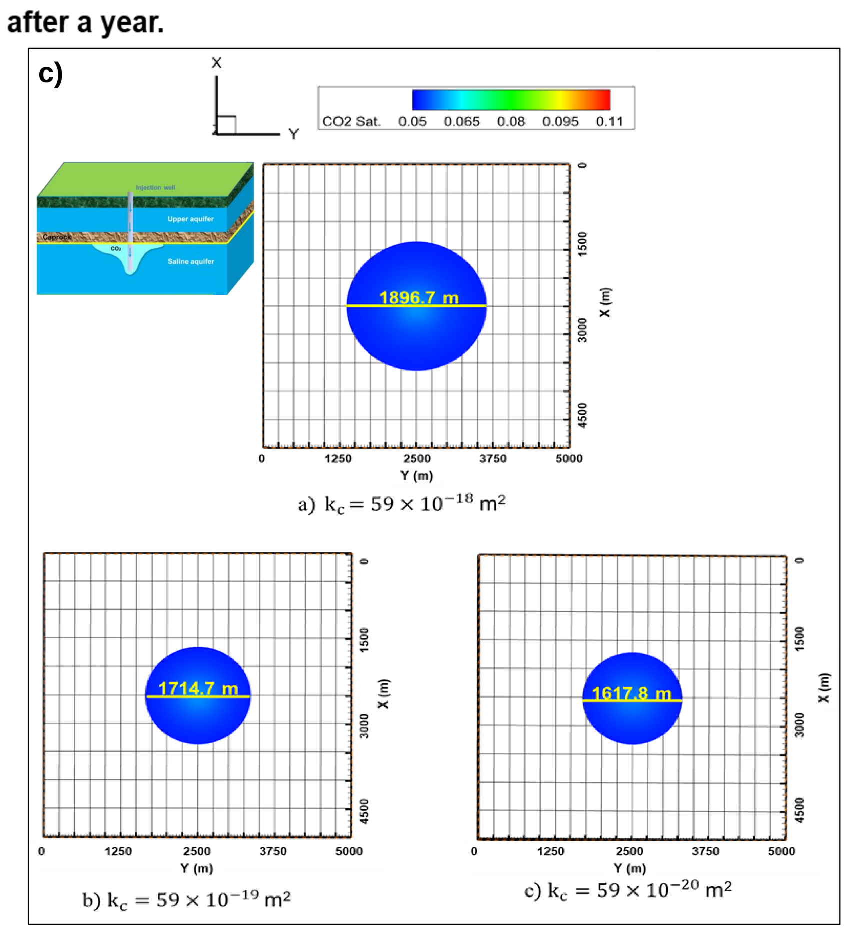
d) This comparison **underscores the importance of selecting suitable** to ensure secure and effective CO_2 storage.

CO_2 saturation distribution with different caprock permeability after a year.



a) $k_c = 59 \times 10^{-18}$ m²
b) $k_c = 59 \times 10^{-19}$ m²
c) $k_c = 59 \times 10^{-20}$ m²

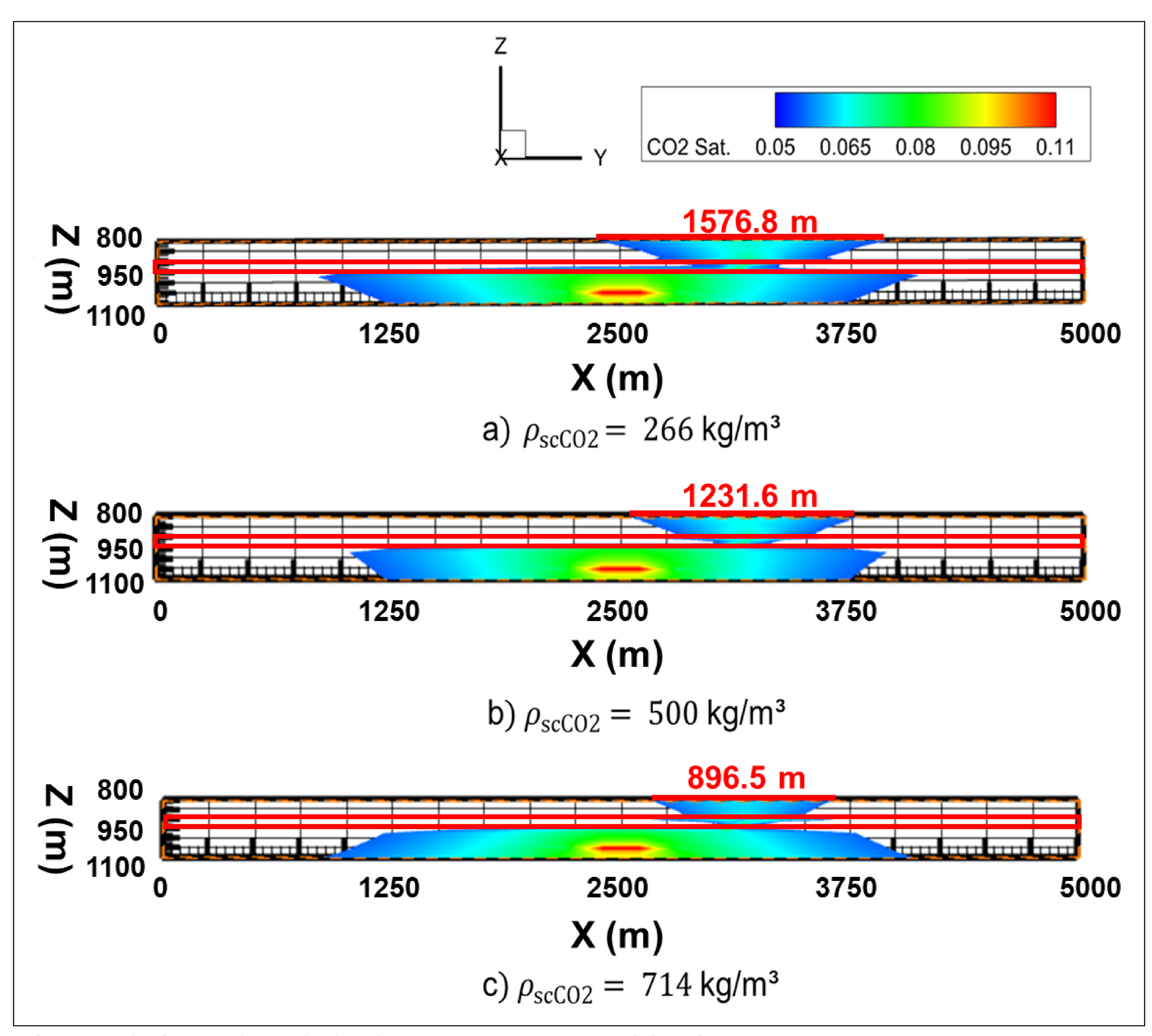
CO_2 saturation distribution in the injection plane in saline aquifer after a year.



a) $k_c = 59 \times 10^{-18}$ m²
b) $k_c = 59 \times 10^{-19}$ m²
c) $k_c = 59 \times 10^{-20}$ m²

The CO_2 saturation distribution at the contact area after a year.

Effect of different CO_2 densities to the CO_2 leakage along fault



a) $\rho_{scCO2} =$ 266 kg/m³
b) $\rho_{scCO2} =$ 500 kg/m³
c) $\rho_{scCO2} =$ 714 kg/m³

The CO_2 leakage along fault after a year represented by the CO_2 saturation

1. High difference of density induce more potential risk of leakage.
2. CO_2 plume was formed different due to the significant difference of diferent density.
3. Lower difference of density ensure the safety and less CO_2 leakage along fault.

Considering the appropriate geological formations for CO_2 storage beneath the subsurface in long-term.

CONCLUSIONS

- **The caprock layer acts as a strong seal** due to the significant permeability difference between the caprock and the saline aquifer.
- A **lower density difference** between supercritical CO_2 and brine **enhances long-term storage** by controlling migration and **reducing leakage risks** along faults. In contrast, a **higher density difference increases leakage risks** due to stronger buoyancy forces.
- **Deeper storage reservoirs** provide enhanced safety due to the favorable conditions resulting from the density difference between supercritical CO_2 and brine.
- **A high permeability contrast** and **a low density difference** contribute to **greater stability** in CO_2 migration within the storage reservoir.

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5. ...