國立中央大學

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

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  - CO_2 leakage along the fault
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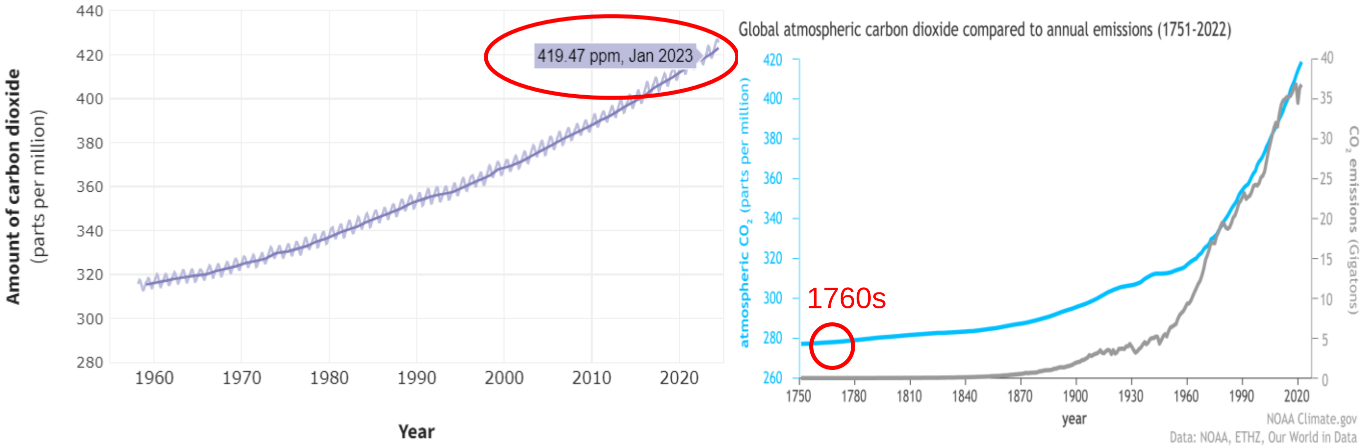
GLOBAL ISSUE OF CO_2 EMISSION

Anthropogenic CO_2

- Power generation
- Transportation
- Industries
- Deforestation
- Land use changes
- Waste management
- ...



The annual report (NOAA's Global Monitoring Lab, 2023)

Global Carbon Budget (2023):

- CO_2 concentrations **419.47 ppm**
- **51% increased** compared to the stage of pre-industrial (1760s)
- Temperature increased **1.1℃**

The impacts if global warming exceed 1.5 ℃

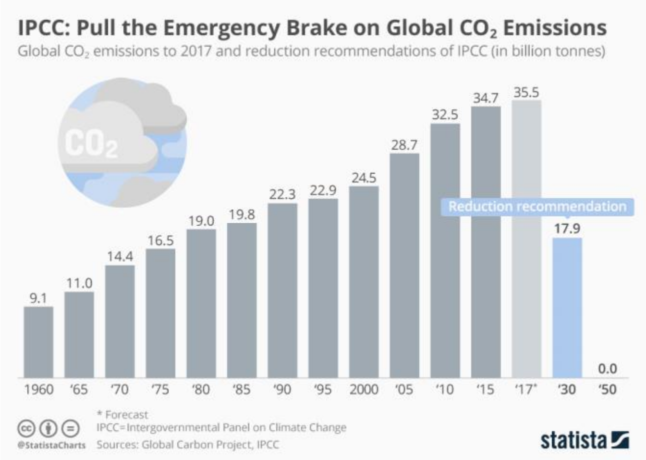
- Extreme weather events
- Sea-level rise
- Biodiversity loss
- Food and water security

GLOBAL RESPONSES AND SOLUTIONS

2017 CO_2 emission were 35.5 billion tonnes

2030 Drop by 45 %to 17.9 billion

2050 Come down to 0.0



The global carbon project (IPCC, 2017)

Rapid Decarbonization
(renewable energy sources, energy efficiency, electrifying transportation)

Nature-based solutions
(Protecting and restoring forests, wetlands, and other ecosystems)

Technology innovations
(Carbon Capture and Storage (CCS))

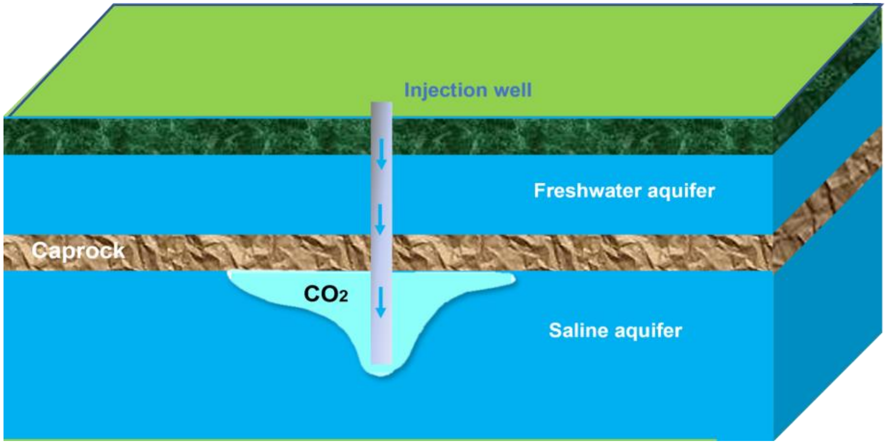
International Cooperation
(Strengthening international climate agreements)

Public Engagement and Policy
(Raising awareness about climate change)

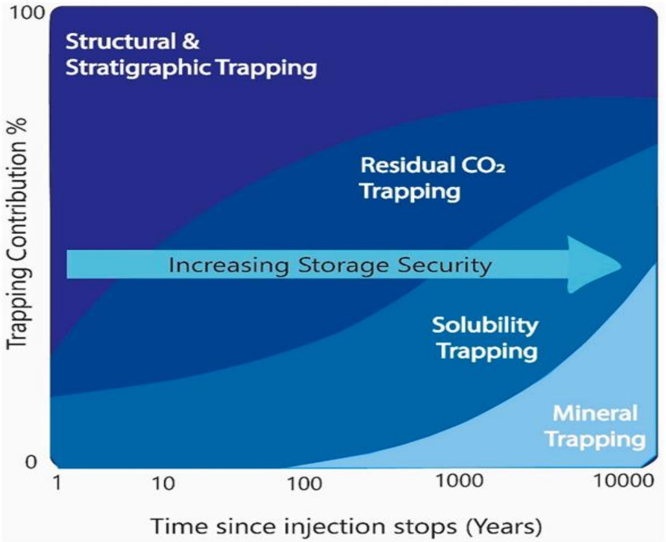
Climate change and sustainability initiatives (NETzero, COP26, COP28)

REDUCING CO_2 EMISSIONS

- ✓ **Essential for mitigating climate change**
- ✓ **Preserving ecosystems**
- ✓ **Ensuring a sustainable future**



CO2 storage in saline aquifer



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

CO_2 GEO-SEQUESTRATION

"Carbon dioxide (CO_2) capture and storage (CCS) is a process consisting of the separation of CO_2 from industrial and energy-related sources, transport to a storage location and long-term isolation from the atmosphere" - Metz, B *et al.* (2005)

FAULT/ REACTIVATED FAULT

CO_2 leakage along the fault was the largest risk of CO_2 sequestration (Miocic *et al.* (2016)).

DEEP SALINE AQUIFERS

- ✓ **Large storage capacity**
- ✓ **Depth**
- ✓ **Natural Trapping Mechanisms**

Deep saline aquifers are one of the main candidates to cut anthropogenic CO_2 emissions.

LITERATURE REVIEW

- Newell *et al.* (2020) considered both vertical and horizontal wellbore orientations for CO2 injection, but using quarter- and half-symmetry domains impacted the accuracy of the results.

- Zhang, L. *et al.* (2018) and Zhang, L. *et al.* (2024) investigated the fluid exchange due to CO2 leakage in geological storage but did not consider the densities of CO2, fresh water, and brine.

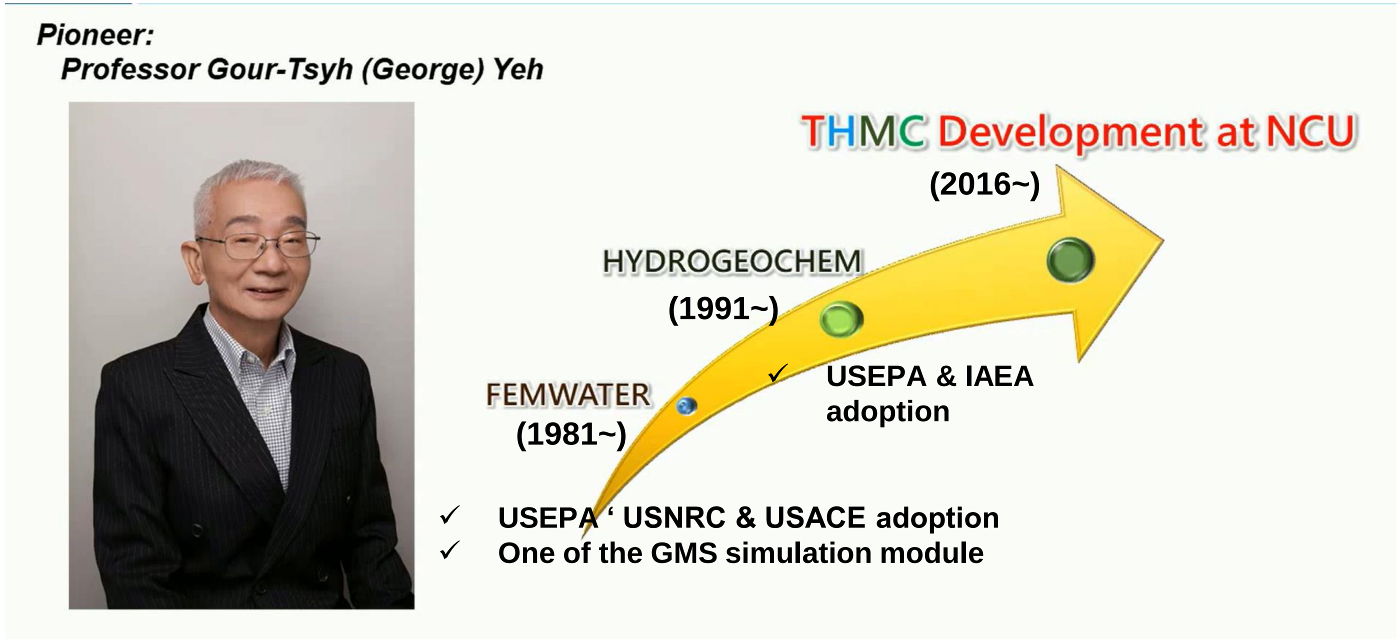
- Nordbotten, J. M. *et al.* (2011) provide a comprehensive synthesis of geological storage of CO2 modeling, with reliable data serving as the basis for simulation.

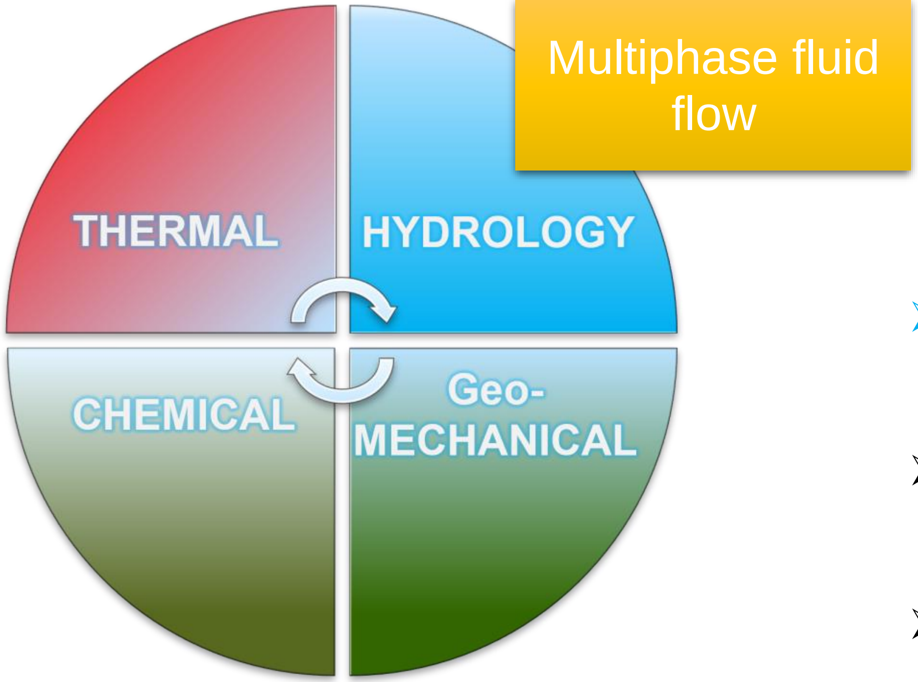
- Several studies have researched CO2 storage and CO2 leakage, but the fundamental concepts remain unclear.

THMC7.1

Thermal Hydrology Geo-Mechanics
Reactive Chemical Model

THMC7.1 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.





- Revolutionizes the user experience within the complex groundwater simulation process.
- With userfriendly interface can facilitate the modeling and analysis of complex THMC systems.
- Allowing engeneers to tackle larger scale problem.

OBJECTIVE

This study employed the $THMC_{7.1}$ model to observe the movement and stabilization of CO_2 within the aquifer under different CO_2 density and caprock permeability conditions, and then assess the potential for CO_2 leakage along faults in caprock layers

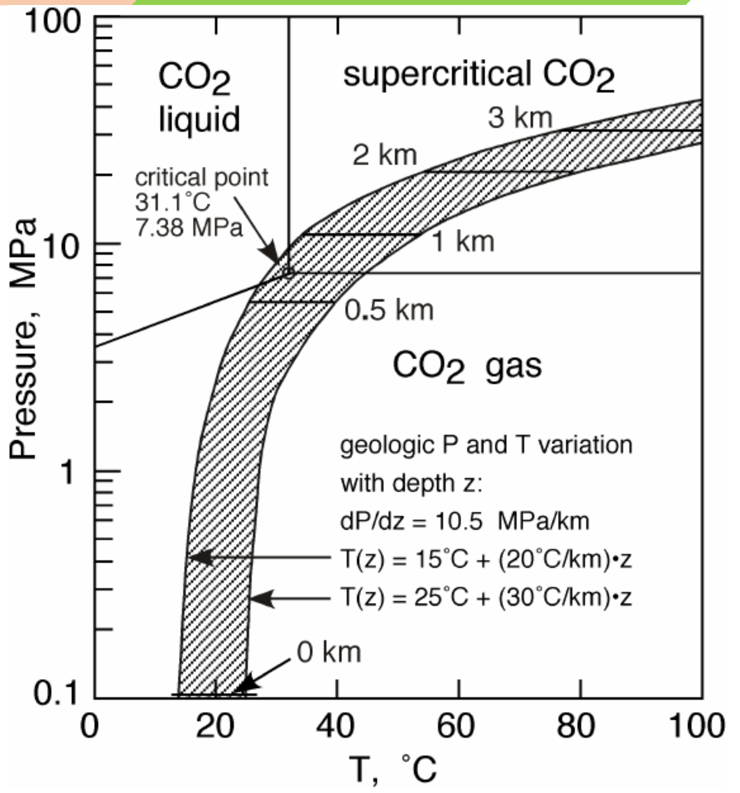
CO2 SUPERCRITICAL PHASE

Typical temperature and pressure

- Critical pressure (>= 7,38 MPa)
- Critical temperature (>= 31.1°C)
- In this phase, CO_2 can move through small spaces like a gas but also can dissolve materials like a liquid

Appropriate for CO_2 geo-sequestration

- Increased storage capacity due to high density
- Improved mobility due to low viscosity
- This phase of CO_2 can react with minerals in the storage formation



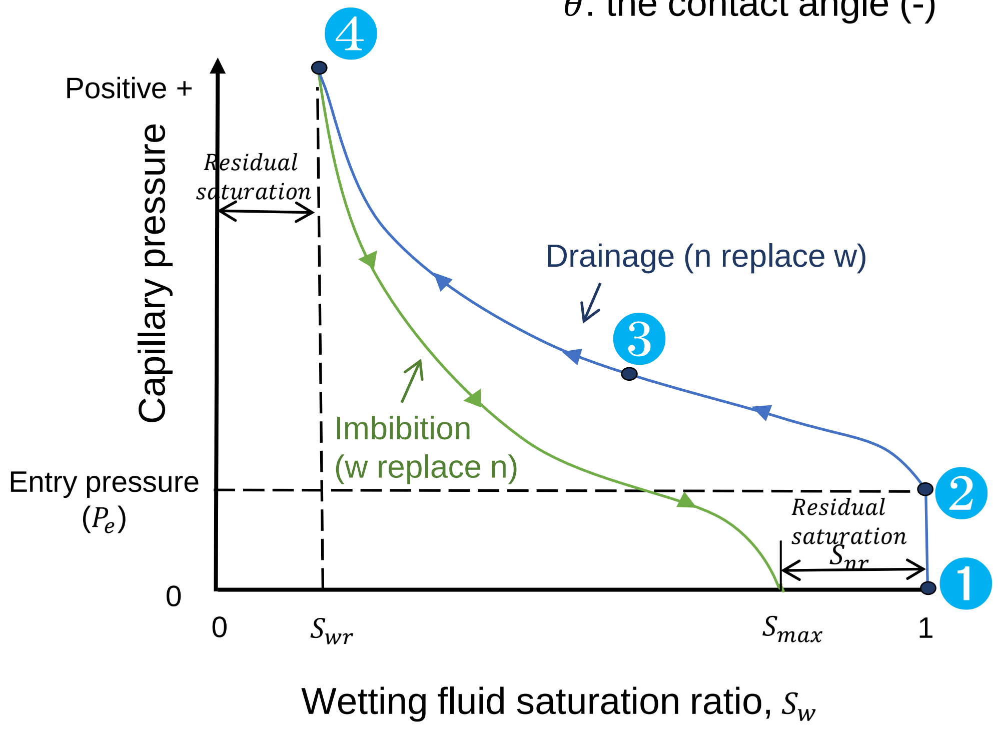
Phase diagram of CO2, showing typical ranges of T and P variation with depth (modified from Celia 2008)

Concept of multiphase fluid & saturation

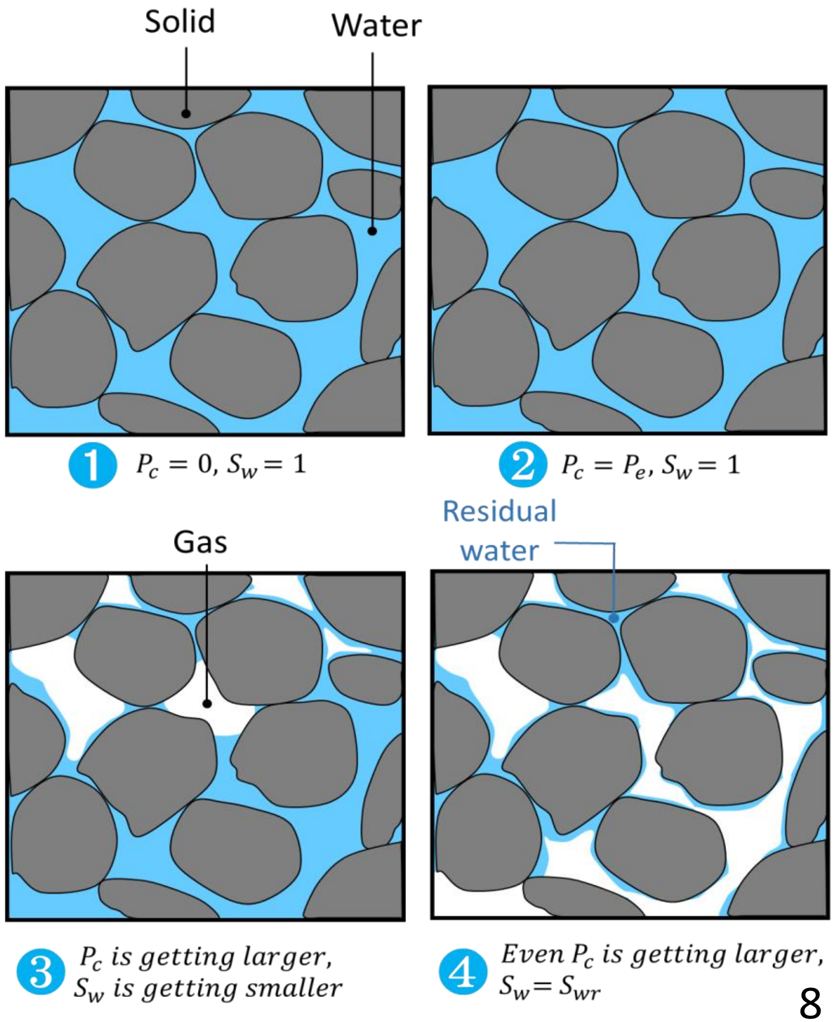
Multiphase fluid flow refers to the simultaneous flow of two or more fluids that are in NAPL *(Non-Aqueous Phase Liquid)* or APL *(Aqueous Phase Liquid)*, gas, and/or solid through a medium, such as a porous rock formation.

$$Pc = Pn - Pw = \frac{2\sigma cos\theta}{r_{tu}} = f(S)$$

Pn: the pressure of nonwetting phase (kg/dm/day^2)
Pw: the pressure of wetting phase (kg/dm/day^2)
r_{tu}: the radius of tube (dm)
σ: the interfacial tension (N/dm)
θ: the contact angle (-)



Relationship between capillary pressure & saturation



THMC7.1 model: Multiphase fluid flow (H) module

- 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)

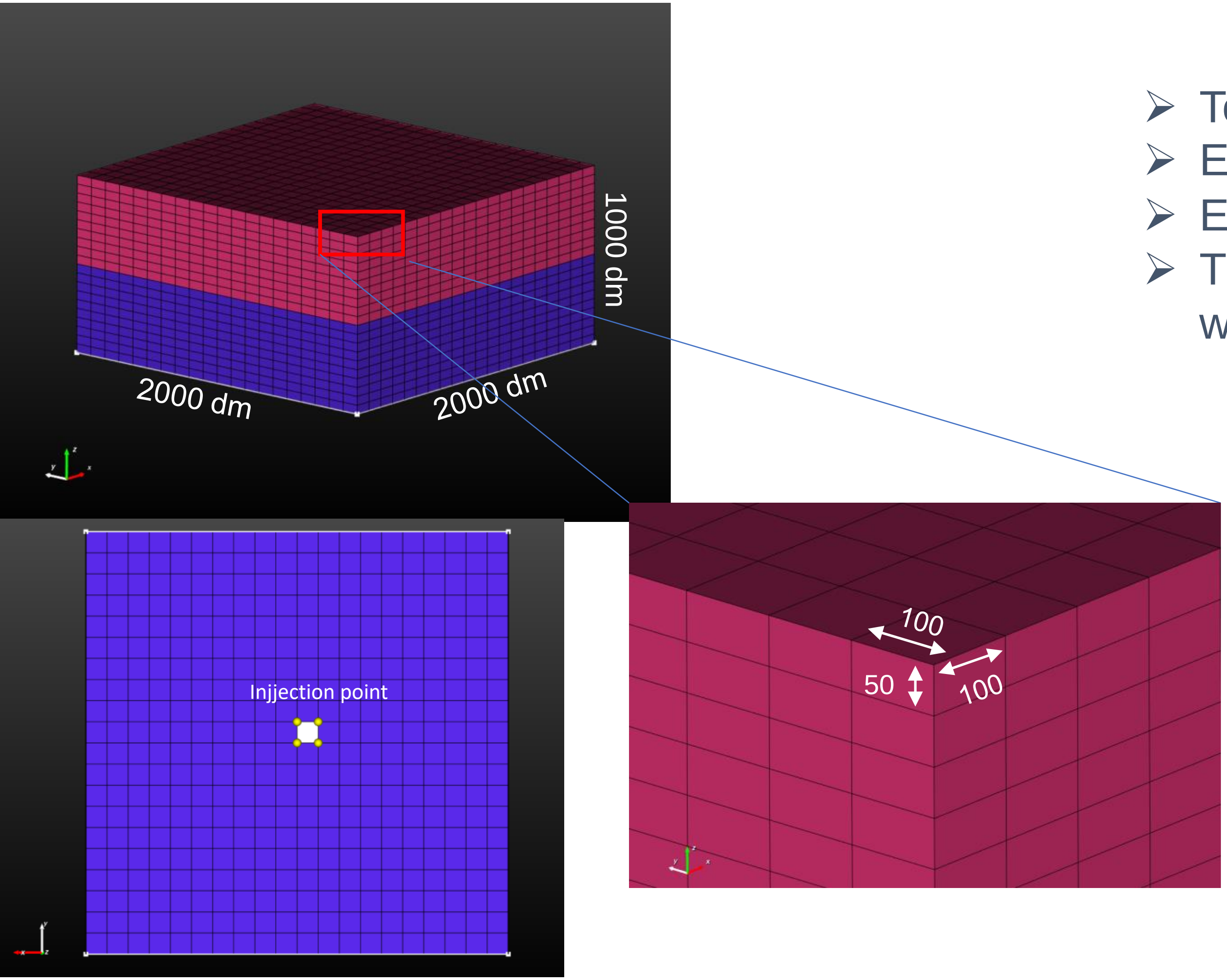
Depends on porous medium

$$K = \frac{\boxed{k}\,\rho\, g}{\mu}$$

Depends on the fluid

K: the hydraulic conductivity (dm/day)
k: the permeability of porous medium (dm²)
ρ: the density of fluid (kg/dm³)
μ: the viscosity of fluid (kg/dm/day)
g: the gravitational constant (dm/day²)

MODEL SETTING



SETTING OF GEOMETRY

- Total nodes: 9261 (21*21*21)
- Elements consisted: 8000 (20*20*20)
- Elements size of the saline aquifer: 100*100*50 (dm^3)
- The injection point placed at the center of the saline aquifer with depth of 10000 dm

INITIAL CONDITION

Parameter	Unit	value
Temperature	℃	49
Porewater pressure	MPa	9
Resedual gas saturation	-	0.01
Salt mass fraction	%	0.6
Injection rate	kg/s	10

PARAMETERS COLLECTION

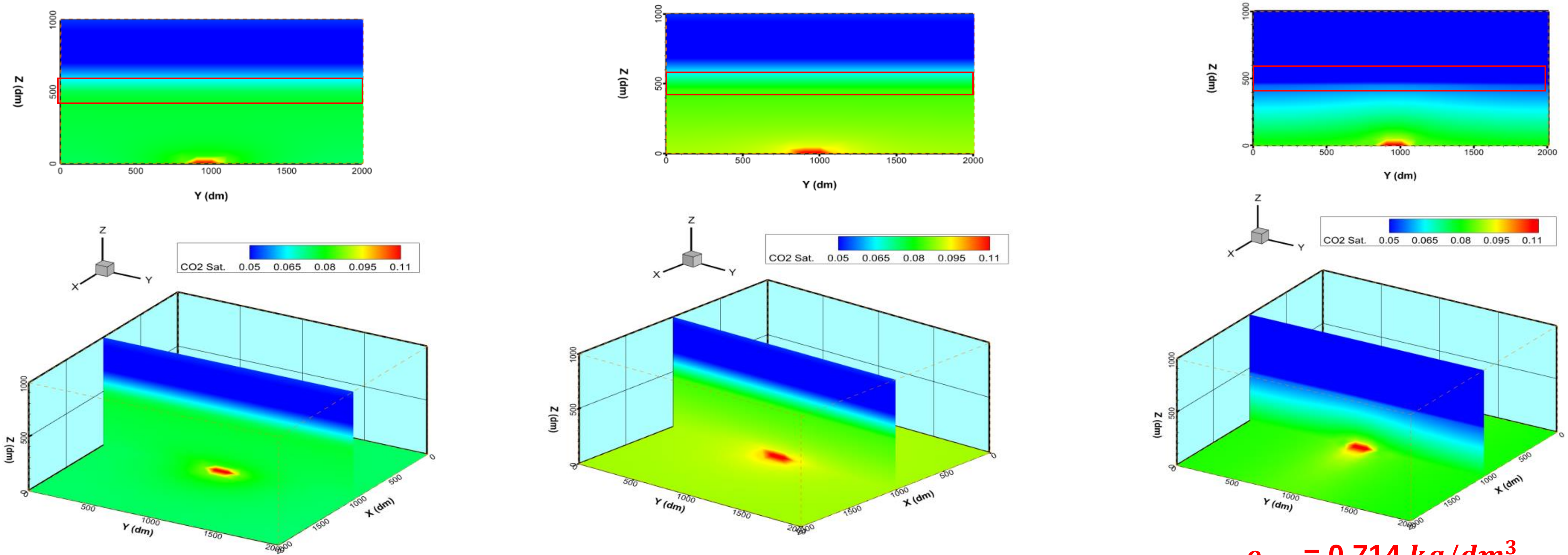
Table 1. Parameters of multiphase flow of formation

Parameter	Unit	Caprock	Saline aquifer	fault	Reference
Intrinsic permeability, k	dm^2	5.9*10^{-17}	5.9*10^{-12}	5.9*10^{-11}	Zhang, L. *et al.* (2018).
Porosity, ϕ	-	0.06	0.15	0.3	Zhang, L. *et al.* (2018).

Table 2. Parameters of multiphase flow of different phases

Parameter	Unit	CO_2	Brine	Caprock	Reference
Density, ρ	$\mathrm{kg/dm}^3$	0.266 – 0.714	1.23	2.6	Nordbotten, J.M. *et al.* (2011).
Viscosity, μ	$\mathrm{kg/(dm * day)}$	0.498528	13.6512		Nordbotten, J.M. *et al.* (2011).
Compressibility, β	$\mathrm{(dm * day^2)/kg}$	1.5*10^{-18}	6.7*10^{-19}	5.9*10^{-19}	Zhang et al. (2018), Nordbotten, J. M. *et al.* (2011)

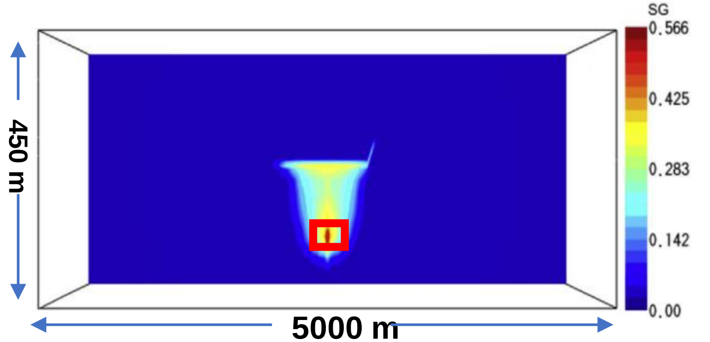
Different densities of CO_2 supercritical phase



ρ_{CO_2} = 0.0714 kg/dm^3 ρ_{CO_2} = 0.266 kg/dm^3 ρ_{CO_2} = 0.714 kg/dm^3

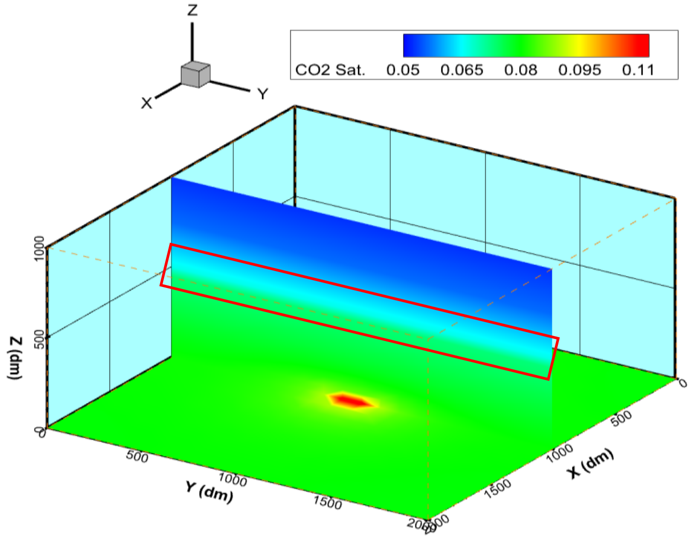
The CO_2 saturation distribution in saline aquifer after 30 days injection

- Low density combined with low viscosity leads to a stronger buoyant force.
- Higher density combined with anisotropic permeability induces the expandation of the CO_2 plume.
- Higher density is more stable and appropriate for CO_2 storage in the long term.

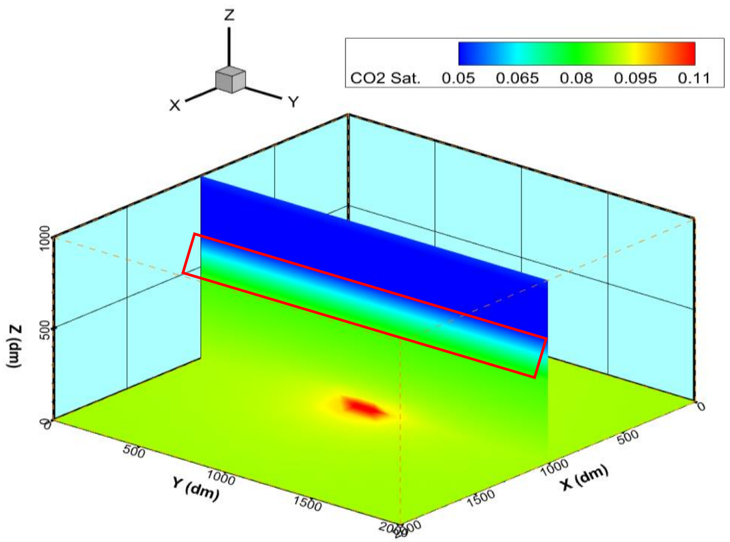


The CO_2 saturation distribution after 5 years, L = 5000 m (Zhang *et al.* (2018))

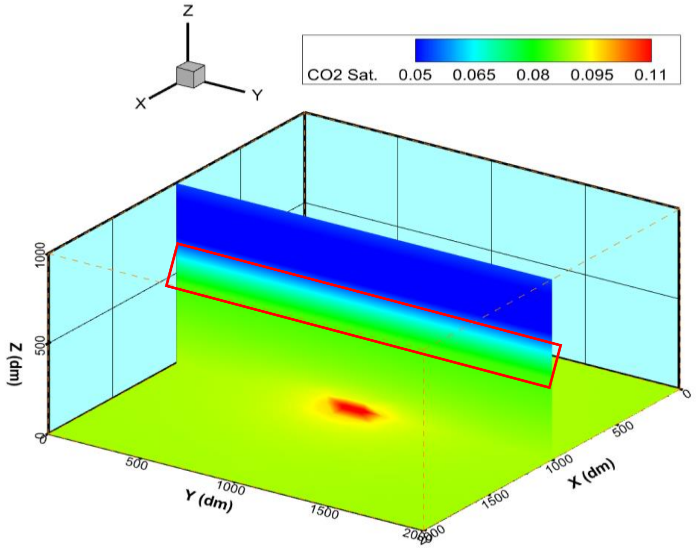
Difference of caprock permeability



k_{cap}= 5.9*10^{-16}



k_{cap}= 5.9*10^{-17}



k_{cap}= 5.9*10^{-18}

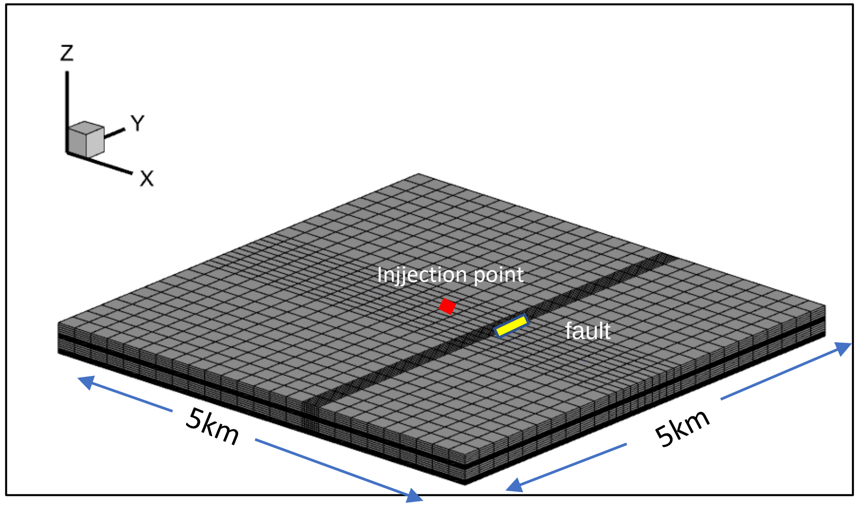
The CO_2 saturation distribution in saline aquifer after 30 days injection ρ_{CO2}= **0.266 kg/dm^3**

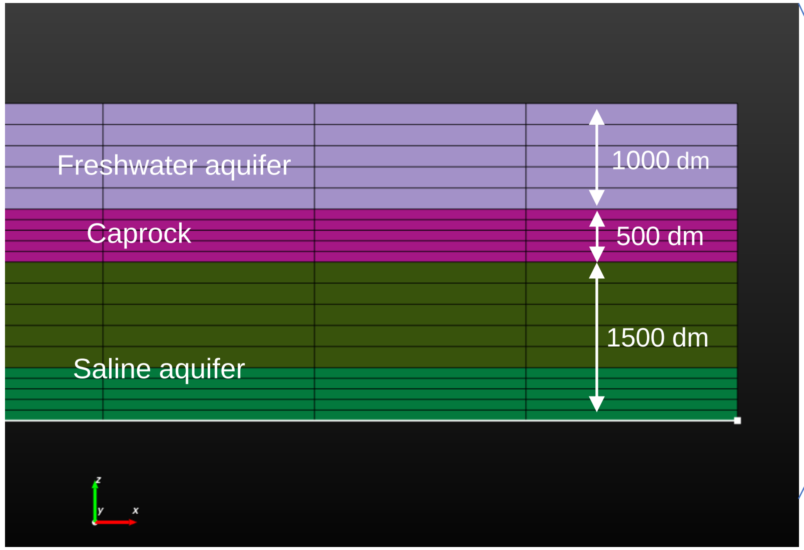
Different permeability levels in the caprock layer will significantly impact CO_2 storage and the potential for leakage:

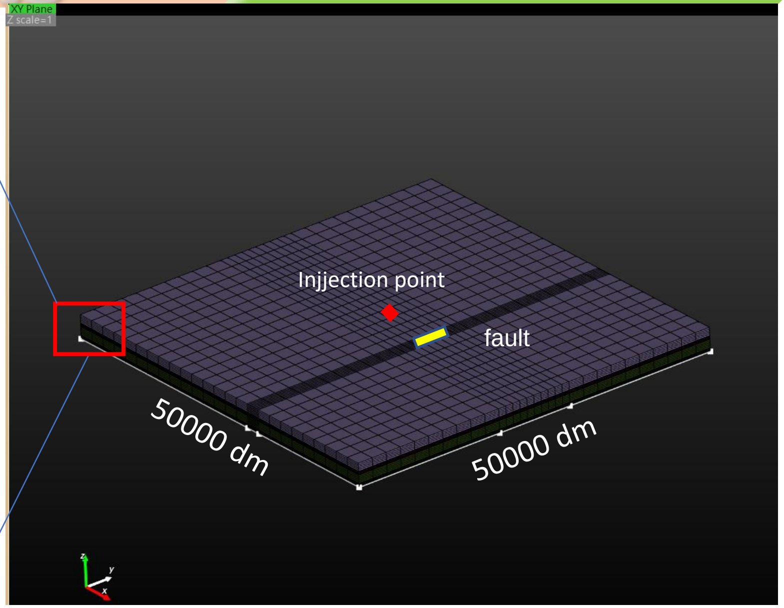
- Low permeability:
  + Enhanced containment
  + Cappilary sealing
  + Long-term stability

- Higher permeability:
  + Increased Leakage Risks
  + Faults and Fractures

APPLY THE FAULT TO SIMULATION

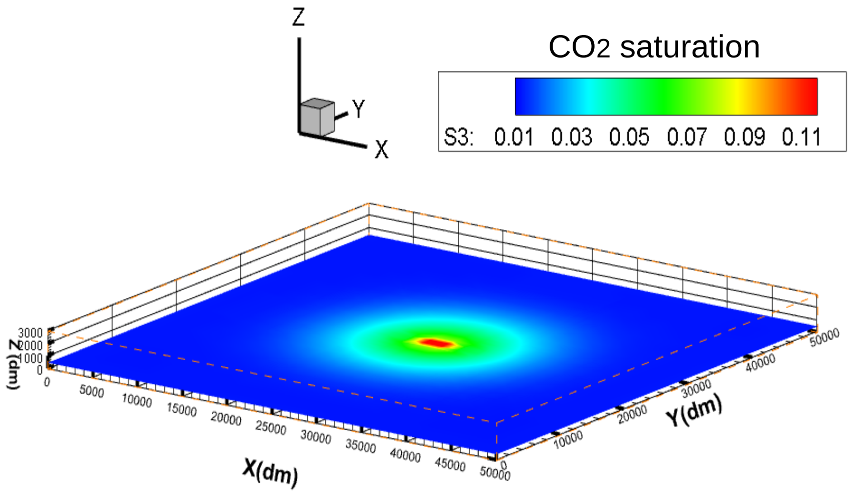


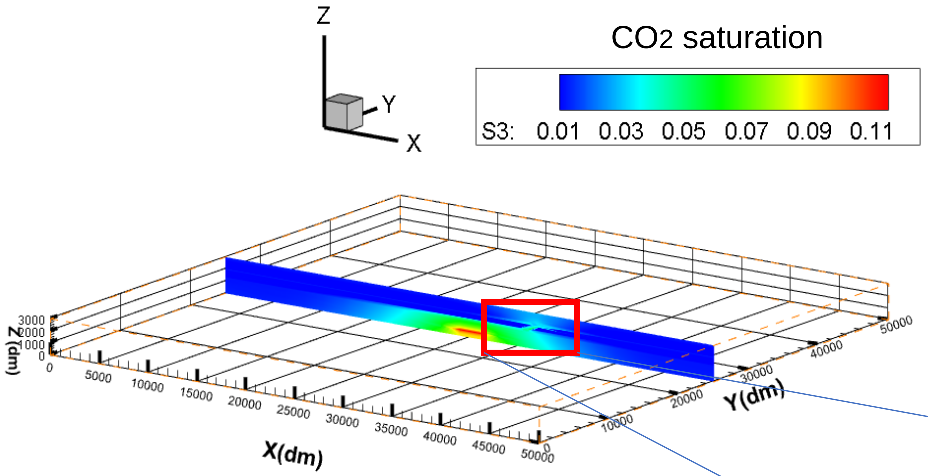




- Volume: 50000*50000*3000 (dm^3)
- Total nodes: 21483 (31*33*21)
- Elements consisted: 19200 (30*32*20)
- The injection point places at the center of saline aquifer with depth of 10000 dm
- Injection surface place at the center: 1000*2000 (dm^2)
- Fault: length: 1000 dm
  thickness: 250 dm
- Distance from an injection well to the fault: 5000 dm

The CO_2 saturation distribution and leakage along fault

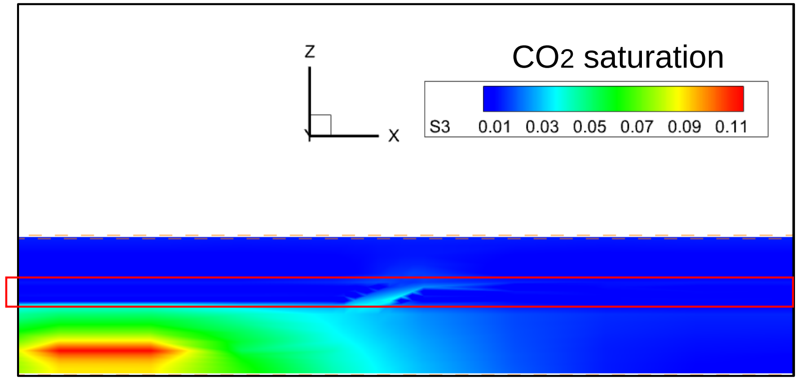




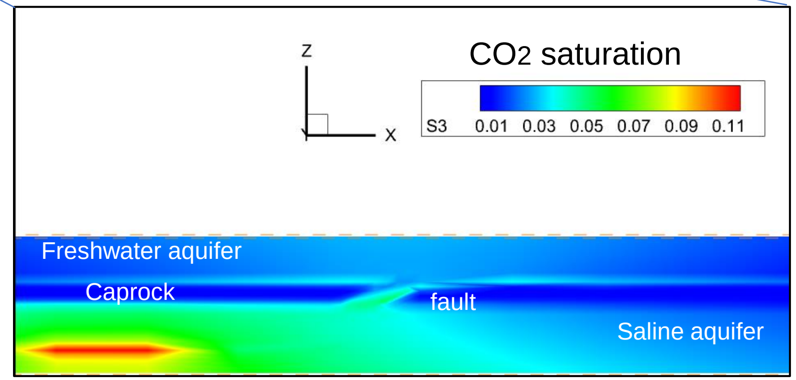
The CO2 saturation distribution in saline aquifer

ρ_{CO2}= 0.266 kg/dm^3

- Firstly, low density induces high migration of CO_2 plume.
- This density definitely affects the high risk of leakage in long-term storage.



The CO_2 plume reaches the fault at first stage

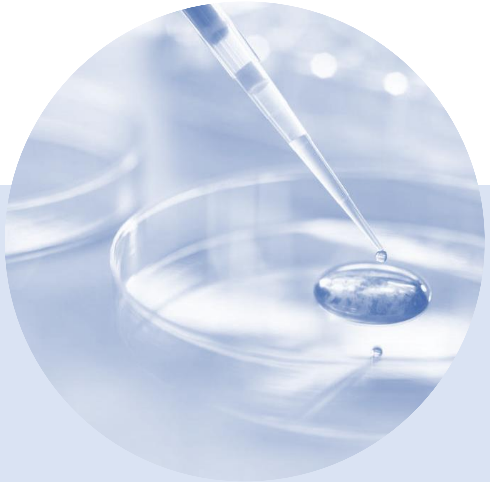


The CO_2 plume has reached and completely covered the fault at the last time

- ✓ THMC7.1 successfully simulation CO_2 storage in saline aquifer and CO_2 leakage along fault of caprock layer.
- ✓ With different density of CO_2 supercritical phase can appropriate for different scenerious of CO_2 trapping mechanism.
- ✓ With lower caprock permeability signigicantly enhance the ability of caprock to effectively trap and contain CO_2. Higher permeability can lead to increased risks of CO_2 leakage from the storage reservoir.

FUTURE WORK

- ☐ Try to simulate CO_2 storage and the effect of the fault in a long time to prove this study more convincing.
- ☐ Consider the connection of flow rate and leakage rate, which affect the safety and stabilization during CO_2 storage time.



Thank you for your listening!