NUMERICAL MODELING OF THE IMPACT OF HYDRATE FORMATION DURING GEOLOGICAL CARBON STORAGE (GCS)

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OUTLINE

- Introduction
    - General context
    - CO2 storage in depleted gas reservoir
    - CO2 storage in deep ocean sediments

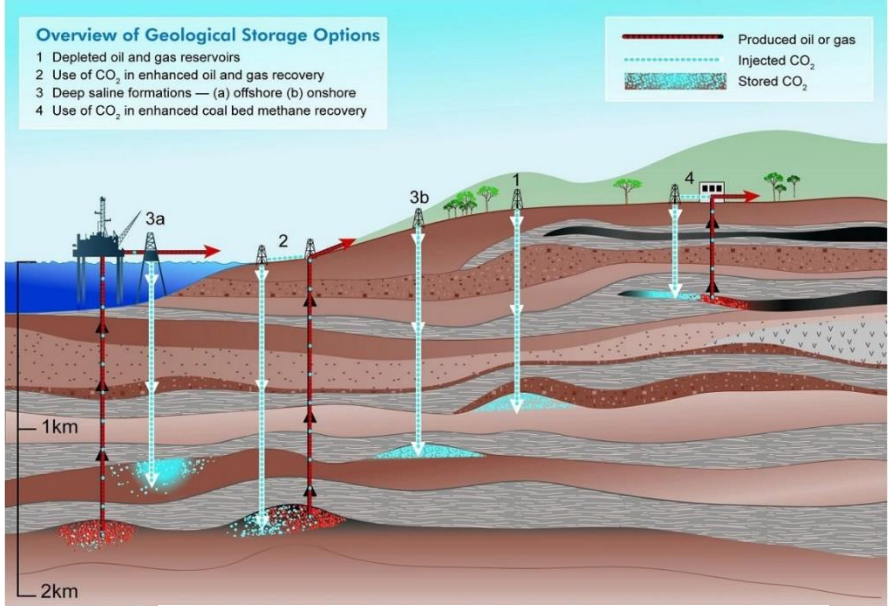
- Mathematical model
    - Non-isothermal reactive compositional multiphase flow in porous media
    - Hydrate kinetic reaction
    - Joule-Thomson effect

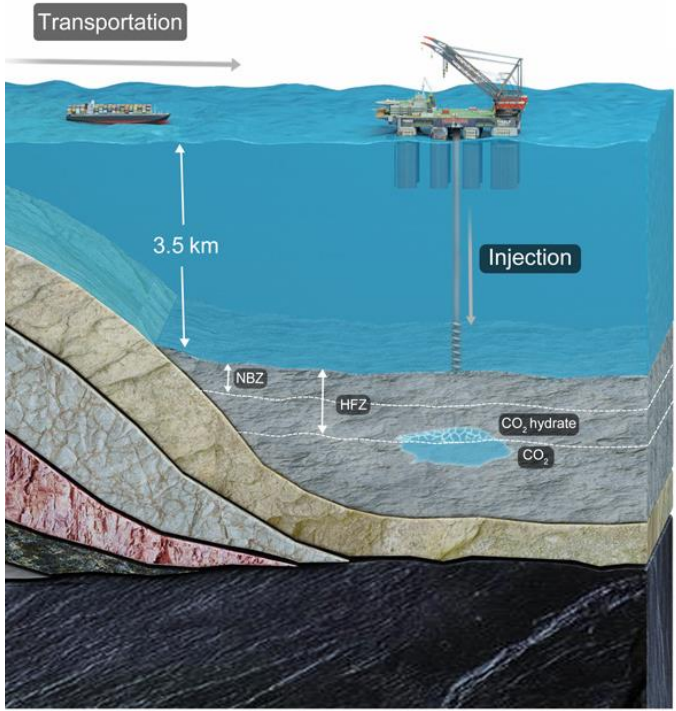
- Numerical simulation

INTRODUCTION

CONTEXT

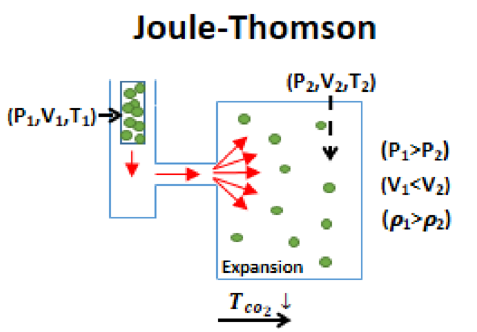
- In the last decades, the CO2 concentration in the atmosphere has dramatically increased due to excessive burning of fossil fuels.
- This greenhouse gas has an important impact on climate change.
- A solution to reduce the concentration of CO2 in the atmosphere is the ***storage in geological formations***:
  - In deep saline aquifers
  - In unmineable coal seams
  - **In depleted oil or gas reservoirs**
  - **In deep ocean sediments**

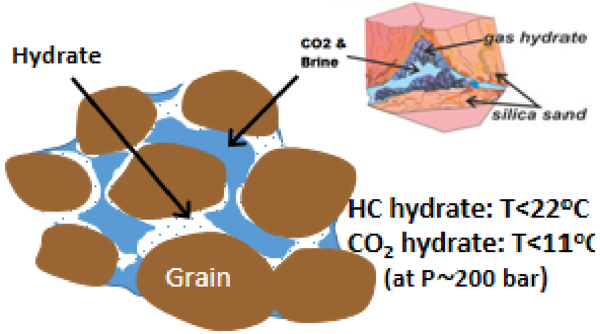




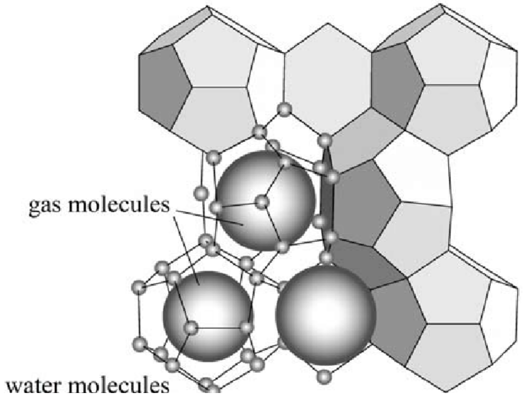
CO_2 STORAGE IN DEPLETED GAS RESERVOIR

- High pressure injection in low pressure reservoir
- Expansion of the gas near the wellbore area: Pressure decreases
- Temperature decreases due to **the Joule-Thomson (JT) effect**
- Possibility of **hydrate formation**
- ***Loss of injectivity***


Joule-Thomson


Hydrate formation

HC hydrate: T<22°C
CO_2 hydrate: T<11°
(at P~200 bar)



Gas hydrate

CO_2 STORAGE IN DEEP OCEAN SEDIMENTS

- **High pressure** and **low temperature** in deep ocean environnement
  - *Hydrate Cap: Hydrate formation may block the CO2 plume*
  - *Gravitational Trapping : Negative buoyancy may seal the CO2 plume*

$$\rho_{CO_2} > \rho_{H_2O} \iff \rho_{H_2O} - \rho_{CO_2} < 0$$

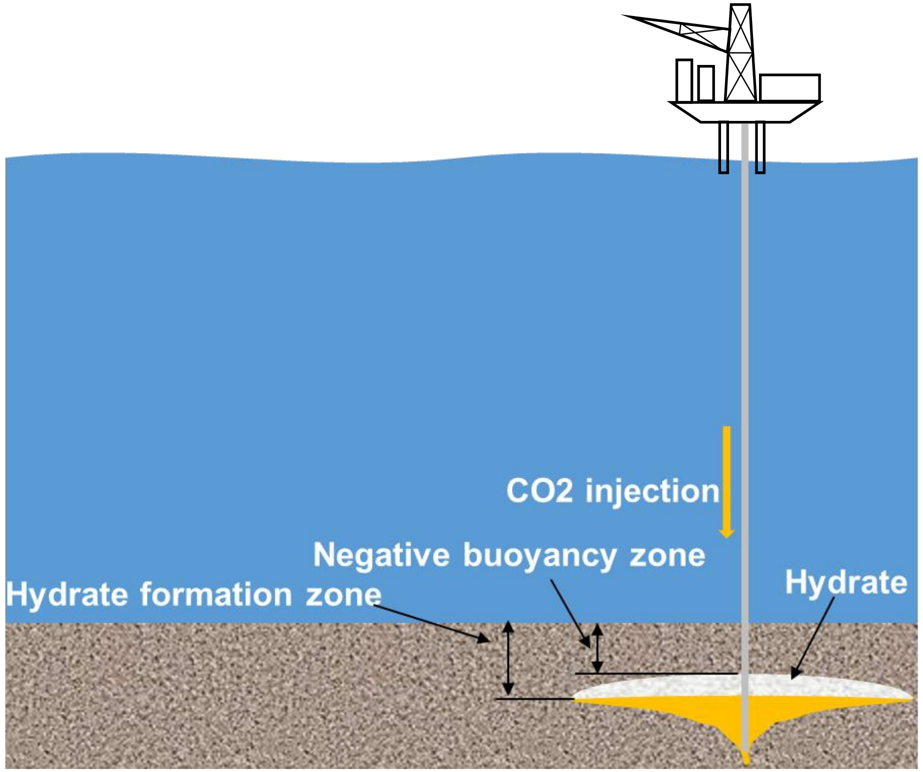


Figure: Injecting and storing CO2 in the deep ocean sediment

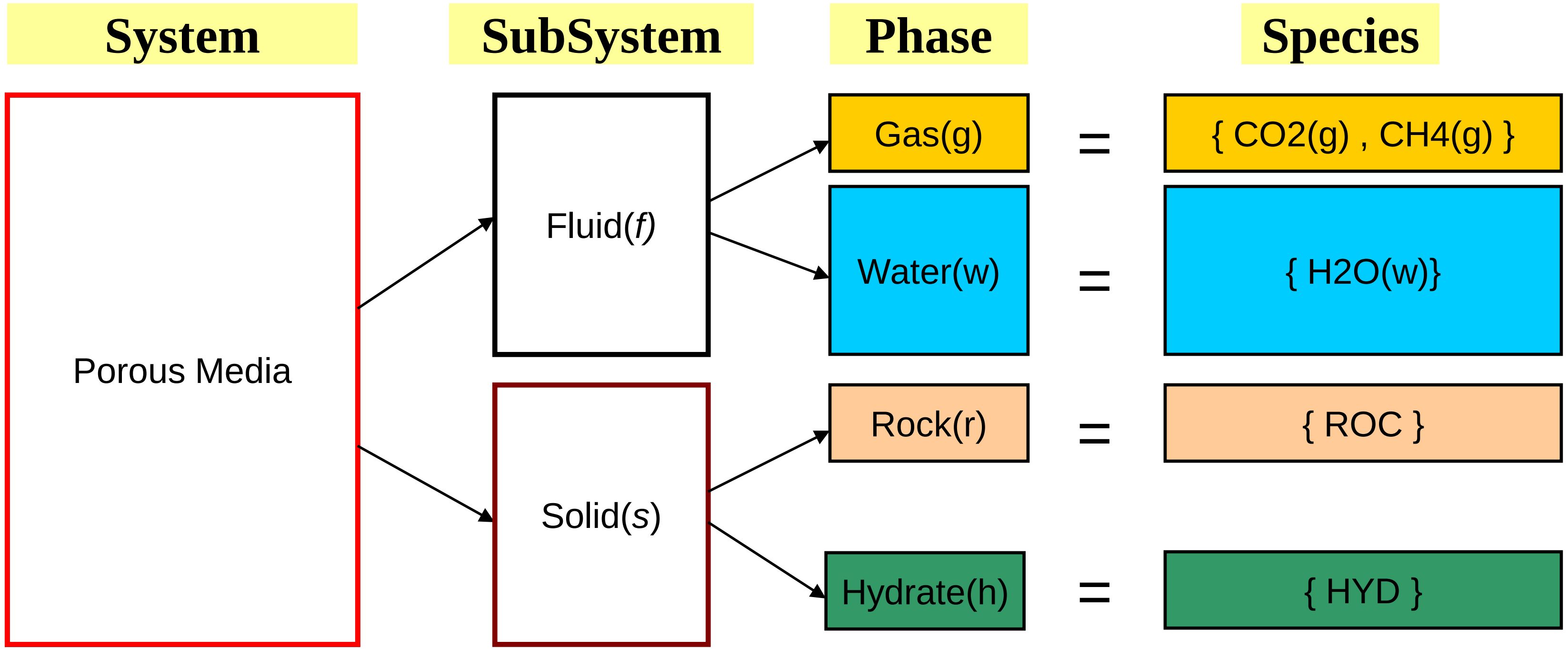
- A more detailed study can be found in [1]

[1] A numerical model for offshore Geological Carbon Storage (GCS) undergoing hydrate formation
Yufei Wang Eric Flauraud, Anthony Michel, Véronique Lachet and Clémentine Meiller,
Computational Geosciences, July 2024

MATHEMATICAL MODEL

NON-ISOTHERMAL REACTIVE COMPOSITIONAL MULTIPHASE FLOW IN POROUS MEDIA

- Example of multiphase compositional system formulation



System **SubSystem** **Phase** **Species**

Porous Media

Fluid(*f*)

Solid(*s*)

Gas(g) = { CO2(g) , CH4(g) }

Water(w) = { H2O(w)}

Rock(r) = { ROC }

Hydrate(h) = { HYD }

NON-ISOTHERMAL REACTIVE COMPOSITIONAL MULTIPHASE FLOW IN POROUS MEDIA

Conservation equations

$$\frac{\partial}{\partial t}\left(\phi_f S_g \rho_g X^g_{CO2}\right) + div\left(\rho_g X^g_{CO2} \vec{v}_g\right) + Q_{CO_2} + {\color{red}R_{CO_2}} = 0 \qquad (CO_2)$$

$$\frac{\partial}{\partial t}\left(\phi_f S_g \rho_g X^g_{CH_4}\right) + div\left(\rho_g X^g_{CH_4} \vec{v}_g\right) + Q_{CH_4} = 0 \qquad (CH_4)$$

$$\frac{\partial}{\partial t}\left(\phi_f S_w \rho_w X^w_{H_2O}\right) + div\left(\rho_w X^w_{H_2O} \vec{v}_w\right) + Q_{H_2O} + {\color{red}R_{H_2O}} = 0 \qquad (H_2O)$$

$$\frac{\partial}{\partial t}\left(\phi_s S_r \rho_r X^r_{ROC}\right) = 0 \qquad (ROC)$$

$$\frac{\partial}{\partial t}\left(\phi_s S_h \rho_h X^h_{HYD}\right) + {\color{red}R_{HYD}} = 0 \qquad (HYD)$$

Closure equations

$$\phi_f + \phi_s = 1$$

$$S_w + S_g = 1 \qquad S_r + S_h = 1$$

$$X^w_{H_2O} = 1 \qquad X^g_{CO2} + X^g_{CH_4} = 1$$

$$X^r_{ROC} = 1 \qquad X^h_{HYD} = 1$$

Darcy law

$$\vec{v}_\alpha = -K \frac{kr_\alpha}{\mu_\alpha}\left(\vec{\nabla} P_\alpha - \rho^m_\alpha \vec{g}\right) \qquad \alpha = w, g$$

Permeability law

$$K(\phi_f) = K_0 e^{\left(c\left(\frac{\phi_f}{\phi_0} - 1\right)\right)}$$

CO_2 HYDRATE KINETIC FORMATION/DISSOCIATION

- Chemical reaction: $$n_h\ H_2O(w) + CO_2(g) \leftrightarrow HYD$$

where n_h is the hydrate number $n_h \approx 6$

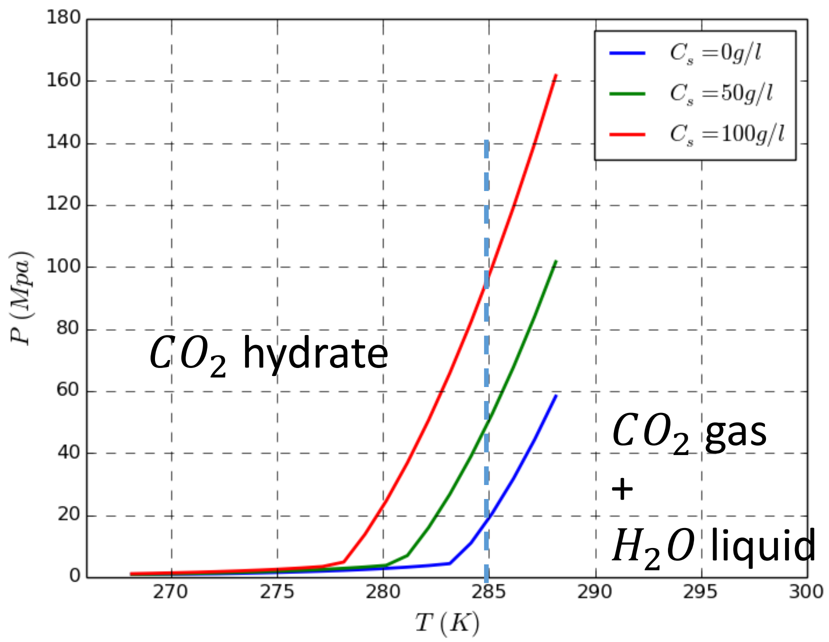
- Reaction rate τ: $$\tau = -k_r A_r (P_h(T,C_s) - P)$$
  - k_r is the kinetic rate constant: $k_r = k_{r0} e^{-\frac{E_a}{RT}}$
  - A_r is the reaction surface: $A_r = A_0\ \Gamma_r$
    - A_0 is the pore surface area
    - Γ_r is the active fraction of the pore surface area

      $\Gamma_r = S_w S_g X^w_{H_2O}\ X^g_{CO_2}$ (hydrate formation)

      $\Gamma_r = S_h$ (hydrate dissociation)
  - $P_h(T,C_s)$ is the equilibrium pressure of hydrate
  - $P_h(T,C_s) - P$ measures the deviation from equilibrium
    - if $P_h(T,C_s) < P \implies \tau > 0$: ***Formation***
    - if $P_h(T,C_s) > P \implies \tau < 0$: ***Dissociation***
    - if $P_h(T,C_s) = P \implies \tau = 0$: ***Equilibrium***

- $$R_{HYD} = -\tau,\ R_{CO_2} = \tau \text{ and } R_{H_2O} = n_h \tau$$

$P_h(T,C_s)$



NON-ISOTHERMAL REACTIVE COMPOSITIONAL MULTIPHASE FLOW IN POROUS MEDIA

- Energy balance equation:

$$\frac{\partial}{\partial t}\left(\phi_f \sum_{\alpha\in\{w,g\}} S_\alpha \rho_\alpha u_\alpha + \phi_s \sum_{\beta\in\{r,h\}} S_\beta \rho_\beta u_\beta\right) + div\left(\sum_{\alpha\in\{w,g\}} \rho_\alpha h_\alpha \vec{v}_\alpha - \Lambda_E \vec{\nabla} T\right) + Q_E = 0$$

- Specific internal energy:

$$u_\alpha = h_\alpha - \frac{P}{\rho_\alpha} \qquad \alpha \in \{w,g\} \qquad\qquad u_\beta = h_\beta \qquad \beta \in \{r,h\}$$

- Specific enthalpy:
  - Simple linear law : $\boxed{h_\alpha(T,P) = h_{ref,\alpha} + C_{p,\alpha}\left(\left(T - T_{ref}\right) - \mu_{JT,\alpha}\left(P - P_{ref}\right)\right)}$
    - $h_{\alpha,ref}$, T_{ref} and P_{ref} are the reference enthalpy, the reference temperature and the reference pressure. $C_{\alpha,p}$ is the heat capacity factor and $\mu_{JT,\alpha}$ is the Joule-Thomson coefficent.
  - Equation of state (EOS) : $\boxed{h_\alpha(T,P,X) = h_{id,\alpha}(T,X) + h_{res,\alpha}(T,P,X)}$
    - Ideal enthalpy: $h_{id,\alpha}(T,X) = \sum_i X_i^\alpha h_{id}^i(T)$
    - Residual enthalpy (EOS): $h_{res,\alpha}(T,P,X) = \sum_i X_i^\alpha h_{res}^i(T,P,X)$

JOULE-THOMSON EFFECT

- Joule-Thomson coefficient

$$\mu_{JT} = \frac{dT}{dP} = \frac{1}{C_p}\left(T\left(\frac{\partial V_g}{\partial T}\right)_P - V_g\right) = -\frac{1}{Cp.\rho_g}\left(\frac{T}{\rho_g}\left(\frac{\partial \rho_g}{\partial T}\right)_P + 1\right)$$

- Joule-Thomson effect
  - For a gas expansion: $dP < 0$
    - If $\mu_{JT} > 0 \Rightarrow dT < 0$: The gas expansion leads to a cooling.
    - If $\mu_{JT} < 0 \Rightarrow dT > 0$: The gas expansion leads to a warming up.
  - For a gas compression: $dP > 0$
    - If $\mu_{JT} > 0 \Rightarrow dT > 0$: The gas compression leads to a warming up.
    - If $\mu_{JT} < 0 \Rightarrow dT < 0$: The gas compression leads to a cooling.

MATHEMATICAL FORMULATION: COATS FORMULATION

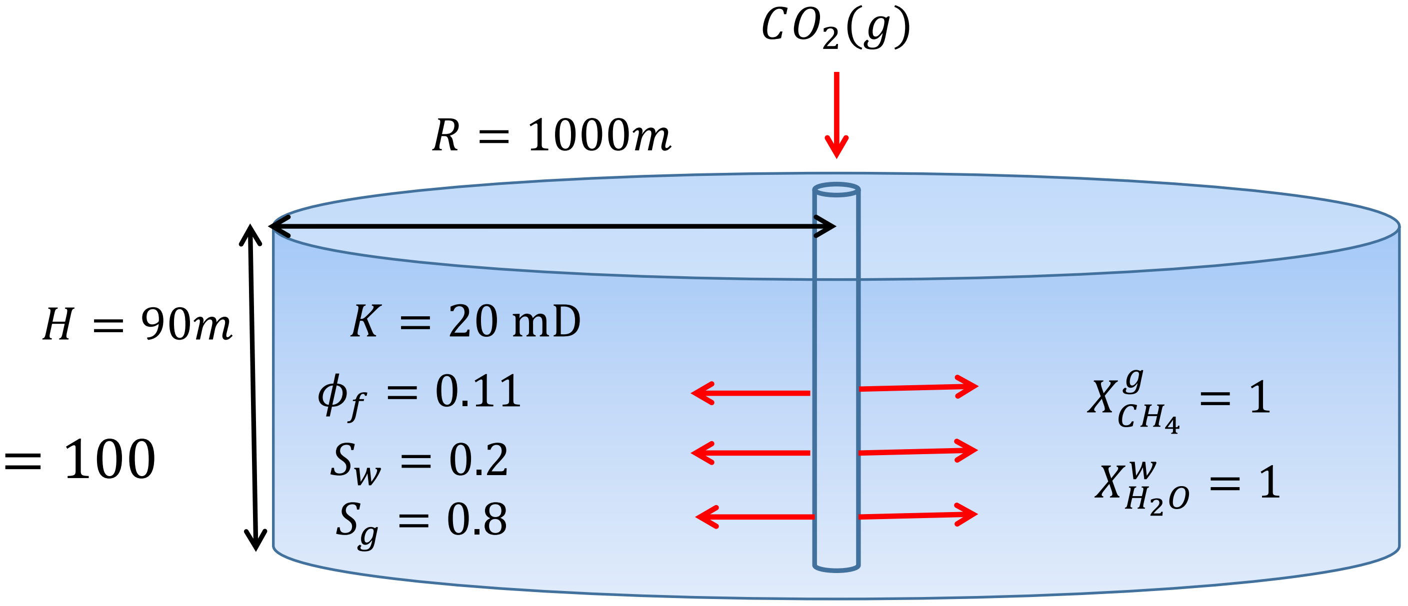
- The unknowns are:

$$P, T, \quad S_w, S_g, S_h, S_r, \phi_f, \phi_s, \quad X^w_{H_2O}, X^g_{CO_2}, X^g_{CH_4}, X^r_{Roc}, X^h_{HYD}.$$

- The equations are discretized with a fully implicit two-point flux finite volume scheme.
- The resulting nonlinear system is solved using the Newton method.
- The size of the system is reduced by pre-eliminating all local equations.
- The set of unknowns is subdivided into a set of primary and secondary unknowns whose definition depends on the local context (variable switching).
- The context is defined at each Newton iteration by using a flash calculation to predict the appearance of a phase and by using the sign of the saturations to predict the disappearance of a phase.

NUMERICAL SIMULATION

INJECTION OF CO_2 IN A GAS (CH_4) DEPLETED RESERVOIR



- 1D radial geometry
- Radial mesh ($\Delta r, \Delta\theta$):

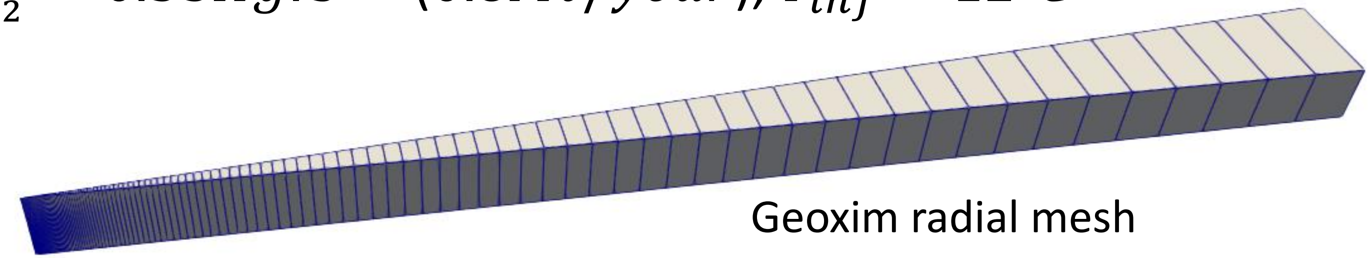
$0{,}002\text{m} < \Delta r < 48m,\ \Delta\theta = 5°, Ncells = 100$

- Using EOS for fluid properties
- Initial conditions:

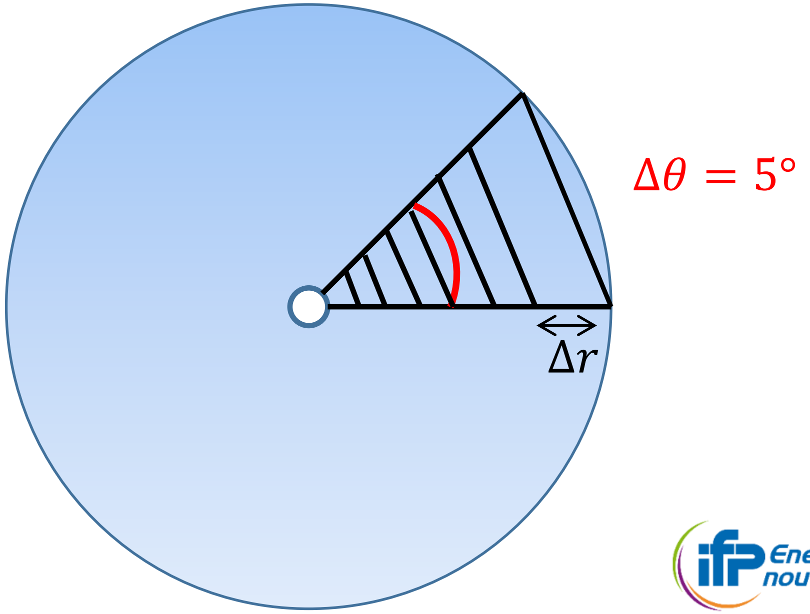
$P_{res} = 20bar, T_{res} = 105°C, C_s = (0\ g/l\ , 30\ g/l)$

- Injection conditions for 5 years:

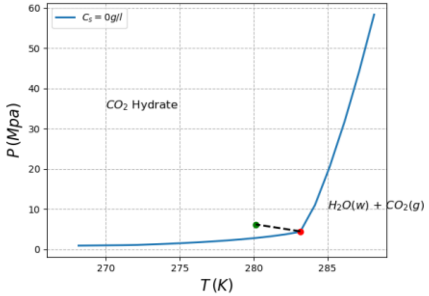
$Q_{CO_2} = 0.35Kg.s^{-1}$ $(0.8Mt/year), T_{inj} = 12°C$



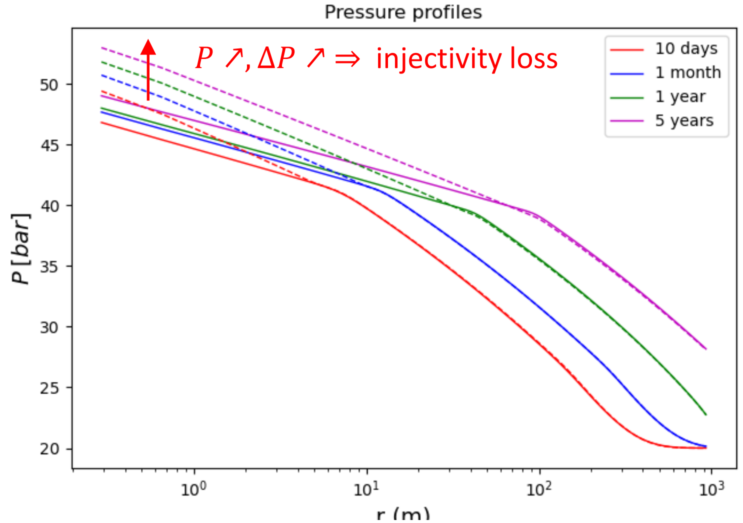
Geoxim radial mesh

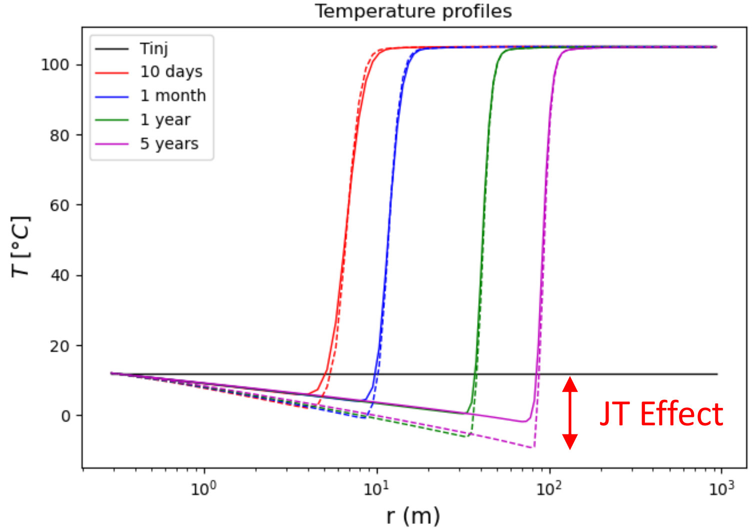


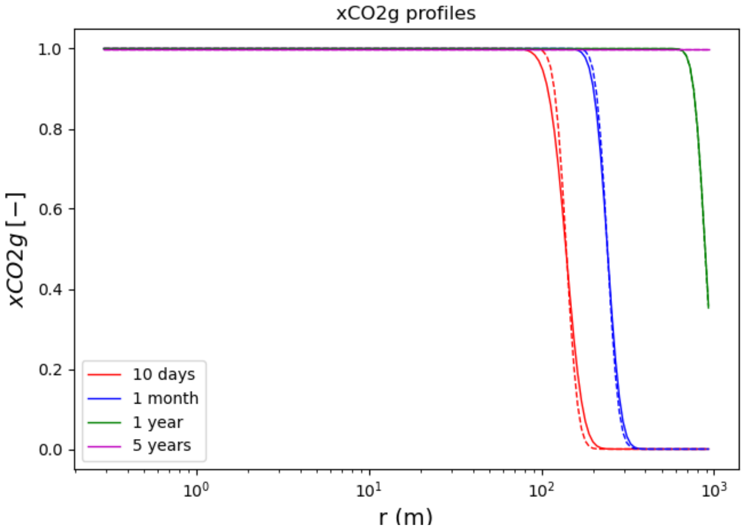
NUMERICAL RESULTS WITHOUT SALINITY ($C_s = 0\ g/l$)

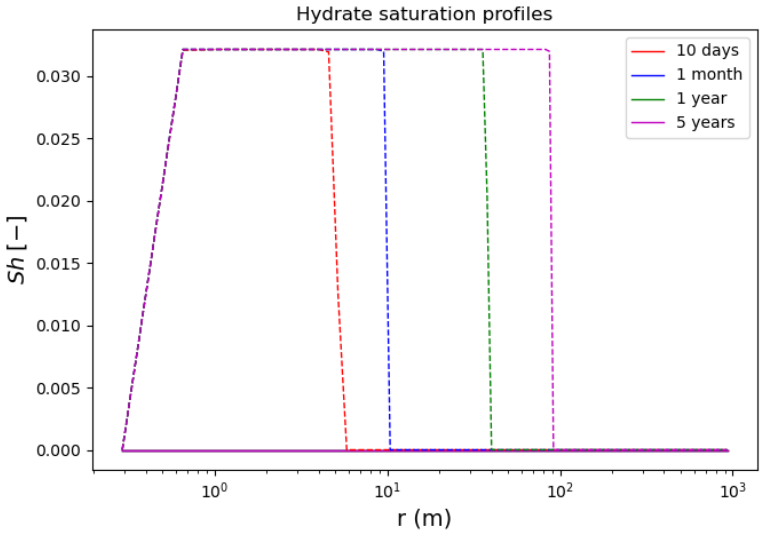


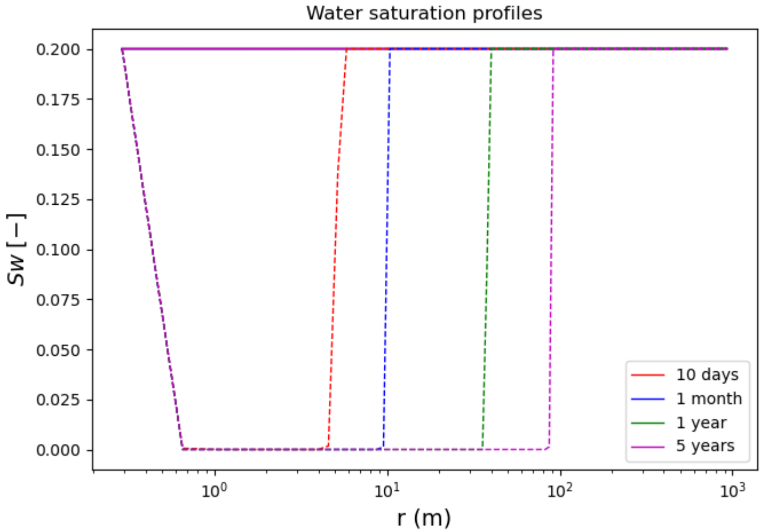
—— (without hydrate formation) ----- (with hydrate formation)

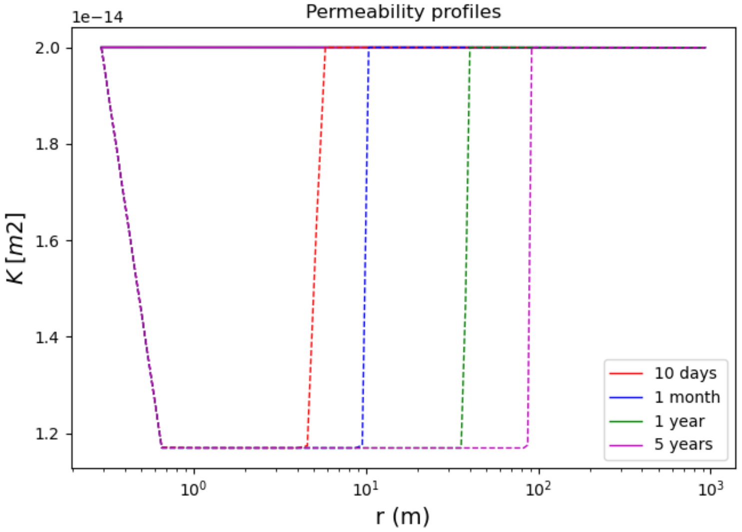




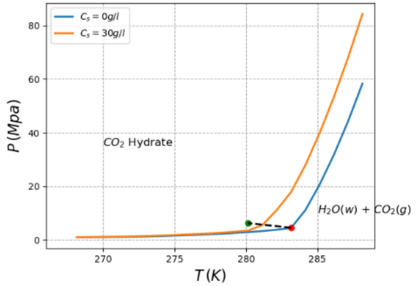


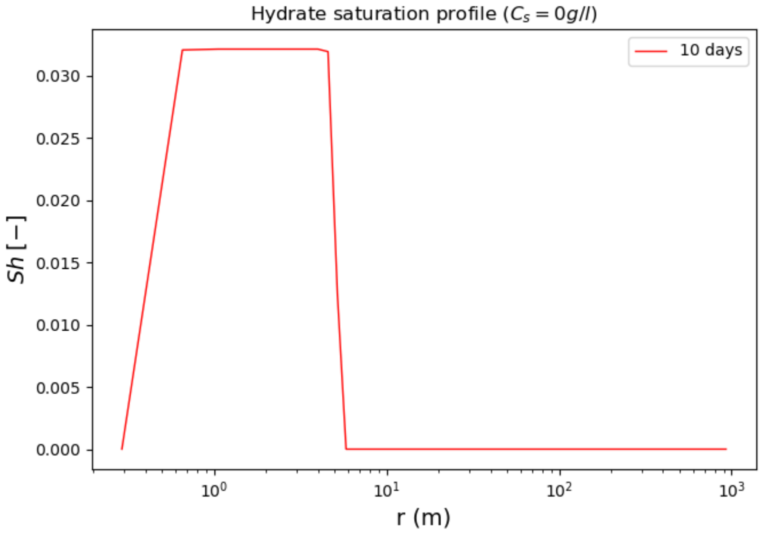


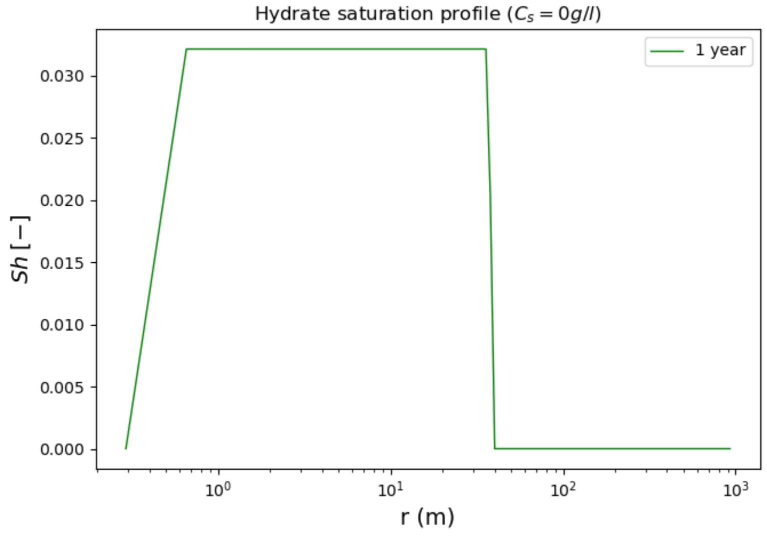


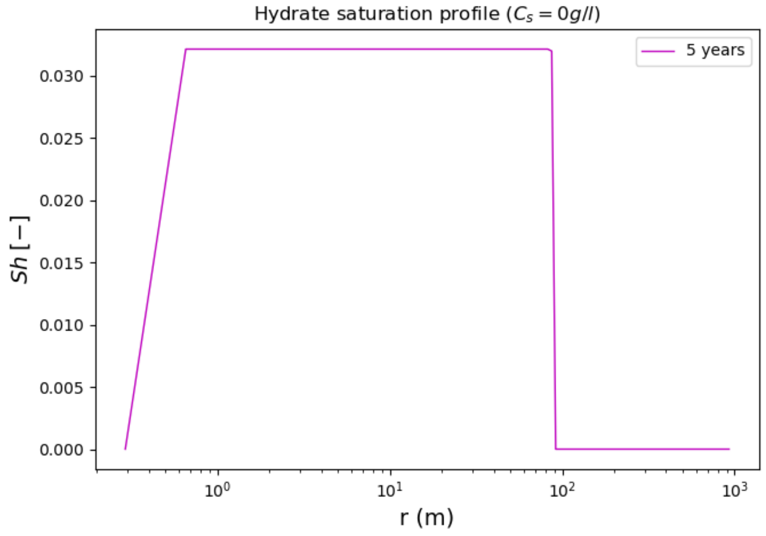


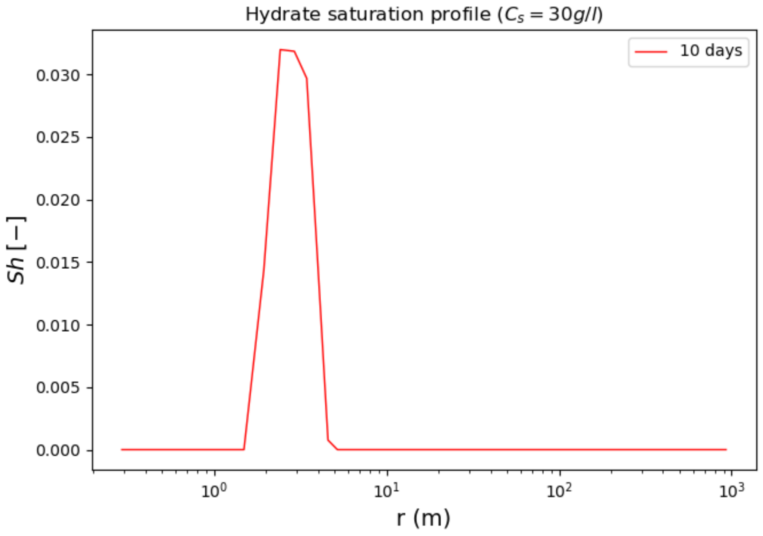
NUMERICAL RESULTS WITH SALINITY $(C_s = 30\ g/l)$

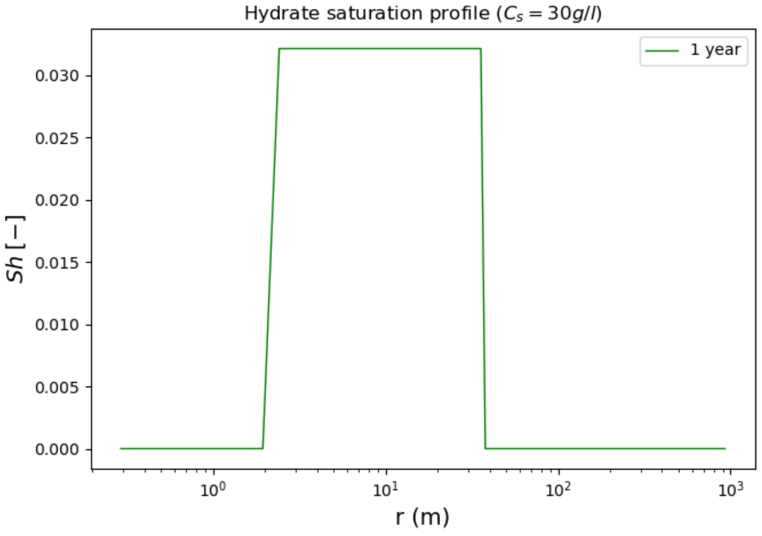


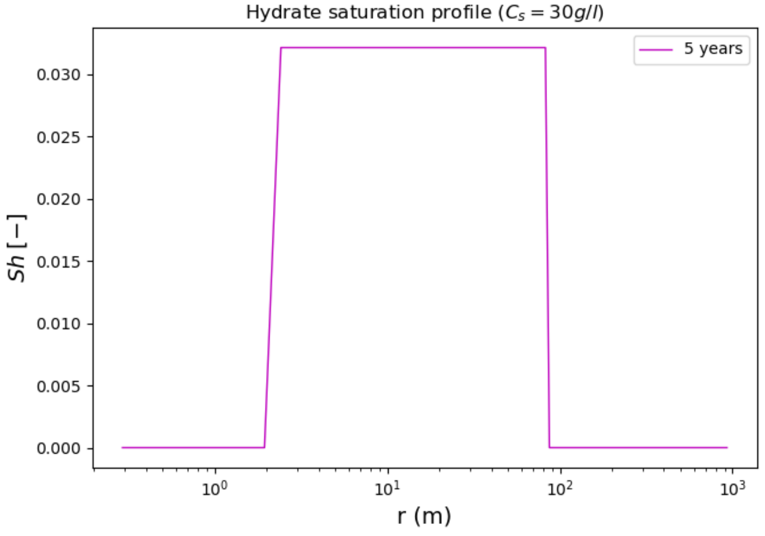

Hydrate saturation profile ($C_s = 0g/l$)


Hydrate saturation profile ($C_s = 0g/l$)

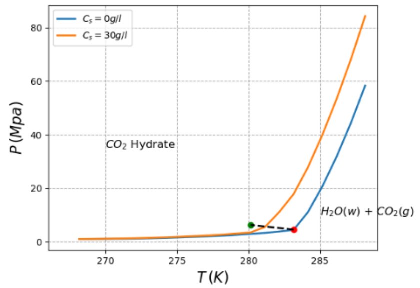

Hydrate saturation profile ($C_s = 0g/l$)


Hydrate saturation profile ($C_s = 30g/l$)

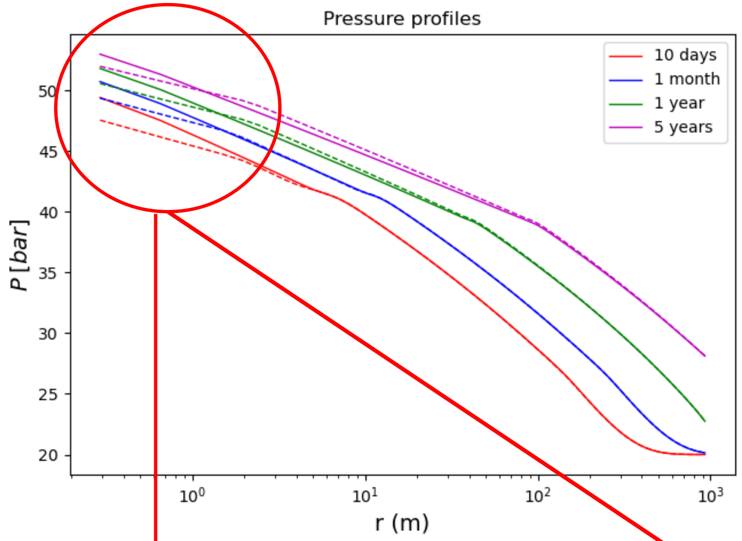

Hydrate saturation profile ($C_s = 30g/l$)

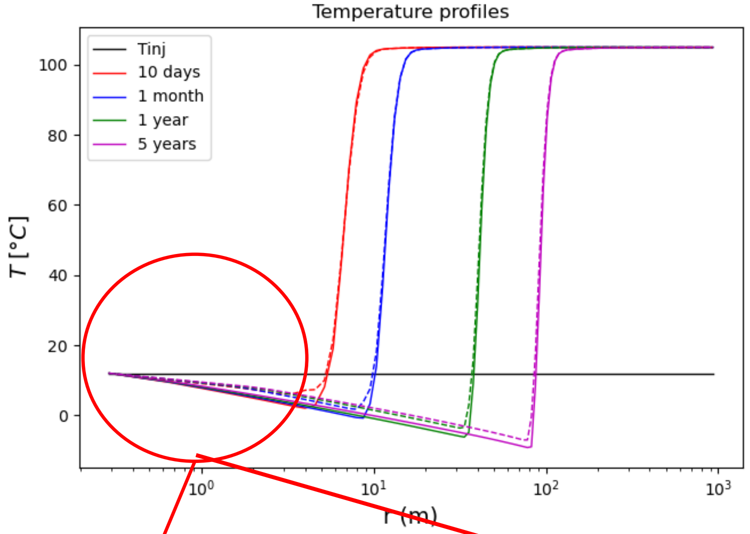

Hydrate saturation profile ($C_s = 30g/l$)

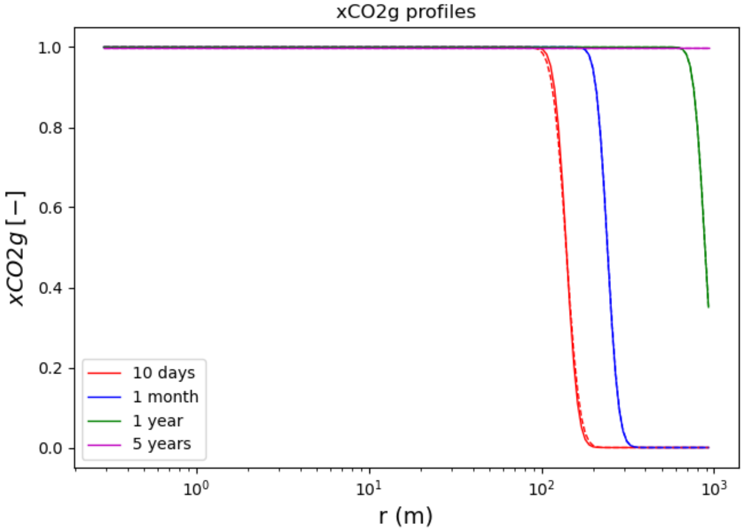
NUMERICAL RESULTS WITH SALINITY $(C_s = 30\ g/l)$

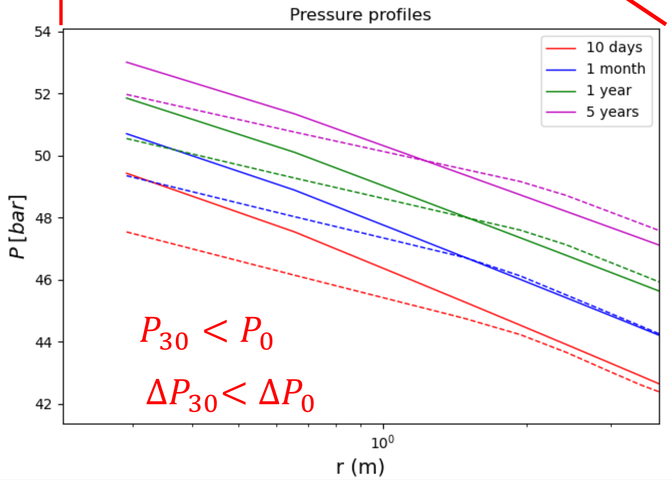


——— $(C_s = 0g/l)$ ----- $(C_s = 30g/l)$



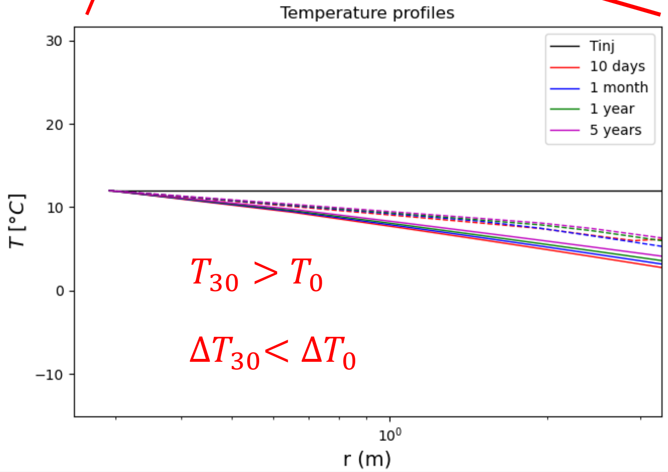






$P_{30} < P_0$

$\Delta P_{30} < \Delta P_0$



$T_{30} > T_0$

$\Delta T_{30} < \Delta T_0$

NUMERICAL RESULTS - CONCLUSION

- These numerical simulations of CO_2 injection into a depleted reservoir have verified that:
  - EOS can well reproduce the Joule-Thomson cooling effect close to the well
  - JT cooling effect ⇒ CO_2 hydrate formation
  - CO_2 hydrate formation ⇒decrease in porosity and permeability ⇒ loss of injectivity
  - But increasing salinity reduces the formation of hydrates
- Future works:
  - Porosity and permeability sensitivity analysis
  - Tacking into account the dissolution of CO_2 and CH_4 in water and water vaporization
  - …

INJECTION OF CO_2 IN DEEP OCEAN SEDIMENTS

- Injection of CO_2 in deep ocean sediments
- 2D radial geometry (R,Z)
- Regular radial mesh $(\Delta r, \Delta z)$:

$$Nr = 50,\ Nz = 100$$

$$\Delta r = 20m,\ \Delta z = 4m$$

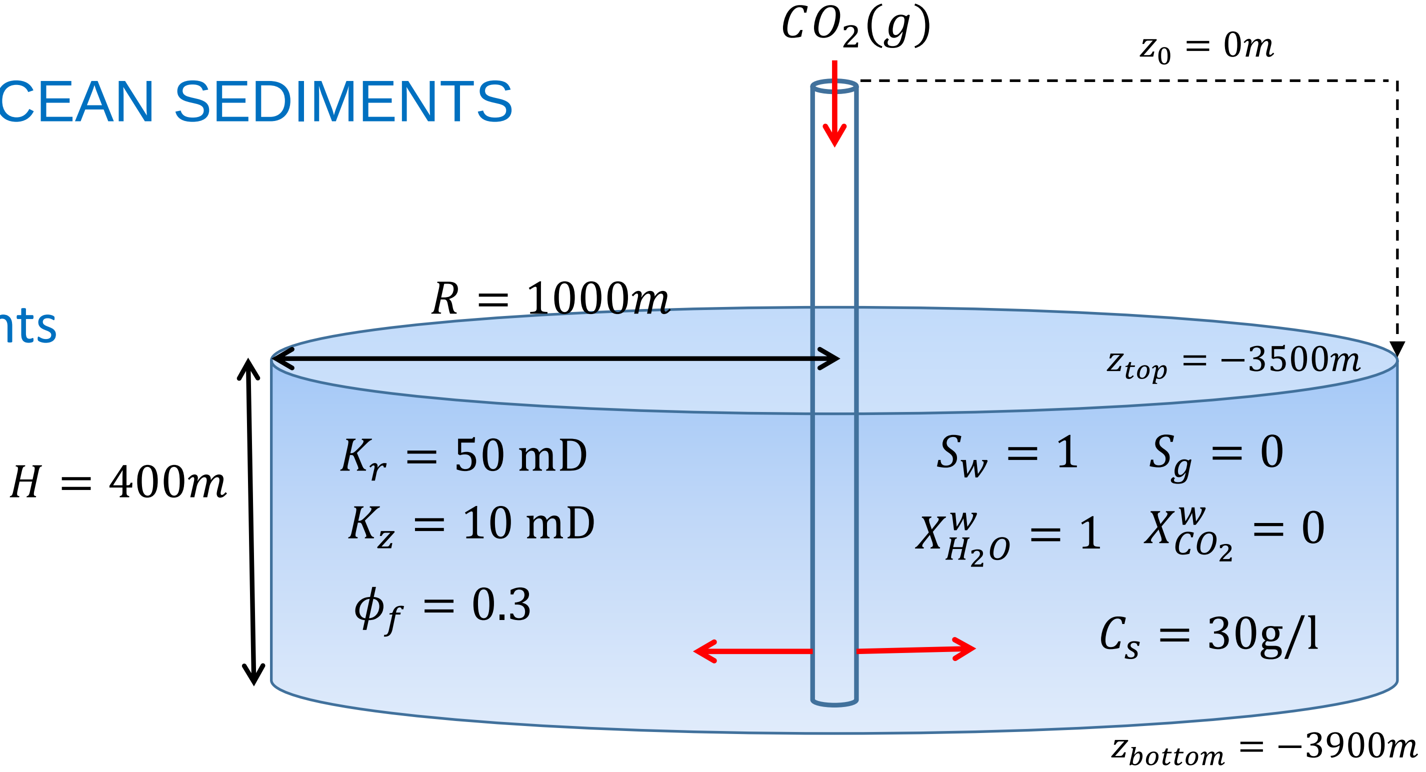
- Dissolution of CO_2 in water
- Initial hydrostatic conditions:

$$P_{top} = 380bar, T_{top} = 3°C$$

$$P_{bottom} = 420bar, T_{bottom} = 15°C$$

- Injection conditions:

$$Q_{CO_2} = 0.44Kg.s^{-1}\ (1\,Mt/year)\ , T_{inj} = 14°C$$



$CO_2(g)$

$z_0 = 0m$

$R = 1000m$

$z_{top} = -3500m$

$H = 400m$

$K_r = 50$ mD

$K_z = 10$ mD

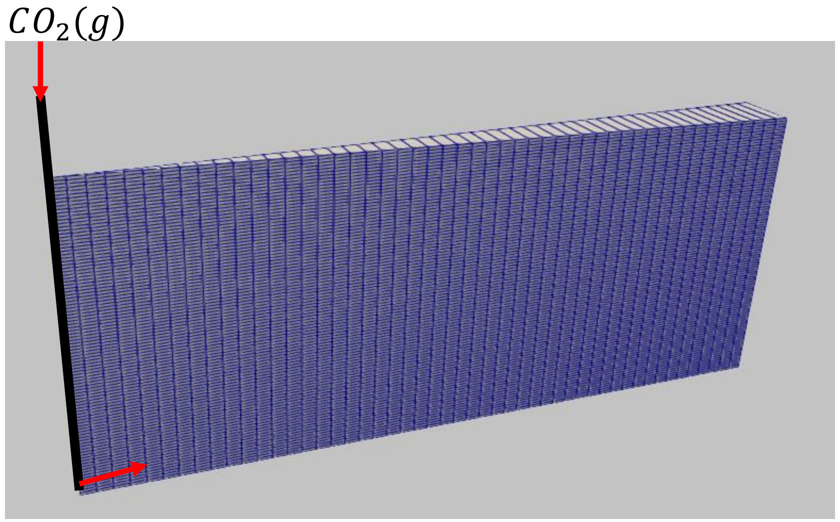
$\phi_f = 0.3$

$S_w = 1 \quad S_g = 0$

$X^w_{H_2O} = 1 \quad X^w_{CO_2} = 0$

$C_s = 30$g/l

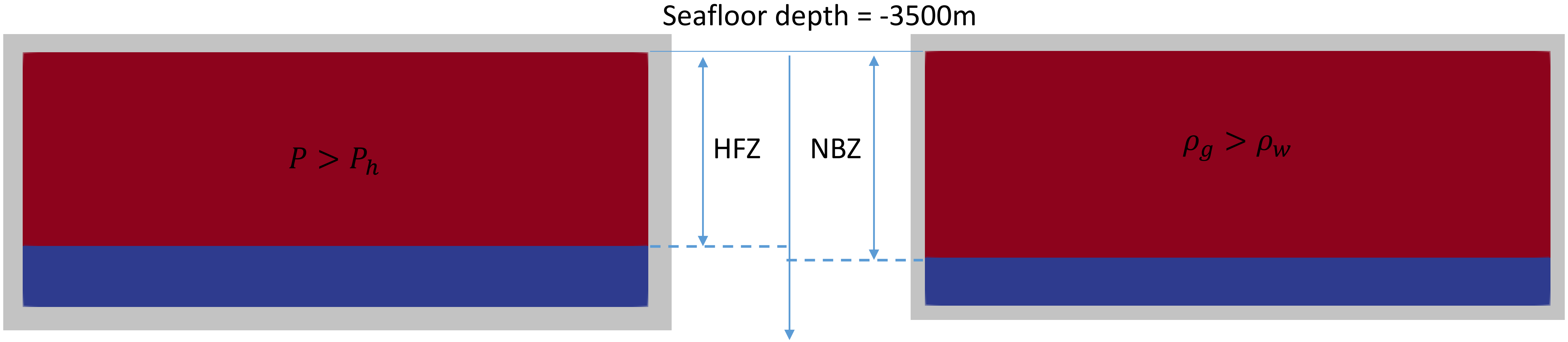
$z_{bottom} = -3900m$



Geoxim 2D radial mesh

NUMERICAL RESULTS WITH $Z_{top} = -3500m$

- Initial Hydrate Formation Zone (HFZ) and initial Negative Buoyancy Zone (NBZ)



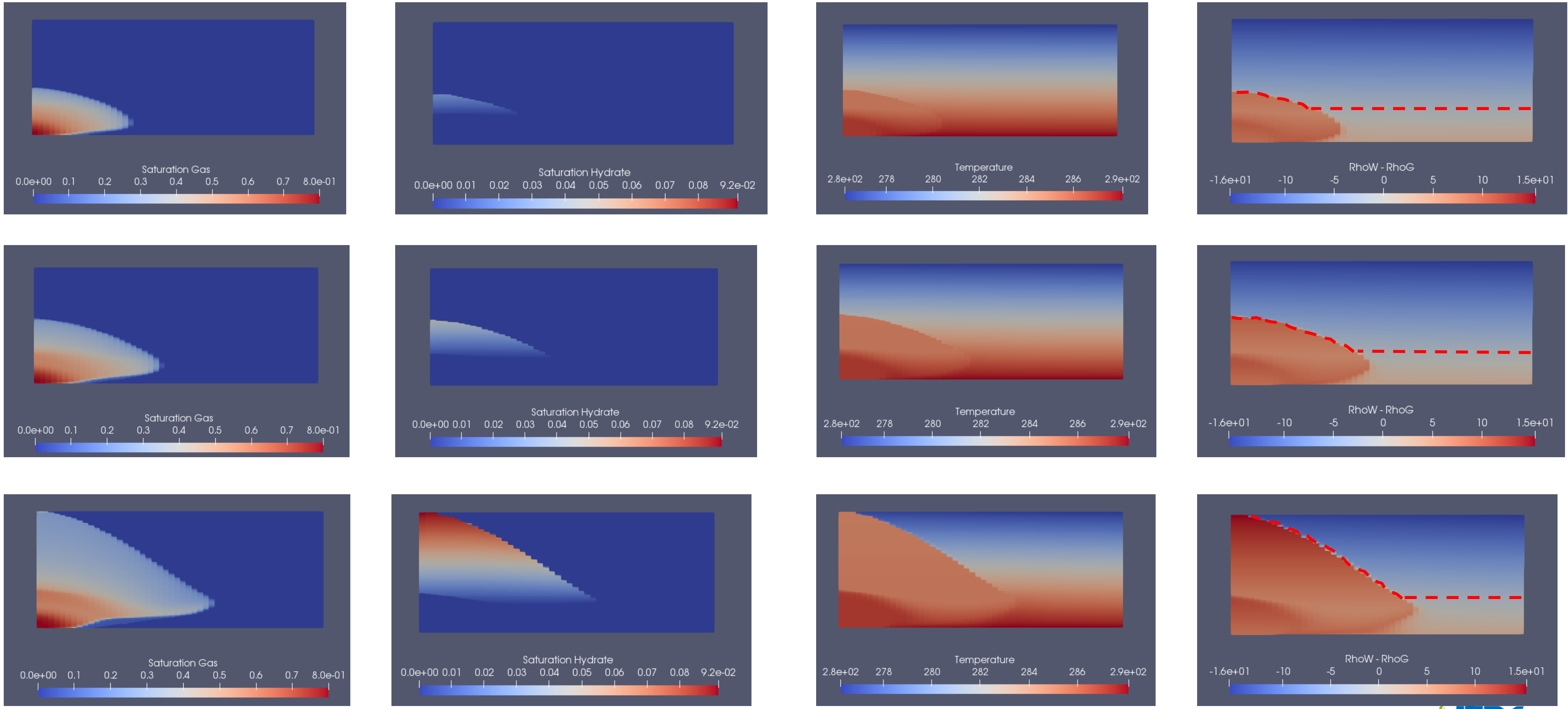
NUMERICAL RESULTS WITH $Z_{top} = -3500m$

S_g | S_h | T | $\rho_w - \rho_g$

$T = 5\ years$

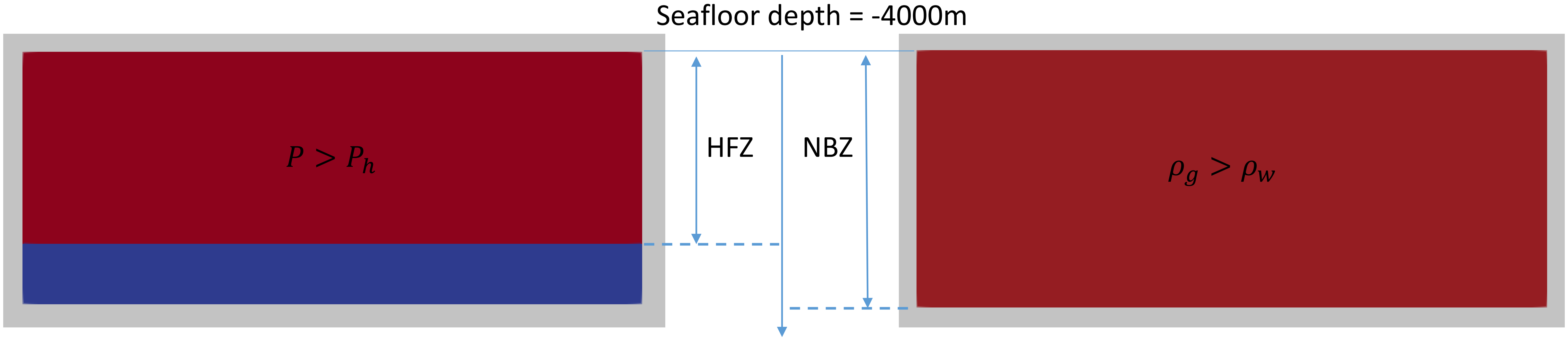
$T = 10\ years$

$T = 25\ years$



NUMERICAL RESULTS WITH $Z_{top} = -4000m$

- Initial Hydrate Formation Zone (HFZ) and initial Negative Buoyancy Zone (NBZ)



Seafloor depth = -4000m

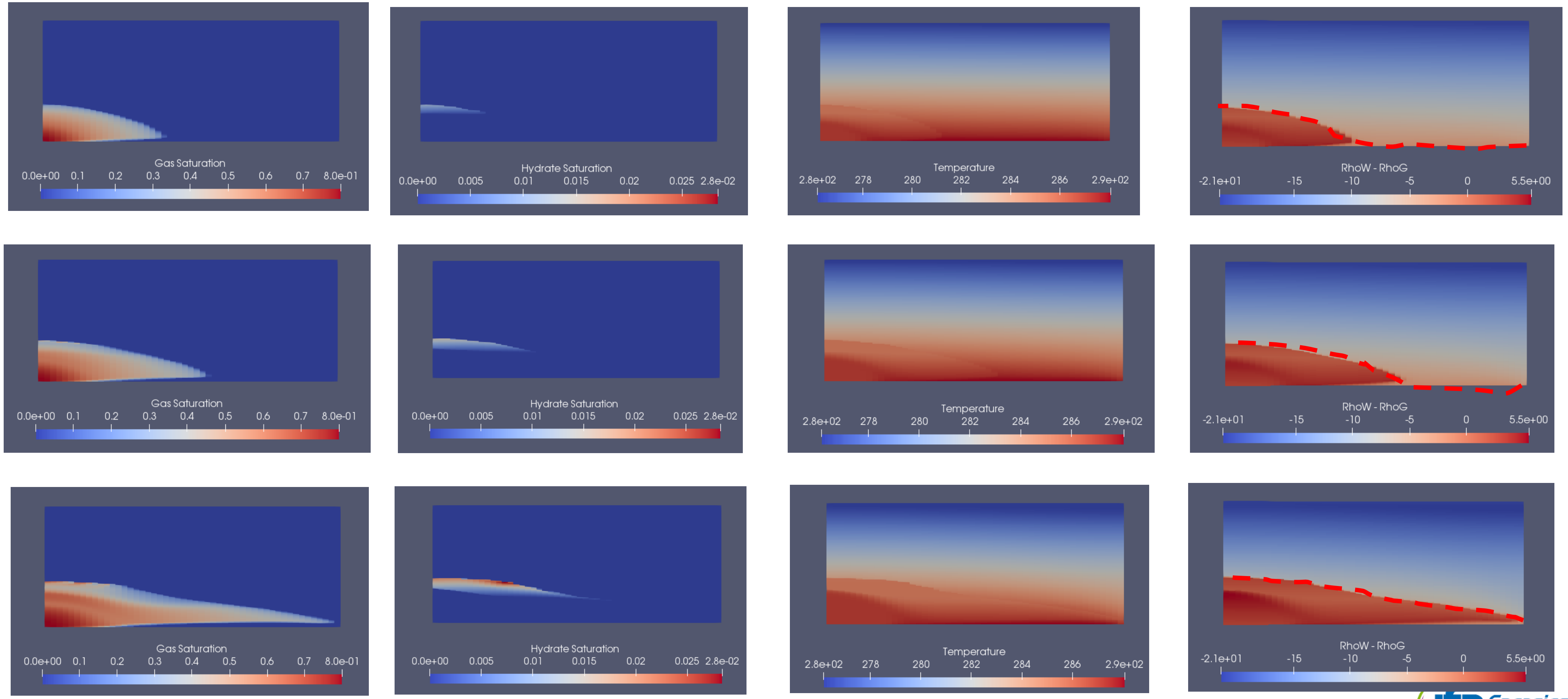
NUMERICAL RESULTS WITH $Z_{top} = -4000m$

S_g | S_h | T | $\rho_w - \rho_g$

$T = 5\ years$

$T = 10\ years$

$T = 25\ years$



NUMERICAL RESULTS - CONCLUSION

- Storing CO2 in deep ocean sediments is not safe:
  - An amount of CO_2 leaks out of the sediments.
  - The amount of hydrate formation is too small to block the CO_2 plume.
  - The Negative Buoyancy zone decreases due to rising temperatures and dissolution of CO_2 in water.

- Permanent CO_2 storage can exist in super deep ocean high permeability sediments which may bring high costs.

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