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Sensitivity Analysis and Validation of the FluidFlower Benchmark Applied to CO_2 Storage

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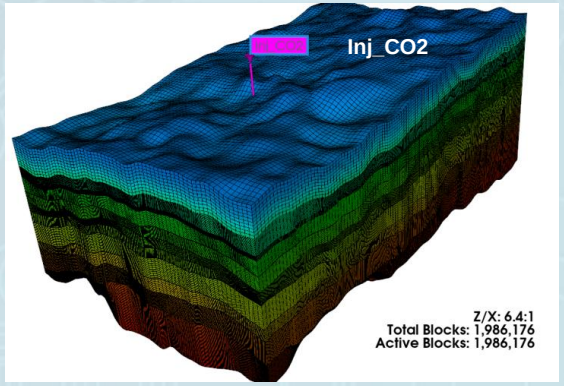
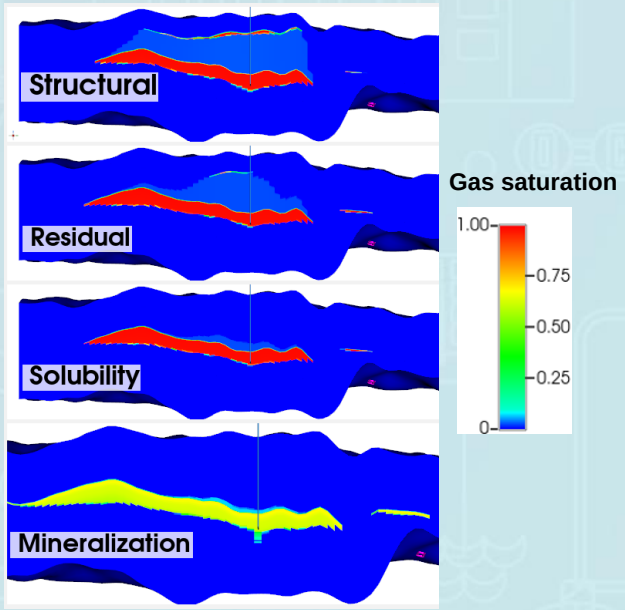
CONTENTS

INTRODUCTION

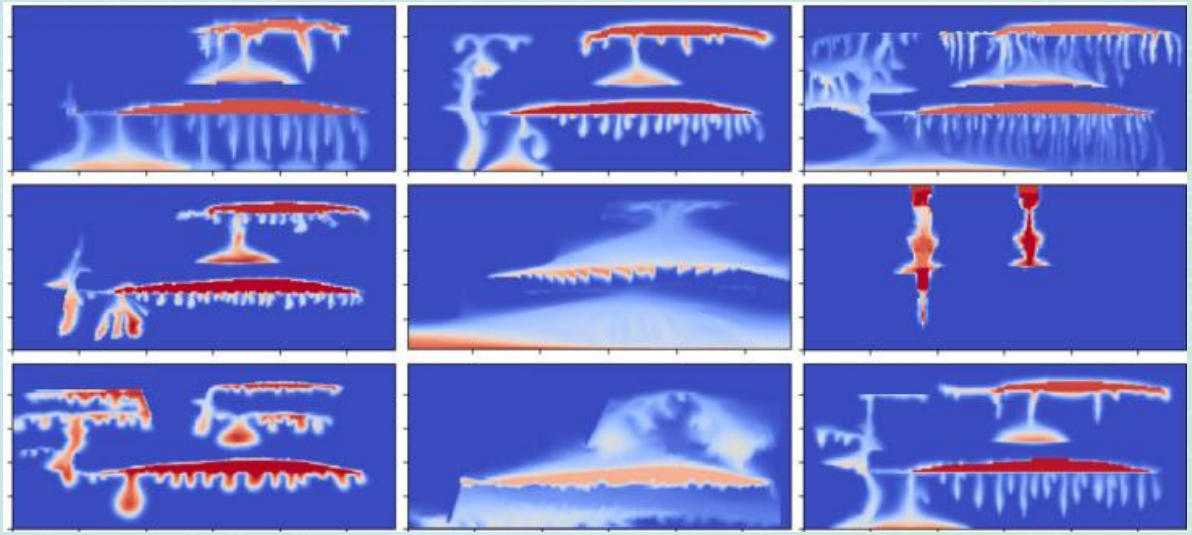
The geological storage of carbon dioxide introduces new challenges related to CO_2 trapping mechanisms, fluid models, reactive transport processes and CO_2 plume formation.



Model area 18.88 km²



Trapping mechanisms Sleipner, Ortega et al. (2024)



Forecasts of concentration of CO_2 with different approaches Bernd F. et al. 2024

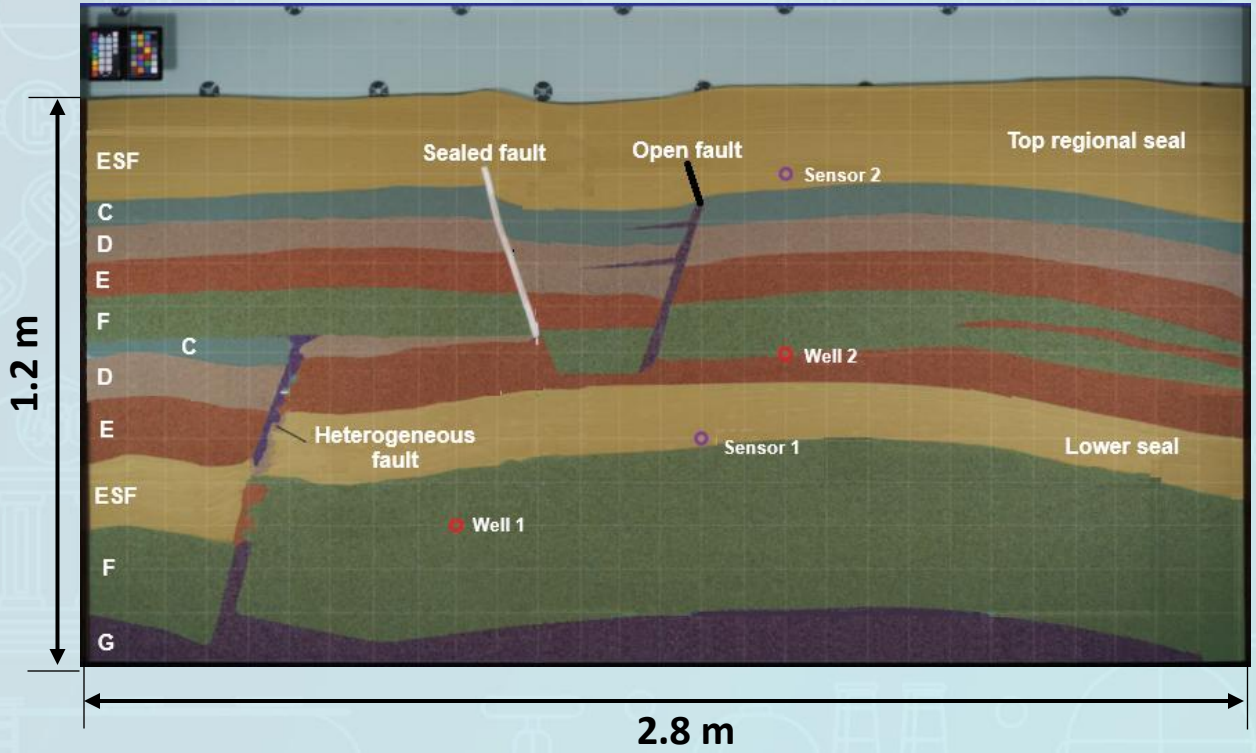
OBJETIVES

- The validation of the simulation model using the experimental data of benchmark “FluidFlower”, case 11A.

- The sensitivity analysis to assess the impact of solubility mechanism, reactive transport process of diffusion and dispersion and dynamic viscosity correlation to understand how these parameters affect finger formation.

FLUIDFLOWER BENCHMARK

This model represents a typical North Sea reservoir at laboratory scale, filled with six different types of unconsolidated sand.



Facies properties

Facies	k (m²)	Φ (-)	$S_{w,imm}$ (-)	P_{entry} (bar)	D_w (m²/s)	E (m)
ESF	$4{\cdot}10^{-11}$	0.44	0.32	1.5E-02	10^{-9}	$1.0E^{-2}$
C	$5{\cdot}10^{-10}$	0.43	0.14	3.0E-03	10^{-9}	$1.0E^{-2}$
D	$1{\cdot}10^{-9}$	0.44	0.12	1.0E-03	10^{-9}	$1.0E^{-2}$
E	$2{\cdot}10^{-9}$	0.45	0.12	2.5E-04	10^{-9}	$1.0E^{-2}$
F	$4{\cdot}10^{-9}$	0.43	0.12	2.5E-04	10^{-9}	$1.0E^{-2}$
Barrier	$1{\cdot}10^{-8}$	0.45	0.08	5.0E-05	10^{-9}	$1.0E^{-2}$
G	0	0	N/A	N/A	0	0

Operational conditions

Parameters	Values
CO_2 injection in Well 1 (m^3/day), continuous for 5 hours.	0.007355
CO_2 injection in Well 2 (m^3/day), start after 2.5 hours, end 2.5 hours later.	0.007355
Reservoir temperature (°C)	20
Pressure at the top of the reservoir (bar)	1.01325
Simulation time (days)	5

Nordbotten eta al., “The 11th Society of Petroleum Engineers Comparative Solution Project: Problem Definition", SPE Journal, Vol. 29, (2024).

METHODOLOGY

A multiphase compositional flow simulator is adopted for solving the mass conservation, solubility, diffusion and dispersion equations.

- ***Mass conservation equation for component 'k':***

$$\frac{\partial}{\partial t}\left(\phi S_\alpha \rho_\alpha \boldsymbol{\omega_{\kappa,\alpha}}\right) = -\nabla \cdot \left[\rho_\alpha \omega_{\kappa,\alpha} \vec{u}_\alpha - S_\alpha \phi D_{\kappa,\alpha} \cdot \nabla(\rho_\alpha \omega_{\kappa,\alpha})\right] + C^*_{\kappa,\alpha} \tilde{q}_\alpha$$

Were α = water or gas phase

- ***Darcy's law:***

$$\vec{v} = -\frac{\mathrm{K}}{\mu}(\nabla p - g\rho\nabla z)$$

- ***Henry's law :***

$$f_{kg} = \boldsymbol{\omega_{\kappa,\alpha}} \cdot H_k$$

- ***Harvey's model:***

$$ln\boldsymbol{H_k} = lnH_k^s + \frac{1}{RT}\int_{p^s_{H_2O}}^{p} \overline{v}_k \, dP$$

Henry's law constant for component:

$$ln\boldsymbol{H_k^s} = lnp^s_{H_2O} + A\left(T_{r,H_2O}\right)^{-1} + B\left(1 - T_{r,H_2O}\right)^{0.355}\left(T_{r,H_2O}\right)^{-1} + C\left[\exp\left(1 - T_{r,H_2O}\right)\right]\left(T_{r,H_2O}\right)^{-0.41}$$

***Water saturation pressure* (Saul and Wagner):**

$$\ln\frac{p^s_{H_2O}}{P_c} = \frac{T_c}{T}\left(a_1\tau + a_2\tau^{1.5} + a_3\tau^3 + a_4\tau^{3.5} + a_5\tau^4 + a_6\tau^{7.5}\right)$$

Partial molar volume (Duan and Sun):

$$\bar{v}_{CO_2} = 47.75418 - 4.336 \times 10^{-1}T - 5.945 \times 10^{-4}T^2$$

Harvey, A.H., "Semiempirical Correlation for Henry's Constants over Large Temperature Ranges", AIChE Journal, Vol. 42, (May 1996), pp. 1491-1494.

METHODOLOGY

The finite difference method is used to solve the system of equations, the fugacity f_{kg} is calculated with Peng-Robinson EOS and relative permeability is modeled with Brooks-Corey correlations.

- ***Mass conservation equation for component 'k':***

$$\frac{\partial}{\partial t}\left(\phi S_\alpha \rho_\alpha \boldsymbol{\omega_{\kappa,\alpha}}\right) = -\nabla \cdot \left[\rho_\alpha \omega_{\kappa,\alpha} \vec{u}_\alpha - S_\alpha \phi D_{\kappa,\alpha} \cdot \nabla(\rho_\alpha \omega_{\kappa,\alpha})\right] + C^*_{\kappa,\alpha} \tilde{q}_\alpha$$

- ***Henry's Law :*** $f_{kg} = \boldsymbol{\omega_{\kappa,\alpha}} \cdot H_k$

- ***Li and Nghiem model:*** $lnH_k = ln\boldsymbol{H_k^0} + \frac{v_i^\infty (P - P_i^0)}{RT}$

$$ln\boldsymbol{H_k^0} = lnp^s_{H_2O} + A\left(T_{r,H_2O}\right)^{-1} + B\left(1 - T_{r,H_2O}\right)^{0.355}\left(T_{r,H_2O}\right)^{-1} + C\left[\exp\left(1 - T_{r,H_2O}\right)\right]\left(T_{r,H_2O}\right)^{-0.41}$$

The molar volume $[v_i^\infty]$***:***

$$\frac{\mathrm{P_{ci}}\mathbf{V_i^\infty}}{\mathrm{RT_{ci}}} = 0.05 + 2.35\left(\frac{\mathrm{TP_{ci}}}{\mathrm{CT_{ci}}}\right)$$

The cohesive energy density of water:

$$C = (h_w^0 - h_w^s - P_w^s v_w^s + RT)/v_w^s$$

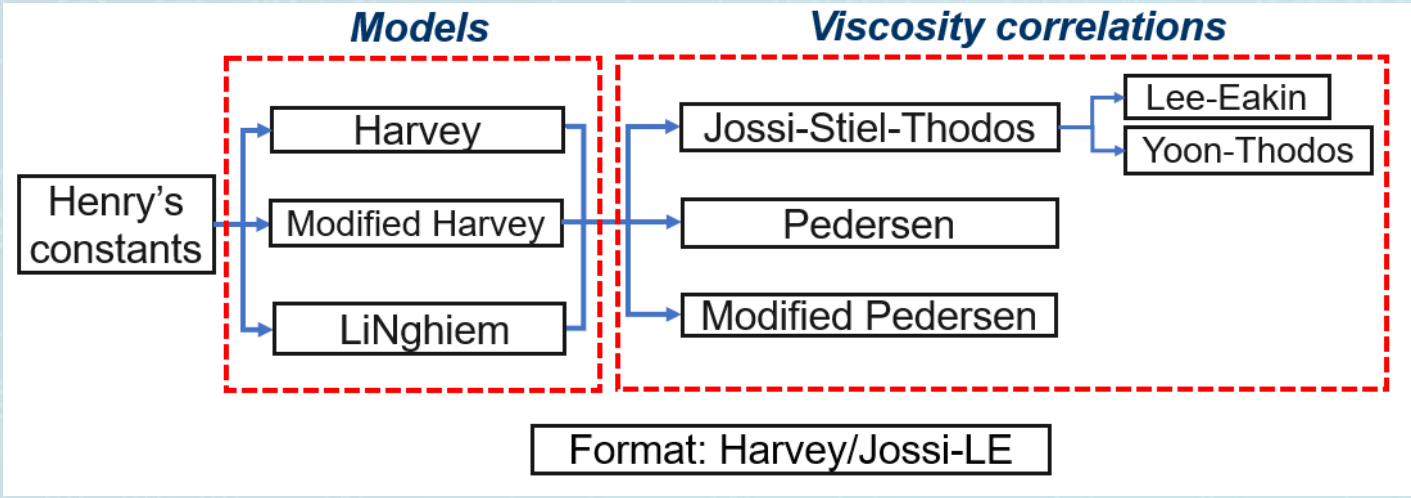
where P_w^s is the water saturation pressure at temperature T, v_w^s is the molar volume of water at P_w^s and T, and $h_w^0 - h_w^s$ is enthalpy departure of liquid water at P_w^s and T.

Li, Y.-K. and Nghiem, L.X., "Phase Equilibria of Oil, Gas and Water/Brine Mixtures from a Cubic Equation of State and Henry's Law", Can. J. Chem. Eng., (1986).

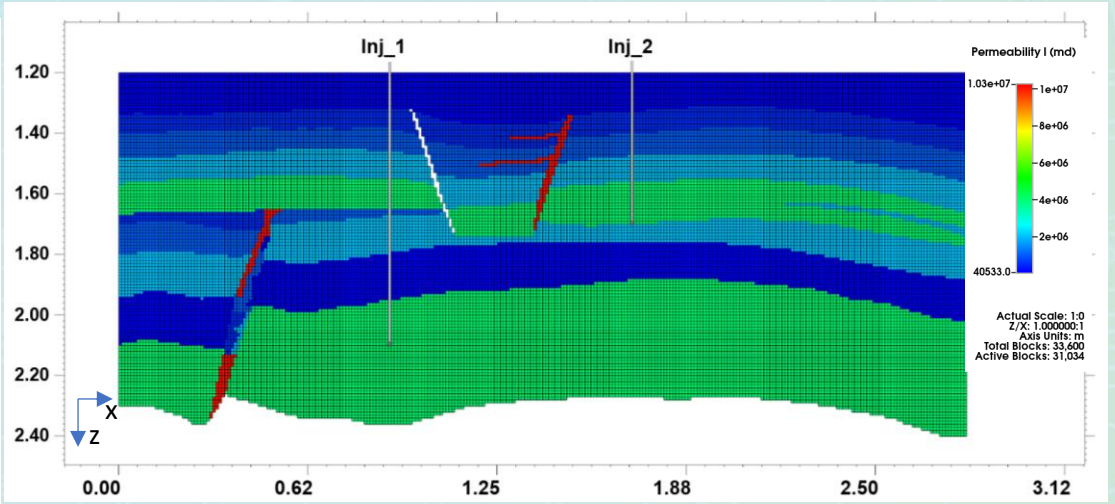
METHODOLOGY

The following figure shows the combinations of models and correlations employed in this study to estimate the amount of CO_2 captured by the aqueous medium.

$$\vec{v} = -\frac{K}{\mu}(\nabla p - g\rho\nabla z)$$



Cartesian grid (2.5D) ***Number of cell (280,1,120)***

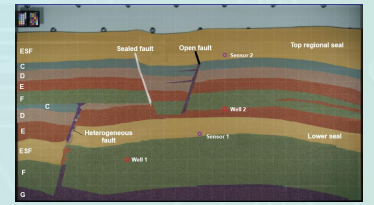


Dimension cell (1 cm x 1 cm)

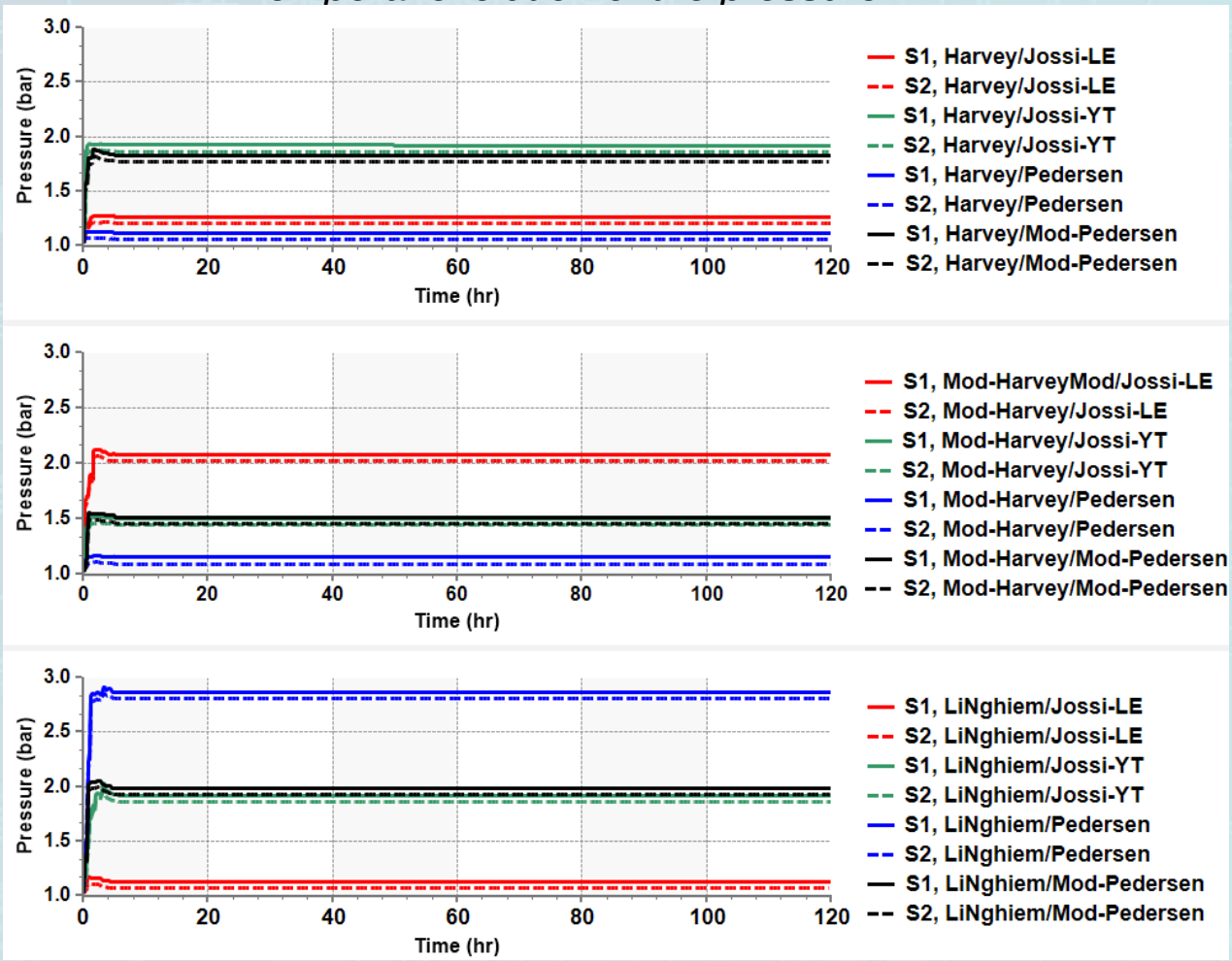
Jossi, J.A., Stiel, L.I. and Thodos, G., "The Viscosity of Pure Substances in the Dense Gaseous and Liquid Phases", AIChE Journal, Vol. 8, (1962).
Pedersen, K.S., Fredenslund, A., Christensen, P.L. and Thomassen, P., "Viscosity of Cruse Oils", Chemical Eng. Science, Vol. 39, (1984).
Yoon, P. and Thodos, G., "Viscosity of Nonpolar Gaseous Mixtures at Normal Pressures", AIChE Journal, Vol. 16, (1970).

SIMULATION RESULTS

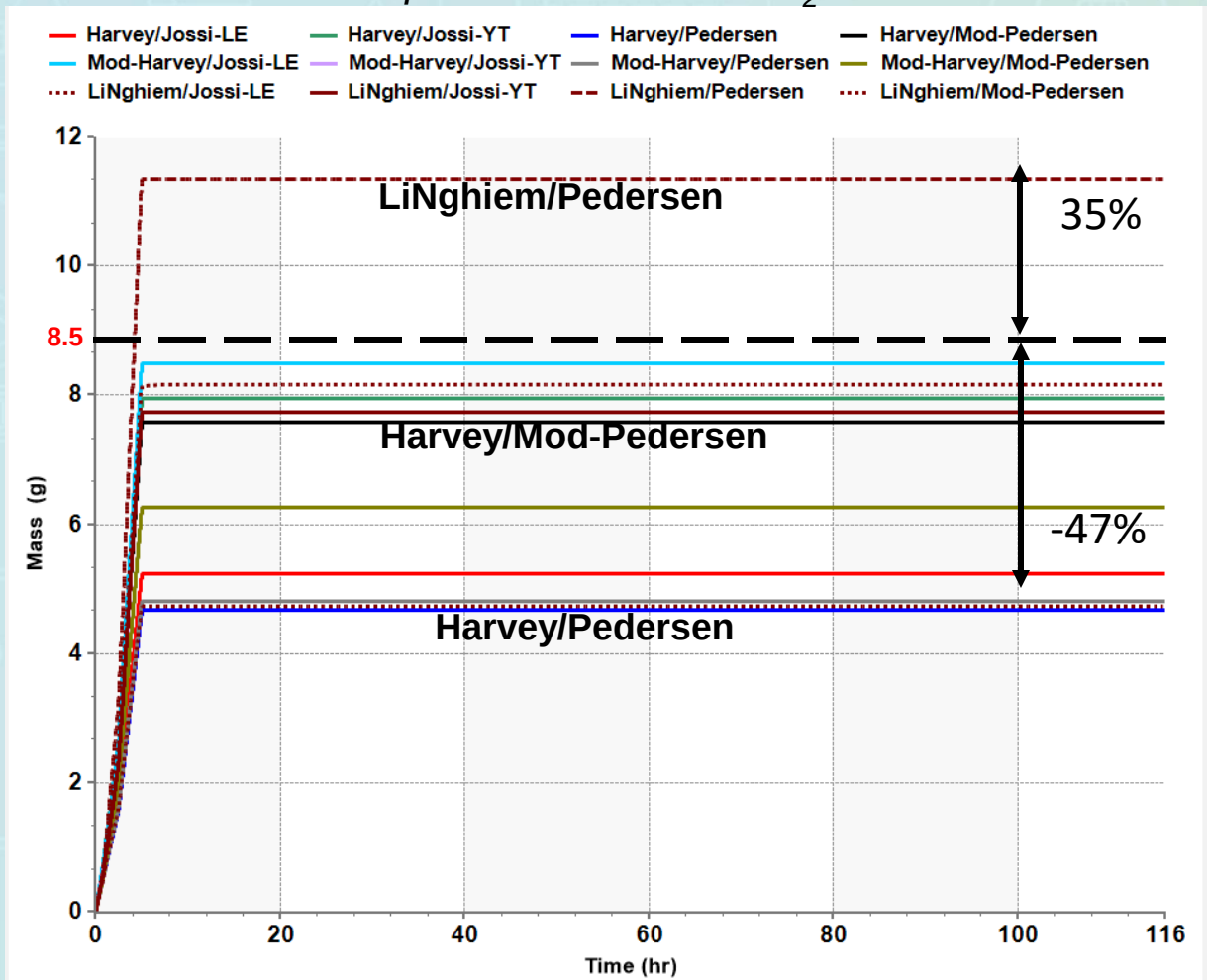
A) Combinations of models and correlations



Temporal evolution of the pressure



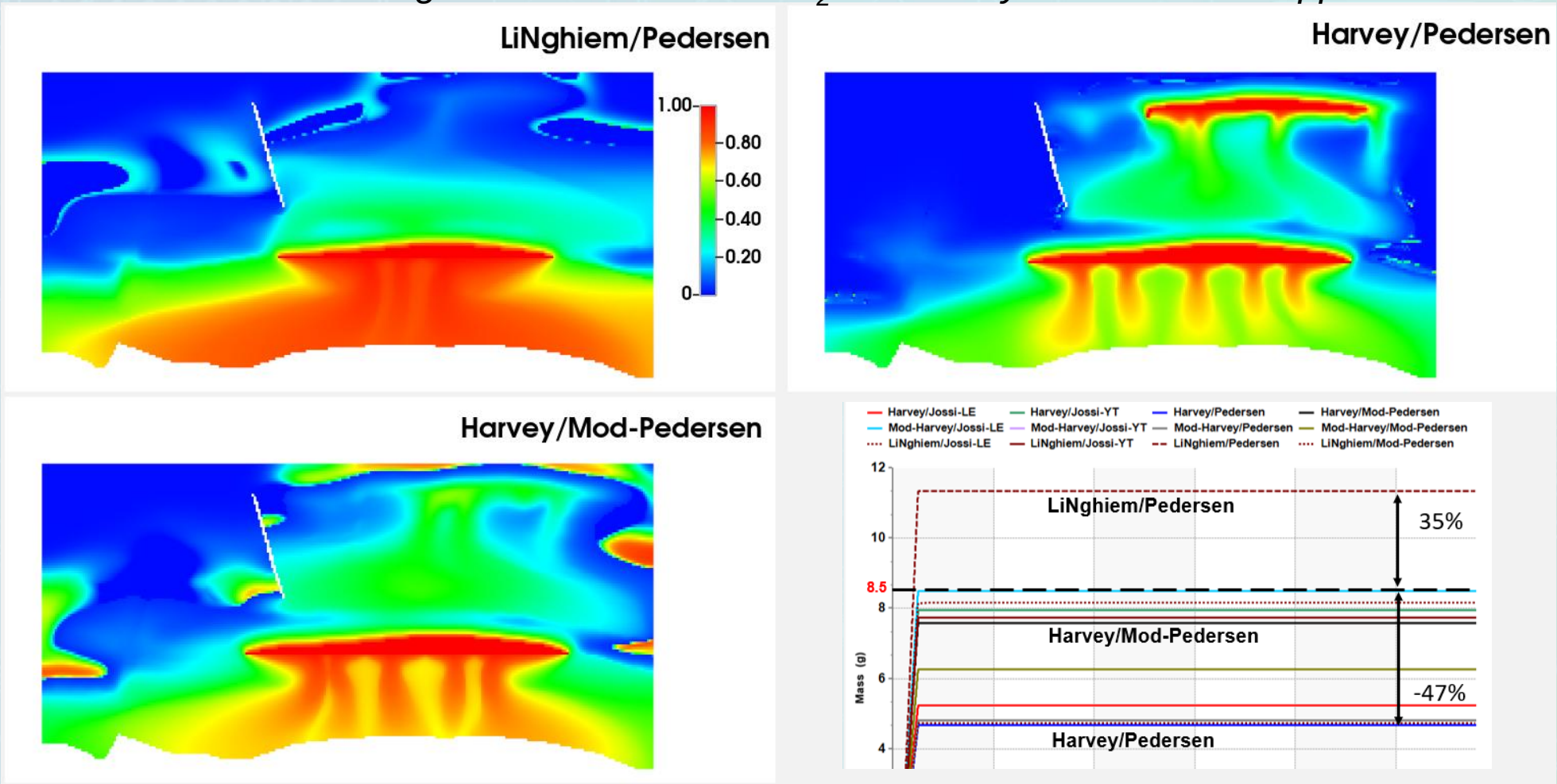
Temporal evolution of CO_2 mass

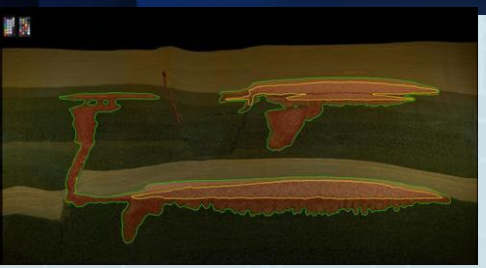


SIMULATION RESULTS

A) Combinations of models and correlations

Numerical results of gas mole fraction of CO_2 after 5 days with different approaches

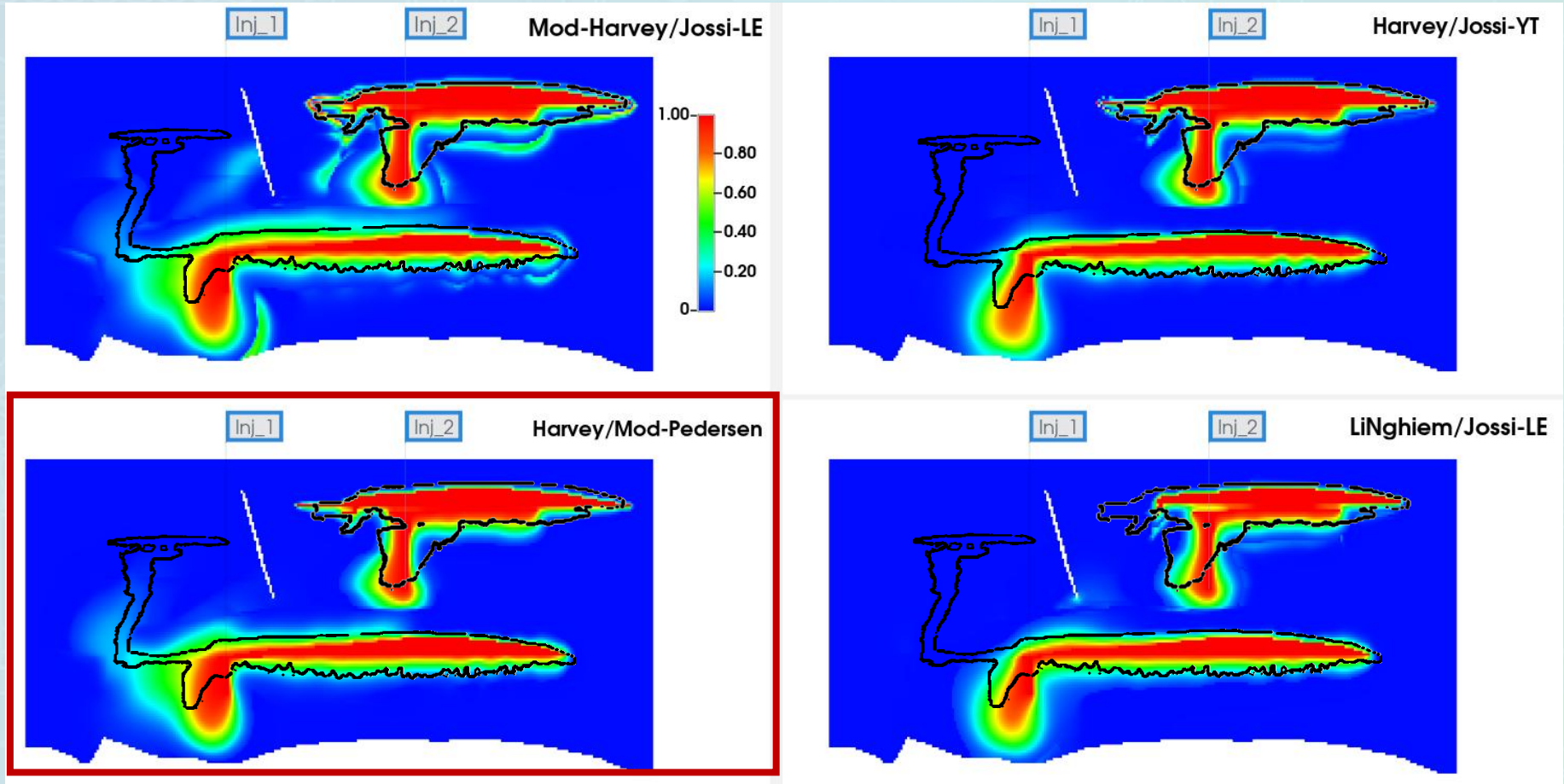


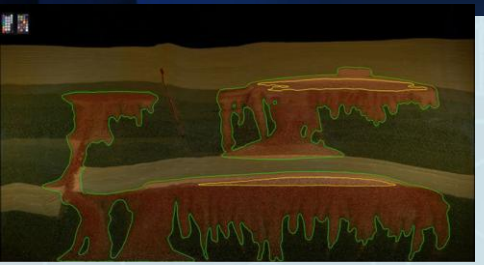


SIMULATION RESULTS

B) The validation of the simulation model:

Comparison numerical results of gas mole fraction of CO_2 after 5 about hours

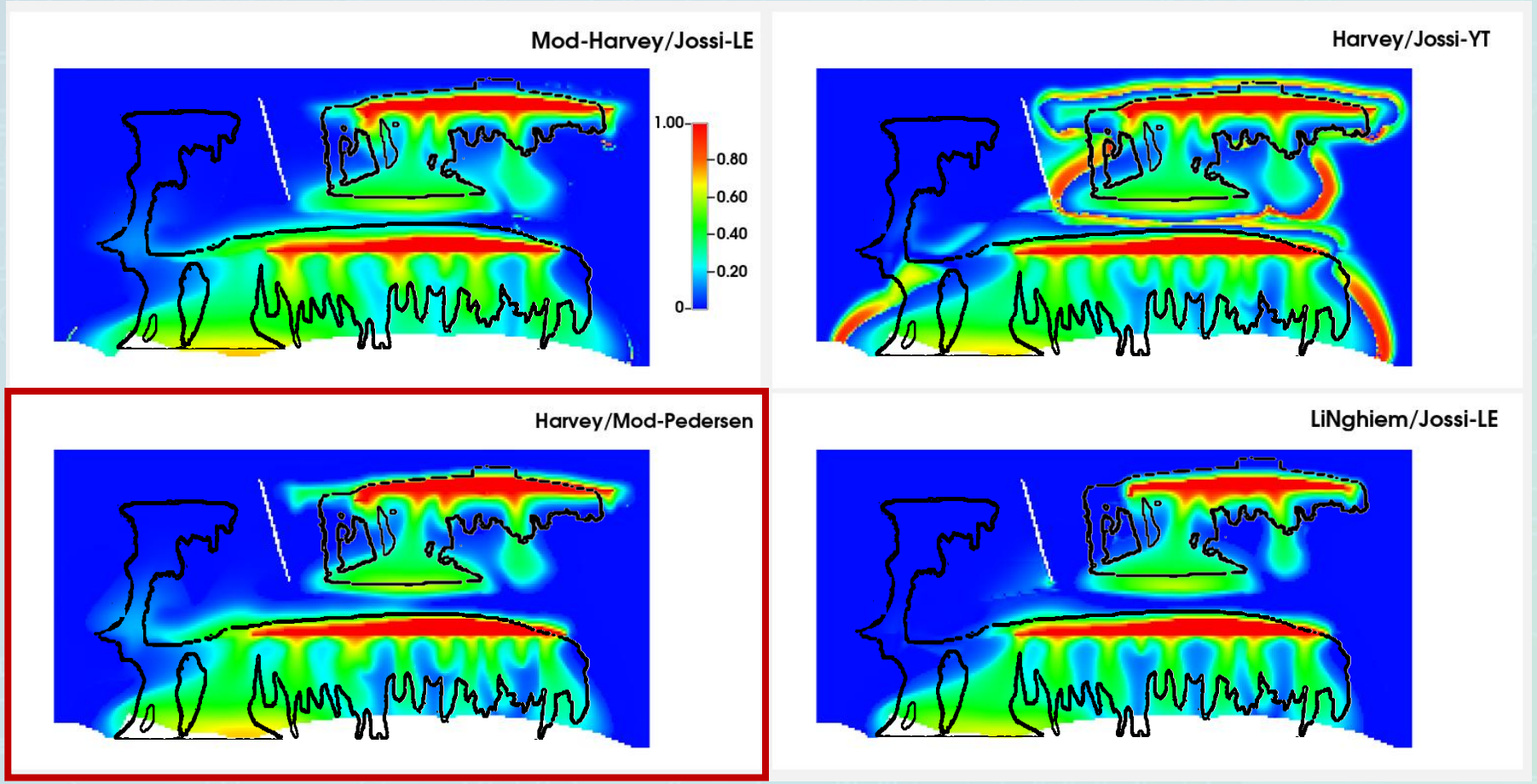




SIMULATION RESULTS

B) The validation of the simulation model

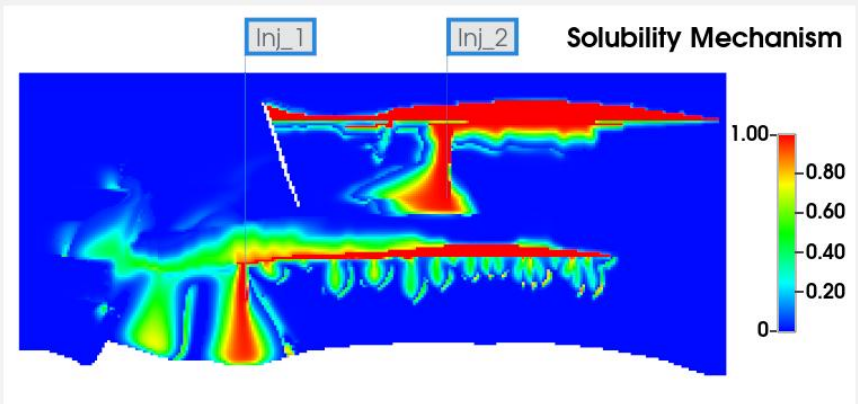
Comparison numerical results of gas Mole Fraction of CO_2 after 24 about hours

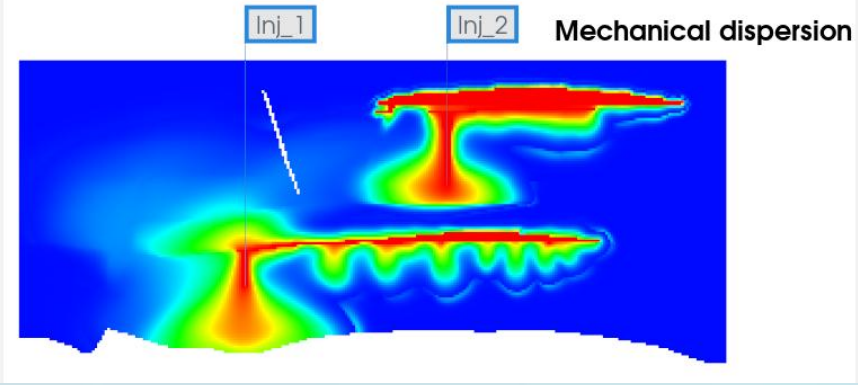


SIMULATION RESULTS

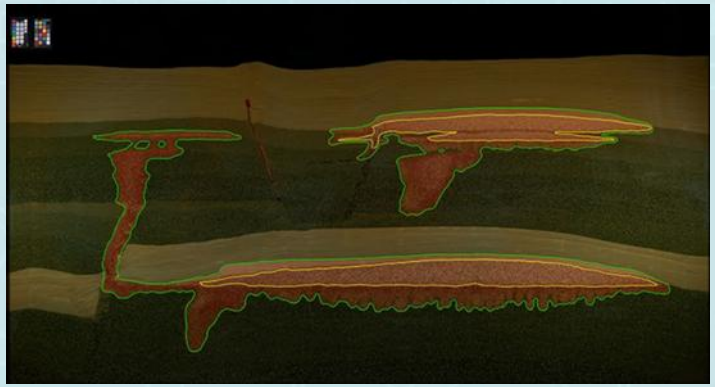
C) Mechanism of the simulation model:

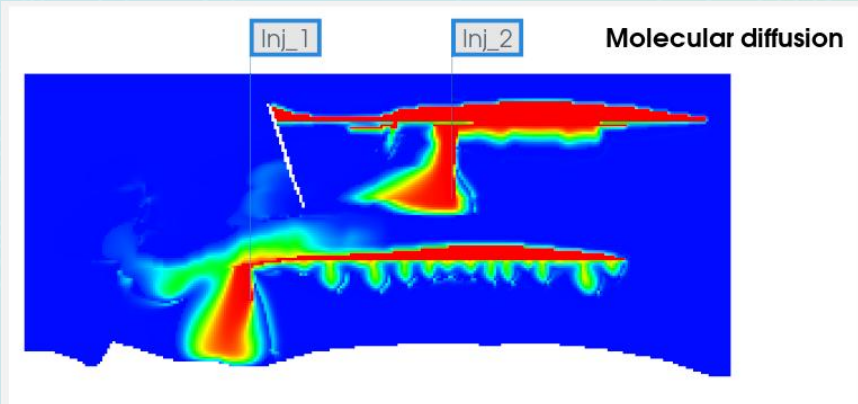
The gas mole fraction of CO_2 after 5 about hours

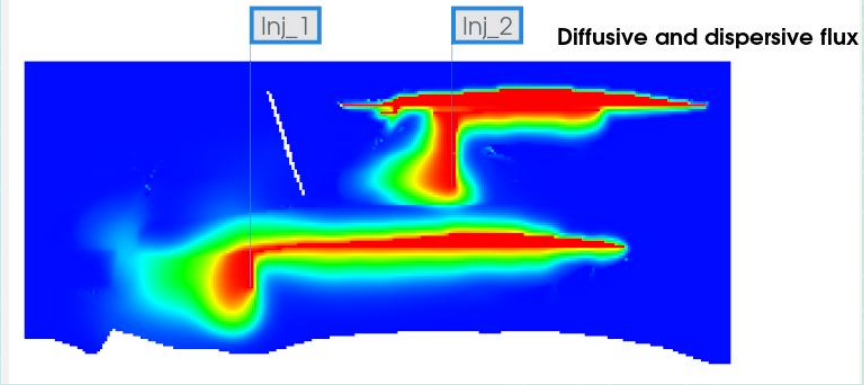




Laboratory spatial distribution of CO_2



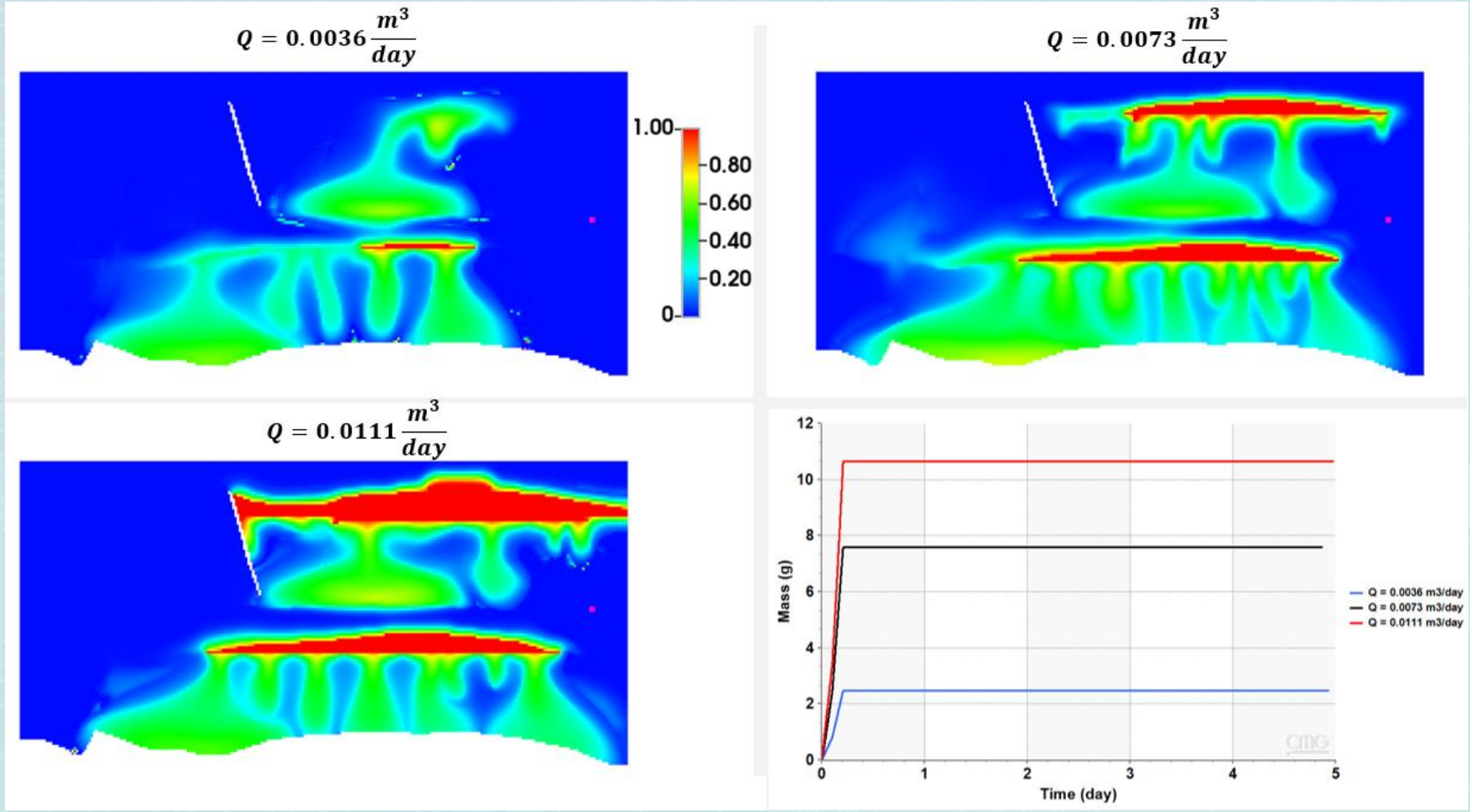




SIMULATION RESULTS

D) Sensitivity analysis of volumetric mass flow:

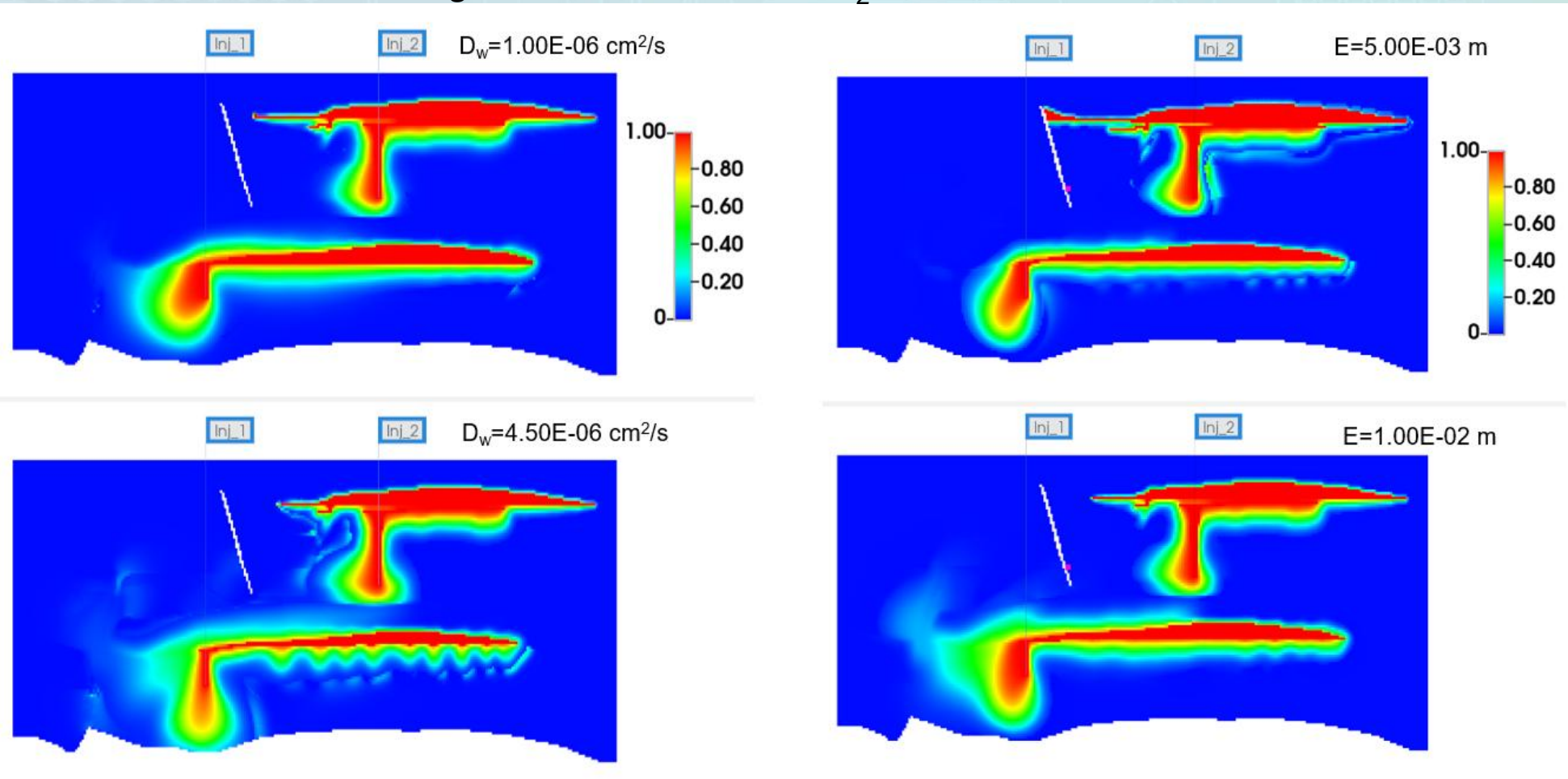
The gas mole fraction of CO_2 after 5 about hours



SIMULATION RESULTS

D) Sensitivity analysis of diffusion *(D_w)* and dispersion constants *(E)*:

The gas mole fraction of CO_2 after 5 about hours



CONCLUSIONS

- In CCUS project modeling, the choice of the solubility model for estimating the amount of CO_2 dissolved in water is a critical factor because, the results can be overestimated by up to 35% or underestimated by up to 47%.

- The Harvey solubility model and the modified Pedersen correlation, used in the simulation, provide the best prediction for the spatial distribution of CO_2, with results close to the experimental data.

- The sensitivity analysis show that molecular diffusion and dispersion have different effects on finger formation. An increase in the diffusion constant of CO_2 in water increase finger. On the other hand, an increase in the constant of dispersivity predominantly acts as a mixing mechanism, smoothing concentration gradients and delaying finger formation.

Thank you!!

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Additional information

Viscosity correlations: Jossie-Stiel-Thodos (1962)

$$[(\mu - \mu_o) \cdot \xi + 1.0e-4]^{\frac{1}{4}} = coef(1) + coef(2) \cdot dr + coef(3) \cdot dr^2 + coef(4) \cdot dr^3 + coef(5) \cdot dr^4$$

where

μ = phase viscosity, cp

μ_o = low-pressure fluid viscosity, cp, calculated internally from the Herning-Zipperer and Yoon-Thodos formulas

$$\xi = tc^{\frac{1}{6}} / \left(mw^{\frac{1}{2}} \cdot pc^{\frac{2}{3}} \right)$$

tc = fluid pseudo-critical temperature, deg K

mw = fluid molecular weight, g/gmol;

pc = fluid pseudo-critical pressure, atm

dr = fluid reduce-molar density (= den * vc);

den = fluid molar density, kmol/m^3;

Yoon and Thodos correlation (1970)

$\mu(low,i)$ = (4.610 * Tr * *0.618 - 2.040 * exp (-0.449 * Tr)

+ 1.94 * exp (-4.058 * Tr) + 0.1 * 10 * * (-4) / μp

where Tr = $Tabs$ / Tc is the reduced temperature of the component and μp is the viscosity parameter μp = (Tc / (M * *3 * Pc * *4)) * *4)) * * (1/6). Here Tc is in K, Pc in atm, M in g/gmol and $\mu(low,i)$ is given in centipoise by this formula.

Lee-Eakin's correlation (1984)

$\mu(low,mix)$ =

(10 * * (-4) * (17.94 + 0.0321 M) * T * * (3/2)) / (1.8 T + 75.4 + 13.9 * M)

where $T(K)$ is the absolute temperature and M is the average molecular weight of the mixture (g/gmol).

Coefficients	Value
coef (1)	0.1023
coef (2)	0.023364
coef (3)	0.058533
coef (4)	-0.040758
coef (5)	0.0093324

Additional information

Viscosity correlations: Pedersen (1984)

$$\frac{\mu_{mix}(P,T)}{\mu_o(P_o,T_o)} = \left(\frac{T_{c,mix}}{T_{c,o}}\right)^{-1/6}\left(\frac{P_{c,mix}}{P_{c,o}}\right)^{2/3}\left(\frac{MW_{mix}}{MW_o}\right)^{1/2}\left(\frac{a_{mix}}{a_o}\right)$$

where

- μ = Viscosity
- T_c = Critical temperature
- P_c = Critical pressure
- MW = Molecular weight
- a = Rotational coupling coefficient

The mixture critical temperature and pressure are calculated using mixing rules that are a function of the component critical temperatures and pressures, and mole fractions. The molecular weight of the mixture is determined from:

$$MW_{mix} = coef(1) \times \left(MW_w^{coef(2)} - MW_n^{coef(2)}\right) + MW_n$$

where MW_w is the weight fraction averaged molecular weight, and MW_n is the mole fraction averaged molecular weight.

The rotational coupling coefficient is calculated as follows:

$$a = 1 + coef(3) \times \rho_r^{coef(4)} MW^{coef(5)}$$

where ρ_r is the reduced density of the reference substance.

Coefficients	Pedersen	Pedersen modify
coef (1)	0.291	0.0001304
coef (2)	1	2.303
coef (3)	7.747E-05	0.007378
coef (4)	4.265	1.847
coef (5)	0.8579	0.5173

Additional information

Salinity

Irrespective of the Henry constant correlation, the effect of salinity on is calculated as described in *Cramer (1982):*

$$\log_{10}\left(\frac{H_{salt,i}}{H_i}\right) = k_{salt,i}\, m_{salt}$$

$H_{salt,i}$	=	Henry's constant of component i in brine (salt solution)
H_i	=	Henry's constant of component i at zero salinity
$k_{salt,i}$	=	salting-out coefficient for component i
m_{salt}	=	molality of the dissolved salt (mol/kg H_2O)

Cramer, S.D., "The Solubility of Methane, Carbon Dioxide and Oxygen in Brines from 0o to 300oC", US Bureau of Mines, Report No. 8706, USA, 16 pp., (1982)