AMPHOS 21
SCIENTIFIC AND STRATEGIC ENVIRONMENTAL CONSULTING

CO2 Storage Trapping Mechanisms Quantification

COMSOL
CONFERENCE
ROTTERDAM2013

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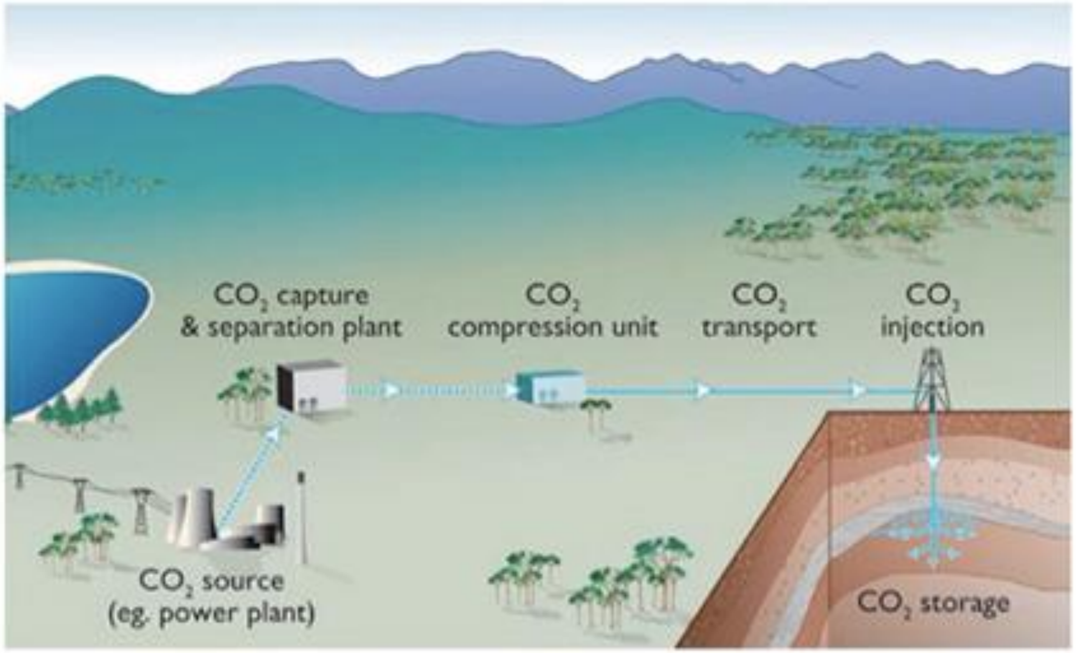
CO2 storage

- The capture and storage of CO_2 in deep geological formations is one of the proposed solutions to reduce CO_2 emissions to the atmosphere.

CARBON CAPTURE AND STORAGE (CCS) PROCESS



Source: Cooperative Research Center for Greenhouse Gas Technologies (CO2CRC)

CO2 storage

- CO_2 is injected as a supercritical fluid deep below a confining geological formation that prevents its return to the atmosphere.

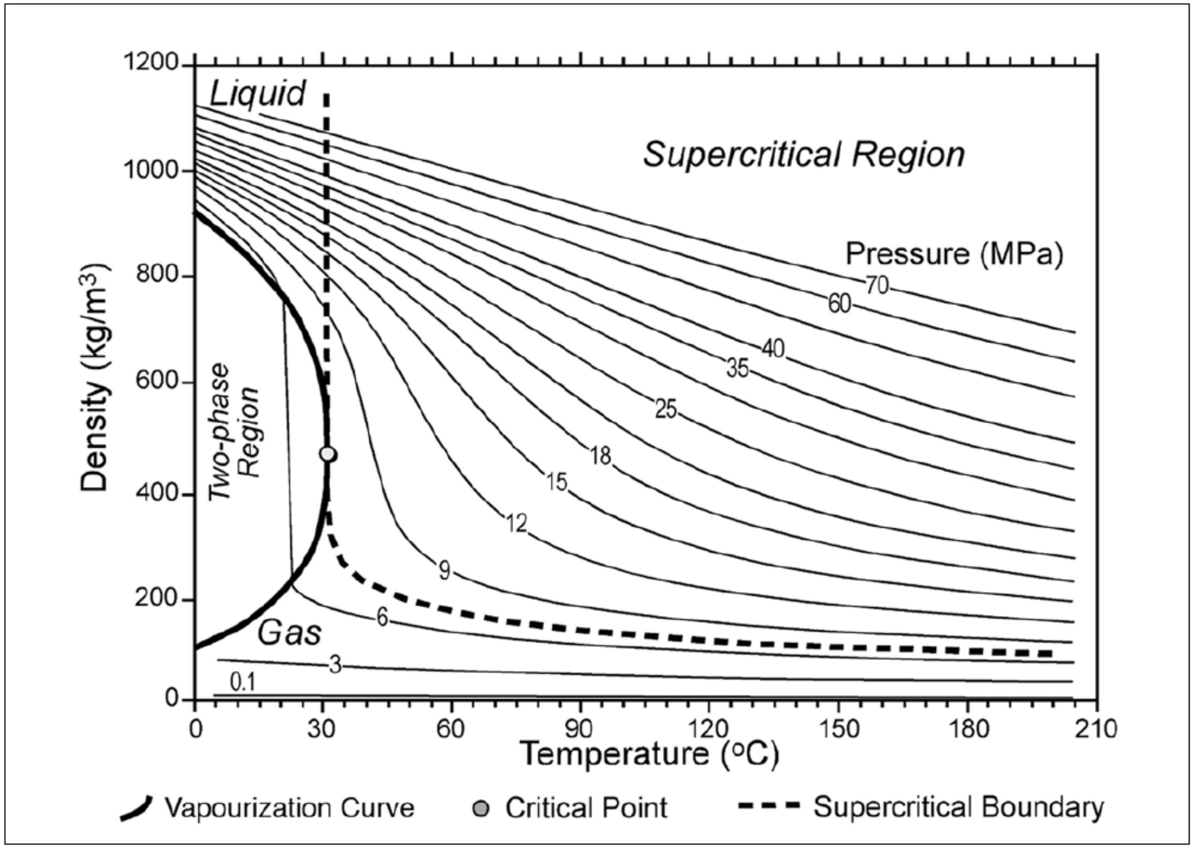
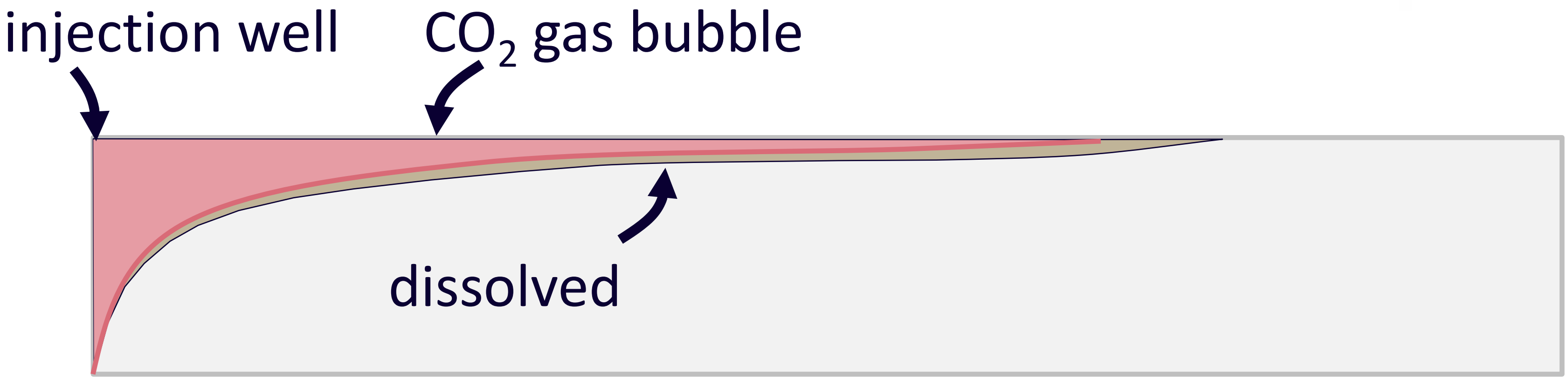


Figure AI.2 Variation of CO_2 density as a function of temperature and pressure (Bachu, 2003).

CO2 storage

- Four trapping mechanisms are expected, which are of increasing importance through time (1) structural, (2) residual saturation, (3) dissolution, and (4) mineral trapping.



CO2 storage

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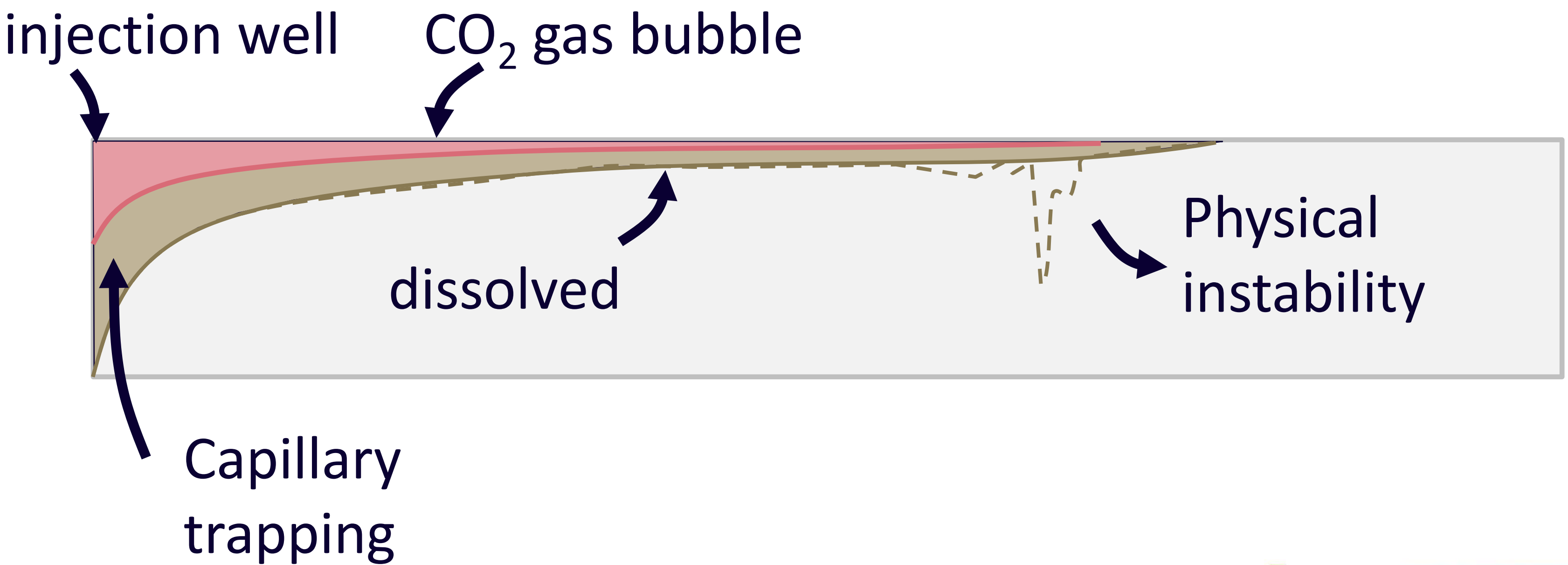


injection well

CO_2 gas bubble

dissolved

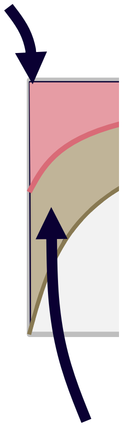
Physical instability

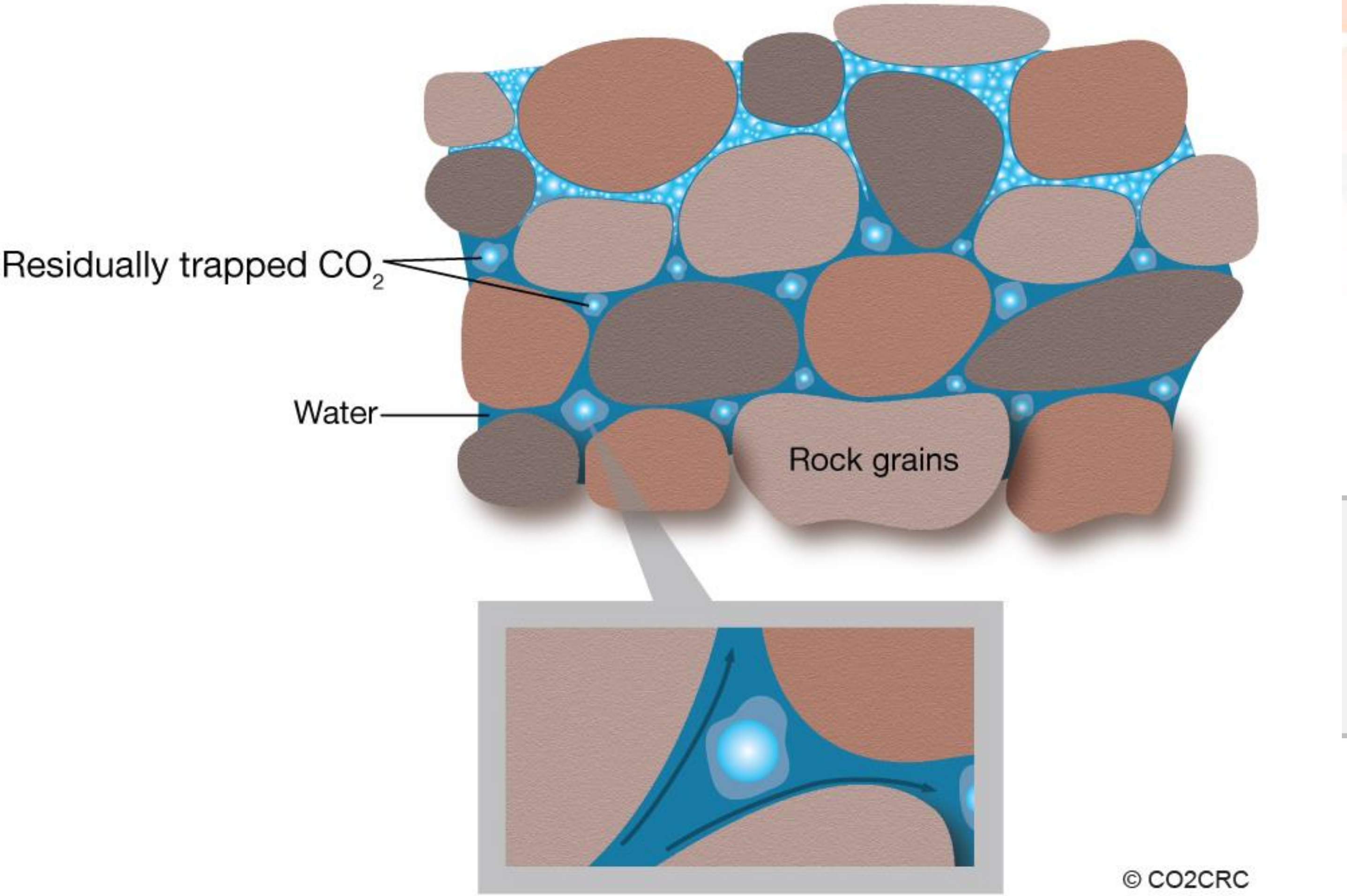
Capillary trapping

CO2 storage

- Fou
  incr
  resi
  trap

injecti

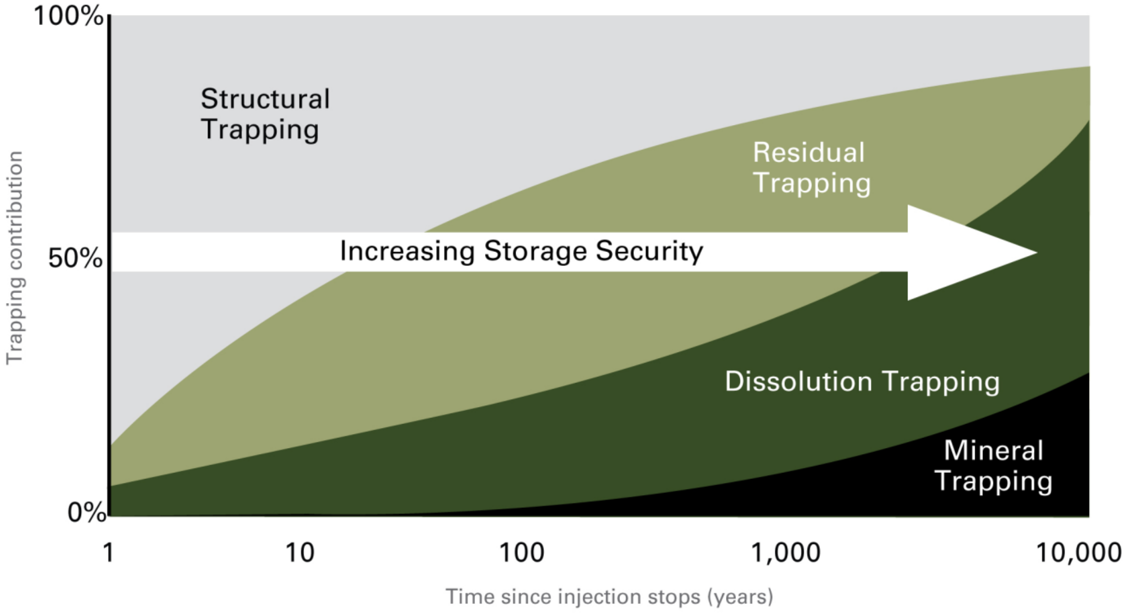




Source: Cooperative Research Centre for Greenhouse Gas Technologies (CO2CRC)

CO2 storage

- The prediction of the mass of CO_2 stored through time in storage systems is an essential parameter in the pre-injection assessment of a geological storage. For safety reasons, it is relevant to know the mass of CO_2 trapped under these different trapping mechanisms.



Source: Intergovernmental Panel on Climate Change, 2008

Objective

- Identify and quantify the different Co2 trapping mechanisms in a saline aquifer

Mathematical description

mass species conservation

$$\partial_t(\phi s_\alpha \rho_\alpha m_\alpha^\kappa M^\kappa) = -\nabla(\boldsymbol{q}_{\boldsymbol{\alpha}} \rho_\alpha m_\alpha^\kappa M^\kappa - \phi s_\alpha \rho_\alpha \boldsymbol{D}_{\boldsymbol{\alpha}} \nabla(m_\alpha^\kappa M^\kappa)) + Q_\alpha^\kappa + T_\alpha^\kappa$$

$$\alpha = l, g \qquad \kappa = CO_2, w$$

Darcy's law

$$\boldsymbol{q}_{\boldsymbol{\alpha}} = -\frac{k k_{r,\alpha}}{\mu_\alpha}(\nabla p_\alpha - \rho_\alpha \boldsymbol{g})$$

Mathematical description

[1] Brooks, R. H. & Corey, A. T., 1964. Hydraulic properties of porous media. Hydrology Papers, Colorado State University, Issue March.

sum of phase saturations

$$s_g + s_l = 1$$

pressure equilibria

$$p_c = p_g - p_l$$

constitutive relations

retention curve

effective saturation

$$s_e = \frac{s_l - s_l^r}{1 - s_l^r - s_g^r}$$ [1]

capillary pressure

$$p_c = p_t s_e^{-1/\omega}$$ [1]

relative liquid permeability

$$k_l^r = s_e^{\frac{2+3\omega}{\omega}}$$ [1]

relative gas permeability

$$k_g^r = (1 - s_e)^2 \left(1 - s_e^{\frac{2+\omega}{\omega}}\right)$$ [1]

Mathematical description

constitutive relations

gas properties

volume $$V_g = V_g\left(p_g, T, m_l^{CO_2}, m_s^{NaCl}\right)$$ [2]

phase composition $$\overline{m}_l^{CO_2} = \overline{m}_l^{CO_2}\left(p_g, T, V_g, m_s^{NaCl}\right)$$ [2]

density $$\rho_g = \frac{M^{CO_2}}{V_g}$$ [3]

viscosity $$\mu_g = \mu_g\left(p_g, T, m_l^{CO_2}, m_s^{NaCl}\right)$$ [4]

enthalpy $$h_g = h_g\left(p_g, T, m_l^{CO_2}, m_s^{NaCl}\right)$$ [5]

[2] Spycher, N. & Pruess, K., 2005. CO2-H2O mixtures in the geological sequestration of CO2. II. Partitioning in chloride brines at 12--100°C and up to 600 bar. Geochimica et Cosmochimica Acta, 69(13), pp. 3309-3320.

[3] Nickalls, R., 1993. A new approach to solving the cubic: Cardan's solution revealed. The Mathematical Gazette, pp. 354-359.

[4] Altunin, V. & Sakhabetdinov, M., 1972. Application of orthogonal expansions to construct a single equation of state for substances on the basis of various experimental data by means of a digital computer(Orthogonal polynomials for computerized construction of equations of state for substances under thermodynamic restrictions). Teplofizika Vysokikh Temperatur, Volume 10, pp. 1195-1202.

[5] Redlich, O. & Kwong, J., 1949. On the Thermodynamics of Solutions. V. An Equation of State. Fugacities of Gaseous Solutions. Chemical Reviews, 44(1), pp. 233-244.

Mathematical description

constitutive relations

liquid properties

density $\rho_l = \rho_l(\rho_b, \rho_{CO_2})$ [6]

$\rho_b = \rho_b(p_l, T, m_l^{CO_2}, m_s^{NaCl})$ [7]

$\rho_{CO_2} = \rho_b(p_l, T, m_l^{CO_2}, m_s^{NaCl})$ [6]

viscosity $\mu_g = \mu_g(p_l, T, m_l^{CO_2}, m_s^{NaCl})$ [8]

enthalpy $h_g = h_g(p_l, T, m_l^{CO_2}, m_s^{NaCl})$ [9]

[6] Garcia, J. E., 2001. Density of aqueous solutions of CO2.

[7] Haas, J., 1976. Physical Properties of the Coexisting Phases and Thermochemical Properties of the H2O Component in Boiling NaCl Solutions. USGS Bulletin 1421-A, Washington, DC, p. 73.

[8] Phillips, S. L. et al., 1981. A technical databook for geothermal energy utilization. s.l.:Lawrence Berkeley Laboratory, University of California.

[9] Pruess, K., 2005. ECO2N: A TOUGH2 fluid property module for mixtures of water, NaCl, and CO2. Lawrence Berkeley National Laboratory Report LBNL-57592, Berkeley, CA.

Formulation used

In this work it will be assumed that water miscibility in gas phase is negligible ($m_g^w = 0$). This is quite reasonable since water dissolution is on the order of tan per mil (Spycher & Pruess, 2005). These restricts the system Eq.[1] to three equations.

For the derivation of the equations notice the following relationships:

$$\sum_{c=CO_2,w} M^c m_\alpha^c = 1$$

$$\sum_{\alpha=l,g} T_\alpha^c = 0$$

$$\sum_{c=CO_2,w} Q_\alpha^c = Q_\alpha$$

Formulation used

The linear combination of the three equations done is the following. A total mass conservation

Eq.[a] is obtained by summing over all the phases and components.

$$\partial_t\left(\phi s_l \rho_l + \phi s_g \rho_g\right) = -\nabla\left(\boldsymbol{q_l}\rho_l + \boldsymbol{q_g}\rho_g\right) + Q_g + Q_l \qquad [a]$$

A CO2 equation mass conservation Eq.[6b] is obtained by summing the Co2 chemical component equations over the two phases.

$$\partial_t\left(\phi s_l \rho_l m_l^{CO_2} M^{CO_2} + \phi s_g \rho_g\right) = -\nabla\left(\boldsymbol{q_l}\rho_l m_l^{CO_2} M^{CO_2} + \boldsymbol{q_g}\rho_g - \rho_l \boldsymbol{D_l}\nabla\left(m_l^{CO_2} M^{CO_2}\right)\right)$$
$$+Q_g^{CO_2} + Q_l \qquad [b]$$

Finally, subtracting the equation Eq.[6a] times $m_l^{CO_2} M^{CO_2}$ to the liquid-CO2 equation we find Eq.[6c]:

$$\phi s_l \rho_l \partial_t\left(m_l^{CO_2} M^{CO_2}\right) - m_l^{CO_2} M^{CO_2} \partial_t\left(\phi s_g \rho_g\right) =$$
$$-\boldsymbol{q_l}\rho_l \nabla\left(m_l^{CO_2} M^{CO_2}\right) + m_l^{CO_2,*} M^{CO_2} \nabla\left(\boldsymbol{q_g}\rho_g\right) + \nabla\left(\rho_l \boldsymbol{D_l}\nabla\left(m_l^{CO_2} M^{CO_2}\right)\right)$$
$$-\boldsymbol{q_l}\rho_l M^{CO_2}\left(m_l^{CO_2} - m_l^{CO_2,*}\right) + Q_l^{CO_2} + T_l^{CO_2} \qquad [c]$$

where $m_l^{CO_2,*}$ is the prescribed concentration of the inflow fluid in the boundaries and $m_l^{CO_2,*} = m_l^{CO_2}$ in the interior domain.

Formulation used

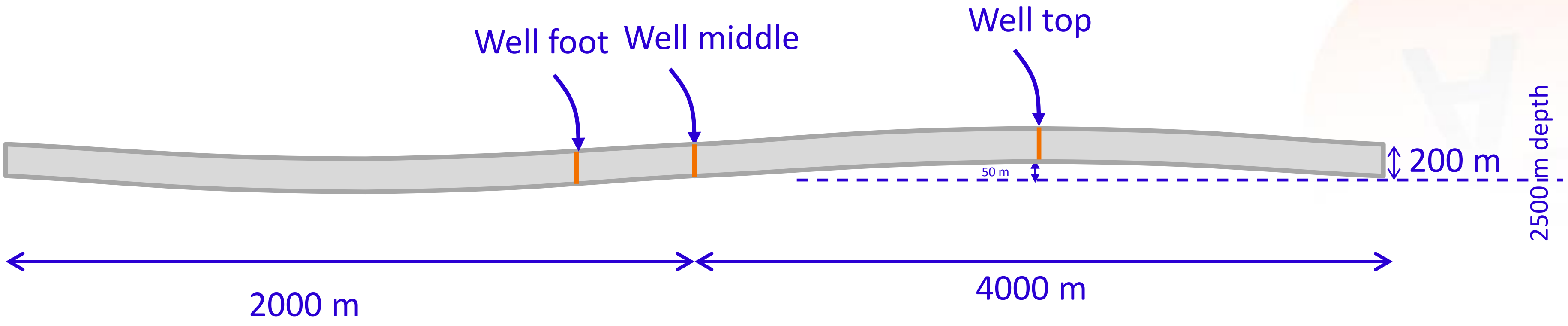
The unknowns for Eq.a, Eq.b, Eq.c chosen are p_l, S_g, $m_l^{CO_2}$ respectively. A conditional kinetic interphase mass transfer is considered.

$$c_1 = \begin{cases} if\,(\,S_g > S_{r,g}), & 1 \\ if\,(\,S_g \leq S_{r,g}), & 0 \end{cases}$$

$$c_2 = \begin{cases} if\,\left(m_l^{CO_2} > \overline{m}_l^{CO_2}\right), & 0 \\ if\,\left(m_l^{CO_2} \leq \overline{m}_l^{CO_2}\right), & 1 \end{cases}$$

$$T_l^{CO_2} = \phi S_l \rho_l k_{kin} \left(\, c_1\left(m_l^{CO_2} - \overline{m}_l^{CO_2}\right) + (1 - c_1)c_2\left(m_l^{CO_2} - \overline{m}_l^{CO_2}\right)\right)$$

2D synthetic dome problem



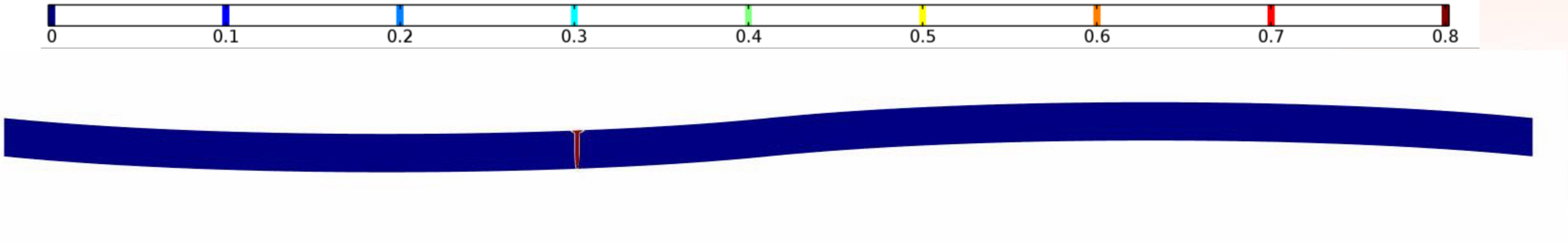
ϕ	0.15	$(m^3 \cdot m^{-3})$
$d_l = d_m$	40	(m)
κ	1e-11	(m^2)
p_t	1e5	(Pa)
ω	2	$(-)$
s_l^r	0.05	$(m^3 \cdot m^{-3})$
s_g^r	0.1	$(m^3 \cdot m^{-3})$
m_s^{NaCl}	1	$(mol \cdot kg^{-1})$

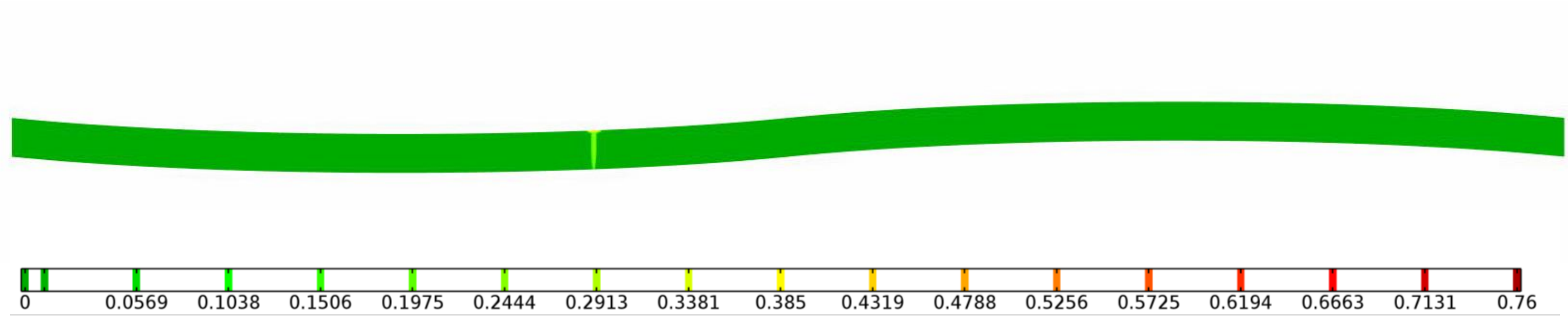
Pumping rate

$$Q_g^{CO_2} = 0.3\ (kg \cdot s^{-1})\ \text{(during 180 days)}$$

Results (well foot)

Co2 molality on liquid

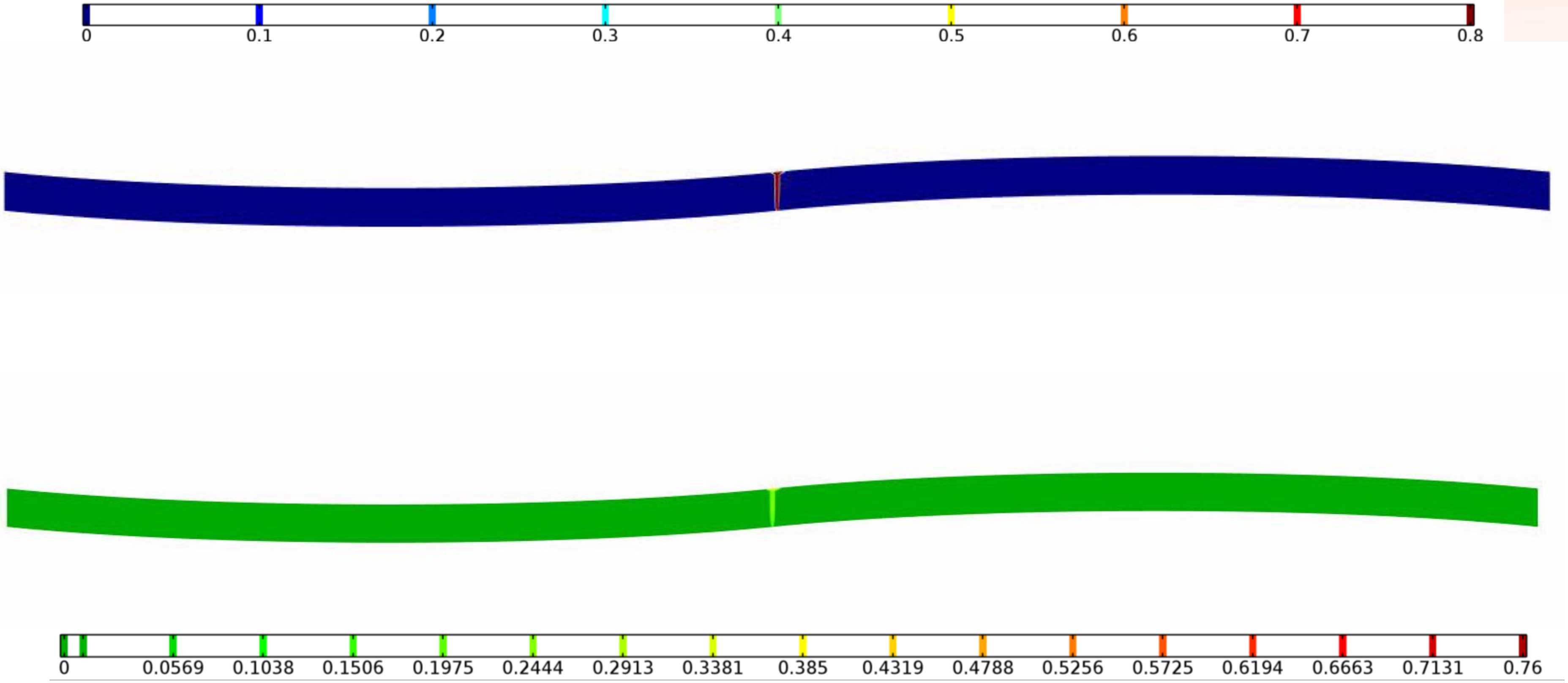




Gas saturation

Results (well middle)

Co2 molality on liquid



Gas saturation

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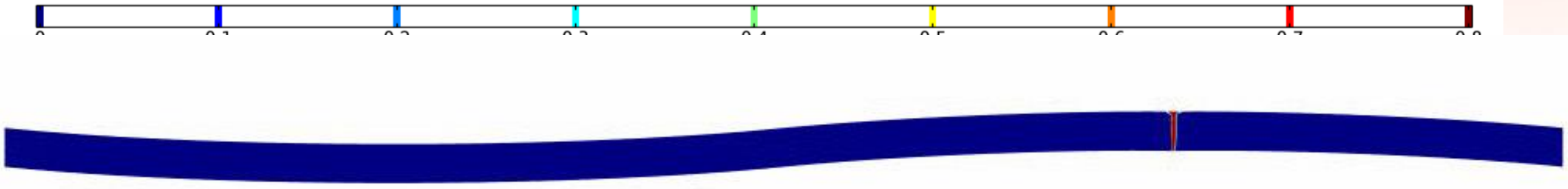
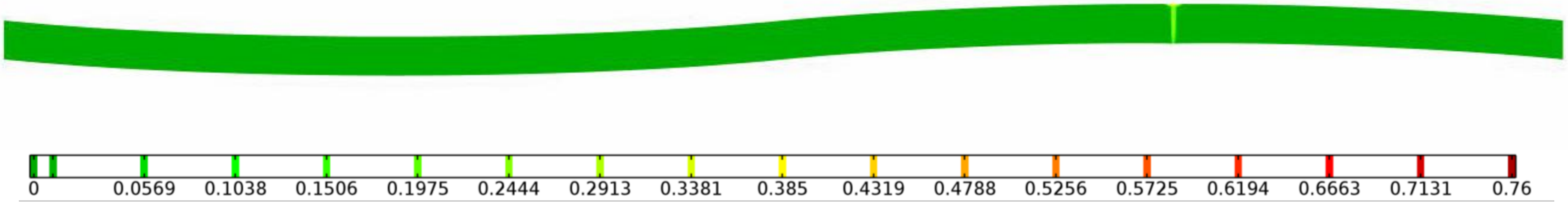
Results (well top)

Co2 molality on liquid

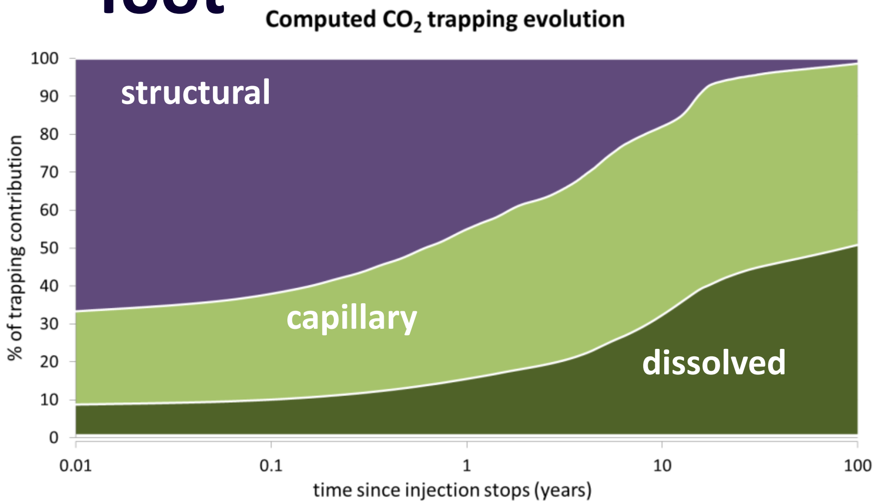




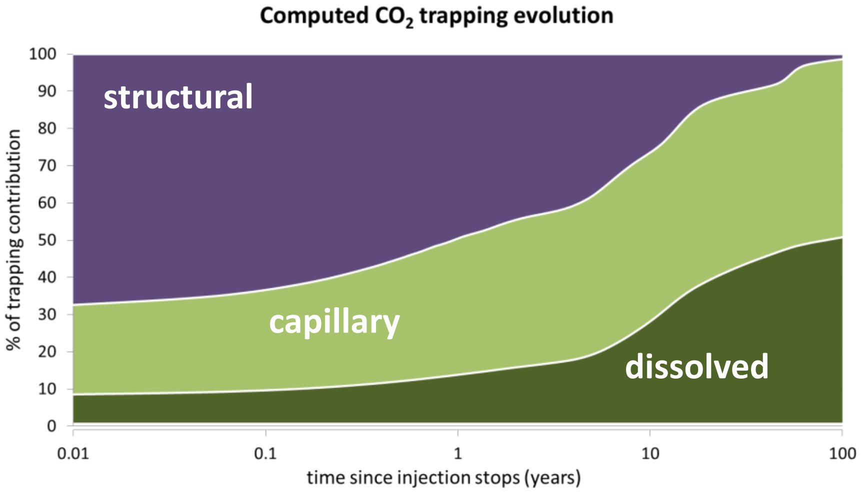
Gas saturation

Results

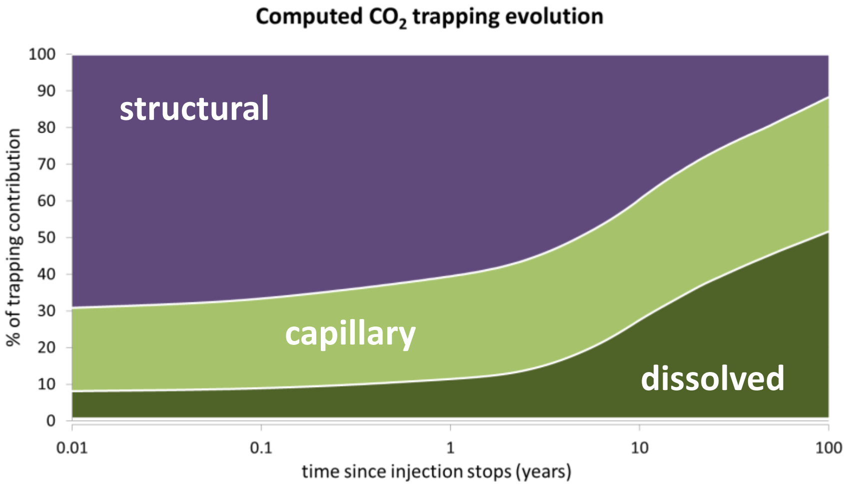
foot



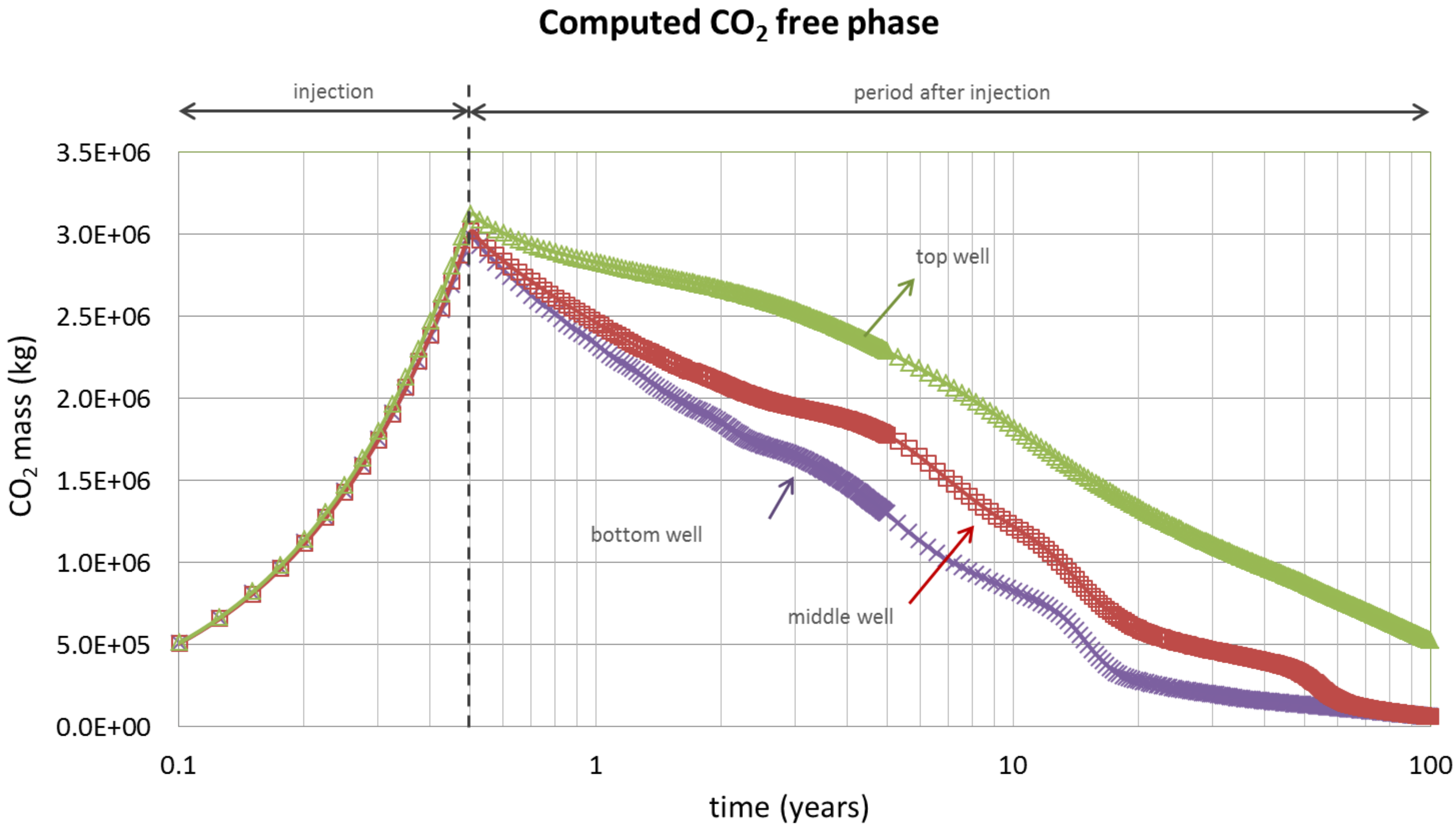
middle



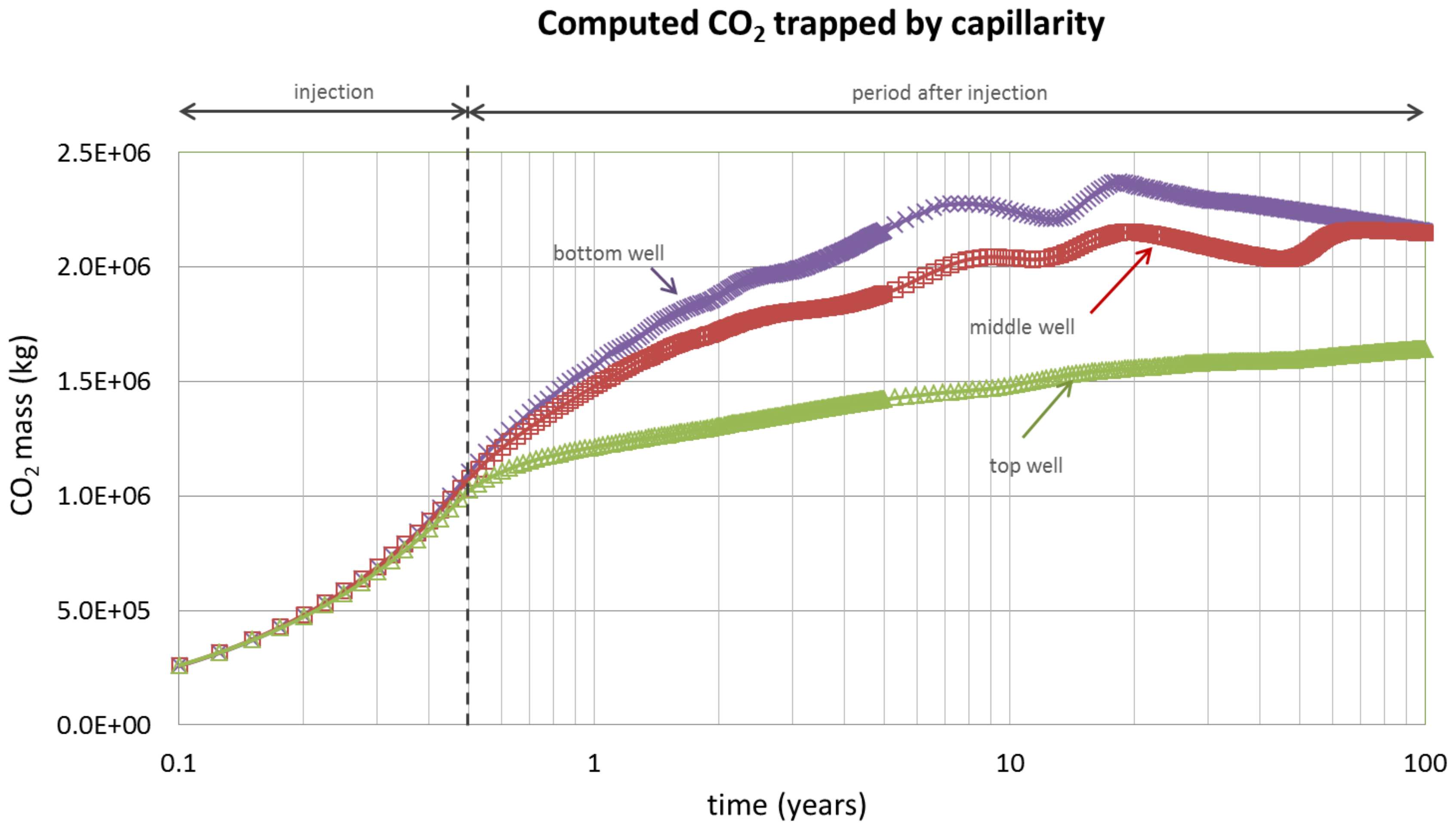
top



Results


Computed CO_2 free phase
injection
period after injection
3.5E+06
3.0E+06
2.5E+06
2.0E+06
1.5E+06
1.0E+06
5.0E+05
0.0E+00
CO_2 mass (kg)
0.1
1
10
100
time (years)
top well
bottom well
middle well

Results



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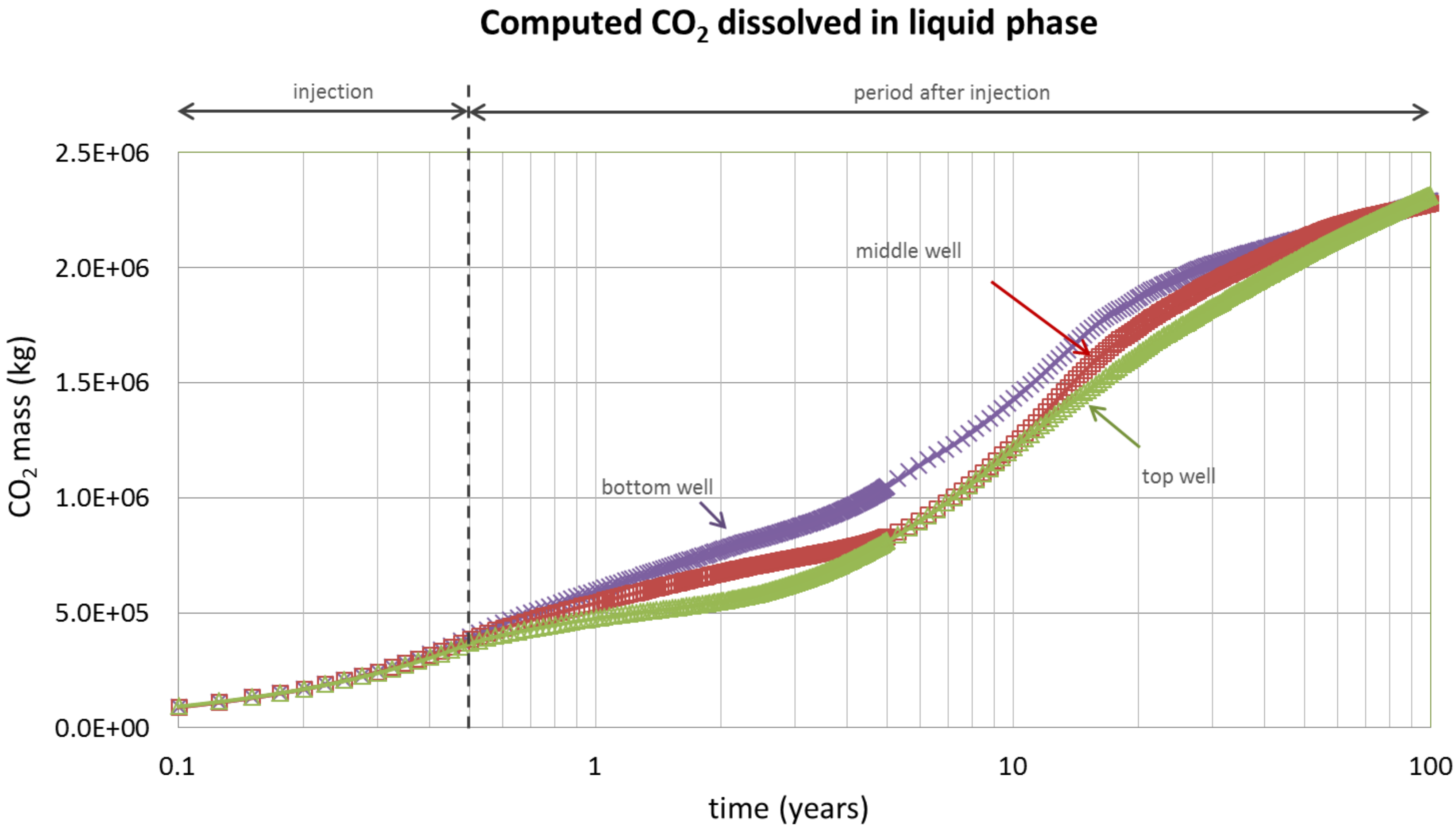
Results


Computed CO2 dissolved in liquid phase
injection
period after injection
2.5E+06
2.0E+06
1.5E+06
1.0E+06
5.0E+05
0.0E+00
CO2 mass (kg)
middle well
bottom well
top well
0.1
1
10
100
time (years)

Conclusions

- Expected Co2 storage systems can be reproduced in a model
- Quantification of this systems is numerically feasible
- The position of the well in a synclinal formation affects the trapping mechanisms.

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