Experimental Investigation of Enhanced CO_2 Mass Transfer in Water-saturated Porous Media

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Introduction

Carbon Dioxide (CO_2) is one of the major greenhouse gases blamed for causing global warming. The dissolution of CO_2 increases the density of brine. This density increase together with temperature fluctuations in the aquifer (which may be only partially compensated by pressure gradients) destabilize the CO_2-brine interface and accelerate the transfer rate of CO_2 into the brine by natural convection. The occurrence of natural convection significantly increases the total storage rate in the aquifer since convection currents bring the fresh brine to the top. Hence, the quantification of CO_2 dissolution in water andunderstanding the transport mechanisms are crucial in predicting the potential and long-term behavior of CO_2 in aquifers. Furthermore, accurate modeling of the experimental data is required to fully understandthe underlying mass transfer mechanisms and to predict the behavior of injected CO_2 in the aquifer.

Mathematical Model

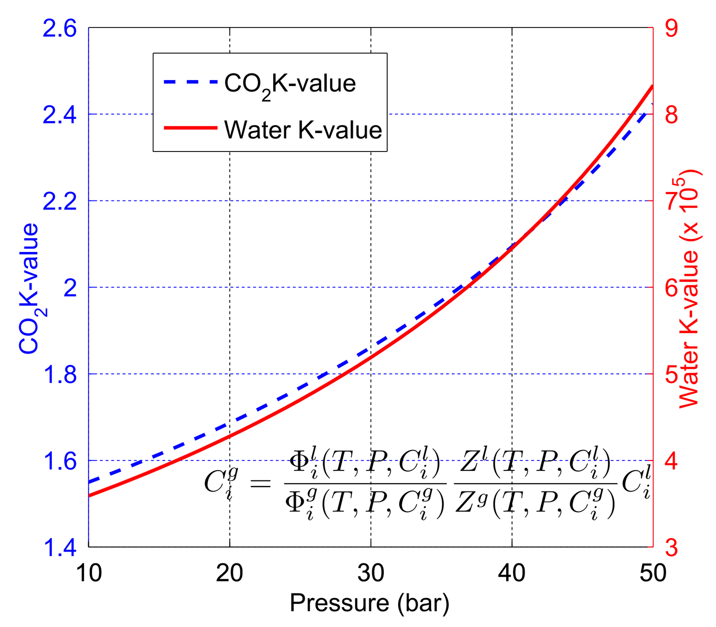
Z

0.245 m

$$-D_i^g \nabla C_i^g = \begin{cases} \frac{P_0 L_{void}}{ZRT\Delta t_0} & t \leq 900[s] \\ 0 & t > 900[s] \end{cases}$$

Gas

$$\frac{\partial C_i^g}{\partial t} + \nabla.\left(-D_i^g \nabla C_i^g\right) = 0$$



$$-D_i^g \nabla C_i^g = 0$$

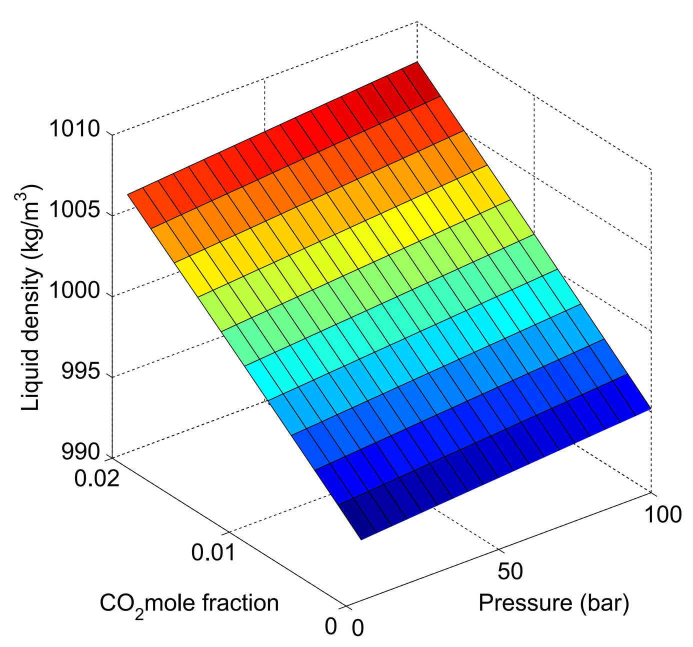
Interface

$$C_i^g = K_i C_i^l$$

0.274 m

$$P = (C_{CO_2}^g + C_{water}^g) ZRT$$

$$-\phi D_i^l \frac{\partial C_i^l}{\partial z} = -D_i^g \frac{\partial C_i^g}{\partial z}$$



Porous media

$$\phi \frac{\partial C_i^l}{\partial t} + \nabla.\left(-\phi D_i^l \nabla C_i^l + u C_i^l\right) = 0$$

$$u = -\frac{\kappa}{\mu}\left(\nabla P + \rho g \nabla z\right)$$

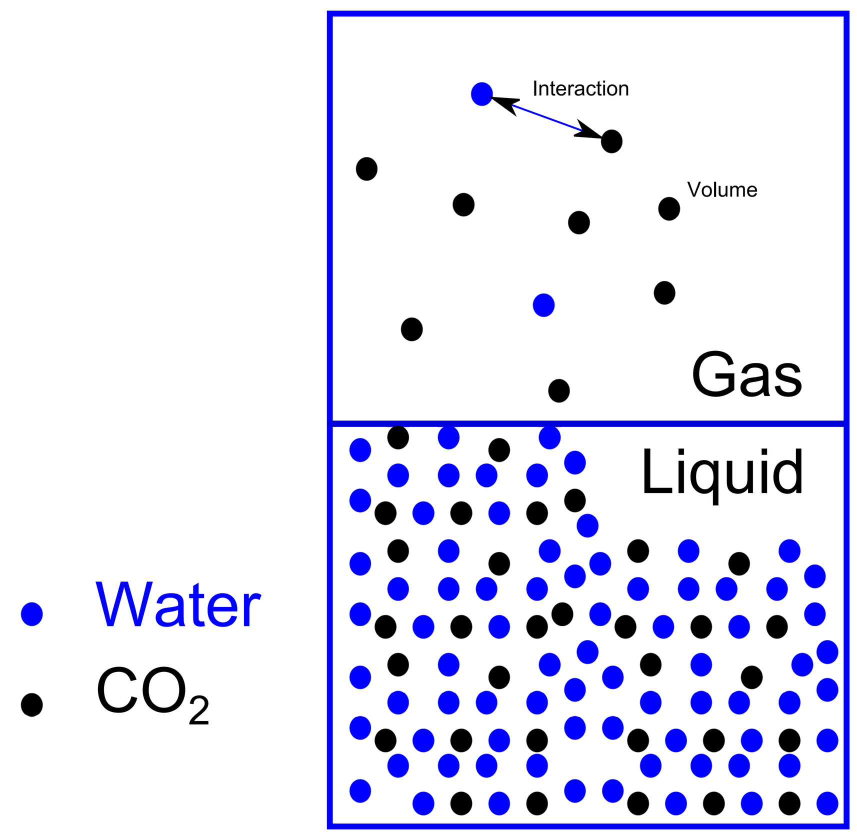
$$\frac{\partial}{\partial t}(\rho\phi) + \nabla.(\rho u) = 0$$

$$-\phi D_i^l \nabla C_i^l + u C_i^l = 0$$

0.076 m

r

Phase Equilibria



Equilibrium Constraint

$$y_i \Phi_i^g (y_i, T, P) = x_i \Phi_i^L (x_i, T, P)$$

Equations

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b) + b(v-b)}$$

- Accurate dedicated model for the phase equilibrium of CO_2-water and CO_2-water-salt exist.
- Dedicated model are not general and extendable.
- We focused on the general cubic equation of states.
- Simple van der Waals mixing rule is not suitable for the attractive term of the PR EOS.
- Correction of Stryjek-Vera on the parameter α that counts for the vapor pressure of each species generates more accurate result for the composition of vapor phase in the VLE calculation than the original PR EOS.
- To model the non-ideality in the liquid phase, NRTL activity coefficient model is used in combination with the modified Harun-Vidal second order mixing rule. We assumed that NRTL parameters are a linear function of temperature.
- The volume shift parameter corrects the EOS predicted liquid density.
- This model is general, easily extendable, computationally efficient, and can be easily tuned to the experimental phase equilibrium and density data.

Objective functions

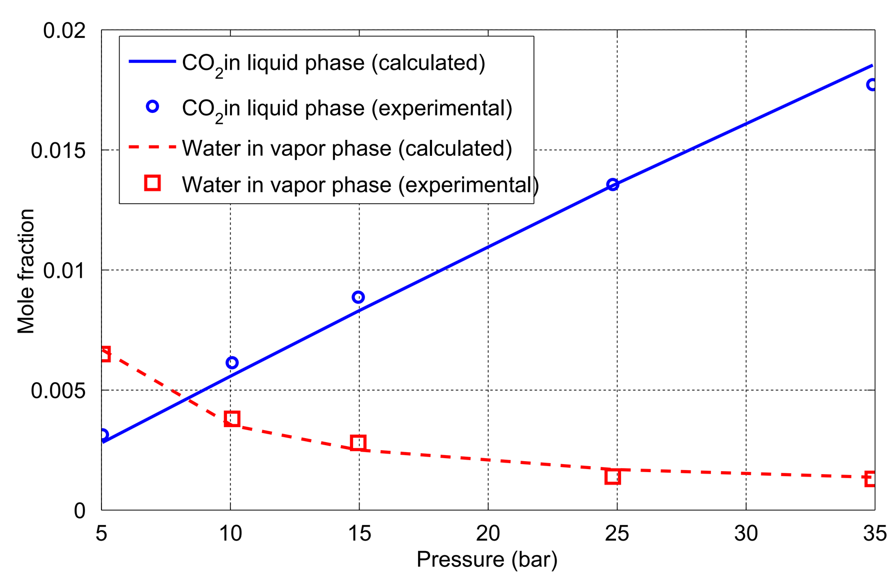
$$OF\left(\Delta G_{12}^0, \Delta G_{12}^1, \Delta G_{21}^0, \Delta G_{21}^1\right) = \frac{100}{N}\left(\sum_{i=1}^{N} \frac{\left|x_{CO_2,i}^{exp} - x_{CO_2,i}^{cal}\right|}{x_{CO_2,i}^{exp}} + \sum_{i=1}^{N} \frac{\left|y_{water,i}^{exp} - y_{water,i}^{cal}\right|}{y_{water,i}^{exp}}\right)$$

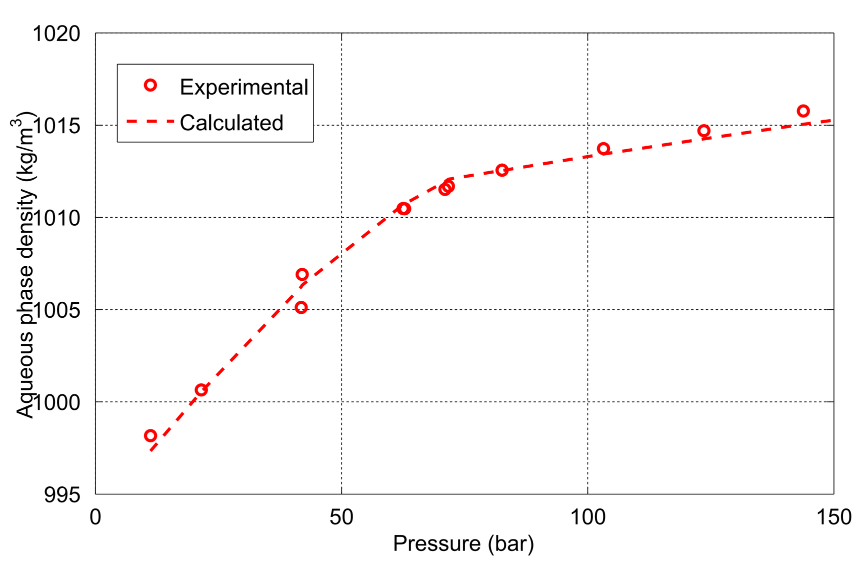
$$\Delta G_{12} = \Delta G_{12}^0 + \Delta G_{12}^1 T,\ \Delta G_{21} = \Delta G_{21}^0 + \Delta G_{21}^1 T$$

$$OF\left(c_{CO_2}^0, c_{CO_2}^1, c_{water}^0, c_{water}^1\right) = \frac{100}{N}\sum_{i=1}^{N}\left(\left|\frac{x_{CO_2,i} M_{CO_2} + x_{water,i} M_{CO_2}}{v_i^{cal}} - \rho_i^{exp}\right| / \rho_i^{exp}\right)$$

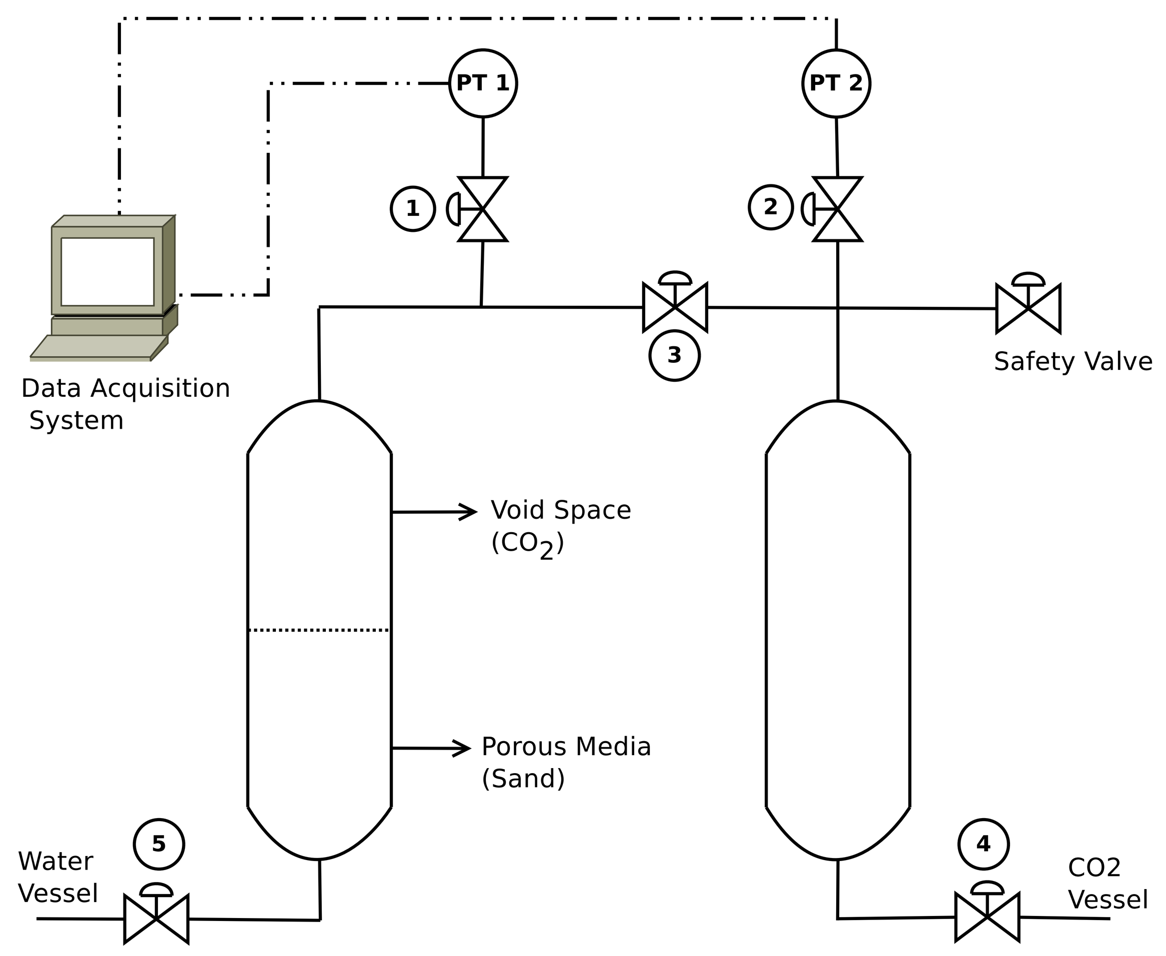
$$c_i = c_i^0 + c_i^1 T$$

Optimization Results

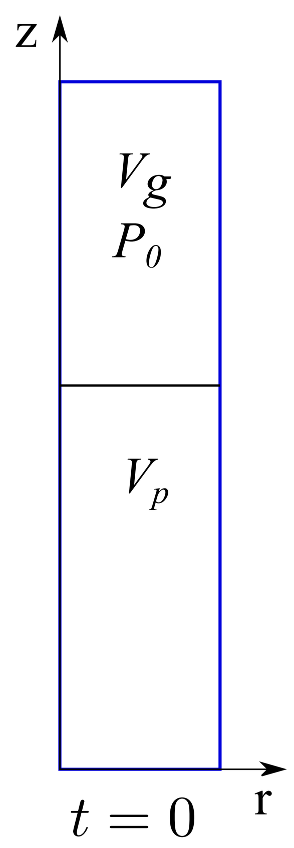




Experimental Set-up



Steady-State Solution



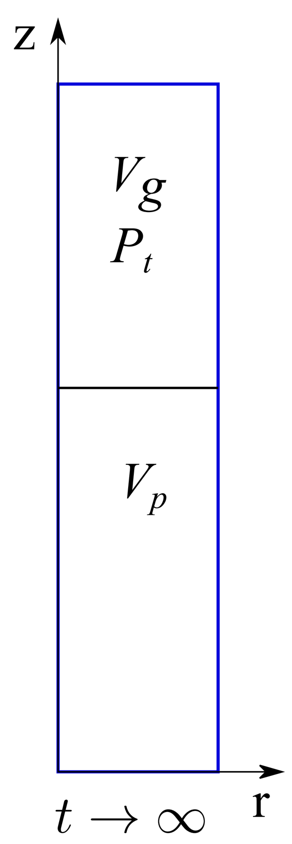
$$N_{i,0} = N_{i,t}$$

$$C_{CO_2,0}^g V_g = C_{CO_2,t}^g V_g + \phi C_{CO_2,t}^l V_p$$

$$\phi C_{water,0}^l V_p = C_{water,t}^g V_g + \phi C_{water,t}^l V_p$$

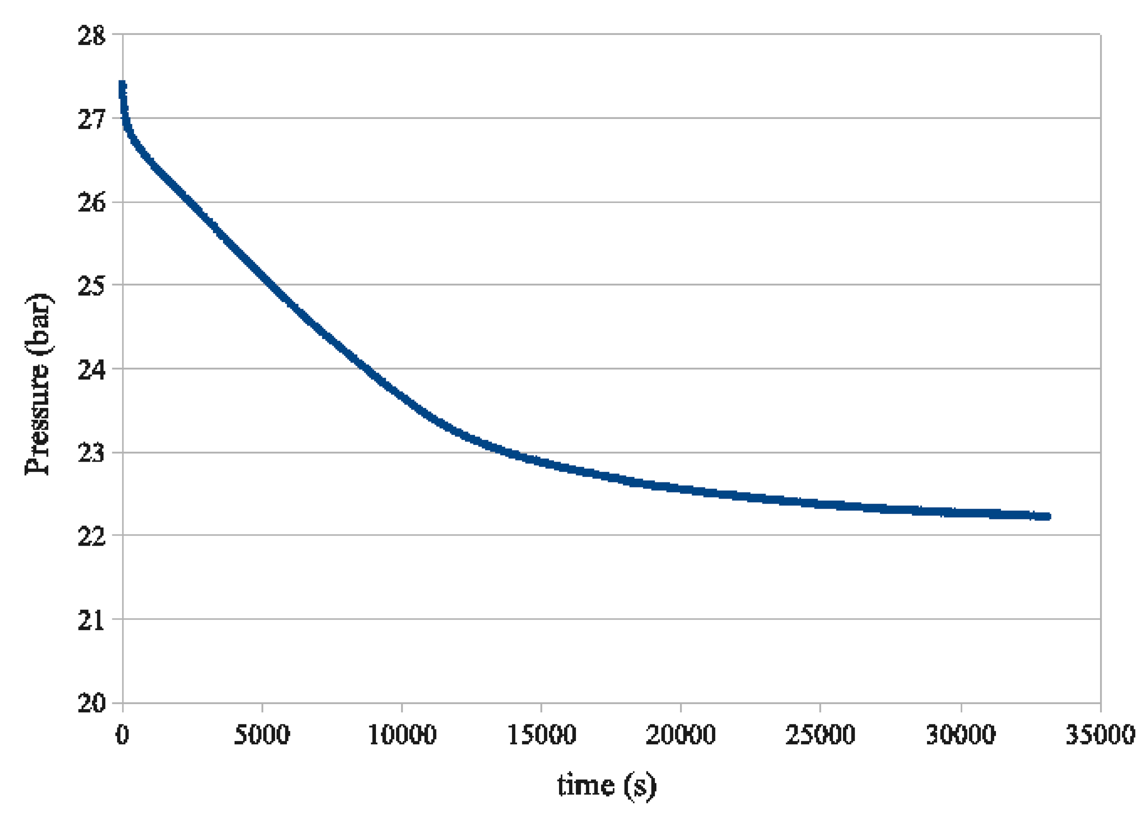
$$C_i^g = \frac{\Phi_i^l(T, P_t, C_i^l)}{\Phi_i^g(T, P_t, C_i^g)} \frac{Z^l(T, P_t, C_i^l)}{Z^g(T, P_t, C_i^g)} C_i^l \qquad i = CO_2,\ water$$

$$P_t = (C_{CO_2,t}^g + C_{water,t}^g) Z^g(T, P_t, C_i^g) RT$$

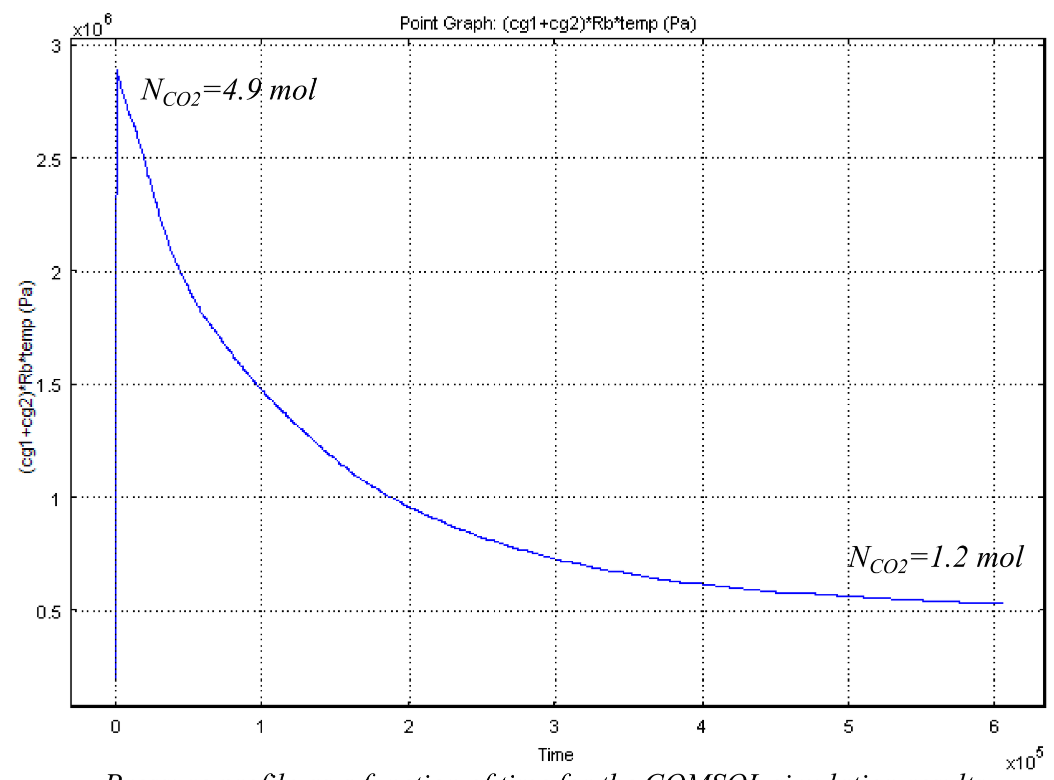


Results

Experimental Results



Model



Pressure profile as a function of time for the COMSOL simulation results