

Sensitivity analysis of CO₂ sequestration in saline aquifers

Zhao Hongjun, Liao Xinwei*, Chen Yanfang and Zhao Xiaoliang

Key Laboratory of Petroleum Engineering, Ministry of Education, China University of Petroleum, Beijing 102249, China

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Abstract: Carbon capture and storage (CCS) technology has been considered as an important method for reducing greenhouse gas emissions and for mitigating global climate change. Three primary options are being considered for large-scale storage of CO₂ in subsurface formations: oil and gas reservoirs, deep saline aquifers, and coal beds. There are very many large saline aquifers around the world, which could make a big contribution to mitigating global warming. However, we have much less understanding of saline aquifers than oil and gas reservoirs. Several mechanisms are involved in the storage of CO₂ in deep saline aquifers, but the ultimate goal of injection of CO₂ into the aquifers containing salt water is to dissolve the CO₂ in the water. So it is important to study the solubility trapping and sensitivity factors of CO₂ in saline aquifers. This paper presents results of modeling CO₂ storage in a saline aquifer using the commercial reservoir simulator ECLIPSE. The objective of this study was to better understand the CO₂/brine phase behavior (PVT properties) and quantitatively estimate the most important CO₂ storage mechanism in brine-solubility trapping. This would provide a tool by performing theoretical and numerical studies that help to understand the feasibility of CO₂ geological storage. A 3-dimensional, 2-phase (water/gas) conceptual reservoir model used finite, homogenous and isothermal formations into which CO₂ is injected at a constant rate. The effects of main parameters were studied, including the vertical to horizontal permeability ratio k_v/k_h , salinity, and residual phase saturations. The results show that the vertical to horizontal permeability ratio has a significant effect on CO₂ storage. Moreover, more CO₂ dissolves in the brine at lower k_v/k_h values.

Key words: CO₂, geologic sequestration, saline aquifer, solubility trapping, numerical simulation

1 Introduction

The concentration of CO₂ in the atmosphere has gradually increased in the last 250 years due to human activities, leading to measurable global warming. The Intergovernmental Panel on Climate Change (IPCC) has projected that for a 'business as usual' energy scenario the atmospheric concentration of CO₂ may double by the middle of the 21st century, and may continue to rise at increasing rates beyond (Houghton, 1996). Climate modeling shows that a rise of 0.3-0.6 °C in the near-earth-surface temperature could result from the increased concentration of CO₂ in the atmosphere during the last 150 years (Ledley et al, 1999). Experts agree that a number of actions should be taken soon in order to reduce the amount of CO₂ entering the atmosphere. One of the important means is to capture millions of tonnes of CO₂ produced by industrial processes and sequester CO₂ deep underground – this is known as CO₂ capture and geological storage (CCS) (IEA, 2007).

Geological storage of anthropogenic CO₂ as a greenhouse gas mitigation option was first proposed in the 1970s, but little research was done until the early 1990s, when the idea gained credibility through the work of individuals and research groups (Marchetti, 1977; Kaarstad, 1992; Koide et al, 1993; van der Meer, 1992; Gunter, 1993; Holloway and Savage, 1993; Bachu et al, 1994; Korbol and Kaddour, 1995). In 1996, the world's first large-scale storage project was initiated by Statoil and its partners at the Sleipner Gas Field in the North Sea (IPCC, 2005).

Three main alternatives have been considered for large-scale storage of CO₂ in subsurface formations (Orr et al, 2003): depleted oil and gas reservoirs, deep saline aquifers, and coal beds. Among these, saline aquifers can effectively contribute to CO₂ sequestration because of their large capacity and broad distribution around the world. However, we know very little about saline aquifers when compared to our understanding of oil and gas reservoirs. In this study we use the ECLIPSE simulator to investigate the flow of CO₂ in brine by considering the solubility effect and the sensitivity analysis of various parameters. It is very important to predict leakage risk and for the implementation of field projects.

*Corresponding author. email: xinwei@cup.edu.cn

Received May 11, 2009

2 Mechanisms of CO₂ sequestration in saline aquifers

Four principal mechanisms for sequestering CO₂ in saline aquifers have been described in the literature.

Hydrodynamic trapping In a storage project, supercritical CO₂ will be injected as a single phase, but once in the geological formation it will partition into free-phase (immiscible) CO₂ and a CO₂-rich brine. The flow of the free-phase CO₂ is dependent on the dip of the sealing horizon and the flow velocity and direction of the in situ formation water. Saline aquifers generally have very low flow velocities, of the order of tens of cm/year. This slow flow velocity leads to residence times of millions of years. This geological time-scale trapping of CO₂ in deep regional aquifers is called hydrodynamic trapping (Finley et al, 2005). In the short term, this is likely to be the most important mechanism for sequestration (Pruess, 2004).

Solubility trapping When CO₂ is injected into a reservoir, a portion of the injected CO₂ will dissolve in the formation water in the aquifer and the dissolution of CO₂ per unit volume of water is a function of pressure, temperature, and salinity of the aqueous phase (Holtz, 2002). The aqueous phase will retain the dissolved CO₂ regardless of being stationary or transported to another location as long as the physical conditions are undisturbed. CO₂-saturated formation water is denser than water not containing CO₂. The difference in density of CO₂-saturated aquifer water and virgin formation water triggers convection currents in the aquifer beneath the CO₂ plume, and accelerate the efficiency of dissolution (Ennis-King and Paterson, 2005).

Residual trapping Most of the CO₂ injected into a saline aquifer migrates upward as a separate CO₂-rich phase. During this upward migration two different displacement processes are active; namely, gravity drainage and imbibition. At the tail of the migrating CO₂ plume, formation water invades the CO₂ plume. Due to relative permeability and capillary hysteresis a fraction of the non-wetting phase is trapped in the imbibition process. When the concentration of CO₂ falls below a certain level CO₂ becomes trapped by capillary pressures and ceases to flow. This process is commonly referred to as residual trapping (Felett et al, 2004; Kumar et al, 2005).

Mineral trapping CO₂ can react with minerals and organic matter in geological formations to form precipitates (Pruess et al, 2003). This trapping will create stable repositories of CO₂ that decreases mobile hazards such as leakage to the surface (Nghiem et al, 2004).

3 Simulation model descriptions

3.1 Model conditions

The purpose of this study was to illustrate the processes occurring during CO₂ injection and investigate the effects of reservoir parameters. The simulations assume an isotropic and homogenous aquifer with a horizontal permeability of 100 mD, porosity of 0.18, and 50 m of thickness. The impermeable top layer of the aquifer is located at a depth of 1,000 m with a corresponding pressure and temperature of 1,500 psi

and 50 °C, respectively. Table 1 summarizes the base case input parameters including aquifer parameters and injection conditions. Pure CO₂ is injected at a constant rate for 15 years. Our simulation domain is in one quarter of a five spot pattern, in which four production wells are located at the corners of a square and the injection well sits in the center. The distance between the injection and production wells is 3,400 m. The production well is controlled by bottom hole pressure (BHP).

The main substances to be taken into account when describing flow and transport during CO₂ sequestration are CO₂, formation water, and salinity (salt), of course, the rock matrix that forms the porous medium. Water and CO₂ are defined as two components. Salts are not considered as an independent component, but considered a corrected coefficient in the equation of state (EOS). Therefore, a two-phase two-component model was chosen (which refers to the water-rich phase as a liquid and the CO₂-rich phase as a gas) for the following study.

Table 1 Summary of the aquifer properties and injection conditions

Reservoir size (m×m×m) (length, width and thickness)		2500×2500×50
Permeability mD	<i>x</i>	100
	<i>y</i>	100
	<i>z</i>	10
Porosity, %		0.18
Top depth, m		1000
Number of grids		50×50×5
Rock compressibility, psi ⁻¹		0.55×10 ⁻⁶
Temperature, °C		50
Residual water saturation		0.3
Residual CO ₂ saturation		0.1
Salinity, mol/kg		0-4
CO ₂ injection rate, Mscf/day		10000
Boundary condition		No-flow
Injection time, Years		15
Simulation time, Years		30
Injection interval		Block (1, 1, 5)
Initial conditions	Initial pressure, psi	1500
	Water saturation <i>S_w</i>	1.0
	<i>X_b^{CO₂}</i>	0

3. 2 Phase properties of CO₂-brine systems

CO₂ has a high solubility in the aqueous phase in saline aquifers due to high pressures. The dissolution of CO₂ in formation water occurs through mass transfer from the CO₂ phase to the aqueous phase whenever the phases are in contact. The excess CO₂ phase and the aqueous phase are thereby assumed to be in thermodynamic equilibrium in the

model. The Peng-Robinson equations of state were modified following the suggestions of Sørense and Whitson (1992) to obtain accurate gas solubility in the aqueous phase (Eclipse Technical Manual, 2005).

Both gas and water density values were obtained from the equation of state. Brine density, which is a function of temperature and pressure as well as the contributions of salinity and dissolved CO₂, was described as the sum of pure water density and additional density caused by salinity and dissolved CO₂.

Brine viscosity is a strong function of temperature. It also depends on salinity, pressure, and dissolved CO₂, the Lorentz-Bray-Clark method was used to calculate the brine viscosity. The viscosity for each phase is given by:

$$\left[(\mu - \mu^0) \cdot \xi + 0.001 \right]^{1/4} = \sum_{i=1}^N a_i b_r^{i-1}$$

where μ is the brine viscosity; μ^0 is the fresh water viscosity; a_i and b_r are coefficients.

μ^0 and ξ are functions of composition x_i (CO₂ and brine), the molecular weight of composition x_i , critical pressure, and critical temperature.

Many relative permeability curves were proposed for CO₂-water-rock systems, the relative permeability curves of Corey type with exponents determined from laboratory measurements were used. This study considered predominantly solubility trapping, so the capillary pressure curve was not considered.

Corey-type model (Brooks and Corey, 1964):

$$k_{rw} = (S_w^*)^\gamma$$

$$S_w^* = \frac{S_w - S_{wir}}{1 - S_{wir}}$$

$$k_{rg} = \left(1 - \tilde{S}_w \right)^2 \left(1 - \tilde{S}_w^\gamma \right)$$

$$\tilde{S}_w = \frac{S_w - S_{wir}}{1 - S_{wir} - S_{gr}}$$

where S_w is the water saturation; S_{wir} is the irreducible water saturation; S_{gr} is the residual gas saturation; exponent values used are $\gamma = 4$ and $\gamma = 0.5$.

4 Sensitivity analysis

The properties of reservoir and fluid strongly influence CO₂ distribution underground and control the destiny of CO₂. In this section we investigated the effects of several parameters on CO₂ distribution and storage efficiency.

4.1 Reservoir properties

4.1.1 Effect of horizontal permeability

The effect of horizontal permeability k_h on CO₂ storage capacity in a saline aquifer with a constant k_v/k_h of 0.1 is shown in Fig. 1. Simulation results show that more gas

dissolves in the formation brine as the horizontal permeability increases, but the effect of horizontal permeability is very small. During the injection period CO₂ migrates mostly as a gas phase and only about 5%-10% of the CO₂ dissolves in brine. The total injection gas (Field Gas in Place Total, FGIT) and the gas dissolved in liquid (Field gas in place liquid, FG IPL) for different horizontal permeability reservoirs are shown in Fig. 1.

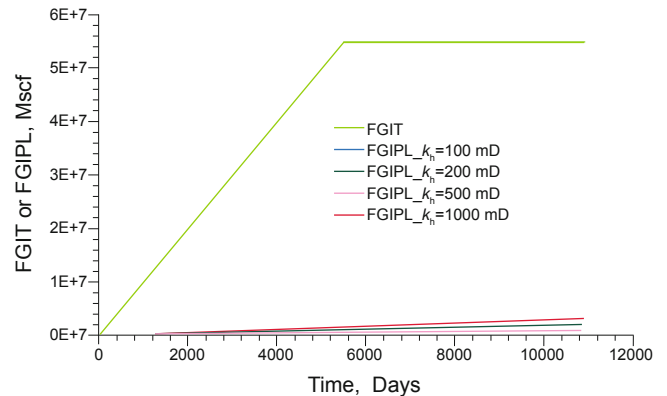


Fig. 1 Amount of CO₂ dissolved in the liquid phase in saline aquifers of different k_h values

4.1.2 Effect of vertical to horizontal permeability ratio

Fig. 2 shows the effect of vertical to horizontal permeability ratio k_v/k_h on the volume of gas dissolved in formation water (the horizontal permeability is 200 mD). It should be pointed out that the amount of dissolved gas increases as the k_v/k_h decreases. The difference is significantly related to the upward migration as mentioned above. The lower vertical permeability (i.e. low k_v/k_h value) prevents CO₂ from migrating up to the cap rock. This is particularly evident in Fig. 4 where for the lower k_v/k_h cases cross flow is observed in the horizontal direction in injection intervals. As mentioned above, convection may strongly enhance the dissolution of CO₂ and in fact be the most important mechanism for gas dissolution.

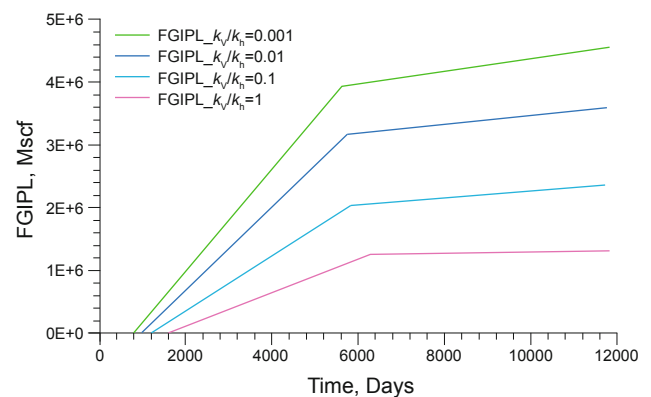


Fig. 2 Effect of k_v/k_h on time development of dissolved gas

Figs. 3 and 4 show the changes of CO₂ saturation profile with time (1, 5, 15, 30 years) for the cases with different vertical to horizontal permeability ratios. The horizontal permeability is kept constant at 200 mD.

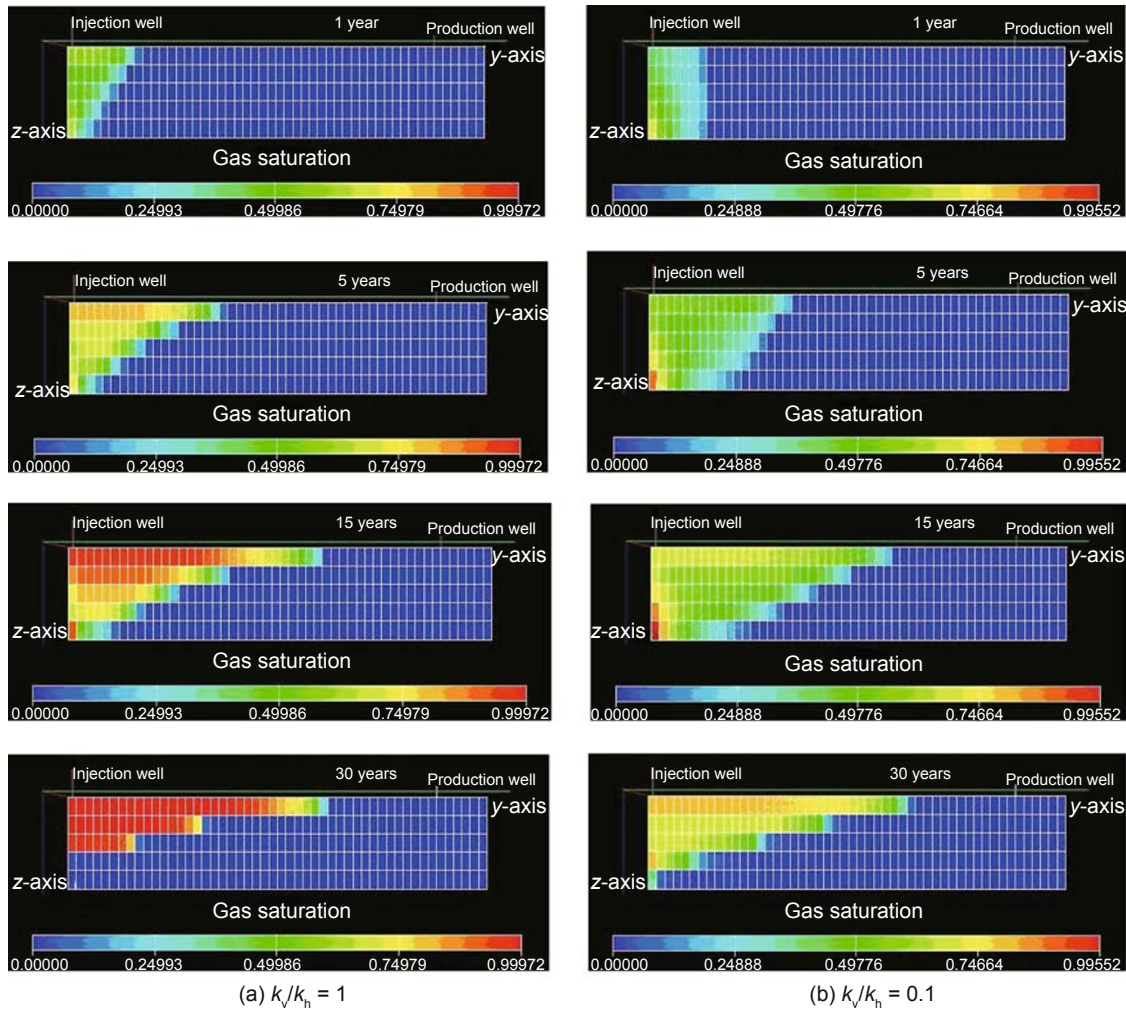


Fig. 3 Cross-section of the distribution of free CO₂ plume for $k_v/k_h = 1$ and 0.1, respectively

Simulation results show that the vertical to horizontal permeability ratio has a strong effect on CO₂ flow distribution. Figs. 3 and 4 show that at very low k_v/k_h values, CO₂ tends to migrate laterally in injection intervals, which would increase the dissolution of CO₂. Whereas an increase in the permeability ratio enhances the vertical migration and CO₂ spreads out laterally underneath the cap rock.

4.2 Phase properties of CO₂-brine

4.2.1 Effect of critical gas saturation

In the simulation we do not consider the hysteresis effect, but some gas may become trapped. This is achieved by setting the critical gas saturation $S_{gc} > 0$. In these cases only the critical gas saturation value is changed and the irreducible water saturation is kept at 0.3. Fig. 5 shows the volume of dissolved gas (FGIPL) for the cases of different critical gas saturations. The dissolution of gas increases as the critical gas saturation decreases. This is due to the fact that during the injection period CO₂ mostly migrates as a gas phase, which increases the contact between CO₂ and brine and thus enhances the dissolution of CO₂. The effect of increasing critical gas saturation is that the gas can be more effectively

trapped as residual gas as the critical gas saturation increases, which reduces dissolution of CO₂ in the aquifer brine.

4.2.2 Effect of irreducible water saturation

Many studies show that the irreducible water saturation S_{wir} influences the dissolution of CO₂ in the aquifer brine (Mo and Akervoll, 2005). As well known, the irreducible water saturation reduces the pore volume. Typical results (Fig. 6) show that an increase in the irreducible water saturation is beneficial in terms of dissolution trapping of more CO₂, we can also see from Fig. 7 that CO₂ tends to migrate upward with increasing irreducible water saturation. In all cases, the critical gas saturation is kept at 0.1.

4.3 Fluid properties

The properties of brine differ significantly from pure water due to its high salinity. The salt content strongly influences the solubility of CO₂, as mentioned above. The salinity (S) is not treated as a third component but as a parameter that can vary in EOS.

The density and viscosity of the aqueous phase are functions of pressure, temperature, salinity of the aqueous phase, and concentration of CO₂ in the aqueous phase. The concentration of CO₂ is also a function of pressure,

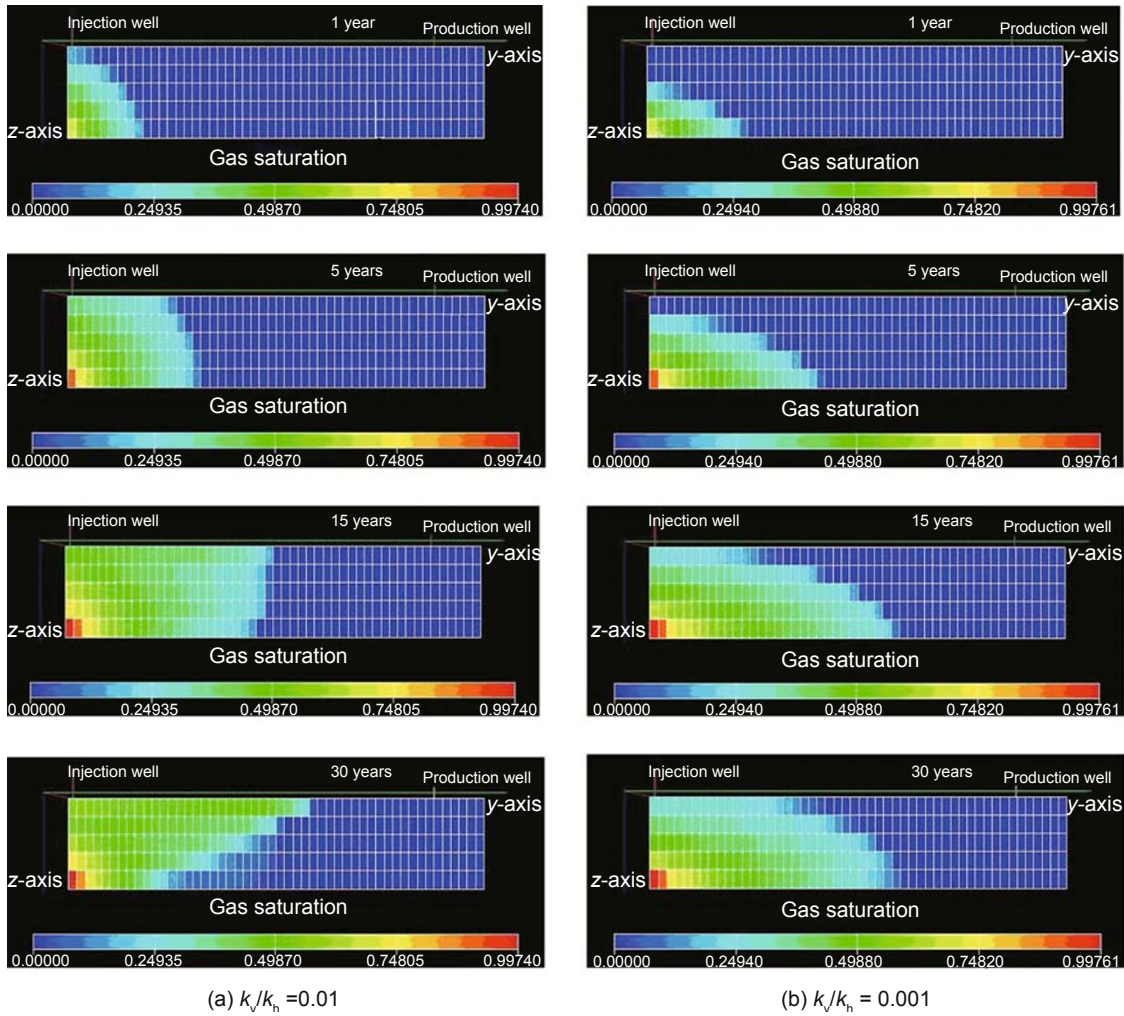


Fig. 4 Cross-section of the distribution of free CO₂ plume for $k_v/k_h = 0.01$ and 0.001 , respectively

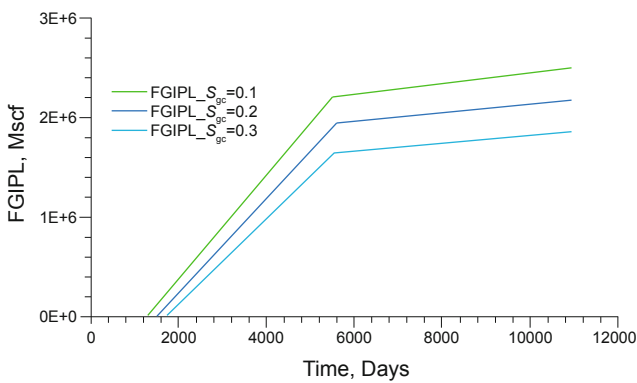


Fig. 5 Effect of critical gas saturation on CO₂ dissolution with time

temperature, and salinity of the aqueous phase. The solubility of CO₂ decreases as the salinity increases, and the efficiency of solubility trapping decreases. Fig. 8 shows the concentration of CO₂ in the aqueous phase varying with time. We can clearly see that the volume of CO₂ dissolved in the aquifer brine is less than that in the fresh water. Fig. 9 depicts the CO₂ plume migration for 1, 15 and 30 years in formation

brines with different NaCl concentrations. The amount of free gas in fresh water is less than that in 4 mol/kg NaCl solution. This is due to smaller buoyancy force acting on the CO₂ bubbles in fresh water, which results in a higher dissolution rate in fresh water aquifer.

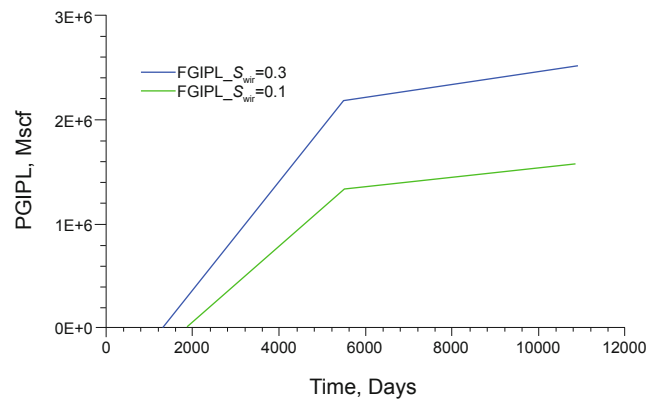


Fig. 6 Effect of irreducible water saturation on CO₂ dissolution in brine

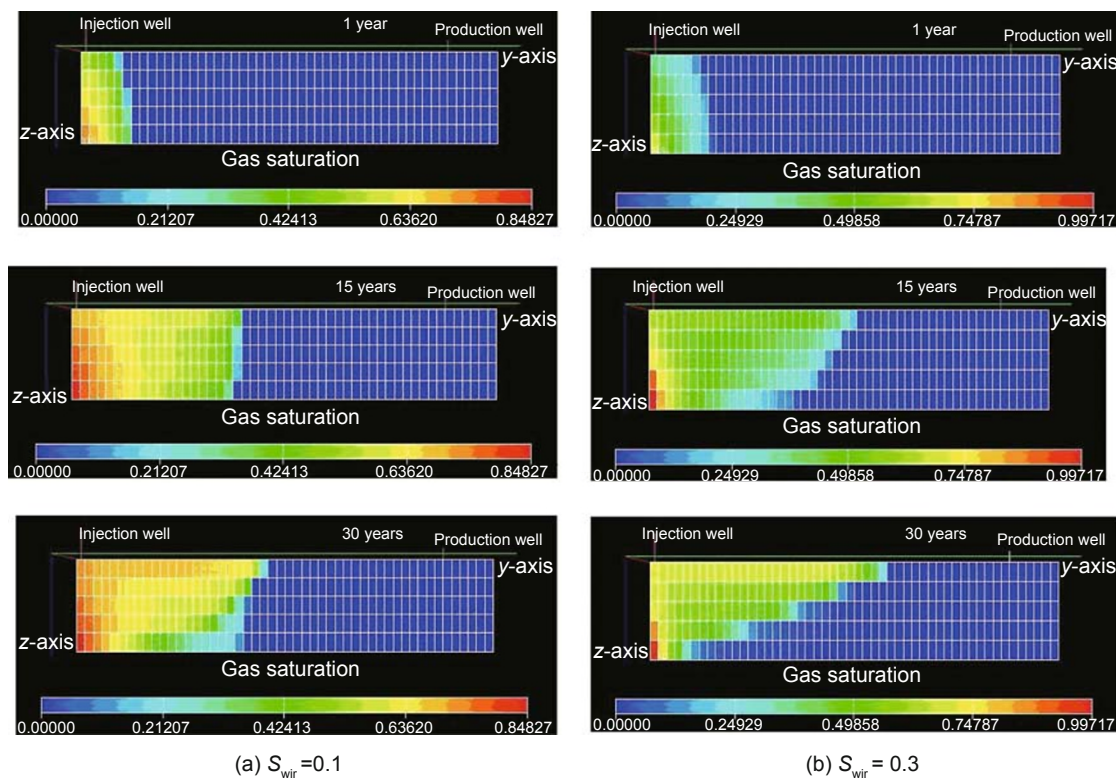


Fig. 7 Cross-section of the distribution of free CO₂ plume for different times (1, 15, 30 years) and for two cases of irreducible wafer saturations

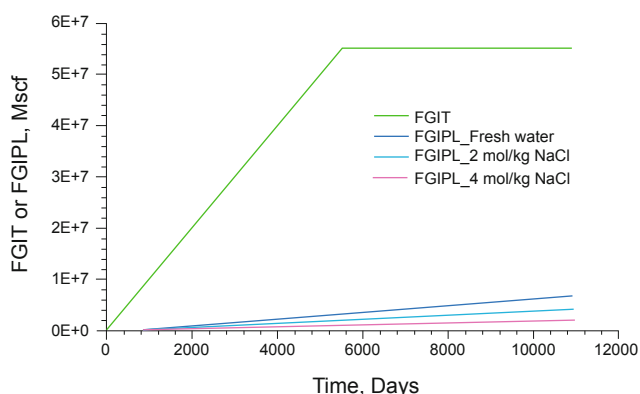


Fig. 8 Effect of salinity on the concentration of CO₂ in the aqueous phase

5 Conclusions

The dissolution of CO₂ in aquifer water is the dominant mechanism of CO₂ storage in saline aquifers. During the injection phase the most CO₂ migrates in the gas phase and only about 5%-10% CO₂ dissolves in the brine. After the termination of injection, CO₂ continues to dissolve mainly due to the contact of gas with brine. Moreover, the efficiency of dissolution depends on many factors, we can draw from this study that the solubility trapping is strongly dependent on the following factors:

- 1) The brine salinity. The dissolution of CO₂ decreases as the salinity increases, and thus the effectiveness of solubility trapping decreases.
- 2) The vertical to horizontal permeability ratio k_v/k_h . For the cases of extremely low k_v/k_h , CO₂ tends to migrate

laterally in the injection intervals, thus increasing the dissolution of CO₂; whereas an increase in the permeability ratio enhances the vertical migration and the gas-phase CO₂ spreads out quickly underneath the cap rock laterally.

3) Residual phase saturations. The amount of dissolved gas in the brine increases as the critical gas saturation decrease. This is due to that fact during the injection period CO₂ mostly migrates as a gas phase, which increases the contact between CO₂ and brine, and thus enhances the dissolution of CO₂.

Meanwhile, hysteresis and mineral trapping are important, and should be investigated further. In the model we proposed, we assume that the aquifers are isotropic and homogenous, so it is important for CO₂ geological storage to consider the effect of temperature and heterogeneity.

Acknowledgments

The authors are grateful for financial support from the National Basic Research Program of China (973 Project, 2006CB705801) and the Program for New Century Excellent Talents in University (2007).

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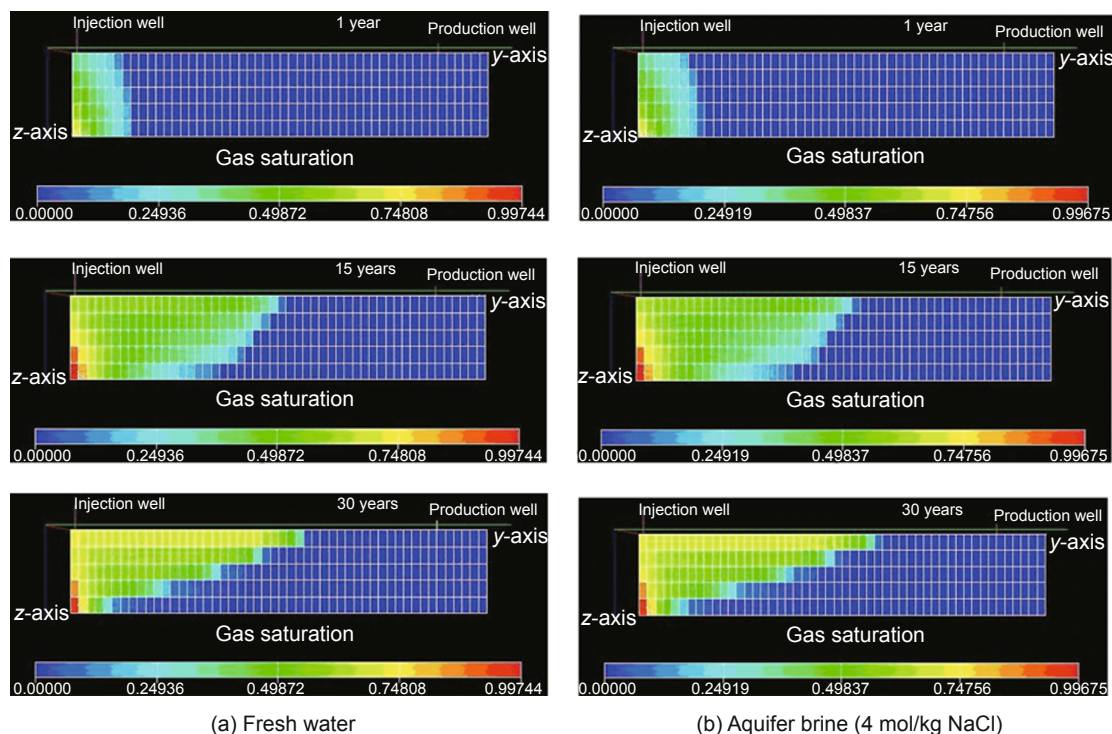


Fig. 9 Cross-section of the distribution of free CO₂ plume in fresh water and aquifer brine at different times

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(Edited by Sun Yanhua)