

# Numeric modeling of carbon dioxide sequestration in deep saline aquifers in Wangchang Oilfield-Jiangnan Basin, China

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## Abstract

Climate change has become one of the most pressing issues globally with the increased emissions of greenhouse gases (GHG) into the atmosphere and the resultant impacts on the environment threatening development and life on Earth. Anthropogenic emissions of carbon dioxide (CO<sub>2</sub>) into the atmosphere are largely blamed for this effect and carbon capture and storage (CCS) in geologic media is an enabling technology that can be utilized to mitigate global warming whilst still continuing to use fossil fuel until the end of the fossil era. Deep saline aquifers in sedimentary basins have a large potential for CO<sub>2</sub> storage. China has a rapidly growing economy with large remaining coal reserves hence her future CO<sub>2</sub> emissions are bound to increase from the present high levels. We have developed a simple 2-dimensional homogenous model to study the spatial and temporal distribution and storage of CO<sub>2</sub> injection into Wangchang Oilfield, Jiangnan Basin, one of China's largest inland sedimentary basins. A 10 year injection phase followed by 90 years shut-in is modeled. During the injection period, most of the gas exists in a supercritical state trapped beneath the caprock. When injection ceases, the gas gradually dissolves into the formation brine. Increase in vertical to horizontal permeability ratio, residual gas saturation and salinity all have different effects on the CO<sub>2</sub> spatial migration, dissolution in brine and overall storage. [Journal of American Science 2010; 6(8):178-187]. (ISSN: 1545-1003).

**Key words:** Geological storage; deep saline aquifers; carbon dioxide; numerical modeling; Wangchang Oilfield-Jiangnan Basin; China.

## 1. Introduction

Climate change has become one of the most pressing issues globally with both the developed and developing countries decrying the increasing emissions of GHG into the atmosphere (IPCC, 2005, Bekker et al, 2009). Combustion of fossil fuel mainly from power production and transportation is largely blamed for this effect with CO<sub>2</sub> being the leading GHG largely responsible for warming in global temperatures with a warming forecast of 1.8-4.0°C if current trends persist (IPCC, 2007). CO<sub>2</sub> emissions in the atmosphere have increased over the past 200 years from about 280 parts per million (ppm) to the current 380 ppm levels, a 30% increase (IPCC, 2007). If effective and urgent mitigation measures are not put in place, under the current "business as usual" scenario, these levels could double over the next 50 years (IPCC, 2007). CCS in geologic media is regarded as one of the possible mitigation options for reducing anthropogenic GHG emissions in the atmosphere (IPCC, 2005). Potential geologic formations include porous and permeable depleting or depleted oil and gas fields, unmineable coal seams and deep saline aquifers in sedimentary basins (IPCC, 2005; Holloway, 2008).

CCS is a process consisting of the separation of CO<sub>2</sub> from industrial and energy-related sources

(capture), transporting it to a storage location and subsequently disposing it in geologic media either permanently (sequestration) or for significant periods of time (storage) (IPCC, 2005, Bachu, 2008). Therefore, CCS can be applied to large sources of CO<sub>2</sub> including large fossil-fuel and biomass energy facilities; major CO<sub>2</sub>-emitting industries; natural gas production plants; synthetic fuel plants and fossil-fuel-based hydrogen production plants, among others. Globally, large-scale field injections are already being done at Alberta, Canada; Sleipner Vest Field, Norway; Gippsland Basin, Australia (Holloway, 2005; Bachu, 2008) and Nagaoka, Japan (Sasaki et al, 2008). Other GHG emission mitigation options include switching to more energy-efficient machinery, use of less carbon-intensive fuels, nuclear power, renewable energy sources, enhancement of biological sinks and the reduction of non-CO<sub>2</sub> GHG emissions in addition to socio-economic and policy changes (IPCC, 2005; IPCC, 2007; Celia and Nordbotten, 2009).

China is the second largest emitter of CO<sub>2</sub> globally after the USA and it is projected to be the world's largest emitter of GHG by 2025, thus China's

action to reduce its emissions is requisite (Meng, et al, 2007, Li et al., 2009). In addition, it has large remaining coal reserves with a rapidly growing economy contributing high amounts of CO<sub>2</sub> emissions into the atmosphere making CCS a viable mitigation option the country. China has 629 power plants emitting 72% of 3,890 million tons CO<sub>2</sub> per annum with the remaining percentage split among 994 sources from other industrial sectors (Li, et al., 2009). These large emitters are concentrated along the heavily industrialized North China plain and the coastal zones (Li, et al., 2009). Fortunately, China has a large CO<sub>2</sub> storage capacity in both onshore and offshore sedimentary basins with continental deep saline aquifers offering over 90 percent of total geological storage (Li, et al., 2009).

CO<sub>2</sub> can be stored in deep saline aquifers by three principle mechanisms. (1) *structural trapping/hydrodynamic trapping* where CO<sub>2</sub> is trapped as a supercritical fluid (hereinafter referred to as 'gas') below a low permeability confining caprock according to the structural lithology of the storage zone or as an immobile phase trapped in the pore spaces of the reservoir rocks (*residual trapping*) (IPCC, 2005; Audigane et al., 2007); (2) *solubility trapping* where CO<sub>2</sub> dissolves *in situ* in the formation brine, a process which increases the brine density and lowers the pH (increases the acidity) (Xu et al., 2004; Ghanbari et al, 2006); and (3) the decreased brine pH induces *mineral trapping* where CO<sub>2</sub> reacts with carbonate minerals such as calcite, magnesite, siderite, dolomite and/or dawsonite through a series of reactions (dissolution and complexing) with the dissolved ions found in the brine aquifer as well as with minerals composing the host rock matrix leading to chemical precipitation of secondary carbonates (Allen et al., 2005; IPCC, 2005; Xu et al., 2005). The interaction of CO<sub>2</sub> with alkali aluminosilicate minerals will result in the formation of dissolved alkali carbonate and bicarbonates thereby enhancing solubility trapping (Xu, et al, 2006, Xu, 2009). These four trapping mechanisms occur at different time scales (see figure 1). Initially, structural trapping is the dominant mechanism but with time, residual and solubility trapping become significant. The advantage of residual, solubility and mineral trapping and is that they do not rely directly on the integrity of the caprock as physical trapping does hence they enhance storage security (Suekane, 2008). The objective of this paper was to numerically simulate the temporal and spatial distribution and storage of CO<sub>2</sub> injection in Wangchang Oilfield, Jiangnan Basin, China. A short-term period of 100 with 10 years injection followed by 90 years shut-in is modeled. Three sensitivity tests are done for permeability, residual gas saturation and salinity.

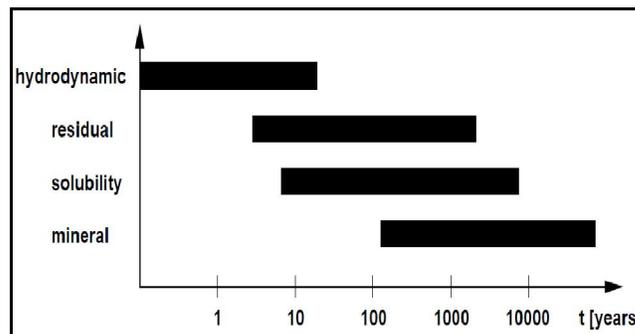


Figure 1. Predominant CO<sub>2</sub> trapping mechanisms and their estimated times within saline aquifers (Bieliski, 2007, p7)

## 2. 0. Numerical method

### 2.1. Simulation tool

Modeling geochemical systems to predict future outcomes is an indispensable tool in geochemical engineering. This is because the geo-environment is highly complex and investigation by laboratory experiments can only apply to subsystems and processes (van Gaans, 1998). For CO<sub>2</sub> sequestration research, numeric simulation is essential prior to experimental and field demonstrations on account of feasibility and cost and also because mineral alteration rates to CO<sub>2</sub> injection in saline aquifers are very slow especially with regard to aluminosilicates which are not amenable to experimental study (Xu, et al, 2007). In our research, simulations were done using TOUGH2 version 2 (Transport of Unsaturated Groundwater and Heat), a general purpose simulator program for multi-dimensional fluid and heat flow of multiphase, multi-component fluid mixtures in 1-, 2- and 3-dimensional porous and fractured media (Pruess, et al, 1999). It is a program that has wide application including geothermal reservoir engineering; nuclear waste isolation studies; environmental assessment and remediation; and flow and transport in variably saturated media and aquifers (Pruess, 1999; Wu and Pruess, 2000).

In our simulation, ECO2N, a fluid and property module of TOUGH2 designed for applications of geologic sequestration of CO<sub>2</sub> in saline aquifers is used (Pruess, 2005). ECO2N gives an ample description of the thermodynamics and thermophysical properties of mixtures of water, brine and CO<sub>2</sub> under conditions typically encountered in saline aquifers targeted for CO<sub>2</sub> disposal and gives results largely within experimental error for

temperature, pressure and salinity conditions within the range of  $10^{\circ}\text{C}$   $T$   $110^{\circ}\text{C}$ ;  $P$  600 bar and salinity of up to full halite saturation (Pruess, 2005). Flow processes may be modeled isothermally or non-isothermally and phase conditions represented may include a single aqueous or  $\text{CO}_2$ -rich phase as well as two-phase mixtures (Pruess and Sypcher, 2007). Solid salt may precipitate or dissolve adding a third active phase in the system (Pruess and Sypcher, 2007). Mutual solubilities for  $\text{CO}_2$  and  $\text{H}_2\text{O}$  in gas and brine phases are calculated from the correlations of Sypcher and Pruess (2005). Spatial discretization is achieved through the Integral Finite Difference method (IFD). Time is discretized fully implicitly as a first-order backward difference (Pruess et al., 1999).

## 2.2. Model setup

A simple two-dimensional radial model with a cylindrical geometric configuration is used to study the temporal and spatial distribution of  $\text{CO}_2$  as injected into the first segment of Qian reservoir of Wangchang Oilfield in Jianghan Basin, Hubei Province, China (hereinafter referred to as Wangchang for simplicity) (PRC, 1987). Jianghan Basin (see figure 2) in Hubei Province is one of China's largest inland petroleum reservoirs with an area of  $28,000\text{km}^2$  (PRC, 1987) and a potential for  $\text{CO}_2$  storage by solubility trapping in deep saline aquifers of 52,800 million tons  $\text{CO}_2$  (Li et al., 2009). Wangchang lies within Qiangjiang depression and is mainly composed of alternating sequence of sandstone and mudstone or sandstone and salt (PRC, 1987). The mudstone and salt offer good sealing conditions while the sandstone are a good storage formation making the Wangchang a suitable reservoir for  $\text{CO}_2$  injection. The salinity at Wangchang ranges between 120 to  $300\text{mg/l}$ . The air permeability of Qian 1 lies within  $1880 \times 10^{-9}$  to  $2537 \times 10^{-9} \text{mm}^2$  and the porosity ranges between 23 to 28.5 percent (PRC, 1987).

In our model,  $\text{CO}_2$  was injected into a homogenous sandstone aquifer of 100 meter thickness. The depth at the top of the reservoir is 1000 meters below the earth surface. The aquifer is discretized into 10 grids of constant 10 meters spacing in the vertical direction while in the horizontal direction, a distance of 10,000 meters is modeled with a radial spacing that increases gradually away from the 0.3 meter injection well positioned at the center of the domain. A total of 65 radial grid elements are used including the injection well. The outer boundary was assumed to be infinite acting by making the last grid inactive while the top and bottom cap-rock layers are assumed to be impermeable. A hydrostatic pressure distribution

over the depth was initially specified and local phase equilibrium is assumed with a constant temperature.  $\text{CO}_2$  is injected at a supercritical state of  $31.04^{\circ}\text{C}$  temperature and 73.82 bar pressure into the lower segment at a constant rate of  $50\text{kg/s}$  for 10 years, equivalent to 1.6 metric tons per year followed by 90 years shut-in period. Other hydrological and thermodynamical parameters used in the simulations are in table 1 below.

## 3. Results and discussion

### 3.1. Base-case

As  $\text{CO}_2$  is injected at the lower segment of the sandstone reservoir, it migrates rapidly upwards by buoyancy forces towards the impermeable cap-rock because the density of supercritical  $\text{CO}_2$  is lower than that of aqueous brine in the formation (Figure 3). Upon reaching the cap-rock, the gas spreads horizontally along the impermeable cap-rock and this upward and horizontal spread continues even after gas injection stops. During the injection phase, most of the free  $\text{CO}_2$  gas accumulates below the cap-rock (hydrodynamic trapping) but in this same upper region, some of gas will dissolve in the formation brine (solubility trapping) thereby increasing the density of the  $\text{CO}_2$ -brine mixture which starts to sink downwards due to gravity (figure 4). The sinking heavier  $\text{CO}_2$ -brine mixture vertically displaces the lower fresh brine which is pushed upwards giving rise to a fluid circulation mixing process that enhances dissolution of free  $\text{CO}_2$  gas in the fresh brine (Ennis-King et al., 2005, Audigane et al., 2007).

This fluid circulation process between fresh formation brine and the  $\text{CO}_2$ -brine mixture is mainly controlled by vertical permeability (Audigane, et al, 2007) and is mainly evident after hundreds of years hence it is not covered in the present work but is nonetheless important in  $\text{CO}_2$  solubility trapping (Audigane et al., 2007 and references therein). Even after injection stops,  $\text{CO}_2$  dissolution in the brine continues trapping the gas in solution thus enhancing solubility trapping. As  $\text{CO}_2$  migration in the media perpetuates, some of it is trapped in the formation interstices between pores of the grains in the rocks leaving a trace of residual saturation (occurring at a residual gas saturation value of less than 0.05) where a certain part of the pore volume is filled with  $\text{CO}_2$  that is immobilized due to the effect of capillary pressure (Bachu, 2008) and interfacial tension (Chalraud, et al, 2009; Suekane, et al, 2008) - residual trapping. Thus with increased time, solubility trapping increases while gas trapping decreases. Mineral trapping is not covered here because it occurs after hundreds of years.

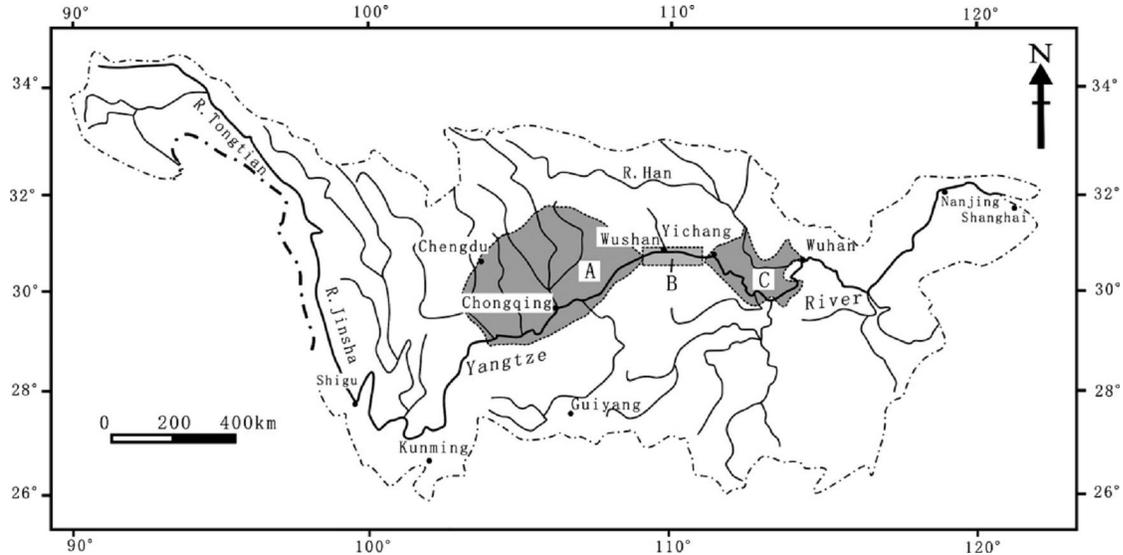


Figure 2. Location map, shaded areas are: A. – Sichuan Basin, B. – Three Gorges, C. – Jiangnan Basin. (Fang, et al., 2007, p250)

Table 1: Hydrogeological and thermodynamical parameters used in the simulations

Rock	specific heat (J/kg °C)	Aquifer
Permeability		
Horizontal		$2 \times 10^{-12} \text{ m}^2$
Vertical		$2 \times 10^{-13} \text{ m}^2$
Porosity (%)		26
Pressure (bar)		110
Temperature (°C)		48
Salinity (% by weight)		12
CO <sub>2</sub> injection rate (kg/s)		50
<i>Relative permeability model:</i>		
Liquid (van Genutchen, 1980)		
$k_{rl} = \sqrt{S^*} \{1 - (1 - [S^*]^{1/m})^m\}^2$		$S^* = (S_l - S_{lr}) / (1 - S_{lr})$
$S_{lr}$ : residual water saturation		$S_{lr} = 0.30$
$m$ : exponent		$m = 0.457$
Gas (Corey, 1954)		
$k_{rg} = (1 - \hat{S})^2 (1 - \hat{S}^2)$		$\hat{S} = (S_l - S_{lr}) / (S_l - S_{lr} - S_{gr})$
$S_{gr}$ : residual gas saturation		$S_{gr} = 0.05$
<i>Capillary pressure model (van Genutchen)</i>		
$P_{cap} = -P_0 ([S^*]^{-1/m} - 1)^{1-m}$		$S^* = (S_l - S_{lr}) / (1 - S_{lr})$
$S_{lr}$ : residual water saturation		$S_{lr} = 0.00$
$m$ : exponent		$m = 0.457$
$P_0$ : strength coefficient		$P_0 = 19.61 \text{ kPa}$
Rock grain density (kg/m <sup>3</sup> )		2600
Formation heat conductivity (W/m °C)		2.51

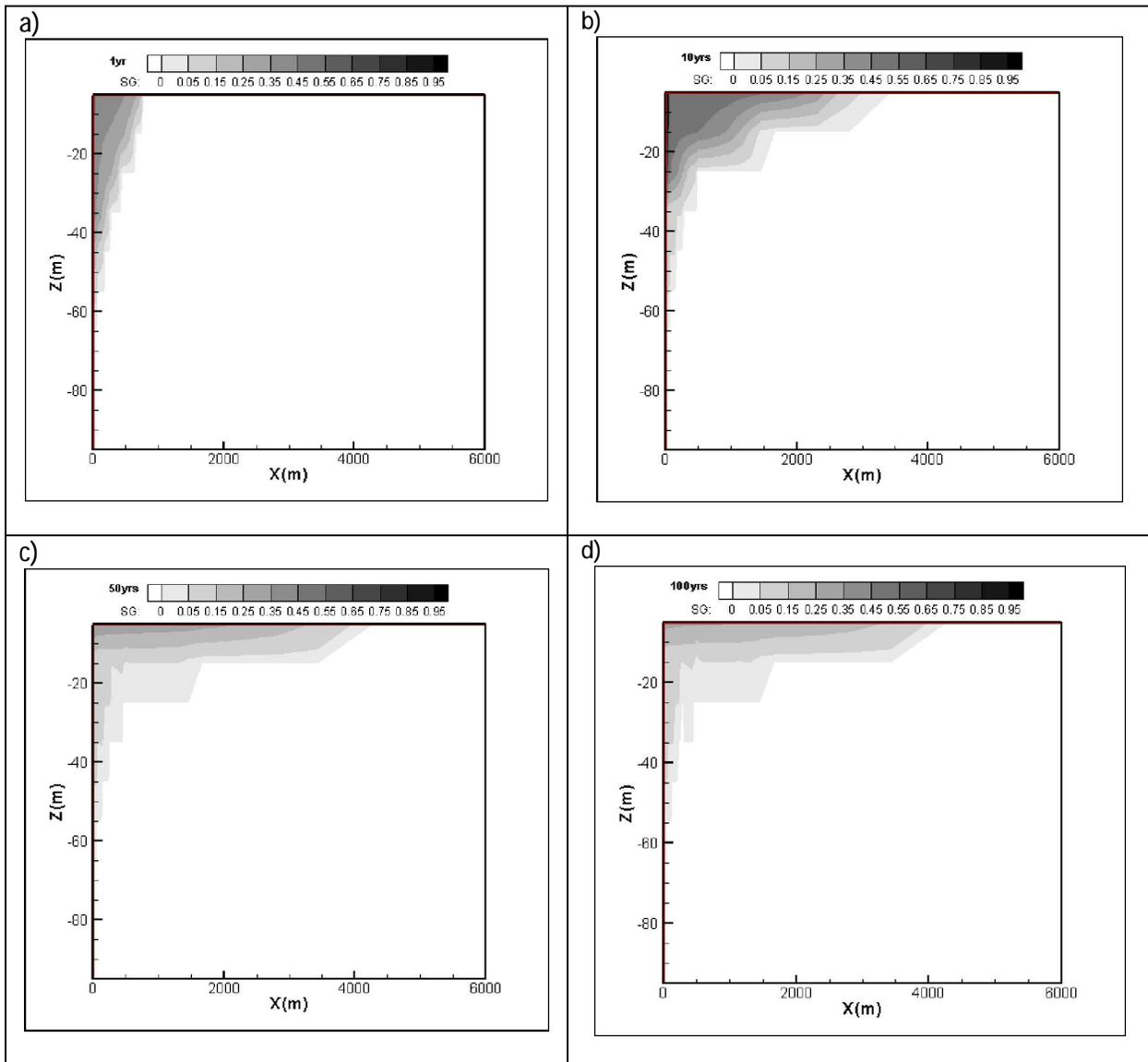


Figure 3 (a-d). Distribution of gas saturation (SG) for 1, 10, 50 and 100 years for base-case

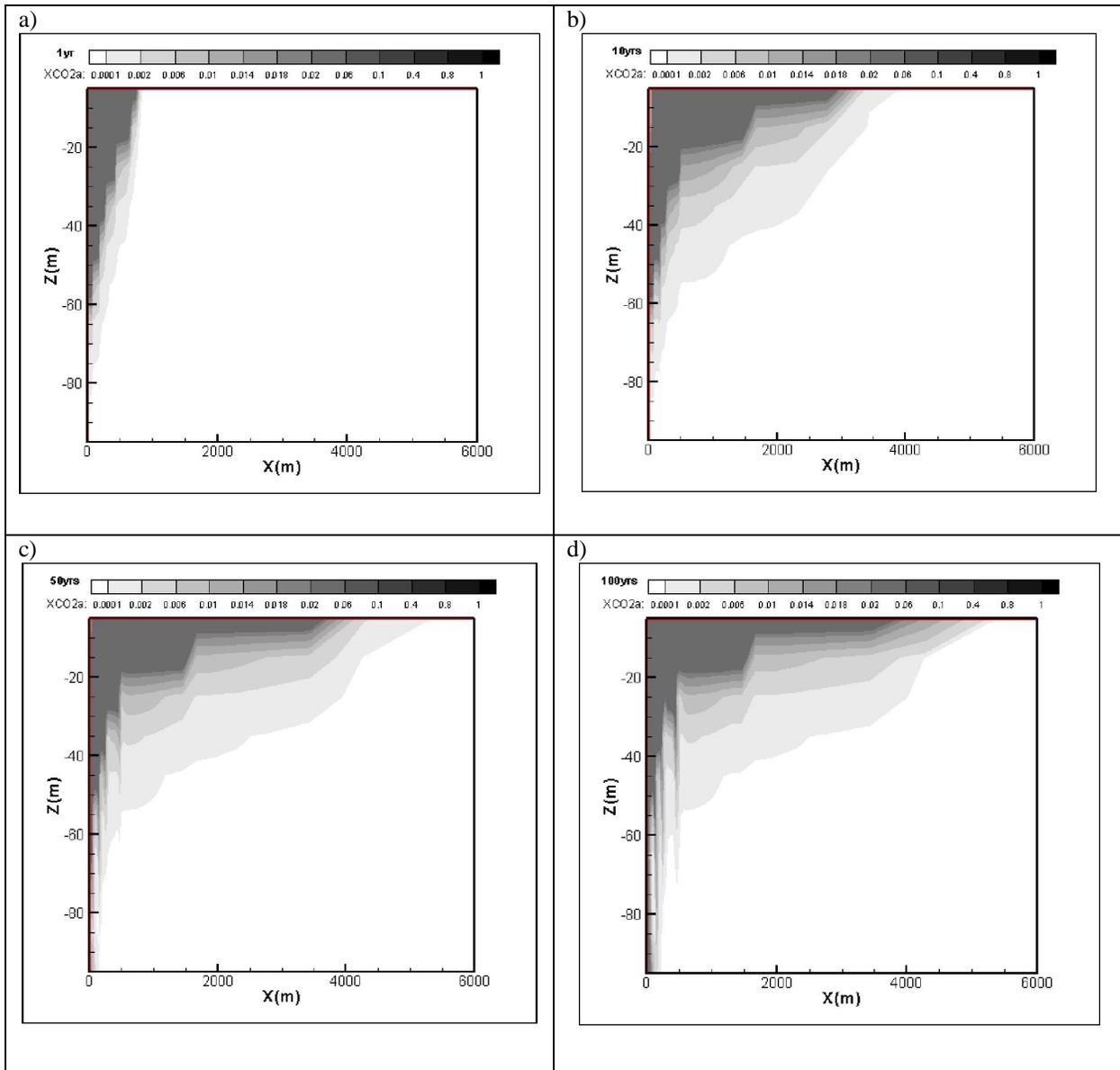


Figure 4(a-d). Distribution of concentration of dissolved CO<sub>2</sub> mass fraction (XCO<sub>2a</sub>) for 1, 10, 50 and 100 years for base-case

Table 2. Values used in sensitivity analysis and impact on dissolved CO<sub>2</sub> after 100 years

Sensitivity test	Parameter	CO <sub>2</sub> dissolved in formation water after 100 years (%)
Vertical permeability(K <sub>v</sub> )	2X10 <sup>-13</sup> (K <sub>v</sub> /K <sub>h</sub> =0.1) base case	33.7
	1x10 <sup>-12</sup> (k <sub>v</sub> /k <sub>h</sub> =0.5) case 2	34.5
Residual gas saturation (S <sub>gr</sub> )	0.05 (base-case)	33.7
	0.25 (case 3)	21.5
Salinity	12% by weight (base case)	33.7
	24% by weight (case 4)	23.2

### 3.2. Sensitivity studies

Accuracy of site-specific parameters is critical if the numeric simulations are to give a true representation of the reality. In this regard, sensitivity tests have been conducted for three parameters which may affect CO<sub>2</sub> spatial distribution and overall storage in the formation. These are vertical to horizontal permeability ratio ( $K_v/K_h$ ) that has been increased from 0.1 (base-case) to 0.5 (case 2); residual gas saturation ( $S_{gr}$ ) that has been raised from 0.05 (base-case) to 0.25 (case 3), and salinity ( $X_{NaCl}$ ) whose value has been increased from 0.12 (base-case) to 0.24 (case 4) - see table 2.

#### 3.2.1. Change in vertical to horizontal permeability ratio – case 2

Increase in the  $K_v/K_h$  ratio (case 2) increases the amount of CO<sub>2</sub> that is trapped by solubility trapping from 33.7% to 34.5% (table 2). In our case, vertical permeability was increased while the horizontal permeability remained unchanged. This in turn leads to greater vertical gas migration during the injection phase (figure 5a). At the end of 100 simulation time, there is greater slumping of the CO<sub>2</sub>-brine mixture due to higher vertical permeability which promotes dissolution of CO<sub>2</sub> in the fresh brine that is displaced by the sinking CO<sub>2</sub>-brine mixture - figure 5b (Ghanbari et al., 2006). However, although higher vertical permeability promotes solubility trapping through enhanced fluid circulation (Audigane et al., 2007), it may increase chances of CO<sub>2</sub> vertical leakage if the caprock has fractures, faults or there exists pre-existing poorly-sealed abandoned oil wells in Wangchang in turn threatening CO<sub>2</sub> storage safety.

#### 3.2.2. Change in residual gas saturation – case 3

Increase in  $S_{gr}$  from 0.05 to 0.25 leads to reduced solubility trapping and increase in gas trapping. At the end of 100 years simulation time, only 21.5% of total CO<sub>2</sub> injected is stored in solution form compared to base-case's 33.7% (table 2). This in turn means that more gas is stored as free gas hydrodynamically or by residual trapping when compared to base-case (figure 5c). Consequently, higher  $S_{gr}$  limits movement in the gas within rock interstices and pores which leads to decreased contact between CO<sub>2</sub> gas and formation brine thereby decreasing dissolution of CO<sub>2</sub> (Zhang, et al., 2009).

#### 3.2.3. Effect of salinity - Case 4

Wangchang has highly halide waters thus a sensitivity test for salinity was done by increasing the base-case value of 12%-by-weight two-fold (case 4). An increase in salinity reduced the amount of CO<sub>2</sub> stored by solubility trapping at the end of the 100 years simulation time with case 4 having 23.2% compared to 33.7% for base-case (table 2 and figure 5d). Increase in salinity increases the partial molar volume of water hence the difference between the partial molar volume of water and CO<sub>2</sub> decreases in turn reducing solubility through convective mixing (Ghanbari et al., 2006). This therefore means that saline aquifers in continental sedimentary basins may be more ideal for CO<sub>2</sub> storage compared to marine sedimentary ones (Zhao et al., 2009).

### Conclusion

A short-term 100 year simulation of CO<sub>2</sub> injection into a deep saline sandstone aquifer has been done using a simple homogenous 2-dimensional radial fluid flow model to study CO<sub>2</sub> spatial and temporal distribution and storage. Parameters from Wangchang have been used in the model and three sensitivity tests have been carried out. Based on our studies, the following conclusions can be drawn out. When CO<sub>2</sub> is injected at the lower segment of the model, it will tend to migrate upwards towards the cap-rock and then horizontally upon reaching the cap-rock barrier driven by buoyancy forces because of density differences between the supercritical CO<sub>2</sub> and aquifer formation brine. Thereafter, the gradually gas dissolves in the formation water even after injection ceases. Increase in ratio of  $K_v/K_h$ ,  $S_{gr}$  and salinity have different effects on overall storage. Increase in  $K_v/K_h$  increases CO<sub>2</sub> dissolution in brine but may be a danger in cases of caprock imperfections leading to vertical leakage of the gas to overlying shallow aquifers. Higher  $S_{gr}$  and increased brine salinity both reduce the amount of CO<sub>2</sub> dissolved in formation brine thus more gas is trapped structurally but at a different degree of effect. Overall, 33.7% of gas is stored in solution form in base-case compared to 33.4% in case 2, 21.5% case 3 and 23.2% in case 4 (table 2).

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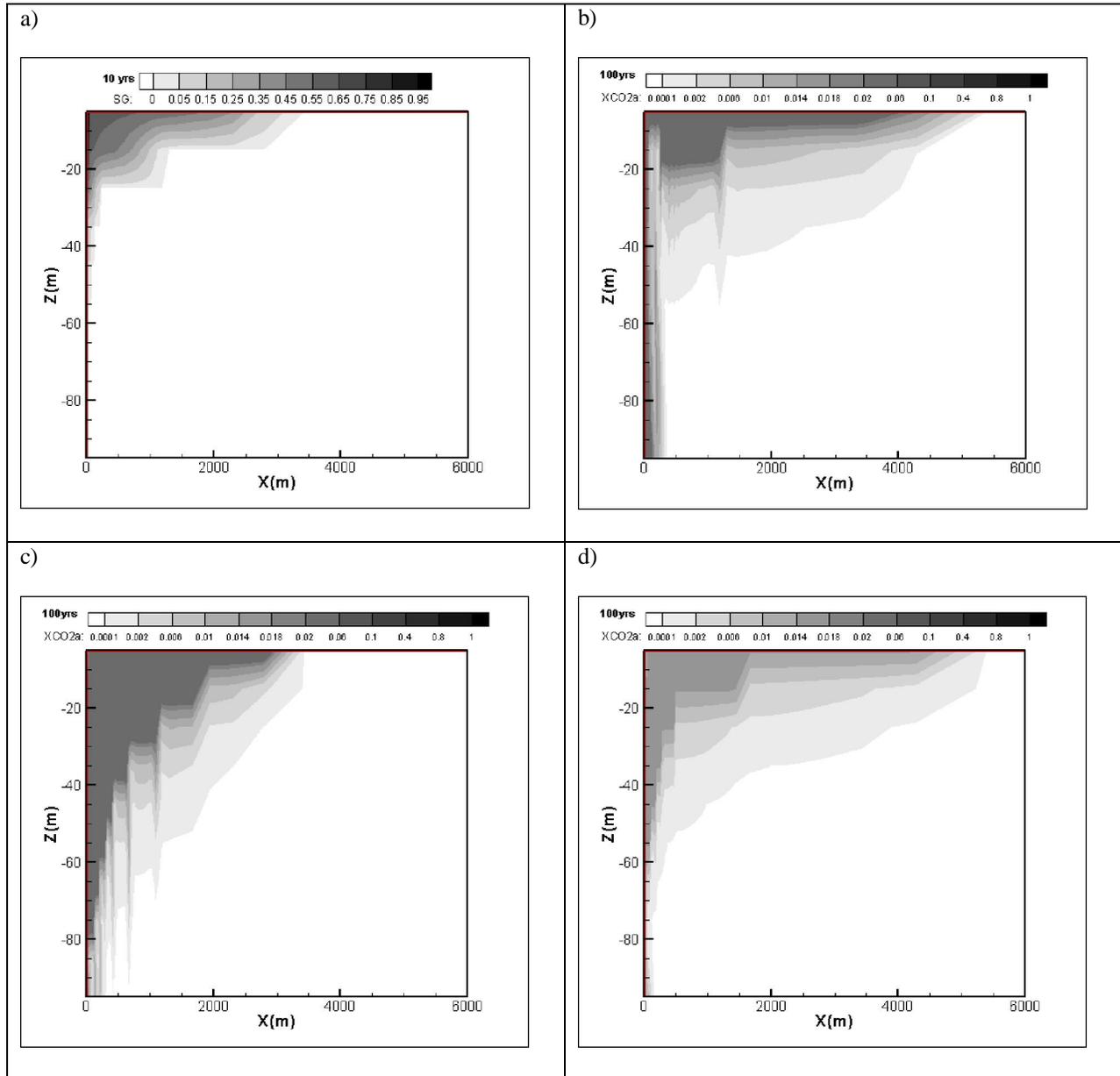


Figure 5a) Gas saturation profile at 10 years for case 2; b to d - spatial distribution of concentration of dissolved CO<sub>2</sub> in brine at 100 years for case 2, 3 and 4 respectively.

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