

**MODELING DENSITY EFFECTS IN CO<sub>2</sub> INJECTION IN OIL RESERVOIRS**  
**AND**  
**A CASE STUDY OF CO<sub>2</sub> SEQUESTRATION IN A QATARI SALINE AQUIFER**

A Thesis

by

TAUSIF KHIZAR AHMED

Submitted to the Office of Graduate Studies of  
Texas A&M University  
in partial fulfillment of the requirements for the degree of  
**MASTER OF SCIENCE**

August 2011

Major Subject: Petroleum Engineering

Modeling Density Effects in CO<sub>2</sub> Injection in Oil Reservoirs and a Case Study of CO<sub>2</sub>  
Sequestration in a Qatari Saline Aquifer  
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Approved by:

Co-Chairs of Committee,	Steve Holditch
	Hadi Nasrabadi
Committee Members,	Maria Barrufet
Head of Department,	Steve Holditch

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## ABSTRACT

Modeling Density Effects in CO<sub>2</sub> Injection in Oil Reservoirs and a Case Study of CO<sub>2</sub>  
Sequestration in a Qatari Saline Aquifer. (August 2011)

Tausif Khizar Ahmed, B.S., Texas A&M University at Qatar

Co-Chair of Advisory Committee: Dr. Steve Holditch  
Dr. Hadi Nasrabadi

CO<sub>2</sub> injection has been used to improve oil recovery for several decades. In recent years, CO<sub>2</sub> injection has become even more attractive because of a dual effect; injection in the subsurface 1) allows reduction of CO<sub>2</sub> concentration in the atmosphere to reduce global warming, and 2) improves the oil recovery.

In this study, the density effect from CO<sub>2</sub> dissolution in modeling of CO<sub>2</sub> injection is examined. A method to model the increase in oil density with CO<sub>2</sub> dissolution using the Peng-Robinson equation of state and the Pedersen viscosity correlation is presented. This method is applied to model the observed increase in oil density with CO<sub>2</sub> dissolution in a West Texas crude oil. Compositional simulation of CO<sub>2</sub> injection was performed in a 2D vertical cross section and a 3D reservoir with the density effect. The results show that the density increase from CO<sub>2</sub> dissolution may have a drastic effect on CO<sub>2</sub> flow path and recovery performance. One main conclusion from this work is that there is a need to have accurate density data for CO<sub>2</sub>/oil mixtures at different CO<sub>2</sub> concentrations to ensure successful CO<sub>2</sub> injection projects.

While CO<sub>2</sub> enhanced oil recovery (EOR) is part of the solution, saline aquifers have the largest potential for CO<sub>2</sub> sequestration. A literature review of the CO<sub>2</sub> sequestration in saline aquifers is performed. The dominant trapping mechanisms and transport processes and the methods used to model them are discussed in detail. The Aruma aquifer, a shallow saline aquifer in southwest Qatar is used as a case study for CO<sub>2</sub> sequestration. A compositional simulation model is prepared for the Aruma aquifer using the available log data and flow test data. It was found that the grid size is a key parameter in modeling CO<sub>2</sub> sequestration accurately. It affects the propagation of the CO<sub>2</sub> plume and amount of CO<sub>2</sub> dissolved in brine.

## **DEDICATION**

To my family, teachers and friends

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## 1. INTRODUCTION: THE PROBLEMS ADDRESSED

### 1.1 Introduction

The combustion and flaring of fossil fuels produces large quantities of CO<sub>2</sub>. The Intergovernmental Panel on Climate Change (IPCC 2007) stress the need to control anthropogenic greenhouse gases in order to mitigate the climate change that is adversely affecting the planet. They report that over the last three decades CO<sub>2</sub> emissions have been growing at a rate of 1.9% per year . Atmospheric CO<sub>2</sub> concentrations have increased by 100 ppm in comparison to its preindustrial level, reaching 379 ppm in 2005. Geologic storage of CO<sub>2</sub> would be to sequester CO<sub>2</sub> captured from anthropogenic sources, such as power plants, oil refineries and chemical plants. Value added geologic sequestration would include injecting CO<sub>2</sub> for enhanced oil recovery. However it is important to understand the dynamics of CO<sub>2</sub>/ crude oil at reservoir conditions and predict fluid properties accurately. The impact of modeling this behavior will be discussed in this study.

The largest, but least defined sources of geologic storage possibilities lies in saline aquifers (Beecy and Kuuskraa 2001). Firoozabadi and Cheng (2010) estimate that about  $2 \times 10^4$  gigatons can be stored in saline aquifers in the United States and Canada alone. These formations have the advantage of being close to many CO<sub>2</sub> emission sources.

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This thesis follows the style and format of *SPE Reservoir Evaluation and Engineering*.

This study briefly reviews density effects and investigates the sequestration potential of CO<sub>2</sub> in a shallow saline aquifer in Qatar.

## **1.2 CO<sub>2</sub> in Enhanced Oil Recovery**

The CO<sub>2</sub> enhanced oil recovery (EOR) has been applied in petroleum production for many years. The first large-scale, commercial CO<sub>2</sub> EOR project began operations in 1972 at the SACROC field in West Texas, and continues to this date (Sweatman et al. 2009). A large number of CO<sub>2</sub> EOR projects have started since then. Based on the 2010 EOR survey by the Oil and Gas Journal there are a total of 129 projects globally (120 of them in the US and Canada). In the US alone, CO<sub>2</sub> injection has accounted for the recovery of about 1.5 billion barrels of oil. CO<sub>2</sub> injection in oil reservoirs (for sequestration purposes) has also become more attractive from a global warming standpoint. The increase in CO<sub>2</sub> concentration in atmosphere due to burning fossil fuels and deforestation may be one of the main causes for the acceleration of global warming. Since fossil fuels will be a critical component of world energy supply for the coming decades, methods for disposal of CO<sub>2</sub> that do not involve long residence of CO<sub>2</sub> in the atmosphere (such as injection in oil and gas reservoirs) are considered as part of a possible solution.

CO<sub>2</sub> injection may improve oil recovery through three main mechanisms: 1) swelling, 2) reducing viscosity, and 3) decreasing residual oil saturation. Diffusion of CO<sub>2</sub> in the oil



phase may also contribute to recovery in highly heterogeneous and fractured reservoirs (Hoteit and Firoozabadi 2009).

In CO<sub>2</sub> injection schemes, the minimum miscibility pressure (MMP) from 1D horizontal slim-tube measurements is often thought to be a key parameter. The MMP is defined as minimum pressure that is required to achieve multiple contact miscibility between the injected fluid and oil at the reservoir temperature. However, the flow path may be very different in a slim tube and in a reservoir.

In a slim-tube experiment, a long (say 10 m or longer) small diameter (say 0.5 cm) tube packed with sand or glass beads is saturated with oil that is then displaced by injection gas at a fixed pressure and temperature. The oil recovery after injection of some fixed amount of gas (usually 1.1 or 1.2 pore volume) is measured at different pressures. Typically, recovery increases with an increase in pressure and then levels off. In a recovery vs. pressure plot, the MMP is usually taken to be the point where the recovery starts to level off. The measured MMP from slim tube is used for the purpose of field evaluation or tuning equations of state.

The question is how relevant slim tube MMP is to performance of CO<sub>2</sub> injection in 2D and 3D reservoirs. The slim tube, because of its small diameter, represents a 1D horizontal flow. The flow in reservoir conditions even in homogenous domains is 2D or 3D. As CO<sub>2</sub> dissolves in the oil, the density often increases. On the other hand, when a

gas phase evolves from mixing of CO<sub>2</sub> and the oil, the gas phase is often lighter than CO<sub>2</sub> and the oil. The evolved gas phase moves upward due to buoyancy. These density effects under the influence of gravity in reservoir conditions will change the flow path from 1D to 2D or 3D. In a 1D slim tube, there is no gravity effect.

There has been extensive research on the effect of CO<sub>2</sub> dissolution on oil viscosity and many correlations have been developed. Density effects from mixing have not been taken into account in the past; they often are ignored in modeling of CO<sub>2</sub> injection (Bangia et al. 1993; Cardenas et al. 1984; Johnston 1988; Palmer et al. 1984; Perry 1982) . A clear example of neglect of density effect is the pilot performance in the Weeks Island from CO<sub>2</sub> injection, which showed an early breakthrough of injected CO<sub>2</sub> (Johnston 1988). A number of other papers which are based on the assumption that when the injected CO<sub>2</sub> is lighter than the oil, the CO<sub>2</sub> injection is a stable gravity drainage process (Bangia et al. 1993; Cardenas et al. 1984). As will be shown in this study, this may not be true when the permeability is high. CO<sub>2</sub> dissolution in water also results in a density increase (Garcia 2001; Han and McPherson 2009; Tabasinejad et al. 2010). The density increase in water may have a significant effect on the mixing and the flow path and affects the sequestration potential (Farajzadeh 2008; Firoozabadi and Cheng 2010).

In this study, literature on change in density from CO<sub>2</sub> dissolution in a petroleum fluid is first briefly reviewed. The procedure to model the density increase from CO<sub>2</sub> dissolution (while preserving the viscosity reduction effect) using the Peng-Robinson equation of

state (Peng and Robinson 1976) is then discussed. The density effect is then examined for CO<sub>2</sub> injection in a 2D vertical cross section and in a 3D reservoir and the results are compared for cases with and without the density increase. This effect is investigated in: homogenous 2D domains with two different permeabilities and a heterogeneous 3D domain with random permeability distribution.

### **1.3 CO<sub>2</sub> Sequestration in Saline Aquifers**

Studies on CO<sub>2</sub> sequestration in saline aquifers have been performed since the early 90's. The first study of the reservoir simulation of CO<sub>2</sub> sequestration in a saline aquifer reported by van der Meer (1992). In the geological considerations for the storage site, he stated that an aquifer must be at a depth of at least 800 m for the injected CO<sub>2</sub> to remain in the supercritical state. This constraint has been followed in all the published work since. Gravity segregation and viscous fingering were found to be dominant CO<sub>2</sub> water displacement mechanisms.

Holt et al. (1995) used a black oil simulator to model CO<sub>2</sub> sequestration. Their aquifer model consisted of 4800 grid blocks and permeabilities ranged from 100-2000 mD with an average of 340 mD. The ratios between vertical and horizontal permeabilities varied from 0.02 to 0.045. The reservoir pressure and temperature was set to 2900 psi and 144 °F. The base case model has a CO<sub>2</sub> injection rate of 1.6 PV/year and the injection well was perforated through all layers. Based on the simulation results, they concluded that CO<sub>2</sub> storage in a heterogeneous aquifer depends strongly on injection rate and

permeabilities. An injection rate below 0.4% PV/year gave gravity stabilized displacement and high storage capacity (>30%). At rates of 1.6% PV/year and higher, the storage capacity became 16% PV and was rate independent.

Pruess et al. (2003) studied the amount of CO<sub>2</sub> that can be trapped into the various phases (gas, aqueous, and solid) for a range of conditions encountered in typical disposal aquifers. They estimated the combined storage capacity of CO<sub>2</sub> at 30 kg per unit of reservoir volume.

Kumar et al. (2005) performed simulation studies using the GEM compositional simulator to study CO<sub>2</sub> storage in saline aquifers. Simulations of a few decades of CO<sub>2</sub> injection followed by several thousand years of natural gradient flow were done. They concluded that the effect of residual gas on CO<sub>2</sub> storage was significant compared to storage in brine or minerals. Injecting CO<sub>2</sub> from the bottom half of the aquifer enhanced residual trapping and reduced the amount of mobile gas before it migrated to the aquifer seal. They also found that injecting water after the CO<sub>2</sub> injection period increases the storage capacities of solubility and mineral trapping.

Ennis-King and Paterson (2005) studied the role of convective mixing in the long-term storage of CO<sub>2</sub> in deep saline aquifers. The density of formation water increases upon dissolution with CO<sub>2</sub> which creates density instability. They used linear stability analysis to estimate when this instability would occur in anisotropic systems. This was

compared with numerical simulations performed using the TOUGH2 simulator. The simulator used a detailed equation of state (EOS) for CO<sub>2</sub>-brine systems on a 2D grid 500 m wide (50 grid blocks) and 400 m thick (100 blocks refined to 0.5 m at the top). The pressure at the top was 2610 psi and the temperature was 172 °F. They found that the time required for the convective instability to begin ranges from less than a year to hundreds of years depending on the permeability. This time is less than the total time required to dissolve CO<sub>2</sub> in a typical storage project, which can be up to tens of thousands of years.

Bryant et al. (2008) investigated whether the intrinsic instability of buoyancy driven flow leads to fingering of CO<sub>2</sub>. The mechanisms governing this type of displacement were studied in a series of fine grid simulations with a finite volume of CO<sub>2</sub> placed at the bottom of a 2D aquifer and only buoyancy driving the displacement. The GEM-GHG simulator was used in this study and simulation used 40,000 grid blocks. There were several fine-scale geostatistical realizations of permeability and the effect of capillary pressure and dip angle were also investigated. They found that CO<sub>2</sub> rises along preferential flow paths that are a consequence of rock properties (permeability, drainage capillary pressure curve and anisotropy). Capillary pressure broadens the lateral extent of the flow paths.

Burton et al.(2008) developed an analytical model using Darcy's Law and a modified form of the Buckley-Leverett theory. The long term injection of CO<sub>2</sub> dries out the near-

wellbore region. Drying removes the water from the near wellbore region but also precipitates salts altering the permeability. From their model, they concluded that quantifying the relative permeability curve is very important in determining achievable injection rate and therefore determining the well count for CO<sub>2</sub> sequestration projects. The well count in return strongly affects the economics of sequestration projects.

More recently, storage in shallow saline aquifers has also been investigated. Tiamiyu et al. (2010) used CMG-GEM in a study to find the optimal combination of operational parameters: injection rates, well completion types, and brine withdrawal strategy to harness CO<sub>2</sub> storage potential and leakage risk mitigation in shallow saline aquifers. The motivation behind this study was that deep saline aquifers may not always be present near the CO<sub>2</sub> source. The aquifer top was set at 550 m (1804 ft.) and the initial reservoir pressure of 810 psi was used. This is well below the critical pressure of CO<sub>2</sub>. They found that the potential of CO<sub>2</sub> storage in shallow saline aquifers can be greatly enhanced using brine withdrawal. Using horizontal wells that completed in the bottom of a moderately heterogeneous aquifer helps mitigate CO<sub>2</sub> leakage through the cap rock. Well perforation and orientation while having a negligible effect on CO<sub>2</sub> injectivity, extended the injection period until the aquifer reached the maximum allowable injection pressure.

Many of the studies discussed above assume a constant pressure outer boundary. Economides and Ehlig-Economides (2009) through a simple analytical model showed that assuming a constant pressure boundary neglects the critical point that reservoir

pressure will build up under a constant injection rate. They concluded that CO<sub>2</sub> can occupy no more than 1% of the pore volume. Barrufet et al. (2010) performed a comparison study of the CO<sub>2</sub> storage capacity between a depleted gas condensate reservoir and equivalent saline aquifer. They found that due to the low overall compressibility of aquifers, the mass of CO<sub>2</sub> sequestered per pore volume is approximately 13 times lower than that of a depleted gas condensate model. However, due to their large extent, aquifers still can provide storage for significant volumes of CO<sub>2</sub>.

First-order finite difference methods present numerical dispersion errors unless very fine gridding is used. This can be computationally expensive. Moortgat and Firoozabadi (2010) modeled two phase compositional flow in anisotropic media using a combination of high-order finite element methods. They used the mixed hybrid finite element method to solve for pressure and fluxes, and the discontinuous Galerkin method to update the mass transport. This method reduced numerical dispersion, captured shock fronts more accurately and lowered the dependence on mesh quality and orientation. By using this higher-order method, coarser meshes can be used at a lower CPU cost, compared to traditional finite difference methods. In a later work (Moortgat et al. 2011), they also suggested the use of cubic-plus-association (CPA) equation of state, instead of Henry's law to more accurately model the effect of cross association of water and CO<sub>2</sub> molecules on phase behavior.

### ***1.3.1 Field Injection Studies***

The Sleipner project in offshore Norway is the world's first commercial-scale CO<sub>2</sub> storage project injecting CO<sub>2</sub> in the sands of the Utsira formation at 1million tons per year (Gale et al. 2001). The Utsira formation is a moderately sorted, uncemented sand that has a high porosity The Saline Aquifer Carbon Dioxide Storage (SACS) project consisted of the Statoil and partners along with several independent research organizations to plan and monitor the storage of CO<sub>2</sub>. They performed a simulation study using a modified black oil simulator. The reservoir pressure ranged from 8 to 10 MPa (1160 - 1450 psi) and temperature of 37 °C (98.6 °F). The formation porosity ranged from 27 to 30 % and permeability from 1 to 8 Darcy. Results of the injection planning studies revealed that CO<sub>2</sub> should be injected near the bottom of the formation to minimize areal distribution and maximize the dissolution in formation water. Up to 18% of the CO<sub>2</sub> injected was dissolved in the formation water. They predicted that the maximum extension of CO<sub>2</sub> after 20 years would be 3 km and supercritical conditions resulted in wider distribution of free CO<sub>2</sub>.

### ***1.3.2 Sources of CO<sub>2</sub> in Qatar***

In 2009, Qatar produced 3,154 billion cubic feet (Bcf) of natural gas which is approximately 8.6 bcf/day. The natural gas produced from the North field, Qatar's largest gas field, consists of 3.5 wt% CO<sub>2</sub> (Whitson and Kuntadi 2005). If the average gas density is 0.05 lb/ft<sup>3</sup>, then this translates to 2.54 million metric tons (tonnes) of CO<sub>2</sub> produced every year. The average daily design injection rate for CO<sub>2</sub> sequestration in



this case would need to be 132 million SCF/day. This rate was calculated by noting that 1 million tons is 50,045,455 lbmoles of CO<sub>2</sub>, and 1 lbmole of CO<sub>2</sub> occupies 379.4 SCF at standard conditions (House et al. 2003).

Real estate development in Qatar during recent years has also led to an increase in cement production. Producing 1 tonne of cement generates 0.83 tonnes of CO<sub>2</sub>. But fossil fuel combustion still remains the largest source of CO<sub>2</sub> emissions. According to the Carbon Dioxide Information Analysis Center (CDIAC), Qatar produced 17.1 million tonnes of CO<sub>2</sub> in 2007 (Fig. 1.1), out of which 10 million tonnes were produced from combustion of gas fuels. Cement production emitted 340,000 tonnes of CO<sub>2</sub>. Qatar has the highest per capita emissions of CO<sub>2</sub> in the world (14.02 tonnes). Comparatively, the US ranks as the 11<sup>th</sup> highest CO<sub>2</sub> emitter per capita (5.2 tonnes). There is a need for CO<sub>2</sub> mitigation in Qatar.

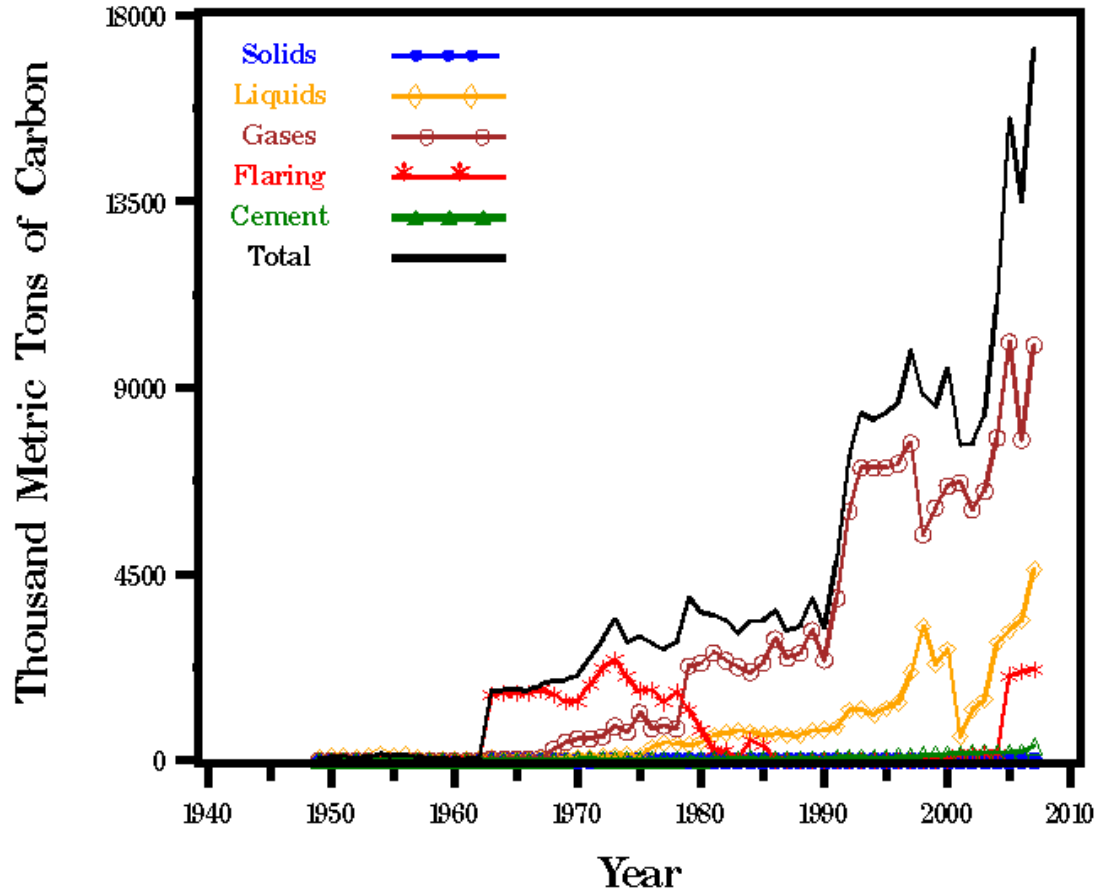


Fig. 1.1 —Fossil-Fuel CO<sub>2</sub> Emissions for Qatar from 1949 to 2007. (CDIAC 2007)

#### 1.4 Review of Sections

Section 2 describes the process of modeling the abnormal density behavior seen in CO<sub>2</sub>/crude oil mixtures. A brief literature review about effect of CO<sub>2</sub> solubility on oil density is presented. A fluid model for the GEM compositional simulation is then developed.

Section 3 describes the 2D and 3D models developed for the GEM simulator. The fluid model capturing the density increase is compared with the default model. The effect of injection depth is also investigated in homogenous and heterogeneous models.

Section 4 discusses the transport processes and trapping mechanisms involved in CO<sub>2</sub> sequestration.

Section 5 discusses the development of a CO<sub>2</sub> sequestration reservoir model for a saline aquifer in Qatar. The geology of the Aruma aquifer along with the data used to build the base case model is described briefly. The effects of diffusion are also investigated.

Section 6 outlines conclusions and recommendations for further work.

## **2. MODELING THE ABNORMAL DENSITY BEHAVIOR IN CO<sub>2</sub>/CRUDE OIL MIXTURES**

### **2.1 Effect of CO<sub>2</sub> Solubility on Oil Density**

There are several published data that report an increase in liquid hydrocarbon density upon CO<sub>2</sub> dissolution. Lansangan and Smith (1993a) have found that mixtures of CO<sub>2</sub> and a West Texas crude oil show monotonic viscosity decrease and the density increase with increased CO<sub>2</sub> concentration. They suggest that the increase in density might be caused by strong intermolecular Coulombic interactions between CO<sub>2</sub> and hydrocarbon molecules.

DeRuiter et al. (1994) studied the solubility and displacement of viscous crudes with CO<sub>2</sub> and have found that the oils exhibit an increase in density due to CO<sub>2</sub> solubility. The two samples in their study with API gravities of 18.5 and 14 exhibited an increase in density upon CO<sub>2</sub> dissolution. In a study of a West Texas crude oil, Grigg (1995) observed a 2% increase in oil density (after the addition of CO<sub>2</sub> and before the phase split) while the viscosity decreased. After the phase split, the traditional viscosity-density relationship was observed; viscosity increased (decreased) when density increased (decreased).

Ashcroft and Ben-Isa (1997) report on the effect of dissolved air, nitrogen, oxygen, methane, and carbon dioxide on the densities of liquid hydrocarbons. The hydrocarbons

include heptanes, octane, nonane, decane, dodecane, tetradecane, hexadecane, cyclohexane, methylcyclohexane, and methylbenzene (toluene). Their data shows that saturation of hydrocarbon liquids with gases other than CO<sub>2</sub> results in a decrease in density while saturation with CO<sub>2</sub> causes an increase in density.

## **2.2 Fluid Selection**

As discussed in the previous section, there may be an increase in oil density and a decrease in viscosity with CO<sub>2</sub> dissolution. Lansangan and Smith (1993b) report density and viscosity measurement trends for oil samples from West Texas. The fluid sample (RO-B) from their paper was used in this study as it shows relatively high increase in density (about 5%) with CO<sub>2</sub> dissolution. They report a density of 0.74 g/cc and viscosity of 0.77 cp at 1700 psia and 116 °F for this fluid.

## **2.3 Fluid Characterization**

The CMG WINPROP software is used to match the density and viscosity of the oil sample by performing regression on critical properties, binary interaction coefficients, and shift parameters for the heavy fractions and viscosity correlation parameters. In this work, the Peng-Robinson EOS is used to calculate phase behavior, and density (with volume shift parameters) and the Pedersen et al. (1987) correlation to calculate viscosity. To improve the accuracy of predictions, the original C<sub>7+</sub> heavy fraction (reported by Lansangan and Smith (1993b)) was split into three pseudo-components.

Table 2.1 lists the fluid composition with the heavy fraction split and Table 2.2 shows the measured density and viscosity with CO<sub>2</sub> dissolution in single phase. The calculated density and viscosity of the CO<sub>2</sub>/oil mixtures for increasing CO<sub>2</sub> solubility using the tuned EOS parameters are reported in Table 2.3. To predict the increasing density trend, the volume shift parameter of CO<sub>2</sub> was modified. By changing the CO<sub>2</sub> volume shift parameter, the density increase in the fluid from CO<sub>2</sub> dissolution can be modeled without affecting the calculated viscosity. This is due to the fact that in the Pedersen correlation the viscosity of the mixture depends on the viscosity (and density) of a reference component (usually methane) and other factors that are independent of mixture density. Therefore, modifying the shift parameter of CO<sub>2</sub> does not affect the viscosity of the mixture.

<b>Table 2.1 – Fluid composition (Fluid ‘RO-B’ from Lansangan and Smith (1993b))</b>	
Components	Initial composition (mole fraction)
CO <sub>2</sub>	0.0220
C <sub>1</sub>	0.2228
C <sub>2</sub>	0.1285
C <sub>3</sub>	0.1235
C <sub>4</sub>	0.0819
C <sub>5</sub>	0.0386
C <sub>6</sub>	0.0379
C <sub>7-12</sub>	0.1301
C <sub>13-21</sub>	0.1085
C <sub>22+</sub>	0.1062

**Table 2.2 – Measured density and viscosity vs. CO<sub>2</sub> composition in CO<sub>2</sub>/oil mixture (Fluid ‘RO-B’ from Lansangan and Smith (1993b))**

CO <sub>2</sub> composition	measured viscosity (cp)	measured density (g/cc)
0.022	0.770	0.744
0.034	0.683	0.745
0.1506	0.530	0.749
0.3498	0.419	0.761
0.5482	0.380	0.782

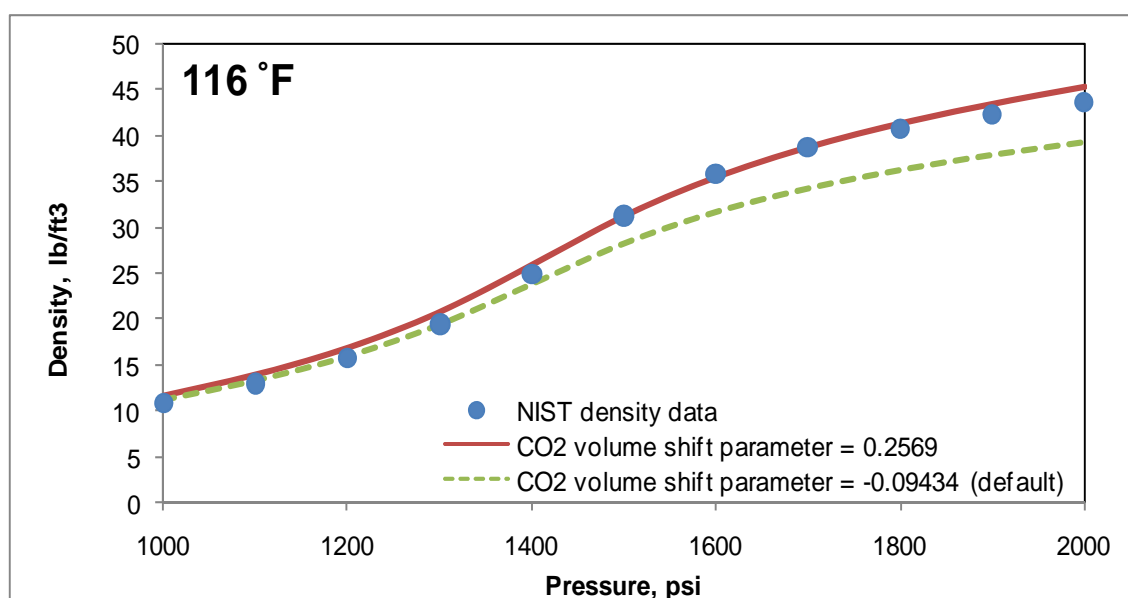
**Table 2.3 – Fluid critical properties and other relevant data**

Components	T <sub>c</sub> (K)	P <sub>c</sub> (atm)	MW (g/mole)	$\omega$	B/C CO <sub>2</sub> -comp <sub>i</sub>	B/C C <sub>1</sub> -comp <sub>i</sub>
CO <sub>2</sub>	304.2	73.76	44.01	0.2250	0.000	0.100
C <sub>1</sub>	190.6	46.00	16.04	0.0080	0.100	0.000
C <sub>2</sub>	305.4	48.84	30.07	0.0980	0.100	0.003
C <sub>3</sub>	369.8	42.46	44.10	0.1520	0.100	0.009
C <sub>4</sub>	425.2	38.00	58.12	0.1930	0.100	0.015
C <sub>5</sub>	469.6	33.74	72.15	0.2510	0.100	0.021
C <sub>6</sub>	507.5	32.89	86.00	0.2750	0.100	0.025
C <sub>7-12</sub>	569.6	21.11	126.19	0.3462	0.100	0.038
C <sub>13-21</sub>	790.3	15.00	218.64	0.4636	0.080	0.070
C <sub>22+</sub>	1075.4	9.65	442.38	0.8050	0.100	0.129

### **2.3.1 Basis for Modification of CO<sub>2</sub> Volume Shift Parameter**

The CO<sub>2</sub> density is calculated using the Peng-Robinson EOS with the default volume shift parameter that WINPROP uses. This data is compared to the isothermal CO<sub>2</sub> density data at 116 °F from the National Institute of Standards and Technology (NIST).

NIST uses an equation of state developed for CO<sub>2</sub> by Span and Wagner (1996) with estimated density uncertainty ranging from 0.03% to 0.05%. The correlation of Jhaveri and Youngren (1988), used in many commercial simulators (including WINPROP) to calculate the volume shift parameters, may not be accurate for CO<sub>2</sub>. The default volume shift parameter by the Jhaveri and Youngren correlation underestimates the density as the pressure increases (Fig. 2.1). At 1700 psi and 116 °F, the correct CO<sub>2</sub> volume shift parameter is found to be 0.2569 which is significantly different from the value given by the Jhaveri and Youngren correlation (-0.09434). To model the increasing oil density with CO<sub>2</sub> dissolution, the initial oil density (without CO<sub>2</sub>) is first matched by adjusting the volume shift parameters of the heavy fractions. Then the CO<sub>2</sub> volume shift parameter is adjusted based on the pure CO<sub>2</sub> density.



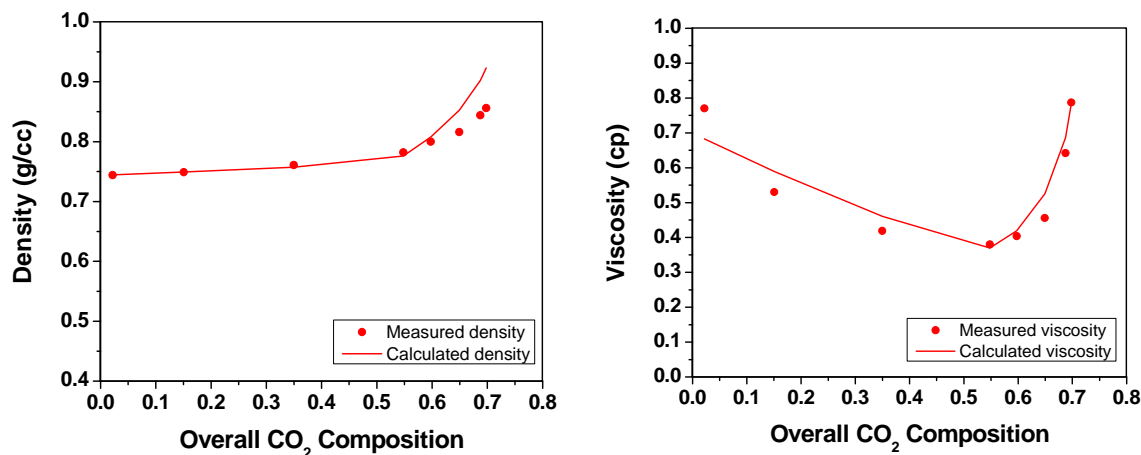
**Fig. 2.1 —Density of pure CO<sub>2</sub> at 116 °F from 1000-2000 psi (from the NIST Chemistry WebBook). The CO<sub>2</sub> density calculated with the Peng-Robinson EoS using the default volume shift parameter and an optimum value are compared against the NIST data.**



Table 2.4 lists the volume shift parameters of different components for the default case (decreasing density with CO<sub>2</sub> dissolution) and for the proper prediction of density (increasing density with CO<sub>2</sub> dissolution). Using the default CO<sub>2</sub> volume shift parameter gives an 11.7% difference in the value of pure CO<sub>2</sub> density at 1700 psia and 116 °F as can be seen in Fig. 2.1. Table 2.5 lists the Pedersen et al. correlation for viscosity model parameters. The results of density and viscosity predictions using parameters listed in Tables 2.3-2.5 are compared with measured values in Fig. 2.2. The densities and viscosities shown in Fig. 2.2 are the single phase liquid and two-phase liquid densities and viscosities. The phase-split occurs when the overall CO<sub>2</sub> mole composition is approximately 0.55. The calculated data match the increasing density trend in the single phase quite well but deviate when in the two-phase liquid region (max error of 7.8%). This can also be partially due to error in the two-phase composition measurements and limited available data to characterize EOS parameters.

<b>Table 2.4 – Volume shift parameters</b>		
Components	Default (decrease in density with CO <sub>2</sub> dissolution)	Adjusted (increase in density with CO <sub>2</sub> dissolution)
CO <sub>2</sub>	-0.09434	0.2569
C <sub>1</sub>	-0.15386	-0.15386
C <sub>2</sub>	-0.1021	-0.1021
C <sub>3</sub>	-0.0733	-0.0733
C <sub>4</sub>	-0.05706	-0.05706
C <sub>5</sub>	-0.03446	-0.03446
C <sub>6</sub>	-0.00499	-0.00499
C <sub>7-12</sub>	0.065225	0.1000
C <sub>13-21</sub>	0.14672	0.1900
C <sub>22+</sub>	0.06936	0.4700

<b>Table 2.5 – Parameter values for Pedersen et al. (1987) viscosity correlation</b>				
MW mixing rule coefficient	MW mixing rule exponent	Coupling factor correlation coefficient	Coupling factor correlation density exponent	Coupling factor correlation MW exponent
0.0001304	2.303	0.007378	1.847	0.5173

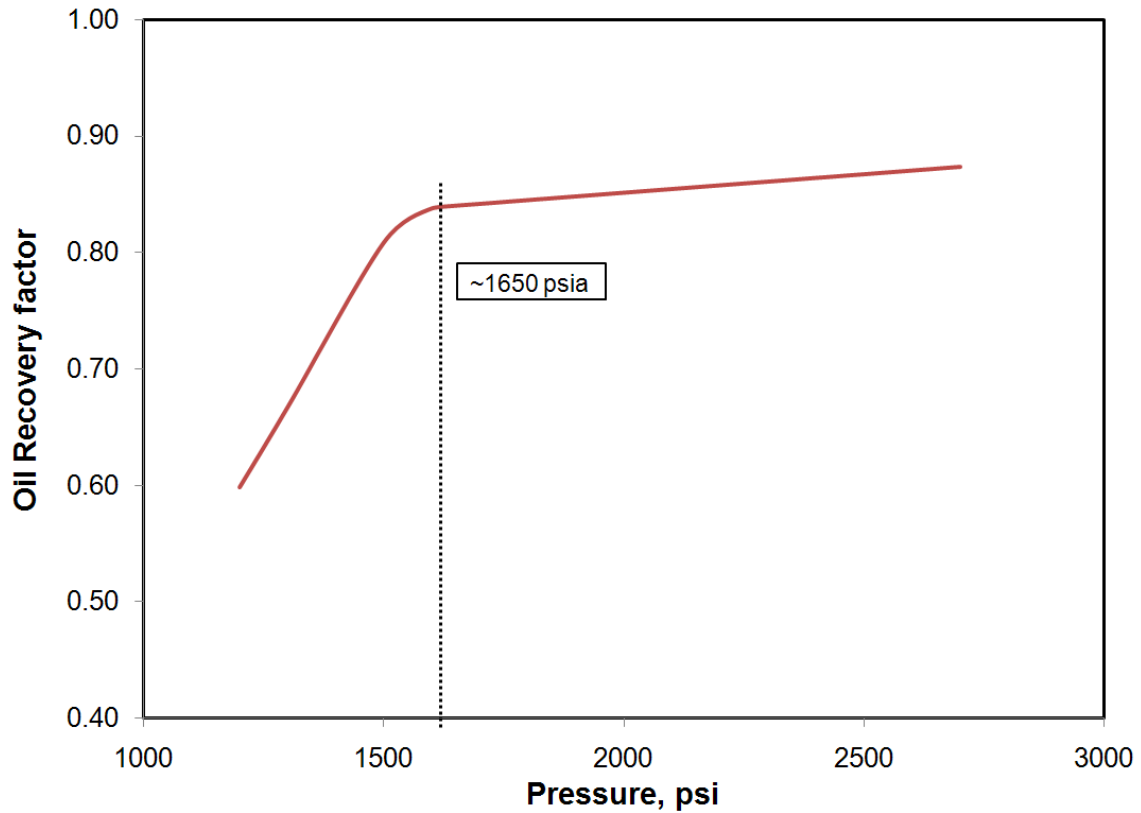


**Fig. 2.2 —Variation of density and viscosity with overall CO<sub>2</sub> composition (mole fraction) in CO<sub>2</sub>/oil mixtures for: Oil 'RO-B' (Table 2.1),  $P = 1700$  psi,  $T = 116$  °F. Measured values are from Lansangan and Smith (1993b). Computed density values are based on adjusted volume shift parameters.**

## 2.4 Validation of the Fluid Model through MMP Simulation

The characterized fluid is used to saturate a slim tube simulation model to validate the MMP. Data from Yellig and Metcalfe (1980) are used to simulate the slim-tube experiment. These authors employ a stainless steel tube with length of 40 ft (12.2 m) and diameter of 1/4-in. (6.3 mm) packed with 160-200 mesh sand. They report a permeability of approximately 2.5 Darcy and pore volume of 85 cm<sup>3</sup>. A constant injection rate of 0.00305 ft<sup>3</sup>/day is used (Yellig and Metcalfe 1980) to carry out the simulation runs for pressures ranging from 1100-2500 psi. Uniform initial composition and initial pressure are assumed. The oil recoveries at 1.2 PVI are plotted for each pressure (Fig. 2.3). A MMP of around 1650 psi is obtained. This is very close to the reported value of 1700 psi for this oil sample. Lansangan and Smith (1993b) do not report other measurements

related to fluid properties such as saturation pressure but based on the density, viscosity, and MMP comparisons between experimental and simulated data, the characterized fluid is representative of the original reported fluid.



**Fig. 2.3 —MMP validation of the characterized reservoir fluid RO-B in a slim tube simulation model. Simulated oil recoveries for different pressures are plotted at 1.2 PVI.**

### 3. 2D AND 3D SIMULATION RUNS

#### 3.1 Model Descriptions

To study the effect of density increase from mixing in flow path and recovery, CO<sub>2</sub> is injected in a 2D vertical cross-section and in a 3D domain. A commercial compositional simulator (CMG GEM) with a fully-implicit scheme is used for simulations.

##### *3.1.1 2D Model Description*

A domain with a length of 1200 ft (365 m) and depth of 200 ft (61 m) and width of 16.4 ft (5 m) is used in the 2D model. There are 240 grids in the  $x$ -direction (length) and 40 grids in  $z$ -direction (depth). Grid sensitivity tests show that the gridding is adequate for the 2D examples. The use of finer gridding also corrected the numerical diffusion seen in the CO<sub>2</sub> flow path. A constant porosity of 22.35% is used in this model.

##### *3.1.2 3D Model Description*

In the 3D domain, a  $\frac{1}{4}$  five-spot pattern with an injector-producer spacing of 1200 ft (365 m) and a depth of 200 ft (61 m) is modeled. The total pattern area is 60 acres and the length and width of the  $\frac{1}{4}$  five-spot pattern is 848 ft (258 m). This model has the same porosity as the 2D domain except for the random heterogeneity example. In 3D examples, there are 21 grids in  $x$ -direction, 21 grids in  $y$ -direction (width), and 20 grids in  $z$ -direction. Grid sensitivity tests showed that this level of gridding was accurate.

### 3.1.3 Well Constraints

In both 2D and 3D examples, the injector is located at the top (bottom) on one side of the formation and the producer is located at the bottom (top) on the opposite side. In these examples, the injection rate is constant (approximately 0.05 PV/year) and the pressure at the producing well is set equal to 1700 psi, the reported reservoir pressure of the fluid.

### 3.1.4 Rock-Fluid Data

The gas and oil relative permeability data used in all the examples are listed in Table 2.6.

The capillary pressure is assumed to be zero.

<b>Table 2.6 – Gas and oil relative permeabilities</b>		
<u>Oil Saturation</u>	<u><math>k_{ro}</math></u>	<u><math>k_{rg}</math></u>
0.3	0	1
0.344	0.003	0.879
0.388	0.011	0.766
0.431	0.025	0.660
0.475	0.044	0.563
0.519	0.068	0.473
0.563	0.098	0.391
0.606	0.134	0.316
0.650	0.175	0.250
0.694	0.221	0.191
0.738	0.273	0.141
0.781	0.331	0.098
0.825	0.394	0.063
0.869	0.462	0.035
0.913	0.536	0.016
0.956	0.615	0.004
1	0.7	0

### 3.1.5 Numerical Model Parameters

Initial runs with fine grids gave a high material balance error. Therefore the following steps were taken to reduce the material balance error in GEM:

- The maximum change in pressure, saturation and global composition were changed to account for the high flow rates at the wellbore. The keywords associated with this are *NORM* (*\*PRESS*, *\*SATUR*, and *\*GMOLAR*).
- The convergence tolerance for the linear solver was reduced. (*PRECC*).
- The minimum time-step size (*DTMIN*) was reduced. The default maximum time-step (*DTMAX* = 365 days) was used.
- The calculation settings for GMRES were changed. GMRES is an acceleration procedure to solve the linear systems in compositional simulations. The keywords associated this are *NORTH* and *ITERMAX*.

The detailed values of the parameters stated above can be found in the example data file in Appendix A. This numerical scheme gave material balance errors of less than 1% for all of the simulation runs.

## 3.2 Simulation Results

To show the effect of density on CO<sub>2</sub> flow path and oil recovery, a number of 2D and 3D simulations were performed. In each case, there were two different density change case as CO<sub>2</sub> dissolved in oil. The reference case has the default volume shift parameters (used in the commercial simulator) where there is a decrease in oil density with CO<sub>2</sub> dissolution. In the other case, the modified CO<sub>2</sub> shift parameter (as in Table 2.4) is used,

where the oil density increases with CO<sub>2</sub> dissolution. In both 2D and 3D examples it is observed that the effect of increasing density with CO<sub>2</sub> dissolution can have a significant effect on the flow path, time of breakthrough and recovery. The results are presented in the sections below.

### ***3.2.1 Homogenous Domains***

In the first example a constant permeability of 100 mD was used in the domain. Fig. 3.1 compares CO<sub>2</sub> composition profiles in the domain at 0.05, 0.1, 0.3, and 0.7 PV injection for both the default case (where oil density decreases with CO<sub>2</sub> dissolution) and for the case with increasing oil density with CO<sub>2</sub> dissolution. The injector is located at the top-left corner and the producer is located at the right-bottom corner of the domain. The results show the effect of increasing density on CO<sub>2</sub> composition in flow path and front shape. There is a slight difference in the flow path between the increasing density and decreasing density cases when CO<sub>2</sub> is injected from the top.



There is, however, a drastic change in the flow path when CO<sub>2</sub> is injected from the bottom and produced at the top. Fig. 3.2 depicts simulation results for this case with  $k = 100$  mD. In some CO<sub>2</sub> injection schemes the density of CO<sub>2</sub> is close to the oil density and CO<sub>2</sub> may be injected in the bottom. At the injection point, the CO<sub>2</sub> density ranges from 0.59 to 0.63 g/cc; the oil density is approximately 0.74 g/cc before mixing with CO<sub>2</sub>. Unlike the decreasing density case in Fig. 3.1 where CO<sub>2</sub> tends to move upward and then right towards the producer at the top, with increasing density, there is a tendency for CO<sub>2</sub> to move along the bottom/middle of the domain. Results at 0.7 PVI show a high CO<sub>2</sub> sweep efficiency with increasing density. The high sweep efficiency results in a significantly longer breakthrough time and ultimate recovery (Fig. 3.3). For bottom injection, with increasing density, the predicted recovery is 59% whereas for the decreasing density, the predicted recovery is 51%. In the top injection, with increasing density, the predicted recovery is 52% whereas for the decreasing density, the predicted recovery is 53%. In this example, bottom injection (including the density effects) resulted in more recovery than top injection which is a common industry practice. The GEM simulation data file used for the 100 mD case is provided in Appendix A.

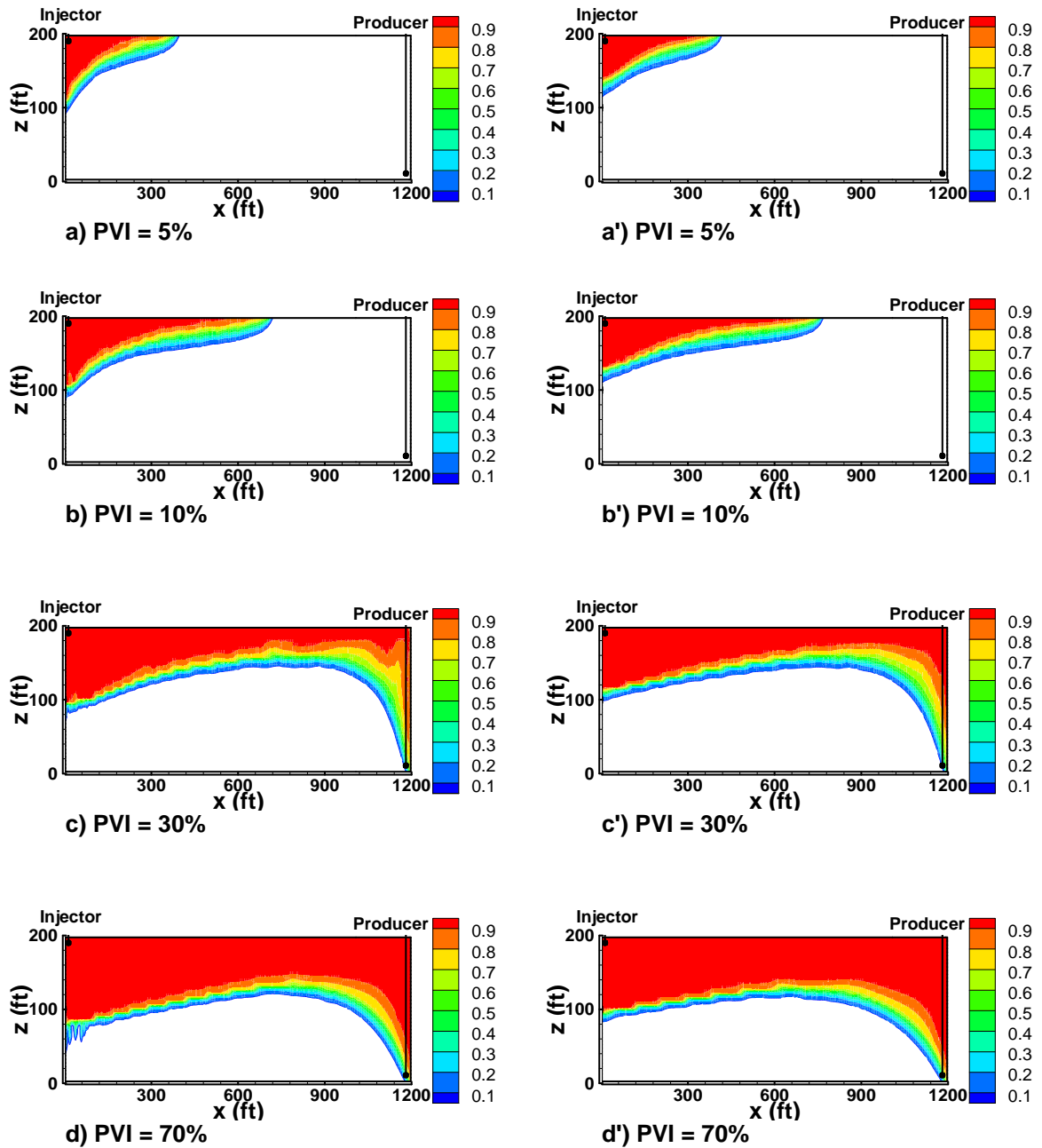
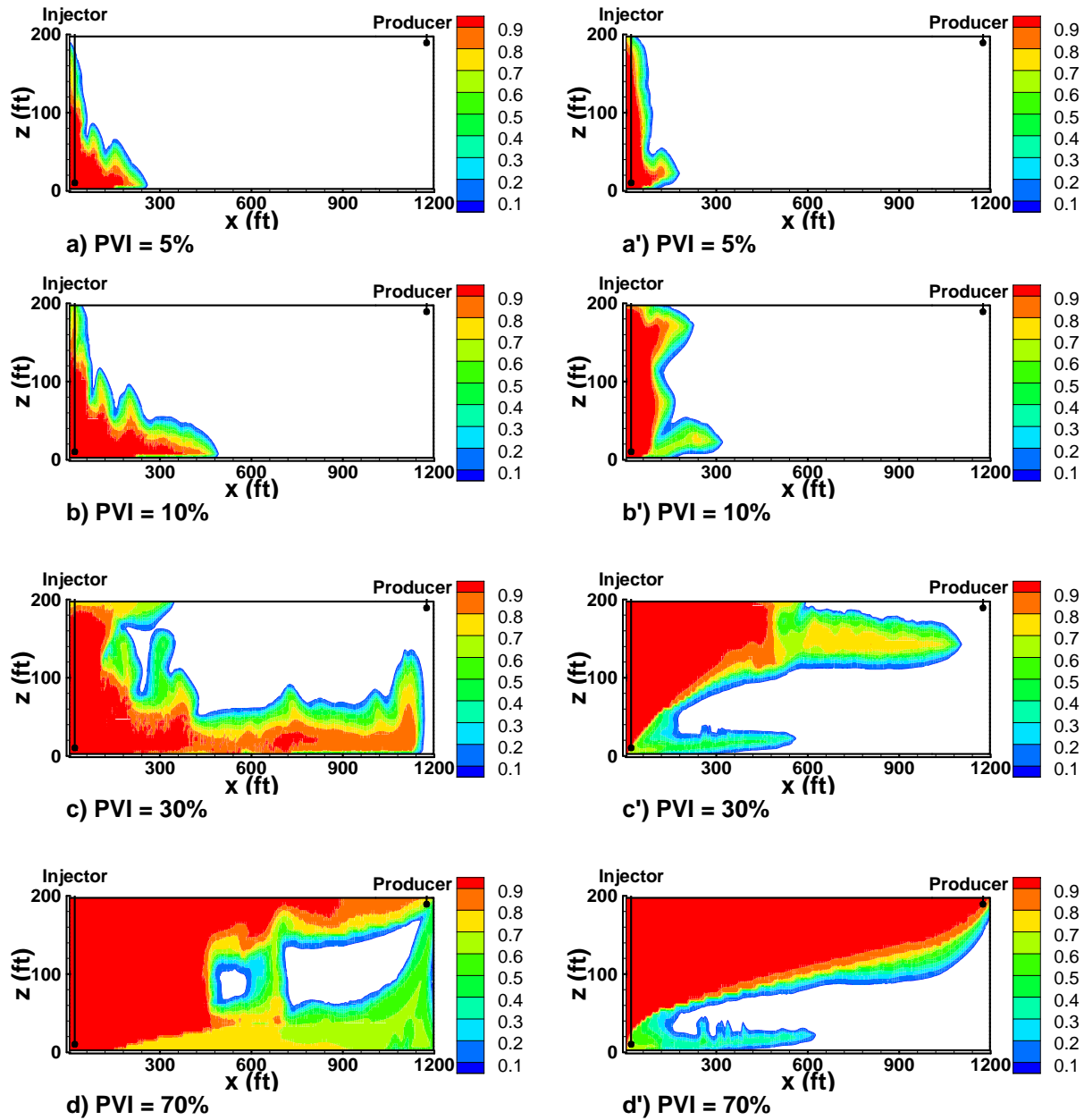
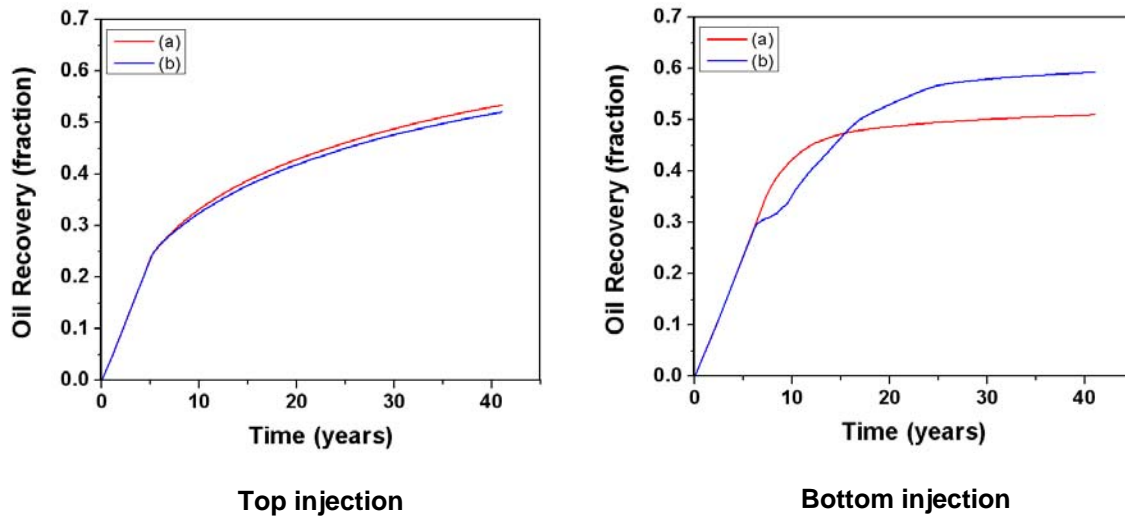


Fig. 3.1 —Overall CO<sub>2</sub> composition (mole fraction) at different PVI for (a, b, c, d) increasing density with CO<sub>2</sub> dissolution and (a', b', c', d') decreasing density with CO<sub>2</sub> dissolution: top injection, homogenous 2D media,  $k = 100$  mD.



**Fig. 3.2 —Overall CO<sub>2</sub> composition (mole fraction) at different PVI for (a, b, c) increasing density with CO<sub>2</sub> dissolution and (a', b', c') decreasing density with CO<sub>2</sub> dissolution: bottom injection, homogenous 2D media,  $k = 100$  mD.**



**Fig. 3.3 —Oil recovery vs. time for (a) decreasing density with CO<sub>2</sub> dissolution and (b) increasing density with CO<sub>2</sub> dissolution: homogenous 2D media,  $k = 100$  mD.**

For a permeability of 1000 mD, there is a pronounced occurrence of gravity fingers especially for the top injection case with increasing density (Fig. 3.4). If the producer well is located below the injector well, there will be a breakthrough as was the case for CO<sub>2</sub> injection in the Weeks Island study (Johnston 1988). There is also an increase in density for the case of decreasing density with CO<sub>2</sub> dissolution due to vaporization of methane from the liquid phase in the gas phase giving rise to gravity fingers as can be seen in Fig. 3.4 c'. Due to the position of the producer, the breakthrough time and recovery for the two cases is nearly the same. The 3D results in the homogeneous domain with  $k = 100$  mD and  $k = 1000$  mD are qualitatively similar in 2D and 3D and are not discussed for the sake of brevity.

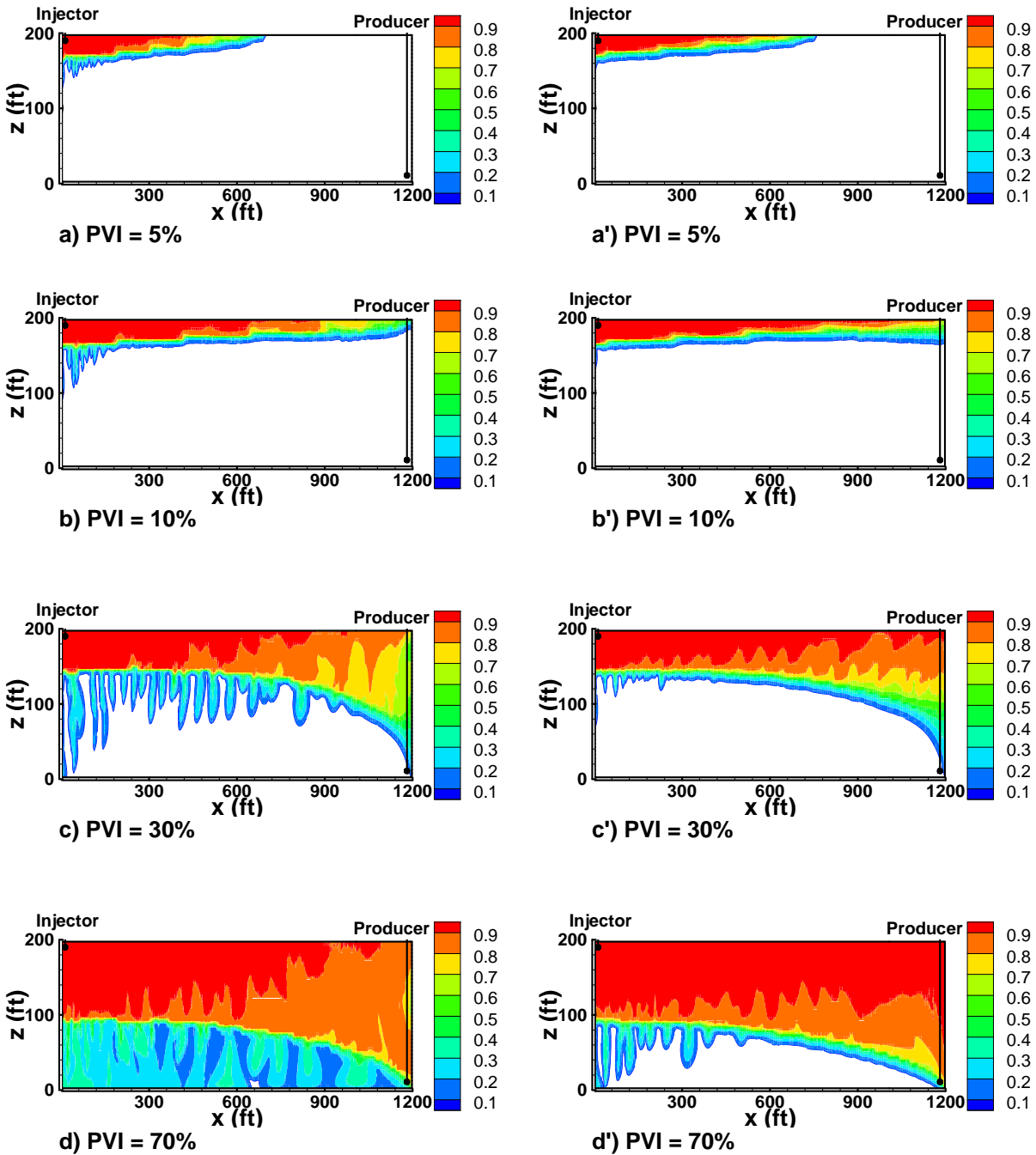


Fig. 3.4 – Overall CO<sub>2</sub> composition (mole fraction) at different PVI for (a, b, c) increasing density with CO<sub>2</sub> dissolution and (a', b', c') decreasing density with CO<sub>2</sub> dissolution: top injection, homogenous 2D media,  $k = 1000$  mD.

### 3.2.2 Heterogeneous Domains

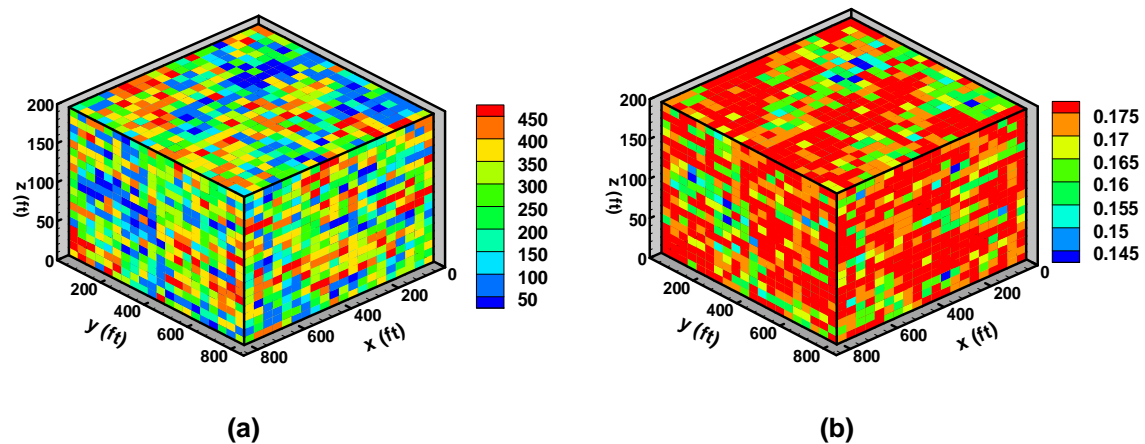
To study the density effect in heterogeneous domains, two examples are considered. Both examples have random permeability distribution and differ only in the degree of heterogeneity. In the first example, Gaussian geostatistical simulation is used to assign permeabilities to the grid blocks ranging from 10 mD to 500 mD (Fig. 3.5a). The porosity (Fig. 3.5b) in each grid block is related to permeability by:

$$\phi_i = 0.11889 + 0.02277 \log(k_i) \quad (k_i \text{ in mD}).$$

This method produces a highly heterogeneous domain. Fig. 3.6 shows the density effect on CO<sub>2</sub> flow path for the top and bottom injection scenarios; both exhibit better vertical sweep efficiency when the increasing density is modeled. Fig. 3.7 shows the recovery profiles for the top and bottom injection scenarios. For both cases, the recovery with density increase is higher than that with density decrease. The recovery from bottom injection is about 48% with density increase while it is 31% with density decrease. The breakthrough time for bottom injection is extended by 2 years when the density effect is included. There is less gas production in the top injection cases than the bottom injection cases.

In the next example, ordinary kriging is used to assign permeabilities to the grid blocks ranging from 10 mD to 500 mD (Fig. 3.8a). The porosity is related to the permeability using the same expression as the previous example (Fig. 3.8b). Even though the

permeability distributions in the two examples are quite different, the density effects on flow path are very similar (Fig. 3.9). Fig. 3.10 shows the recovery profiles for the top and bottom injection scenarios. For both cases, the recovery with density increase is higher than that with density decrease. The recovery from bottom injection is about 47% with density increase while it is 30% with density decrease. Breakthrough occurs after 2 years with density decrease, while it occurs after 4 years with density increase.



**Fig. 3.5 —Distribution of (a) permeability (mD) and (b) porosity( fraction) in the heterogeneous 3D media using Gaussian geostatistical simulation.**

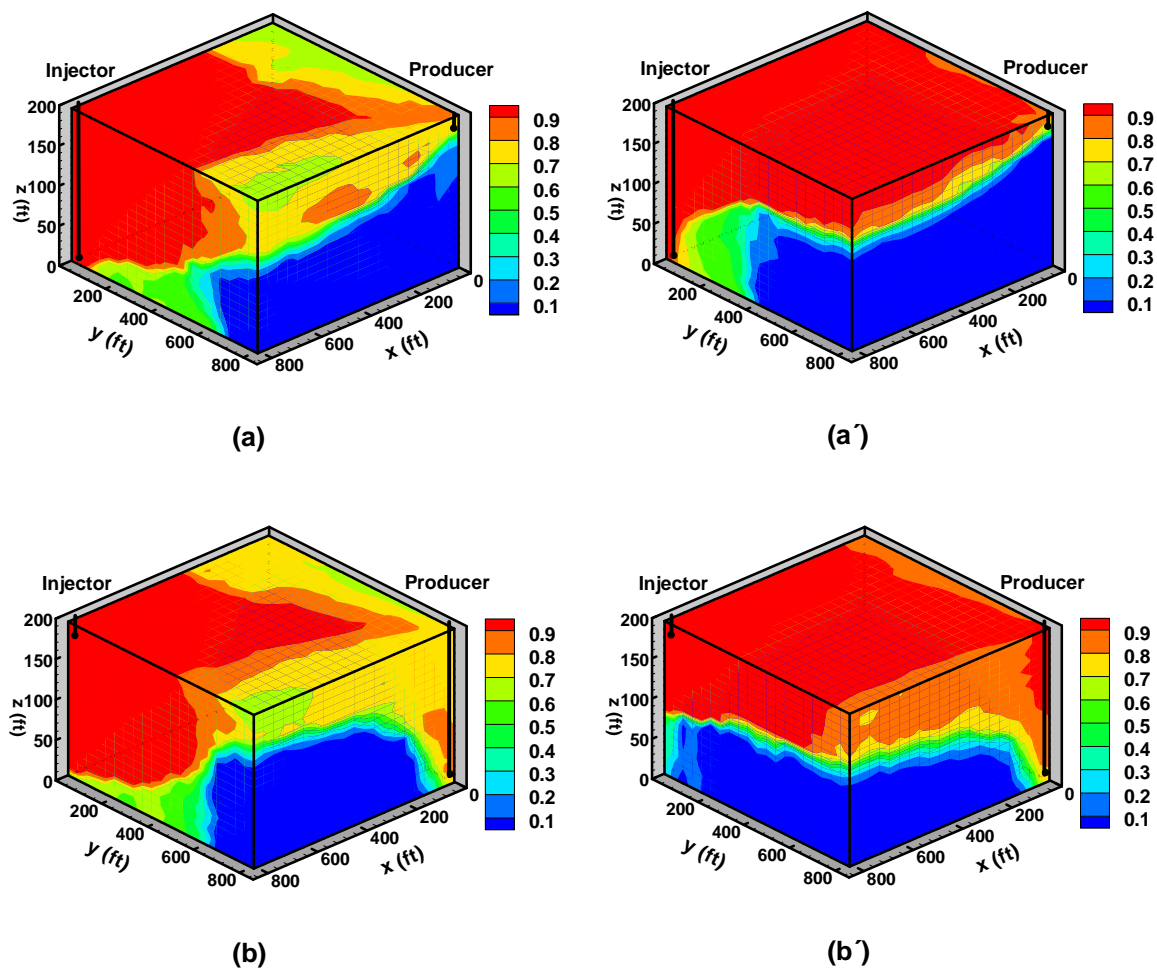


Fig. 3.6 —Overall CO<sub>2</sub> composition (mole fraction) at 70% PVI for (a, b) increasing density with CO<sub>2</sub> dissolution and (a', b') decreasing density with CO<sub>2</sub> dissolution: heterogeneous 3D media using Gaussian geostatistical simulation.



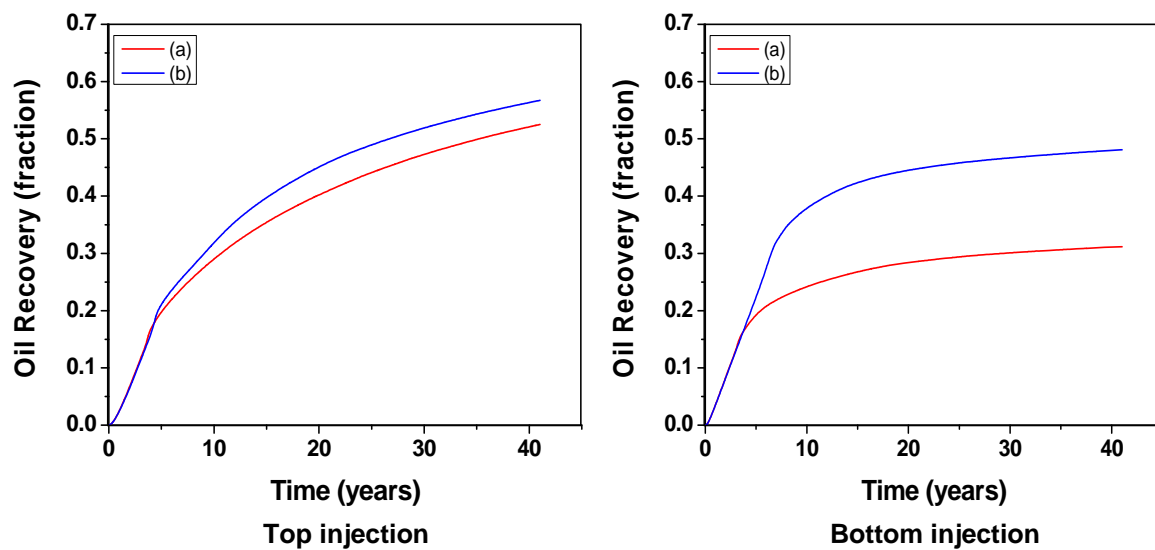


Fig. 3.7 —Oil recovery vs. time for (a) decreasing density with CO<sub>2</sub> dissolution and (b) increasing density with CO<sub>2</sub> dissolution: heterogeneous 3D media using Gaussian geostatistical simulation.

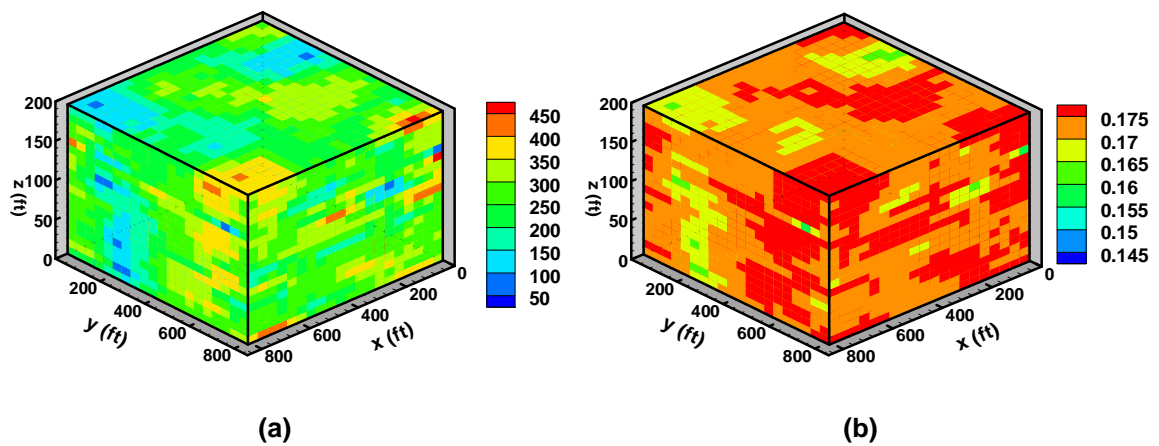


Fig. 3.8 —Distribution of (a) permeability (mD) and (b) porosity(fraction) in the heterogeneous 3D media using ordinary kriging.

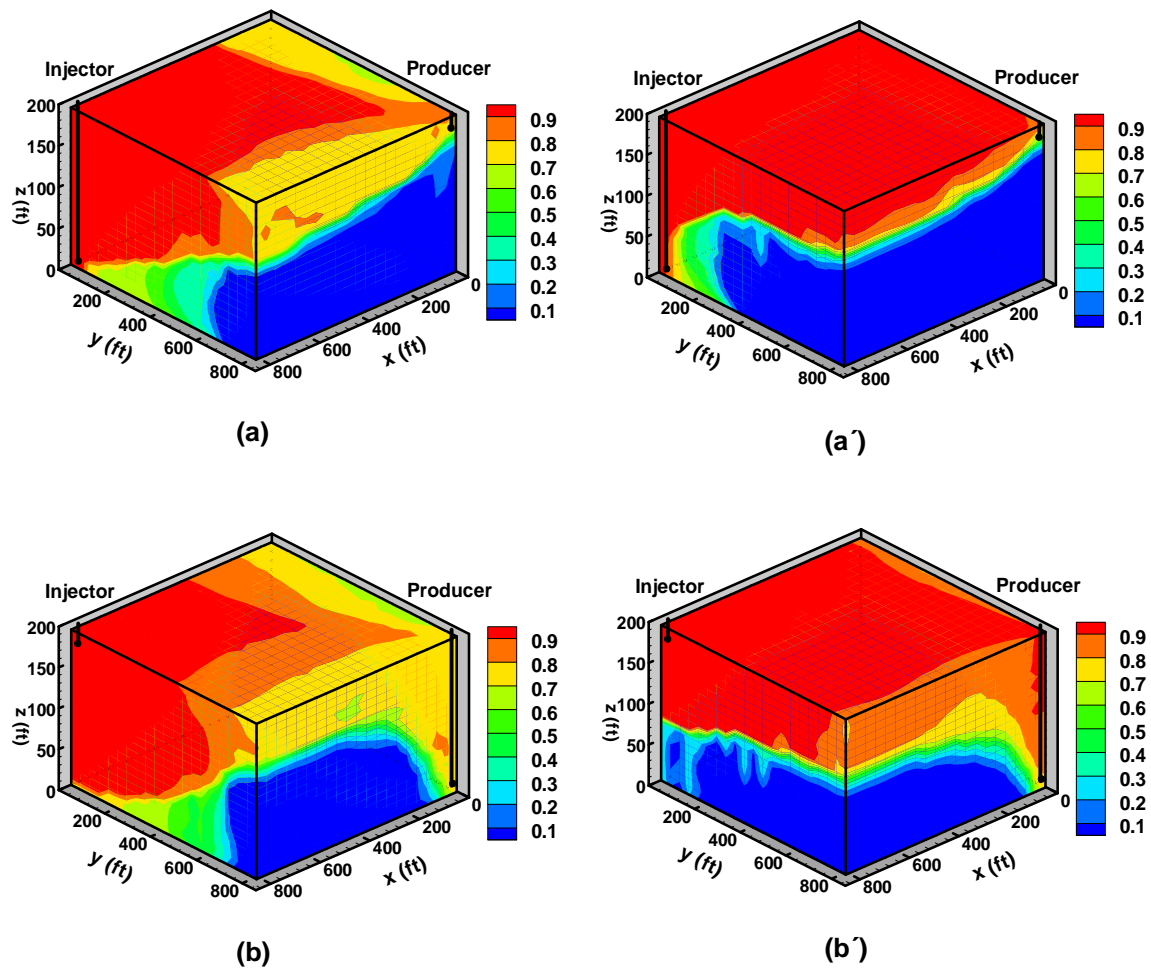
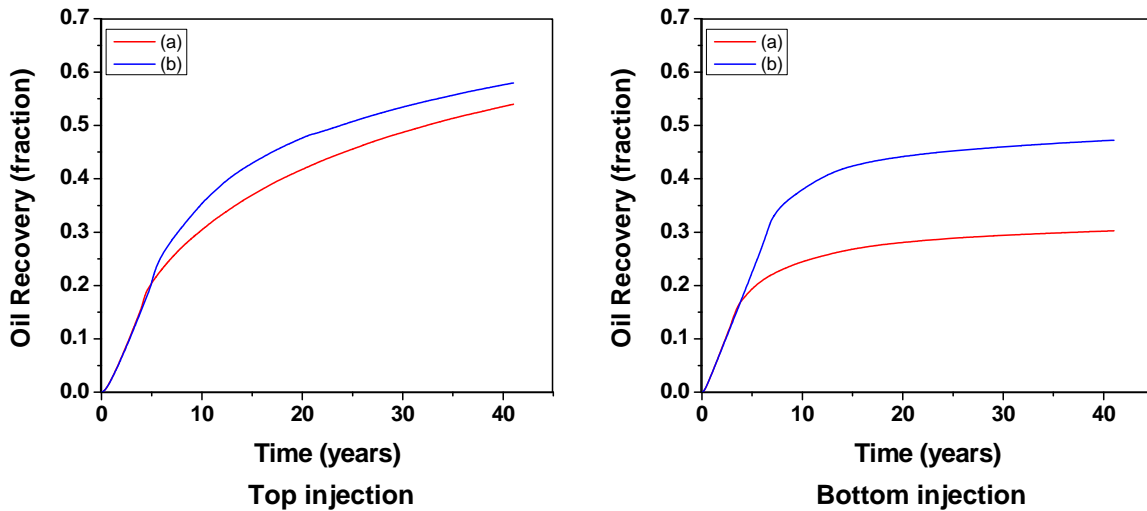


Fig. 3.9 —Overall  $\text{CO}_2$  composition (mole fraction) at 70% PVI for (a, b) increasing density with  $\text{CO}_2$  dissolution and (a', b') decreasing density with  $\text{CO}_2$  dissolution: heterogeneous 3D media using ordinary kriging.



**Fig. 3.10 —Oil recovery vs. time for (a) decreasing density with CO<sub>2</sub> dissolution and (b) increasing density with CO<sub>2</sub> dissolution: heterogeneous 3D media using ordinary kriging.**

### 3.3 Section Summary

A simple approach to model the increase in oil density with CO<sub>2</sub> dissolution using the Peng-Robinson EOS and the Pedersen viscosity correlation is presented. By changing the volume shift parameter of CO<sub>2</sub>, one can model the increase in oil density with CO<sub>2</sub> dissolution while preserving the viscosity match. The Peng-Robinson EOS can predict the density of pure CO<sub>2</sub> by adjusting the CO<sub>2</sub> volume-shift parameter. The use of the existing correlations for predicting the volume-shift parameters do not perform well for CO<sub>2</sub> injection at high pressures. While the slim tube MMP is independent of density effects, the oil density change from CO<sub>2</sub> dissolution can have a drastic effect on recovery performance as seen in the simulation results. Due to the 1D nature of flow in slim tube experiments, the density effect is not taken into account. In 2D and 3D, when injected

CO<sub>2</sub> is lighter than the oil phase, there may be no gravity stable displacement due to increase in oil density from solubility. When the density of the injected gas is less than the oil density, CO<sub>2</sub> injection may result in unstable gravity drainage. Past literature has neglected density effects in the study and evaluation of CO<sub>2</sub> injection. Density measurements for CO<sub>2</sub>/oil mixtures at different CO<sub>2</sub> compositions and prediction of these results in the fluid model can increase the reliability of the simulation results and decrease the degree of uncertainty. Heterogeneity may also have a significant effect as would be expected. The depth of injection and production wells with respect to the top of the reservoir may also have a major impact on recovery.

## CO<sub>2</sub> SEQUESTRATION IN SALINE AQUIFERS

In this section, the processes involved in CO<sub>2</sub> sequestration are discussed. Section 4.1 discusses the transport processes involved in CO<sub>2</sub> sequestration, followed by Section 4.2 discussing the various trapping mechanisms.

### 4.1 Transport Processes

The following transport processes are relevant to CO<sub>2</sub> storage in saline aquifers (Ukaegbu et al. 2009):

1. Advection is the movement of CO<sub>2</sub> caused by pressure gradients. When CO<sub>2</sub> is injected into saline aquifers, it flows away from the high-pressure injection points in a radial direction towards areas of low pressure according to Darcy's Law.
2. Buoyancy is caused by the density differences between the gas and the liquid phases. CO<sub>2</sub> being less dense will rise upwards as the brine sinks.
3. Diffusion is caused by the concentration gradients. Molecules of CO<sub>2</sub> will migrate from regions of higher concentration to regions of lower concentration to achieve equilibrium in chemical potential.

Advection is dominant during the injection period. Buoyancy is also an important transport mechanism since CO<sub>2</sub> is typically 40-60% less dense than the formation brine. Including diffusion in the modeling of CO<sub>2</sub> sequestration can have a significant effect on the storage of CO<sub>2</sub>. This is addressed in this study.

## **4.2 Trapping Mechanisms**

When injected in saline aquifers, CO<sub>2</sub> can be trapped through a combination of one or more chemical and physical processes. Orr et al. (2005) tried to postulate the time and length scales that characterize the sequestration of CO<sub>2</sub> and introduced two time periods: injection period and post-injection period. During the injection period, advection and gravity segregation are the dominant transport mechanisms. Heterogeneity determines the movement of low viscous CO<sub>2</sub> and appropriate representation of heterogeneity is important. Structural trapping of CO<sub>2</sub> and CO<sub>2</sub> trapping as a residual gas (hysteresis) are the main sequestration mechanisms during this phase. In the post-injection period (100 to 10000 years), buoyancy and capillary forces dominate over the viscous forces. Dissolution of CO<sub>2</sub> in brine and mineralization of CO<sub>2</sub> become more important as time progresses. These trapping mechanisms are discussed in detail below.

### ***4.2.1 Structural Trapping***

Structural trapping consists of trapping CO<sub>2</sub> in a flow system with low flow velocity over geologic periods of time (Nghiem et al. 2004). Being less dense than brine, CO<sub>2</sub> will rise upwards as a plume until it encounters the low permeability cap rock. CO<sub>2</sub> will then migrate laterally up dip along the seal if it is not horizontal. This is the first and most basic screening criteria for CO<sub>2</sub> sequestration in saline aquifers.

#### ***4.2.2 Residual Trapping***

Residual trapping is another effective trapping mechanism and is also most effective when the immobile gas is away from the cap rock. CO<sub>2</sub> trapped in pore spaces, from which water was displaced, will remain locked in place because of the capillary effect and cannot be displaced by imbibitions of any fluid (Tiamiyu et al. 2010). Kumar et al. (2005), through an inject low and let rise approach, have shown that residual trapping plays a dominant role in CO<sub>2</sub> storage. Bryant et al. (2008) further investigated whether the intrinsic instability of buoyancy driven flow leads to fingering of CO<sub>2</sub>. The mechanisms governing this type of displacement were studied in a series of fine grid simulations with a finite amount of CO<sub>2</sub> at the bottom of a 2D aquifer and only buoyancy driving the displacement. There were several fine-scale geostatistical realizations of permeability and the effect of capillary pressure and dip angle were also investigated. They found that CO<sub>2</sub> follows preferential flow paths that are a consequence of rock properties (permeability, drainage capillary pressure curve and anisotropy). Capillary pressure broadens the lateral extent of the flow paths.

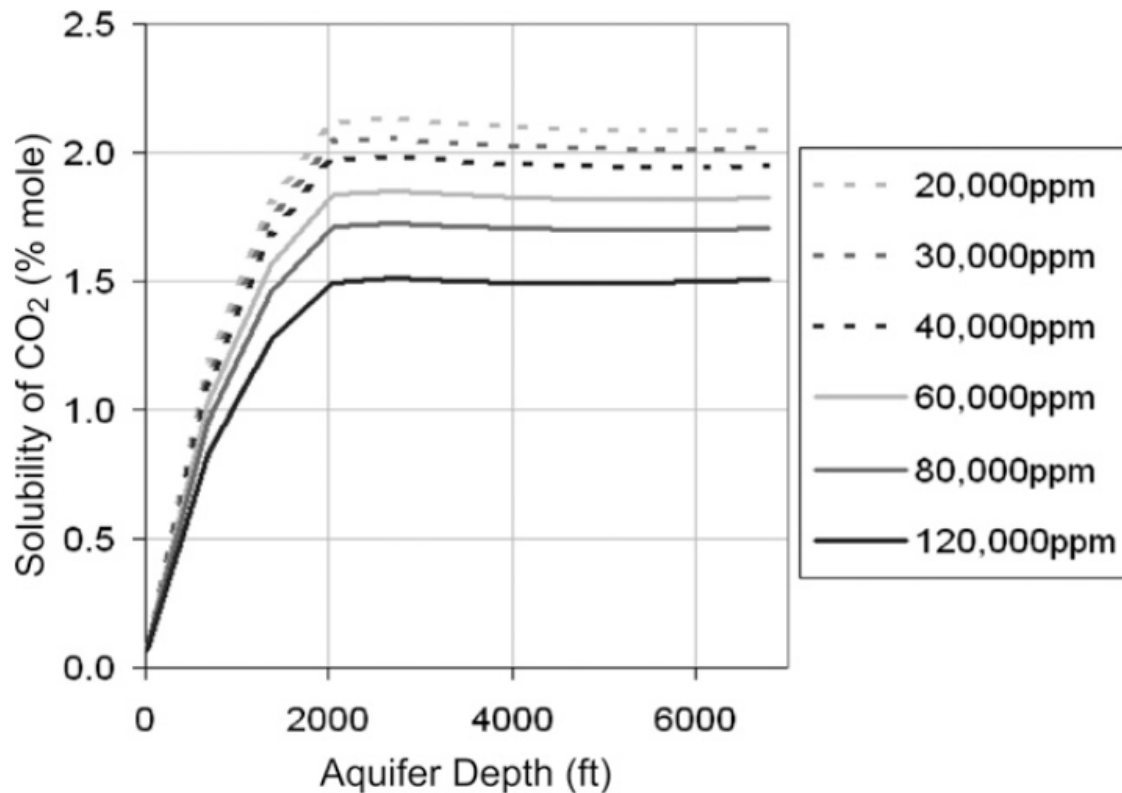
#### ***4.2.3 Solubility Trapping***

Solubility trapping involves the dissolution of CO<sub>2</sub> in the formation brine. The mixture of CO<sub>2</sub> and brine is denser than the fresh brine and this sets up a convective process in which the denser brine sinks to the bottom. The percentage of CO<sub>2</sub> dissolved in brines during the upward migration of CO<sub>2</sub> is typically less than 10%. Over a long period of time, the injected CO<sub>2</sub> will form a thin layer of CO<sub>2</sub> free phase which will slowly

dissolve in the underlying brine. There are several correlations available to calculate the density of CO<sub>2</sub> dissolved brine. Duan and Sun (2003) have the most comprehensive model for calculating CO<sub>2</sub> solubility in pure water and NaCl solutions from 273 to 533 K and 0 to 2000 bar. Their model is based on the equation of state of Duan et al. (1992) and the work on thermodynamics of electrolytes by Pitzer (1973). Comparison of their equation of state predictions with experimental data show that their results are close to experimental uncertainty which is about 7% in CO<sub>2</sub> solubility. The model is also extended to model CO<sub>2</sub> solubility in complex brines such as seawater with good accuracy.

Using the equation of state developed by Duan and Sun (2003), Burton and Bryant (2009) calculated the solubility of CO<sub>2</sub> in brine as a function of depth with the temperature and pressure gradients assumed to be 0.01 °F/ft and 0.44 psi/ft respectively. They found that beyond 2000 ft the solubility in brine remains constant (Fig. 4.1). Thus the formation depth presents neither advantage nor disadvantage for this process. They found the solubility of CO<sub>2</sub> at aquifer conditions to be around 2.1 mol%. This can be achieved with several combinations of pressure and temperature.





**Fig. 4.1 —The solubility of CO<sub>2</sub> in brine as a function of temperature pressure and salinity determined by the Duan and Sun EOS (Burton and Bryant 2008). Solubility increases with depth to ~2000 ft, and then remains constant. A geothermal gradient of 0.01 °F/ft and a hydrostatic gradient of 0.44 psi/ft are used. Brine salinity effects the plateau solubility.**

Fig. 4.1 cannot be reproduced directly by the Peng Robinson EOS. The solubility is tuned by the binary interaction coefficients (BICs), which are functions of temperature and salinity (Kumar 2004). If one set of BICs are used, the solubility will continue to increase even after 2000 ft, failing to capture the plateau. Recalculating the BICs at each depth captures the plateau, but this is a very inefficient process. Therefore the Peng Robinson EOS cannot model solubility in thick aquifers and aquifers with large temperature or salinity variations.

#### ***4.2.4 Aqueous Phase Diffusion***

Molecular diffusion describes the passive movement of molecules, due to random motion (Brownian motion), or due to a compositional gradient in the mixture, and is quantified by molecular diffusion coefficients (Leahy-Dios and Firoozabadi 2007). To include the effect of molecular diffusion, the diffusion coefficients of CO<sub>2</sub> in water are required. There is a lot of experimental data available for measuring molecular diffusion. Tamimi et al.(1994) reported the diffusion coefficients of CO<sub>2</sub> in water from 298 to 368K. For this study, (~313K) the diffusivity reported was  $2.93 \times 10^{-5} \text{ cm}^2/\text{s}$ . Frank et al. (1996) measured the diffusion coefficients and viscosities for CO<sub>2</sub>/H<sub>2</sub>O systems. At 318K, they reported a diffusion coefficient of  $3.07 \times 10^{-5} \text{ cm}^2/\text{s}$ . Renner (1988) developed a novel in-situ method to calculate the diffusion coefficients of CO<sub>2</sub> and other solvent gases in consolidated media at high pressures. The diffusion coefficient of CO<sub>2</sub> in 0.25 M NaCl brine at 100 F and pressures ranging from 647 to 846 psi was reported to be ranging from  $3.64 - 7.35 \times 10^{-5} \text{ cm}^2/\text{s}$ . Renner concluded that the diffusion coefficient of CO<sub>2</sub> in water or brine was an empirical function of liquid and CO<sub>2</sub> viscosities.

There have been diverging opinions in the literature on the effect of diffusion on the CO<sub>2</sub> sequestration process. Ukaegbu et al. (2009) found through a simulation study that the diffusion of CO<sub>2</sub> in the aqueous phase increases the amount of dissolved CO<sub>2</sub>. This increase was as much as 18% after 20 years into the simulation. They explained that the increase in CO<sub>2</sub> concentration in the gridblock cause CO<sub>2</sub> to migrate to areas of lower concentration to reduce the concentration difference, which allows greater dissolution.

On the other hand, Ennis-King and Paterson (2005) have shown through linear stability analysis that the dominant mechanism for dissolution of  $\text{CO}_2$  in water is convective mixing rather than diffusion. Moortgat and Firoozabadi (2010) state that current correlations used assume an effective diffusivity in which the diffusive flux of the component  $i$  only depends on its own compositional gradient. This could lead to an oversimplification, especially for 3 component systems. They suggest the use of Fickian diffusion.

### **4.3 Section Summary**

There has been a lot of work on  $\text{CO}_2$  sequestration in recent years. Researchers have investigated the dominant physical and chemical processes involved. Solubility and mineral trapping are the most desirable trapping mechanisms because the  $\text{CO}_2$  is sequestered in a form that is safe for the environment. The Peng Robinson EOS is not a suitable method to model  $\text{CO}_2$  solubility in brine. The literature discussed in this section along with published experimental data will be used in the development of a simulation model in the next section.

## **CO<sub>2</sub> SEQUESTRATION CASE STUDY: ARUMA AQUIFER**

### **5.1 Aquifer Description and Hydrogeology**

The Aruma aquifer is located in southwest Qatar. It occupies an area of about 1985 km<sup>2</sup> on land which is approximately 16% of Qatar's area. The Qatar Department of Agricultural and Water Research have drilled four deep wells in this aquifer to characterize it better. Regional monitoring of the groundwater levels and comprehensive logging were performed to better understand the aquifer. Water quality analysis was also performed at the four deep wells. Details of the drilling report completed by Al-Baida Technical Services (ATS) are presented in the next section (ATS 2004).

The Aruma aquifer comprises approximately 130 m (426 ft) of granular limestone belonging to the Aruma Formation. The top of the aquifer ranges from 380 to 550 m within southwest Qatar. The aquifer is overlain by thick relatively impermeable deposits of the lower Umm Er Radhuma (UER) aquifer and is underlain by a sequence of shales of up to 100 m thickness belonging to the lower Aruma Formation. These strata bound the aquifer and serve to isolate it from groundwater movement in other formations. The aquifer is highly confined within its bounding strata and this is confirmed by a very low "storativity" value. The storativity of an aquifer is a dimensionless number that equals to the volume of water released from a unit volume of aquifer per unit decline in pressure. There was also no evidence of leakage or drainage while testing. The overall thickness of the Aruma formation declines moving northwards from approximately 265 m in the

south to less than 240 m in the north. Within the formation, the upper limestone becomes thicker moving northwards while the shales at base become thinner.

## **5.2 Data Processing**

The approximate limits of the project area are shown in Fig. 5.1. There are 11 pre-existing deep wells in the project area numbered DW-1 through to DW-11. The new deep wells drilled were numbered DW-12, DW-13, DW-14 and DW-15. DW-12 and DW-13 were located adjacent to existing wells DW-03 and DW-11 in order to perform aquifer tests while observing water levels in the nearby deep wells. The new wells are located around the flanks of the Dukhan anticline which has a dip that exceeds  $0.5^\circ$ . DW-14 and DW-15 are located in the neighboring syncline while DW-12 and DW-13 are located on the anticlinal crest. Detailed logging was performed at each new deep well location. This data along with the limited log data of the existing deep wells was used to map the Aruma aquifer top and bottom. The log data of the wells available and those that are used in this study are provided in the Table 5.1. Table 5.2 provides a summary of the aquifer properties measured from log data and flow tests.

Using the log data and the results of the flow tests, maps were created for porosity, permeability, formation depth and thickness. Geographix software was used for the log analysis and creating the maps. These maps were then exported to CMG to create the static reservoir model. SI units were used in the static reservoir model as most of the data was reported in SI units. The results are reported in field units for ease of understanding.

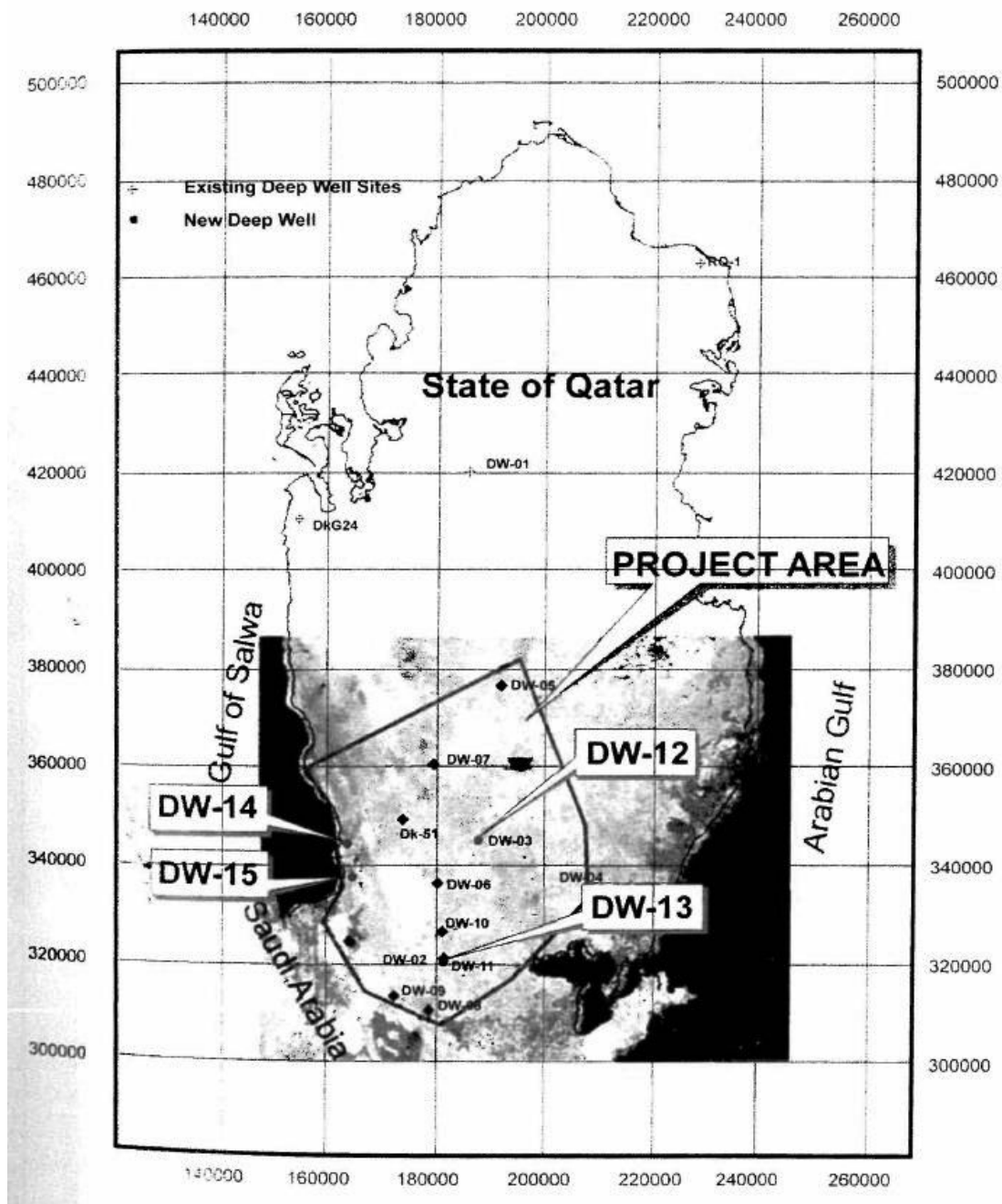


Fig. 5.1 —The project area and location of the deep wells (ATS 2004)

**Table 5.1 – Log data available for the Aruma aquifer**

Well	Gamma Ray	Sonic Log	Neutron Log	Density Log	Temperature	Resistivity
DW-6	X					X
DW-7	X					X
DW-8	X					X
DW-10	X					X
<b>DW-12 *</b>	X	X	X	X	X	X
<b>DW-13 *</b>	X	X	X	X	X	X
<b>DW-14 *</b>	X	X	X	X	X	X
<b>DW-15 *</b>	X	X	X	X	X	X
<b>* = newly drilled wells</b>						

**Table 5.2 – Aruma Aquifer properties**

Well	Top (ft)	Bottom (ft)	Thickness (ft)	Porosity (fraction)	Permeability (mD)	Temperature (°F)
DW-12	1585	2028	443	0.162	4187	112.8
DW-13	1503	1936	433	0.149	3395	115.5
DW-14	1880	2388	509	0.111	2263	116.9
DW-15	1854	2336	482	0.123	3508	118.2
Total Dissolved Solids, ppm			5000			
$k_v/k_h$			0.1			

It is important to note that the Aruma aquifer is highly permeable (Table 5.2). Firoozabadi and Cheng (2010) emphasize the selection of high permeability aquifers to store CO<sub>2</sub> because they aid in the rapid dissolution of CO<sub>2</sub> in brine.

### 5.3 Base Case Model Description

A three dimensional corner point fine grid was used to model the project area. The model consists of 106 grids in the  $x$ -direction, 145 grids in the  $y$ -direction (width), and 7 grids in the  $z$ -direction. The Aruma aquifer is modeled with five layers in the  $z$ -direction. The two layers above it represent the seal and the overlying UER formation. Each gridblock is 500 meters in the  $x$ - and  $y$ -directions. Isopachs generated from the log analysis were used to assign thickness for each layer in the  $z$ -direction. The permeability of the seal is assumed to be 0.01 mD due to a lack of permeability measurements of the seal rock. A  $k_v/k_h$  value of 0.1 was used. Null blocks were assigned to cells outside the project area. The eight existing deep wells shown in Table 5.1 were converted to CO<sub>2</sub> injectors. They were all set to inject equal amounts of CO<sub>2</sub> in the bottom layer for 30 years. The simulation stops after 200 years to observe the gradient flow. Fig. 5.2 shows the reservoir model with the well locations. The selection of the injection rates and well constraints are discussed in the next section.



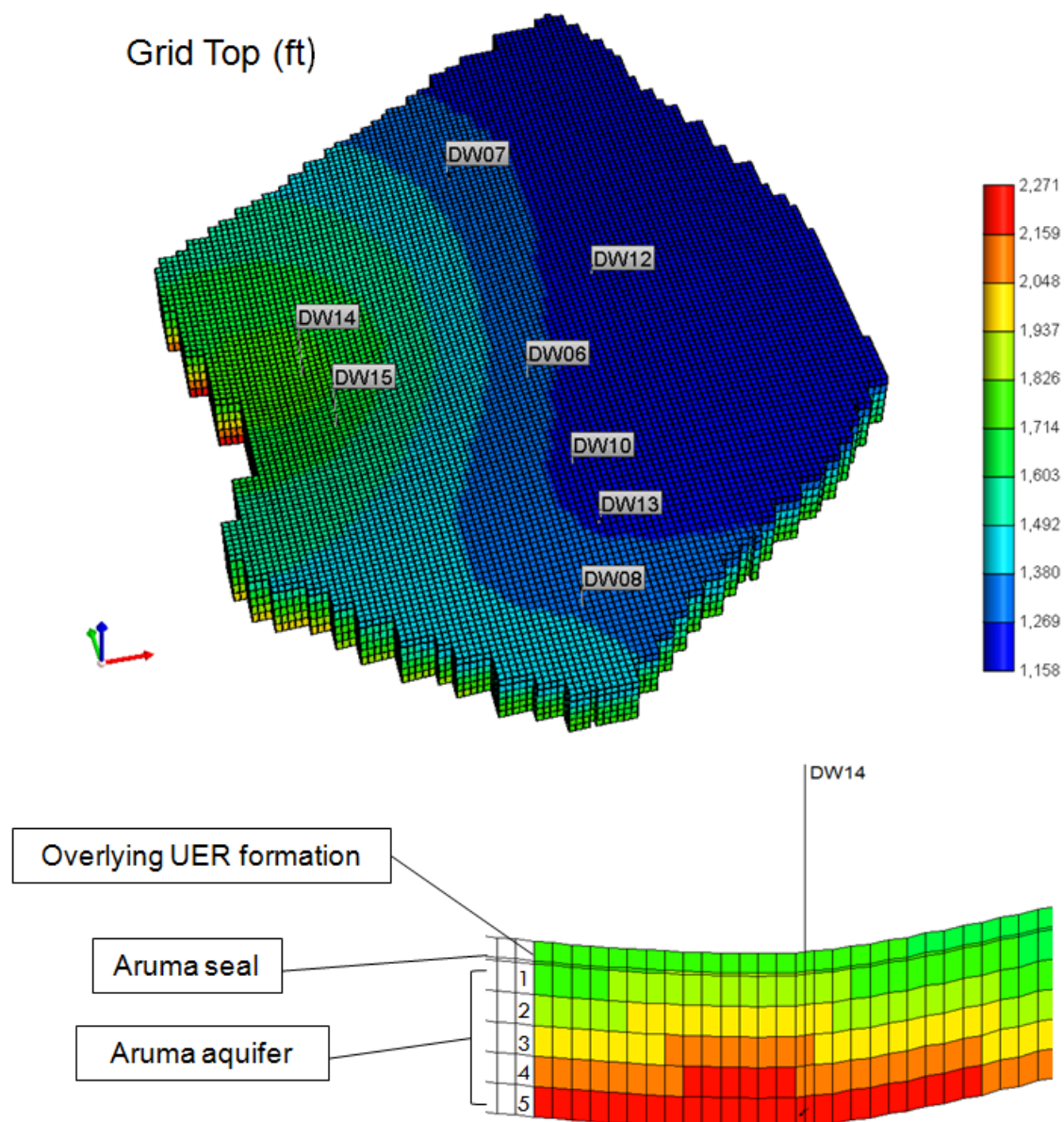


Fig. 5.2 —The reservoir model showing well locations and the description of the layers.

### ***5.3.1 Injection Design and Well Constraints***

A realistic injection scenario is developed taking into account existing sequestration projects. The Sleipner project was chosen as a facilities design analog. In terms of pore volume, the Utsira formation is 10 times larger than the Aruma formation modeled. CO<sub>2</sub> is being injected into the Utsira Formation at a rate of 1 million tonnes/year. This translates to average daily injection rate of 52 million SCF/day. Since the Aruma formation is 10 times smaller, a daily injection rate of 5.2 million SCF/day is used. This rate is divided equally among the eight wells giving each an injection rate of 650000 SCF/day (18406 sm<sup>3</sup>/day). CO<sub>2</sub> is injected through perforations made in the bottom layer of the Aruma aquifer.

The change in pressure at the well will have an impact on the pressure at the caprock, which affects the seal integrity. The bottomhole pressure constraint was set such that injection pressure would not exceed the fracture gradient. Using the formula proposed by Eaton (1969) to predict fracture gradient, a fracture gradient of 0.68 psi/ft (15.7 kPa/m) was obtained. This means that at a depth of 500 m (1640 ft), the fracture pressure of the rock is 1115 psia. All the wells are present at depths exceeding 500 m. The ideal injection wells are located in the syncline (DW-14 and DW-15). Injection from these points allows the gas to migrate up dip and get trapped under the anticline.

### 5.3.2 Fluid Phase Behavior

The Peng-Robinson EOS was used to model phase behavior. The model consists of CO<sub>2</sub>, H<sub>2</sub>O and C<sub>1</sub> as pure components. Table 5.3 shows the different property values used by the Peng-Robinson EOS. It should be noted that the Peng-Robinson EOS is only used to calculate the gas phase behavior. C<sub>1</sub> is used as a trace component to add compressibility to the near incompressible system. This helps in the convergence of the equations in the reservoir simulator. The aqueous phase density is calculated from the Rowe and Chou correlation, while aqueous viscosity is calculated using the Kestin correlation. These correlations are built into GEM and are functions of pressure, temperature and salinity. The Peng-Robinson EOS predicts the CO<sub>2</sub> gas density accurately within the pressure range of this study when a volume shift parameter of zero is used. The Pedersen correlation is used to calculate the viscosity of the components. The values of the five coefficients used in this study were those obtained by Kumar (2004) after matching experimental data (Table 5.4).

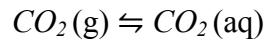
Table 5.3 – Component properties used in the aquifer model						
Components	T <sub>c</sub> (K)	P <sub>c</sub> (atm)	MW (g/mole)	$\omega$	<i>BIC</i> CO <sub>2</sub> -comp <sub>i</sub>	Volume Shift
CO <sub>2</sub>	304.2	73.76	44.01	0.2250	0.000	0.000
C <sub>1</sub>	190.6	46.00	16.04	0.0080	0.103	0.000
H <sub>2</sub> O	647.3	217.60	18.01	0.3440	0.200	0.000

**Table 5.4 – Parameter values for Pedersen et al. (1984) viscosity correlation for a CO<sub>2</sub> – brine system obtained by Kumar (2004)**

MW mixing rule coefficient	MW mixing rule exponent	Coupling factor correlation coefficient	Coupling factor correlation density exponent	Coupling factor correlation MW exponent
0.291	1.4	0.0005747	4.265	1.0579

### 5.3.3 CO<sub>2</sub> Solubility in Brine

In this study, Henry's Law is used to model CO<sub>2</sub> solubility in brine. The solubility of CO<sub>2</sub> in brine is a reversible reaction given by:



Thermodynamic equilibrium between the gas and aqueous phase requires that the fugacities of CO<sub>2</sub> in the gas and aqueous phase be equal:

$$f_{CO_2(g)} = f_{CO_2(w)}$$

The gas fugacity,  $f_{CO_2(g)}$  is calculated using the Peng-Robinson EOS. But the equation of state fails to model the behavior of the aqueous phase properly. Therefore the fugacity of CO<sub>2</sub> in the aqueous phase is calculated using Henry's Law, i.e.

$$f_{CO_2(w)} = y_{CO_2(w)} H_{CO_2(w)}$$

The Henry's constant,  $H_{CO_2(w)}$ , is calculated at the reservoir temperature is also dependent on salinity (Nghiem et al. 2004). It is calculated at the reservoir pressure,  $P$ , as follows:

$$\ln(H) = \ln(h) + \frac{v^\infty (P - P_{ref})}{RT}$$

where  $P_{ref}$  is the reference pressure

$v^\infty$  is the partial volume at infinite dilution

$h$  is the Henry's constant at  $P_{ref}$

Accurate correlations for the Henry's constants of CO<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>S and CH<sub>4</sub> have already been implemented in GEM. These correlations take into account the pressure, temperature and salinity. The Harvey model (1996) for calculating the Henry's constant of CO<sub>2</sub> is activated with the keyword *HENRY-CORR-CO2*.

### 5.3.4 Rock-Fluid Data

Relative permeability data was obtained by using the following equations and parameters (Table 5.5)(Anchliya 2009; Kumar 2004):

For  $S_g \leq S_{gcr}$  :  $k_{rg} = 0$

For  $S_g > 1 - S_{wrg}$  :  $k_{rwg} = 0$

For  $S_g \geq S_{gcr}$  :

$$k_{rg} = k_{rg}^\circ \left( \frac{S_g - S_{gcr}}{1 - S_{wrg} - S_{wirg}} \right)^{N_g}$$

For  $S_g \leq 1 - S_{wrg}$  :

$$k_{rwg} = k_{rw}^{\circ} \left( \frac{S_g - S_{gcon}}{1 - S_{wrg} - S_{gcon}} \right)^{N_w}$$

where  $k_{rg}^{\circ}$  is gas end point relative permeability

$k_{rw}^{\circ}$  is water end point relative permeability

$S_g$  is gas saturation

$S_{gcr}$  is critical gas saturation

$S_{wirg}$  is irreducible water saturation

$S_{wrg}$  is residual water saturation during gas flood

$S_{gcon}$  is connate gas saturation

$N_g$  is gas relative permeability exponent

$N_w$  is water relative permeability exponent

**Table 5.5 – Relative permeability parameters for the base case (Kumar 2004)**

Gas end point relative permeability	1.0
Water end point relative permeability	0.334
Connate gas saturation	0.25
Critical gas saturation	0.25
Residual water saturation	0.25
Irreducible water saturation	0.25
Water relative permeability exponent	2
Gas relative permeability exponent	2.5

Relative permeability data published by Bennion and Bachu (2008) was not used as it was obtained using highly saline brine and supercritical CO<sub>2</sub>. The capillary pressure for the base case was assumed to be zero from the lack of experimental data. Other works have used the Brooks-Corey approach (Brooks and Corey 1966) to predict capillary pressure. The Brooks-Corey relation is given by:

$$P_c = P_d S_w^{*-1/\lambda}$$

where  $P_d$  is threshold or displacement pressure

$\lambda$  is pore geometric factor

$S_w^*$  is effective water saturation

The effective water saturation,  $S_w^*$  is calculated by

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

where  $S_{wr}$  is irreducible water saturation

The pore geometric factor and displacement pressure are determined experimentally. Values of  $\lambda = 2$  and  $P_d = 10$  Pa are used in the literature for CO<sub>2</sub> sequestration (Bielinski et al. 2008; Ukaegbu et al. 2009).

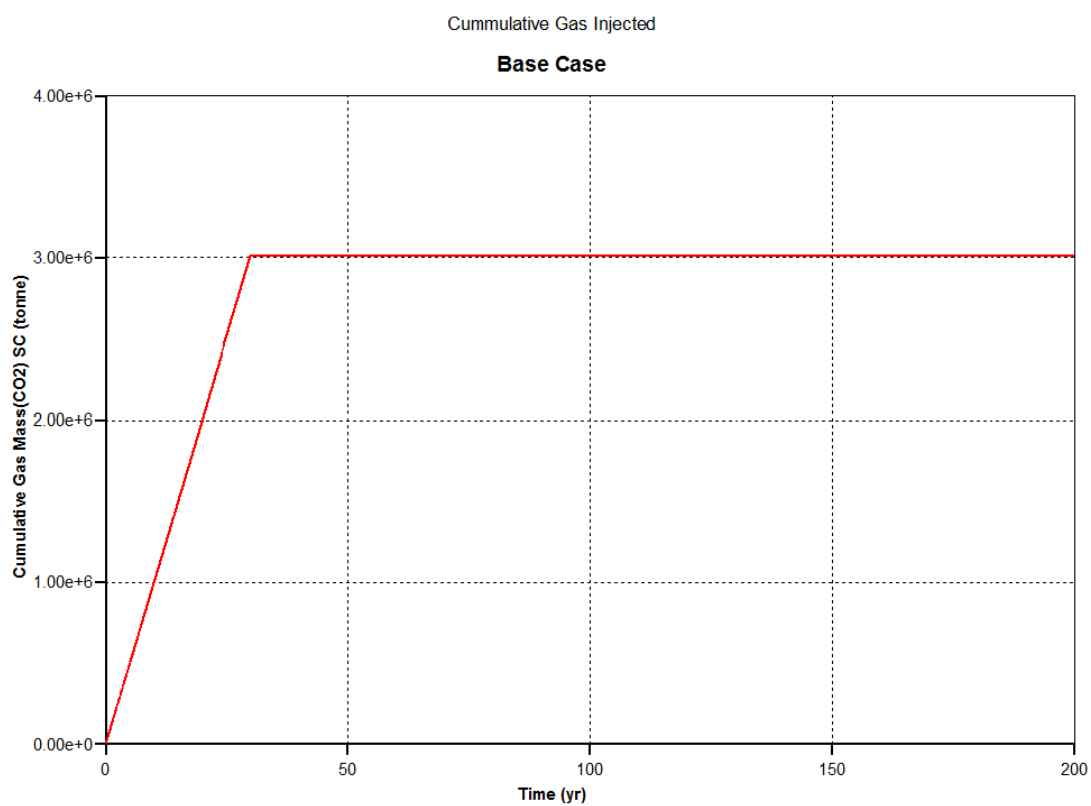
### **5.3.5 Initial Conditions**

The initial overall mole fraction of CO<sub>2</sub> in the aquifer is zero, where the global mole fraction of water is one. The initial reservoir pressure at 500 m (1640 ft) is 721 psi, which is calculated using a hydrostatic gradient of 0.44 psi/ft. Pure CO<sub>2</sub> is not in a supercritical state when it is injected into this aquifer.

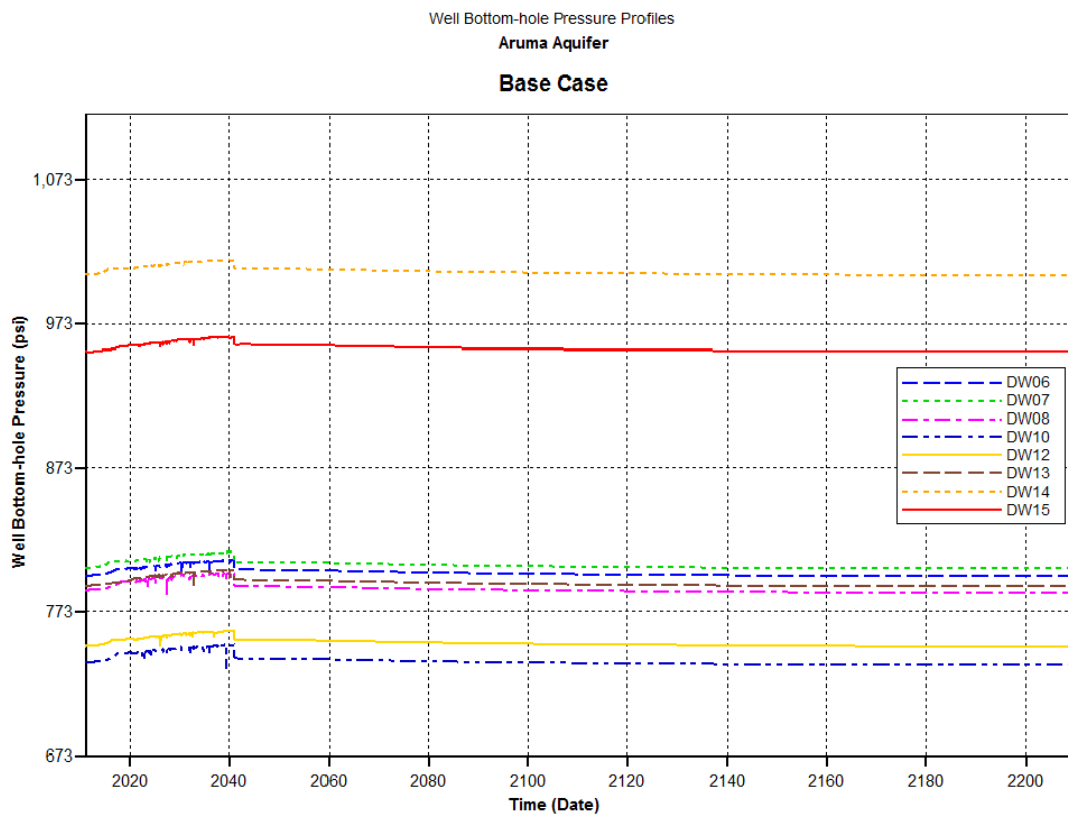
## **5.4 Simulation Results for the Base Case**

Fig. 5.3 shows the cumulative gas injected with time. At shut-in (30 years), approximately 57 BSCF of gas has been injected, translating to 3 million tonnes. After injecting a constant rate for a period of 30 years the average aquifer pressure has increased only by 7 psia. The well bottom-hole pressure profiles in Fig. 5.4 show that average increase in bottom-hole pressure during the injection period was only about 17 psia. The overall difference in pressure between the wells is due to the fact they are all injecting from different depths into the lowest layer of the Aruma aquifer. DW-14 and DW-15, located in a syncline as mentioned previously, have the highest bottom-hole pressure. Due to the size of the aquifer, the increase in pressure is negligible with respect to the fracture pressure of the rock. The GEM data file for the base case is provided in Appendix B.





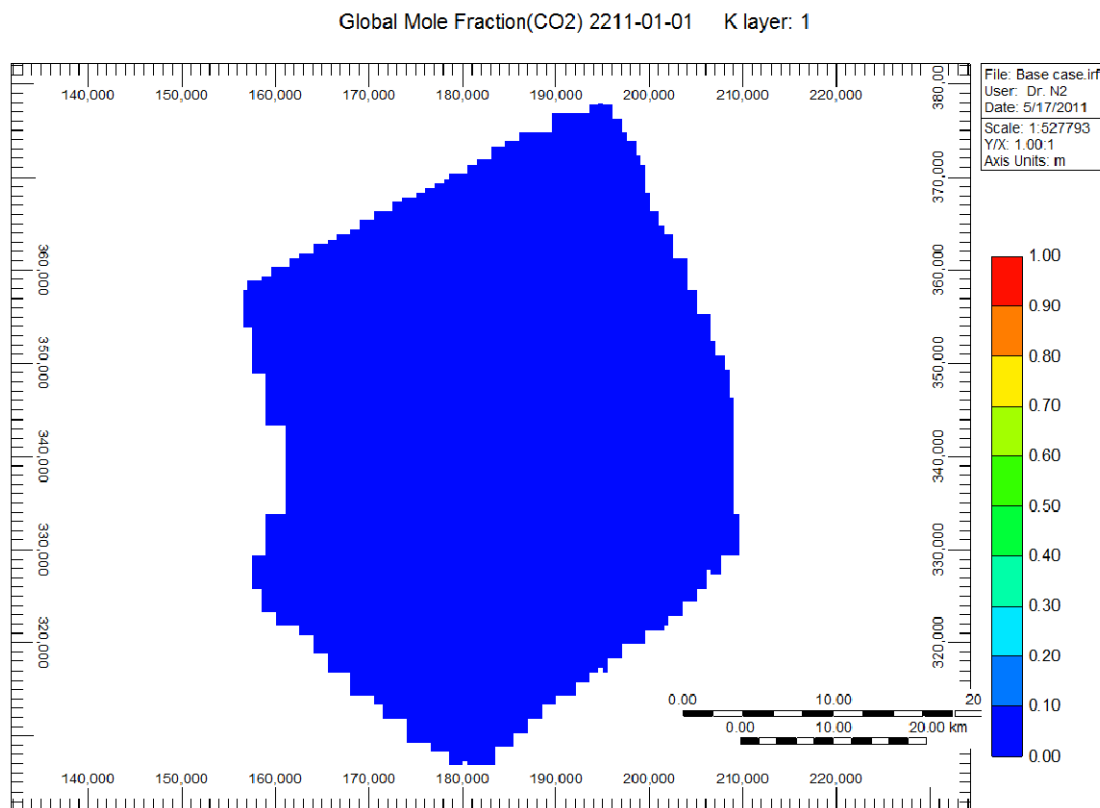
**Fig. 5.3 —Cumulative gas injected with time for the base case. Approximated 3 million tonnes are injected at the end of a 30 year injection period.**



**Fig. 5.4 —Well Bottom-hole Pressure profiles for the base case.**

Fig.5.5 shows the global mole composition of CO<sub>2</sub> in the overlying UER formation. It is interesting to note that CO<sub>2</sub> does not breakthrough into the UER and the seal manages to contain the CO<sub>2</sub>. The selection of the injection rate also plays an important role on the effect of seal integrity. If a very high CO<sub>2</sub> injection rate is used, the pressure under the seal will rapidly increase surpassing the fracture pressure and causing leakage of CO<sub>2</sub>. It should be noted that CO<sub>2</sub> cannot be prevented from reaching the seal in this case. The average permeability of the Aruma aquifer is 3340 mD. Assuming a kv/kh value of 0.1, there is still a vertical permeability of 334 mD. It has also been speculated that the seal

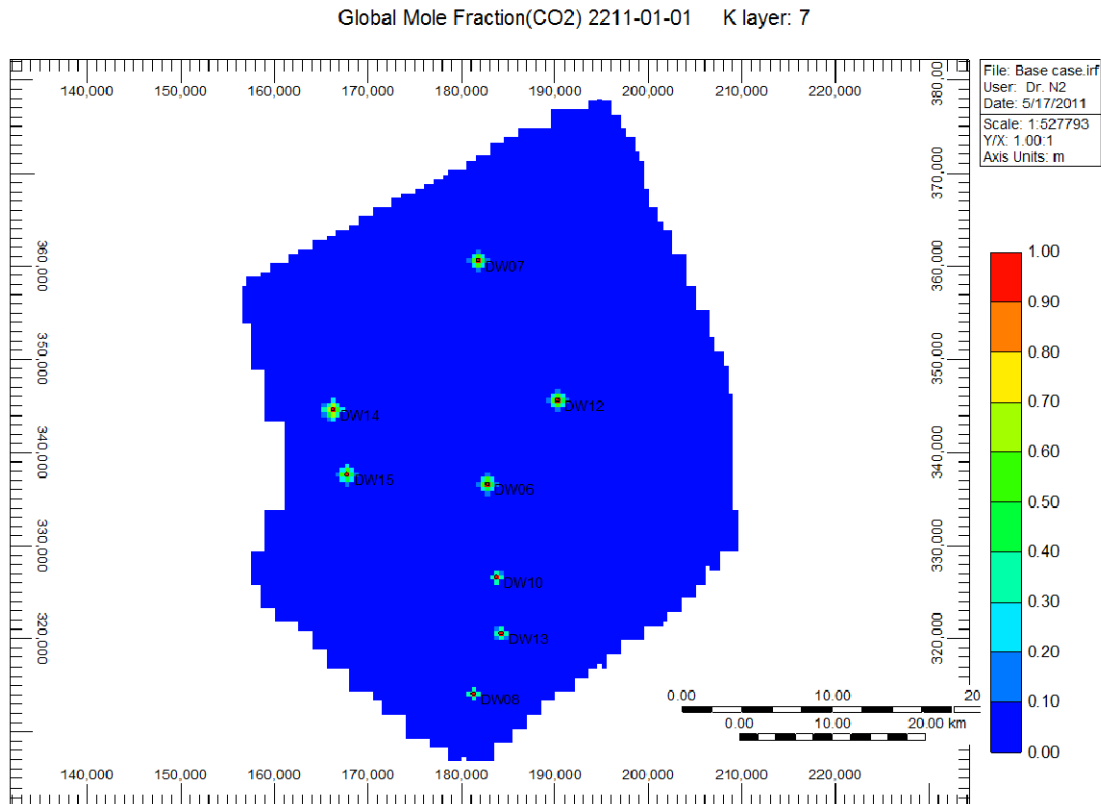
rock may have a higher capillary pressure than the reservoir rock. Bryant et al. (2008) have shown that if the rising  $\text{CO}_2$  encounters a layer whose capillary pressure exceeds the capillary pressure of  $\text{CO}_2$  phase, then the  $\text{CO}_2$  is completely diverted to flow up dip in the layer beneath the barrier. This process is not modeled in this study due to lack of capillary pressure data.



**Fig. 5.5 —The  $\text{CO}_2$  global mole fraction in the overlying formation at the end of the simulation. There is no leakage for  $\text{CO}_2$  into the UER after 200 years with the proposed injection scheme.**

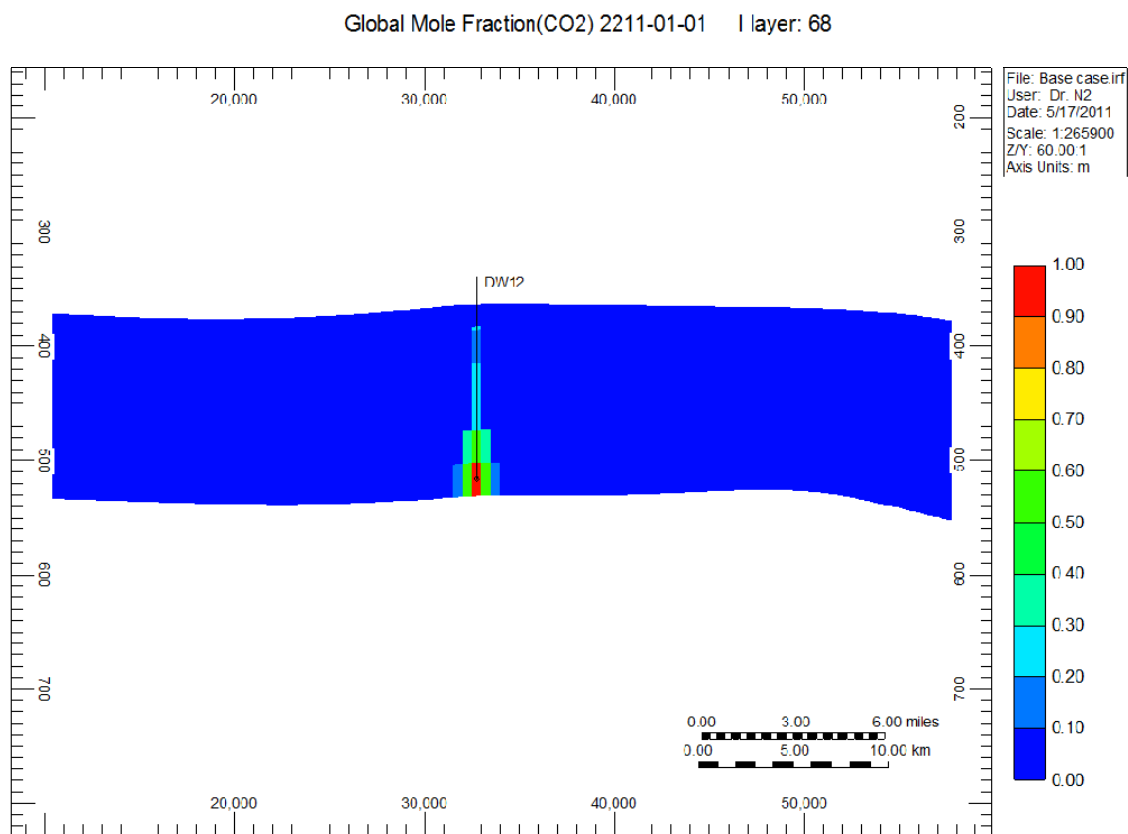
The  $\text{CO}_2$  global mole fraction in the lowest layer of the aquifer (layer 7) is shown in Fig. 5.6. We observe that due to high permeability, there is a greater radial spread of  $\text{CO}_2$  at

bottom of the aquifer. A vertical cross section around the well DW-12 shows the shape and propagation of the CO<sub>2</sub> plume.



**Fig. 5.6 —The CO<sub>2</sub> global mole fraction in the lowest layer of Aruma aquifer. CO<sub>2</sub> is being injected in this layer.**

It is observed from Figs. 5.6 and 5.7 that a large portion of the Aruma aquifer has still not been affected by 30 years of CO<sub>2</sub> injection. A closed boundary system was modeled in order to represent a confined aquifer.



**Fig. 5.7 —Propagation of the CO<sub>2</sub> plume from DW-12.**

### 5.5 Including Diffusion in the Base Case

The keyword in GEM to model diffusion in the aqueous phase is *DIFFC-AQU*. The diffusion coefficient of the components in cm<sup>2</sup>/s must be provided to use this option. GEM has the Sigmund (1976) correlation and the Wilke-Chang (1955) correlation built in to calculate the diffusion coefficient in oil and gas phases. Previous works to model diffusion have used a CO<sub>2</sub> diffusion coefficient of  $2 \times 10^{-5}$  cm<sup>2</sup>/s (Anchliya 2009; Ukaegbu et al. 2009). The diffusion coefficient is primarily a function of temperature. The average temperature of the Aruma aquifer is 115 °F (319 K). Based on

experimental data (Frank et al. 1996; Tamimi et al. 1994) a  $\text{CO}_2$  diffusion coefficient of  $3 \times 10^{-5} \text{ cm}^2/\text{s}$  is used in this study.

### 5.5.1 Simulation Results

The same injection scheme as the base case was used in the simulation run. There was almost no difference in the bottom-hole pressure profiles. Fig. 5.8 compares the number of moles of  $\text{CO}_2$  in the aqueous phase with and without diffusion. It was found that diffusion enhances the solubility of  $\text{CO}_2$  in brine.

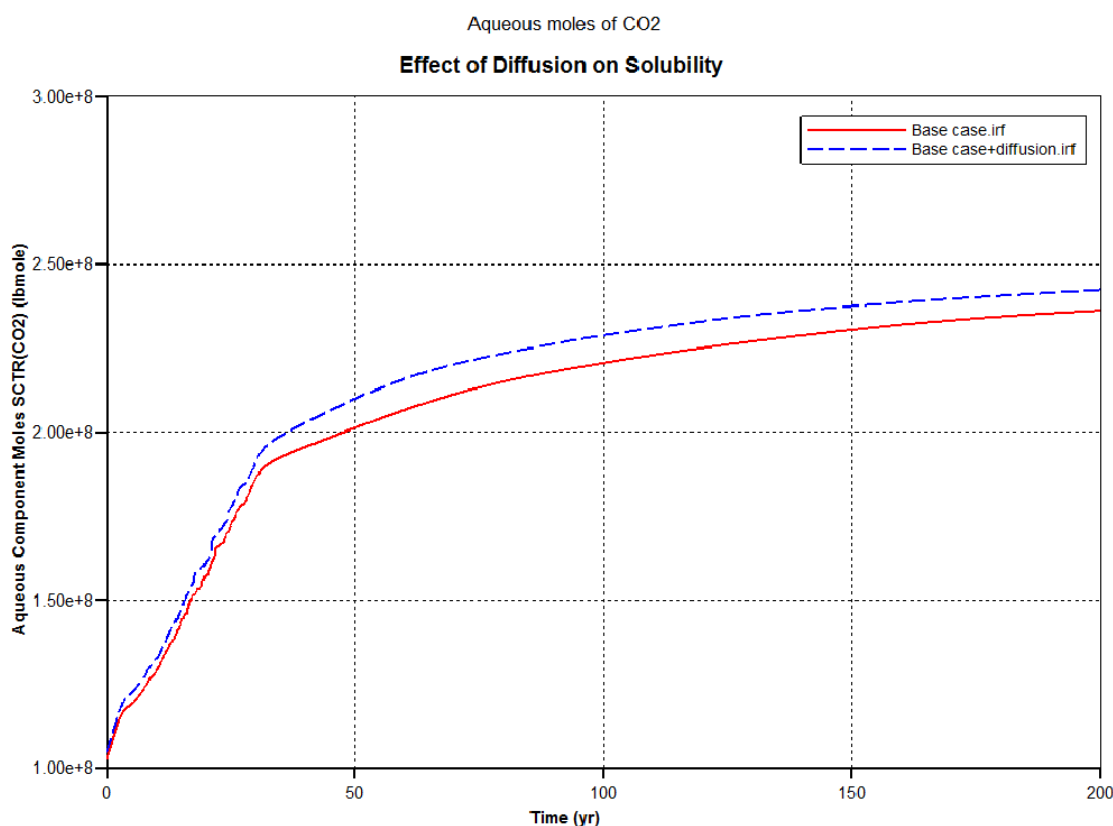
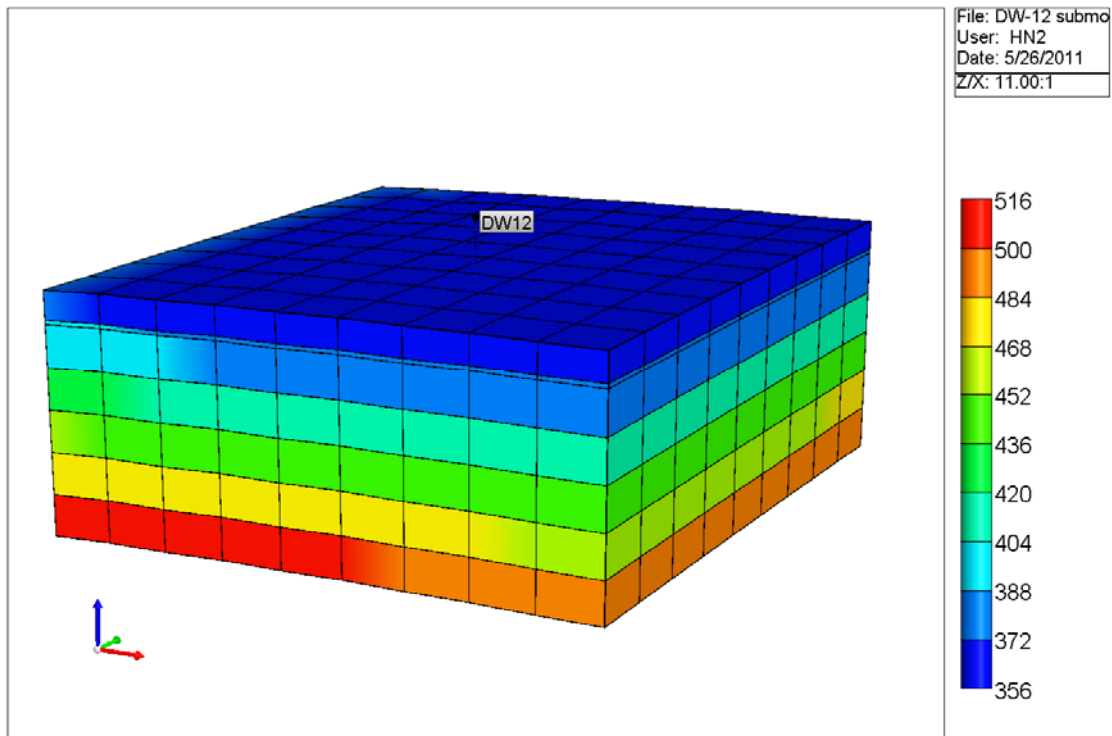


Fig. 5.8 —The effect of diffusion on the solubility of  $\text{CO}_2$  in brine.

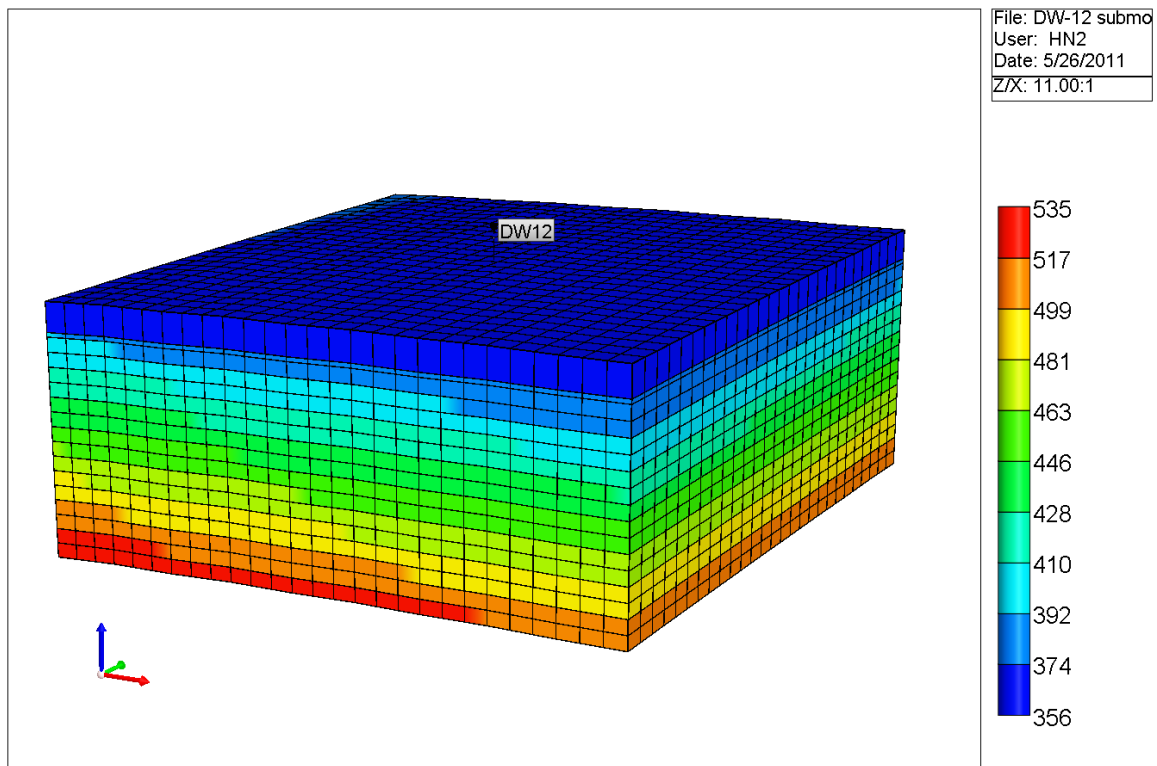
## 5.6 Grid Sensitivity Analysis

The current dimensions of each grid block in the base case are 500 m in the  $x$ - and  $y$ -directions. To study the effect of the gridding size on the propagation of the CO<sub>2</sub> plume, a sub-model containing a single well (DW-12) was used. The sub-model dimensions are 4500 m in the  $x$ - and  $y$ -directions with the well placed in the center. The dimensions of the grid blocks are the same as the base case (Fig. 5.9). The sub-model contains 567 cells.



**Fig. 5.9 —Extraction of a sub-model containing the well DW-12 for grid sensitivity tests. The current gridding dimensions are used in the base case. The sub-model contains 567 grids.**

In the fine grid sub-model, the dimensions of the grid blocks representing the Aruma aquifer are reduced by one-third in each direction. The grid blocks of the seal and the overlying UER formation are reduced by one-third in the  $x$ - and  $y$ -directions. This model now contains 12960 cells (Fig. 5.10). The effect of grid size on diffusion is also investigated.

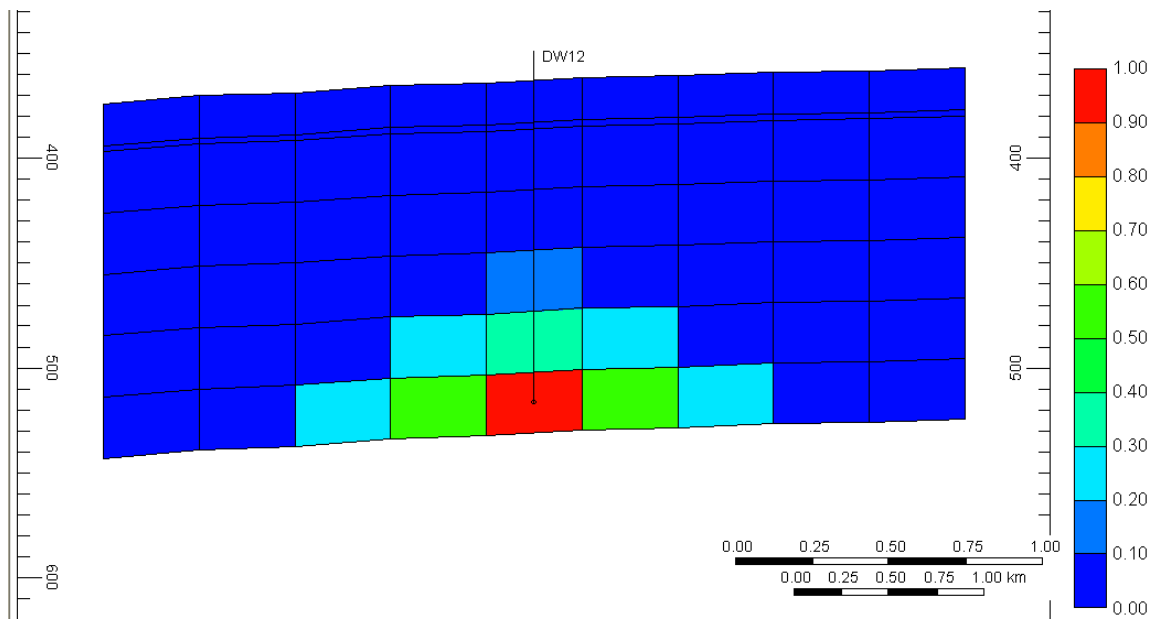


**Fig. 5.10 —The fine grid sub-model containing the well DW-12 for grid sensitivity tests. The sub-model contains 12960 grid blocks.**

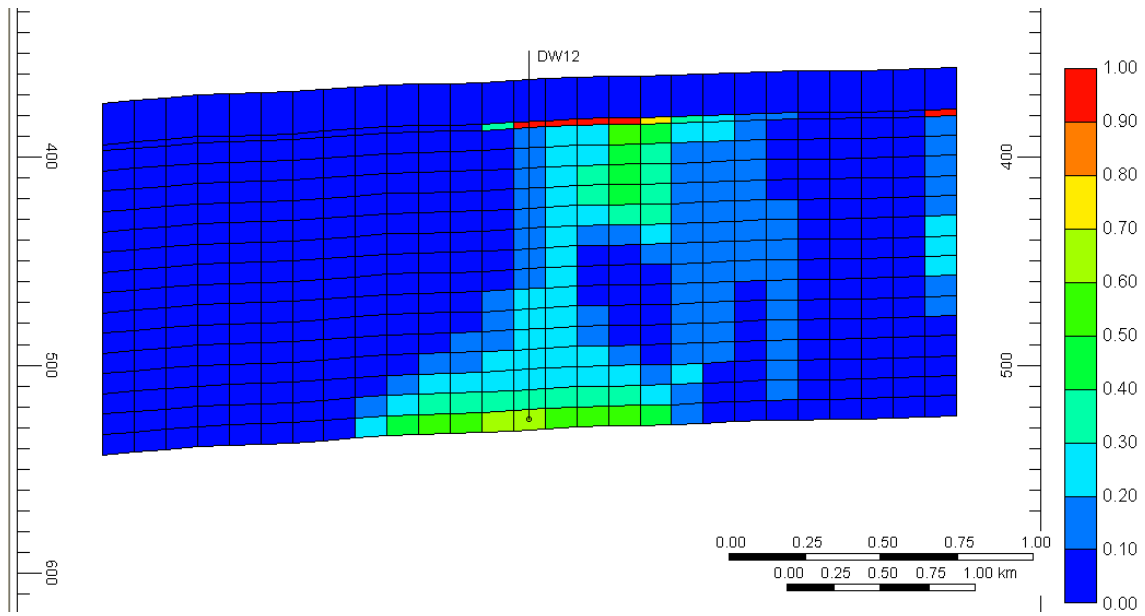
### ***5.6.1 Grid Sensitivity Results***

The use of finer grids shows a significant difference in the propagation of CO<sub>2</sub> plume. Fig. 5.11 compares the global mole fraction of CO<sub>2</sub> between the two cases after 200 years.





(a)



(b)

**Fig. 5.11 —Comparison of CO<sub>2</sub> plume propagation after 200 years: (a) coarse gridding and (b) fine gridding.**

With coarse gridding, upward movement of CO<sub>2</sub> is limited. CO<sub>2</sub> spreads radially from the injection point. The use of fine grids shows the CO<sub>2</sub> plume reaching the seal and beginning to move up dip below the seal. As the CO<sub>2</sub> dissolves in the brine below the seal, the increase in the brine density triggers convective mixing of CO<sub>2</sub>. The use of coarse grids also overestimates the amount of CO<sub>2</sub> dissolved in brine as can be seen in Fig. 5.12.

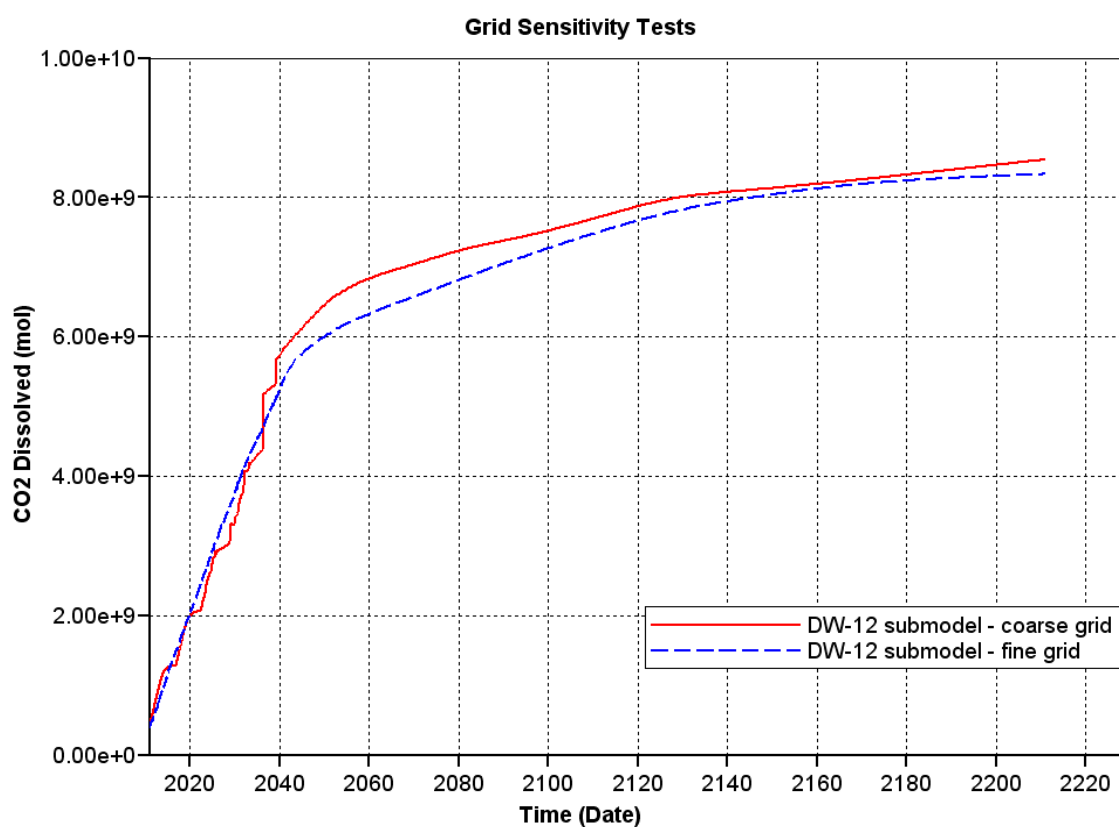
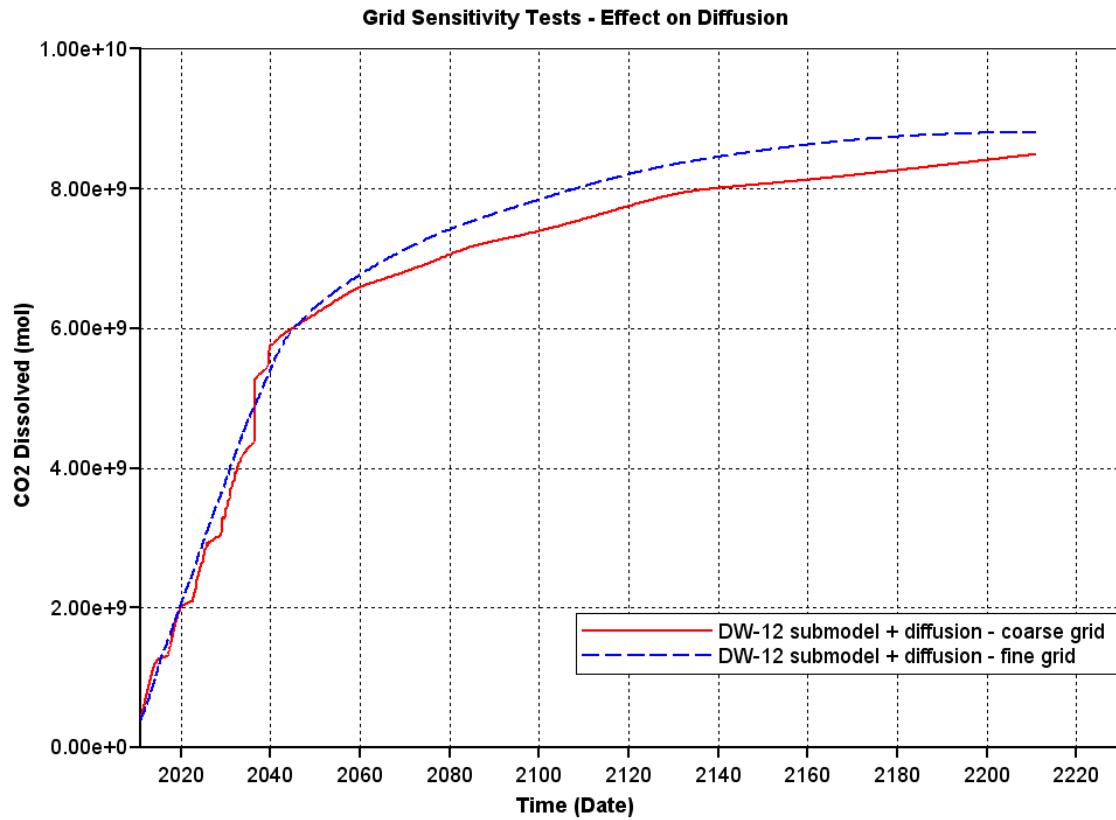


Fig. 5.12 —Effect of grid size on CO<sub>2</sub> solubility in brine – base case.

When diffusion is included in the models, the use of fine grids enhances the effect of diffusion. Fig. 5.13 shows an increase in the rate of dissolved  $\text{CO}_2$  when fine grids are used.

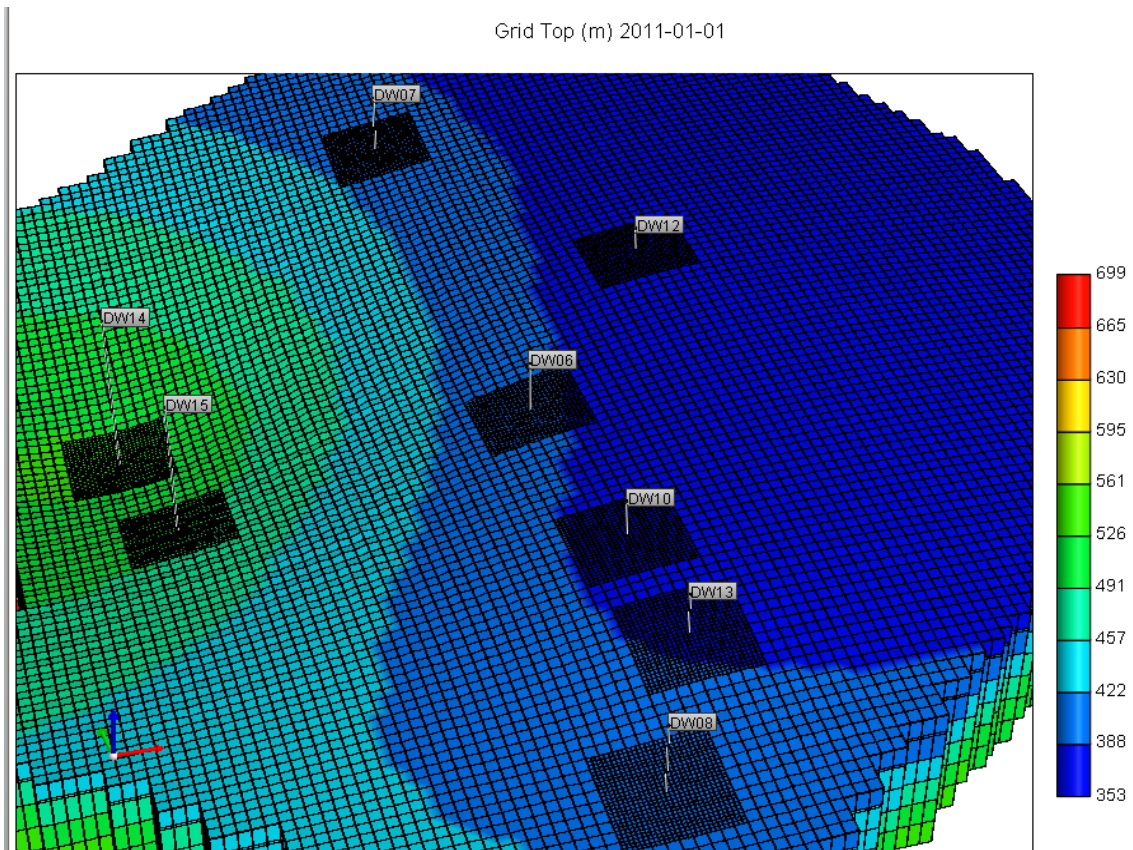


**Fig. 5.13 —Effect of grid size on  $\text{CO}_2$  solubility in brine – with diffusion.**

In the case where finer grids were used, the CO<sub>2</sub> dissolved in brine increased by 3.6%. Selection of the right grid size is very important for accurate modeling of CO<sub>2</sub> sequestration. However, the use of fine grids is computationally expensive. The simulation run time increased by factor of 92 when finer grids are used in the sub-model. Local grid refinement is a useful technique for increasing the numerical accuracy of the simulations without refining the entire grid, which would take more simulation time. This feature is available in GEM, and is described in the next section.

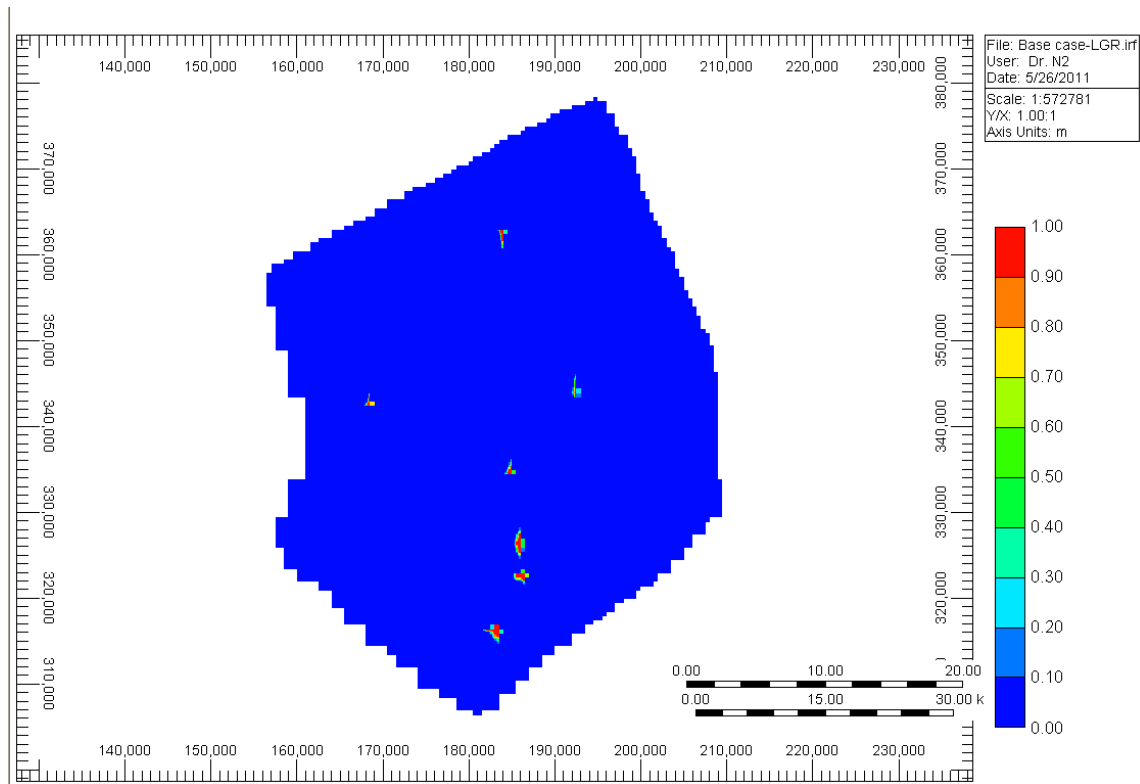
### **5.7 Including Local Grid Refinement in the Aquifer Modeling**

Based on the results of Section 5.6, local grid refinement (LGR) was used in the Aruma model (Fig. 5.14). Grid refinement was done around the wellbore, in the region where CO<sub>2</sub> was expected to migrate, based upon the results presented in Section 5.4. Approximately 5000 acres around the wellbore were refined. The grid size along all three dimensions was reduced by a factor of three for the bottom five layers representing the Aruma aquifer. The grid size in the top two layers was reduced by a factor of three only along the  $x$ - and  $y$ -directions.



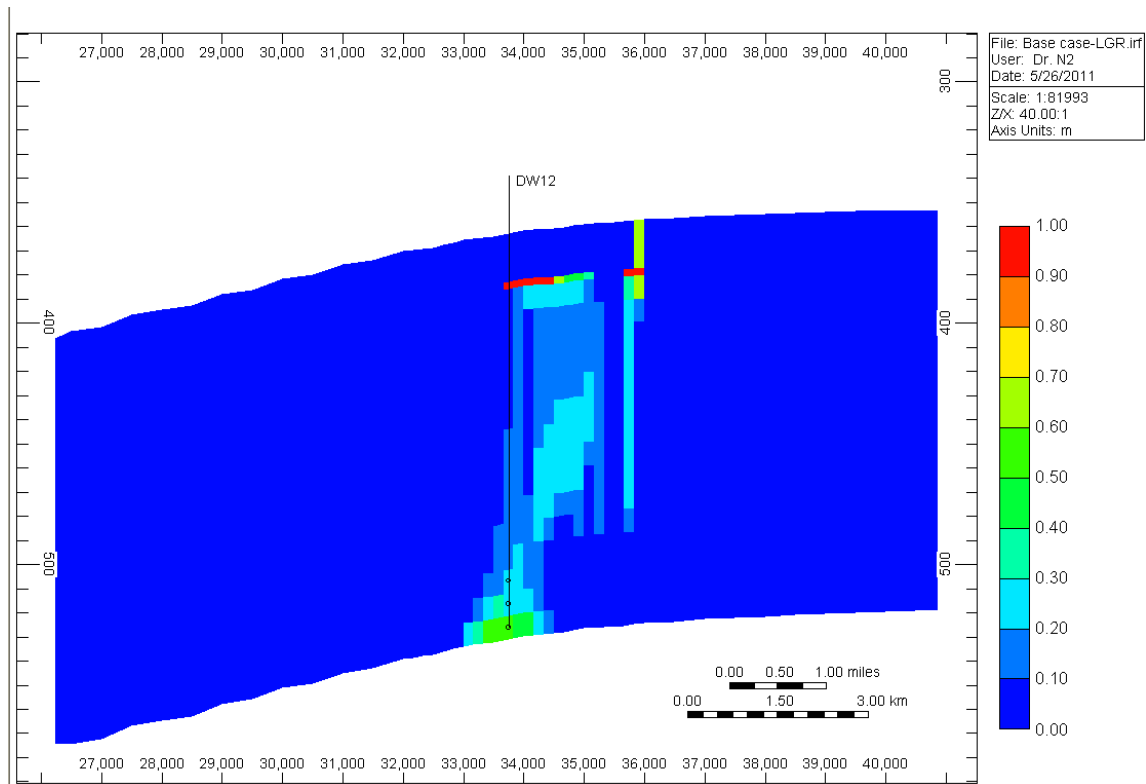
**Fig. 5.14 —Including local grid refinement to the Aruma aquifer model.**

Fig. 5.15 shows the global mole composition of  $\text{CO}_2$  in the overlying UER formation (layer 1). The use of LGR shows that  $\text{CO}_2$  breakthrough occurs in the UER at the end of the simulation run. This was not observed when coarser grids were used.



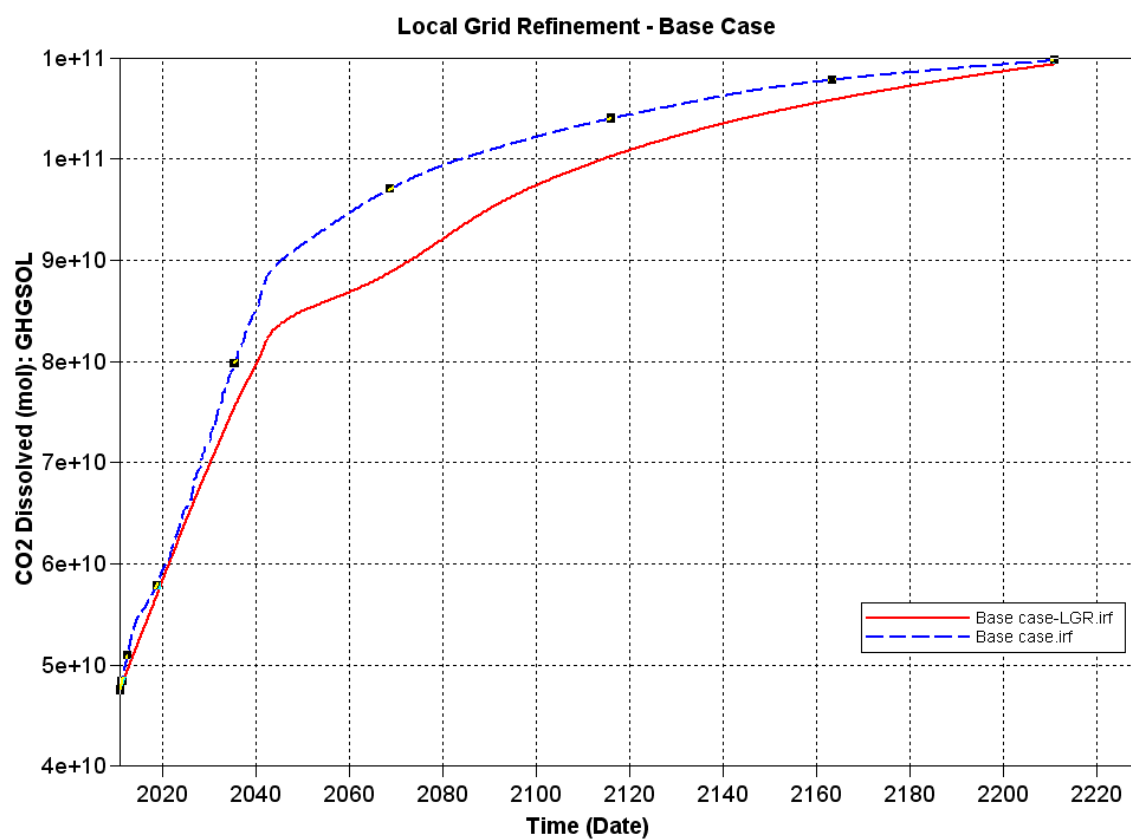
**Fig. 5.15 —The CO<sub>2</sub> global mole fraction in the overlying formation at the end of the simulation. There is CO<sub>2</sub> leakage into the UER after 200 years when local grid refinement is used.**

Fig. 5.16 shows the movement of CO<sub>2</sub> around the well DW-12 after 200 years. Greater vertical movement of CO<sub>2</sub> is observed in this case. The profile of the plume is very different of that which is seen when course grids are used throughout the aquifer.



**Fig. 5.16 —Cross-section of DW-12 showing the CO<sub>2</sub> global mole fraction after 200 years. Vertical movement of CO<sub>2</sub> is observed.**

As seen in the previous section, when diffusion is not included, the model without LGR overestimates the amount of CO<sub>2</sub> dissolved (Fig. 5.17). When diffusion is included, the model without LGR underestimates the amount of CO<sub>2</sub> dissolved (Fig. 5.18).



**Fig. 5.17—Comparison of the CO<sub>2</sub> dissolved with local grid refinement – without diffusion.**



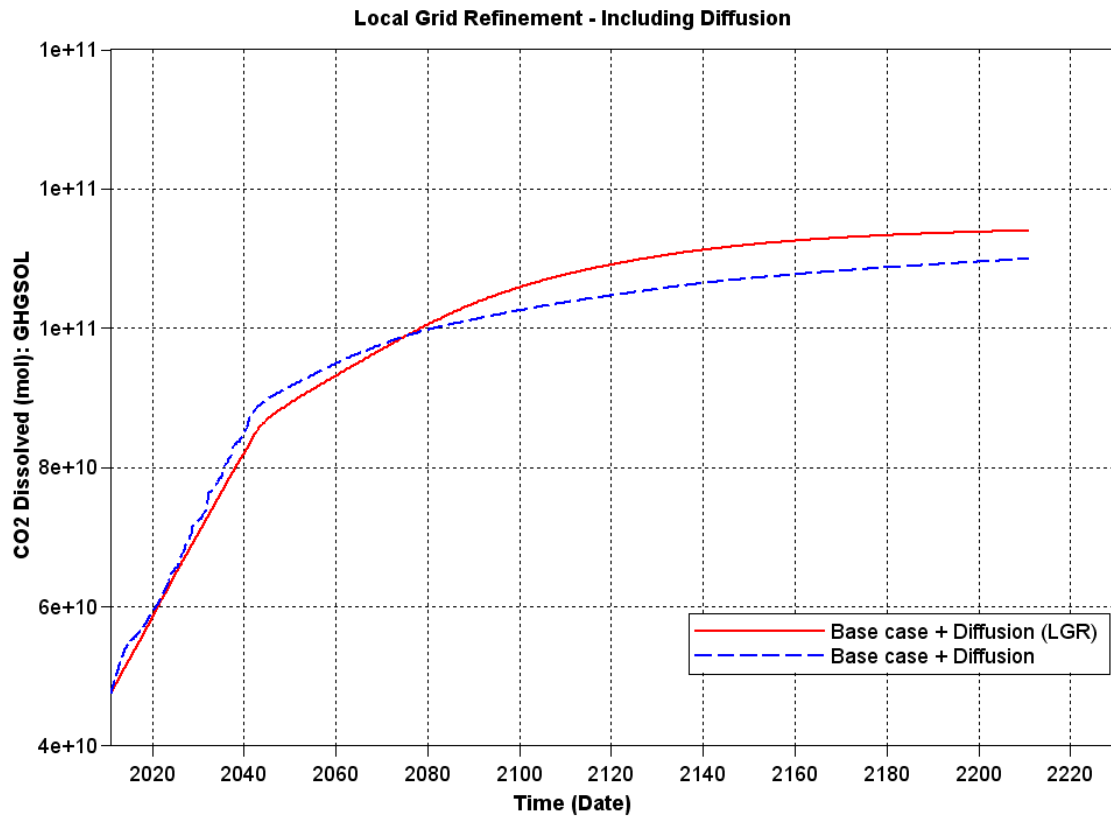


Fig. 5.18 —Comparison of the CO<sub>2</sub> dissolved with local grid refinement – with diffusion.

### 5.8 Section Summary

A simulation model is prepared for the Aruma aquifer using the available log data and flow test data. The existing deep wells were converted to CO<sub>2</sub> injectors. CO<sub>2</sub> was injected at a constant rate for a period of 30 years. The inclusion of diffusion enhances the rate of CO<sub>2</sub> dissolution in brine. The grid size affects the movement of the CO<sub>2</sub> plume and the propagation of vertical fingers (caused by the density instability).

## 4. CONCLUSIONS AND RECOMMENDATIONS

### 6.1 Conclusions

To address the issue of including abnormal density effects arising from CO<sub>2</sub> solubility in crude oils, a simple approach to model the increase in oil density with CO<sub>2</sub> dissolution using the Peng-Robinson EOS and the Pedersen viscosity correlation is presented. By changing the volume shift parameter of CO<sub>2</sub>, the increase in oil density with CO<sub>2</sub> dissolution can be modeled while preserving the viscosity match. The Peng-Robinson EOS can predict the density of pure CO<sub>2</sub> by adjusting the CO<sub>2</sub> volume shift parameter. The use of the existing correlations for predicting the volume shift parameters do not perform well for CO<sub>2</sub> injection at high pressures. Due to 1D nature of flow in slim tube experiments, the density effect is not taken into account. In 2D and 3D, when injected CO<sub>2</sub> is lighter than the oil phase, there may be no gravity stable displacement due to increase in oil density from solubility. CO<sub>2</sub> injection when the density of the injected gas is less than the oil density may result in unstable gravity drainage.

Past literature has neglected density effects the study and evaluation of CO<sub>2</sub> injection in the crest. Density measurements for CO<sub>2</sub>/oil mixtures at different CO<sub>2</sub> compositions and prediction of these results in the fluid model can significantly increase the reliability of the simulation results and decrease the degree of uncertainty. Heterogeneity may also have a significant effect as expected. The depth of injection and production wells with respect to the top of the reservoir may also have a large impact on recovery.

Saline aquifers hold a lot of potential for sequestering CO<sub>2</sub>. The important transport processes and trapping mechanisms are identified and discussed. A simulation model is prepared for the Aruma aquifer using the available log data and flow test data. The existing deep wells were converted to CO<sub>2</sub> injectors. CO<sub>2</sub> was injected at a constant rate for a period of 30 years. There was no leakage of CO<sub>2</sub> through the seal using the proposed injection scheme. The inclusion of diffusion increased the amount of CO<sub>2</sub> dissolved in brine.

## **6.2 Recommendations**

The acquisition of more experimental data that captures the density effect would greatly help in modeling this phenomenon. The creation of a database with experimental data would be the next step. Though Lansangan and Smith (1993) proposed a theory that increase in density might be caused by strong intermolecular Coulombic interactions between CO<sub>2</sub> and hydrocarbon molecules, this would need to be verified at a molecular level. There is a lot we still need to understand about these complex fluid systems.

The Aruma aquifer in Qatar, though being a shallow saline aquifer, has been shown to have potential in CO<sub>2</sub> sequestration. A seismic study should be conducted to obtain a more detailed structure of the aquifer. This would also help in the prediction of the CO<sub>2</sub> migration flow paths. There is also a possibility that discovery of extensive faults could greatly increase the leakage risk of this project. More data needs to be collected to make a thorough and informed decision. The diffusion coefficients and rock capillary pressure

data should be determined experimentally. Including geochemistry in the aquifer model and its effect on CO<sub>2</sub> injectivity would be the next step.

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## APPENDIX A

### EXAMPLE CO<sub>2</sub>/OIL DATA FILE

Following in the GEM input file used for simulating the CO<sub>2</sub> injection from the bottom of a 2D domain that has a homogenous permeability of 100 mD.

```

-----
RESULTS SIMULATOR GEM 200800

DIM MDV 57600
DIM MDLU 2684304
DIM MDALP 5448984
DIM MDDD 691200

INUNIT FIELD
WSRF WELL 1
WSRF GRID TIME
OUTSRF GRID DENG DENO K 'C1' K 'CO2' KRG KRO PRES SG SO SW
TSO
          X 'C1' X 'CO2' Y 'C1' Y 'CO2' Z 'C1' Z 'CO2'
OUTSRF RES NONE
OUTSRF WELL ZWEL 'CO2' 'Well-2'
WPRN GRID 0
OUTPRN GRID NONE
OUTPRN RES NONE
**$ Distance units: ft
RESULTS XOFFSET          0.0000
RESULTS YOFFSET          0.0000
RESULTS ROTATION          0.0000 **$ (DEGREES)
RESULTS AXES-DIRECTIONS 1.0 -1.0 1.0

**----- RESERVOIR DATA -----
GRID VARI 240 1 40

```

```

KDIR DOWN
DI IVAR 240*5
DJ JVAR 16.4042
DK ALL 9600*5
DTOP 240*1000
**$ Property: NULL Blocks Max: 1 Min: 1
**$ 0 = null block, 1 = active block
NULL CON 1
**$ Property: Porosity Max: 0.2235 Min: 0.2235
POR CON 0.2235
**$ Property: Permeability I (md) Max: 100 Min: 100
PERMI CON 100
PERMJ EQUALSI
PERMK EQUALSI
**$ Property: Pinchout Array Max: 1 Min: 1
**$ 0 = pinched block, 1 = active block
PINCHOUTARRAY CON 1
CPOR 3e-5

**----- FLUID COMPONENT DATA -----

MODEL PR
NC 10 10
COMPNAME 'CO2' 'C1' 'C2' 'C3' 'NC4' 'NC5' 'FC6' 'C7+'
'C13+' 'C22+'
HCFLAG
0 0 0 0 0 0 0 0 0 0
VISCOR MODPEDERSEN
VISCOEFF 1.3040000E-04 2.3030000E+00 7.3780000E-03
1.8470000E+00 5.1730000E-01
MW
4.4010000E+01 1.6043000E+01 3.0070000E+01 4.4097000E+01
5.8124000E+01 7.2151000E+01 8.6000000E+01 1.2619000E+02
2.1864000E+02 4.4238000E+02
AC
0.225 0.008 0.098 0.152 0.193 0.251 0.27504 0.34615 0.46364
0.80496
PCRIT
7.2800002E+01 4.5400051E+01 4.8200051E+01 4.1900026E+01
3.7500026E+01 3.3299977E+01 3.2460006E+01 2.0830990E+01
1.4803850E+01 9.5238099E+00
VCRIT

```

9.4000000E-02 9.9000000E-02 1.4800000E-01 2.0300000E-01  
 2.5500000E-01 3.0400000E-01 3.4400000E-01 4.6250000E-01  
 8.1500000E-01 1.8580000E+00

TCRIT

3.0420000E+02 1.9060000E+02 3.0540000E+02 3.6980000E+02  
 4.2520000E+02 4.6960000E+02 5.0750000E+02 5.6964311E+02  
 7.9025476E+02 1.0754300E+03

PCHOR

78 77 108 150.3 189.9 231.5 250.1 361.2 589.6 986.9

SG

0.818 0.3 0.356 0.507 0.584 0.631 0.69 0.71224 0.78276  
 0.84911

TB

-109.21 -258.61 -127.57 -43.69 31.19 96.89 146.93 239.189  
 480.328 921.603

OMEGA

0.457236 0.457236 0.457236 0.457236 0.457236 0.457236  
 0.457236 0.457236 0.457236 0.457236

OMEGB

0.0777961 0.0777961 0.0777961 0.0777961 0.0777961 0.0777961  
 0.0777961 0.0777961 0.0777961 0.0777961

VSHIFT

-0.0943467 -0.153861 -0.102103 -0.0733009 -0.0570559 -  
 0.0344627 -0.004992 0.1 0.19 0.47

BIN

1.0000000E-01  
 1.0000000E-01 2.6890022E-03  
 1.0000000E-01 8.5370405E-03 1.6620489E-03  
 1.0000000E-01 1.4748531E-02 4.9143360E-03 8.6625350E-04  
 1.0000000E-01 2.0640839E-02 8.5779330E-03 2.7121325E-03  
 5.1467786E-04  
 1.0000000E-01 2.5345101E-02 1.1747825E-02 4.6198099E-03  
 1.4920539E-03 2.5462307E-04  
 1.0000000E-01 3.8419394E-02 2.1279999E-02 1.1202389E-02  
 5.8809841E-03 2.9279823E-03 1.4586581E-03  
 1.0000000E-01 7.0018325E-02 4.6738564E-02 3.1412902E-02  
 2.2113722E-02 1.6006595E-02 1.2281260E-02 5.3273178E-03  
 8.0000000E-02 1.2883664E-01 9.8473647E-02 7.6801306E-02  
 6.2529225E-02 5.2384492E-02 4.5721369E-02 3.1440562E-02  
 1.1219313E-02

TRES 116

\*\*----- ROCK FLUID -----



ROCKFLUID

RPT 1

SWT

**\$	Sw	krw	krow
	0	0	0.7
0.04375	0.00390625	0.615234	
0.0875	0.015625	0.535937	
0.13125	0.0351562	0.462109	
0.175	0.0625	0.39375	
0.21875	0.0976563	0.330859	
0.2625	0.140625	0.273438	
0.30625	0.191406	0.221484	
0.35	0.25	0.175	
0.39375	0.316406	0.133984	
0.4375	0.390625	0.0984375	
0.48125	0.472656	0.0683594	
0.525	0.5625	0.04375	
0.56875	0.660156	0.0246094	
0.6125	0.765625	0.0109375	
0.65625	0.878906	0.00273437	
0.7	1	0	

SLT

**\$	S1	krq	krog
	0.3	1	0
0.34375	0.878906	0.00273437	
0.3875	0.765625	0.0109375	
0.43125	0.660156	0.0246094	
0.475	0.5625	0.04375	
0.51875	0.472656	0.0683594	
0.5625	0.390625	0.0984375	
0.60625	0.316406	0.133984	
0.65	0.25	0.175	
0.69375	0.191406	0.221484	
0.7375	0.140625	0.273438	
0.78125	0.0976563	0.330859	
0.825	0.0625	0.39375	
0.86875	0.0351562	0.462109	
0.9125	0.015625	0.535937	
0.95625	0.00390625	0.615234	
1	0	0.7	

\*\*----- INITIAL CONDITION -----

INITIAL

```

USER_INPUT
**$ Property: Pressure (psi)    Max: 1700  Min: 1700
PRES CON          1700
**$ Property: Water Saturation  Max: 0    Min: 0
SW CON           0
**$ Property: Global Composition(NC5)  Max: 0.0386  Min:
0.0386
ZGLOBALC 'NC5' CON          0.0386
**$ Property: Global Composition(C1)  Max: 0.2228  Min:
0.2228
ZGLOBALC 'C1' CON          0.2228
**$ Property: Global Composition(CO2)  Max: 0.022  Min:
0.022
ZGLOBALC 'CO2' CON         0.022
**$ Property: Global Composition(C2)  Max: 0.1285  Min:
0.1285
ZGLOBALC 'C2' CON          0.1285
**$ Property: Global Composition(C3)  Max: 0.1235  Min:
0.1235
ZGLOBALC 'C3' CON          0.1235
**$ Property: Global Composition(NC4)  Max: 0.0819  Min:
0.0819
ZGLOBALC 'NC4' CON         0.0819
**$ Property: Global Composition(FC6)  Max: 0.0379  Min:
0.0379
ZGLOBALC 'FC6' CON         0.0379
**$ Property: Global Composition(C13+)  Max: 0.10851  Min:
0.10851
ZGLOBALC 'C13+' CON        0.10851
**$ Property: Global Composition(C7+)  Max: 0.13008  Min:
0.13008
ZGLOBALC 'C7+' CON         0.13008
**$ Property: Global Composition(C22+)  Max: 0.10621  Min:
0.10621
ZGLOBALC 'C22+' CON        0.10621

```

```

**----- NUMERICAL -----

```

```

NUMERICAL
*NORM *PRESS  500.0
*NORM *SATUR   0.1    ** expected changes in one time-step
*NORM *GMOLAR  0.1

*DTMIN 1.0E-3          ** timestep size
*PRECC 1.0D-04         ** set convergence tolerance

```

\*ITERMAX 50

\*NORTH 20

\*\*----- WELL DATA -----

RUN

DATE 2009 1 20

\*\*\$

WELL 'Well-1'

INJECTOR 'Well-1'

INCOMP SOLVENT 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.

OPERATE MAX BHG 126.66 CONT

\*\*\$ rad geofac wfrac skin

GEOMETRY K 0.25 0.37 1. 0.

PERF GEOA 'Well-1'

\*\*\$ UBA ff Status Connection

1 1 40 1. OPEN FLOW-FROM 'SURFACE'

\*\*\$

WELL 'Well-2'

PRODUCER 'Well-2'

OPERATE MIN BHP 1700. CONT

\*\*\$ rad geofac wfrac skin

GEOMETRY K 0.25 0.37 1. 0.

PERF GEOA 'Well-2'

\*\*\$ UBA ff Status Connection

240 1 1 1. OPEN FLOW-TO 'SURFACE'

\*\*\$ Property: Implicit flag Max: 3 Min: 3

AIMSET CON 3

DATE 2009 4 20.00000

DATE 2009 7 20.00000

DATE 2009 10 20.00000

DATE 2010 1 20.00000

DATE 2010 4 20.00000

DATE 2010 7 20.00000

DATE 2010 10 20.00000

DATE 2011 1 20.00000

DATE 2011 4 20.00000

DATE 2011 7 20.00000

DATE 2011 10 20.00000

DATE 2012 1 20.00000

DATE 2012 4 20.00000

DATE 2012 7 20.00000

DATE 2012 10 20.00000

DATE 2013 1 20.00000

DATE 2013 4 20.00000

DATE 2013 7 20.00000  
DATE 2013 10 20.00000  
DATE 2014 1 20.00000  
DATE 2014 4 20.00000  
DATE 2014 7 20.00000  
DATE 2014 10 20.00000  
DATE 2015 1 20.00000  
DATE 2015 4 20.00000  
DATE 2015 7 20.00000  
DATE 2015 10 20.00000  
DATE 2016 1 20.00000  
DATE 2016 4 20.00000  
DATE 2016 7 20.00000  
DATE 2016 10 20.00000  
DATE 2017 1 20.00000  
DATE 2017 4 20.00000  
DATE 2017 7 20.00000  
DATE 2017 10 20.00000  
DATE 2018 1 20.00000  
DATE 2018 4 20.00000  
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DATE 2019 1 20.00000  
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DATE 2023 4 20.00000  
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DATE 2030 4 20.00000  
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DATE 2045 1 20.00000  
DATE 2045 4 20.00000  
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DATE 2045 10 20.00000  
DATE 2046 1 20.00000  
DATE 2046 4 20.00000  
DATE 2046 7 20.00000  
DATE 2046 10 20.00000  
DATE 2047 1 20.00000

DATE 2047 4 20.00000  
DATE 2047 7 20.00000  
DATE 2047 10 20.00000  
DATE 2048 1 20.00000  
DATE 2048 4 20.00000  
DATE 2048 7 20.00000  
DATE 2048 10 20.00000  
DATE 2049 1 20.00000  
DATE 2049 4 20.00000  
DATE 2049 7 20.00000  
DATE 2049 10 20.00000  
DATE 2050 1 20.00000  
STOP

\*\*----- SIMULATION STOP -----

## APPENDIX B

### BASE CASE CO<sub>2</sub> SEQUESTRATION DATA FILE

Following in the GEM input file used for simulating the CO<sub>2</sub> injection in the Aruma aquifer. This is a base case data file; diffusion and local grid refinement are not modeled here. The SI units are used in all the sequestration data files in this study. The depth, permeability, and porosity data are not a part of the main data file, and are included separately. The author may be contacted if those files are required.

-----

RESULTS SIMULATOR GEM 200800

\*\* This is a base case. Henry's Law is used to model  
solubility  
\*\* Diffusion and Hysteresis are not modeled here.

INUNIT SI  
WSRF WELL 1  
WSRF GRID TIME



```

OUTSRF GRID SG SW PRES DENW DENG Z 'CO2' W 'CO2' Y 'H2O' W
'H2O'
OUTSRF WELL PAVG GHGTHY GHGSCRIT GHGSOL GHGLIQ GHGGAS
OUTSRF RES NONE
WPRN GRID 0
OUTPRN GRID NONE
OUTPRN RES NONE
WRST 10000
INVENTORY-CO2
**$ Distance units: m
RESULTS XOFFSET 156547.0000
RESULTS YOFFSET 378337.0000
RESULTS ROTATION 0.0000 **$ (DEGREES)
RESULTS AXES-DIRECTIONS 1.0 -1.0 1.0

```

```

**----- RESERVOIR DATA -----

```

[illegible]





22:43	10:18	1:7	= 0
31:48	9:16	1:7	= 0
1:15	26:33	1:7	= 0
1:25	25:28	1:7	= 0
1:6	33:38	1:7	= 0
1:10	30:36	1:7	= 0
1:2	38:39	1:7	= 0
3:4	39:39	1:7	= 0
11:23	29:29	1:7	= 0
10:18	27:31	1:7	= 0
18:20	29:30	1:7	= 0
56:66	1:7	1:7	= 0
54:76	1:3	1:7	= 0
50:59	2:9	1:7	= 0
26:28	25:26	1:7	= 0
33:37	19:21	1:7	= 0
38:39	20:20	1:7	= 0
38:41	19:19	1:7	= 0
11:11	34:34	1:7	= 0
12:12	34:34	1:7	= 0
1:1	40:40	1:7	= 0
33:34	22:22	1:7	= 0
54:56	10:10	1:7	= 0
49:50	14:14	1:7	= 0
44:44	17:17	1:7	= 0
105:105	64:64	1:7	= 0
87:106	1:20	1:7	= 0
96:106	19:41	1:7	= 0
91:97	18:29	1:7	= 0
88:91	18:24	1:7	= 0
82:88	1:9	1:7	= 0
80:81	2:4	1:7	= 0
93:97	29:34	1:7	= 0
90:90	25:27	1:7	= 0
101:106	42:52	1:7	= 0
98:106	34:46	1:7	= 0
104:106	52:58	1:7	= 0
102:106	51:55	1:7	= 0
105:106	57:62	1:7	= 0
85:85	10:12	1:7	= 0
86:86	9:14	1:7	= 0
82:82	8:9	1:7	= 1
75:76	2:3	1:7	= 1
79:82	1:1	1:7	= 0
106:106	64:89	1:7	= 0

106:106	63:63	1:7	= 0
105:105	63:63	1:7	= 0
87:104	119:145	1:7	= 0
100:106	121:142	1:7	= 0
98:105	106:117	1:7	= 0
100:106	113:122	1:7	= 0
98:105	135:143	1:7	= 0
101:103	140:145	1:7	= 0
104:105	142:145	1:7	= 0
77:88	135:144	1:7	= 0
68:79	139:145	1:7	= 0
64:73	142:145	1:7	= 0
91:105	114:123	1:7	= 0
79:90	130:138	1:7	= 0
2:23	124:145	1:7	= 0
1:4	126:144	1:7	= 0
2:5	60:98	1:7	= 0
1:2	50:63	1:7	= 0
6:9	71:89	1:7	= 0
2:4	106:129	1:7	= 0
1:2	63:124	1:7	= 0
3:7	111:126	1:7	= 0
23:35	134:145	1:7	= 0
77:77	123:123	1:7	= 0
82:102	118:122	1:7	= 0
106:106	108:119	1:7	= 0
103:106	99:114	1:7	= 0
100:100	102:102	1:7	= 0
100:104	103:106	1:7	= 0
106:106	143:145	1:7	= 0
80:93	143:145	1:7	= 0
82:87	123:130	1:7	= 0
76:84	129:136	1:7	= 0
70:81	134:144	1:7	= 0
63:69	140:145	1:7	= 0
48:48	143:143	1:7	= 0
55:65	140:145	1:7	= 0
62:75	134:140	1:7	= 0
68:81	129:134	1:7	= 0
77:84	124:131	1:7	= 0
79:84	121:126	1:7	= 0
59:61	137:139	1:7	= 0
65:67	131:133	1:7	= 0
72:76	126:128	1:7	= 0
35:57	144:145	1:7	= 0

75:76	124:126	1:7	= 0
87:90	115:117	1:7	= 0
92:97	109:113	1:7	= 0
92:94	109:111	1:7	= 1
5:15	114:125	1:7	= 1
1:15	114:127	1:7	= 0
18:28	129:133	1:7	= 0
12:18	120:124	1:7	= 0
34:40	139:145	1:7	= 0
38:44	141:143	1:7	= 0
28:30	131:133	1:7	= 0
13:15	114:115	1:7	= 1

\*\*\$ Property: Porosity Max: 0.268061 Min: 0.0574038  
 POR ALL  
 INCLUDE "POR.IN"  
 \*\*\$ Property: Permeability I (md) Max: 4177.73 Min: 0.01  
 PERMI ALL  
 INCLUDE "PERMI.IN"  
 PERMJ EQUALSI  
 PERMK EQUALSI \* 0.1  
 \*\*\$ Property: Pinchout Array Max: 1 Min: 1  
 \*\*\$ 0 = pinched block, 1 = active block  
 PINCHOUTARRAY CON 1  
 PRPOR 4130  
 CPOR 4.38e-07

\*\*----- FLUID COMPONENT DATA -----

MODEL PR  
 NC 3 3  
 COMPNAME 'CO2' 'C1' 'H2O'  
 HCFLAG 0 0 0  
 VISCOR PEDERSEN  
 MIXVC 1  
 VISCOCOEFF 0.291 1.4 0.0005747 4.265 1.0579  
 MW 4.4010000E+01 1.6043000E+01 1.8015000E+01  
 AC 0.225 0.008 0.344  
 PCRIT 7.2800000E+01 4.5400000E+01 2.1760000E+02  
 VCRIT 9.4000000E-02 9.9000000E-02 5.6000000E-02  
 TCRIT 3.0420000E+02 1.9060000E+02 6.4730000E+02  
 PCHOR 78 77 52  
 SG 0.818 0.3 1  
 TB -78.45 -161.45 100

OMEGA 0.457236 0.457236 0.457236  
 OMEGB 0.0777961 0.0777961 0.0777961  
 VSHIFT 0 0 0  
 HEATING\_VALUES 0 890773 0  
 VISVC 9.4000000E-02 9.9000000E-02 5.6000000E-02

BIN  
 1.0300000E-01  
 2.0000000E-01 4.9070000E-01

TRES 46.1111  
 PHASEID GAS  
 PSAT -1  
 DENW 1036.3  
 CW 4.45E-07  
 REFPW 5882  
 VISW 0.61  
 SOLUBILITY HENRY  
 DERIVATIVEMETHOD NUMERALL  
 H2O\_INCLUDED  
 HENRY-CORR-CO2  
 TRACE-COMP 2  
 SATWCUTOFF 0.0  
 SWR-H2OVAP 0.0  
 OGW\_FLASH ON  
 METHOD-OGW 1  
 NC-AQUEOUS 1  
 COMPNAME-AQUEOUS 'NaCl'  
 AQFILL OFF  
 SALINITY PPMVOL 5000  
 SALINITY-CALC OFF  
 AQUEOUS-DENSITY ROWE-CHOU  
 AQUEOUS-VISCOSITY KESTIN

\*\*----- ROCK FLUID -----

ROCKFLUID

RPT 1

SWT

\*\*\$                Sw                krw                krow

0.25	0	0.741513
0.259	0.00100683	0.721249
0.268	0.00180539	0.704854
0.295	0.0038533	0.641721
0.322	0.0079916	0.581367
0.349	0.0128232	0.501012
0.376	0.0193238	0.421985
0.40092	0.0294565	0.363937
0.421	0.0387603	0.319328
0.448	0.051718	0.259998
0.475	0.070279	0.207043
0.502	0.093775	0.164473
0.529	0.11933	0.123684
0.556	0.149558	0.0883395
0.583	0.186321	0.0615307
0.61	0.227836	0.039882
0.63416	0.266466	0.0212892
0.655	0.306498	0.00995504
0.67532	0.35208	0.00545978
0.7	0.408888	0
0.71648	0.448173	0
0.74392	0.519642	0
0.77136	0.607685	0
0.7988	0.695778	0
0.82624	0.777445	0
0.85368	0.852026	0
0.88112	0.92274	0
0.90856	0.98431	0
0.936	1	0

SLT

\*\*\$

S1	krq	krog
0.25	1	0
0.2602	0.951272	0.000408816
0.2704	0.902544	0.000817632
0.2908	0.810565	0.00265018
0.3112	0.723454	0.00542236
0.3316	0.642796	0.00933594
0.352	0.567034	0.0142417
0.3724	0.497842	0.0204728
0.3928	0.432889	0.027559
0.4132	0.374559	0.0360611
0.4336	0.319843	0.0454498
0.454	0.271738	0.0560851
0.4744	0.226656	0.0675863
0.4948	0.188098	0.0805607



0.5152	0.152006	0.0941881
0.5356	0.122259	0.109483
0.556	0.0944639	0.125456
0.5764	0.0727291	0.142851
0.5968	0.0524727	0.161062
0.6172	0.0378599	0.180665
0.6376	0.0242972	0.20085
0.658	0.015786	0.222925
0.6784	0.00794832	0.245442
0.6988	0.00430131	0.269631
0.7192	0.00101088	0.294517
0.7396	0.000449725	0.320785
0.76	0	0.347774
0.7864	0	0.38488
0.8162	0	0.428813
0.846	0	0.474841
0.8758	0	0.523413
0.9056	0	0.57472
0.9354	0	0.628123
0.9652	0	0.683586
0.995	0	0.741513

\*\*----- INITIAL CONDITION -----

INITIAL

VERTICAL DEPTH\_AVE WATER\_GAS

ZGAS

.001 .999 0.0

REFPRES

4975

REFDEPTH

500

DWGC

250

SWOC

0.995

GASZONE NOOIL

\*\*----- NUMERICAL -----

NUMERICAL

DTMAX 1

DTMIN 0.001

NORM PRESS 3450

MAXCHANGE GMOLAR 0.5

MAXCHANGE SATUR 0.5

CONVERGE PRESS 3.55

\*\*----- WELL DATA -----

RUN

DATE 2011 1 1

\*\*\$

WELL 'DW06'

INJECTOR 'DW06'

INCOMP SOLVENT 1. 0.

OPERATE MAX STG 18406. CONT

\*\*\$ rad geofac wfrac skin

GEOMETRY K 0.0762 0.37 1. 0.

PERF GEOA 'DW06'

\*\*\$ UBA ff Status Connection

53 84 7 1. OPEN FLOW-FROM 'SURFACE'

\*\*\$

WELL 'DW07'

INJECTOR 'DW07'

INCOMP SOLVENT 1. 0.

OPERATE MAX STG 18406. CONT

\*\*\$ rad geofac wfrac skin

GEOMETRY K 0.0762 0.37 1. 0.

PERF GEOA 'DW07'

\*\*\$ UBA ff Status Connection

51 36 7 1. OPEN FLOW-FROM 'SURFACE'

\*\*\$

WELL 'DW08'

INJECTOR 'DW08'

INCOMP SOLVENT 1. 0.

OPERATE MAX STG 18406. CONT

\*\*\$ rad geofac wfrac skin

GEOMETRY K 0.0762 0.37 1. 0.

PERF GEOA 'DW08'

\*\*\$ UBA ff Status Connection

```

      50 129 7 1. OPEN FLOW-FROM 'SURFACE'
**$
WELL 'DW10'
INJECTOR 'DW10'
INCOMP SOLVENT 1. 0.
OPERATE MAX STG 18406. CONT
**$      rad geofac wfrac skin
GEOMETRY K 0.0762 0.37 1. 0.
PERF GEOA 'DW10'
**$ UBA      ff Status Connection
      55 104 7 1. OPEN FLOW-FROM 'SURFACE'
**$
WELL 'DW12'
INJECTOR 'DW12'
INCOMP SOLVENT 1. 0.
OPERATE MAX STG 18406. CONT
**$      rad geofac wfrac skin
GEOMETRY K 0.0762 0.37 1. 0.
PERF GEOA 'DW12'
**$ UBA      ff Status Connection
      68 66 7 1. OPEN FLOW-FROM 'SURFACE'
**$
WELL 'DW13'
INJECTOR 'DW13'
INCOMP SOLVENT 1. 0.
OPERATE MAX STG 18406. CONT
**$      rad geofac wfrac skin
GEOMETRY K 0.0762 0.37 1. 0.
PERF GEOA 'DW13'
**$ UBA      ff Status Connection
      56 116 7 1. OPEN FLOW-FROM 'SURFACE'
**$
WELL 'DW14'
INJECTOR 'DW14'
INCOMP SOLVENT 1. 0.
OPERATE MAX STG 18406. CONT
**$      rad geofac wfrac skin
GEOMETRY K 0.0762 0.37 1. 0.
PERF GEOA 'DW14'
**$ UBA      ff Status Connection
      20 68 7 1. OPEN FLOW-FROM 'SURFACE'
**$
WELL 'DW15'
INJECTOR 'DW15'
INCOMP SOLVENT 1. 0.

```

```

OPERATE  MAX  STG  18406.  CONT
**$      rad  geofac  wfrac  skin
GEOMETRY K  0.0762  0.37  1.  0.
PERF  GEOA  'DW15'
**$  UBA      ff  Status  Connection
      23 82 7  1.  OPEN      FLOW-FROM  'SURFACE'
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DATE 2011 9  1.00000
DTMAX 10
DATE 2012 1  1.00000
DATE 2012 5  1.00000
DATE 2012 9  1.00000
DATE 2013 1  1.00000
DATE 2013 5  1.00000
DATE 2013 9  1.00000
DATE 2014 1  1.00000
DATE 2014 5  1.00000
DTMAX 20
DATE 2014 9  1.00000
DATE 2015 1  1.00000
DATE 2015 5  1.00000
DATE 2015 9  1.00000
DATE 2016 1  1.00000
DTMAX 30
DATE 2016 5  1.00000
DATE 2016 9  1.00000
DATE 2017 1  1.00000
DATE 2017 5  1.00000
DATE 2017 9  1.00000
DATE 2018 1  1.00000
DATE 2018 5  1.00000
DATE 2018 9  1.00000
DATE 2019 1  1.00000
DATE 2019 5  1.00000
DATE 2019 9  1.00000
DATE 2020 1  1.00000
DATE 2020 5  1.00000
DATE 2020 9  1.00000
DTMAX 40
DATE 2021 1  1.00000
DATE 2021 5  1.00000
DATE 2021 9  1.00000
DATE 2022 1  1.00000
DATE 2022 5  1.00000
DATE 2022 9  1.00000

```

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DATE 2023 9 1.00000
DATE 2024 1 1.00000
DATE 2024 5 1.00000
DTMAX 100
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DATE 2025 9 1.00000
DATE 2026 1 1.00000
DATE 2026 5 1.00000
DATE 2026 9 1.00000
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DATE 2027 9 1.00000
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DATE 2030 1 1.00000
DATE 2030 5 1.00000
DATE 2030 9 1.00000
DATE 2031 1 1.00000
DATE 2031 5 1.00000
DATE 2031 9 1.00000
DATE 2032 1 1.00000
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DATE 2034 9 1.00000
DATE 2035 1 1.00000
DTMAX 300
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DATE 2036 1 1.00000
DATE 2036 5 1.00000
DATE 2036 9 1.00000
DATE 2037 1 1.00000
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DATE 2040 9 1.00000
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SHUTIN 'DW06'
SHUTIN 'DW07'
SHUTIN 'DW08'
SHUTIN 'DW10'
SHUTIN 'DW12'
SHUTIN 'DW13'
SHUTIN 'DW14'
SHUTIN 'DW15'
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DATE 2049 1 1.00000

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STOP

\*\*----- SIMULATION STOP -----

## VITA

Tausif Khizar Ahmed received his Bachelor of Science degree in petroleum engineering from Texas A&M University at Qatar in 2009. He entered the petroleum engineering distance learning program at Texas A&M University in September 2009. He completed his research at Texas A&M University at the Qatar campus and received his Master of Science degree in August 2011.

His research interests include CO<sub>2</sub> crude oil fluid characterization and CO<sub>2</sub> sequestration.

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