

# Predictions of long-term behavior of a large-volume pilot test for CO<sub>2</sub> geological storage in a saline formation in the Central Valley, California

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## Abstract

The long-term behavior of a CO<sub>2</sub> plume injected into a deep saline formation is investigated, focusing on mechanisms that lead to plume stabilization. Key measures are plume migration distance and the time evolution of CO<sub>2</sub> phase-partitioning, which are examined by developing a numerical model of the subsurface at a proposed power plant with CO<sub>2</sub> capture in the San Joaquin Valley, California, where a large-volume pilot test of CO<sub>2</sub> injection will be conducted. The numerical model simulates a four-year CO<sub>2</sub> injection period and the subsequent evolution of the CO<sub>2</sub> plume until it stabilizes. Sensitivity studies are carried out to investigate the effect of poorly constrained model parameters permeability, permeability anisotropy, and residual gas saturation.

*Keywords: geologic CO<sub>2</sub> storage; multi-phase flow modeling; CO<sub>2</sub> trapping mechanism; plume stabilization*

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## 1. Introduction

Understanding the long-term behavior of large-volume CO<sub>2</sub> plumes is critical for advancing the technology of geologic carbon storage in deep saline formations. This behavior is examined by developing a numerical model of the subsurface at the proposed nominal-50 MW Kimberlina advanced oxy-combustion power plant with CO<sub>2</sub> capture in the southern San Joaquin Valley, California. For its first four years of operation, the power plant will provide 250,000 metric tons of CO<sub>2</sub> per year for a large-volume CO<sub>2</sub> geologic storage pilot. Thereafter, the captured CO<sub>2</sub> will be sold locally for enhanced oil recovery operations. The model simulates the four-year injection period, in which a total of 1 million metric tons of CO<sub>2</sub> are injected, and the subsequent evolution of the CO<sub>2</sub> plume for hundreds of years. Key measures of CO<sub>2</sub> plume stabilization are the migration distance of the plume and the time evolution of the partitioning of CO<sub>2</sub> between phases – dissolved, immobile gas, and mobile gas. At formation depth, the immiscible phase is supercritical, but it has gas-like properties so it is commonly referred to as gas.

The target storage region is the Vedder Formation, a high-permeability sand about 150 m thick, located at a depth of 2 km. The model grid covers an area of 125 km<sup>2</sup> of the Vedder formation, which dips 7° to the southwest. The Vedder Formation is over- and underlain by low-permeability shales. Within the formation itself, sands and shales are interleaved in a lenticular fashion, with typical lens size 15 m thick and 5 km in lateral extent. This geological setting provides an ideal situation for examining the interplay of buoyancy flow, CO<sub>2</sub> dissolution, capillary trapping, and geologic heterogeneity in controlling the long-term fate of the injected CO<sub>2</sub> plume. At the location of the proposed injection well, the Vedder formation consists of five sand layers with total thickness 79 m, separated by four shale layers with total thickness 79 m. In the model, injection is distributed among the sand layers, with injection strength proportional to layer thickness.

Because trapping mechanisms are scale-dependent, understanding large-volume pilots is a necessary step between existing studies involving small-scale CO<sub>2</sub> injection tests and actual commercial CO<sub>2</sub> storage operations. Additionally, predicting the spatial and temporal evolution of the CO<sub>2</sub> plume and the attendant pressure increase can help optimize design of the monitoring methods used for the pilot.

## 2. Model Development

Numerical modeling is conducted using TOUGH2 [1], a general-purpose numerical simulator for multi-phase, multi-component fluid and heat flow in porous and fractured media. TOUGH2 uses a multi-phase extension of Darcy's law that includes relative permeability and capillary-pressure effects and incorporates accurate phase-partitioning and thermophysical properties of all fluid phases and components. At depths commonly considered for CO<sub>2</sub> storage (>800 m), CO<sub>2</sub> primarily exists as a gas-like supercritical phase, which is the non-wetting phase, while some CO<sub>2</sub> dissolves in the brine, which is the wetting phase. The present studies utilize a hysteretic formulation for capillary pressure and relative permeability [2] and an equation of state package called ECO2N [3], designed to treat a two-phase (liquid, gas), three-component (water, salt, CO<sub>2</sub>) system in pressure/temperature regimes above the critical point of CO<sub>2</sub> ( $P = 73.8$  bars,  $T = 31^\circ\text{C}$ ).

Although TOUGH2 has the capability to solve fully coupled fluid and heat flow problems, temperature is assumed to remain constant for the present simulations, to increase computational efficiency. Additionally, because the numerical simulations discussed here are all of relatively short duration (i.e., on the order of years rather than tens of thousands of years), they emphasize advective processes. The slower flow processes of aqueous-phase diffusion of dissolved species is not included in the numerical model. Salt may precipitate out of the brine, but the rock matrix itself is inert. Thus, chemical reactions between CO<sub>2</sub> and rock minerals are not considered.

Together, capillary pressure  $P_c$ , liquid relative permeability  $k_{rl}$ , and gas relative permeability  $k_{rg}$  variation as a function of saturation are known as characteristic curves; they control the way the brine (the wetting phase, also called the liquid phase) and supercritical CO<sub>2</sub> (the non-wetting phase, also called the gas phase) interact. In a hysteretic formulation,  $P_c$ ,  $k_{rl}$ , and  $k_{rg}$  depend not only on the saturation of the grid block, but also on the history of the saturation of the grid block. When liquid saturation decreases because more CO<sub>2</sub> enters a grid block than leaves it, the process is known as drainage. Alternatively, when liquid saturation increases because more brine enters a grid block than leaves it, the process is known as imbibition. The most critical parameter of the characteristic curves is the residual gas saturation, denoted  $S_{gr}^A$ , which is the saturation below which gas is immobile (i.e., the saturation below which immiscible CO<sub>2</sub> is trapped). We use the conceptualization common in the petroleum literature [4, 5] in which it is assumed that under drainage conditions,  $S_{gr}^A = 0$ , but for imbibition,  $S_{gr}^A$  increases as maximum historical gas saturation increases. Thus, grid blocks that once contained the most CO<sub>2</sub> are those which trap the most CO<sub>2</sub>. During a CO<sub>2</sub> injection period, drainage is the dominant process because the CO<sub>2</sub> plume is growing in all directions, hence  $S_{gr}^A = 0$  and no CO<sub>2</sub> is trapped as residual gas. After injection ends, the leading edge of the CO<sub>2</sub> plume may still undergo drainage as the plume moves upward and up dip by buoyancy forces, but at the trailing edge of the plume imbibition occurs,  $S_{gr}^A \gg 0$ , and a significant fraction of the CO<sub>2</sub> plume may be trapped as residual gas.

A geologic model of the Kimberlina site provides the basis for the TOUGH2 model. The geologic model discretizes the Vedder formation in the vicinity of the Kimberlina power plant into cells, and assigns a facies (either sand or shale) to each cell, based on information interpolated from well logs. The geologic model extends about 6 km laterally in all directions from the power plant with a lateral cell dimension of 250 m in the E-W ( $x$ ) direction and 200 m in the N-S ( $y$ ) direction. The geologic model uses 180 layers to represent the Vedder Formation. Over the entire model, formation thickness ranges from 110 m to 187 m, but within the 2 km surrounding the power plant, thickness only ranges from 150 m to 164 m.

The TOUGH2 model (Figure 1) covers roughly the same spatial extent as the geologic model. Because the formation dip and thickness are nearly uniform in the vicinity of the power plant, the TOUGH2 model is constructed as a tilted plane, with just a single value of thickness (157.5 m) and dip ( $7^\circ$ ). The up-dip direction is  $30^\circ$  counterclockwise from the  $+x$ -axis, corresponding to an ENE strike direction. Each TOUGH2 model layer is formed by combining six geologic model layers, resulting in 30 layers, each 5.25 m thick. This combining scheme results in at least two model layers per sand layer, to enable vertical flow arising from buoyancy forces to be resolved. Laterally, the TOUGH2 model grid block size varies, with finest grid blocks in the vicinity of the injection well (5 m by 5 m), increasing to 50 m by 50 m in the region where the  $\text{CO}_2$  plume is expected to go (roughly an ellipse with major axis of 2 km), and gradually increasing further beyond that region. The lateral extent of the active portion of the TOUGH2 model is 11 km by 11 km, beyond which additional grid blocks are added to represent lateral boundary conditions.

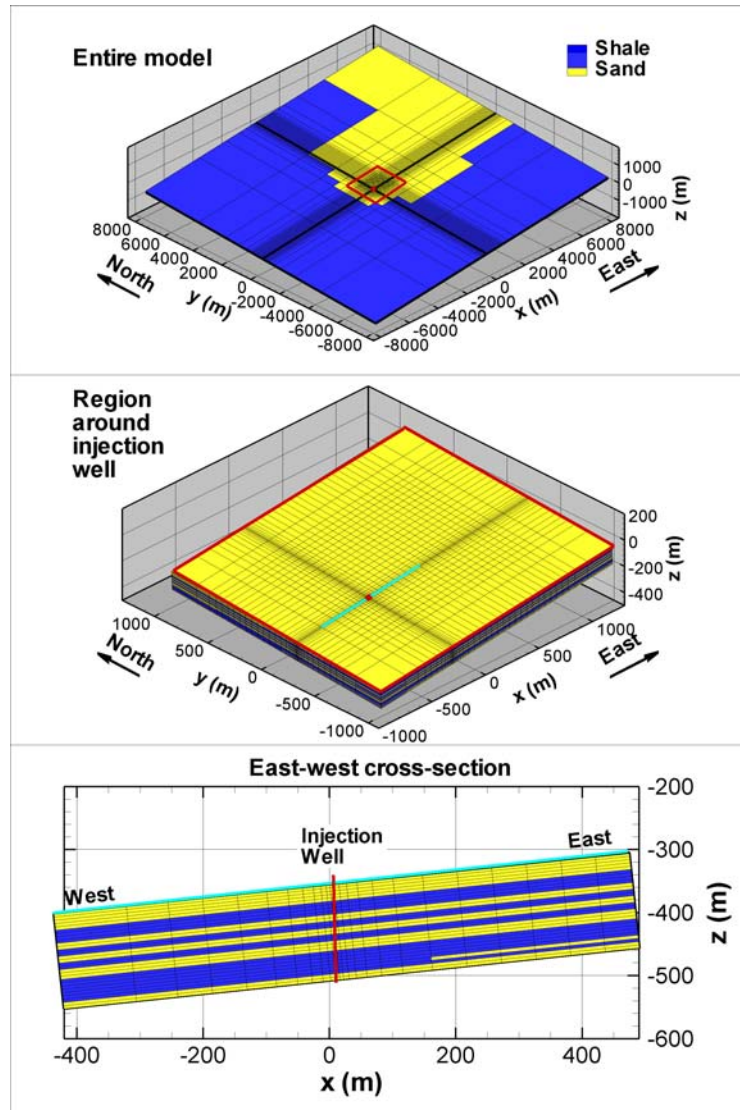


Figure 1. Several views of the TOUGH2 grid for the Vedder Formation at the Kimberlina site.

The top and bottom boundary of the model are no-flow boundaries, to represent regionally extensive, continuous shale layers over- and underlying the Vedder Formation. In the  $x$ -direction the lateral boundaries are constant pressure boundaries and in the  $y$ -direction the lateral boundaries are no-flow boundaries. This choice is primarily made for numerical convenience. The lateral boundaries are so far away from the injection well and the region the  $\text{CO}_2$  plume is expected to occupy that they have little impact on the evolution of the  $\text{CO}_2$  plume. Table 1 summarizes the geometric properties and boundary conditions of the TOUGH2 model.

Table 1. Geometric properties and boundary conditions of the TOUGH2 model for the Vedder Formation at the Kimberlina power plant site.

Parameter	Value	Comment
Depth at injection well (m)	2200	Same as geologic model
Thickness (m)	157.5	Geologic model thickness ranges from 110 m to 187 m
Percent sand/shale	50/50	Sand occurs in five distinct layers, with interleaving shales
Number of model layers	30	Each model layer 5.25 m thick, combines 6 geologic-model layers
Lateral extent (km)	11 by 11	Comparable to geologic model
Lateral grid spacing	Varies	5 m by 5 m at injection well; maximum 50 m by 50 m within $\text{CO}_2$ plume

Formation dip	7°	footprint Up-dip direction is ENE, 30° counterclockwise from +x-axis
Boundary Conditions		
Top and bottom	No flow	Represent continuous, extensive shale layers
Lateral, x-direction	Constant pressure	
Lateral, y-direction	No flow	

The initial conditions for the CO<sub>2</sub> injection are a brine-saturated formation with a hydrostatic pressure distribution, and a pressure of 220 bars at the injection well location. Initial temperature and salinity are uniform at 81°C and 50,000 TDS, respectively. This temperature is calculated assuming a surface temperature of 15°C and a geothermal gradient of 30°C per km, both of which are rough estimates considered reasonable for Southern California. In the absence of specific information on salinity for the Vedder Formation, a moderate value of 50,000 TDS is chosen. Varying this value by a factor of two or three is not expected to have significant impact on the results. The primary impact of the initial pressure and temperature are to define the density and viscosity of the CO<sub>2</sub> plume in the subsurface. Density controls not only the volume of the plume, but the strength of the gravity force, which is proportional to the density difference between injected CO<sub>2</sub> and native brine. In conjunction with permeability, viscosity controls how mobile the CO<sub>2</sub> is. Table 2 summarizes the initial conditions used for the Kimberlina simulations, and the resulting density and viscosity of the injected CO<sub>2</sub> and the native brine. It shows that the injected plume will be strongly buoyant in the subsurface. The effects of initial pressure and temperature on plume migration are examined in another paper in this proceedings [6].

Table 2. Initial conditions and flow properties of CO<sub>2</sub> and brine.

Initial Condition	Value	
Initial pressure	Hydrostatic pressure distribution; average 220 bars at injection well	
Initial temperature	81°C	
Initial salinity	50,000 mg/L	
Flow property	CO <sub>2</sub>	Brine
Density (kg/m <sup>3</sup> )	632	1014
Viscosity (Pa sec)	0.50·10 <sup>-4</sup>	0.39·10 <sup>-3</sup>

The material properties used in the base-case TOUGH2 model are summarized in Table 3. These material properties are not well established for the Kimberlina site, so parameter values are adapted from other studies of CO<sub>2</sub> geologic storage in saline formations [2]. Sensitivity studies then examine the impact of varying permeability, permeability anisotropy (both vertical and lateral), and maximum residual gas saturation. Table 3 shows that the permeability contrast between the sand and shale facies is large; thus CO<sub>2</sub>, which is injected only into sand layers, is expected to remain in the sand layers.

Table 3. Material properties of the base-case TOUGH2 model.

Facies	Porosity	Horizontal Permeability, $k_x, k_y$ *	Vertical Permeability $k_z$ *	Residual Liquid Saturation $S_{lr}$	Maximum Residual Gas Saturation $S_{gmax}$ **
Sand	28%	200 md	20 md	0.2	0.28
Shale	15%	0.1 md	0.01 md	0.3	0.29

\* "Horizontal" means parallel to layering; "vertical" means perpendicular to layering

\*\* Residual gas saturation  $S_{gr}^A$  is zero during drainage and non-zero during imbibition, where it depends on saturation history and has a maximum value of  $S_{gmax}$ .

### 3. Simulation Results

The base-case TOUGH2 model simulates the injection of 250,000 t/yr of CO<sub>2</sub> for four years, then simulates the following 196 years during which CO<sub>2</sub> is subject only to gravity and capillary forces. Figure 2 and Figure 3 show snapshots of the supercritical CO<sub>2</sub> plume at various times. Figure 2 shows a top view of the uppermost layer of the model, which is the layer in which the greatest lateral extent of CO<sub>2</sub> occurs. Figure 3 shows *x-z* cross-sections through the model, and illustrates the formation of five sub-plumes in the five sand layers within the Vedder formation. Note from Figure 2 that the *x-z* plane does not show the maximum lateral extent of CO<sub>2</sub>, which occurs in the up-dip direction. Together, Figure 2 and Figure 3 illustrate the strong buoyancy flow that moves CO<sub>2</sub> to the top of each sand layer, and from there moves the plume up dip. For the present paper, we define plume stabilization as occurring when two successive snapshots show no advance of the leading edge of the plume. Figure 2 shows that the base-case plume has stabilized by 25years.

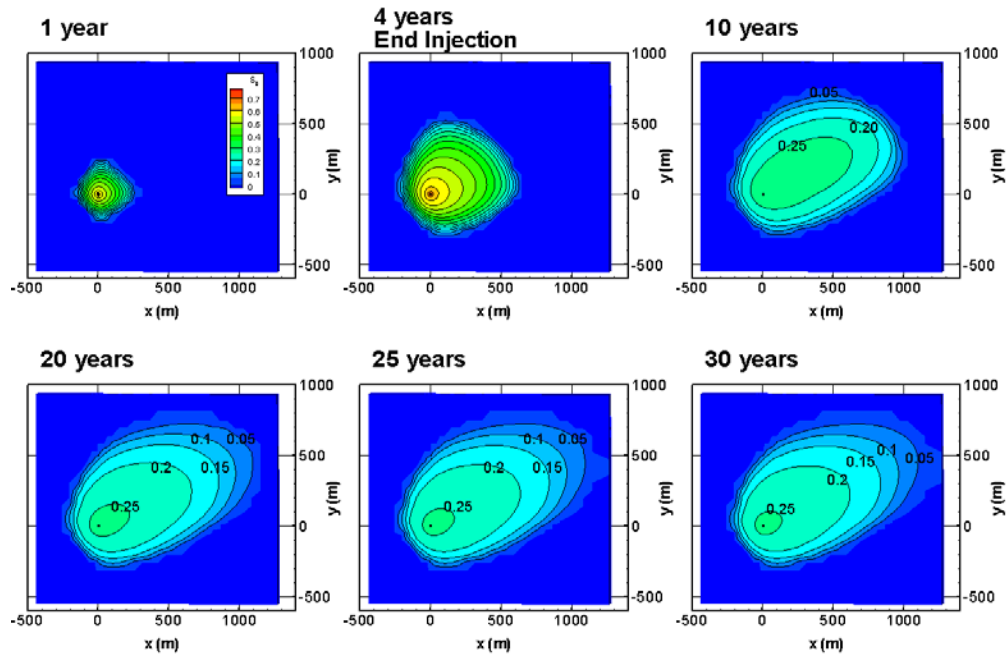


Figure 2. Top view of the base-case CO<sub>2</sub> plume at a series of times. During injection, the rectilinear grid produces numerical artifacts in the plume distribution by enabling enhanced flow along the grid axes directions.

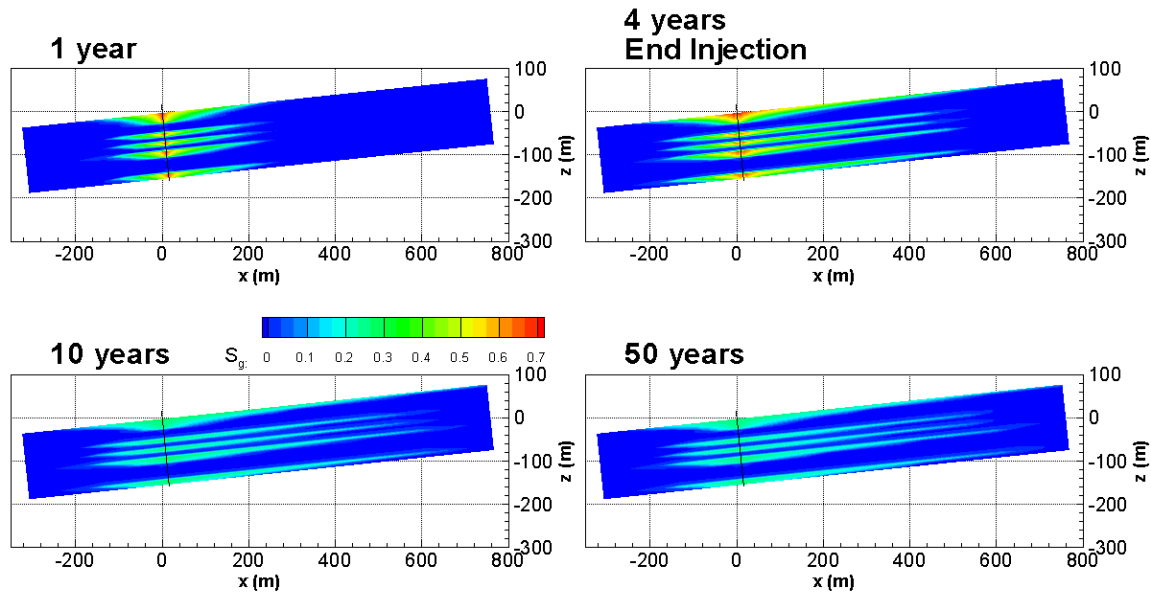


Figure 3. East-west cross-section of the base-case CO<sub>2</sub> plume at a series of times.

Quantification of the trapping and stabilization process is presented in Figure 4, which shows a CO<sub>2</sub> mass balance for the entire model. The total amount of CO<sub>2</sub> injected is divided into two parts: a gas-like supercritical phase and a dissolved phase. The supercritical phase is further divided into mobile and immobile CO<sub>2</sub>, with CO<sub>2</sub> becoming immobile when its saturation drops below residual gas saturation  $S_{gr}^A$ . Throughout the injection period, about 20% of the CO<sub>2</sub> dissolves, while most of the supercritical-phase CO<sub>2</sub> is mobile. After injection ends, the dissolved fraction increases gradually to about 40% as the plume moves up dip and encounters new under-saturated brine. This up-dip movement is accompanied by capillary trapping, and Figure 4 shows how the mobile fraction of supercritical CO<sub>2</sub> decreases concurrent with the increase of the immobile fraction. By 30 years the supercritical CO<sub>2</sub> is largely immobile, coinciding with the stabilization of the plume shown in Figure 2.

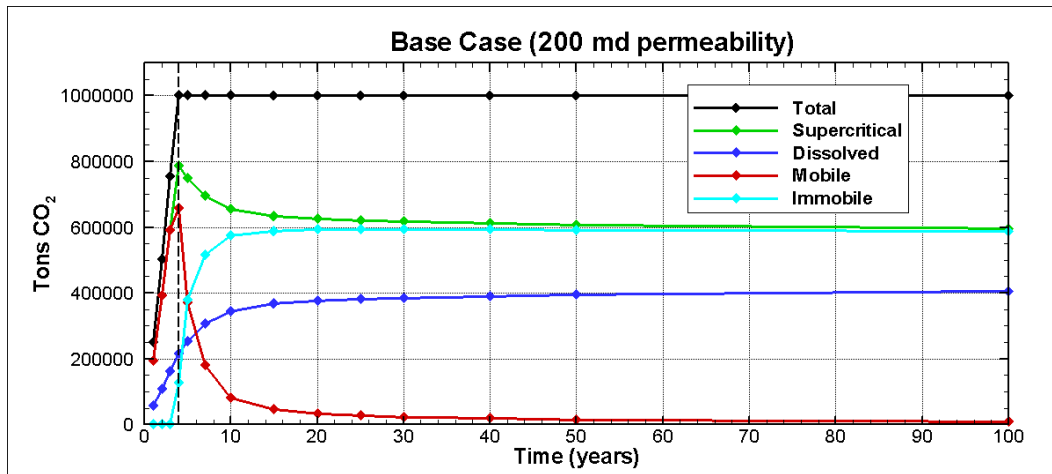


Figure 4. Integrated mass balance for the entire model for the base-case.

Several of the parameters used as input to the numerical simulation are not well known. To assess the impact of parameter uncertainty on plume evolution, sensitivity studies are carried out, using alternative parameter choices for poorly-known parameters. Table 4 summarizes the cases and the key performance measures for each. Figure 5 shows a plan view of the top of the stabilized plume for each case.

Table 4. Summary of sensitivity studies.

Case	Key Features	Time of plume stabilization (years)	Up-dip migration distance at stabilization (km)	Percent dissolved at stabilization
A10	Base case $k_x = k_y = 200$ md, $k_z = 20$ md, $S_{gmax} = 0.28$ <i>Sand Anisotropy Studies</i>	25	1.30	38
A	Isotropic permeability $k_x = k_y = k_z = 200$ md	25	1.35	39
I	Lateral permeability anisotropy $k_x = k_y/3, <k_x, k_y>_g = 200$ md, $k_z = 20$ md	25	1.5	39
H	Lateral permeability anisotropy $k_x = k_y/10, <k_x, k_y>_g = 200$ md, $k_z = 20$ md <i>Sand Permeability Studies*</i>	20	2.50	41
K	Very low permeability $k_x = k_y = 20$ md, $k_z = 2$ md	85	0.70	32
J	Low permeability $k_x = k_y = 66$ md, $k_z = 6.6$ md	50	1.00	34
G	High permeability $k_x = k_y = 500$ md, $k_z = 250$ md	20	2.00	45
E	Very high permeability $k_x = k_y = k_z = 1000$ md <i>Residual Gas Saturation Studies**</i>	15	2.50	52
F	Low residual gas saturation $S_{gmax} = 0.10$	30	1.80	53
N	Medium-low residual gas saturation $S_{gmax} = 0.20$	25	1.45	43
M	Medium-high residual gas saturation $S_{gmax} = 0.30$	25	1.20	37
L	High residual gas saturation $S_{gmax} = 0.40$	15	1.05	32

\*When sand permeability decreases, capillary pressure strength and  $S_{gmax}$  increase

\*\*Here only  $S_{gmax}$  is varied

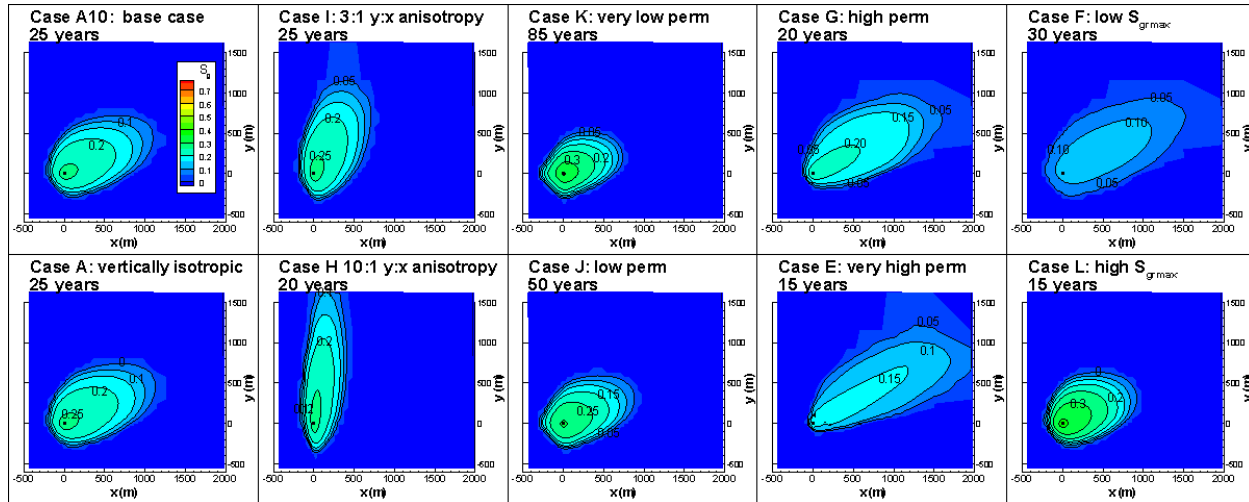


Figure 5. Plan view of stabilized CO<sub>2</sub> plumes for various cases.

The base-case model (A10) assumes vertical permeability is 1/10th of horizontal permeability, a common assumption for sands with permeability in the hundred millidarcy range. Assuming an isotropic medium (Case A), produces only subtly different plume evolution: perhaps 50 m more up-dip migration. This insensitivity largely arises from the sand/shale layering, which creates five sub-plumes in the sand layers, and thereby limits the amount of buoyancy flow that can occur. It is expected that a factor of ten change in permeability anisotropy would have a much greater effect for a homogeneous sand formation.



The region surrounding the Kimberlina site contains numerous small faults, many of which have a north-south orientation. Whether these faults act as conduits or barriers to flow, their net effect is likely to be a lateral ( $x:y$ ) anisotropy in sand permeability with a greater permeability in the north-south ( $y$ ) direction. Cases I and H, with a 3:1 and 10:1  $y:x$  anisotropy ratio, respectively, show that the direction of plume migration shifts dramatically from the up-dip direction ( $30^\circ$  north of due east) toward the north.

Sand-layer permeability (Cases K, J, G, and E) has a strong effect on plume behavior, with plume extent and percent dissolved  $\text{CO}_2$  increasing as permeability increases, whereas stabilization time and maximum  $\text{CO}_2$  saturation decrease as permeability increases. It should be noted that while well logs from the Kimberlina region do show sand permeabilities even higher than 1000 md and even lower than 20 md, it is not known how regionally extensive such extreme features are.

Sand-layer maximum residual gas saturation  $S_{grmax}$  (Cases F, N, M, and L) also has a major impact on long-time plume behavior, with smaller values of  $S_{grmax}$  producing a more spread out plume and higher percent dissolved  $\text{CO}_2$ .

#### 4. Conclusions

Simulation results show that for the base case, about 20% of the injected  $\text{CO}_2$  is in dissolved form at the end of the four-year injection period, and this percent increases to almost 40% by the time the  $\text{CO}_2$  plume stabilizes at 25 years. From this time onward, very little mobile  $\text{CO}_2$  is left in the formation, and plume evolution consists solely of slow dissolution. The plume footprint is roughly elliptical, with a long axis of about 1500 m and a short axis of 900 m. The plume is asymmetric about the injection well, extending 1300 m in the up-dip direction and 200 m in the down-dip direction. Sensitivity studies show that model parameters permeability, permeability anisotropy, and maximum residual gas saturation strongly affect the direction and extent of plume movement, indicating that additional site characterization efforts to better constrain these parameters prior to  $\text{CO}_2$  injection would be beneficial. The effect of in situ temperature and pressure is examined in a companion paper [6].

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