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Introduction

In order to significantly impact increases in atmospheric concentrations of CO₂, an alternative to releasing very large volumes of this gas must be found. Average releases at U.S. power plants are 2.7 million metric tons of CO₂ per year, with large plants releasing more than 18 million metric tons. One attractive option for reducing these emissions is to inject the CO₂ into unused subsurface brine formations below, and hydrologically separated from, potable water. Brine formations provide large volumes of storage space and decrease or eliminate the cost of pipelines for moving CO₂ from the source to the injection site. Technologies for doing this kind of injection are well known because CO₂ has been injected into hydrocarbon reservoirs as part of an enhanced oil recovery (EOR) process for decades. In addition, there is a long operational history for waste-fluid disposal by underground injection, and the technological and regulatory environments for this process are also well known.

For CO₂ to be injected, we assume that there must be (1) extraction of the CO₂ from the waste stream and drying in order to avoid compression costs of the nitrogen and oxygen and equipment being corroded by water vapor, (2) compression to conditions above the critical point, and (3) injection through one or more well bores to the target horizon(s). A typical project's life span might be 30 years. During this time, the CO₂ as a supercritical fluid will immiscibly displace brine in a large area around the injection well, and the pressure within the subsurface injection horizon will increase over a much larger area. We expect, over time, the "bubble" of supercritical CO₂ to migrate under the influence of gravity and the pressure to decrease as CO₂ dissolves into the brine and as brine or CO₂ slowly leaks from the injection horizon into lateral or overlying lower pressure zones.

Objective and Approach

The objective of this phase of our project is to do a series of simulations using realistic geotechnical data to explore the engineering and monitoring issues that can be expected during the active injection period and over the geologic time frame during which CO₂ is stored in the subsurface. Issues to be evaluated with respect to the impact of realistic geologic properties on injection and CO₂ storage processes include pressure increase at the injection well bore, stress changes in the overlying low-permeability horizon that serves as the seal, radial migration of the CO₂ bubble away from the injection well(s), regional distribution of pressure in the brine formation, long-term migration of the CO₂ bubble over geologic time frames, dissolution of CO₂ in the aqueous phase, and rock–water interactions. Our goal is to test the feasibility of high-volume sequestration in a real, nonidealized, brine-bearing formation in a typical area where there are currently large CO₂ emissions to the atmosphere.

The upper Texas Gulf Coast around Houston, Texas, is one of the areas where U.S. CO₂ emissions to the atmosphere are concentrated because of a combination of electric power generation and industrial activity. Within a 7-county area (16,700 km²) centered around Houston, Texas (fig. 1), 10 power plants released an estimated 32 million metric tons of CO₂ in 1996. In addition, more than 100 chemical manufacturing plants and refineries in the same area continue to release an unknown additional volume of CO₂. We selected this area as a representative region in which strategies for emissions reduction must be implemented if U.S. emissions are to be reduced sufficiently to impact atmospheric concentrations.

This area of concentrated emissions in the upper Texas Gulf Coast overlies a thick sedimentary section that provides an attractive target for geologic sequestration. The geologic and petrophysical characteristics of Gulf Coast sands are well known because of a long and intensive history of hydrocarbon exploration and production. Sands are thick, laterally extensive, and permeable and are separated by regionally extensive shales deposited during transgressions. Volumetric estimates of the sequestration capacity of one major stratigraphic interval, the Frio Formation (fig. 2), have been made in Texas according to the following assumptions. The area assessed is the Oligocene Frio Formation as defined by Galloway and

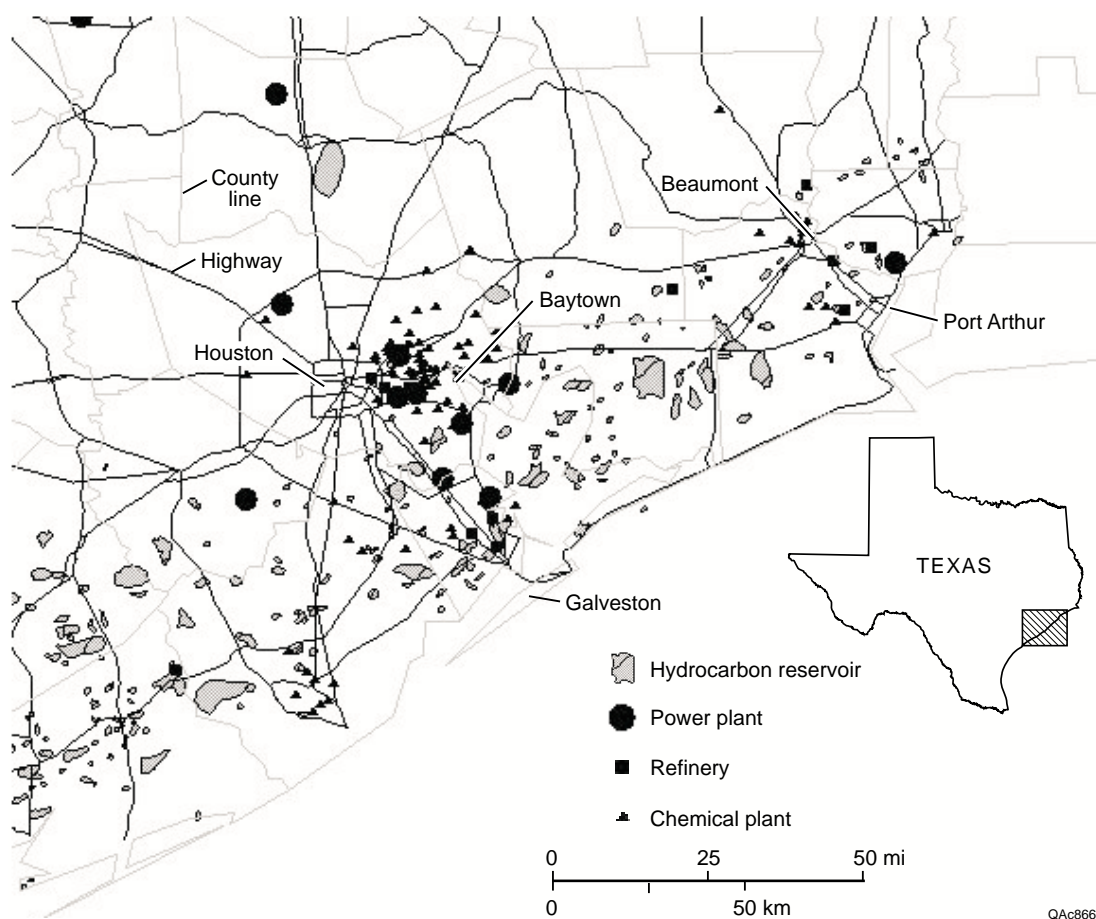


Figure 1. Distribution of representative power plants and industrial and refinery emitters in the upper Texas Gulf Coast.

others (1982) from the Sabine River to the Rio Grande. Pore volume calculations were made by using the net sand thickness of the Frio between 1,000 and 3,000 m below the ground surface and multiplying it by gridded porosity from regional data compiled by Hovorka and others (2000). A CO_2 density of 595 kg/m^3 (corresponding to an average reservoir pressure and temperature of 80°C and 200 bars) and a range of storage efficiency of from 1 to 6 percent, as suggested by Van der Meer (1995), yield a capacity of the Frio of between 208×10^9 and 358×10^9 metric tons of CO_2 .

Geologic complexities that present a challenge for modeling and issues needing to be investigated to determine their impact on sequestration include fluvial, deltaic, and barrier island sands that provide a heterogeneous permeability; regional dip, growth faults, and salt diapirs (Galloway and others, 1984) that supply potential avenues for upward leakage of CO_2 and brine; and producing oil fields and geopressure regimes that create a complex pressure domain (Kreitler and others, 1986).

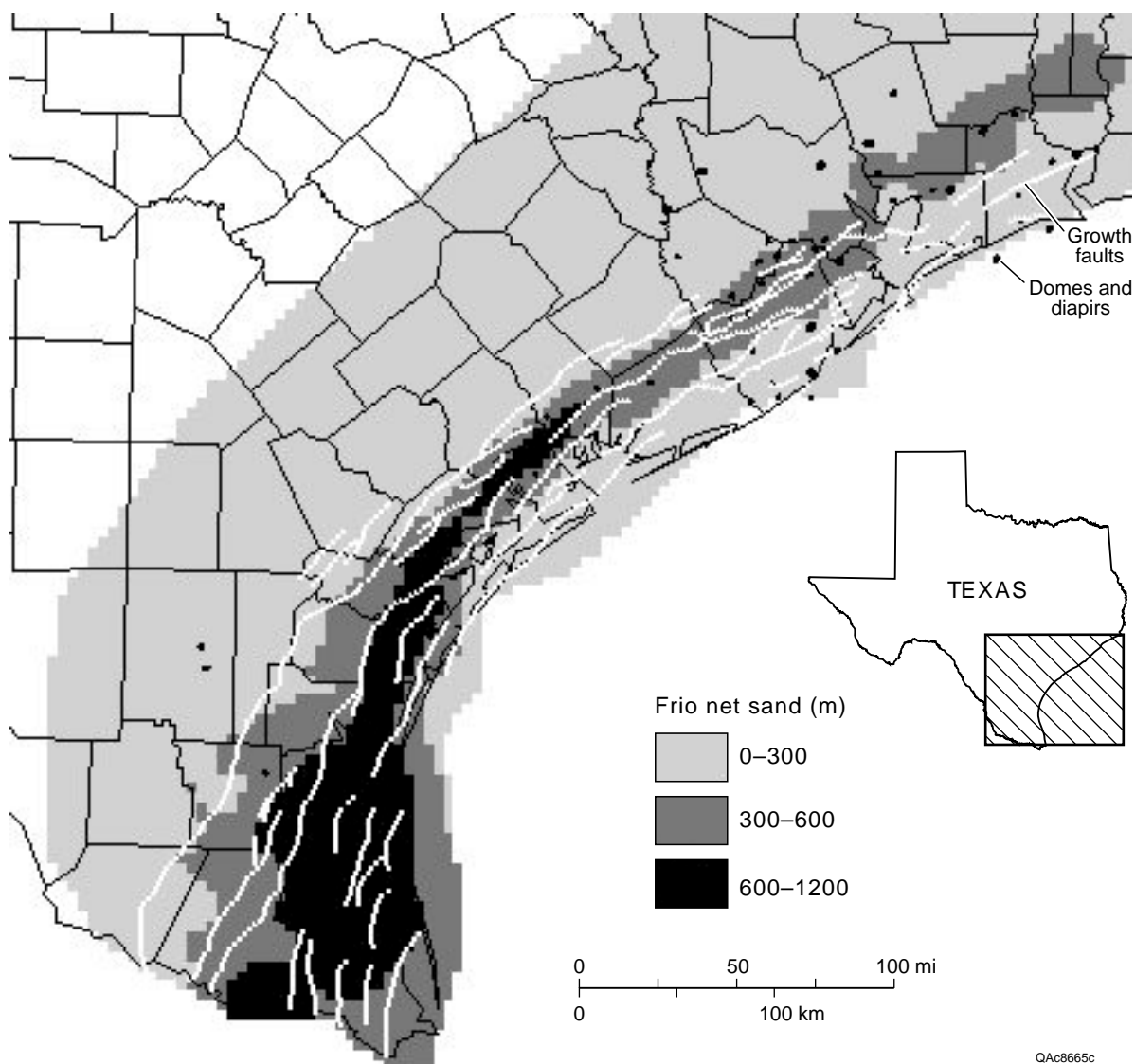


Figure 2. Geologic setting of the Frio Formation in the Texas Gulf Coast.

Project Description

Three types of reservoir simulations are being conducted to address these issues (fig. 3): (a) Small-scale simulations are being developed to assess the effects of vertical and lateral heterogeneity on pressure buildup at CO₂ injection wells, the number of injection wells needed, and the influences of reservoir-scale heterogeneity on CO₂ storage efficiency. (b) A conceptual model and modeling approach are being developed and tested to create reservoir-scale simulations for assessing sequestration performance over a typical 30-year project lifetime. These simulations are needed to provide information

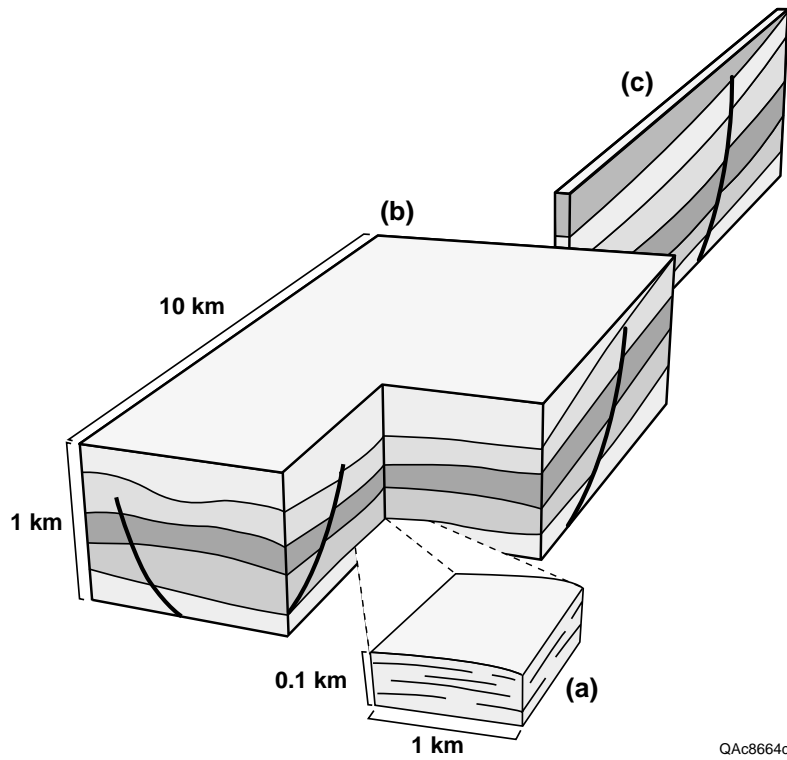


Figure 3. Simulations constructed at three scales: (a) $1 \times 1 \times 0.1$ km, (b) $10 \times 10 \times 1$ km, and (c) regional scale.

on the extent and phase distribution of the CO₂ plume during the injection period, the regional extent and magnitude of pressure buildup, and the displacement of brines into surrounding geological strata. In order to determine the significance of geologic complexities such as growth faults, folds, and facies changes, we must represent them using appropriate space discretization and determine which grid reproduces appropriate flow and pressure conditions at the reservoir scale. Initial goals toward producing this simulation include data compilation, experiments in methods of representing stratigraphically and structurally complex reservoirs in model grids, and testing the sensitivity of CO₂ behavior to these factors. (c) Long-term (10,000 years) regional-scale simulations will assess how residence time is affected by CO₂ buoyancy, large-scale geological features, CO₂–brine interactions, and deep-basin brine migration. These simulations will be carried out by using a very narrow three-dimensional grid that is aligned with buoyancy-driven movement of the CO₂ plume but that still preserves some of the important characteristics of a 3-dimensional flow field.

We selected for our investigation an injection site near the Cedar Bayou power plant (Reliant Energy Houston Power and Light) and adjacent Bayer Refinery. 1997 CO₂ emissions of 4.3 million metric tons of CO₂ have been reported for this 2295 MW gas-fired power plant (U.S. Geological Survey, 2001).

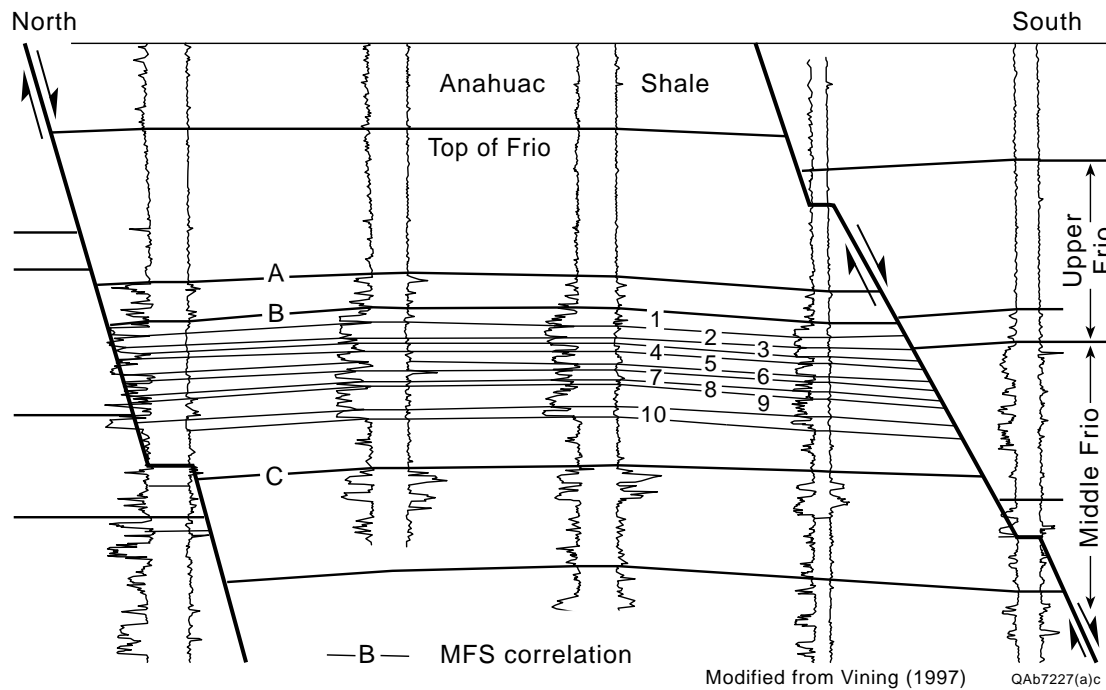


Figure 4. Structural cross section from Umbrella Point field, showing the stratigraphy characteristic of the injection target.

Results

Examination of the selected site shows that the top of the Frio Formation lies at a depth of 1,850 m (Geomap of the Gulf Coast, Inc., 1981). Examination of representative log cross sections and a type log (Vining, 1997) from Umbrella Point, a nearby well-studied reservoir, shows that the middle Frio is a sequence of alternating sands and shales (fig. 4). The first thick sand (stratigraphic interval MFS-B) in the Frio is identified as the target. We classified 10 depositional layers separated by subregionally extensive shales (flooding surfaces) within a 100-m-thick, sand-rich interval, according to depositional facies interpreted from the curve shape on resistivity logs. In the selected injection site, we do not have sufficient well data to map permeability in the injection interval. For this simulation we therefore selected a geologically constrained probabilistic procedure to create a model grid.

For the initial simulation we assessed the general depositional setting of the selected sand on regional, dip-oriented, well log cross sections (Dodge and Posey, 1981) and regional depositional system patterns (Galloway, 1982). After determining that deltaic and barrier strandplain systems were likely settings, we subdivided the selected sand into 10 layers separated by flooding surfaces. Log shape and lateral variability of sands in cross section from adjacent and stratigraphically similar Umbrella Point oil field (Vining, 1997) provided information on probable facies for each layer (fig. 5) and the scale of both

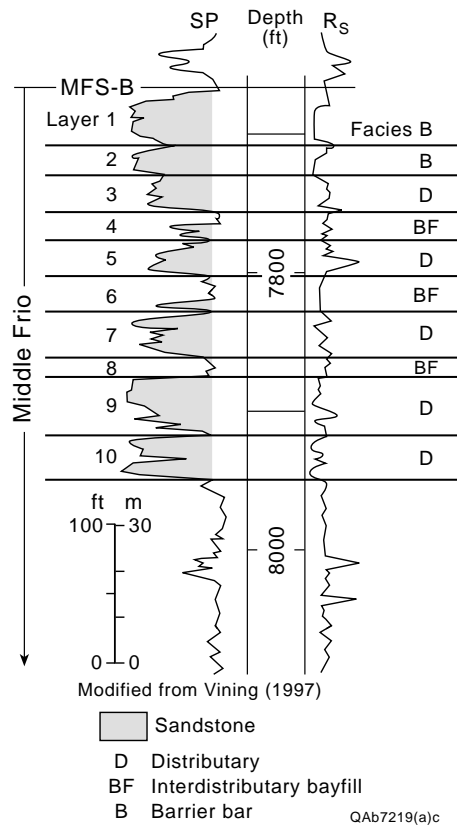


Figure 5. Log showing stratigraphic and facies subdivisions of Umbrella Point field used for the detailed model.

sandy and muddy depositional features (distributary channels, bayfill shales, barrier bars, etc.). The various depositional features were oriented in map view by using regional trends from Galloway and others (1982). Numerous past detailed studies of Frio sandstones in the Texas Gulf Coast (Galloway, 1982; Galloway and Cheng, 1985; Knox and others, 1996; Knox and Barton, 1999) provided the background needed to interpret depositional features from limited site-specific information. The result was idealized facies maps, 1.4 km on a side, for three depositional settings: distributary channel, interdistributary bayfill (narrow channel and splays), and barrier bar. A total of 10 stochastic realizations were then created from each idealized facies map using TProGS (Transition Probability Geostatistics), a 3-D geostatistical simulation software package (Carle, 1996; Carle and Fogg, 1996; Carle, 1997; Carle and Fogg, 1997; Carle and others, 1998). TproGS uses transition probabilities to preserve cross-correlations, such as upward-fining sequences, that traditional geostatistical approaches typically neglect. Such cross-correlations may be important factors in the interconnectivity of high-conductivity zones (Fogg and others, in press), which affects mass-transfer rates. Realizations for each layer of the final model were then selected, with different realizations of a particular facies being used for different layers.

Other modeling parameters were selected through examination of reservoir characteristics in similar facies in adjacent reservoirs (McConnell, 1962; Pace, 1962; Quinn, 1962; Steer, 1962; Surber, 1962).

Table 1. Typical reservoir characteristics for each facies

Facies	Porosity (%)	Horizontal permeability (md)	Vertical permeability (md)
Shale	10	0.001	0.0001
Splay-1	28	150	30
Channel	30	400	100
Splay-2	30	250	100
Barrier core	32	700	700
Washover	29	200	50

The regional geothermal gradient above geopressure is 32.6°C/1000 m (Loucks and others, 1984). For Frio water chemistry at these depths, reasonable values are TDS 100,000 ppm, Na 35,000 ppm and Cl 45,000 ppm (Kreitler and others, 1988; Macpherson, 1992). The injection interval is nonproductive of hydrocarbons. We selected an injection rate of 0.75 million metric tons of CO₂ per well per year by considering the injection rate in thicker, more permeable sands in the Sliepner CO₂ injection interval and by making an optimistic assessment of gas-production rates from Frio reservoirs.

The numerical simulations presented in this paper were performed by using TOUGH2, a general-purpose simulator for multiphase flows in porous and fractured media (Pruess and others, 1999). TOUGH2 solves mass-balance equations (optionally also an energy balance) for multicomponent fluid mixtures in which the components can partition into several fluid and solid phases. Flow is represented by a multiphase version of Darcy's law that includes relative permeability and capillary-pressure effects. The continuum equations are discretized by means of an integral finite difference method, which for systems of regularly shaped grid blocks is mathematically equivalent to conventional finite differences (Narasimhan and Witherspoon, 1976). For numerical stability, time is discretized fully, implicitly as a first-order backward finite difference. Time steps are automatically adjusted (increased or reduced) during the course of a simulation, to cope with variable nonlinearities and convergence rates, especially during appearance or disappearance of phases. Discretization results in a system of coupled nonlinear algebraic equations that are solved by Newton-Raphson iteration. The linear equations arising at each iteration step are solved by means of preconditioned conjugate gradient methods or sparse direct solvers (Moridis and Pruess, 1998).

The fluid-property description is based on correlations originally developed for geothermal applications (Battistelli and others, 1997) and subsequently enhanced to more accurately represent phase partitioning and thermophysical properties of water–CO₂–NaCl mixtures at near-ambient temperatures and

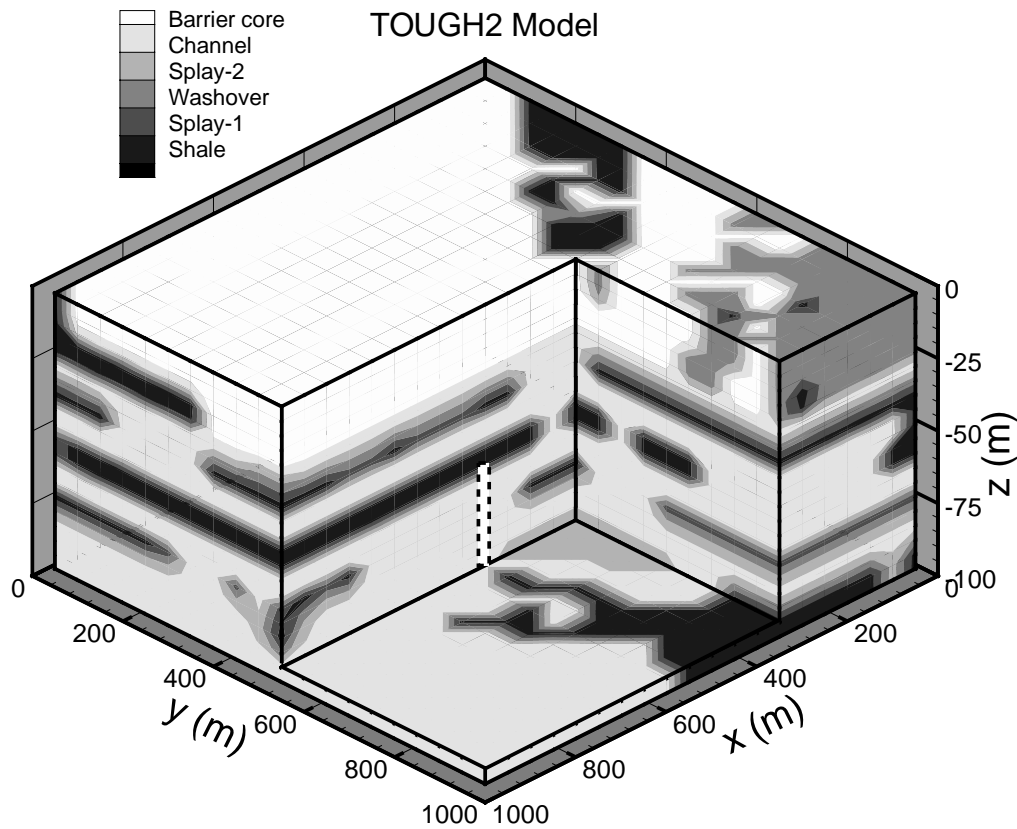


Figure 6. The TOUGH2 model created using the TPGS algorithm. Materials are listed in order of decreasing permeability. The injection interval is shown as a dashed rectangle.

supercritical CO₂ pressures (Pruess and Garcia, in press). Densities, viscosities, and enthalpies of CO₂ are calculated from correlations developed by Altunin (1975) and his associates, as implemented in a computer program kindly provided to us by V. Malkovsky. Dissolution of CO₂ in NaCl brines is described in an extended version of Henry's law that accounts for effects of CO₂ fugacity, temperature, and salinity. Details of the fluid-property model are given in Pruess and Garcia (in press).

A cutaway view of the TOUGH2 model created from the TProGS algorithm is shown in figure 6. The model extends over 1 km² and is 100 m thick. It contains 10 layers that range in thickness from 4 to 15 m. Each layer includes 400 grid blocks having lateral dimensions of 50 m. Six material types are represented, with permeabilities ranging from 0.001 to 700 md and porosities ranging from 10 to 32 percent (table 1).

The model, bounded above and below by impermeable layers, has constant-pressure lateral boundaries. Initial conditions include brine having a TDS content of 100,000 ppm under hydrostatic condi-

Modeled Gas Saturation

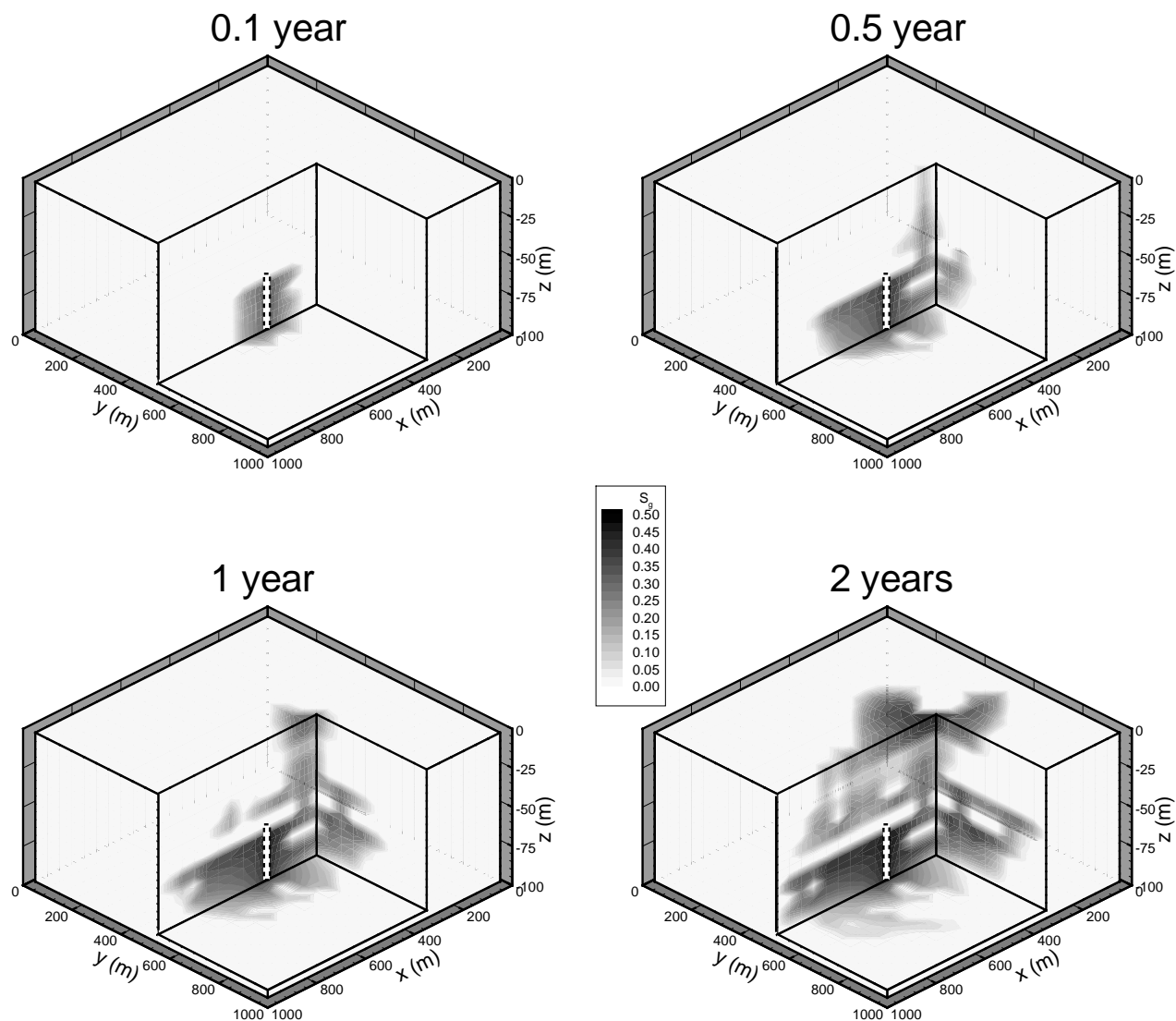


Figure 7. Modeled CO₂ distribution after 0.1, 0.5, 1.0 and 2.0 years of injection.

tions. CO₂ is injected at a constant rate of 750,000 metric tons per year into a single well open over the lower half of the model. The top of the model lies at a depth of 1,860 m, and at ambient pressure and temperature conditions, CO₂ is in a supercritical state.

Model results presented in figure 7 show CO₂ saturations at a series of times during the injection period. Preferential flow through higher permeability materials and buoyancy flow of the immiscible CO₂ are readily apparent.

Application and Future Activities

This numerical study provides an essential test of the feasibility and issues surrounding the injection of large volumes of CO₂ into the subsurface. If geologic sequestration is to be used to reduce carbon emissions at many power plants, large volume and wide availability of brine formations will make the formations an attractive option for sequestration of CO₂. This first series of simulations highlights the critical parameters that must be considered in site selection, injection design, and short- and long-term monitoring and verification.

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