

Numerical Simulations of Fluid Leakage from a Geologic Disposal Reservoir for CO₂

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Introduction

Among the different concepts currently being studied for reducing atmospheric emissions of greenhouse gases, primarily carbon dioxide (CO₂), one of the more promising ones involves disposal into deep geologic formations. Containment of CO₂ in geologic structures is not expected to be perfect. CO₂ may leak along pre-existing faults or fracture zones, and an assessment of the feasibility of geologic disposal requires an understanding of the manner in which CO₂ may escape and ultimately be discharged at the land surface. The behavior of CO₂ depends on the hydrogeologic properties of the pathways along which it migrates, on the thermodynamic regime encountered (temperature and pressure conditions), and on the thermophysical properties of CO₂ and resident aqueous fluids.

In a previous study the pathway for CO₂ escape from the storage reservoir was modeled as a circular vertical channel of 3 m radius, embedded in a porous medium of lower permeability, and extending from 1000 m depth straight up to the ground surface (Pruess, 2003). In the present paper we consider migration along a 2-D planar feature that is intended to represent a generic fault or fracture zone (Fig. 1). Our main interest is in the thermodynamic regime and the coupled fluid flow and heat transfer effects during migration of CO₂.

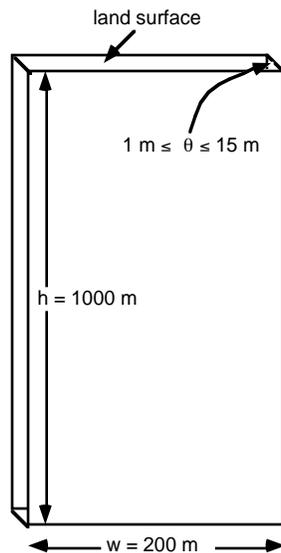


Figure 1. Simple model of a fracture zone used for modeling CO₂ escape from a geologic disposal reservoir. A rectangular high-permeability zone of 200 m width is assumed to extend from a CO₂ reservoir at 1000 m depth all the way to the land surface. CO₂ migration was studied for different thicknesses of this zone in the range from 1 to 15 m.

Thermodynamic Issues

The thermodynamic issues relevant to upflow of CO₂ from a deep storage reservoir are illustrated in Fig. 2a. The saturation pressure of CO₂ as a function of temperature is shown along with two hydrostatic pressure profiles, calculated for a typical geothermal gradient of 30 °C per

km, for two average land surface temperatures of 5 °C and 15 °C, respectively. Both profiles pass in the vicinity of the critical point of CO₂ ($T_{crit} = 31.04$ °C, $P_{crit} = 73.82$ bar), and the one for 5 °C surface temperature intersects the CO₂ saturation line. In the latter case a bubble of CO₂ that is migrating upward would undergo a phase transition from liquid to gas at a pressure of approximately 63 bars, corresponding to a depth of approximately 630 m. Leakage of CO₂ from a deeper brine formation may induce some overpressure, which would shift the pressure profiles towards higher values. Phase change from liquid to gas is to be expected if CO₂ escapes upward at rates large enough so that not all of the leaking CO₂ dissolves in the aqueous phase. Boiling of liquid CO₂ may have large effects on leakage rates, because CO₂ density is much lower for the gaseous than for the liquid state (Fig. 2b). At subsurface (T, P) conditions, CO₂ is always less dense than aqueous phase and thus is subject to upward buoyancy force. A transition to gaseous conditions would greatly enhance the buoyancy forces and accelerate fluid leakage, as well as causing a rapid increase in fluid pressures at shallower horizons. This in turn could open pre-existing faults and fractures, enhancing their permeability and further increasing leakage rates.

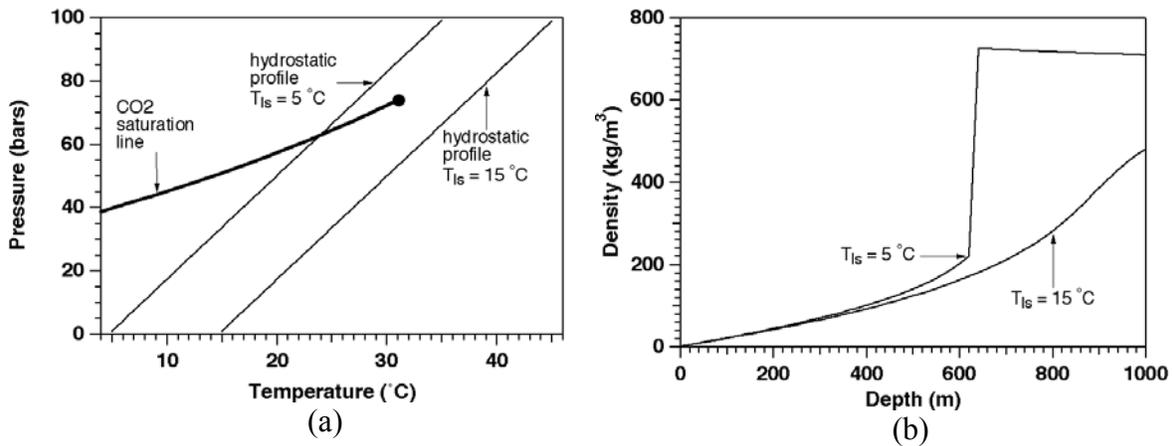


Figure 2. (a) CO₂ saturation line and hydrostatic pressure-temperature profiles for typical continental crust; (b) density of CO₂ vs. depth for the two hydrostatic profiles shown in Fig. 2a.

The specific enthalpy of CO₂ increases upon decompression, even if no phase change occurs, so that CO₂ migrating upward towards lower pressures would tend to undergo cooling as it expands. Inside a porous medium, the temperature decline is buffered by heat transfer from the solids. Heat transfer between rocks and fluids occurs locally on the pore scale, and also over larger distances by means of heat conduction from the low-permeability country rock towards the CO₂ pathway. Additional thermal effects occur when advancing CO₂ partially dissolves in aqueous fluids, giving rise to a small temperature increase from heat-of-dissolution effects.

Approach

The fracture zone considered in this paper is shown in Fig. 1, and is modeled as a porous medium sandwiched between impermeable walls. Permeability is assumed as 10^{-13} m², and porosity is taken as 0.35. Initial conditions are prepared by allowing a water-saturated system to run to steady state corresponding to land surface conditions of $T_{ls} = 15$ °C, $P_{ls} = 1.013 \times 10^5$ Pa, and a geothermal gradient of 30 °C/km (see Fig. 2a). Boundary conditions at 1000 m depth are a temperature of 45 °C, and a hydrostatic pressure of 98.84×10^5 Pa. Leakage is initiated by applying CO₂ at a slight overpressure of 99.76×10^5 Pa over a width of 6 m at the bottom left

hand side of the fracture zone. Boundary conditions at the top are maintained unchanged throughout the simulation. Lateral boundaries are "no flow." The walls bounding the fracture zone are assumed impervious to fluids but are participating in conductive heat exchange with the fluids in the fracture.

All simulations were performed with our general-purpose code TOUGH2 (Pruess et al., 1999), using a newly developed fluid property module that treats all seven possible phase combinations in the three-phase system aqueous - liquid CO₂ - gaseous CO₂ (Pruess, 2003). Thermophysical properties of CO₂ are represented, within experimental accuracy, by the correlations of Altunin (Altunin, 1975; Pruess and García, 2002). Conductive heat exchange with the impermeable wall rocks is modeled with the semi-analytical method of Vinsome and Westerveld (1980). This obviates the need to explicitly include the wall rocks into the definition domain of the numerical model, reducing the dimensionality of the flow problem to 2-D. Salinity effects were neglected. As will be seen below, there is a tendency for thermodynamic conditions to be drawn towards the critical point during the system evolution, and to remain very close to the CO₂ saturation line for extended periods of time, in some cases undergoing frequent changes between all gas or all liquid conditions. These features make the calculation quite challenging, requiring special techniques to avoid time steps being reduced to impractical levels.

Results

The CO₂ entering the column partially dissolves in the aqueous phase, but most of it forms a separate supercritical phase. Cross sections of CO₂ plumes for the case of a 15 m thick fracture zone are shown in Fig. 3 at two different times. A three-phase zone forms which initially is thin and of limited areal extent. With time this zone becomes thicker, broader, and migrates towards shallower elevations. Fluid mobility is reduced from interference between the three phases. This tends to divert upflowing CO₂ sideways, broadening the three-phase zone. Continuing heat loss resulting from boiling also causes this zone to become thicker with time and to migrate towards shallower elevations. Temperatures attain a local minimum at the top of the three-phase zone, where boiling rates are largest, and over time decrease to low values, approaching the freezing point of water (Fig. 4). Our simulator currently has no provisions to treat solid ice, but there is little doubt that for the conditions investigated in this simulation, water ice and hydrate phases would form at later time. Discharge of CO₂ at the land surface begins after approximately 6 years, first by exsolution of dissolved CO₂ from water that is flowing out at the top, and followed within a few months by a free CO₂-rich gas phase reaching the top boundary of the fracture zone. Fig. 4 also shows that at early time there is a temperature increase of approximately 2-3 °C, which is due to heat-of-dissolution effects.

It is instructive to plot thermodynamic conditions in a temperature-pressure diagram. Fig. 5 shows such a diagram for the leftmost column of grid blocks above the CO₂ injection region at different times. Initial conditions are represented by the line labeled "hydrostatic profile." After 6.07 yr the CO₂ injection has caused temperatures to decline in the high (T, P)-region, at the bottom of the fracture zone. The underlying mechanism is cooling from expansion of CO₂. At the lowest pressures (shallow elevations) temperatures have increased due to heat-of-dissolution effects. After a three-phase zone has formed, thermodynamic conditions track the CO₂ saturation line (15.65 and 30.69 yr in Fig. 5).

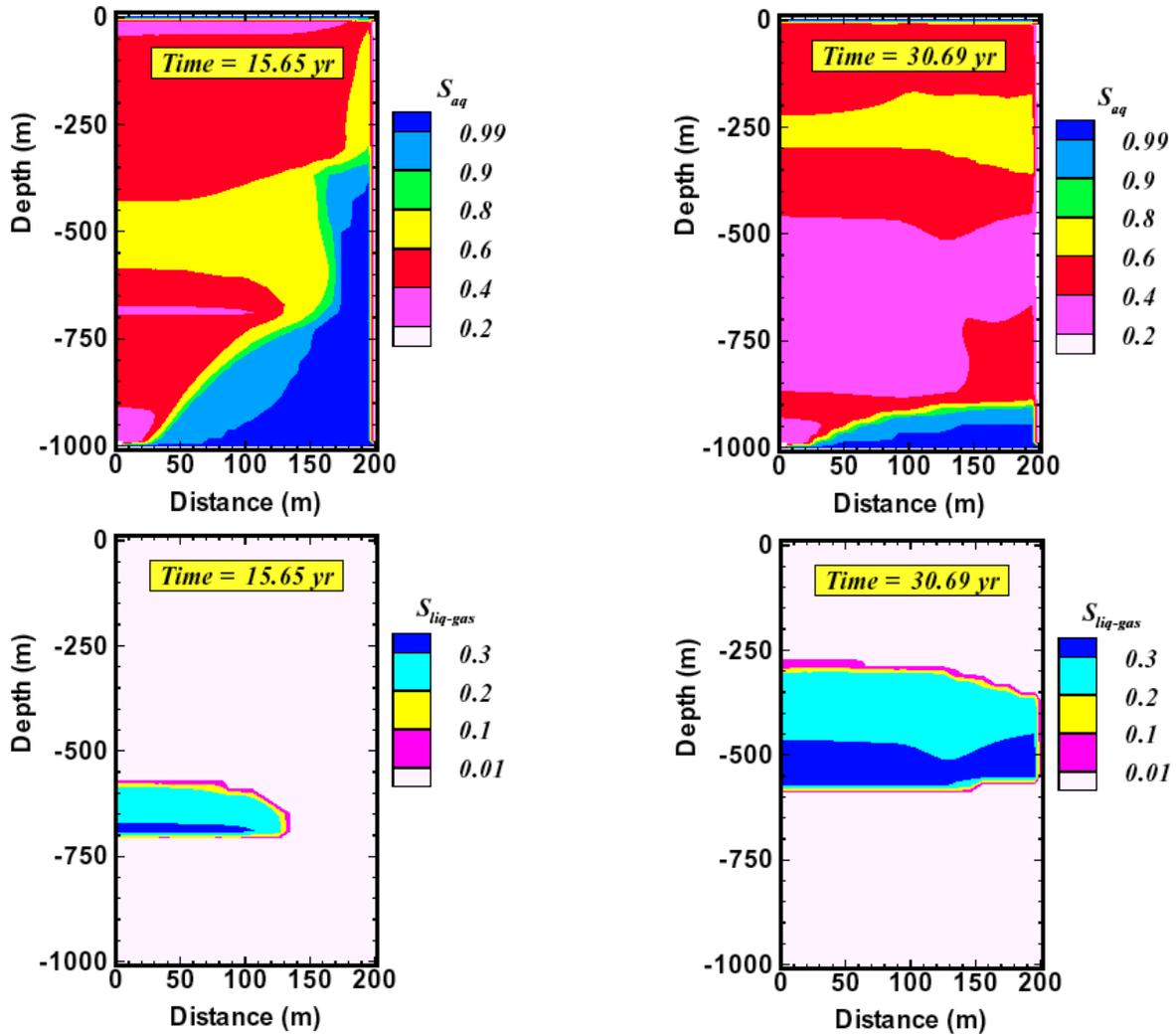


Figure 3. Snapshots of system evolution at two different times, showing CO_2 plumes (top) and extent of three-phase zone (bottom). The parameter $S_{liq-gas}$ is defined as $\sqrt{S_{liq} \cdot S_{gas}}$, which is non-zero only for three-phase conditions.

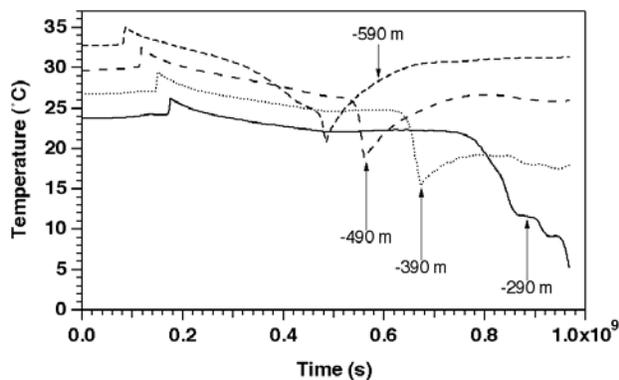


Figure 4. Temperatures at four different elevations in the leftmost column of grid blocks for a fault zone of 15 m thickness.

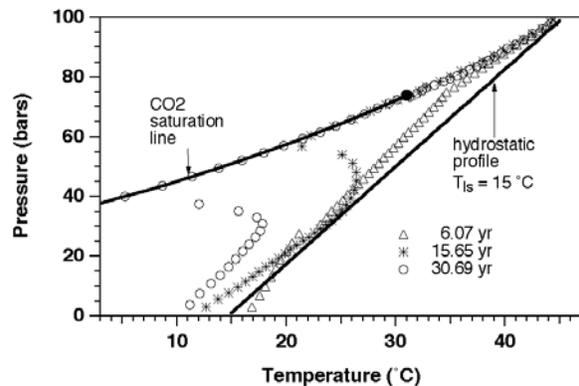


Figure 5. Pressure-temperature profiles in the leftmost column of grid blocks for a fault zone of 15 m thickness at different times.

Concluding Remarks

CO₂ migration behavior depends on relative rates of fluid flow and heat transfer. Simulation results presented above and additional results not shown here demonstrate the following.

- Upward migration of CO₂ along a fracture zone is strongly affected by heat transfer effects. Limited cooling occurs from expansion, while much stronger cooling takes place when liquid CO₂ boils into gas.
- CO₂ migration to elevations shallower than about 750 m may generate a three-phase aqueous - liquid CO₂ - gaseous CO₂ fluid system, even if the initial hydrostatic-geothermal profile does not intersect the CO₂ saturation line.
- There is a strong tendency for thermodynamic conditions to be drawn towards the critical point of CO₂ ($T_{\text{crit}} = 31.04 \text{ }^{\circ}\text{C}$, $P_{\text{crit}} = 73.82 \text{ bar}$), and to remain close to the CO₂ saturation line. This gives rise to severely non-linear behavior and makes numerical simulations of leakage processes very challenging.
- The tendency towards development of three-phase zones increases with increasing thickness of the fracture zone (increasing rate of CO₂ discharge). When CO₂ migrates through thin fracture zones, three-phase zones may not form at all or may form and dissolve in a transient manner.
- Fluid mobility is reduced in three-phase zones, due to interference between the phases. This impedes upflow, diverting CO₂ sideways and making these zones areally more extensive.
- Continued heat loss in boiling causes temperatures to decline over time, so that three-phase zones tend to grow in thickness and advance towards shallower elevations. Depending on the fracture zone thickness and permeability (CO₂ discharge rate), temperatures may reach the freezing point of water, and water ice and hydrate phases may form.
- The interplay between multiphase flow effects, phase change, and heat transfer may give rise to non-monotonic flow and temperature behavior.

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