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## Modeling Leakage through Faults of CO<sub>2</sub> Stored in an Aquifer

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### Abstract

For secure storage of CO<sub>2</sub> within geologic formations, the integrity of caps – overlying strata that are impervious to CO<sub>2</sub> – is an important factor. Geologic structures, notably faults and the damage zones surrounding them may provide a conduit for CO<sub>2</sub> to escape through a cap. If the fault encounters shallower permeable formations, the CO<sub>2</sub> rising along the fault can enter them. This lateral migration would attenuate the rate at which CO<sub>2</sub> enters sensitive formations such as aquifers used for drinking water. Thus, CO<sub>2</sub> leakage along faults will have three behaviors: upward migration from the storage formation along a fault, lateral movement from the fault into permeable layers, and a continued but attenuated CO<sub>2</sub> flux along the fault above the layers.

Here we develop a quasi-1D single-phase flow model for these three behaviors. The model is highly simplified and intended to be suitable for inclusion in a certification framework for geologic storage projects. The model accounts for flow from the fault into a permeable formation using a leakoff coefficient. The coefficient can vary spatially and depends on the geometry and petrophysical properties of the formation. We apply a commercial simulator to verify the quasi-1D model. A series of examples illustrates the controlling mechanisms for leakage rate from the reservoir and its attenuation by flux into shallower layers.

Nonlinearities arise even in this simple model. For example, leakage flux and the degree of attenuation vary nonlinearly with the permeability of the fault and the permeability of the shallower layer(s) intersected by the fault. Layers nearest the CO<sub>2</sub> storage formation produce the most attenuation. But the percentage of CO<sub>2</sub> entering overlying formations from the fault varies linearly with the ratio of fault permeability to leakoff coefficient. A simple estimate of the leak-off coefficient compares favorably with 2D, full-physics simulations. If the permeable layer is dipping, CO<sub>2</sub> enters it asymmetrically and estimating the leakoff coefficient is less straightforward. The difference arises because of preferential flow within the layer (CO<sub>2</sub> in the upper part, water below).

### Introduction

If society elects to reduce anthropogenic emissions of CO<sub>2</sub>, geologic storage will be one of the key technologies for achieving this goal. In the standard approach to storage, CO<sub>2</sub> is captured from fixed sources such as coal-fired power plants, compressed and injected at supercritical conditions into a suitable target formation. For typical geothermal gradients, suitable formations are found at depths of 800 m (2600 ft) or more, as their temperatures and pressures will be above the critical point of CO<sub>2</sub>. Trapping the injected CO<sub>2</sub> involves one or more mechanisms (Bachu *et al.* 1994; IPCC 2006): (1) permeability trapping by an impervious confining layer or cap rock; (2) solubility trapping by CO<sub>2</sub> dissolution into the aqueous phase in the pore space; (3) mineralogic trapping by chemical reaction of cations with dissolved CO<sub>2</sub> to precipitate carbonate minerals; (4) residual phase trapping as the nonwetting CO<sub>2</sub> phase becomes disconnected in pores or small clusters of pores; (5) stratigraphic trapping below a formation whose capillary entry pressure is greater than the capillary pressure of the CO<sub>2</sub> phase. An intact confining layer is necessary for several trapping mechanisms. However, sedimentary basins often contain geological discontinuities which are potential pathways for leakage through the confining layer. Faults are one such discontinuity and are prevalent in many regions where CO<sub>2</sub> storage is likely to be implemented. Wells are a man-made discontinuity, likewise prevalent in likely storage regions. We do not treat them here, but the conceptual model for faults provides a foundation for assessing leakage along wells (Huerta *et al.* 2008).

It is therefore important to examine the consequences if injected CO<sub>2</sub> encounters a fault. Figure 1 illustrates the situation of interest. A conductive fault can be a major pathway for the CO<sub>2</sub> plume due to its large transfer capacity. However CO<sub>2</sub> leaking

from the main target formation does not necessarily reach the Earth's surface. It may not even reach shallower formations of economic interest (mines, hydrocarbon reservoirs, aquifers that serve as underground sources of drinking water (USDW)). Instead, the rising CO<sub>2</sub> can be secondarily trapped by shallow subsurface structures, dissolution and residual phase creation (Lindeberg 1997). It can also migrate into permeable formations encountered by the conductive fault. On one hand, this migration attenuates the upward flux. On the other, it spreads the influence of the CO<sub>2</sub> across a wider area. The near-surface zone can also attenuate CO<sub>2</sub> leaks and decrease CO<sub>2</sub> concentration reaching the surface. The attenuation rate is sensitive to the subsurface properties (Oldenburg and Unger 2003). Thus, the effect of a conductive fault on net CO<sub>2</sub> storage needs to be analyzed based on the geometric and petrophysical properties of the formation, of the fault and of the overlying permeable layer, and on the boundary conditions (pressure in the storage formation and in the overlying layers).

The physics of a CO<sub>2</sub> plume rising long vertical distances through the Earth's crust can be complex (Pruess 2003). Here we present a highly simplified model, motivated by two considerations. One is geological: in many sedimentary basins, a fault is unlikely to be conductive continuously from depth to the shallow subsurface. Leakage to surface or to USDW will involve a sequence of upward (along a fault) and lateral (within a permeable layer) migrations. Thus we will consider moderate conduit lengths of 1000 meters or less. The other consideration is practical: for CO<sub>2</sub> storage to be implemented broadly and rapidly enough to mitigate anthropogenic emissions, thousands of storage projects will be needed. Each will have to be permitted by regulators in a streamlined yet robust and transparent way. Unfortunately the physical properties of most storage formations – deep saline aquifers – will be poorly constrained prior to injection. In light of this uncertainty, simple models that allow adequate physics-based risk assessment will be valuable tools for operators, regulators and policymakers.

The model presented here was developed to be applicable within the Certification Framework (CF) for geologic storage (Oldenburg and Bryant 2007, Oldenburg *et al.* 2008). The purpose of the CF is to provide a framework for project proponents, regulators, and the public to analyze the risks of geologic CO<sub>2</sub> storage in a simple and transparent way. The risk analysis would be performed to certify the startup and decommissioning of sites for geologic CO<sub>2</sub> storage. The CF currently emphasizes risks associated with subsurface processes and excludes compression, transportation, and injection-well leakage risk. The CF is designed to be simple by (1) using proxy concentrations or fluxes, rather than complicated exposure functions, for quantifying impact; (2) using a catalog of pre-computed CO<sub>2</sub> injection results (Kumar 2008), and (3) using a simple framework for calculating leakage risk. For transparency, the CF endeavors to be clear and precise in terminology in order to communicate to the full spectrum of stakeholders. One concept of the CF is that leakage occurs along conduits from the storage volume to “compartments” such as hydrocarbon reservoirs or USDW. The risk associated with leakage is the product of the probability of leakage and the impact of that leakage. The flux of CO<sub>2</sub> contributes to impact. Thus the goal of the fault-leakage model is to estimate flux at an “outlet” of a conductive fault, once CO<sub>2</sub> has arrived at the “inlet”.

The overarching criteria of the CF and the models within it are simplicity, transparency and acceptability. Here we emphasize the requirement of simplicity. The subsurface data available as input to any numerical model in the CF will always be limited. This limitation is especially troublesome in the case of injection into saline aquifers. Saline aquifers provide large storage capacity but are not well characterized due to the small number of existing wells which could provide geologic information about that particular region of the subsurface. The flow properties of faults are even more uncertain, at least before injection begins. In principle the required properties could be obtained from appropriate measurement campaigns. In practice, measurement will increase the cost of storage, and cost minimization will be a high priority for any greenhouse gas mitigation strategy. Moreover, the most reliable measurements would come from wells drilled into the formation or through the fault. These wells would themselves be potential pathways for leakage. The philosophy of the fault-leakage model is thus to identify the key physical phenomena controlling leakage flux. The sensitivity of the flux to physical parameters provides insight as to which aquifer properties should be measured when designing or monitoring a storage project.

In subsequent sections we present a quasi-1D mathematical description of CO<sub>2</sub> flux using the “leaky conduit” model. The leaks correspond to permeable formations intersected by the conduit. A “leakoff coefficient” is used to control the rate of leakage. We describe a method for estimating these coefficients from the properties of the formations. To test whether these idealizations are reasonable, we carry out simulations of the full physics of the problem in a 2D domain.

### Quasi-1D Modeling Approach

**Assumptions.** We assume that the CO<sub>2</sub> storage reservoir is located at sufficient depth for the carbon dioxide to be modeled as a slightly compressible fluid. Intersecting this storage volume is a fault, either vertical or at a fixed angle to the storage reservoir (Fig. 1). The most stringent assumption of the model is that we only consider the flow of a single fluid, namely CO<sub>2</sub>, along the fault. Leakage of CO<sub>2</sub> from saline aquifers will involve cocurrent and countercurrent flow of two fluid phases (brine and carbon dioxide), and relative permeability and capillary pressure play critical roles in buoyancy driven flow (e.g. Lakshminarasimhan *et al.* (2006) and Saadatpoor *et al.* (2008)). However, for the purposes of quantifying leakage mechanisms, single phase flow of CO<sub>2</sub> (Darcy's law) is assumed to capture the relationship between flux and driving force. We test this idealization later in this paper via two-phase flow simulations carried out using the GEM commercial simulator (Nghiem *et al.* 2006).

We treat the fault as a one-dimensional conduit with spatially varying permeability. Thus the complexities of the fault core and the damage zone surrounding it are averaged into a single array of permeability values. This simplification is extreme but it is consistent with concepts such as the shale gouge ratio (Yielding *et al.* 1997). Permeability in the direction of the fault throw is likely to be small in regions where sufficient shale is entrained in the fault. The existence of such a region will control CO<sub>2</sub> flux along the fault. This is true even in a long fault that elsewhere juxtaposes sand against sand and is very conductive.

Accounting for permeability variation along the fault will be important in estimating the risks associated with faults for a geologic storage project.

We further assume that the CO<sub>2</sub> remains slightly compressible as it rises along the fault. If the CO<sub>2</sub> moves slowly enough to equilibrate with the pressure and temperature of the surrounding formations, slight compressibility is a reasonable assumption for two situations. One is for deep leaks, those along faults beginning and ending at depths greater than about 1200 m (3500 ft). The other situation is shallow leaks, along faults less than 600 m (2000 ft) in depth. The density of CO<sub>2</sub> for hydrostatic pressure gradient and a representative geothermal gradient (29.2°C/1 km or 1.6°F/100 ft,  $T_{surface} = 15^\circ\text{C}$  or 59°F) is shown as a function of depth in Fig. 2a. The combined variation of pressure and temperature yields an almost linear variation of CO<sub>2</sub> density with depth for  $D > 3500$  ft and for  $D < 2000$  ft. The variation in each region can be approximated well with a slightly compressible model with constant compressibility (Table 1). Leaks which rise through intermediate depths, 2000 ft <  $D < 3500$  ft, could also be approximated with a slightly compressible model, and long leakage paths could be modeled by piecing together the appropriate behavior. We do not explore that possibility here. All results are for a single value of compressibility. For simplicity we assume constant viscosity. Figure 2b shows that this is a reasonable assumption if we take a value around 0.000018 Pa-s (0.018 cp) in the “shallow leak” region and 0.00006 Pa-s (0.06 cp) in the “deep leak” region, respectively. This simplification of the phase behavior also assumes that the pressure-temperature profile does not cross the gas/liquid phase boundary. As indicated in Fig. 2c, this assumption is valid for typical geothermal gradients and surface temperatures.

The model is “quasi”-1D because CO<sub>2</sub> is allowed to enter neighboring strata lateral to the fault (Fig. 3), but flow in these lateral formations is not explicitly modeled. Because we represent the fault as a “leaky conduit”, we refer to flow into these strata as “leakage”. The connotation of “leakage,” that is, flow from the fault vs. flow from the storage formation, should be clear from the context. We will also use the term “attenuation” to indicate CO<sub>2</sub> leaving the fault and entering a permeable layer. We model leakage from the fault via a specially designed source term. The lateral formations may be horizontal or inclined. The angle of inclination adds buoyancy to the driving force for leakage into the lateral formation.

We assume that the fault contains water initially (implemented by assuming the initial pressure along the fault is hydrostatic). The top of the fault is assumed to be at hydrostatic pressure. The bottom boundary of the fault is set to a pressure above hydrostatic. The value of this over-pressurization is proportional to the height of the column of stored CO<sub>2</sub>. The pressure in the CO<sub>2</sub> phase is taken to be hydrostatic at the base of the column. The thicker the column, the higher the pressure in the CO<sub>2</sub> at the location where the fault intersects the storage formation. This high pressure at the bottom of the fault (along with buoyancy) is the driving force for flow along the fault.

**Mathematical Model.** The single-phase flow equation derived from conservation of mass and Darcy’s law is given by Ewing (1983):

$$\frac{\partial}{\partial t}(\phi\rho) = \nabla \cdot \frac{\rho k}{\mu} (\nabla p - \rho g \nabla D) + q \quad (1)$$

where  $\phi$  is porosity,  $\rho$  is fluid density,  $p$  is pore pressure,  $k$  is vertical permeability of the fault,  $\mu$  is fluid viscosity,  $g$  is the gravitational constant,  $D$  is the depth vector, and  $q$  denotes the source or sink term.

Mathematically, the boundary and initial conditions described in the previous subsection are modeled as follows. If  $p_z$  denotes hydrostatic pressure then our initial condition along the fault at initial time  $t_0$  is  $p(z, t_0) = p_z(z)$ . The pressure at the top of the fault is given by  $p(z_{top}, t) = p_z(z_{top})$ , and the pressure at the bottom of the fault is  $p(z_{bottom}, t) = p_z(z_{bottom}) + X$  where  $X$  is an additional pressure due to the CO<sub>2</sub> storage compartment below the fault. Finally the source term is modeled by a vector of “leakoff coefficients”  $q_{leak}$  times a potential difference. The coefficients and the potential difference vary along the fault. Physically these leakoff values are only nonzero at depths  $z$  corresponding to leaks from the fault into lateral strata. The leakage source term is, therefore, described by

$$q(z, t) = q_{leak}(z) [p(z, t) - p_z(z) - \rho(z) g \sin \gamma] \quad (2)$$

Here in the gravity term, the gradient of the depth vector has been evaluated in the direction of the permeable formation. It is zero for horizontal formations and equal to  $\sin \gamma$  for formations inclined at angle  $\gamma$  to the horizontal.

Equation 1 is a single equation in two unknowns (density  $\rho$  and pressure  $p$ ). To reduce this equation to one equation in one unknown we make use of the equation of state which relates density to pressure via the differential equation (Chen *et al.* 2006):

$$\frac{\partial \rho}{\partial t} = c_f \rho \frac{\partial p}{\partial t} \quad (3)$$

The end result is that our one-dimensional model requires solution of the following equation for fluid pressure along the fault (Chen *et al.* 2006):

$$\rho \phi c_t \frac{\partial p}{\partial t} = \frac{\partial}{\partial z} \frac{\rho k}{\mu} \left( \frac{\partial p}{\partial z} - \rho g \sin \theta \right) + q \quad (4)$$

Here the angle  $\theta$  is the dip angle for the fault measured from horizontal (so a vertical fault has  $\sin \theta = 1$ ). We have introduced the total compressibility  $c_t$  defined by  $c_t = c_f + \frac{\phi_0}{\phi} c_r$ , where  $\phi_0$  is a reference porosity at reference pressure  $p_0$ ,  $c_f$  is fluid compressibility, and  $c_r$  is rock compressibility. For a slightly compressible fluid we approximate the exponential solution of the equation of state by a linear Taylor series, namely, that

$$\rho \approx \rho_0 [1 + c_f (p - p_0)] \quad (5)$$

which then requires solution of a nonlinear flow equation of the form of Eq. 4. The values of  $c_f$  for CO<sub>2</sub> in the “shallow leak” and “deep leak” regions are given in Table 1. We solve this system numerically by discretizing the spatial derivatives using Galerkin finite elements and using backward Euler for the time derivative.

**Leakoff Coefficients.** The leakoff coefficient  $q_{leak}$  in the source term can be estimated from the formation and fluid properties. The estimate is based on the Darcy’s law and the modeling assumptions described above. Assuming further that flow into the layer is steady, linear and one-dimensional flow, we write

$$Q = \frac{k_r k_{layer} A}{\mu} \left( \frac{\Delta \Psi}{L} \right) \quad (6)$$

where  $Q$  is volumetric flow rate of CO<sub>2</sub> (reservoir conditions),  $k_r$  is relative permeability,  $k_{layer}$  is absolute permeability of the layer into which CO<sub>2</sub> enters,  $A$  is cross-sectional area for leakage (i.e. the area of the intersection between fault and layer) and  $L$  is the distance between fault and the far boundary of the layer, where the pressure is hydrostatic. The potential difference is given by

$$\Delta \Psi = (p_1 - p_2) + (\rho_1 z_1 - \rho_2 z_2) g \sin \gamma \quad (7)$$

Subscripts ‘1’ and ‘2’ define locations; at location ‘1’ the fault intersects the permeable layer and at location ‘2’ the hydrostatic boundary is located. Fig. 4 shows the schematic description. For horizontal layer(s) we have  $\gamma = 0$  and the driving force is only the pressure difference between fault and far-field. We neglect the variation in CO<sub>2</sub> density between locations ‘1’ and ‘2’. To obtain leakoff coefficients, we rewrite Eq. 6 in the form

$$\Phi(z) = \rho(z) \frac{Q(z)}{A} = q_{leak}(z) \Delta \Psi(z) \quad (8)$$

where  $\Phi$  is the mass flux into the layer and  $q_{leak}$  is the leakoff coefficient:

$$q_{leak} = \frac{\rho(z) k_r k_{layer}}{\mu L} \quad (9)$$

The leakoff coefficient consists of five parameters: CO<sub>2</sub> density, relative permeability and viscosity, permeability of layer, and a distance from a fault to hydrostatic boundary. The absolute permeability of the layer differs in general from the fault permeability at the same depth. The relative permeability is evaluated at the CO<sub>2</sub> saturation at the Buckley-Leverett front. The rationale for this choice is discussed below. The frontal saturation is easily computed graphically from an extension of fractional flow theory that accounts for the mutual solubility of water and CO<sub>2</sub> (Noh *et al.* 2007). The distance  $L$  measures the extent of the pressure perturbation within the layer.

## Results and Discussion

**Quasi-1D Results.** In the following section we detail results derived from the one-dimensional fault model. Specifically we describe fundamental mechanisms that can be illustrated with this simple model and which are of interest for assessing leakage of CO<sub>2</sub> from storage sites. In these simulations we consider a 1000 m (3280 ft) long vertical fault extending from a depth of 1000 m (3280 ft) down to 2000 m (6560 ft) into the earth. We will assume in all of the simulations except the last that the CO<sub>2</sub> storage reservoir abuts the bottom of the fault and that the storage compartment is 500 m (1640 ft) thick (resulting in an overpressurization of 5 MPa (725 psi) at the top of the reservoir (bottom of the fault)). In the final simulation discussed in this section we consider the effect of the pressure value at the bottom of the fault. The reservoir is assumed to have constant CO<sub>2</sub>

viscosity of 0.00005 Pa-s, an initial reservoir porosity of 20%, an initial fluid pressure of 18 MPa (2611 psi), and an initial CO<sub>2</sub> density of 647 kg/m<sup>3</sup> (40.39 lb/ft<sup>3</sup>). The rock compressibility is  $1 \times 10^{-11}$  Pa<sup>-1</sup>. Our mathematical model assumes the fluid is only slightly compressible. This assumption allowed us to replace the exponential relationship between density and pressure by the linear Taylor series approximation (Eq. 5). In Fig. 5 we see that values of fluid compressibility which are smaller than about  $1 \times 10^{-9}$  Pa<sup>-1</sup> result in small variations in density along a fault at steady state flow conditions. However, when the compressibility reaches values of  $5 \times 10^{-9}$  Pa<sup>-1</sup> the fluid density varies by about 10% along the length of a 1000 m (3280 ft) long vertical fault. In Fig. 6 we illustrate the effect of compressibility on mass flux. The fault permeability is uniform at 1 D, and we assume there is a single leak along the fault at a depth of 1400-1450 m (4600-4760 ft). The source coefficient  $q_{leak}$  at this depth takes the value  $-1.5 \times 10^{-8}$  sec/m. (The negative sign ensures that the leakage flux is out of the fault and into the permeable layer.) In Fig. 6 we see that for this leak the effect of compressibility is minor. The main effect of larger values for compressibility (and hence a bigger range of density values) is the time needed to reach steady state. As the value of compressibility increases more time steps are needed to reach a steady state solution.

Having illustrated a range of plausible values for which the small compressibility assumption holds, we now turn to simulations that illustrate fundamental conclusions we can make about leakage. We assume in all simulations that follow that fluid compressibility,  $c_f$  is  $1 \times 10^{-9}$  Pa<sup>-1</sup>. Our first conclusion is that *Leaks near the bottom of the fault have a greater impact than leaks which occur at shallower depths*. We again consider a 1000 m (3280 ft) long vertical fault which extends from 1000-2000 m (3280-6560 ft) in depth. CO<sub>2</sub> viscosity, reservoir porosity, rock compressibility, and initial fluid density are all taken to have the same values as those given in the last simulation. The fault permeability is again uniform at 1 D. In these simulations the leakoff coefficient is non-zero along two sections of the fault: namely from 1100-1150 m (3600-3770 ft) and from 1800-1850 m (5900-6070 ft) depth. At these two locations  $q_{leak}$  is assigned the value  $-1.5 \times 10^{-9}$  sec/m. So the value of the leakoff coefficient is the same at these two leakage depths.

In Fig. 7 we show the steady state mass flux along the fault. Escaping from the storage formation is 0.26 kg CO<sub>2</sub>/m<sup>2</sup>-s. Most of this flux (about 80%) enters the deeper permeable formation at 1800 m (5900 ft). Relatively little attenuation (about 5% of the escape flux) occurs in the shallower permeable formation. Thus only 15% (0.07 kg CO<sub>2</sub>/m<sup>2</sup>-s) of the CO<sub>2</sub> escaping the storage formation reaches the top of the fault. In contrast in Fig. 8 we have simulated the same situation but with only the shallow leak. The flux escaping the storage formation is less than half the value with the deeper leak, about 0.12 kg CO<sub>2</sub>/m<sup>2</sup>-s. This flux undergoes only 30% attenuation into the shallow permeable formation, even though the leakoff coefficient is identical at both depths. Thus the flux of CO<sub>2</sub> at the top of the fault is 0.08 kg CO<sub>2</sub>/m<sup>2</sup>-s. Although much less CO<sub>2</sub> escapes the storage formation, more CO<sub>2</sub> reaches the top of the fault when the leakage layer is near the top of the fault. This counterintuitive result is the consequence of the decrease in driving force for leakage (CO<sub>2</sub> pressure in fault less hydrostatic water pressure in the formation) as CO<sub>2</sub> rises. From the perspective of risk assessment, the CO<sub>2</sub> reaching the top of the fault is the greatest concern. Thus a corollary of our first conclusion is that *attenuation can reduce risk even if more CO<sub>2</sub> leaves the storage formation*.

A second major conclusion is that *the attenuation is proportional to the ratio of fault permeability to leakoff coefficient ( $k/q_{leak}$ )*. Figure 9 shows mass flux for a single permeable layer between 1700-1750 m (5580-5740 ft) depth with a leakoff coefficient of  $-1.5 \times 10^{-8}$  sec/m. The fault permeability is uniform at 10 D. We see that the flux of CO<sub>2</sub> out the top of the fault is  $(-0.75 \text{ kg/m}^2\text{-s})/(-2.1 \text{ kg/m}^2\text{-s})$  or approximately 0.36 the flux escaping the storage formation. The attenuation is thus 64%. In Fig. 10 the fault permeability is 10× smaller (1 D) and the leakoff coefficient is also a factor of 10 smaller ( $-1.5 \times 10^{-9}$  sec/m). The flux out the top of the fault now  $-0.075/-0.21 \approx 0.36$  of the escape flux. Finally, in Fig. 11 we have again reduced the fault permeability and leakoff coefficient by a factor of 10 each and the attenuation into the permeable layer remains 64%.

In the next set of simulations we examine the effect of permeability variation within the fault. In these simulations the fault and fluid properties are largely the same as in the previous simulations. We assume one lateral leakage pathway exists along the fault between 1700-1750 m. Different values of the leakoff coefficient are chosen, from  $-1.5 \times 10^{-8}$  sec/m to  $-1.5 \times 10^{-11}$  sec/m. Figure 12 gives the mass flux along the fault with fault permeability fixed at 1 D (blue curve) and the mass flux when the fault permeability is 1 D except between 1400 (4590) and 1500 m (4920 ft) where it is taken to be very small (i.e., 0.0001 D) (magenta curve). We refer to this section of the fault as a choke point. In this simulation the leak has value  $-1.5 \times 10^{-8}$  sec/m (i.e., a big leak). Figure 13 shows the final pore pressure at the end of simulation in red and hydrostatic pressure in blue. Figures 14 and 15 give the mass flux when the leakoff coefficient is one and two orders of magnitude smaller respectively (i.e.,  $-1.5 \times 10^{-9}$  sec/m and  $-1.5 \times 10^{-10}$  sec/m). And finally, Fig. 16 gives the mass flux when the leakoff coefficient is smaller still ( $-1.5 \times 10^{-11}$  sec/m). The gap between the constant and variable permeability curves widens, and the influence of the choke point becomes greater, as the leakoff coefficient becomes smaller. The attenuation into the permeable layer is close to 100% if the fault has a choke point above the layer.

Clearly if one is doing inventory on CO<sub>2</sub> in the storage formation, these results suggest that one could not tell just from the rate of escape whether the CO<sub>2</sub> is going into a harmless formation or rising up to the shallower subsurface. As was the case with the depth of the leakage layer, large fluxes of CO<sub>2</sub> can escape the storage formation without reaching the top of the fault, and on the other hand, relatively small fluxes may escape and undergo minimal attenuation, resulting in significant flux at the top of the fault. Our conclusion is, therefore, that *the leakage layer permeability (or leakoff coefficient) and the fault permeability distribution together dictate where leakage will occur. For large leakage layer permeability (i.e.,  $q_{leak} = 1 \times 10^{-8}$  sec/m), escape from the storage formation is almost independent of whether choke exists. For very small leakage layer permeability, the fault permeability dictates escape rate*. However, whether the fault has a choke point or not, the escape flux does not vary linearly with leakage layer permeability.

While layer dip angle  $\gamma$  does not appear to affect mass flux, the angle  $\theta$  of fault inclination away from vertical does have some impact. In Fig. 17 we see three mass flux plots. In all cases there is a single leak from 1700–1750 m (5580–5740 ft) depth with leakoff coefficient of  $-1.5 \times 10^{-11}$  sec/m. The fault permeability is constant at 1 D. All other parameters are as in previous simulations. The blue curve corresponds to a vertical fault. The magenta and red curves correspond to fault inclined at 45 and 60 degree angles from the vertical respectively. Buoyancy has less effect on attenuation in the inclined faults than in the vertical fault. Finally in Fig. 18 we show results from an identical simulation except that the over-pressurization at the bottom of the fault is taken to be 10× smaller, i.e.,  $X = 0.5$  MPa (72.5 psi) rather than  $X = 5$  MPa (725psi). This change corresponds to a thinner CO<sub>2</sub> storage formation. We see negligible attenuation into the horizontal layer when we reduce the overpressure. Moreover, though the driving force is reduced by 10×, the flux escaping from the storage reservoir only changes by a factor of 2.

## 2D Modeling Approach

**Overview.** We develop a 2D model to test the assumptions in the quasi-1D model. Figure 19 describes the base case, which accounts for two fluid phases and a homogeneous storage formation at a depth of 1615 m (5300 ft). Initially the storage formation, surrounded by an impermeable formation, is saturated fully with CO<sub>2</sub> ( $S_g = 1.0$ ). The intersection with a conductive fault on the top seal of the CO<sub>2</sub> reservoir allows leakage along the fault. To simulate geometric and petrophysical properties of a fault we set transmissibility multipliers on a series of grid blocks assigned to have fault characteristics. The fault is assigned isotropic permeability ( $k_v/k_h=1$ ), while the matrix and the permeable layer(s) have anisotropic permeability ( $k_v/k_h < 1$ ). The storage formation is set at higher initial pressure (3.45 MPa or 500 psi more) than the surrounding formation. This is intended to account for the larger pressure during CO<sub>2</sub> injection and for the smaller pressure gradient (5.61 kPa/m or 0.248 psi/ft) in the CO<sub>2</sub> column. Outside the storage reservoir, the pressure gradient is taken to be hydrostatic (9.79 kPa/m or 0.433 psi/ft). Production wells at side boundaries are held at hydrostatic pressure. In effect, these wells establish an open boundary that does not perturb the pressure field. The worst-case leakage condition is that pressure at the bottom of the fault does not decrease. Thus we placed injection wells within the storage formation to replace CO<sub>2</sub> that escapes along the fault, thereby maintaining constant pressure within the storage formation (22.06 MPa or 3200 psi). We assume the whole domain is isothermal. To compare with the quasi-1D model, we place a constant-bottomhole-pressure producer (set to hydrostatic pressure) in the grid block at the top of the fault.

We compare the rates of escape from the storage formation and the rate of attenuation from quasi-1D and 2D simulation results. To do so, the leakoff coefficient in the quasi-1D model is computed directly from Eq. 9. For this calculation the density and viscosity of CO<sub>2</sub> are taken at the initial conditions in the storage compartment. The rates of escape and attenuation must be derived from the 2D simulation output. To do so, the values of CO<sub>2</sub> phase velocity and density at appropriate grid blocks are extracted from the output files. The CO<sub>2</sub> mass flux is the product of phase velocity and density; we neglect the mass of water dissolved in the CO<sub>2</sub> phase.

We then examine the effect of two-phase composition and geometric properties on the leakoff coefficient. The goal here is to ensure that the simple estimate of Eq. 9 does not neglect any essential phenomena. We conduct 2D simulations with different values of permeability, thickness and dip angle of the permeable layer and the relative permeability curve for matrix rocks. The leakoff coefficient is derived from simulation output. The mass flux of CO<sub>2</sub> into the permeable layer is computed from the CO<sub>2</sub> phase density and velocity in a layer grid block adjacent to the fault grid block. The potential difference between the fault/layer intersection and the domain boundary, Eq. 7, is also extracted from the output. As shown in Eq. 8, the ratio of these quantities,  $u\rho/\Delta\Psi$ , is the apparent leakoff coefficient, i.e. the value of  $q_{leak}$  that should enable the quasi-1D model to reproduce the 2D results.

**Comparison of Quasi-1D and 2D Results.** Table 2 summarizes the properties of the test case. The 2D model, Fig. 19, was set up to mimic the assumptions of the quasi-1D model (hydrostatic pressure in the layers outside the fault, constant pressure at bottom and top of fault, distance  $L$  between fault and far-field boundary fixed by the positioning of constant-pressure wells at the domain boundary). The 2D model further assumes that the matrix other than the leakage layer has small permeability, so it does not affect the behavior. For convenience a vertical fault and horizontal permeable layer were assumed. (A dipping layer turns out to add a degree of complexity, discussed below.) The discretization was different in the two models, with 1 m spacing in the 1D model and  $0.61\text{m(W)} \times 0.61\text{m(L)} \times 3.05\text{m(H)}$  (2 ft × 2 ft × 10 ft) elements in the 2D simulation. Thus the permeable layer was represented by a single grid block in the vertical direction. Subsequently we refined the grid in the vertical direction to 0.61 m (2 ft); the results are presented below.

As Fig. 20 and Table 3 show, the quasi-1D, single phase flow model and the 2D, full-physics model have the same trend of CO<sub>2</sub> fluxes. The rate of CO<sub>2</sub> escape from the storage formation is essentially the same for both models, 0.095 kg/m<sup>2</sup>·s in 1D and 0.099 kg/m<sup>2</sup>·s in 2D when the leakage layer has 1 darcy permeability. The 1D model correctly captures the nonlinear change in escape flux when the permeability of the leakage layer is changed: a ten-fold reduction in layer permeability reduces the escape flux only about 10%. The attenuation predicted by the 1D model, 46% of the escape flux for a 1 darcy leakage layer, is less accurate; the full-physics code indicates a 68% attenuation. However, the 1D model does estimate the nonlinear change in attenuation with layer permeability reasonably well. A ten-fold reduction in layer permeability reduces attenuation by a factor of six in the 1D model and by a factor of 4.5 in the 2D model.

We conclude that the 1D model captures the basic physics of the escape/attenuation process for short to moderately long faults. One qualification to this assertion is that the parameter  $L$  is well defined in the 2D simulation. For a fault intersecting an unbounded aquifer, a procedure to identify the appropriate value of  $L$  to enter into Eq. 9 needs to be developed.

**Factors Controlling Leakoff Coefficient.** As defined in Eq. 9, the leakoff coefficient will be determined by four parameters: CO<sub>2</sub> density and viscosity, subsurface permeability and a distance from the fault to the hydrostatic boundary of the layer. Here we examine the sensitivity of the behavior to these factors in full 2D simulations in order to validate our method of estimating  $q_{\text{leak}}$ , i.e. Eq. 9. Every case is based on two-phase flow and homogeneous reservoir as our 2D base model does. Also, the vertical fault has  $9.87 \times 10^{-13} \text{ m}^2$  (1 Darcy) of permeability.

**Layer Properties (Permeability, Thickness & Dip Angle).** The layer permeability is one of the main factors which determine the attenuation rate of CO<sub>2</sub> flowing in a fault. On the other hand the geometric properties of layer such as thickness (cross-sectional area) and dip angle should not influence leakoff coefficient. Table 4 shows that leakoff coefficients remain constant in spite of layer thickness variation while they vary proportionally according to layer permeability. This result is consistent with our analytic formula.

Table 5 show that the leakoff coefficient does depend on dip angle. Tilting the layer by 14 degrees reduces the coefficient by a factor of two to three relative to the horizontal case. The dip also increases the sensitivity of the leakoff coefficient to the layer permeability slightly. Recall that in the 1D single-phase flow results we did not see this impact from the dip angle of the layer. Moreover the primary effect of dip angle should be accounted for in the potential difference term, Eq. 7, and the leakoff coefficient should be independent of dip angle.

To investigate these unexpected factors, we carried out a grid refinement study. With the two-phase, 2D model the dip results in counter-current flow within the layer. Only part of the layer accommodates CO<sub>2</sub> flux, while water moves in the remainder of the layer. Thus the leakoff coefficient could be correctly characterizing the conductivity of the layer for CO<sub>2</sub>; the problem is that as far as CO<sub>2</sub> is concerned, the layer is in effect thinner than its nominal thickness. To account for this dip effect in the 1D model we could reduce the thickness of the interval where the leakoff coefficient is applied. A horizontal layer intersecting a fault at 1700–1750 m might be represented instead as a tilted layer intersecting a fault from 1700–1720 m.

**Rock Property (Relative Permeability Data).** Figure 21 shows the relative permeability curves used to test sensitivity. The CO<sub>2</sub> phase endpoint relative permeabilities were changed, while the shape of the curves and the endpoint saturations were kept the same. Changing the CO<sub>2</sub> relative permeability by a factor of three has only a slight effect on the observed leakoff coefficient (Table 6). This is not obvious; it happens because CO<sub>2</sub> establishes a front with a characteristic saturation as it rises, analogous to the Buckley-Leverett front saturation (Lakshminarasimhan *et al.* 2006). The value of the frontal saturation in turn determines the relative permeability characterizing the CO<sub>2</sub>/brine displacement (Kumar *et al.* 2008). Decreasing the CO<sub>2</sub> phase relative permeability increases this frontal saturation (Fig. 22). Consequently, the relative permeability that is characteristic of the CO<sub>2</sub> leaking into the layer is larger. The net result is that the leakoff coefficient is relatively insensitive to changes in the relative permeability.

**Countercurrent Flow in Permeable Layer.** We examine the behavior in dipping leakage layers more closely. The 2D full physics simulations show that less CO<sub>2</sub> enters a dipping layer than the 1D model predicts, but the models agree for horizontal layers. Fig. 23 shows how refined grids compose the permeable strata. The coordinate of a grid consists of two parts: the first one indicates mother grid and the later one defines finer grids.

Figure 23 shows CO<sub>2</sub> occupying the upper three or four sublayers of the leakage layer. The CO<sub>2</sub> saturation in the bottom sublayer is much smaller. The CO<sub>2</sub> has invaded less into the downdip zone due to its buoyancy. As shown in Fig. 24, larger dip amplifies the CO<sub>2</sub> override in the downdip direction. As a result, downdip leakoff coefficient decreases as dip angle increases.

Figure 25 introduces the CO<sub>2</sub> phase velocities overlaid on the CO<sub>2</sub> saturation profile. The velocity vectors distribute exactly the same way as we define three typical behaviors: CO<sub>2</sub> escapes from storage, attenuated CO<sub>2</sub> enters the permeable layer, and CO<sub>2</sub> leaks past layer. Figure 26 shows the water velocity distribution overlaid on CO<sub>2</sub> saturation. Brine inside the permeable strata is displaced by CO<sub>2</sub> entering the strata. But brine also sinks (slowly) in the updip part of the layer, occupying the bottom sublayer.

The modified leakoff coefficient obtained from these refined grid simulations is more consistent with the expectation from Eq. 9, though some dependence on dip angle persists (Table 7). We remark that the 1D model is necessarily symmetric with regard to the leakage layer; it cannot account for different behavior in the downdip and updip sides of the layer.

## Conclusion

Leakage of CO<sub>2</sub> along a conductive fault that intersects a deep saline aquifer in which the CO<sub>2</sub> is stored can be treated with a quasi-1D “leaky conduit” model. We present a highly simplified version of this model suitable for incorporation in a risk assessment framework. The idealizations capture some of the essential physics and thereby provide insight on important couplings within the system. The model is an attempt to enable assessments of leakage fluxes when the flow properties of formations and faults intersecting them are poorly constrained.

The analytical leakoff coefficient approach assumes 1D, single phase and slightly compressible flow. The leakoff coefficient based on Darcy's law consists of five characteristic parameters: density and viscosity of CO<sub>2</sub>, relative permeability, absolute permeability of the layer, and the distance from attenuation point to hydrostatic boundary. Full-physics simulations in 2D indicate that this simple estimate is reasonable, and that the quasi-1D model captures key features of CO<sub>2</sub> migration in faults over moderate distances (< 1 km). The assumption of slight compressibility is the main limitation on applicability to longer distances.

The results from the quasi-1D model study show that the location of permeable layer(s) plays a significant role in determining the rate of attenuation of the rising CO<sub>2</sub> flux. Deeper layers provide much more attenuation than shallower layers. Ironically, more CO<sub>2</sub> escapes from the storage formation, but less CO<sub>2</sub> reaches the top of the fault, if the leakage layer is deeper. This nonlinearity is exacerbated if the fault has a low permeability section above the leakage layer. Thus attenuation can reduce risk associated with CO<sub>2</sub> reaching the top of the fault, even if more CO<sub>2</sub> leaves the storage formation. Attenuation is proportional to the ratio of fault permeability to leakoff coefficient. The interaction between CO<sub>2</sub> and water phases complicates attenuation behavior in the dipping layer. Denser fluid (brine) will occupy the lower part of a permeable zone depending on the dip angle. Consequently, applying the leakoff coefficient to the entire thickness of the layer will overestimate the attenuation.

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### Nomenclature

$A$	= cross-sectional area of layer, ft <sup>2</sup> or m <sup>2</sup>
$c_f$	= fluid compressibility, psi <sup>-1</sup> or Pa <sup>-1</sup>
$c_r$	= rock compressibility, psi <sup>-1</sup> or Pa <sup>-1</sup>
$D$	= depth vector
$F_i$	= driving force on refined layer $i$ , lb/ft sec <sup>2</sup> or kg/m sec <sup>2</sup> ( $i$ = layer index)
$g$	= gravitational acceleration, ft/sec <sup>2</sup> or m/sec <sup>2</sup>
$k_{layer}$	= absolute permeability of layer, md or m <sup>2</sup>
$L$	= distance between fault and hydrostatic boundary, ft or m
$p$	= pressure, psi or Pa
$q$	= flow rate, ft <sup>3</sup> /sec or m <sup>3</sup> /sec
$q_{leak}$	= leakoff coefficient, sec/ft or sec/m
$q_{leak,i}$	= leakoff coefficient for refined $i^{\text{th}}$ layer, sec/ft or sec/m
$q_{leak,total}$	= total leakoff coefficient (summation of $q_{leak,i}$ ), sec/ft or sec/m
$r_i$	= radial distance for boundary $i$ , ft or m
$z$	= depth, ft or m
$\varphi$	= mass flux, lb/ft <sup>2</sup> sec or kg/m <sup>2</sup> sec
$\varphi_{\text{Attenuation}}$	= mass flux of attenuated CO <sub>2</sub> leaks, lb/ft <sup>2</sup> sec or kg/m <sup>2</sup> sec
$\varphi_i$	= mass flux for refined layer $i$ , lb/ft <sup>2</sup> sec or kg/m <sup>2</sup> sec
$\mu_{CO_2}$	= viscosity of carbon dioxide, cp or Pa-s
$\gamma$	= dip angle of layer, degree
$\theta$	= inclination angle of fault, degree
$\rho_{CO_2}$	= density of carbon dioxide, lb/ft <sup>3</sup> or kg/m <sup>3</sup>
$\Psi$	= potential

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**Table 1—Carbon dioxide compressibility values for the slightly compressible model of CO<sub>2</sub> density, Eq. 5. In our simulation works, we consider only “deep leak.”**

Region	Range of depths	$c_r \text{ Pa}^{-1}$
“shallow leak”	$0 < z < 600 \text{ m}$	$1.66 \times 10^{-7}$
“deep leak”	$1100 \text{ m} < z$	$1.82 \times 10^{-8}$

**Table 2—Description of model properties and parameters for analytical leakoff coefficient; both quasi-1D and 2D models involves the same properties of reservoir and structures.**

Property	Value	
Location	Fault	In the middle of reservoir
	Layer	5800 ft (below the earth)
Permeability	Fault	$9.87 \times 10^{-13} \text{ m}^2$
	Layer	$9.87 \times 10^{-13} \text{ or } 10^{-14} \text{ m}^2$
Pressure gradient		9.79 kPa/m
Compressibility		$1.82 \times 10^{-8} \text{ Pa}^{-1}$
1D Leakoff coefficient	1000 md Layer	$5.24 \times 10^{-9} \text{ sec/m}$
	100 md Layer	$5.24 \times 10^{-10} \text{ sec/m}$
Parameters for 2D Analytical Leakoff Coefficient	Relative Permeability ( $k_r$ )	0.157
	Density ( $\rho_{CO_2}$ )	643.30 kg/m <sup>3</sup>
	Viscosity ( $\mu_{CO_2}$ )	$6.81 \times 10^{-5} \text{ Pa-s}$
	Distance (L)	304.8 m

**Table 3—Comparison of CO<sub>2</sub> escape flux from storage formation and attenuation into a single permeable layer from quasi-1D and 2D simulation outputs (assuming the same reservoir properties).**

Layer permeability, m <sup>2</sup>		Escape Rate from Storage, kg/m <sup>2</sup> s	Attenuation, %
$9.87 \times 10^{-13}$	1D	$9.18 \times 10^{-2}$	46
	2D	$10.00 \times 10^{-2}$	68
$9.87 \times 10^{-14}$	1D	$8.20 \times 10^{-2}$	8
	2D	$8.49 \times 10^{-2}$	15

**Table 4—Comparison of leakoff coefficients from a series of simulation results; the variable parameters are thickness and absolute permeability of the layer. Leakoff coefficients are consistent to the variation of layer permeability, while they are not affected by the variation of layer thickness. This result validates our simple analytical approach of leakoff coefficient.**

Layer Permeability, m <sup>2</sup>	Layer Thickness, m	Leakoff Coefficient, sec/m
9.87×10 <sup>-13</sup>	3.05	5.24×10 <sup>-9</sup>
	9.14	4.92×10 <sup>-9</sup>
	15.24	4.95×10 <sup>-9</sup>
Analytical Solution		4.79×10 <sup>-9</sup>
	3.05	5.12×10 <sup>-10</sup>
	9.14	5.18×10 <sup>-10</sup>
Analytical Solution	15.24	5.05×10 <sup>-10</sup>
		4.79×10 <sup>-10</sup>
	3.05	5.15×10 <sup>-11</sup>
9.87×10 <sup>-15</sup>	9.14	5.05×10 <sup>-11</sup>
	15.24	4.92×10 <sup>-11</sup>
	Analytical Solution	4.79×10 <sup>-11</sup>

**Table 5—Comparison of leakoff coefficients from a series of simulation outputs; The variable parameters are dip/non-dip, dipping status and layer permeability (assuming dip angle is constant, 14°). For horizontal layer leakoff coefficient is proportional to layer permeability, while for tilted layer leakoff coefficient varies according to dipping status. The dipping condition causes inconsistency of analytical estimation of leakoff coefficient due to the interaction between brine and CO<sub>2</sub> phases.**

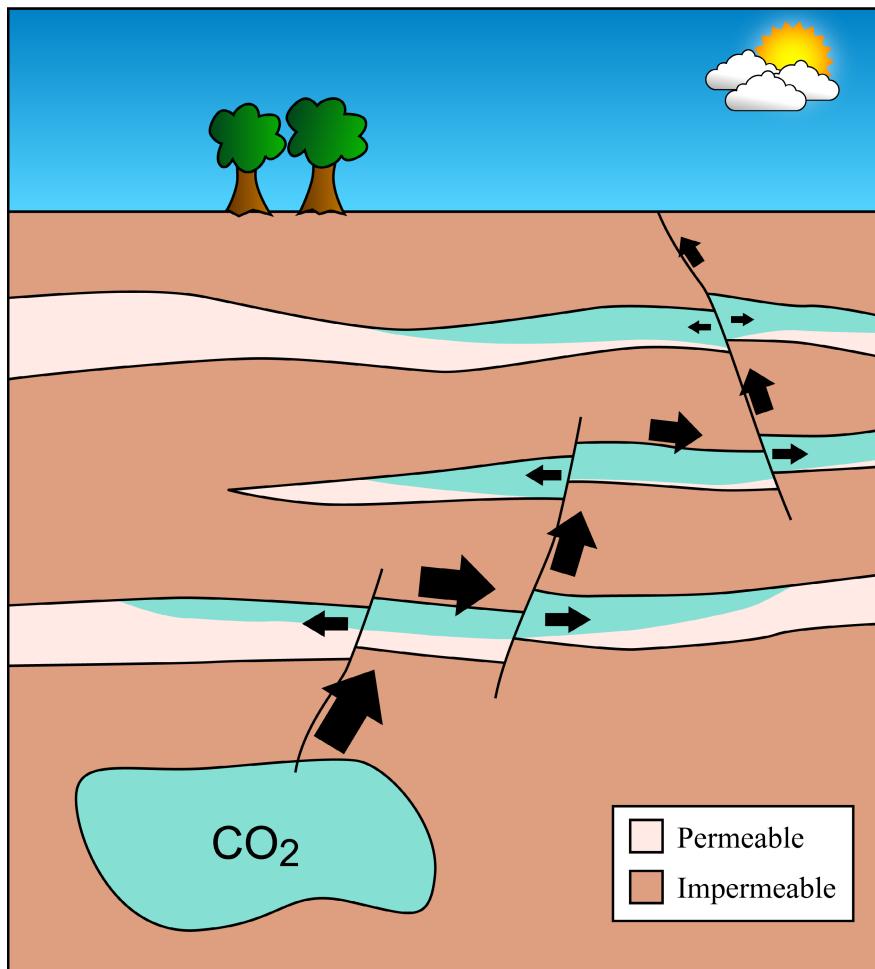
Layer Permeability, m <sup>2</sup>	Layer Geometry	Leakoff Coefficient, sec/m
		Horizontal
9.87×10 <sup>-13</sup>	Tilted	5.24×10 <sup>-9</sup>
		Downdip
		3.18×10 <sup>-9</sup>
9.87×10 <sup>-14</sup>	Tilted	Updip
		1.74×10 <sup>-9</sup>
		Horizontal
9.87×10 <sup>-14</sup>	Tilted	5.12×10 <sup>-10</sup>
		Downdip
		2.79×10 <sup>-10</sup>
9.87×10 <sup>-15</sup>	Tilted	Updip
		1.93×10 <sup>-10</sup>
		Horizontal
9.87×10 <sup>-15</sup>	Tilted	5.15×10 <sup>-11</sup>
		Downdip
		1.57×10 <sup>-11</sup>
		Updip
		2.89×10 <sup>-11</sup>

**Table 6—Comparison of leakoff coefficients; the variable parameter is relative permeability data. This table shows the leakoff coefficient is affected by relative permeability curve.**

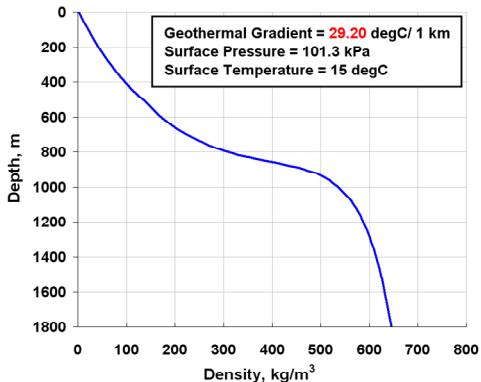
Relative Permeability	Layer Permeability, m <sup>2</sup>	Leakoff Coefficient, sec/m	
		Simulation	Analytical
BASE	9.87×10 <sup>-13</sup>	4.85×10 <sup>-9</sup>	4.79×10 <sup>-9</sup>
	9.87×10 <sup>-14</sup>	4.82×10 <sup>-10</sup>	4.79×10 <sup>-10</sup>
	9.87×10 <sup>-15</sup>	5.05×10 <sup>-11</sup>	4.79×10 <sup>-11</sup>
BASE ÷ 2	9.87×10 <sup>-13</sup>	4.20×10 <sup>-9</sup>	3.74×10 <sup>-9</sup>
	9.87×10 <sup>-14</sup>	4.39×10 <sup>-10</sup>	3.74×10 <sup>-10</sup>
	9.87×10 <sup>-15</sup>	4.49×10 <sup>-11</sup>	3.74×10 <sup>-11</sup>
BASE ÷ 3	9.87×10 <sup>-13</sup>	3.97×10 <sup>-9</sup>	3.05×10 <sup>-9</sup>
	9.87×10 <sup>-14</sup>	3.87×10 <sup>-10</sup>	3.05×10 <sup>-10</sup>
	9.87×10 <sup>-15</sup>	4.23×10 <sup>-11</sup>	3.05×10 <sup>-11</sup>

**Table 7—Comparison of leakoff coefficient from simulation outputs using refined grid blocks and analytical estimation using mass flux derivation. The variable partaker is dip angle of layer. The leakoff coefficient derivation using refined gridding will be reasonable to estimate CO<sub>2</sub> leaks and its attenuation. This table also shows leakoff coefficients vary corresponding to layer dip and dipping status (updip & downdip). As we expected from simulation outputs, downdip leakoff coefficient decreases as dip angle increase.**

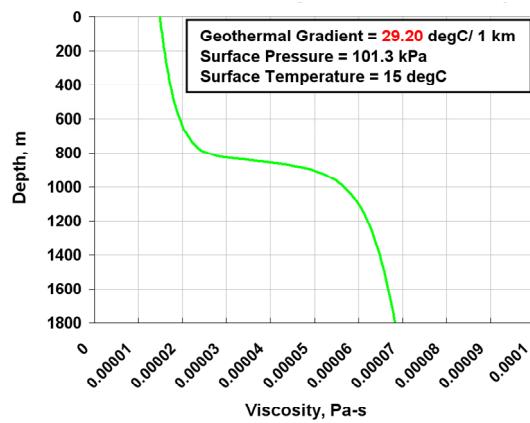
Refined Grids System	Leakoff Coefficient, sec/m	
Analytical Solution	$2.39 \times 10^{-9}$	
Simulation Horizontal Case	$2.46 \times 10^{-9}$	
14°	Downdip	$3.02 \times 10^{-9}$
	Updip	$2.10 \times 10^{-9}$
19°	Downdip	$1.31 \times 10^{-9}$
	Updip	$1.97 \times 10^{-9}$



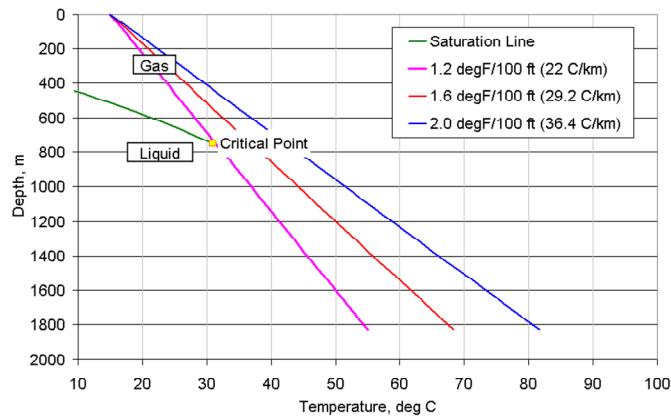
**Fig. 1—Conceptual illustration for risks of underground CO<sub>2</sub> leakage along faults. Our model focuses on the fault zone encountering permeable layer(s). Injected CO<sub>2</sub> migrates and meets a conductive fault. The combination of fluid pressure and buoyancy drives CO<sub>2</sub> up the fault. The presence of permeable layer(s) attenuates the upward flux of CO<sub>2</sub>. Continued leakage from fault into permeable layers can lead to encounter with another fault, and the process of upward migration and attenuation into permeable layers continues.**



(a)



(b)



(c)

Fig. 2—(a) Density of pure CO<sub>2</sub> varies almost linearly with depth for depths greater than about 1200 m, assuming a constant hydrostatic pressure gradient and geothermal gradient. Values used in this plot are 9.79 kPa/m for pressure gradient and 29.20°C/km for geothermal gradient with surface conditions of 101.3 kPa and 15°C. (b) For the same conditions as (a), the viscosity of the CO<sub>2</sub> phase does not vary greatly for depths below 1200 m. (c) For typical geothermal and hydrostatic gradients (surface conditions of 101.3 kPa and 15°C), and for all depths below 800 m, CO<sub>2</sub> exists as a single phase.

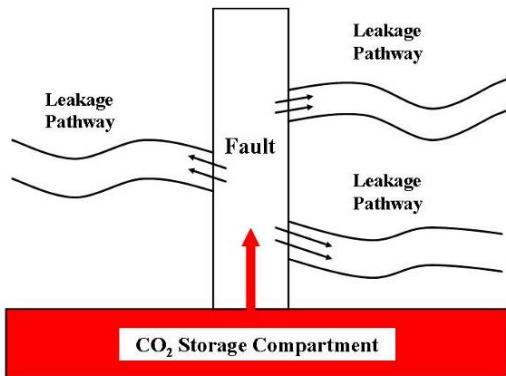


Fig. 3—Schematic illustration of fault leakage model. CO<sub>2</sub> plume escapes the storage formation through a conductive fault. It migrates up the fault. If the fault intersects permeable layer, the CO<sub>2</sub> can leak from the fault into the layer, resulting in attenuation of the escape flux.

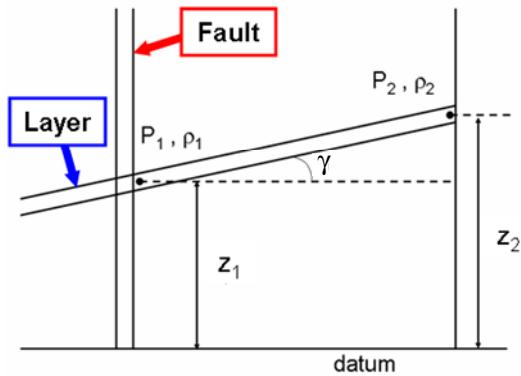


Fig. 4—Schematic illustration for potential derivation.

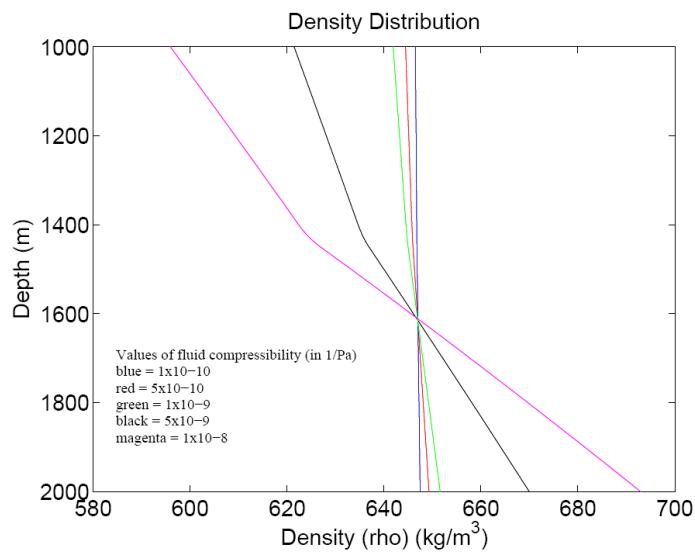


Fig. 5—Density of  $\text{CO}_2$  along fault at steady state flow with different compressibility values used in Eq. 5. Simulation models a fault with a single leak between 1400-1450 m. Magenta curve: fluid compressibility =  $1 \times 10^{-8} \text{ Pa}^{-1}$ ; Black curve:  $c_f = 5 \times 10^{-9} \text{ Pa}^{-1}$ ; Green curve:  $c_f = 1 \times 10^{-9} \text{ Pa}^{-1}$ ; Red curve:  $c_f = 5 \times 10^{-10} \text{ Pa}^{-1}$ ; Blue curve:  $c_f = 1 \times 10^{-10} \text{ Pa}^{-1}$ .

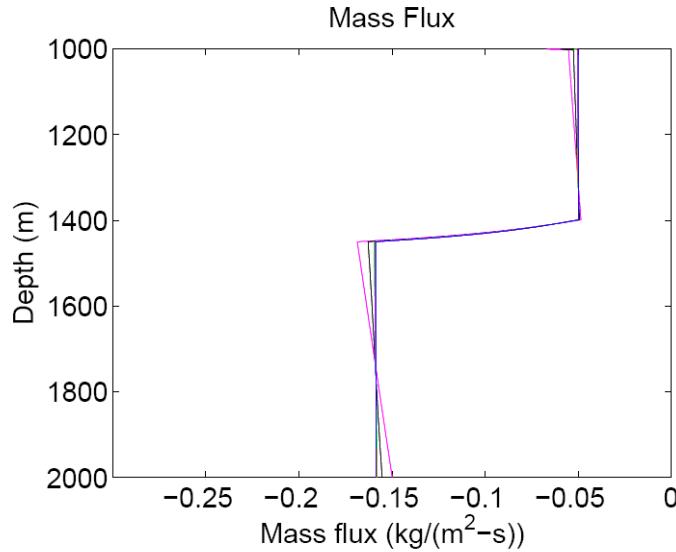


Fig. 6—Steady state mass flux along fault when fluid compressibility varies. In this simulation we consider a single leak between 1400–1450 m. Magenta curve: fluid compressibility =  $1 \times 10^{-8} \text{ Pa}^{-1}$ ; Black curve:  $c_f = 5 \times 10^{-9} \text{ Pa}^{-1}$ ; Green curve:  $c_f = 1 \times 10^{-9} \text{ Pa}^{-1}$ ; Red curve:  $c_f = 5 \times 10^{-10} \text{ Pa}^{-1}$ ; Blue curve:  $c_f = 1 \times 10^{-10} \text{ Pa}^{-1}$ .

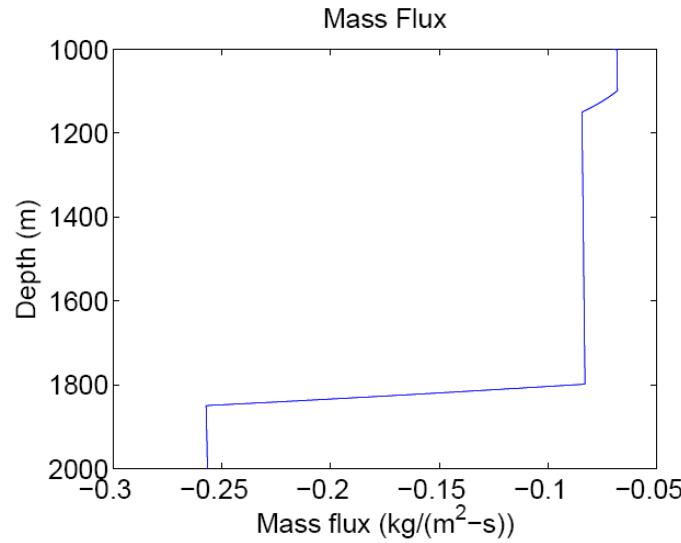


Fig. 7—Mass flux along fault for simulation with two identical permeable layers (same leakoff coefficients) at different depths. Fault permeability is uniform at 1 D. The leaks occur at 1100–1150 m and from 1800–1850 m depth. In these two intervals  $q_{\text{leak}}$  takes the value  $-1.5 \times 10^{-9} \text{ sec/m}$ .

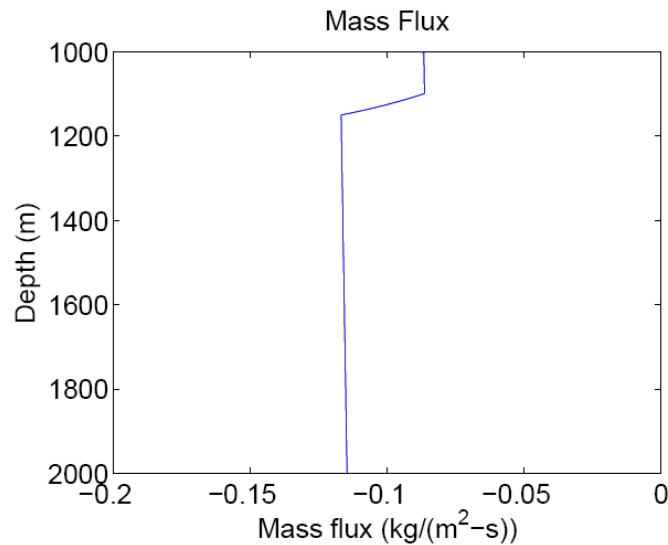


Fig. 8—Mass flux along fault for a simulation with a single shallow permeable layer at a depth of 1100–1150 m of size  $q_{leak} = -1.5 \times 10^{-9}$  sec/m.

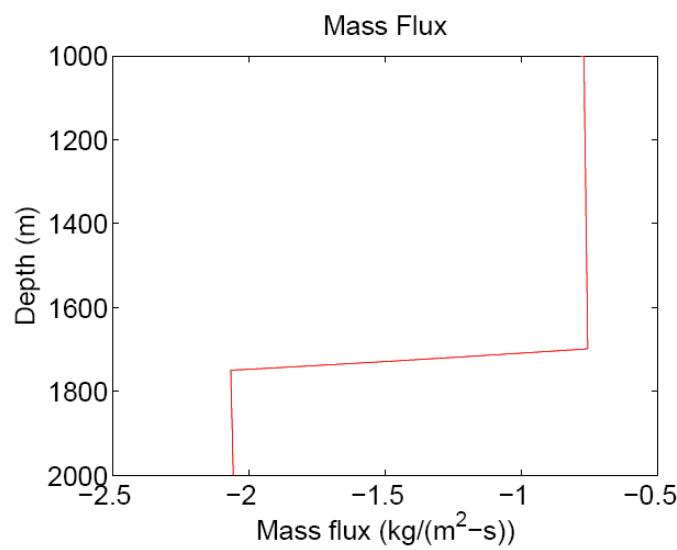


Fig. 9—Mass flux along fault for a simulation with a single permeable layer between 1700–1750 m depth with leakoff coefficient of  $-1.5 \times 10^{-8}$  sec/m. The fault permeability is uniform at 10 D.

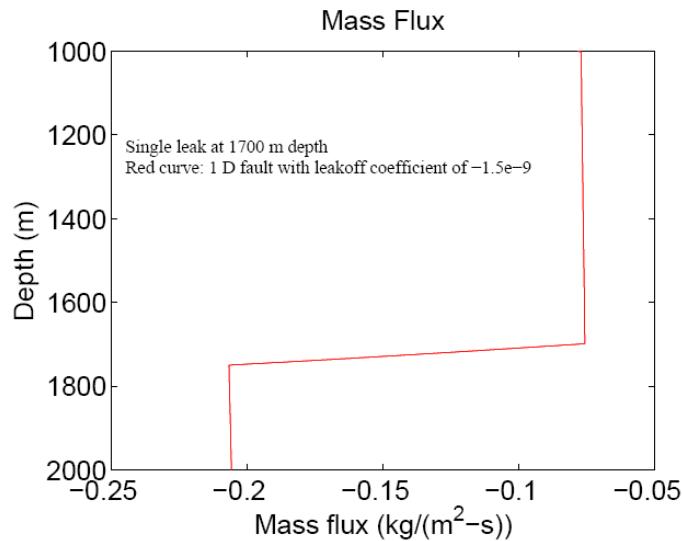


Fig. 10—Mass flux along fault for a simulation in which the fault permeability is 1 D and the leakoff coefficient is  $-1.5 \times 10^{-9}$  sec/m.

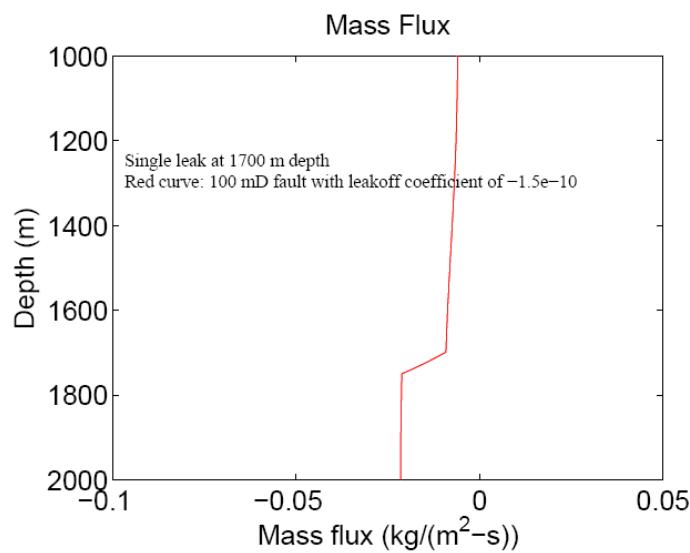


Fig. 11—Mass flux along fault for a simulation in which the fault permeability is 100 mD and the leakoff coefficient is  $-1.5 \times 10^{-10}$  sec/m.

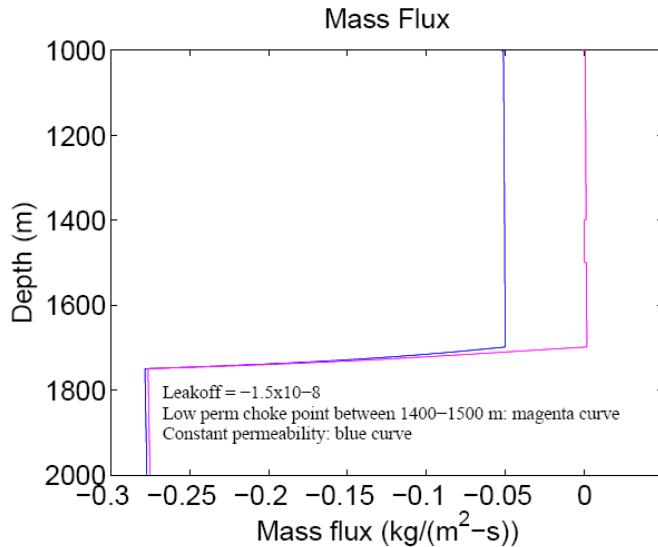


Fig. 12—Mass flux along fault for simulations with one permeable layer between 1700–1750 m. The leakoff coefficient is  $-1.5 \times 10^{-8}$  sec/m (i.e., a big leak). Blue curve: mass flux with fault permeability fixed at 1 D. Magenta curve: The fault permeability is 1 D except between 1400 and 1500 m where it is taken to be very small (i.e., 0.0001 D).

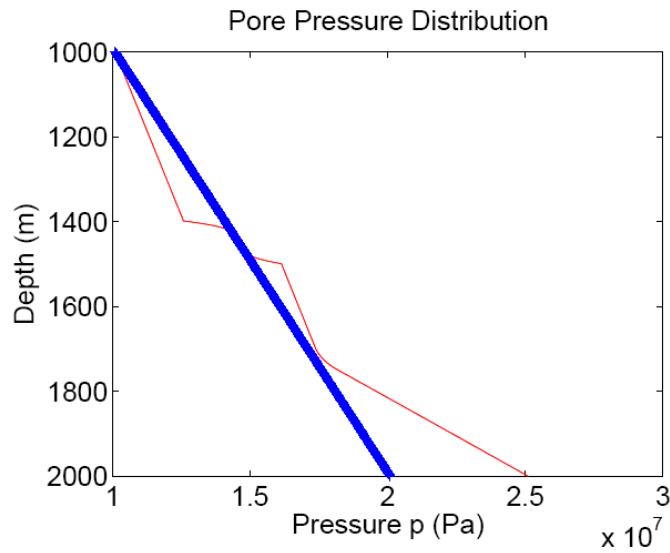


Fig. 13—Pore pressure at the end of simulation for the simulation described in Figure 12. One permeable layer is between 1700–1750 m. The leakoff coefficient is  $-1.5 \times 10^{-8}$  sec/m with fault permeability fixed at 1 D except between 1400 and 1500 m where it is taken to be 0.0001 D. The red curve gives the final pore pressure at the end of simulation and the blue curve is hydrostatic pressure.

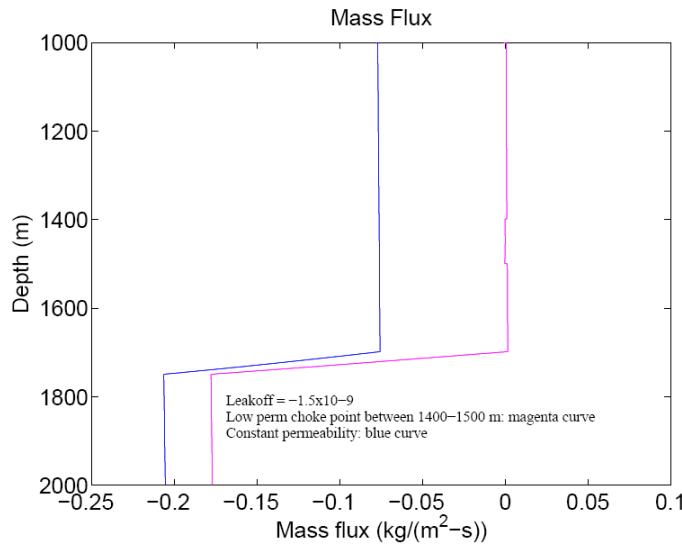


Fig. 14—Mass flux values for simulations with one leakage pathway between 1700–1750 m. The leak has value  $-1.5 \times 10^{-9}$  sec/m. Blue curve: mass flux with fault permeability fixed at 1D. Magenta curve: mass flux when the fault permeability is 1D except between 1400 and 1500 m where it is taken to be very small (i.e., 0.0001D).

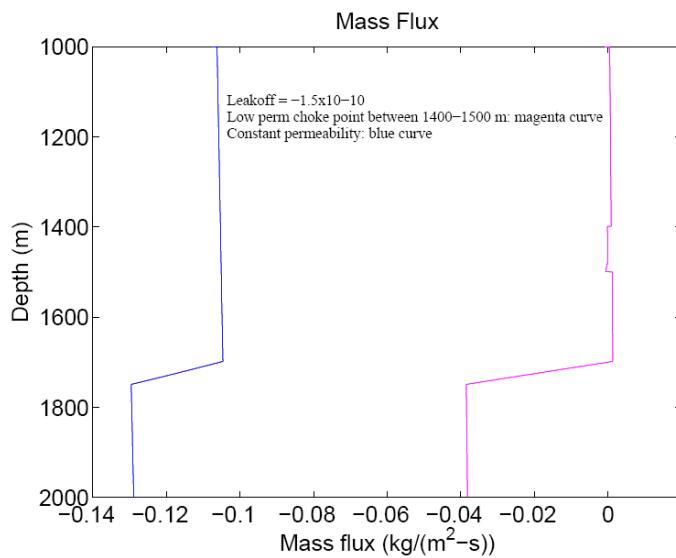


Fig. 15—Mass flux values for simulations with one leakage pathway between 1700–1750 m. The leak has value  $-1.5 \times 10^{-10}$  sec/m. Blue curve: mass flux with fault permeability fixed at 1D. Magenta curve: mass flux when the fault permeability is 1D except between 1400 and 1500 m where it is taken to be very small (i.e., 0.0001D).

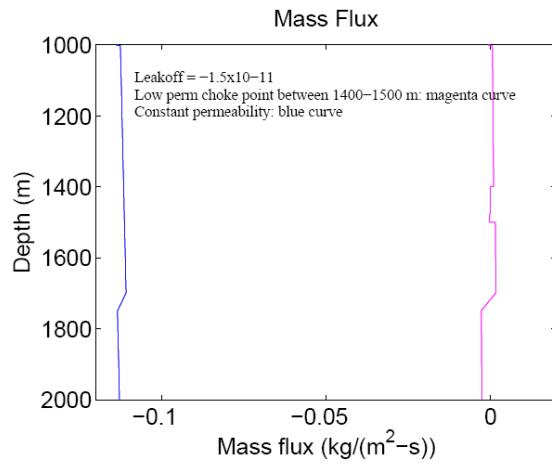


Fig. 16—Mass flux values for simulations with one leakage pathway between 1700–1750 m. The leak has value  $-1.5 \times 10^{-11}$  sec/m. Blue curve: mass flux with fault permeability fixed at 1D. Magenta curve: mass flux when the fault permeability is 1D except between 1400 and 1500 m where it is taken to be very small (i.e., 0.0001 D).

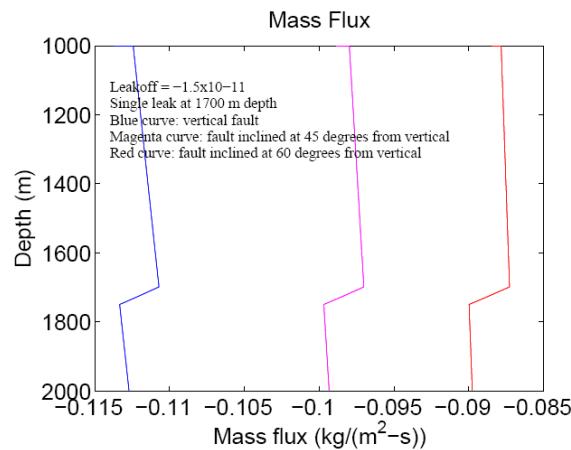


Fig. 17—Mass flux for simulations with a single leak from 1700–1750 m depth with leakoff coefficient of  $-1.5 \times 10^{-11}$  sec/m. Constant fault permeability of 1D. Blue curve corresponds to a vertical fault. The magenta and red curves correspond to faults inclined at 45 and 60 degree angles from the vertical respectively. Here the overpressurization due to the CO<sub>2</sub> storage compartment is 5 MPa at the bottom of the fault.

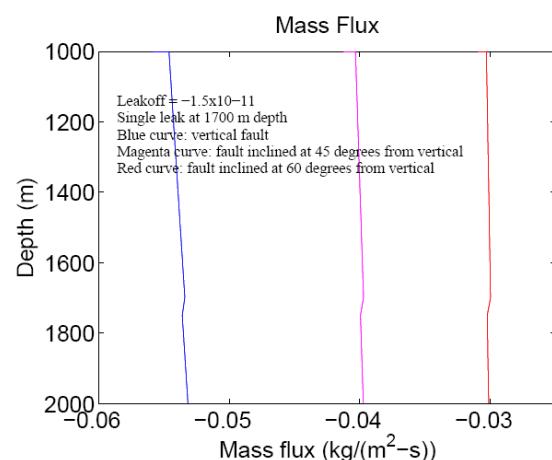


Fig. 18—Mass flux for simulations with a single leak from 1700–1750 m depth with leakoff coefficient of  $-1.5 \times 10^{-11}$  sec/m. Constant fault permeability of 1D. Blue curve corresponds to a vertical fault. The magenta and red curves correspond to faults inclined at 45 and 60 degree angles from the vertical respectively. Here the overpressurization due to the CO<sub>2</sub> storage compartment is 0.5 MPa at the bottom of the fault.

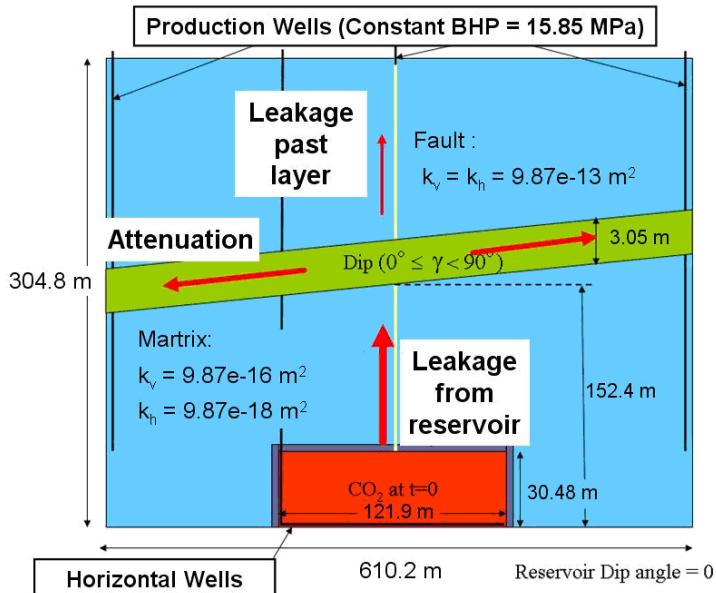


Fig. 19—Schematic description of 2D model assuming homogeneous reservoir with hydrostatic boundaries. The top of this model domain is located 1615 m (5300 ft) below the surface. The red lines represent  $\text{CO}_2$  plume migration through permeable structures.

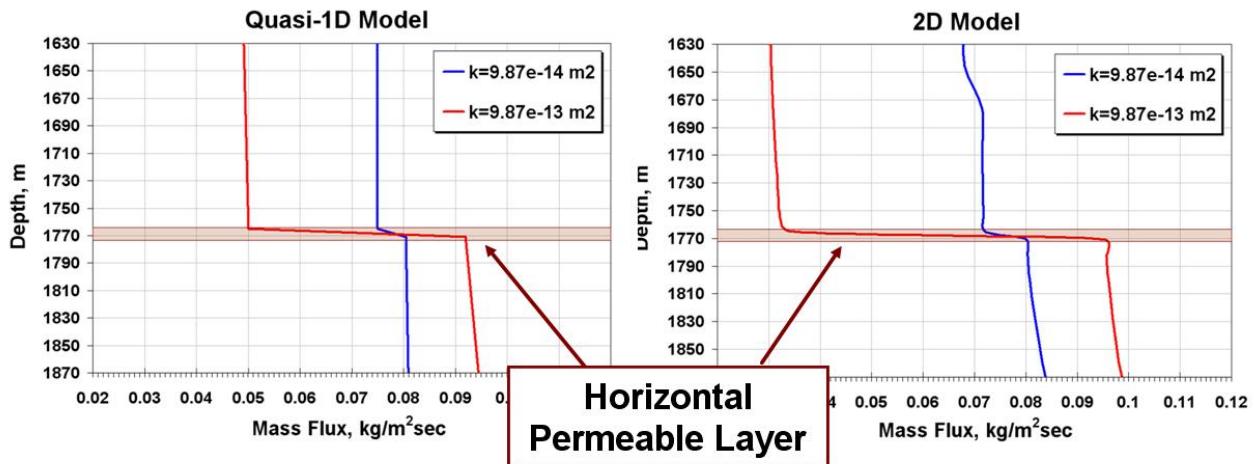


Fig. 20—Comparison of mass flux distribution from quasi-1D and 2D simulation outputs. Both show quite similar trend, initially  $\text{CO}_2$  leak happens and then the leak is attenuated into the permeable layer.

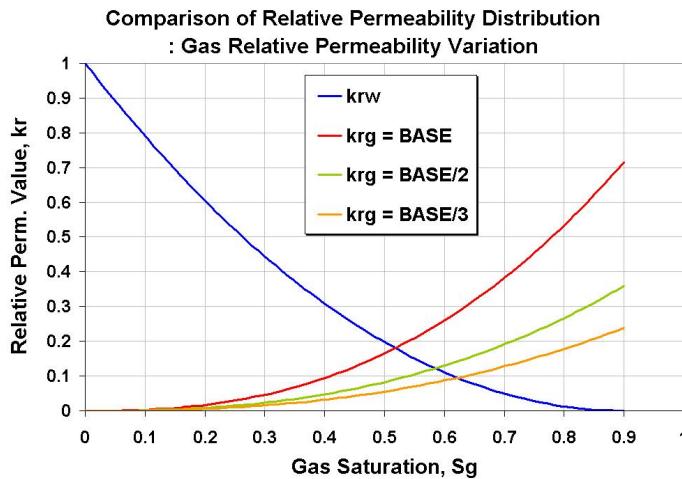


Fig. 21—Artificial relative permeability curve distribution; Only drainage curves for gas phase vary proportionally. Other values associated with hysteresis or water phase are fixed for this simulation study.

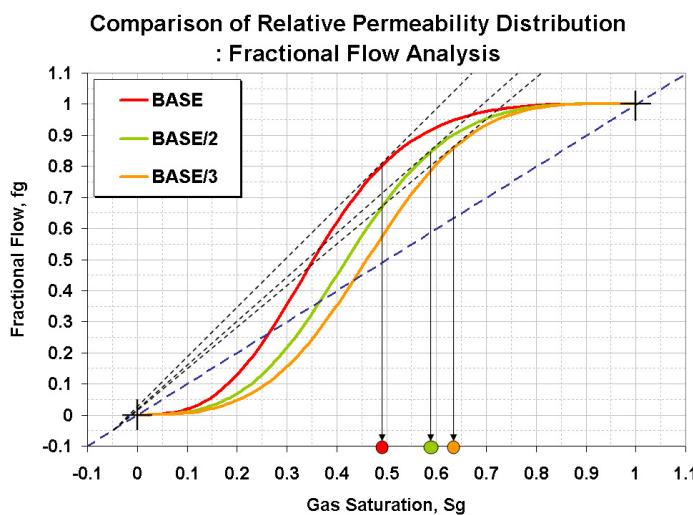


Fig. 22—Fractional Flow Curves with end-point saturation variation; Decreasing CO<sub>2</sub> phase saturation results in increasing its frontal saturation (Buckley-Leverett front). Then relative permeability of CO<sub>2</sub> plumes increases corresponding to given relative permeability curve.

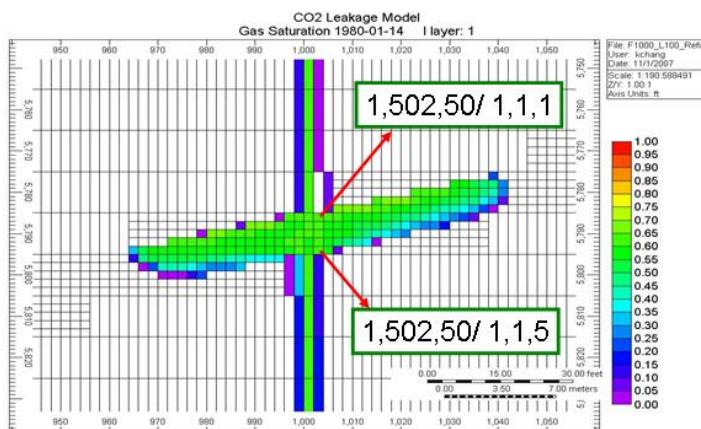


Fig. 23—Gas saturation profile of tilted model using refined grid blocks, which divide the layer into five separated layers. The coordinates in green boxes represent refined grid blocks. Mass fluxes for each layer are different, and the summation of them defines total mass flux of attenuated CO<sub>2</sub> inside the layer.

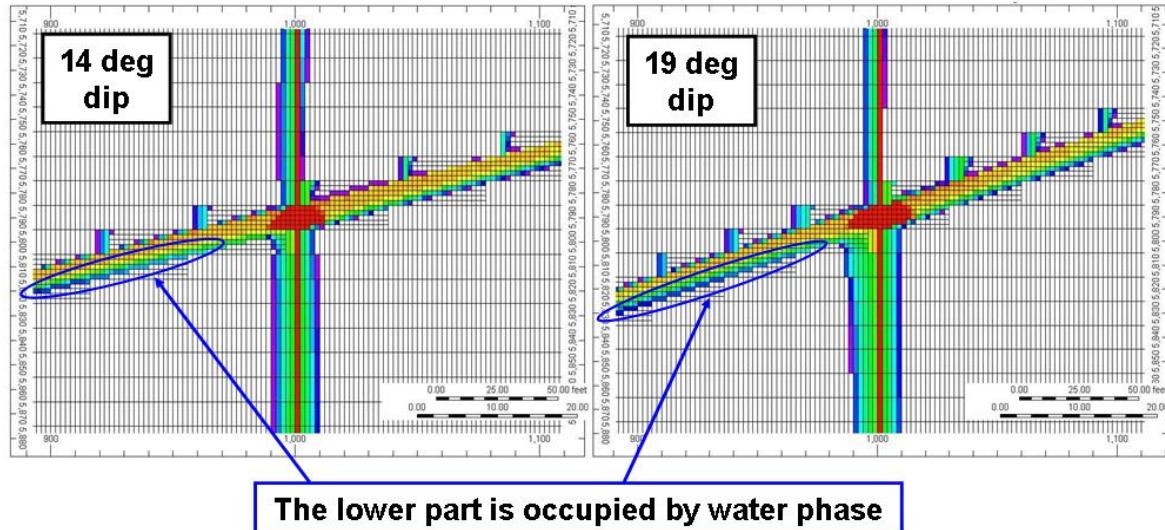


Fig. 24—Saturation profiles for comparison of layer dip angle variation. The downdip zone of more tilted layer is occupied more by brine phase. Thus, leakoff coefficient for downdip will be less than for updip.

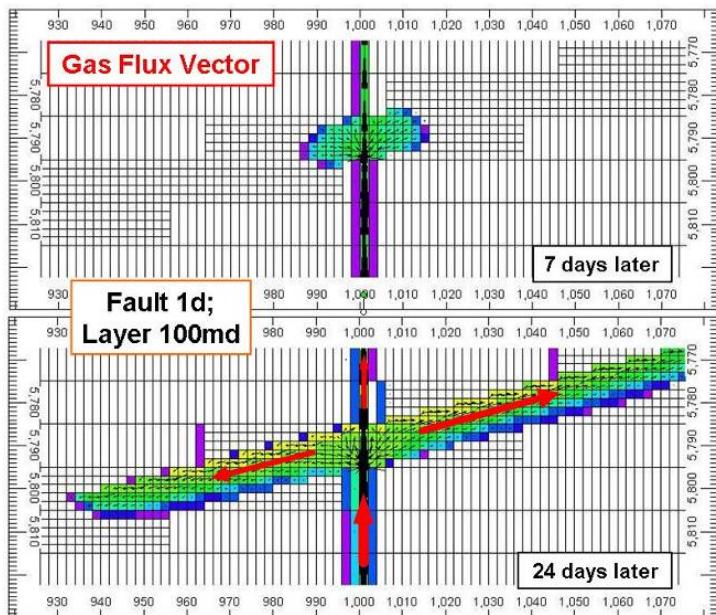


Fig. 25—Gas flux vector distribution superimposed on gas saturation profile. Larger flux of gas phase flows through updip.

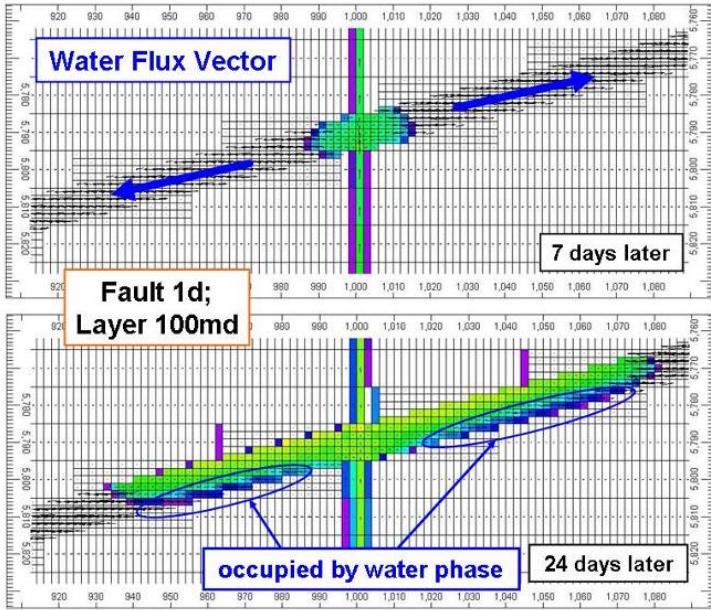


Fig. 26—Water flux vector distribution overlapped with gas saturation profile (tilted layer case, dip angle is 14°). In the upper figure, blue arrows represent that attenuated CO<sub>2</sub> pushes pre-occupied brine inside the layer. In the lower figure, the bottom part of the layer is occupied by brine, which means less dense fluids (CO<sub>2</sub>) migrate through the upper part of the layer while denser fluids (brine) occupy the lower part. In addition, according to dipping status (updip and downdip) the region at which CO<sub>2</sub> migrates is different. Buoyant force make CO<sub>2</sub> migrate upward so that the updip zone of the layer is invaded by CO<sub>2</sub> rather than the downdip zone.