Dissolution Potential of SO₂ Co-Injected with CO₂ in Geologic Sequestration

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Sulfur dioxide is a possible co-injectant with carbon dioxide in the context of geologic sequestration. Because of the potential of SO₂ to acidify formation brines, the extent of SO₂ dissolution from the CO₂ phase will determine the viability of co-injection. Pressure-, temperature-, and salinity-adjusted values of the SO₂ Henry’s Law constant and fugacity coefficient were determined. They are predicted to decrease with depth, such that the solubility of SO₂ is a factor of 0.04 smaller than would be predicted without these adjustments. To explore the potential effects of transport limitations, a nonsteady-state model of SO₂ diffusion through a stationary cone-shaped plume of supercritical CO₂ was developed. This model represents an end-member scenario of diffusion-controlled dissolution of SO₂ to contrast with models of complete phase equilibrium. Simulations for conditions corresponding to storage depths of 0.8–2.4 km revealed that after 1000 years, 65–75% of the SO₂ remains in the CO₂ phase. This slow release of SO₂ would largely mitigate its impact on brine pH. Furthermore, small amounts of SO₂ are predicted to have a negligible effect on the critical point of CO₂ but will increase phase density by as much as 12% for mixtures containing 5% SO₂.

Introduction

Geologic sequestration of carbon dioxide is emerging as a promising carbon mitigation strategy (1–3). Electric power plants, which are the largest point sources from which CO₂ will be captured, emit other important pollutants such as sulfur dioxide, and there is the possibility that such pollutants could be disposed of by co-injection with CO₂ into deep geologic formations. Every year, the electric power industry collectively spends more than $5 billion on permits for the right to emit SO₂ (4). Given the environmental and human health benefits of controlling SO₂ emissions (5), it may be economically advantageous to dispose of SO₂ with CO₂. However, the effects that impurities in the CO₂ stream will have on injection and long-term storage are largely unknown. Regulations governing the injection of CO₂ have been proposed by the U.S. EPA; however, there has been no specification of the required purity of the injected stream except that it must not meet the definition of a hazardous waste (6). John Gale, of the IEA, recently commented on the need to understand the effects of impurities on capture, transport, and storage before setting purity regulations (7).

In aqueous solution, SO₂ may form sulfuric acid, sulfuric acid, and even H₂S (8). With the exception of H₂S, these are acids stronger than carbonic acid, formed from aqueous CO₂. Acidity in the context of geologic CO₂ sequestration will accelerate mineral dissolution and precipitation, which may affect formation porosity and permeability, integrity of wellbore cements, and caprock integrity (9–13). Gunter et al. (11) examined water-rock reactions for injection streams of CO₂, H₂SO₄, and H₂S and predicted that these acids could be effectively buffered by the formation mineralogy, thus reducing the potential for long-term brine acidification. However, other geochemical modeling studies (14–16) predict that storage of sulfur co-injectants with CO₂ would create persistent, highly acidic conditions. Knauss et al. (15) used a reactive transport simulation and predicted that even small amounts of SO₂, such as 10⁻⁶ bar partial pressure, would create pH conditions near unity. Under these acidic conditions, porosities will be increased because of mineral dissolution and carbonate mineral precipitation will be inhibited. Similarly, Xu et al. (16) predicted that co-injection of SO₂ would create a larger and more acidic zone than injection of CO₂ alone and would increase porosity in the acidic zone due to mineral dissolution and decrease porosity at the acid front due to sulfate precipitation.

The magnitude of brine acidification will depend on the extent and rate of dissolution of SO₂ out of the injected CO₂. One of the objectives of this work was to determine a means of predicting the solubility of SO₂ in formation brines under geologic sequestration conditions. Solubility of CO₂ under these conditions has been fairly well examined (17–19); however, little is known of SO₂ solubility at high temperature, pressure, and salinity conditions. At injection depths below 800 m, where CO₂ would exist as a supercritical fluid (20), temperatures are greater than 30°C, and pressures are greater than 74 bar. The solubility of SO₂ in pure water has been determined at temperatures up to 130°C, but at pressures up to only 25 bar (21–23). Furthermore, at depths relevant for geologic sequestration, brine salinity in sedimentary basins is as high as 225 g/L (approximately 3.8 M) (20). SO₂ solubility has been measured in 0.1–6 M NaCl solutions (24–26), and in mixed electrolyte solutions (27–29) but not at the pressures relevant for geologic sequestration.

In this work, we present a means of determining the phase partitioning of SO₂ from supercritical CO₂ (scCO₂) by using pressure-, temperature-, and salinity-adjusted parameters including the Henry’s Law constant and the CO₂-phase fugacity coefficient. We examine how these parameters and the resulting SO₂ brine concentrations would vary with depth, in comparison to CO₂ concentrations. Additionally, densities of CO₂–SO₂ mixtures under relevant pressure and temperature (PT) conditions, along with mixture critical points, are calculated. These properties are important to demonstrate the effects of SO₂ additives on CO₂ injection depth and migration potential. Finally, the diffusivity of SO₂ in scCO₂ is estimated, and its variation with depth and PT conditions is examined.

In addition to the need to quantify the potential for equilibrium phase partitioning of SO₂, there is a need to estimate the flux of SO₂ from the injected CO₂ to the bulk brine phase. Previous modeling studies (15, 16) of co-injection of SO₂ with CO₂ assume sustained phase equilibrium between all the scCO₂ and brine. This is an extreme case scenario in which there is no limitation on contact of SO₂ with the brine. The opposite extreme case is a scenario in which SO₂ is limited by diffusion through a stationary scCO₂ phase. These two extremes bound reality in which the actual rate of SO₂ contact...
with brine is controlled by process complexities and system heterogeneities.

To address the need to understand the diffusion-limited bounding scenario, the second major objective of this work was to describe diffusion-limited dissolution behavior of SO$_2$ into brines in the context of co-injection with CO$_2$ in geologic sequestration. A nonsteady-state model of SO$_2$ diffusion through a stationary cone-shaped plume of scCO$_2$ was developed and used to simulate fluxes of SO$_2$ into the brine outside the scCO$_2$ plume. Pressure- and temperature-adjusted binary diffusion coefficients of SO$_2$ in scCO$_2$ were estimated. A variety of depths were considered to determine how changes in temperature and pressure affect the properties. Two different mixture compositions, 1 and 5% SO$_2$, were considered, corresponding to moderate-to-high ratios of SO$_2$ to CO$_2$ in emissions from electric power plants.

Methods

CO$_2$–SO$_2$ Mixture Properties. Critical points for mixtures of CO$_2$ and SO$_2$ were estimated by using the corresponding states method as given by Lee and Kesler (30). Yang et al. (31) examined the accuracy of this method in describing CO$_2$ densities of pure CO$_2$ despite the availability of CO$_2$ equations of state. This method was also used to estimate the densities of pure CO$_2$ despite the availability of CO$_2$ equations of state (33). Densities were calculated at PT conditions corresponding to a variety of depths, based on gradients from reported data (31–34) (Supporting Information, Table S1).

The densities of mixtures of CO$_2$ and SO$_2$ were estimated by using the method given in Lee and Kesler (30). For consistency, this method was also used to estimate the densities of pure CO$_2$ despite the availability of CO$_2$ equations of state (33). Densities were calculated at PT conditions corresponding to a variety of depths, based on gradients from reported data (36, 37) as described in the Supporting Information (Section S-1).

Partitioning into Brine. For the case of phase equilibrium partitioning of SO$_2$ between scCO$_2$ and brine, the convention of the infinite-dilution reference state for the aqueous phase is adopted. This results in an expression relating the SO$_2$ concentration in the brine phase, C[M], to the partial pressure in the scCO$_2$ phase, P$_{SO2}$ [atm]:

\[
C = \phi_{SO2} P_{SO2} K_H
\]

where \(\phi_{SO2}\) is the fugacity coefficient of SO$_2$ in the scCO$_2$ phase and \(K_H\) is the Henry’s Law constant in [M/atm].

The adjustment of the Henry’s Law constant for high pressures was done by using the Krichhevsky–Ilinskaya equation, which also adjusts for variation in activity coefficient, important for highly soluble gases (38). This equation relates the Henry’s law constant, \(K_{H,P}\), at system pressure, \(P\), to the Henry’s law constant at a lower reference pressure, \(K_{H,L}\), through

\[
\ln K_{H,P} = \ln K_{H,L} - \frac{A}{RT} (x^2 - 1) - \frac{\nu_{SO2}(P - P^*)}{RT} + \ln \left( \frac{V_{brine}}{V_P} \right)
\]

where \(A\) is the Margules constant, \(x_j\) is the mole fraction of water in the brine phase, \(V_{SO2}\) is the partial molar volume of SO$_2$ at infinite dilution, \(P^*\) is the reference pressure, \(R\) is the universal gas constant, \(T\) is the temperature, and \(V_P\) is the molar volume of water. In this work, the last term is ignored because changes in the molar volume of water with pressure are assumed negligible. Henry’s Law constants for SO$_2$ at 1 bar were taken from Rabe and Harris (21) for several temperatures representative of geologic sequestration conditions (given in Table S2 in the Supporting Information).

These values of \(K_{H,P}\) refer to aqueous SO$_2$ in the unreacted form, as opposed to the total SO$_2$ in solution. Partial molar volumes of SO$_2$ at infinite dilution (Table S1 in the Supporting Information) were taken from Brelvi and O’Connell (39). The Margules constants were estimated via regression of measurements of SO$_2$ solubility in pure water at pressures up to 11 bar (22).

The Henry’s Law constants were adjusted for saline conditions by using the Schumpe model (27) for mixed electrolyte solutions with an adjusted gas-specific parameter given by Rodriguez-Sevilla et al. (24). A 1 M NaCl solution was selected to represent the brine.

The fugacity coefficient for SO$_2$ in the scCO$_2$ was determined from the second virial coefficients, determined from the reduced-virial-coefficient method in Tarakad and Danner (40).

SO$_2$ Diffusivity in scCO$_2$. The diffusion coefficient for SO$_2$ in scCO$_2$, \(D_{SO2,CO2}\), at high pressures was estimated by using the Takahashi correlation (41) as described in the Supporting Information (Section S-4). Values of \(D_{SO2,CO2}\) at relevant conditions are also given in the Supporting Information (Section S-4).

Model System and Simplifications. A model system was conceptualized to represent an extreme-end-member scenario in which SO$_2$ contact with the bulk brine is entirely diffusion-limited within the scCO$_2$ phase. By “bulk brine” we refer to the brine phase outside the scCO$_2$ plume. The system is a scCO$_2$ phase within a geologic formation after the injection period (Figure 1). We selected a cone as simplified geometry to mimic the shape of a CO$_2$ plume trapped underneath a caprock seal. For simplicity, the scCO$_2$ is assumed to be stationary. During the injection process, pressure will force the CO$_2$ to flow into the formation (see e.g. refs 42–44). Post-injection, however, these pressures will dissipate, and CO$_2$ flow will be slower, driven only by buoyancy override and hydrodynamic flow. Furthermore, in deep aquifers, the flow of water is slow, 1–10 cm/yr (45), which means that hydrodynamic forces are minimal.

The other type of CO$_2$ flow, which is not considered here, is the flow driven by the new density gradients that will be created because of spatial differences in SO$_2$ concentrations within the scCO$_2$ phase. A circulation pattern may emerge in which SO$_2$-rich CO$_2$ near the top, center of the cone will exchange with the less dense CO$_2$ that is depleted of SO$_2$. (Note that this does not affect mixing between the brine phase and the scCO$_2$ phase because the density of the SO$_2$-rich scCO$_2$ phase is still significantly less than the density of the brine phase.) This advective transport is one of the processes that will enhance SO$_2$ flux relative to the extreme case of diffusion in a stagnant fluid, modeled here.

Another process not considered is partitioning of SO$_2$ into residual brine trapped within the volume of the cone. Partitioning to residual brine may be significant. The effect, relative to what is modeled here, is that the diffusive flux to the bulk brine would be diminished because of the reduced SO$_2$ concentrations in the scCO$_2$ phase.

A cone volume of 6.1 × 10$^8$ m$^3$ was calculated on the basis of a CO$_2$ density of 750 kg/m$^3$, an aquifer porosity of 20%, and a 50 year injection period at a rate of 1.83 Mton/year.
By assuming a formation thickness of 75 m and by assuming that the height of the cone equals this thickness, a cone with the selected injection volume would extend to a radius of 2.8 km.

**SO₂ Diffusion Modeling.** The cone radius was discretized in radial coordinates by first dividing it into wedges with angle θ. The wedges with total height Z were divided into slices with thickness Δz. Slices were then divided into segments with width Δr, as shown in Figure 1. The derivation of the equation for diffusive mass transport of SO₂ in scCO₂ in a differential volume element is presented in detail in the Supporting Information (Section S-5). The resulting model equation is

\[
\frac{\partial C}{\partial t} = D_{\text{eff}} \left( \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial C}{\partial r} \right) + \frac{\partial^2 C}{\partial z^2} \right)
\]

(3)

where \( C \) is the concentration of SO₂ and \( D_{\text{eff}} \) is the effective diffusion coefficient. The effective diffusion coefficient is calculated from \( D_{\text{SO₂,CO₂}} \), formation porosity, \( n \), and tortuosity, \( \sigma \) (47).

\[
D_{\text{eff}} = D_{\text{SO₂,CO₂}} \frac{n}{\sigma}
\]

(4)

For this work, tortuosity was selected as \( \sigma = 2 \) to represent high diffusive flux.

The initial condition assumes a spatially uniform concentration of 1 or 5% SO₂ within the scCO₂. A no-flux boundary was assumed at the top of the cone, representing an aquifer bounded by an impermeable caprock. Diffusion within the cone is driven by a concentration gradient created by preferential dissolution of SO₂ into the bulk brine at the cone boundary. SO₂ dissolution was predicted by using eq 1 and the estimated Henry’s Law constant and fugacity coefficient. The model does not account for dissolution of CO₂. In Ellis et al. (8), we describe this process and examine the change in the scCO₂ plume size by considering different scenarios for brine-phase transport. To create a maximum driving force for dissolution, at each time step, the brine at the cone boundary was reset to have a zero concentration of SO₂. This is a realistic condition because dissolved SO₂ will quickly convert to acid reaction products (see Ellis et al. (8)). The diffusion equation was numerically solved by using a time-split explicit difference method as described in the Supporting Information (Section S-5).

**Results and Discussion**

**CO₂—SO₂ Mixtures.** The critical points estimated for mixtures of CO₂ and SO₂ are shown in the phase diagram in Figure 2. For reference, gas–liquid phase boundaries for pure CO₂ and SO₂ are also shown. Published correlations were used for the phase boundaries for CO₂ (48) and SO₂ (34). Whereas the critical temperature of SO₂ is much higher than that of CO₂, pure SO₂ and pure CO₂ have similar critical pressures. Also, critical points for mixtures of SO₂ and CO₂ are predicted to be fairly constant in pressure. This implies that, in the context of injection, to ensure a supercritical mixture, less than an additional 1 m depth is required for 1% SO₂ mixtures and an additional 3.5 m for 5% SO₂ mixtures.

Estimated densities are shown in Figure 3, along a trajectory corresponding to a surface temperature of 10 °C. Uncertainties are 5.3% (see Supporting Information). The density of pure CO₂ ranges from 754 to 759 kg/m³ from depths of 0.8 to 2.4 km (Figure 3a). This variation is small because, coincidentally, the PT depth trajectory is closely aligned with an iso-density (isopycnic) line in the supercritical regime. Densities of mixtures of CO₂ and SO₂ (Figure 3b,c) are larger than those of pure CO₂. For the conditions of interest, densities are up to 3% larger for 1% SO₂ mixtures and up to 12% larger for 5% SO₂ mixtures. This increase is expected given the larger density of pure SO₂. For pressures and temperatures that correspond to depths between 0.8 and 2.4 km, the density of SO₂ as measured by Ihmels (49), ranges from 1373 to 1300 kg/m³. Thus, small amounts of SO₂ have a large effect on the mixture density. In the context of geologic sequestration, this may be beneficial. The densities of brines vary from 950 to 1200 kg/m³ (50). A decrease in the density difference between the two phases would decrease the buoyancy of scCO₂ and may decrease leakage potential.

**Equilibrium Partitioning of SO₂ into Brine.** Salinity-adjusted values of the Henry’s Law constant for SO₂ were determined at 20, 40, 60, and 70 °C, for pressures from 1 to 260 bar, corresponding to depths up to 2.4 km. These values have estimated errors of 14% (see Supporting Information). For example, at 1.2 km depth, the Henry’s Law constant is predicted to be 0.58 ± 0.08 M/atm. Interpolations of the computed values are shown as contours in a PT plot in the Supporting Information (Section S-6). Values of \( K_{\text{H,SO₂}} \) decrease with temperature and pressure. Therefore, the Henry’s Law constant decreases with increasing injection depth such that SO₂ solubility at geologic sequestration conditions is less than that under conditions at the land surface (value given in Table S1 in the Supporting Information).

The depth variations of all the factors that govern SO₂ equilibrium phase partitioning into brine (eq 1) are shown in Figure 4. Partial pressure increases linearly with depth, but \( \phi_{\text{SO₂}} \) and \( K_{\text{H,SO₂}} \) decrease nonlinearly. At shallow depths, SO₂ would behave ideally in the CO₂ phase, with \( \phi_{\text{SO₂}} \) approximately equal to unity, and at greater depths, substantial negative deviations from ideality are predicted. Also shown in Figure 4 is the resulting molar concentration of SO₂ in brine and its variation with depth. This was computed with the simplifying assumptions that, over the entire depth, the aqueous phase is a 1 M NaCl brine, and the brine is in equilibrium with scCO₂ containing 1 or 5% of SO₂. Also, this calculation does not account for the fact that phase partitioning of a finite mass of SO₂ would deplete it from the scCO₂ phase, and the resulting concentration of SO₂ in the brine would be much smaller than what is computed here. (This more realistic case is considered in Ellis et al. 2009 (8).) However, this simplified case is examined for the sake of illustration. At land-surface conditions of 1 bar and 10 °C, the solubility of SO₂ would be 0.02 M for 1% SO₂ and 0.09 M for 5% SO₂. As depth increases, the increase in partial pressure causes phase partitioning to increase by one-to-two orders of magnitude to a maximum of 0.45 M at 0.8 km.
for 1% SO2 and 2.2 M at 0.6 km for 5% SO2. At greater depths, the effects of increasing nonideality in the scCO2 phase and decreasing Henry’s Law constant reverse the trend, causing the phase partitioning of SO2 to decrease with depth.

SO2-phase partitioning can be compared with the solubility of CO2 by using the values calculated by Duan and Sun (18). A major difference between the two cases is that SO2 is a minor mixture component with significant nonideal solution behavior and CO2 is a nearly pure component with less extreme deviations from ideality. Consequently, the value of $\phi$ is not as important for CO2 as it is for SO2. At PT conditions representative of the land surface, the solubility of CO2 in 1 M NaCl is 0.04 M, and it increases by two orders of magnitude to a value of 1.06 M at a depth of 1.2 km (Figure 4d). This similarity to our findings for SO2 at shallow depths is expected because the determining factor is the change in pressure. Beyond a depth of 1.2 km, the solubility of CO2 levels off (Figure 4d), which is explained mostly by the increasing importance of the Henry’s Law constant. By using the $K_H$ correlations presented by Bachu and Adams (17) and correcting them for salinity by using the Schumpe model (27), the pressure-adjusted Henry’s Law constants for CO2 were calculated. These values were found to decrease from 0.053 M/atm at the surface to 0.009 M/atm at a depth of 2.4 km (Figure 4c). In comparison with SO2, values of $K_H$ for CO2 are always smaller, reflecting the higher aqueous solubility of SO2. In fact, the solubility of SO2 is so much higher that its concentration in the brine phase is comparable to that of CO2 despite the fact the mole fraction of SO2 is so small. At 1.2 km, the equilibrium concentration in the brine
is 0.38 and 1.8 M for 1 and 5% SO₂, respectively and 1.03 M for CO₂ at 1.2 km (Figure 4d).

**SO₂ Diffusion through scCO₂.** The predicted diffusion of SO₂ through the model scCO₂ cone is shown in Figure 5, for the case of 1% SO₂, as concentration profiles through a vertical section of the cone. The concentration of SO₂ near the cone boundary decreases early on because of the relatively high solubility of SO₂ in the bulk brine. The resulting depletion of SO₂ at this boundary creates a concentration gradient within the scCO₂ that causes diffusive flux of SO₂ from the center of the plume. The simulations predict that the concentration contours are roughly parallel with the cone boundary. The parallel contours establish a “zone of depletion” of fairly uniform thickness at the boundary of the cone. If we arbitrarily define the zone of depletion to be bounded by where the SO₂ concentration equals 0.999%, after 100 years, it is 15 m thick, and after 1000 years, it is approximately 41 m thick. Even after 1000 years, the concentration of SO₂ in a large portion of the center of the cone remains unchanged.

The effective flux of SO₂ from the entire cone over time is shown in Figure 6a for depths of 0.8 and 2.4 km. Initially, the flux of SO₂ into the bulk brine is limited mostly by solubility, and later, the thick zone of depletion acts as a barrier for diffusion. For both PT conditions, after the first 200 years, the flux is two orders of magnitude less than the flux during the initial years. If the model allowed for SO₂ to accumulate in the bulk brine, the flux of SO₂ from the cone would be even slower (see Ellis et al. (8)). Slower flux would also be predicted in the case of a model that described SO₂ partitioning to a residual brine phase within the scCO₂ cone.

Figure 6b shows the total amount of SO₂ that remains in the cone over time. Even though the effective flux in the case of 5% SO₂ is consistently five times larger than the effective flux for the 1% case (Figure 6a), this difference has a negligible effect on the percent of SO₂ remaining. In the first few years, nearly 5% of the SO₂ leaves the cone. After this, there is a more gradual change in the percent of SO₂ removed because of a slower flux of SO₂ from the cone during these years. After 1000 years, 64–75% of SO₂ still remains in the cone for all of the PT conditions simulated.

The variation in flux with depth seen in Figure 6 is due to the variation in the diffusion coefficient of SO₂ in scCO₂. For 1% SO₂, at 0.8 km, the diffusion coefficient is $4.76 \times 10^{-8}$ m²/sec, compared with $1.9 \times 10^{-8}$ m²/sec for the 2.4 km depth, both with error of ±7% (see Supporting Information). As shown in Figure S-1 in the Supporting Information, at shallower depths, there is little change in $D_{SO2,CO2}$ with temperature, and values are quite sensitive to changes in pressure. A pressure increase from 80 bar to only 100 bar produces a decrease in $D_{SO2,CO2}$ from $6 \times 10^{-8}$ to $3 \times 10^{-8}$ m²/sec. At greater depths, $D_{SO2,CO2}$ values decrease slightly with pressure, and the increase with temperature is more substantial than at shallower depths. The balance of these two effects means that, for depths of 1.2–2.4 km, $D_{SO2,CO2}$ contours align with the PT gradient such that there is little change in $D_{SO2,CO2}$ values.

**Implications for Geologic CO₂ Sequestration.** As mentioned in the Introduction, prior co-injection modeling studies predicted low pH conditions because of the formation of sulfur-containing acids and that these conditions would be sustained for decades. It is certainly the case that SO₂ is
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Supporting Information Available

Supporting Information includes sedimentary basin PT gradients, data used to estimate Henry’s Law constants and mixture properties, PT contour plot of adjusted Henry’s Law constants for SO2, derivation of the diffusion model equations, diffusion coefficients for SO2 in scCO2 and error propagation for calculations of Henry’s law constant, mixture density, and the diffusion coefficient. This material is available free of charge via the Internet at http://pubs.acs.org.

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