



Prediction of carbon dioxide dissolution in bulk water under isothermal pressure decay at different boundary conditions



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ABSTRACT

In this work, dissolution of CO₂ in bulk water is simulated under isothermal pressure decay. Different boundary conditions (BCs) including equilibrium, semi-equilibrium and non-equilibrium are examined at gas/liquid interface. Comparison of our simulated and measured experimental data shows that the non-equilibrium BC can predict dissolution behavior reliably. Other boundary conditions show considerable deviation between model predictions and experimental measurements. On the other side, convective dissolution is found much more active than diffusive mixing, so that the role of diffusive transport is overshadowed. Mass transfer coefficient is highest at the start of dissolution and decreases with time. Results show that when convection is the active mechanism even at late times, it interferes with diffusivity measurements and makes interpretation of diffusion experiment results difficult both at early and later times.

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1. Introduction

Transfer of gases, tracers, and concentrated species into solvents is controlled by the mechanisms of mass transfers i.e. convection and diffusion. For a system like CO₂ and water, as CO₂ is dissolved in water, a heavier layer forms at an interface and causes CO₂ to dissolve rapidly in the form of instabilities. This process has a direct application in CO₂ geological storage where free phase gas is dissolved in brine after a long time. Modeling of miscible gas injection in all types of crude oil is analogous to CO₂ injection.

The main difference in modeling such processes refers to the presence of convection [1], liquid swelling [2], solubility [3], and dependence of parameters (such as diffusivity, viscosity) on pressure or temperature or time [4,5]. As it is mentioned, when CO₂ dissolves in water, heavier water saturated with CO₂ at the interface tends to sink down the water column by making instabilities.

The similar steady-state problem in heat transfer is known as Rayleigh–Bénard convection in which fluid is confined between two parallel horizontal plates with hot fluid rising and cold fluid falling [6]. In our study, CO₂ concentrated water is falling due to gravity effect while fresh water rising to reach an equilibrium state in CO₂-saturated water. Thus, the same criteria of the Rayleigh–Bénard convection can be used for our study by using the analogy. However, due to differences

in boundary conditions and time conditions, results can be expected different.

Modeling instabilities caused by density difference has been considered for a long time. The works of Rayleigh and Taylor on modeling instability stand out as the problem named after them [7,8]. After that, many works tried to model, simulate and perform the experimental design of Hele-Shaw [9], Rayleigh–Bénard [10,11], Rayleigh–Taylor and Saffman–Taylor [12] problems.

However, few works can be cited to discuss instability growing for two miscible phases when one phase dissolves from the interface.

In this study, numerical and experimental dissolution of CO₂ in water is evaluated under pressure decay. The dissolution sequences are distinguished based on the trend of the Sherwood number like Hassanzadeh et al. [13]. However, our discussion includes dissolution in both porous media and bulk water. Many other works can be referred that modeled or simulated convective dissolution in porous media for reservoir applications such as Ghesmat et al. [14], Ouakad and Nasrabadi [15] and Szulczewski et al. [16].

While, experimental applications imply simulation of convective mixing in bulk fluid which is the main topic of our work. Farajzadeh et al. [17] simulated CO₂ dissolution in bulk water in axisymmetric coordination. They used equilibrium boundary condition (BC) at the interface and observed instabilities in the form of Rayleigh–Taylor problem.

Although, more perturbed results are expected. In another work, Haugen and Firoozabadi [18] studied the effect of bulk flow due to non-ideality and compressibility on dissolution. They showed that neglecting bulk flow results in fitting of Fick's second law with higher diffusion

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coefficients. We know that natural density-driven convective flux is much more significant than the so-called mechanisms of non-ideality or compressibility addressed in the work of Haugen and Firoozabadi [18].

Another criterion for modeling the gas dissolution is choosing the proper boundary condition at gas/liquid interface. In literature, different boundary conditions are used for modeling. Most works considered a saturated interface i.e. equilibrium or semi-equilibrium BC [19–22].

Recently some authors have considered other forms of boundary conditions rather than simple equilibrium BC [23–25]. They used a Neumann boundary condition type at gas/liquid interface accounting for the effect of declining pressure versus time. Non-equilibrium BC is another form of boundary condition standing for the effect of interface resistance.

The pioneer works of Civan and Rasmussen [2,3,26] illustrates this BC. However, a more general form is described by Etminal et al. [27] in which a sharp concentration change across the interface is considered. In the following sections, we first explain experimental procedure briefly and then present our assumptions, equations and boundary conditions.

After that, convective dissolution of CO₂ in water under pressure decay is modeled. We used the experimental data obtained from a PVT cell and the data of Rongy et al. [28] to see validity of our model. Concluding remarks appear at the end of the paper.

2. Material and methods

A PVT cell is filled with liquid (water) sample up to a special height (H) (see Fig. 1). Details of experimental setup used here were described by Azin et al. [29] in which a certain amount of gas is brought into contact with water and pressure is recorded as gas is dissolving in water.

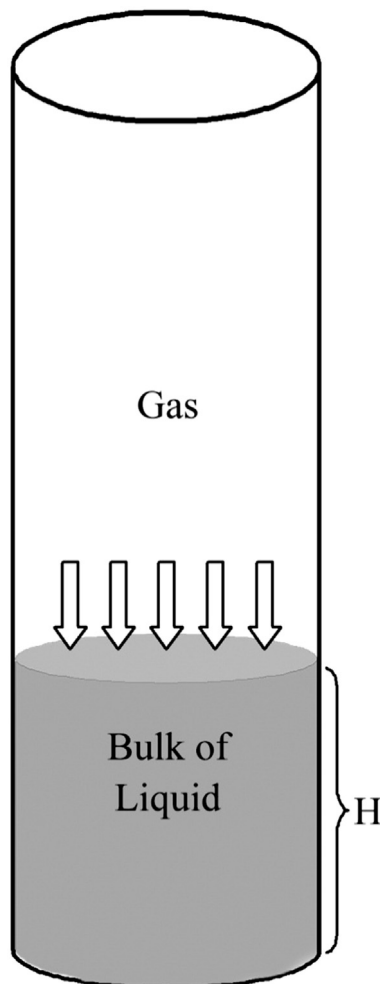


Fig. 1. A PVT cell shows the initial state of fluids for conducting a pressure decay test.

The same approach is used by many authors to calculate diffusion coefficient in oil as an inverse problem based on Fick's second law of diffusion [19,21,30,31]. The cell is mounted under the injection line and gas is injected from top of the cell. The gas injection process continues to reach the required initial pressure.

Then, the injection line is shut off and the test starts by recording pressure versus time periodically. The whole cell is put through a thermal air bath to keep the temperature constant. All the connecting valves are tested frequently to prevent any leakage. The tests are conducted until a steady pressure is reached.

The steady pressure is the same as the equilibrium pressure. Depending on the method of diffusivity calculation, this equilibrium pressure can have significant effect on the results. The high pressure cell has inner dimensions of 3.81 cm in diameter and 31 cm in height. The CO₂ gas cylinder was obtained from domestic suppliers and has 99.99% purity. Distilled water was provided from a generator in the chemistry laboratory, which filled 10 cm height of high pressure cell.

3. Mathematical modeling

Mathematical modeling is based on the experimental conditions. Our modeling uses the following assumptions:

1. There is no chemical reaction in the system.
2. Two dimensional and Cartesian coordinate describe our geometry.
3. Evaporation of water into the gas phase is negligible [17,32].
4. Resistance of mass transfer at water/CO₂ interface can be neglected (Equilibrium or Semi-equilibrium boundary condition) or considered (Non-equilibrium boundary condition).
5. There is no pressure gradient in the CO₂ phase [32].
6. Swelling of water due to dissolution of CO₂ is negligible [29]. Thus, interface position during the run is constant [32,33].
7. Due to low solubility of CO₂ in water (compared to CO₂ in hydrocarbons) diffusion coefficient versus time and position is assumed to be constant.
8. The whole process is isothermal.
9. Viscosity of water does not change due to CO₂ dissolution.
10. Boussinesq approximation is valid.

Assumptions 5 and 6 imply that the geometry is a regular rectangle with the diameter and height of high pressure cell filled with water. Fig. 2 shows a schematic of the model geometry. It should be added that however experiments are conducted in a cylindrical PVT diffusion cell, a Cartesian geometry is used here. Axisymmetric coordinates result in symmetric fingers which are not of interest. The similar problem is modeled in a 2-D Cartesian geometry by Rongy et al. [28].

From the real gas law, the number of CO₂ gaseous moles at a specified pressure can be calculated:

$$PV = znRT \Rightarrow n_g = \frac{PV_g}{ZRT} \quad (1)$$

Pressure change among the runs is not that much (<5% of the initial pressure) to use more complicated equation of states. The prescribed equation will be used for conversion between gas pressure and aqueous CO₂ concentration, which is a simple linear relationship. Assuming that gas compressibility factor is constant as pressure decays, the difference between initial and current gaseous CO₂ can be written:

$$\Delta n_g = \frac{\Delta PV_g}{ZRT} \quad (2)$$

The change in CO₂ moles can be written in terms of the average concentration in bulk liquid, \bar{c}_{CO_2} ($\frac{\text{mol}}{\text{m}^3}$):

$$\Delta n = -V_l \Delta \bar{c}_{CO_2} \quad (3)$$

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