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Numerical investigation of double diffusive natural convection of CO_2 in a brine saturated geothermal reservoir

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ABSTRACT

In geologic sequestration or in CO_2-based geothermal systems, CO_2 is present on top of the brine phase. In this study we performed a numerical analysis of a geothermal reservoir that is impermeable from the sides and is open to CO_2 at the top. For this configuration, double diffusive natural convection due to density and temperature differences across the height enhance the mass transfer rate of CO_2 into the initially stagnant brine. The analysis is done using mass, momentum, energy conservation laws, and the Darcy laws. The objective is to understand the diffusion of CO_2 over long periods of time after sequestration into a subsurface porous media geothermal aquifer. The problem parameters are the solutal Rayleigh number ($100 \le Ra_s \le 10{,}000$), the buoyancy ratio ($2 \le N \le 100$), the cavity aspect ratio ($0.5 \le A \le 2$), and a fixed Lewis number ($Le = 301$). Numerical computations do not exhibit natural convection effects for homogeneous initial conditions. Hence a sinusoidal perturbation is added for the initial top boundary condition. It is found that the CO_2 plumes move faster when Ra_s is increased, however they slow down with decreasing N. For every simulation run, the average CO_2 concentration ($\bar{S} = (\sum_i^{n_i} \sum_j^{n_j} c_{i,j}/n_i \times n_j)$) is computed. Higher concentration rates in laterally wide reservoirs make better candidates than deeper aquifers for CO_2 sequestration.

1. Introduction

In order to control carbon emissions, the use of technologies to capture and store CO_2 has rapidly emerged as an important physically and economically viable method these days. Various CO_2 storage methods in geological formations, such as depleted oil and gas fields, un-mineable coal seams, saline-filled basalt formations, have been suggested (Bryant, 2007; Hassanzadeh et al., 2005a; Hovorka, 2010; Ruhl, 2007). CO_2 has also been proposed as a working fluid in Enhanced Geothermal Systems, EGS (Pan et al., 2013; Pistone et al., 2011; Pruess, 2006). Geological storage in underground saline formations or its use as a working fluid involves injecting supercritical CO_2 at high pressure into a saline aquifer capped by a rock formation. Following injection, CO_2 accumulates between the cap and aquifer surface. Eventually, the CO_2 is trapped by two different mechanisms, namely; capillary trapping and solubility trapping. In capillary trapping, part of the CO_2 rises through porous rock formations above due to buoyancy and capillary forces and gets trapped in the rock pores (Han et al., 2010; Ide et al., 2007; Juanes et al., 2006). On the other hand, at the interface between the CO_2-rich phase and brine (Farajzadeh et al., 2009), dissolution of CO_2 into the brine starts with molecular diffusion. This process increases the brine density by about 1% (Duan et al., 2008; Islam and Carlson, 2012; Spycher and Pruess, 2010) on the aquifer top surface, which then sinks into the brine by natural convection due to the solute gradient. This phenomenon is termed solubility trapping. Another destabilizing agent is the naturally occurring geothermal temperature gradient (typically ∼3 °C/100 m depth), which induces upward natural convection of the brine. The interaction of these two opposing processes, termed double diffusive transport, determines the resultant rate of concentration of the CO_2 in the brine. The geothermal gradient is partially compensated by the geo-pressure gradient (Lindeberg and Wessel-berg, 1997) (normally ∼10 bar/100 m depth). The convective mixing enhances dissolution of CO_2 by continuously removing CO_2-rich brine from the top layer and bringing under-saturated brine into contact with the downward advancing CO_2 plume. For the design, operation, and maintenance of such a geologic CO_2 storage facility, it is very important to quantify the rate of dissolution and understand the transport mechanisms. The time scale of the solubility trapping is very large ranging from hundreds to thousands of years. During this time, the high pressure free phase CO_2 that accumulated between the aquifer free surface and the top rock formation may leak out through rock fractures (Ennis-King and Paterson, 2003;

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Notations

A	aspect ratio, H/L
c	concentration [mol/m^3]
C_p	heat capacity at constant pressure [J kg^{-1} K^{-1}]
D	diffusion coefficient [m^2/s]
g	acceleration due to gravity [m/s^2]
H	porous medium height [m]
k	permeability [m^{-2}]
L	porous medium length [m]
n	number of nodes
p	pressure [Pa]
Le	Lewis number
Pe	Peclet number
Pr	Prandtl number
Ra	Rayleigh number
Ra_e	equivalent Rayleigh number
$\bar{S}$	average concentration
t	time [s]
u	velocity [m/s]
x	distance along x-axis
z	distance along z-axis

Greek letters

α	thermal diffusivity
β_c	coefficient of density increase by concentration [m^3/mol]
β_T	coefficient of thermal expansion [K^{-1}]
φ	porosity
μ	viscosity [kg m^{-1} s^{-1}]
κ	thermal conductivity
ρ	density [kg/m^3]
ψ	stream function [m^3/m^{-1} s^{-1}]

Superscript

*	Dimensionless quantity

Subscripts

0	initial value
c	concentration
i	node in x-direction
j	node in z-direction
r	reference value
s	solutal
T	temperature
x	x-coordinate
z	z-coordinate

Hassanzadeh et al., 2005b; Kumar et al., 2004; Lindeberg and Wessel-berg, 1997; Taheri et al., 2012). In a very recent study Taheri et al. (2012) concluded the dissolution process is very slow and the pure CO_2 phase would remain mostly intact for about 10,000 years unless other processes occur. The chance of leakage is reduced when a significant amount of CO_2 dissolves in the brine.

The importance of double-diffusive convection is generally recognized from the dynamics and associated flow patterns that develop, in particular the phenomena of fingers and layered convection. Comprehensive investigations in which heat and solute are the diffusive components have been conducted by Oldenburg and Pruess (1998), and Stern (1975). Green (1984) described scales for double diffusive fingering. The author examined the influence of double diffusion on vertical transport using oceanic salt finger theory. A three dimensional numerical study of a cubic enclosure subject to opposing and horizontal gradients of heat and solute was conducted by Sezai and Mohamad (2000). They concluded that that double diffusive flow in enclosures with two opposing buoyancy forces is strictly three dimensional for a certain range of parameters of Ra_s, N, and Le. Cooper et al. (1997, 2001) described the effects of the buoyancy ratio on the development of double-diffusive finger convection in a Hele-Shaw cell. They presented the results of a set of experiments that considered the system's evolution after the onset of instability for NaCl and sucrose systems. Strong (2009) analyzed the effects of vertical harmonic vibrations, which was first noticed by Mojtabi et al. (2005) These vibrations develop upon the onset of convection in an infinite horizontal layer of a binary fluid mixture saturating a porous medium. Pau et al. (2010) showed that the CO_2 mass flux due to density driven convection process is 25% higher when the simulations are performed for a 3-dimensional geometry compared to that for a 2-dimensional cavity. Their finding strongly warrants 3-dimenaional studies, which target to perform in future. Several studies investigating the effects of solutal and thermal gradients on the onset of convection, preferred wavelengths and growth rates of the convective fingers in natural convection processes, have been published over the years (Bhadauria, 2006; Gunter et al., 1997; Poulikakos, 1986; Sodha and Kumar, 1985). Linear stability analysis of double-diffusive convection process with thermal and solutal gradients were conducted by Javaheri et al. (2010) for CO_2–brine system in porous media. However, they did not present any simulation results.

The long time scale of the storage process renders experimental investigations impractical. Although some laboratory studies (Ennis-King and Paterson, 2005; Kneafsey and Pruess, 2010; Moghaddam et al., 2012; Watson et al., 2012) have been conducted to evaluate density driven natural convection processes. They cannot replicate reservoir size, e.g., the geometry of the experiment by Kneafsey and Pruess (2010) was 25.4 cm × 30.5 cm whereas reservoirs can be several hundreds to thousands of square meters in area. The viable alternatives are numerical simulations, which is the motivation behind this work. The use of modeling and simulations to make predictions on realistic timescale is obviously impossible to validate, since even in field operations one cannot historically match more than a small increment of the relevant time period (Ennis-King and Paterson, 2003).

CO_2 is being considered as a working fluid in Enhanced Geothermal System (EGS) reservoirs, because of its heat extraction properties (Pan et al., 2013; Pistone et al., 2011; Pruess, 2006). Consequently processes related to CO_2 dissolution, including the time and length scale of dissolution and diffusion during natural convection is of particular significance. This paper describes numerical experiments on double diffusive convection of CO_2 in brine under vertical thermal and solutal gradients appropriate for geologic sequestration in geothermal reservoirs. Results are presented graphically in terms of the propagation of the CO_2 front through the aquifer with time for various cavity configurations ($0.5 \le A \le 2$) and for a range of the solutal Rayleigh number ($100 \le Ra_s \le 10{,}000$) and buoyancy ratio ($2 \le N \le 100$). The occurrence of convection is closely related to the Rayleigh number, which provides an indication on whether convection occurs under the conditions of interest. The Rayleigh number compares the rate of fluid convection with the rate of diffusive transport. The buoyancy ratio is defined mathematically in the next section. The effects of varying these geometric and hydrodynamic parameters on the CO_2 propagation front and dissolution are analyzed and evaluated.

2. Description of the problem and the governing equations

The geometry under consideration is a two-dimensional rectangular cavity reservoir (Fig. 1), filled with a porous medium saturated with brine (H_2O + NaCl), and with a height H and length L. The