

# The diffusion of CO<sub>2</sub>-brine storage based on stochastic partial differential equations

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**Abstract.** The migration of CO<sub>2</sub> is stochastic in heterogeneous porous media. This paper considers the CO<sub>2</sub> diffusion with the case of steady flow in heterogeneous porous media. The partial differential equations of CO<sub>2</sub> diffusion in random velocity field are established based on the mass conservation equations of CO<sub>2</sub>-brine two-phase flow with the change of time scale and spatial scale under the influence of heterogeneity such as permeability and porosity. The random travel process of CO<sub>2</sub> is quantified by joint probability distributions and joint statistical moments (mean and variance), and the diffusion model of CO<sub>2</sub> particle in random velocity field is established under the condition of non-linear and immiscibility in heterogeneous porous media. The micro mechanism of diffusion in heterogeneous porous media is revealed by numerical simulation. The general conclusion of steady state flow of CO<sub>2</sub> diffusion in heterogeneous porous media was verified by simulating Sleipner CO<sub>2</sub>-brine storage in Norway.

## 1 Introduction

Over the past few decades, CO<sub>2</sub> concentration will increase by 2.1% per year due to human activities, and the CO<sub>2</sub> emissions are expected to increase to 3.72 billion tons per year by 2035 from global energy<sup>[1]</sup>. According to the latest report, the global average temperature has risen by 1°C compared with that before the industrial revolution due to the greenhouse effect caused by CO<sub>2</sub> emissions. It is predicted that the global average temperature will rise to 1.5°C in 2030-2050 and 3°C in the end of this century<sup>[2]</sup>. The climate change caused by CO<sub>2</sub> and its impact on the earth's ecosystem are becoming the main environmental challenges in this century<sup>[3]</sup>. In order to avoid this increasing trend and its consequences, CCS (carbon capture and storage) is the technology that stabilizes and reduces the concentration of carbon dioxide in the atmosphere.

In order to ensure that CO<sub>2</sub> can be safely stored in the formation for a long time, it is necessary to know the migration mechanism of CO<sub>2</sub> in geological structures. There are two main phenomena that occur including diffusion and advection with the process of CO<sub>2</sub> migration in brine. Diffusion and advection will accelerate the rate of CO<sub>2</sub> dissolution in brine, so that CO<sub>2</sub> can be effectively and safely stored for a long time. Therefore, the analysis of multiphase flow in porous media is of great significance. In the geological structure, although the geological structure is certain, there is heterogeneity in the spatial scale due to the formation. The characteristics of the formation will be caused by the influence of random factor, and this factor will lead the randomness of CO<sub>2</sub> migration. Therefore, the

nonlinear analysis of multiphase flow must be carried out according to the randomness of formation parameters for the migration of CO<sub>2</sub> in heterogeneous porous media.

The analysis of multiphase flow in heterogeneous porous media is usually more difficult than that of single-phase flow. Therefore, a more efficient solution is to use random processes to estimate the mean behaviour of CO<sub>2</sub>-brine two-phase flow<sup>[4]</sup>. The significant advantage of stochastic method is that the spatial heterogeneity of any reservoir is described by limited statistical properties such as mean and variance.

## 2 Diffusion Equations

The simultaneous flow of two immiscible and incompressible fluids in heterogeneous porous media is considered below. According to the mass conservation equation of CO<sub>2</sub>-brine two-phase flow<sup>[5]</sup>:

$$\phi(x) \frac{\partial S_i(x,t)}{\partial t} - \nabla \cdot \frac{k(x)k_n}{\mu_i} \left( \frac{\partial P}{\partial x} - \rho_i g \frac{\partial D}{\partial x} \right) = 0, i = CO_2, water \quad (1)$$

Here porosity  $\phi$ , absolute permeability  $k$  are all random space functions. The control equations of CO<sub>2</sub>-brine two-phase flow is changed into the stochastic partial differential equations of CO<sub>2</sub>-brine two-phase flow, and  $f_{CO_2}$  is the fractional flow function defined as:

$$f_{CO_2} = \frac{\lambda_{CO_2}}{\lambda_w + \lambda_{CO_2}} = \frac{kk_{rCO_2} / \mu_{CO_2}}{kk_{rw} / \mu_w + kk_{rCO_2} / \mu_{CO_2}} \quad (2)$$

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$$q_{\text{CO}_2} = f_{\text{CO}_2} \left\{ q + \lambda_w \left[ \frac{dP_c}{dS_{\text{CO}_2}} \nabla S_{\text{CO}_2} + (\rho_{\text{CO}_2} - \rho_w) g \right] \right\} \quad (3)$$

$\phi$  is porosity,  $x$  is any point in coordinate( $x,y,z$ ),  $\mu$  is viscosity,  $\rho$  is density,  $kr$  is absolute permeability,  $k$  is relative permeability,  $dP/dx$  is pressure gradient,  $q$  is volume rate of flow,  $S$  is saturation,  $f$  is fractional flow,  $\lambda$  is mobility. Equation (1) becomes:

$$\phi(x) \frac{\partial S_{\text{CO}_2}(x,t)}{\partial t} - \nabla \cdot f_{\text{CO}_2} \left\{ q + \lambda_w \left[ \frac{dP_c}{dS_{\text{CO}_2}} \nabla S_{\text{CO}_2} + (\rho_{\text{CO}_2} - \rho_w) g \right] \right\} = 0 \quad (4)$$

Equation (4) is the stochastic partial differential equation of CO2 diffusion by the influence of heterogeneity in the reservoir. The influence of capillary pressure and gravity on CO2 diffusion is less than that of CO2 particle velocity, so it can be ignored. In order to study the influence of particle velocity on CO2 diffusion, the stochastic partial differential equations of particle velocity and CO2 saturation is needed. In the absence of capillary and gravitational effects, CO2 fractional flow  $f$  can be replaced by CO2 saturation  $S$ :

$$\nabla f_{\text{CO}_2} = f'_{\text{CO}_2}(S_{\text{CO}_2}) \nabla S_{\text{CO}_2} = \left( \frac{df_{\text{CO}_2}}{dS_{\text{CO}_2}} \right) \nabla S_{\text{CO}_2} \Leftrightarrow \frac{\partial f_{\text{CO}_2}}{\partial x} = \frac{\partial f_{\text{CO}_2}}{\partial S_{\text{CO}_2}} \cdot \frac{\partial S_{\text{CO}_2}}{\partial x} \quad (5)$$

Equation (4) can rewrite as:

$$\frac{\partial S_{\text{CO}_2}(x,t)}{\partial t} + f'_{\text{CO}_2}(S_{\text{CO}_2}) \frac{q(x,t)}{\phi(x)} \nabla S_{\text{CO}_2}(x,t) = 0 \quad (6)$$

$v(x) = q(x,t)/\phi(x)$  is CO2 particle velocity, Equation (6) is a nonlinear stochastic partial differential equation composed of random variables. It can be seen as a stochastic process of CO2 diffusion in heterogeneous porous media. It can be described by probability density function and joint probability density moment (mean and variance) in order to quantify the stochastic process:

$$v_{\text{CO}_2}(S_{\text{CO}_2}, x, t) = \langle v_{\text{CO}_2}(S_{\text{CO}_2}, x, t) \rangle + v'_{\text{CO}_2}(S_{\text{CO}_2}, x, t) \quad (7)$$

$$S_{\text{CO}_2}(x, t) = \langle S_{\text{CO}_2}(x, t) \rangle + S'_{\text{CO}_2}(x, t) \quad (8)$$

$\langle \rangle$  represents ensemble mean, the first derivative represents variance, which is the range.

### 3 Diffusion of Sleipner

#### 3.1 Geological Characteristics

Utsira reservoir in Sleipner project in Norway is selected as the research object in order to study the diffusion of CO2-brine two-phase flow in heterogeneous actual formation. It is 450km long, 75-130km wide, with an area of about 26100km<sup>2</sup>, and located between 700m and 1000m below sea level[6]. The formation composition of the target block is mainly sandstone[7]. The results of modal analysis on core of Utsira reservoir show that the porosity of the reservoir is generally between 27% and

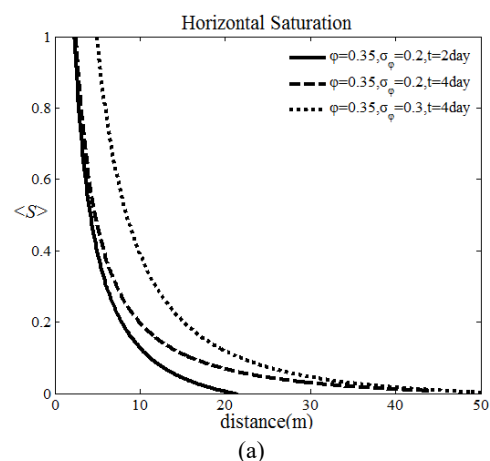
42%[8]. The permeability of Utsira reservoir measured by horizontal and vertical core samples is between 1.5D and 3.2D[9]. Thus, the initial conditions, fluid and reservoir properties are shown in Table 1:

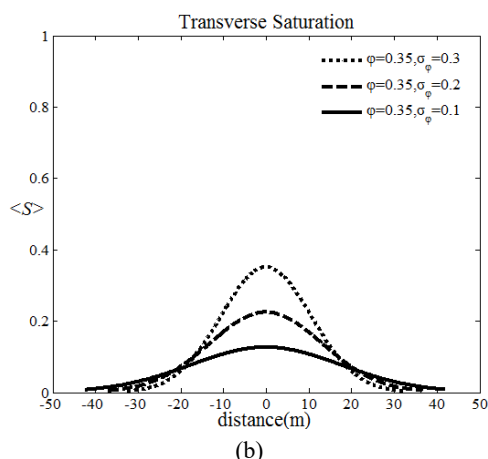
**Table 1.** The initial conditions, fluid and reservoir properties<sup>[6-9]</sup>

Parameter	Value	Unit
Length of formation	50	[m]
Cross-section area	1	[m <sup>2</sup> ]
Temperature	40	[°C]
Pressure	10	[MPa]
Viscosity of brine	6.6×10 <sup>-3</sup>	[Pa•s]
Viscosity of CO <sub>2</sub>	1.3×10 <sup>-3</sup>	[Pa•s]
The mean of porosity	0.35	[-]
The variance of porosity	0.1-0.3	[-]
The correlation scale of porosity	(1-2)×10 <sup>-4</sup>	[m]
Absolute permeability	1-2	[D]
Injection rate	5×10 <sup>-3</sup>	[m <sup>3</sup> /s]
Velocity	1×10 <sup>-3</sup>	[m/s]
Time	96	[h]

#### 3.2 Numerical Simulation

In Utsira reservoir, the joint probability distribution and the joint statistical moment (mean value and variance) were used to quantify the change process of brine saturation under the influence of formation heterogeneity. The mathematical model of CO2 diffusion travel at the case of two-dimensional steady-state flow is established, and it is assumed that brine fills the reservoir. The simulation results are shown as follow:





**Fig. 1.** (a) the horizontal saturation profile of CO<sub>2</sub> particle travel and (b) shows the transverse saturation profile of CO<sub>2</sub> particle travel. The diffusion of CO<sub>2</sub> in Utsira reservoir.

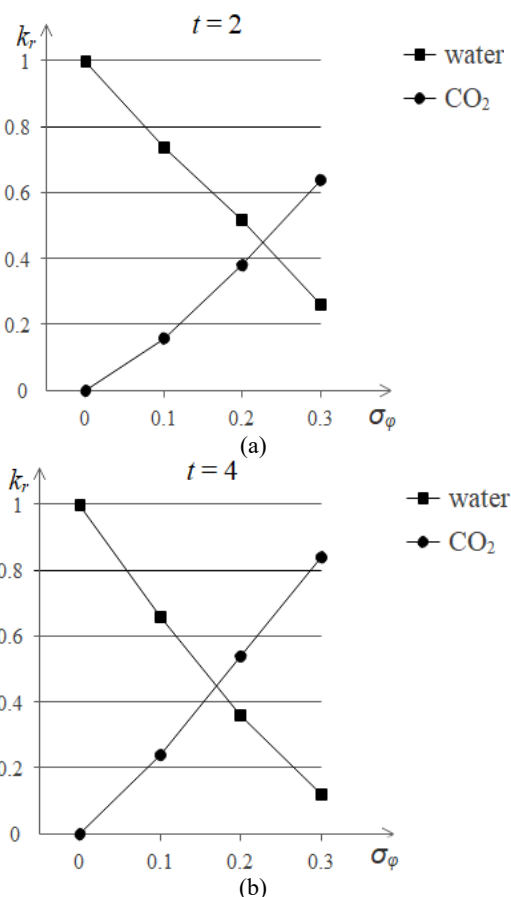
It can be seen from figure (a), when the average porosity is 0.35 and the porosity variance is 0.2, CO<sub>2</sub> particle travels for 2 days with the diffusion distance of 21m, and CO<sub>2</sub> particle travels for 4 days with the diffusion distance of 44m. When the variance of porosity is changed to 0.3, the CO<sub>2</sub> particle travels for 4 days and the diffusion distance increases to 50m. It is indicated that the heterogeneity of the pores affects the CO<sub>2</sub> diffusion farther away with the time increases. When the variance of porosity was 0.3, the saturation starts to change later than when the variance of porosity was 0.2. This indicates the effect of the heterogeneity of the pores on the occurrence time of the diffusion of CO<sub>2</sub>. The later CO<sub>2</sub> diffusion occurs due to the increase of the variance of porosity. It is affected by the heterogeneity of pore, such as the size of pore, the trajectory of CO<sub>2</sub> particle, and the friction between CO<sub>2</sub> particle and the pore.

It can be seen from figure (b), when the average value of porosity is 0.35, the variance of the porosity are 0.1, 0.2 and 0.3 respectively, and the normal distribution formed by the transverse saturation profile increases gradually. As the CO<sub>2</sub> particle diffusion began, the increase of variance of porosity leads to the increase of its saturation variation. All these prove that the heterogeneity of porous media quantified by mean and variance has a significant effect on the diffusion of CO<sub>2</sub>.

### 3.3 Analysis of influencing factors of storage

#### 3.3.1 Analysis of Relative Permeability

In this section, the rules of relative permeability in diffusion were quantitatively analyzed through the simulation results of the saturation changes in heterogeneous actual formation. The simulation is carried out for different variances of porosity, and the simulation results are shown as follows:

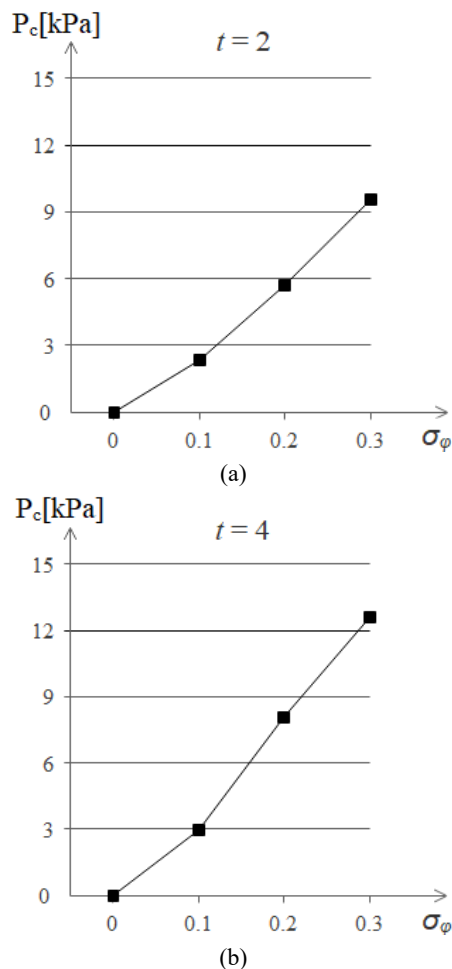


**Fig. 2.** (a)  $t = 2$  day CO<sub>2</sub> diffusion and (b)  $t = 4$  day CO<sub>2</sub> diffusion. Relative permeability curves.

It can be seen from the estimated results that when  $t = 2$  day, the relative permeability of CO<sub>2</sub> diffusion is gradually increasing with the increase of variance of porosity, and when  $t = 4$  day, the relative permeability of CO<sub>2</sub> diffusion is increasing more rapidly with the increase of variance of porosity compared with  $t = 2$  day. This indicates that the diffusion of CO<sub>2</sub> is accelerated with the increase of variance of porosity in the porous media, and the fluidity of CO<sub>2</sub> is improved. This causes more unsaturated brine is in contact with CO<sub>2</sub>, and more CO<sub>2</sub> is dissolved in the brine so that improve the CO<sub>2</sub> dissolved storage.

#### 3.3.2 Analysis of Capillary Pressure

In this section, the rules of capillary pressure in diffusion were quantitatively analyzed through the simulation results of the saturation changes in heterogeneous actual formation. The simulation is carried out for different variances of porosity, and the simulation results are shown as follows:



**Fig. 3.** (a)  $t = 2$  day CO<sub>2</sub> diffusion and (b)  $t = 4$  day CO<sub>2</sub> diffusion. Capillary pressure curves.

It can be seen from the estimation results that when  $t = 2$  day, the capillary pressure of CO<sub>2</sub> diffusion gradually increases with the increase of variance of porosity, and finally reaches 9.6kPa. When  $t = 4$  day, capillary pressure curve of CO<sub>2</sub> diffusion increases faster and finally reaches 12.6kPa compared with  $t = 2$  day. It shows that with as time goes on, the spread of CO<sub>2</sub> is more and more extensive, and more and more CO<sub>2</sub> is dissolved in brine. CO<sub>2</sub> dissolved in brine will increase the concentration of brine and accelerate the diffusion. The change of porosity accelerates the diffusion of CO<sub>2</sub> in the porous media, promotes the contact between CO<sub>2</sub> and more brine. This will increase the dissolution rate of CO<sub>2</sub> in brine, and increase the capillary pressure in the pore. Finally, the amount of CO<sub>2</sub> stored increases in the porous media, and then the residual storage of CO<sub>2</sub> increases.

## 4 Summary

The diffusion of CO<sub>2</sub> particle in heterogeneous porous media is studied in this paper. The equations of CO<sub>2</sub> diffusion in heterogeneous porous media are established at the case of CO<sub>2</sub>-brine two-phase steady flow. The average behaviour of CO<sub>2</sub> diffusion is estimated by stochastic process. The randomness of the mean and variance of CO<sub>2</sub>-brine two-phase flow saturation was

quantified by stochastic process analysis with joint density distribution and joint statistical moment. The general conclusion of steady state flow of CO<sub>2</sub> diffusion in heterogeneous porous media was verified by simulating Sleipner CO<sub>2</sub>-brine storage in Norway.

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## References

1. Cambridge University Press. "Climate change 2007: impacts, adaptation and vulnerability." *journal of environmental quality* 37.6(2007):2407
2. Edenhofer, O., R. Pichs-Madruga, Y. Sokona, E. Farahani, S. Kadner, K. Seyboth, A. Adler, I. Baum, S. Brunner and P. Eickemeier. "IPCC, 2018: Climate change 2018: Mitigation of climate change." *Presentación en Edenhofer, Co-presidente, IPCC Working Group III.* (2018)
3. Allen, Simon K , et al. "Climate Change 2013: The Physical Science Basis. An overview of the Working Group 1 contribution to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change (IPCC)." *computational geometry* 18.2(2007):95-123
4. Evangelos, K., and Paleologos. "Stochastic Methods for Flow in Porous Media, Coping With Uncertainties." *Eos Transactions American Geophysical Union* (2003)
5. Bear, and Jacob. "Dynamics of Fluids in Porous Media." *Soil Science* 120.2(1975):162-163
6. Semere Solomon, The Bellona Foundation . "Carbon Dioxide Storage: Geological Security and Environmental Issues – Case Study on the Sleipner Gas Field in Norway Summary." *bellona report* (2006)
7. Eidvin T, Rundberg Y, Smelror M. Revised chronology of Neogene sands (Utsira and Skade Formations) in the central and northern North Sea. *Onshore/offshore relationships on the North Atlantic Margin.* (2002)
8. Pearce J M, Kemp S J, Wetton P D. Mineralogical and Petrographical Characterisation of a 1m Core from the Utsira Formation, Central North Sea: British Geological Survey Report WG/99/024. *British Geological Survey.* (1999)
9. Zweigel, P. , et al. "Reservoir geology of the Utsira Formation at the first industrial-scale underground CO<sub>2</sub> storage site (Sleipner area, North Sea)." *geological storage of carbon dioxide* 523.7558(2004):96-100