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Effects of capillary pressure – fluid saturation – relative permeability relationships on predicting carbon dioxide migration during injection into saline aquifers

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Abstract

Mathematical modeling and numerical simulations on carbon dioxide plume migration in confined saline aquifers have become important approaches to evaluate storage capacity and efficiency for carbon dioxide sequestration and to predict potential risks of leakage during and after carbon dioxide injection into subsurface formations. The effects of the characteristic functions relating capillary pressures and relative permeabilities to fluid saturations are critical in predicting carbon dioxide plume migration in saline aquifers. In this paper, four well known models, i.e. Brooks-Corey-Burdine model (BCB), Brooks-Corey-Mualem model (BCM), Van Genuchten-Burdine model (VGB), and Van Genuchten-Mualem model (VGM), were incorporated with an immiscible displacement process model to simulate carbon dioxide injection into saline aquifers. Parametric analysis was conducted to identify the influences of parameters in the Brooks-Corey based model on the predictions of carbon dioxide plume migration in a confined saline aquifer. A comprehensive comparison was carried out to reveal the different performances of the models with respect to the evolutions and patterns of carbon dioxide plume in the confined saline aquifer. The simulation results indicate that the saturation distributions of carbon dioxide are drastically sensitive to the capillary entry pressure. However, the parameters n and m in the Brooks-Corey based model, which are related to pore size distribution and tortuosity ratio of a porous medium, respectively, have little effects on predicting carbon dioxide plume migration in the saline aquifer. Moreover, different models may cause extensive influences on the carbon dioxide distributions at the region that is close to the injection well and at the leading edges of carbon dioxide plume in the saline aquifer. Hence, the results indicate that for the evaluation of the storage capacity and efficiency of a saline aquifer to trap carbon dioxide, the storage capacity of the saline aquifer could be over-estimated by using the BCB model, whereas it could be underestimated by using the VGM model. On the other hand, for evaluations of potential leakage of carbon dioxide in saline aquifers, where the movement of the leading edge of carbon dioxide

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plume is monitored, the VGM model is a safe choice in simulations. These results have potentially significant implications for estimation of carbon dioxide storage capacity of saline aquifers and assessments on potential risks of leakage.

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Keywords: Capillary pressure, Relative permeability, Fluid saturation, Carbon dioxide plume, Migration, Saline aquifer, Simulation;

1. Introduction

Carbon dioxide capture and geologic storage is a promising technology that can be an effective way to mitigate global warming[1]. Long-term effectiveness and risk management need to be convinced before its large scale application. In the last decade, mathematical modeling and numerical simulations of carbon dioxide sequestration, which are considered powerful tools of safety analysis and assessment, have made significant progresses. Thus the mathematical modeling has gradually been developed from relatively simple models to comprehensive computer-efficient mathematical models. A variety of commercial software packages were therefore employed in the simulations[2], including TOUGH2[3], TOUGHREACT, PHRE-EQC, NUFT, CHRUNCH, DUMUX[4], ChemTOUGH, GEM-GHG, CO2SINK[5], MUFTE-UG[6], ECLIPSE[7], COMSOL Multiphysics[8] and et al. Various simulations have been conducted to evaluate their capabilities concerning carbon dioxide injection into saline aquifers, enhanced oil recovery (EOR), enhanced coal-bed methane (ECBM), and carbon dioxide leakage through multilayer aquifer systems.

The most crucial point for the successful application and prediction accuracy of these simulations is adequate description of the relationships between capillary pressures and relative permeabilities to fluid saturations that characterize behaviors of multi-phase fluids flow in porous media. In numerical simulations of carbon dioxide injection into subsurface formations, precisely evaluating the migration of carbon dioxide plume is dramatically dependent upon the performances of the characteristic functions of capillary pressures and relative permeabilities to fluid saturations. In general, there are four models of capillary pressure - fluid saturation - relative permeability widely used in the simulations of carbon dioxide injection into subsurface formations[9], i.e. Brooks-Corey-Burdine model (BCB), Brooks-Corey-Mualem model (BCM), Van Genuchten-Burdine model (VGB), and Van Genuchten-Mualem model (VGM)..

Class and his co-workers [10] exploited the BCB model to solve the problem of carbon dioxide leakage through an abandoned well. Zhang and his co-workers [11] investigated the trapping mechanism of carbon dioxide injection into Songliao Basin by using the BCB model to calculate the relative permeability of the non-wetting phase and using the VGM model to calculate the relative permeability of the wetting phase under TOUGHREACT environment. To investigate the hysteretic effects in modeling geologic storage of carbon dioxide, Doughty[12] adopted a modified Van Genuchten model[13] to describe the relationship between capillary pressure and fluid saturation, and solved the problem by the software TOUGHT. The simulator TOUGHT2 was used by Giorgis and his co-workers [14] for modeling salt precipitation during the carbon dioxide injection into a depleted gas reservoir, where the BCB model was used to calculate the relative permeability of the non-wetting phase, whereas the VGB model was used to calculate the relative permeability of the wetting phase. Carbon dioxide injection into natural gas reservoirs to enhance methane production has been simulated by Seo and Mamora[15]. In their work, the BCB model was chosen in the simulations. Niessner and Helmig [16] used the VGM model to simulate contaminant migration of NAPL. Class and his co-workers [17] adopted the relative permeability function that was proposed by Fatt[18] to simulate the non-isothermal multi-phase and multi-component flow processes in porous media. Xu and his co-workers [19] used the VGM model to calculate the BCB model to calculate the relative permeability of the non-wetting phase and the relative permeability of the wetting phase to simulate carbon dioxide injection in a reservoir by considering hydraulic processes, thermal gradients and geological chemical reaction phenomena. Chen[20] developed a rapid, reproducible experimental method that yielded the information that is necessary to determine the parameters of the capillary pressure - fluid saturation - relative permeability functions in application to precisely characterizing and modeling subsurface flow in multi-phase fluid flow in soil systems.

Although successful predictions of destiny of carbon dioxide plume in subsurface formations could be crucial, there are no general agreements in choosing the models that describe the relationship of capillary pressures and relative permeabilities to fluids saturations. As mentioned above, adequate description of the relationships between capillary pressures and relative permeabilities to fluid saturations is a critical point that should be determined before modeling and simulations are carried out. Nevertheless different functions of capillary pressures-fluid saturations-relative permeabilities may lead to different results in predicting migration of carbon dioxide plume, and simulation results also vary with the parameters in the characteristic functions for different host fluids and subsurface formations systems. Hence, it is imperative to evaluate the impacts of both different models and their relevant parameters when migration of carbon dioxide plume in saline aquifers during and after injection is of interests. However, there are few comparative studies to clarify the problems so far.

The primary objective of this work is to investigate the effects of different capillary pressure-fluid saturation-relative permeability functions and the influences of the relevant parameters in the models on carbon dioxide migration during injection into saline aquifers. Therefore, this work is divided into two parts: (1) in order to exemplify the impact of the parameters in the capillary pressures-fluid saturations-relative permeabilities functions, sensitivity analysis of the parameters λ and n in the Brooks-Corey model (BC) was carried out; (2) in order to identify the impact of different models on predictions of the evolution of carbon dioxide plume in saline aquifers, a comparative study of carbon dioxide plume in saline aquifers using four well known models, i.e. Brooks-Corey-Burdine model (BCB), Brooks-Corey-Mualem model (BCM), Van Genuchten-Mualem model (VGM), Van Genuchten-Burdine model (VGB), was conducted subsequently.

2. Models of capillary pressure – fluid saturation – relative permeability

Capillary pressures usually depend upon fluid properties, wettability and structure of porous media. The relationship between capillary pressure and fluid saturation represents the static characteristic of a porous medium, whereas the relationship between relative permeability and fluid saturation denotes the hydraulic property of a porous medium. The relative permeability is, therefore, correlated with the capillary pressure by fluid saturation. Typical models include Burdine model and Mualem model[20].

In this section, four well-known models, i.e. Brooks-Corey-Burdine model (BCB), Brooks-Corey-Mualem model (BCM), Van Genuchten-Burdine model (VGB), and Van Genuchten-Mualem model (VGM), are re-visited and reviewed.

2.1. Characteristics functions of capillary pressure and relative permeability to fluid saturation

Table 1 gives the expressions of the BCB model, the BCM model, the VGB model, and the VGM model. This work focuses on these four models that are applied to carbon dioxide storage in subsurface formations, although there are also some other models, such as Leverett model[21], Lenhrd-Parker model[13]

Table 1. Models that describe the relationships between capillary pressure, fluid saturation and relative permeability

Model	Capillary pressure P_c	Relative permeability for non-wetting phase k_{rn}	Relative permeability for wetting phase k_{rw}	Parameters
BCB	$P_d S_e^{-1/\lambda}$	$(1 - S_e)^2 [1 - S_e^{1+2/\lambda}]$	$S_e^{3+2/\lambda}$	
BCM		$(1 - S_e)^\eta [1 - S_e^{1+1/\lambda}]^2$	$S_e^{\eta+2+2/\lambda}$	
VGB	$\alpha^{-1} (S_e^{-1/m} - 1)^{1/n}$	$(1 - S_e)^2 [1 - S_e^{1/m}]^m$	$S_e^2 [1 - (1 - S_e^{1/m})^m]$	$m = 1 - 2/n$
VGM		$(1 - S_e)^\eta [1 - S_e^{1/m}]^{2m}$	$S_e^\eta [1 - (1 - S_e^{1/m})^m]^2$	$m = 1 - 1/n$

The Brooks-Corey (BC) model was first used for simulating multiphase fluid flow and mass transport in unsaturated soil. The BC model is generally obtained on the basis of experimental observations that correlate capillary pressures with fluid saturations.

The capillary pressure in the BC model can be expressed as

$$p_c = p_d S_e^{-1/\lambda} \quad (1)$$

Where p_d is capillary entry pressure, which is the pressure necessary for the non-wetting phase to enter the largest pore of a porous medium. S_e denotes the effective saturation of the wetting phase, i.e. $S_e = (S_w - S_{wr}) / (1 - S_{wr} - S_{nr})$. S_w denotes the saturation of the wetting phase. S_{wr} and S_{nr} stand for the residual saturations of the wetting phase and the non-wetting phase, respectively. λ is a parameter that characterizes the pore-size distribution of a porous medium.

In contrast, the capillary pressure in the Van Genuchten (VG) model is in the form that [22]

$$p_c = \alpha^{-1} (S_e^{-1/m} - 1)^{1/n} \quad (2)$$

Where α stands for the reciprocal of capillary pressure at $S_e = 0.5$ for given m and n , which is inversely proportional to the capillary entry pressure p_d of the non-wetting fluid. The parameter n characterizes the pore size distribution of a porous medium of interest.

Table 2. Overview of relationships of capillary pressure – fluid saturation – relative permeability models adopted in simulations of CO₂ sequestration

Author	Capillary Pressure p_c	Relative Permeability for non-wetting Phase k_{rn}	Relative Permeability for wetting Phase k_{rw}	Parameter	References
Class	BC	BCB	BCB	$p_d = 1.0 \times 10^4$ Pa, $\lambda = 2$	[10, 17]
Zhang	VG	BCB	VGM	$p_0 = 1.961 \times 10^4$ Pa, $\lambda = 2$ $m = 0.457$	[11]
Pruess	VG	BCB	$k_{rw} = S_e^4$	$p_0 = 6.734 \times 10^5$ Pa, $\lambda = 2$ $m = 0.4438$	[25]
Giorgis	VG	BCB	VGB	$p_c \leq 1.0 \times 10^7$ Pa, $\lambda = 2$	[14]
Mamora	BC	BCB	BCB	$p_d = 1.0 \times 10^4$ Pa, $\lambda = 2$	[15, 26]
Bielinski	BC	BCB	BCB	(1) $p_d = 2.0 \times 10^5$ Pa, $\lambda = 2$	[26-28]
				(2) $p_d = 1.0 \times 10^4$ Pa, $\lambda = 2$	
				(3) $p_d = 1.0 \times 10^3$ Pa, $\lambda = 2$	
Niessner	VG	VG	VG	$\eta = 1/3$	[16]

Likewise, the relationships between permeabilities and fluid saturations can also be given in Table 1. Regarding simulations of carbon dioxide sequestration, different models of capillary pressure - fluid saturation - relative permeability and their parameters adopted in literatures are listed in Table 2. Obviously, both of the models and their parameters used in the literatures are different from each other. And some modified models are used for describing the relationships between capillary pressure and relative permeability. In this work, we simply restrict our attentions to the Brooks-Corey based models and Van Genuchten based models.

2.2. Relationships between capillary pressure and fluid saturation

Although the BC model and the VG model show similar behaviors, the $p_c - S_e$ curve predicted by the BC model presents discontinuity at the fully saturated region. In contrast, the capillary pressure predicted by the VG model reaches zero at the fully saturated region, as shown in Figure 1.

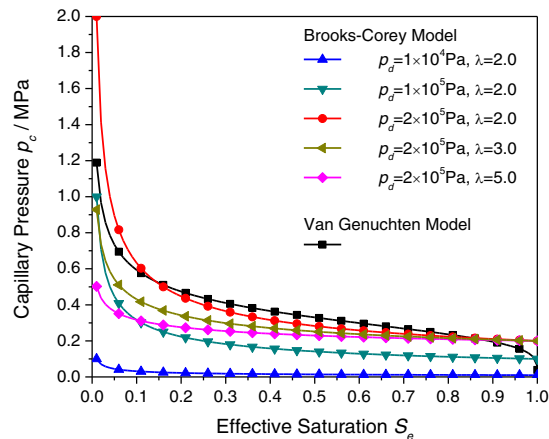


Figure 1. Relationships between capillary pressure and effective saturation

In the BC model, when λ is constant, the $p_c - S_e$ curve becomes plain when p_d is small. It implies that the smaller p_d is, the easier the wetting phase is expelled by non-wetting phase, which is carbon dioxide in the carbon dioxide and brine system. Furthermore, when p_d is constant, the larger λ is, the $p_c - S_e$ curve predicted by the BC model becomes more plain.

However, for a given porous medium, the $p_c - S_e$ curves predicted by of the BC model and the VG model are significantly different at higher saturation region. As shown in Figure 1, the capillary pressure predicted by the VG model reaches zero at the fully saturated region, whereas there exists a leap of pressure at the fully saturated region because of the capillary entry pressure p_d is taken into account in the BC model.

2.3. Relationships between relative permeability and fluid saturation

Figure 2 shows the relationships of relative permeabilities of wetting phase and non-wetting phase with the effective saturations, which are calculated by the BC and VG models, respectively. For the BC model, there is a parameter η , which characterizes the tortuosity of a porous medium. In fact, it may differ for the wetting and non-wetting fluids in practice [23]. We chose the parameter η equal to 0.5 for both of the wetting and non-wetting phases in the calculations.

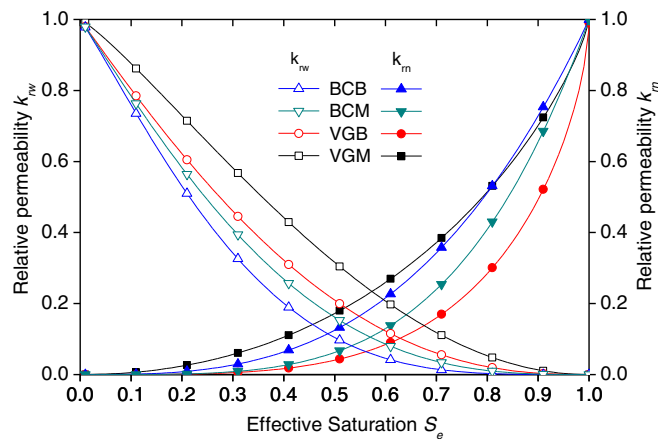


Figure 2. Relationships between relative permeability and effective saturation

It can be seen that the relative permeabilities of wetting phase calculated by the VGM model are always larger than those of the other models, whereas the relative permeabilities of wetting phase calculated by the BCM model are the smallest. Moreover, at the higher saturation region, the relative permeabilities of the non-wetting phase calculated by the VGM and BCB model are the largest, whereas at the lower saturation region, the relative permeabilities of the non-wetting phase calculated by the VGM model are highest, and the relative permeability of the non-wetting phase calculated by the VGB model are the smallest.

3. Mathematical model for carbon dioxide injection into a saline aquifer

3.1. Physical model and simplifications

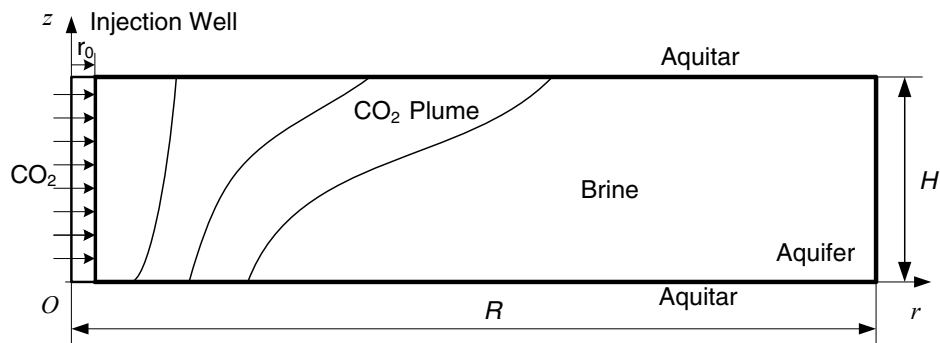


Figure 3. Schematic of CO₂ injection into a confined aquifer

Consider that carbon dioxide is injected into a saline aquifer confined by two parallel aquitars through an injection well with radius r_0 , as shown in Figure 3. The axisymmetric computational domain is taken on the $r-z$ plane of a cylindrical coordinate system. The radial distance of the horizontal aquifer is R with a constant thickness of H . The following assumptions and simplifications are made:

- The injected carbon dioxide is at supercritical state within the entire computational domain;

- In the saline aquifer, carbon dioxide and brine are immiscible phases, and the effect of mutual dissolution is neglected;
- The saline aquifer is a homogeneous porous medium;
- The properties of fluids, such as density and viscosity, are constant.

3.2. Governing equations – Continuity and momentum equations

The governing equations in the general form for two-phase fluids flow in porous media are written as:

Continuity equation

$$\phi \frac{\partial(\rho_i S_i)}{\partial t} + \nabla \cdot (\rho_i \mathbf{u}_i) = 0, \quad i = n, w \quad (3)$$

Momentum equation

$$\mathbf{u}_i = -\frac{k_{ri} \mathbf{K}}{\mu_i} (\nabla p_i + \rho_i \mathbf{g}), \quad i = n, w \quad (4)$$

Where ϕ is the porosity; ρ_i is the density ($\text{kg}\cdot\text{m}^{-3}$); S_i is the saturation; \mathbf{u}_i is the velocity vector ($\text{m}\cdot\text{s}^{-1}$); t is time (s); k_{ri} is the relative permeability; \mathbf{K} is the intrinsic permeability tensor (m^2); μ_i represents the dynamic viscosity ($\text{Pa}\cdot\text{s}$); p_i denotes pressure (Pa); \mathbf{g} is the acceleration due to gravity ($\text{m}\cdot\text{s}^{-2}$); the subscripts w and n denote the wetting and non-wetting fluid, respectively. For the displacement process of a carbon dioxide and brine system in a confined saline aquifer, CO_2 is the non-wetting phase, whereas brine is the wetting phase.

The capillary pressure is equal to the pressure difference between the non-wetting and wetting phases

$$p_c = p_n - p_w \quad (5)$$

The summation of the saturations of the two phases in the saline aquifer satisfies

$$S_w + S_n = 1 \quad (6)$$

3.3. Initial and boundary conditions

The initial conditions and the boundary conditions for each phase are as follows.

Initial conditions are:

for non-wetting phase

$$p_n|_{t=0} = \rho_w g(H-z) + p_d \quad (7)$$

for wetting phase

$$p_w|_{t=0} = \rho_w g(H-z) \quad (8)$$

Boundary conditions are:

for non-wetting phase

$$\mathbf{u}_n|_{r=r_0} = u_0 \quad (9)$$

$$\mathbf{u}_n|_{z=0} = 0, \mathbf{u}_n|_{z=H} = 0 \quad (10)$$

$$p_n|_{r=R} = \rho_w g(H-z) + p_d \quad (11)$$

for wetting phase

$$\mathbf{u}_w|_{r=r_0} = 0, \mathbf{u}_w|_{z=0} = 0, \mathbf{u}_w|_{z=H} = 0 \quad (12)$$

$$p_w|_{r=R} = \rho_w g(H-z) \quad (13)$$

3.4. Solution method

In order to investigate the behaviors of the four characteristic functions with respect to the evolutions of carbon dioxide plume migration in a confined saline aquifer, we solved the aforementioned equations with the corresponding initial and boundary conditions to obtain the saturation distributions of carbon dioxide. The

computations were performed by using a finite element method-based commercial software package COMSOL Multiphysics 3.5a.

In the simulations, we defined the two-phase flow equations by the general form of PDE modes. The mapped meshes consisting of triangle elements were adapted to extremely fine. The solver UMPACK was selected. And the relationships of capillary pressure and relative permeability to fluid saturation were adopted in the simulations as listed in Table 2. The relevant parameters used for the simulations are given in Table 3. The injection durations simulated were up to a hundred years.

Table 3. Properties and operational conditions in the simulations

Parameters	Symbol	Value	Unit
aquifer			
aquifer thickness	H	30	m
intrinsic permeability	K	2.039×10^{-14}	m^2
porosity	ϕ	0.15	
CO ₂			
density	ρ_n	479	$\text{kg} \cdot \text{m}^{-3}$
viscosity	μ_n	3.95×10^{-5}	$\text{Pa} \cdot \text{s}$
brine			
density	ρ_w	1045	$\text{kg} \cdot \text{m}^{-3}$
viscosity	μ_w	2.54×10^{-4}	$\text{Pa} \cdot \text{s}$
gravitational acceleration	g	9.82	$\text{m} \cdot \text{s}^{-2}$
operation parameters			
injection rate	Q_{well}	1600	$\text{m}^3 \cdot \text{day}^{-1}$
injection well radius	r_0	0.15	m

4. Parametric analysis on Brooks-Corey based mode for predicting carbon dioxide plume migration in a confined saline aquifer

In this section, a comprehensive sensitivity analysis was conducted to investigate the primary parameters in the relationships of capillary pressure and relative permeability to fluid saturation that dominate carbon dioxide plume migration in a confined saline aquifer. The Brooks- Corey based model is taken as an example case, in which the parameters, p_d , λ , and η , are involved.

4.1. p_d – Capillary entry pressure

In the BC model, the parameter p_d is the capillary entry pressure characterizing the pressure that is necessary for the non-wetting fluid entering the largest pore of porous media. When the other parameters in the model are constant, the smaller the capillary entry pressure p_d is, the more gentle the capillary pressure - fluid saturation curve is, as shown in Figure 1.

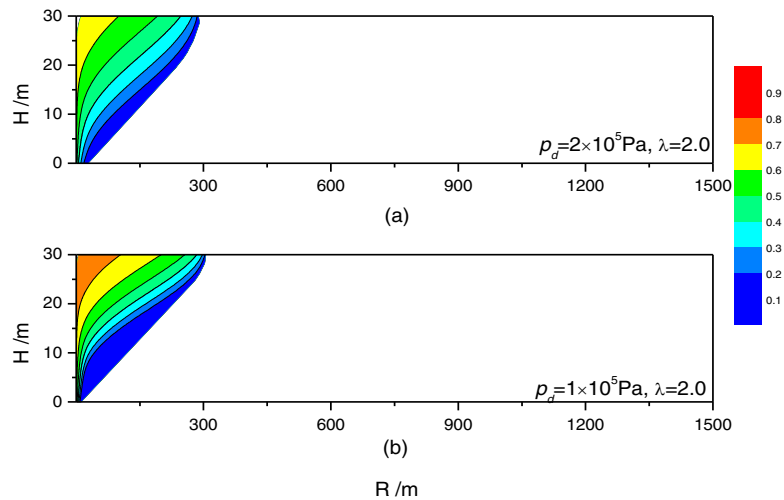


Figure 4. CO₂ saturation distributions for different p_d after 10 years injection

With regard to the simulations of carbon dioxide injection into the saline aquifer, different capillary entry pressures were chosen to observe the evolutions of carbon dioxide plume. Figure 4 shows the saturation distributions of carbon dioxide after 10 years injection at the conditions that $p_d = 2 \times 10^5$ Pa and $p_d = 1 \times 10^5$ Pa [24]. It is readily to seen that the lower p_d is, the larger the saturations of carbon dioxide around the injection well will be although the coverage of the carbon dioxide plumes in the aquifer is similar.

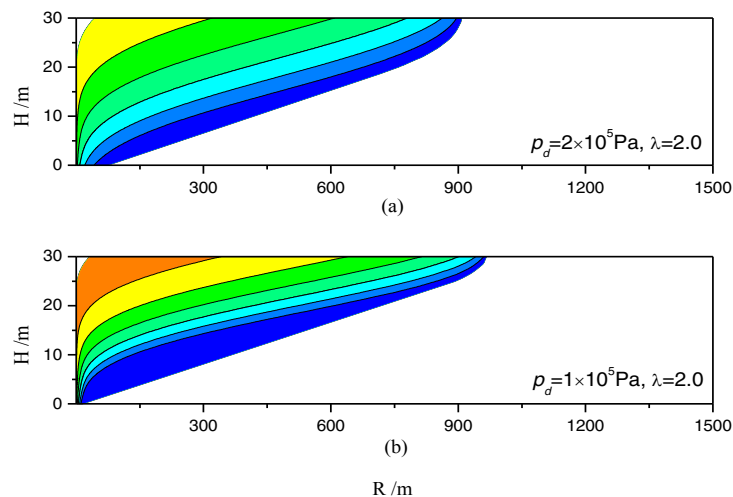


Figure 5. CO₂ saturation distributions for different p_d after 100 years injection

As to a long-term injection, 100 years, for example, the saturation distributions of carbon dioxide are present in Figure 5, where the same capillary entry pressures were chosen in the simulations. It can be seen from Figure 5 that

the trend becomes apparent that the lower p_d is, the larger the saturations of carbon dioxide near the injection well and at the upper part of the aquifer will be. The difference will become much more remarkable as time elapsed. It also presents that when p_d is lower, the carbon dioxide plume tends to move upward in the saline aquifer. Hence, it implies that when p_d is lower, carbon dioxide can be easily injected into the saline aquifer, the carbon dioxide plume, however, tends to accumulate around the injection well and move along the upper region of the aquifer. In contrast, when p_d is higher, carbon dioxide is much easier to be trapped in the aquifer, and the saturation distribution of carbon dioxide is more uniform when compared with the case of lower capillary entry pressure. For the estimation of the storage capacity of the aquifer, it implies that the aquifer can be utilized much more efficiently as the capillary entry pressure is higher.

4.2. λ – Parameter related to pore size distribution

In the BC model, the parameter λ characterizes the pore-size distribution of a porous medium. In general, a smaller value means a heterogeneous porous aquifer, $\lambda = 0.2$, for example, whereas a large value represents a homogeneous porous aquifer, $\lambda = 3$, for example.

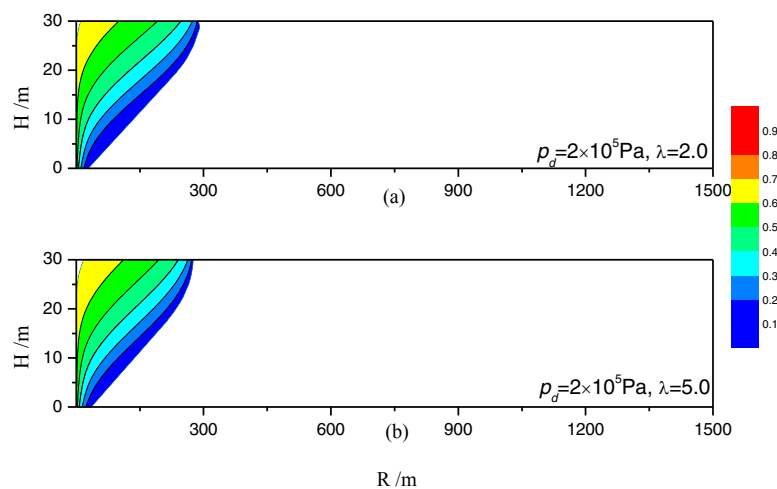


Figure 6. CO₂ saturation distributions for different λ after 10 years injection

With regard to the simulations of carbon dioxide injection into the saline aquifer, different λ was chosen to observe the evolutions of carbon dioxide plume. Figure 6 and Figure 7 show the saturation distributions of carbon dioxide after 10 years and 100 years injection at the conditions that $\lambda = 2$ and $\lambda = 5$, respectively. It can be seen that the saturation distributions of carbon dioxide in the same location of the aquifer do not apparently vary with the different λ , and the coverage of the carbon dioxide plumes in the aquifer is similar. Subsequently, the parameter λ has little effects on the migration of carbon dioxide in the aquifer. Furthermore, it should be noted that the saturations of carbon dioxide near the injection well are not very high, ranging from 0.6 to 0.7 under the given conditions in the simulations. Thus, it implies that the influence of the parameter λ could be overlooked if the exact values of the parameter are difficult to obtain or the information is not available. It would not incur a significant bias when different values of λ are applied to predictions on the evolutions of the carbon dioxide plume.

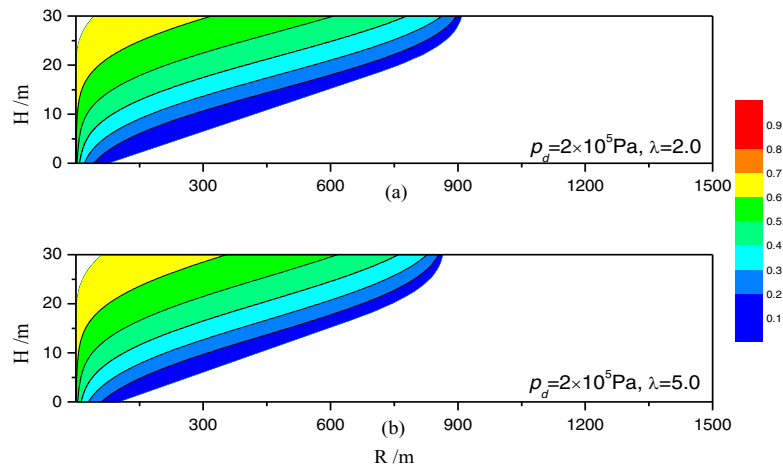


Figure 7. CO₂ saturation distributions for different λ after 100 years injection

4.3. η – Parameter related to tortuosity ratio

The BCB model discriminates against the BCM model only by the parameter η , which is related to a tortuosity ratio of a porous medium. In an immiscible two-phase flow in a porous medium, the parameter η for wetting and non-wetting fluids could be different in practice. For the convenience of comparison in the simulations of carbon dioxide injection, the same value of η for both of the wetting and non-wetting phase was chosen.

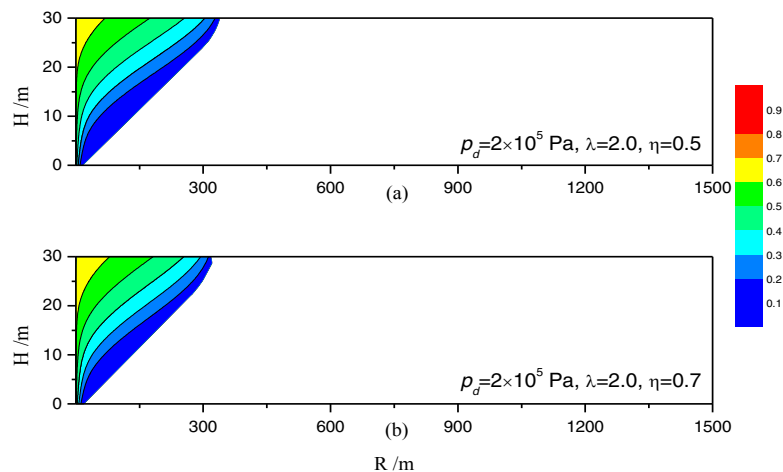


Figure 8. CO₂ saturation distributions for different η after 10 years injection

Figure 8 presents the saturation distributions of carbon dioxide plume after 10 years injection at the conditions

that $\eta = 0.5$ and $\eta = 0.7$. It can be seen that the patterns of carbon dioxide plumes are approximately the same with the different values of η . As the duration of injection is prolonged, Figure 9 shows that the main body of the carbon dioxide plumes is little affected, although the values of η change from 0.5 to 0.7. And the carbon dioxide plume scatters over a limited larger area when the value of η is larger. Thus, the saturation distribution of carbon dioxide is insensitive to the parameter η .

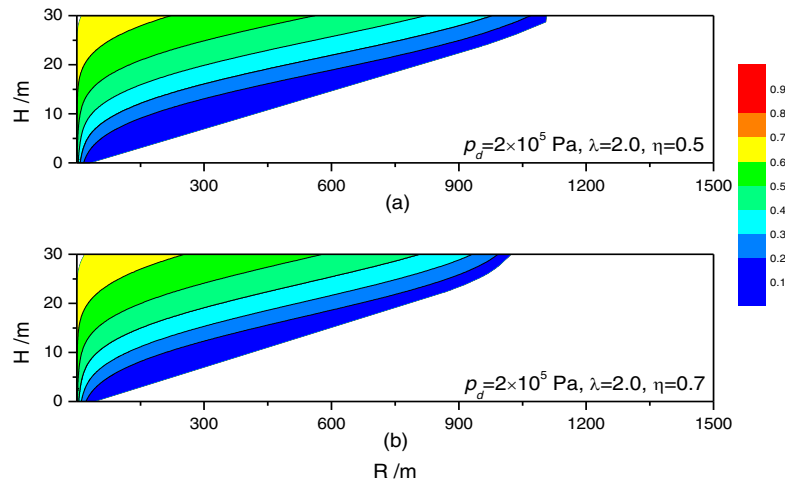


Figure 9. CO₂ saturation distributions for different η after 100 years injection

5. Analysis of carbon dioxide plume migration in a saline aquifer by using BCB, BCM, VGB and VGM models

In order to investigate the effects of different capillary pressure – fluid saturation – relative permeability models on the simulations, in this section, simulations of carbon dioxide injection into the saline aquifer in a short-term and a long-term are performed by using the BCB, BCM, VGB and VGM models. The properties and operational conditions in the simulations are given in Table 3, and parameters used are listed in Table 4.

Table 4. Parameters used in simulations

Model	Parameter	Value
Brooks-Corey Model	p_d	2×10^5 Pa
	λ	2.0
Van-Genuchten Model	α	3.3×10^{-6} Pa ⁻¹
	n	4.367
Residual Saturation	S_{wr}	0.05
	S_{nr}	0.05

Figure 10 presents the saturation distributions of carbon dioxide in the saline aquifer after 10 years injection, in which the BCB, BCM, VGB and VGM models are used to calculate the capillary pressures and relative permeabilities. It appears that the carbon dioxide plume predicted by the VGM model spreads broader than those of the others. Hence, the saturations of carbon dioxide around the injection well are smallest although the same amount of carbon dioxide is injected into the aquifer. In contrast, the saturations of carbon dioxide around the injection well

predicted by the BCB model are the largest. It should also be noted that the migration distance of carbon dioxide plume predicted by the VGB model is practically the farthest. Besides, the area occupied by carbon dioxide saturations less than 0.1 is also the largest.

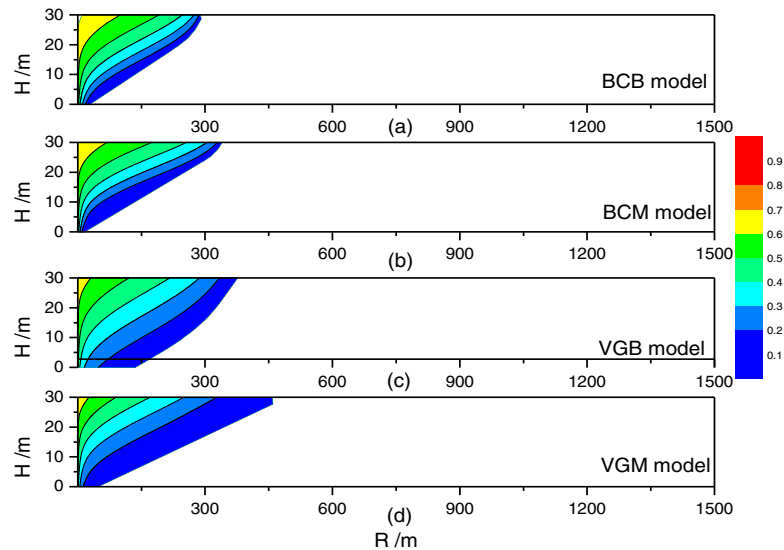


Figure 10. CO₂ saturation distributions after 10 years injection simulated by the BCB, BCM, VGB and VGM models

After 100 years injection, as shown in Figure 11, the invading area of carbon dioxide predicted by the VGM model is still the largest, and the VGB model is at the secondary place. Again, the saturations of carbon dioxide around the injection well are higher no matter which model is used to predict the evolution of carbon dioxide plume. Furthermore, a point worthy of note is that the leading edges of carbon dioxide plume predicted by the VGM model and the VGB model go farther, and most of the area occupied by carbon dioxide holds lower saturations.

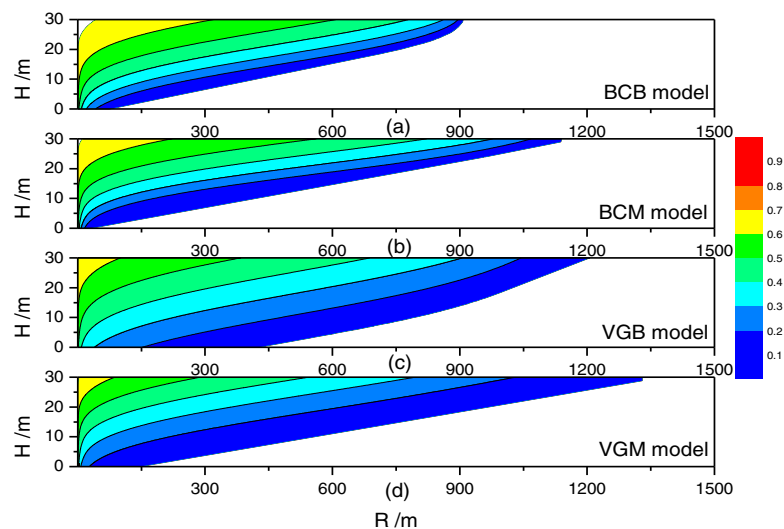


Figure 11. CO₂ saturation distributions after 100 years injection simulated by the BCB, BCM, VGB and VGM models

The aforementioned simulation results reveal that the relationships of the capillary pressure and relative permeability to fluid saturation and the selections of their parameters should be paid sufficient attention in simulations, especially for evaluations of storage capacity and storage efficiency of carbon dioxide in saline aquifers through simulations. In this context, the storage efficiency of a saline aquifer to trap carbon dioxide and the storage capacity of carbon dioxide in the saline aquifer could be overestimated through predictions by using the BCB model, and they could be underestimated by using the VGM model. Nevertheless, it is much safer to calculate the storage capacity of carbon dioxide based on the VGM model. On the other hand, for evaluations of potential leakage of carbon dioxide in saline aquifers, where the movement of the leading edges of carbon dioxide plume is monitored, the VGM model is still a reasonable choice in simulations, and the fronts of carbon dioxide plume predicted by the BCB and BCM models may lag behind the leading edge of carbon dioxide plume in reality.

6. Concluding remarks

Effective assessments of storage capacity and environmental safety of carbon dioxide geological sequestration into subsurface formations have been intimately dependent upon the development of mathematical modeling and simulation techniques. Although simulations of the evolutions of carbon dioxide plume in subsurface formations have been extensively undertaken, the performances of different characteristic functions that describe the relationships of capillary pressures and relative permeabilities to fluids saturations have been paid insufficient attentions. Subsequently, the influences of different models and their relevant parameters on the predictions need to be identified further.

In this paper, the effects of the relationships of capillary pressures and relative permeabilities to fluids saturations on predictions of carbon dioxide plume migration in confined saline aquifers were investigated through an immiscible displacement model for carbon dioxide and brine system, where four commonly used models, including the BCB, BCM, VGB and VGM models, were taken into consideration. Parametric analysis was conducted to illustrate the influences of parameters in the BC model on simulations. Moreover, a comparative study was conducted based on the BCB, BCM, VGB and VGM models to reveal the different behaviors of the four models with respect to the prediction of carbon dioxide migration in confined saline aquifers.

In order to investigate the influences of parameters in the models, the Brooks-Corey model was taken to exemplify the impact of the parameters in the capillary pressures-fluid saturations-relative permeabilities functions on the predictions of carbon dioxide plume migration in the confined saline aquifer. Parametric analysis of the parameters p_d , λ and η in the model shows that the parameters of λ and η in the model have little effects on predicting the evolutions of carbon dioxide plume in the confined saline aquifer. However, the saturation distributions of carbon dioxide are drastically sensitive to p_d . It indicates that the lower the capillary entry pressure p_d is, the larger the saturation of carbon dioxide around the injection well will be. Moreover, at a constant injection rate, the carbon dioxide plume tends to migrate upward, and the leading edge of the carbon dioxide plume reaches farther. Therefore, these results imply that the characteristic parameters related to the capillary entry pressure of subsurface formations should be measured carefully in order to precisely predict the evolutions and patterns of carbon dioxide plume in saline aquifers. In the course of simulations, appropriate estimations of the parameters of λ and η in reasonable ranges for a specific saline aquifer will not necessarily mean the significant differences in the predictions of the evolutions and patterns of carbon dioxide plume.

The simulation results demonstrate that different relationships between capillary pressure relative permeability to fluid saturation may cause significant influences on the carbon dioxide distributions at the regions around the injection well and at the leading edges of carbon dioxide plume that is far away from the injection well. These results have significant implications when simulations results are utilized to assess the storage capacities of saline aquifers and to evaluate the potential risks of leakage. For the assessment of storage capacity and storage efficiency of a saline aquifer for carbon dioxide sequestration, the storage capacity of carbon dioxide in the saline aquifer could be overestimated through predictions by using the BCB model. Nevertheless, it is much safer to estimate the storage capacity of carbon dioxide based on the VGM model. On the other hand, for the evaluations of potential leakage of carbon dioxide in a specific saline aquifer, the movements of the leading edge of carbon dioxide plume should be attached more importance. Under these circumstances, the BCB and BCM model may underestimate the movement of the leading edge of carbon dioxide plume. It will be safe to predict the advance of leading edge by the VGM

model. It should also be pointed out that for numerical simulations of carbon dioxide injection into a specific saline aquifer, of course, the models that describe the relationships of capillary pressure and relative permeability to fluid saturations need to be validated if the experimental data on capillary pressure and relative permeabilities are available.

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