Reservoir Simulation of CO_2 Sequestration in Brine Formation

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Abstract

Considering the long-term and slow processes of CO_2 sequestration in brine formation, it is hard to systematically investigate the underlying mechanisms of CO_2 sequestration in a saline aquifer with bench-scale experiments. In this work, simulation research of CO_2 sequestration in a real saline aquifer was proposed and conducted to investigate the effects of CO_2 injection on the formation and to reveal the mechanisms of CO_2 sequestration. To be specific, the simulation of CO_2 sequestration was carried out with both a homogeneous model and a heterogeneous model. The former model aimed to investigate the effect of CO_2 injection rate on the reservoir conditions and the formation properties. The latter one focused on unveiling the impacts of heterogeneity of formation properties and geological structure, two critical inherent properties of the real saline aquifer, on CO_2 distribution and trapping. The results show that the distribution of pH was affected by the distance to the injector, geological structure, and heterogeneity of permeability. The lowest pH, which was controlled by the maximum formation pressure and corresponding solubility of CO_2, can be found in the location of the CO_2 injector. The porosity changes caused by the reaction with solid minerals in both two models were relatively small after 30 years of CO_2 injection. Meanwhile, the maximum formation pressure was undisputedly located at the CO_2 injector. Then, the formation pressure will gradually decrease with an increase in the distance to the injector satisfying a power function.

Introduction

Due to an increase in consumed amounts of fossil fuels, the content of CO_2 in the atmosphere has risen gradually, which inevitably leads to a serious greenhouse effect on a global scale. How to reduce carbon emissions, while ensuring economic development, has become one of the most important challenges that every country faces. Carbon capture and storage (CCS) is a technology that separates, collects, and compresses CO_2 gas from industrial emissions, and then injects it into places under suitable storage conditions to isolate it from the atmosphere for long-term storage (Rashidi et al. 2020). According to the IEA Report, the contribution of CCS to reducing CO_2 emissions will increase from 3% in 2020 to 10% in 2030 and a further 19% in 2050, making it one of the most attractive technologies to reduce carbon dioxide emissions (Zhao and Liu 2019; James 2020; Li and Qin 2017). CCS mainly includes geological storage, marine storage, mineral storage, ecological storage, and industrial utilization (Liu 2017). Among them, CO_2

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geological sequestration has been of interest to researchers and industries owing to the effectiveness and low cost of reducing CO_2 emissions. The storage sites mainly include deep saline layers, abandoned oil and gas reservoirs or those under development, and unexploitable coal seams. Among them, CO_2 sequestration in the deep underground saline layer has become the most promising CO_2 geological sequestration technology due to its advantages, such as a large volume, a long storage time, and wide distribution of storage sites (Yang 2010; Ma 2010). Therefore, it is pragmatic and theoretical importance to investigate the CO_2 flow behavior and the corresponding effect on the saline aquifer.

The following conditions are commonly required for a success CO_2 sequestration in a saline aquifer (Bentham and Kirby 2005; Zhang et al. 2011; Lee et al. 2012; Chen and Li 2015): (1) a tight cap rock of the saline aquifer, i.e., an impermeable cap rock; (2) a high injectivity of the saline aquifer, i.e., a sufficient capacity to store large. Meanwhile, the mechanisms of CO_2 sequestration in saline aquifer mainly involves four processes: structural sequestration, residual gas sequestration, dissolution sequestration, and mineralization sequestration. These mechanisms, on one hand, improve the sequestration of CO_2 in the formation. However, on the other hand, it will result in (1) an increased formation pressure, (2) a dynamic formation property (porosity and permeability), and (3) a weakened rock strength (Agofacek et al. 2019; Veer et al. 2015; Al-Khdheeawi et al. 2020). All those mechanisms will lead to issues of sealing ability and stability of caprock to some extent because of the reaction between injected CO_2 and formation minerals as well as the potential migration of CO_2 in the caprock.

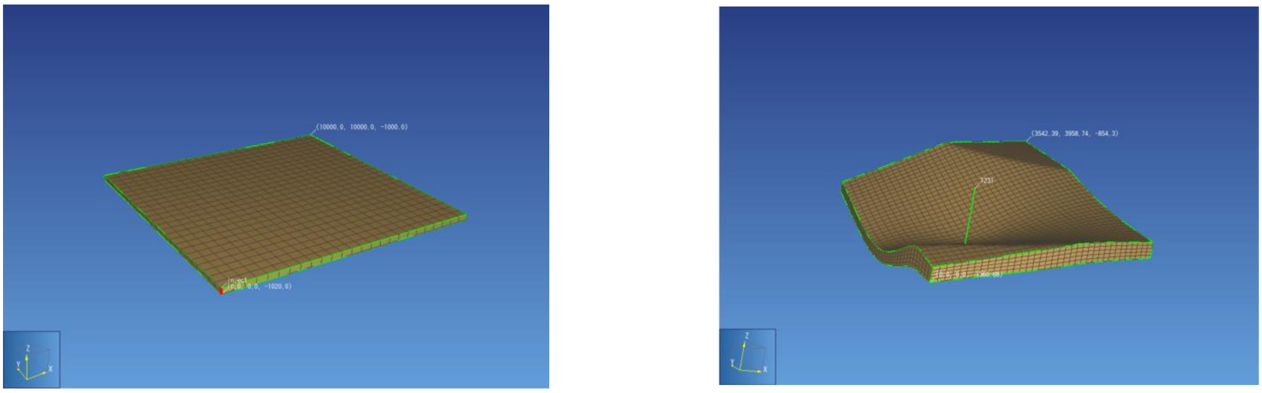
To maintain stable and safe storage and avoid a possible and dangerous leakage, a long-term safety sequestration of CO_2 saline sequestration should be conducted considering that the migration processes of CO_2 and chemical reaction between CO_2 and mineral components of rock is actually quite long and slow process (Zhang 2018; Yu et al. 2015; Winkler et al. 2010; Agofack et al. 2019). Therefore, the numerical simulation is a pragmatic and effective method to assess the above-mentioned long-term CO_2 storage in saline aquifers, especially, compared with bench-scale experimental research (Brantley 2015). In 2011, Tosha (2013) conducted a research aiming to examine the effect of injected CO_2 collected from the refinery on the stability of geological structure of the aquifer via the numerical simulation technique. Ma (2013) took the CO_2 geological sequestration layer in the Ordos Basin demonstration area as the research object and carried out the numerical simulation of carbon dioxide geological sequestration located in the Ordos basin, China. The influence of formation permeability, injection rate, temperature, and cap on formation pressure and mole fraction distribution of CO_2 were calculated and discussed.

In this work, a homogeneous and a heterogeneous simulation model were established to numerically mimic the CO_2 sequestration during a CO_2 injection process lasting for 30/40 years. The effects of three factors, including CO_2 injection rate, amounts of CO_2 injection, and the heterogeneity of saline aquifer on the CO_2 storage, were systematically investigated. Specifically, three parameters, including pH, porosity, and formation pressure, were calculated and analyzed to examine the influences of the above-mentioned three factors on CO_2 sequestration. The results show that the changes in porosity were very slight. The geological structure, heterogeneity of permeability, and CO_2 injection rate imposed a great effect on the formation pressure and pH.

Numerical Simulation Model

Homogeneous model. To investigate the effect of CO_2 injection on the saline aquifer, a CO_2 storage mechanism model was established and shown in **Figure 1a**. Before the CO_2 injection simulation, the initial conditions were analyzed according to the actual situation as shown in **Table 1** (as homogeneous model). The initial formation pressure was 9.6MPa, the initial temperature was 26°C. The porosity and permeability were 0.15 and 2 mD, respectively. The salt mass fraction was 0.05. The sizes of x, y and z directions are 10000m, 10000m and 20m, respectively. Also, the top layer depth of the formation is 1000m. The total number of grids is 625, the injection well is the origin of the model coordinates, the injection rate is unchanged, and the influence of CO_2 on the reservoir at different times was observed.

Heterogeneous model. The geological and physical properties were collected from a saline aquifer located in Xinjiang, China. The initial pressure and temperature were 12.5 MPa and 30 °C, respectively. The average porosity was 5.4%. The salt mass fraction was 0.00253 according to the water analysis report. The length and width of the model block were set as 3600m and 4000m. The average formation thickness was around 40m. The average grid sizes of x, y, and z directions were 100m, 100m, and 10m, respectively. A total of 5760 grids (36×40×4) were involved in the model (**Figure 1b**). **Table 1** also presents the main input parameters for the heterogeneous simulation model.



(a) Homogeneous (b) Heterogeneous

Figure 1—Reservoir model by simulation.

Table 1—Parameters of carbon dioxide-water-rock model

Parameter	Homogeneous model	Heterogeneous model
Formation thickness, m	20	40
Average permeability, mD	2	1.4
Average porosity	0.15	0.054
Coefficient of compressibility, Pa^{-1}	4.5×10^{-10}	$4.5\times10^{-10}pa^{-1}$
Temperature, °C	26	30°C
Pressure, MPa	9.6	10MPa
Salinity, mg/l	0.06	0.00253

Results and Discussion

During the entire simulation process, CO_2 was injected into the reservoir at a constant rate, 10 tons/d for the homogeneous model and 3, 4, and 5 tons/d for the heterogeneous model. Three parameters, including pH, formation pressure, and porosity, strongly related to the safety and effectiveness of CO_2 sequestration were calculated and analyzed to assess the dynamic effect of CO_2 injection on the saline aquifer.

PH. *Homogeneous model.* The pH value of the near wellbore zone decreased rapidly in the first year, which decreased from 7.88 to 5.73, in the near wellbore region. After that, the decline rate of pH gradually slows (**Figure 2**). To be specific, the pH of near wellbore zone was around 4.91 after a constant-rate CO_2 injection of 40 years (**Figure 3**). Meanwhile, one can find that the area with a decreased pH compared with the original pH gradually expanded with an increase in the amount of injected CO_2 or injection time (**Figure 4**). The reason is that minimum pH was dominated by the solubility of CO_2 in the formation water. Generally, the higher solubility of CO_2 in water, the higher pH becomes. In other words, once the maximum solubility reaches under a certain condition (formation pressure and temperature), the pH of the formation fluids will get the smallest value, then be a constant due to the unchanged solubility of CO_2.

Noted that the pH (4.90) of 20 years is slightly lower than that (4.91) of 40 years. The difference between the values was caused by the chemical reaction between the H^+ and mineral components of rock.

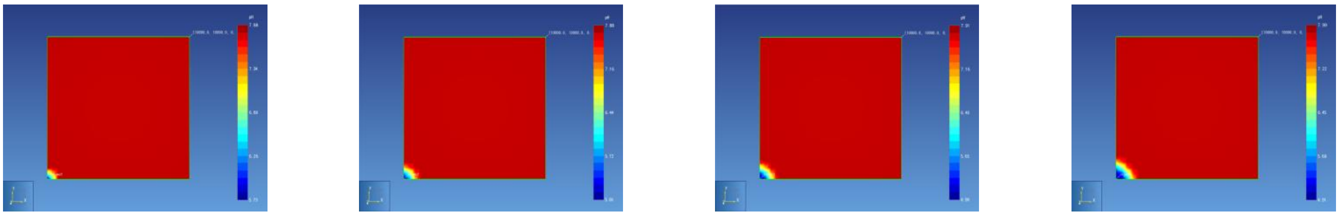

1 year
10 years
20 years
40 years

Figure 2—The pH 2D distribution of homogeneous model at different times.

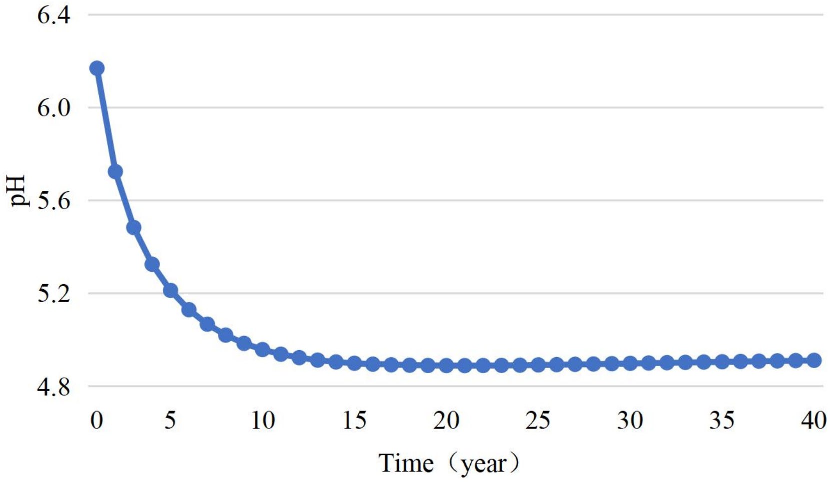


Figure 3—pH of injector at different times.

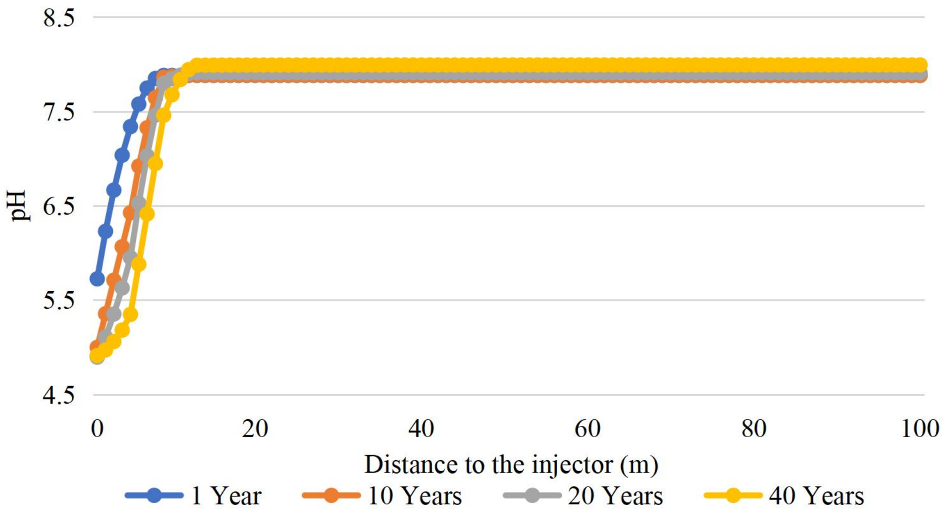
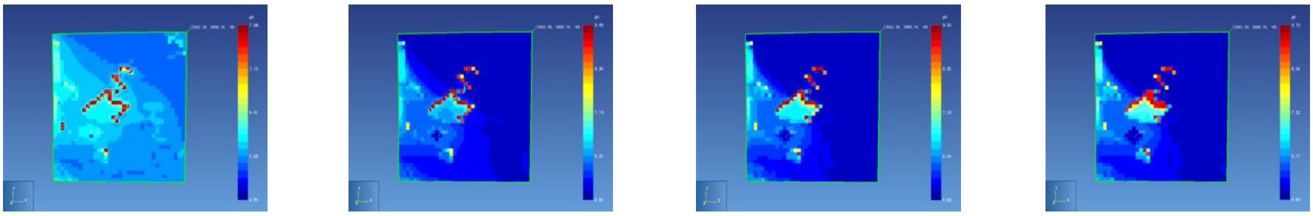


Figure 4—Sectional pH distribution.

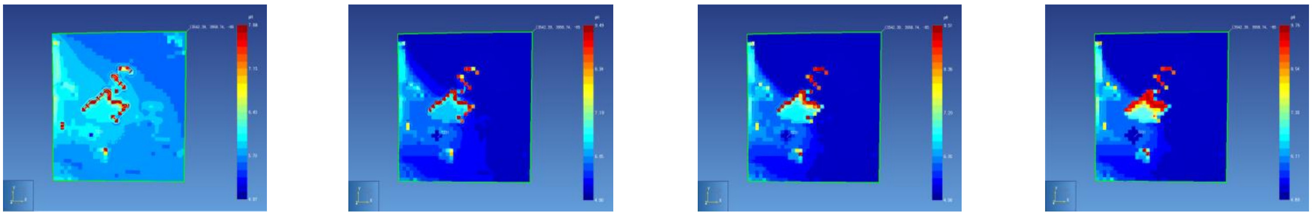
Heterogeneous model. **Figure 5** shows the pH distribution at different injection stages (1, 10, 20, and 30 years) with injection rates of 5, 4, and 3 tons/d. Compared with the pH distribution of the homogeneous model, the pH distribution of the heterogeneous model looks much more complicated. It seems that the pH distribution does not follow the rules that pH gradually increases with an increase in the distance to the well location. Based on Figure 5, the lowest pH is mainly found in the upper right part of the model. Then, the several red points mean the highest pH in the center part of the model. The mechanisms behind such distribution are that the upper right part of the model is the high part of the geological structure, i.e., a low buried depth. Once the $ScCO_2$ is injected into the formation, the CO_2 migrates to the higher part of the geological structure with aid of the buoyancy. Consequently, the reaction between $ScCO_2$ and brine taking place in the zone affected by the migration generates H^+, and consequently, a low pH value of rock.

As shown in **Figure 6**, with CO_2 injection, the wellhead pH changes significantly and the pH near the wellhead decreases as well. The main reason for the rise of pH value in some areas is that carbonate dissolution consumes more H^+ formed by CO_2 dissolved in water.



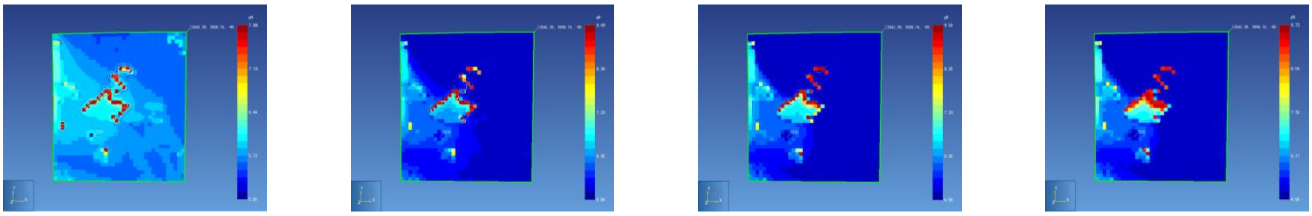
1 year 10 years 20 years 30 years

(a) 5 tons/d



1 year 10 years 20 years 30 years

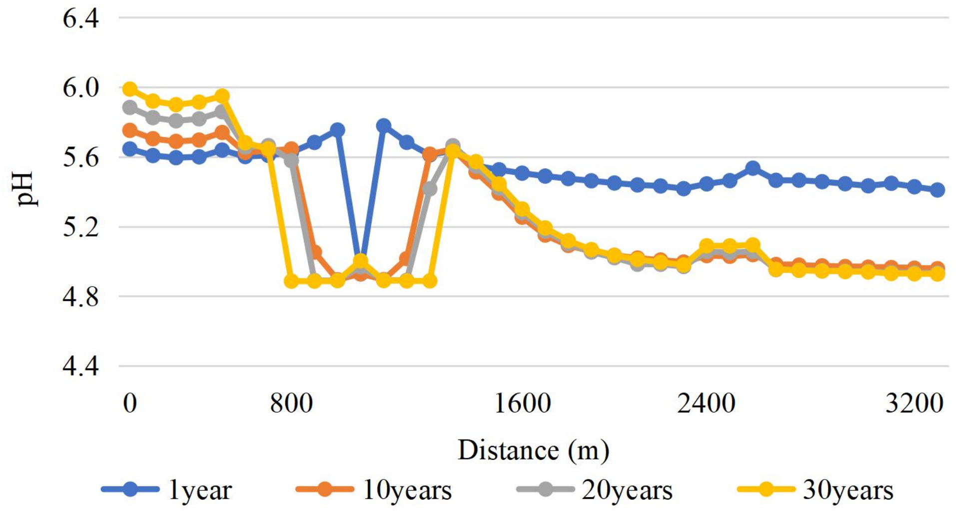
(b) 4 tons/d



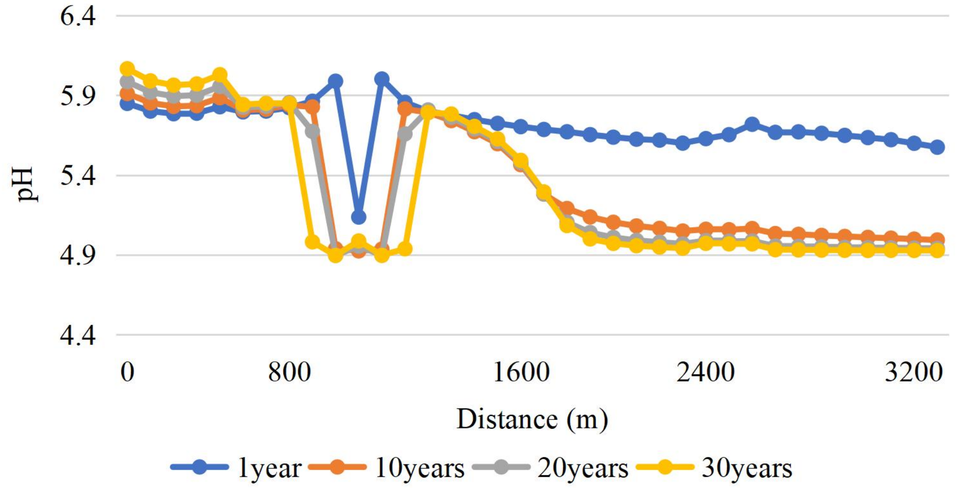
1 year 10 years 20 years 30 years

(c) 3 tons/d

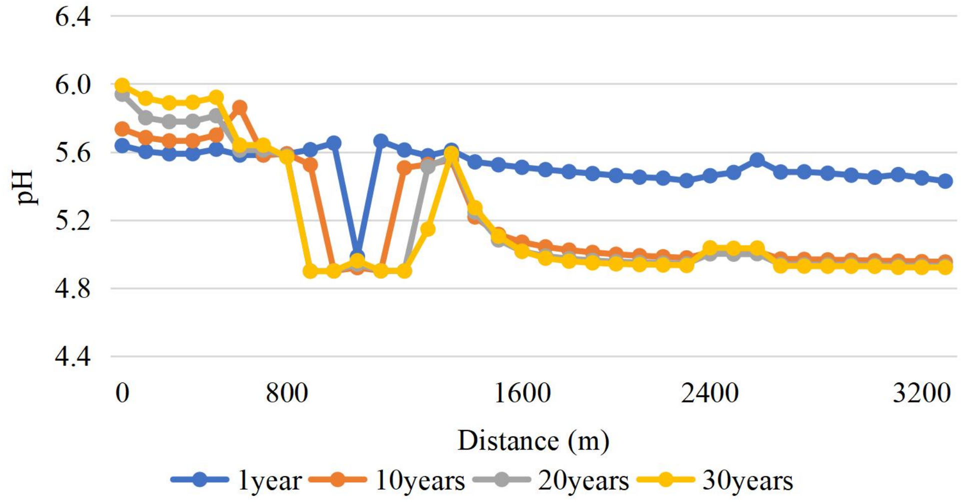
Figure 5—2D pH distribution of heterogeneous model with different injection rates.



(a) 5 tons/d



(b) 4 tons/d



(c) 3 tons/d

Figure 6—The sectional pH distribution with different injection rates.

Formation Pressure. *Homogeneous model.* The injection of supercritical CO_2 undoubtedly would increase the formation pressure and disequilibrate the original state, which imposes a certain impact on the stability of the formation. Apparently, it will be imperative to quantitatively evaluate the impact of the increased formation pressure considering the potential leakage of injected CO_2.

Figure 7 shows the formation pressure distributions with time proceeding at a constant injection rate of 10 tons/d. It can be observed that the reservoir pressure is increased evenly in the horizontal direction from the injection point. Firstly, the pressure at the injection point is the highest during the entire process, with a bottom-hole pressure of 13.7 MPa in the first year, an increase of 4.1 MPa from the initial formation pressure. When the injection time has reached 40 years, and the pressure at the injection point has increased to 23.1 MPa, much larger than the initial pressure of 9.6 MPa.

Secondly, due to an increase in reservoir pressure caused by a continuous CO_2 injection, a high-pressure area with a peak pressure located at the injector position, and pressure gradually decreased to the initial formation pressure with an increase in the distance to the injector. The relationship between the distance to the wellbore and the formation pressure is depicted in **Figure 8**, which actually can be quantified with a logarithm function. The longer the injection time of CO_2 is, the larger the high-pressure area becomes. Figure 8 also indicates the pressure changes from the wellhead location at different times after CO_2 injection. As CO_2 increases, the pressure increases and spreads over a wider area.

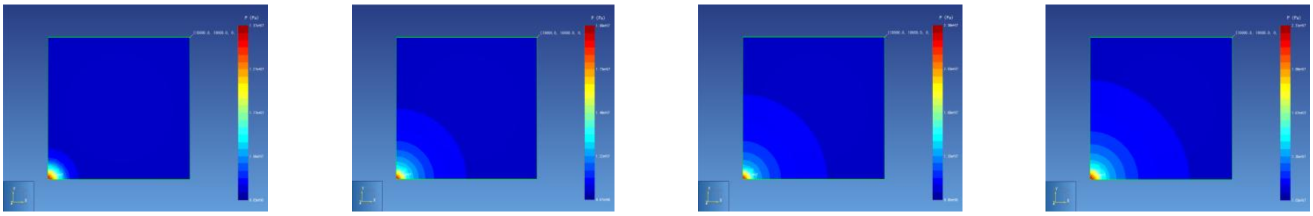

1 year 10 years 20 years 40 years

Figure 7—The formation pressure distributions of homogeneous model at different times.

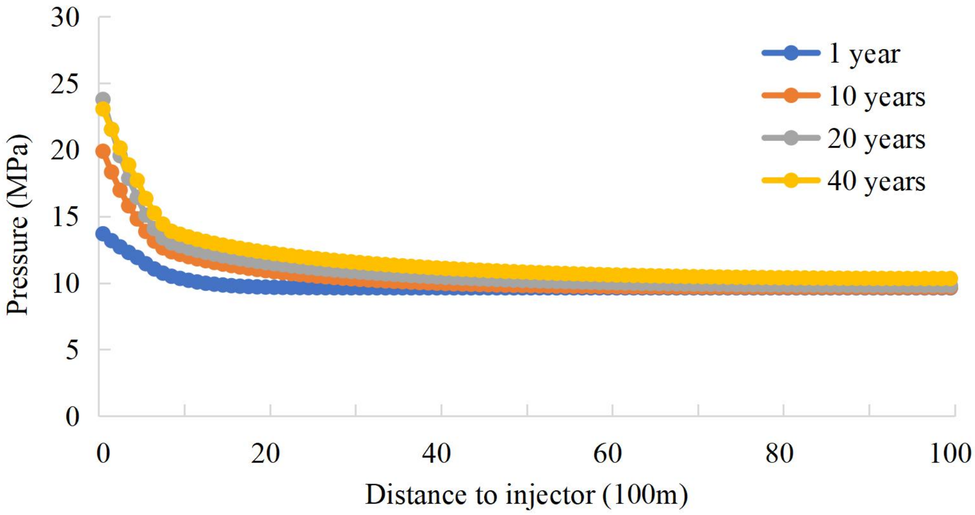
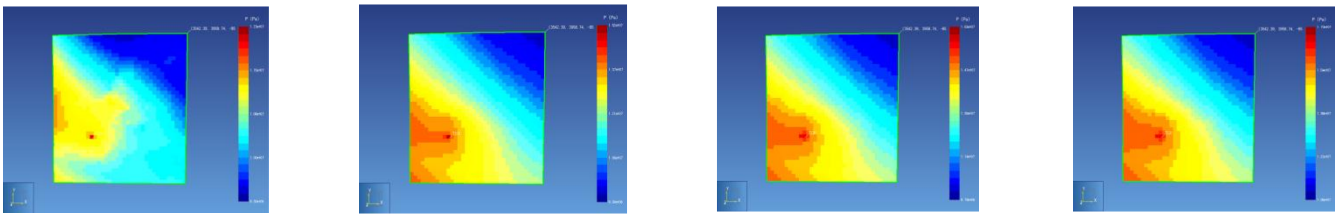


Figure 8—The sectional formation pressure distribution (5 tons/d) at different times.

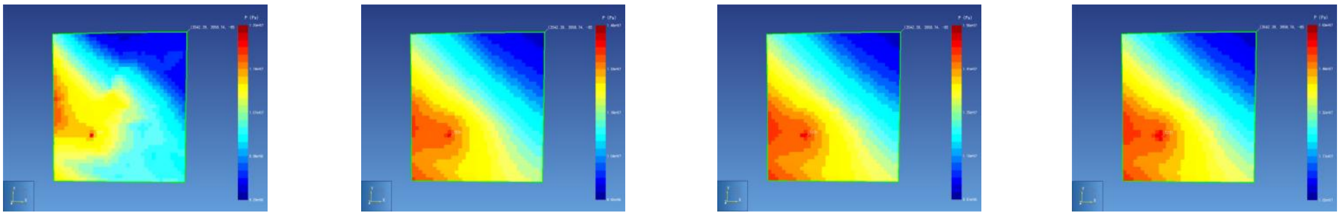
Heterogeneous model. **Figure 9** shows the horizontal pressure distributions at different injection stages (1, 10, 20, and 30 years) with a constant injection rate of 5 tons/d. It can be found that the spatial distribution of the heterogeneous model is remarkably different from that of the homogeneous model, although both the maximum formation pressures are in the position of the injector. The possible reason for such a difference is that the spatial distribution of formation pressure in the heterogeneous model is affected not only by the injected CO_2 but also by the geological structure of the saline aquifer. The formation depth inherently results in different formation pressures and the deviation of pressure distribution between the homogeneous model and the heterogeneous model.

In addition, the increment of formation pressure is strongly pertinent to the amount of injected CO_2. For instance, the pressure at the well position is gradually increased with an increase in CO_2 injection rate. In other words, a large injection rate of CO_2 is, a high formation pressure becomes, according to the simulation results of different injection rates of 5, 4, and 3 tons/d (**Figure 10**).



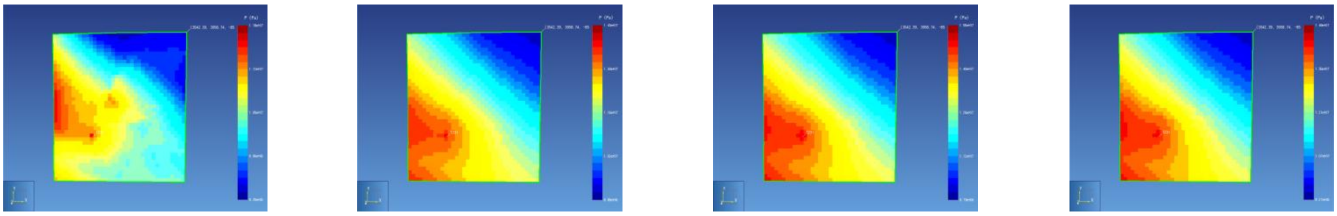
1 year 10 years 20 years 30 years

(a) 5 tons/d



1 year 10 years 20 years 30 years

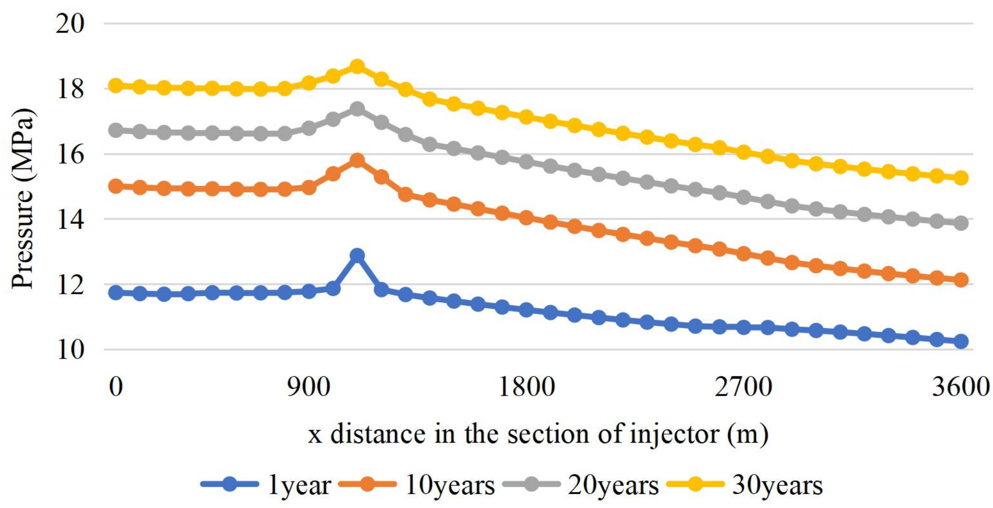
(b) 4 tons/d



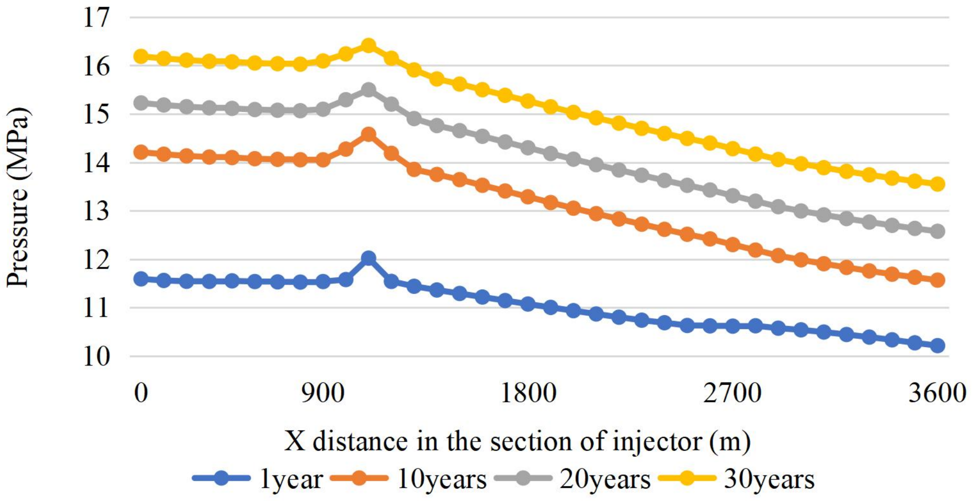
1 year 10 years 20 years 30 years

(c) 3 tons/d

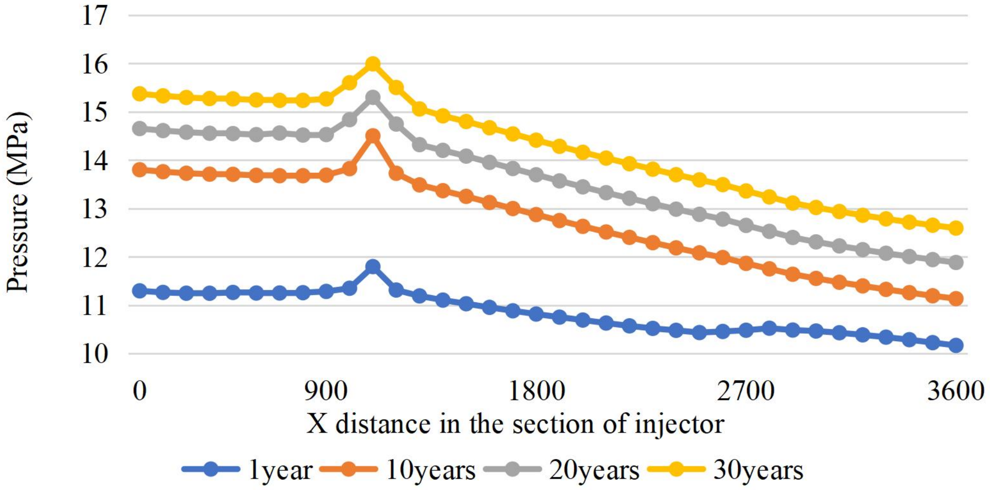
Figure 9—2D formation pressure of heterogeneous model with an injection rate of (a) 5 tons/d; (b) 4 tons/d and (c) 3 tons/d.



(a) 5 tons/d



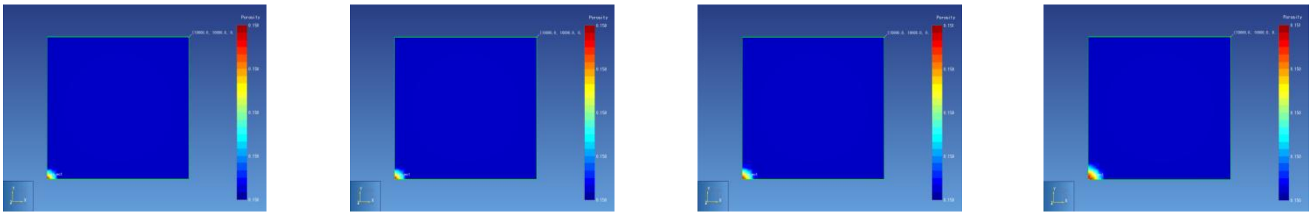
(b) 4 tons/d



(c) 5 tons/d

Figure 10—The sectional formation pressure distribution with CO_2 injection rates of (a) 5 tons/d; (b) 4 tons/d and (c) 3 tons/d at different times.

Porosity. *Homogeneous model*. **Figure 11** shows the dynamic porosity distributions of the homogeneous model with time proceeding. It can be observed that an area with an increased porosity, which surrounds the injector, is formed and gradually enlarged owing to an increase in amounts of injected CO_2. Such changes in porosity have mainly resulted from the chemical reaction between the H+ and minerals, that is to say, the dissolution of minerals in the weak acid formed by the injected CO_2 and formation water. Meanwhile, the spatial distribution of porosity is presented in **Figure 12**. To be specific, the porosity increased from 15% to 15.06% in 40 years, an increase of only about 0.4% compared to the initial value. A minor increase in porosity implies that the reaction of the dissolution of minerals is a gentle and long-term process, which cannot lead to a sharp change in porosity. One can find that the distribution pattern of porosity is similar to that of formation pressure. However, the area with an enlarged porosity is much smaller than that affected by an increased formation pressure, which actually is resulted from the spatial distribution of pH.



1 year 10 years 20 years 40 years

Figure 11—2D porosity distributions of homogeneous model at different times.

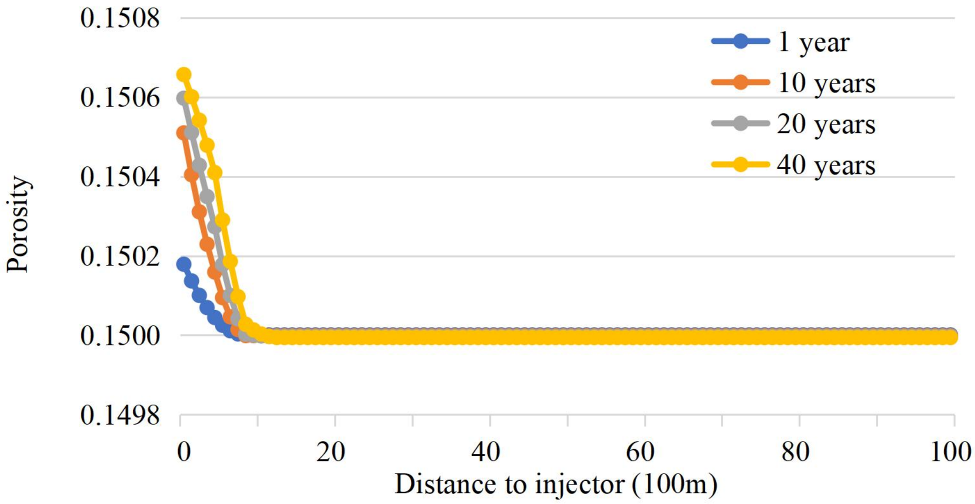
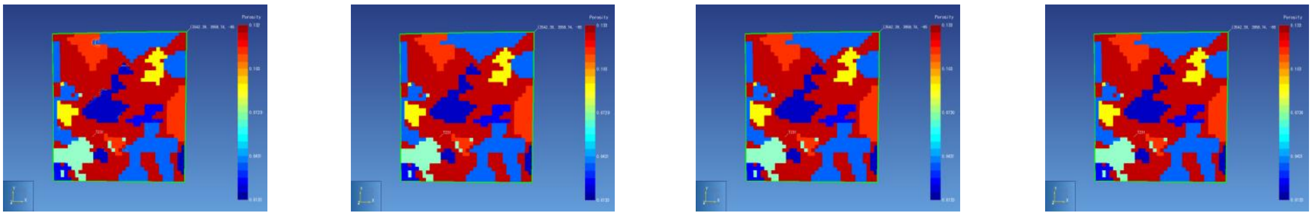


Figure 12—Sectional porosity distribution at different times in homogeneous model.

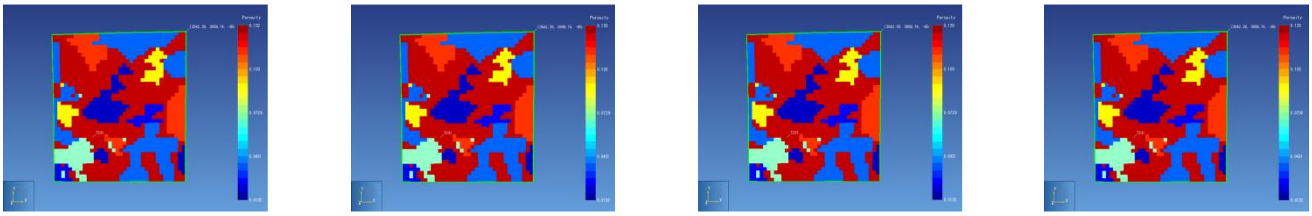
Heterogeneous model. **Figure 13** shows the porosity distribution at different injection stages (1, 10, 20, and 30 years) at an injection rate of 5, 4, and 3 tons/d. According to the figures, one can find that the changes in porosity are very unnoticeable at different times. To be specific, porosity of the formation only increased by 0.000014 in 30 years. Such a small change in porosity implies that the CO_2 sequestration caused by mineral carbonation is not the main contributor to CO_2 trapping in this aquifer.

CO_2 dissolves in water to form a weak acid, leading to carbonate dissolution in the reservoir and an increase in porosity. According to the current simulation (**Figure 14**), this reservoir is less affected by acid dissolution, and its porosity increases only by 0.000014 in 30 years.



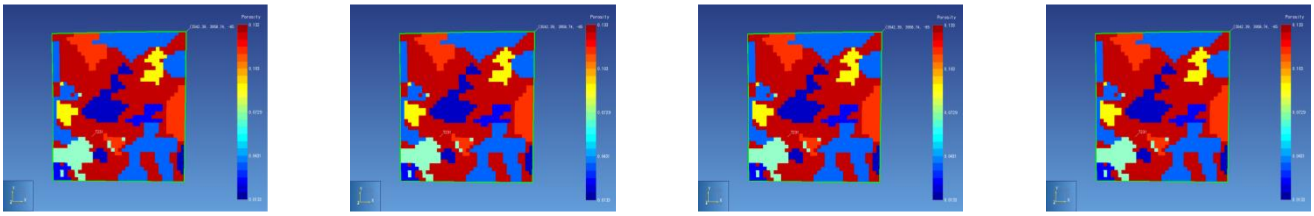
1 year 10 years 20 years 30 years

(a) 5 tons/d



1 year 10 years 20 years 30 years

(b) 4 tons/d



1 year 10 years 20 years 30 years

(c) 5 tons/d

Figure 13—2D formation pressure of heterogeneous model with an injection rate of (a) 5 tons/d; (b) 4 tons/d and (c) 3 tons/d.

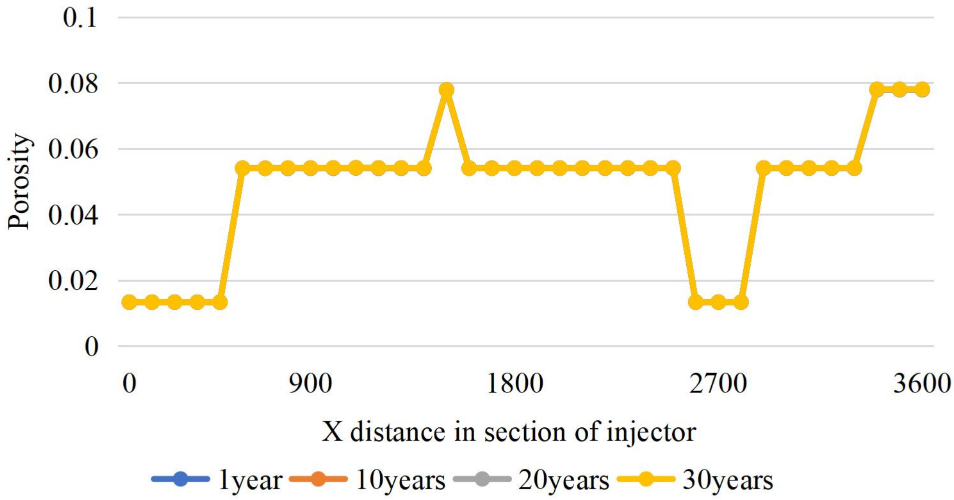


Figure 14—Sectional porosity distribution at different times in heterogeneous model overlaid each other.

Conclusions

In this work, the numerical simulation was carried out to realize the establishment of the heterogeneous model in the actual situation. The influence of CO_2 geological sequestration on reservoirs and cap rocks was studied, and the following conclusions are drawn:

1. The whole process of CO_2 storage changes the original geochemical properties and physical parameters of the reservoir and cap rock, and the CO_2 injection leads to the continuous increase of the pressure in the formation, which may cause vertical differential deformation of the surface, fault activation, and even earthquake; CO_2 escape leads to pollution of freshwater aquifers, and a large amount of gas emission endangers human safety and ecological safety nearby.
2. Through the simulation, the formation of weak acid after CO_2 injection causes the pH value of the formation to change, resulting in the increase of reservoir acidity, especially the injection point and the area around the change range is large, and then promotes the CO_2-water-rock geochemical reaction. The acidity of the formation also leads to the dissolution of minerals and the precipitation of new minerals, and the dissolution is greater than the precipitation in the acidic area, which is also the main reason for the increase in porosity.
3. At present, most of the established numerical models are mean value models and focus on the transport and reaction of CO_2 in the reservoir. This paper has realized the analysis of the physical changes of the reservoir and cap under different conditions of the actual model.

Conflicts of Interest

The author(s) declare that they have no conflicting interests.

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