

Numerical simulation study of CO₂ storage capacity in Deep Saline aquifers

Qigui Wang¹ , Dongxu Zhang^{1,2,*}, Yaqi Li¹, Chengyong Li¹, and Huiying Tang³

¹Energy College, Chengdu University of Technology, 1, Dongsan Road, Erxian Bridge, Chenghua district, Chengdu, Sichuan, PR China

²Geological Resources and Geological Engineering Postdoctoral Research Station, Chengdu University of Technology, 1, Dongsan Road, Erxian Bridge, Chenghua district, Chengdu, Sichuan, PR China

³State Key Laboratory of Oil and Gas Reservoir Geology and Exploitation, Southwest Petroleum University, 8, Xindu Avenue, Xindu District, Chengdu, Sichuan, PR China

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Abstract. The storage of supercritical CO₂ in deep saline aquifers is essential for reducing carbon emissions, and the selection of an appropriate reservoir is a primary consideration for carbon sequestration. To investigate the impact of reservoir physical properties on the CO₂ storage capacity of saline aquifers, this study establishes a numerical simulation model of CO₂ storage in deep saline aquifers and utilizes the MRST toolbox to solve it by the finite volume method. The research thoroughly analyzes the influence of reservoir physical properties on the CO₂ migration process and CO₂ storage capacity of the saline aquifer layer. The results show that prolonged CO₂ injection involves a process of initially suppressing pressure and subsequently slowly diffusing it to the surroundings. Furthermore, the physical properties of the reservoir and the reservoir pressure significantly influence CO₂ burial in deep saline aquifers. Higher reservoir permeability and deeper burial depth result in enhanced CO₂ storage and faster CO₂ plume migration. However, the porosity and temperature of the reservoir have a negligible impact on CO₂ storage. Our research work provides a precise understanding of selecting suitable layers for CO₂ storage in deep saline aquifers, offering strong support for early predictions of carbon capture, utilization, and storage (CCUS).

Keywords: CO₂ storage, Deep Saline aquifers, CO₂ migrates, Numerical simulation.

1 Introduction

The surge in greenhouse gas emissions since the industrial age has led to a substantial global temperature rise, posing a severe threat to the environment on a worldwide scale [1, 2]. In 2018, global CO₂ emissions from fossil fuel combustion reached an estimated 37.1 gigatons (Gt), marking a 2.7% increase from the previous year. If this rate of carbon emissions growth persists, the global average temperature is expected to surpass 1.5 °C shortly [3]. With ongoing economic development and a growing global population, the pressure to reduce carbon emissions is mounting. In this context, carbon capture and storage (CCS) has emerged as a crucial technology for reducing carbon emissions [4]. CCS is considered a critical component in achieving the goal of limiting the increase in global average temperature to within 2 °C of the pre-industrial level. It is regarded as one of the most feasible solutions for effectively mitigating

global warming and significantly reducing CO₂ emissions [5, 6]. After years of theoretical demonstrations and field tests, it has been proven that CCS is an effective method for curbing atmospheric CO₂ levels [7, 8].

The injection of CO₂ into deep saline aquifers is a viable option for reducing CO₂ emissions. Among geological storage mechanisms, deep saline aquifers are known to possess the highest storage capacity for CO₂ [9, 10]. The migration and transformation of CO₂ in deep saline layers can be broadly classified into four types: structural storage, residual gas storage, dissolution migration storage, and mineral storage [11, 12]. The relative contribution of these storage mechanisms dynamically varies over time. Geological structural storage predominantly dominates during the early storage stages, with residual gas and dissolution storage gaining significance over time. Conversely, mineral storage requires a more extended period to become effective [13, 14]. Structural storage has a higher risk of CO₂ Leakage compared to dissolution and bound space storage. Among these mechanisms, mineralization storage is considered the

* Corresponding author: zhangdongxu1992@outlook.com

safest and most long-lasting, although taking hundreds of years to fully occur [15, 16]. The physical properties of the reservoir are essential factors influencing the storage of supercritical CO₂ [17, 18]. When selecting layers for carbon storage, the physical properties of the reservoir are critical factors to consider. However, existing studies focus on specific models to address this issue, with relatively few exploring the impacts of significant changes in reservoir physical properties on CO₂ storage [19–21].

Furthermore, supercritical CO₂ is highly sensitive to changes in reservoir temperature and pressure. The expansion/compression of the CO₂ phase makes it particularly susceptible to alterations in pressure or temperature, significantly impacting CO₂ migration in the reservoir [22, 23]. During the geological storage of CO₂ in saline aquifers, fluctuations in fluid pressure or temperature are anticipated over time [24]. The solubility of the CO₂ component in the water phase and the density of the supercritical CO₂ phase change with reservoir temperature and pressure, leading to significant changes in the two-phase flow migration behavior [25, 26]. While numerous studies have delved into the interfacial tension of the two phases, few have focused on the actual storage capacity and its susceptibility to reservoir temperature and pressure [27, 28].

Mathematical models and numerical simulations are essential tools for better understanding the processes unfolding in the subsurface during and after injection [29–31]. Currently, the primary considerations in CO₂ storage are storage capacity, pressure change, plume migration, and potential CO₂ leakage, factors within the purview of commercial software in the petroleum industry. Many experts and scholars have evaluated and analyzed renowned software such as TOUCH2, ECLIPSE, CMG, etc. These studies encompass multiphase flow simulation, CO₂ dissolution, temperature field changes, and more, providing insights into their efficacy in modeling CO₂ storage [32, 33]. In contrast to typical oil recovery scenarios that involve subterranean reservoirs spanning several kilometers laterally and lasting decades, CO₂ storage scenarios entail migration processes spanning thousands of years and extending hundreds of kilometers [34]. Additionally, carbon dioxide tends to travel underground in long, thin plumes, eventually achieving a thickness measured in centimeters [35]. Representing such a thin plume in a 3D grid on large spatial scales poses computational challenges for traditional simulators, making it complex and computationally slow [36].

Considering the substantial space and time scale inherent in the long-term storage of injected CO₂, this paper establishes a numerical simulation model for CO₂ burial in deep saline aquifers. The model is solved using the finite volume method with the MRST toolbox, simulating the long-term storage of injected CO₂. A sensitivity analysis is conducted to comprehensively understand the influence of reservoir physical properties, temperature, pressure, and other factors on CO₂ geological storage capacity.

2 Methodology

In deep saline aquifers, the injected CO₂ is in a supercritical state and less dense than the brine in the reservoir.

Consequently, the CO₂ migrates upward under the influence of gravity, forming a visible plume in the upper part of the reservoir. The migration process either leads to permanent capture by the storage mechanism or is interrupted due to leakage [37].

2.1 Mathematical model

Based on the continuity equation, flow equation, and state equation of CO₂ and water in the rocky porous medium, the mathematical model for CO₂ seepage in the saline aquifer is established.

The local conservation of mass, a fundamental principle describing the flow of single-phase fluids in porous media, is expressed in the form of a continuity equation:

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla(\rho\mathbf{v}) = q \quad (1)$$

Here, ρ represents the fluid density, ϕ porosity, $\mathbf{v}$ apparent velocity (volumetric fluid flow per unit surface of porous medium), and q source term.

The CO₂ storage system consists of two phases: CO₂ and brine, and independent mass conservation equations can be established for each phase:

$$\begin{aligned} \frac{\partial(\phi\rho_g S_g)}{\partial t} + \nabla(\rho_g v_g) &= q_g \\ \frac{\partial(\phi\rho_w S_w)}{\partial t} + \nabla(\rho_w v_w) &= q_w \end{aligned} \quad (2)$$

Using the multiphase extension of Darcy's law, the velocity of each phase is related to the pressure of each phase:

$$v_\alpha = -\frac{Kk_{r,\alpha}}{\mu_\alpha}(\nabla p_\alpha - \rho_\alpha g). \quad (3)$$

Considering the influence of temperature and pressure, a volume factor is introduced:

$$B_\alpha = \frac{V_\alpha}{V_\alpha^s} \left(= \frac{\rho_\alpha^s}{\rho_\alpha} \right) \quad (4)$$

Here, V_α and V_α^s represent volumes α under storage and standard conditions, respectively. Similarly, ρ_α and ρ_α^s refer to the phase density of the reservoir and standard states. For isothermal models, B_α is simply a function of pressure, and for ease of representation, defined as $b_\alpha = 1/B_\alpha$.

Considering the variation of the pore space of reservoir rock with pore pressure:

$$\phi(p) = \phi_0 e^{c_\phi(p-p_0)} \quad (5)$$

$$c_\phi = \frac{1}{\phi} d\phi/dp. \quad (6)$$

Equation (4) for a carbon dioxide-water system can be rewritten as follows:

$$\frac{\partial}{\partial t}(\phi b_\alpha s_\alpha) + \nabla(b_\alpha \mathbf{v}_\alpha) = b_\alpha q_\alpha. \quad (7)$$

It can be expressed by a simple mathematical model of the power function, that is, hypothetically:

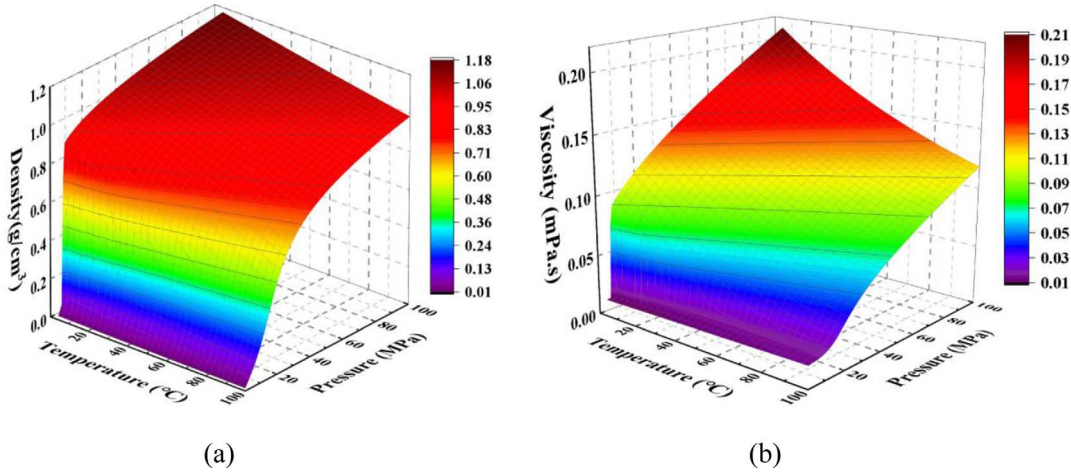


Fig. 1. Relationship between physical properties of CO₂ and temperature and pressure. (a) CO₂ density vs. temperature and pressure. (b) CO₂ viscosity vs. temperature and pressure.

$$k_{r,x}(s_x) = s_x^{N_x}. \quad (8)$$

After considering the effects of bound water and residual gas, the saturation power function of the rescale is α [38]:

$$s_x^* = \frac{s_x - s_{r,x}}{1 - s_{r,x}} \quad (9)$$

The relationship between saturation and capillary pressure was proposed by Brooks and Corey. The parameter p_e represents the entry pressure, MPa.

$$s_w = \begin{cases} (p_c/p_e)^{-n_b}, & \text{if } p_c > p_e \\ 1, & p_c \leq p_e \end{cases} \quad (10)$$

2.2 Fluid properties

In deep geological formations suitable for CO₂ sequestration, temperature, and pressure conditions often exceed the critical point of CO₂, resulting in the occurrence of CO₂ transport and storage under supercritical conditions. Supercritical CO₂ exhibits dual characteristics of both gas and liquid, combining a density close to liquid, viscosity similar to gas, and a diffusion coefficient comparable to gas. These properties contribute to favorable flow and transport characteristics, playing a pivotal role in the geological storage of CO₂. The dual nature of supercritical CO₂ enhances its solubility in saline aquifers, ensuring its fluidity. Therefore, the accuracy of calculating physical property parameters for supercritical CO₂ significantly impacts the precision of research results in the CO₂ storage process.

During actual CO₂ storage, fluid density and viscosity are quantities that vary with external conditions. Fluid density is a thermodynamic property, that could be determined by solving the simultaneous pressure and temperature equation of state [39]. Fluid viscosity, a transport property, correlates with thermodynamic properties and is determined through an experiment-based correlation of fluid properties. In general, equations of state represent mathematical relationships between thermodynamic parameters

of matter [40] and often use cubic equations with fitted parameters to model changes in CO₂ physical properties [41]. These changes include viscosity and density, which are influenced by temperature and pressure.

In this study, physical properties data, such as the density and viscosity of supercritical CO₂ under different temperatures and pressures, are stored in a database to enhance calculation efficiency. Drawing upon this data, relationships between CO₂ physical properties and temperature and pressure are illustrated, as shown in Figure 1.

2.3 Model solution

Numerical simulation models are specified based on discrete data (state variables that divide space into cells and finite time steps). Despite the continuous nature of equations describing the model system across time, some form of discretization is necessary for numerical simulation. The conservation equation is discretized in space using the finite volume method and in time using an implicit first-order discretization.

The block diagram of the solution calculation steps is given in Figure 2.

Finite volume discretization operates by rigorously applying the principle of mass conservation to grid elements. For any given time interval, the change in mass within each grid cell is equated to the change in flux on the grid cell face during the interval, along with the final source term. This ensures flux continuity by associating a distinct flux with each face in the mesh. Any amount flowing out of element A passes through the shared polygon with element B and is equal to the amount flowing into element B through the same face.

In-grid integral control equation:

$$\begin{aligned} \int_t^{t+\Delta t} \int_{\Delta V} \frac{\partial(\rho_x \phi S_x)}{\partial t} dV dt + \int_t^{t+\Delta t} \int_{\Delta V} \text{div}(\rho_x v) dV dt \\ = \int_t^{t+\Delta t} \int_{\Delta V} Q_w dV dt. \end{aligned} \quad (11)$$

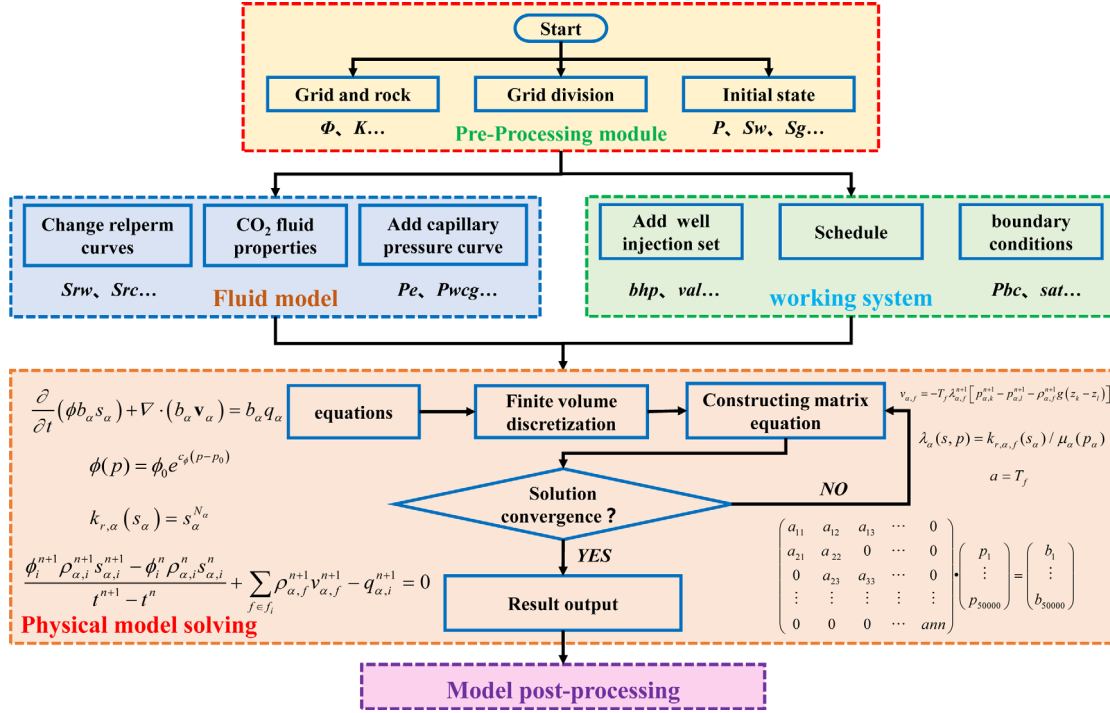


Fig. 2. Discrete solution calculation steps of finite volume method.

Suppose the set of faces on the control body P in the mesh is F_i , the faces are f , and the six faces are assumed to be E, W, N, S, T , and B .

Transient term:

$$\int_t^{t+\Delta t} \int_{\Delta V} \frac{\partial(\rho_\alpha \phi_\alpha S_\alpha)}{\partial t} dV dt = \int_{\Delta V} \left[\int_t^{t+\Delta t} \rho_\alpha \frac{\partial \phi}{\partial t} dt \right] = \rho_p^0 (\phi_p - \phi_p^0) \Delta V. \quad (12)$$

Convection items:

$$\int_t^{t+\Delta t} \int_{\Delta V} \text{div}(\rho_\alpha v_\alpha) dV dt = \int_t^{t+\Delta t} [(\rho_\alpha v_\alpha)_E A_E - (\rho_\alpha v_\alpha)_W A_W + (\rho_\alpha v_\alpha)_N A_N - (\rho_\alpha v_\alpha)_S A_S + (\rho_\alpha v_\alpha)_T A_T - (\rho_\alpha v_\alpha)_B A_B] dt. \quad (13)$$

Using the superscript “n” for the time step and the subscripts ‘i’ and ‘f’ for the grid cell and the mesh surface index, respectively, the time-implicit finite volume discretization of the equation for the grid element ‘i’, can be expressed as follows:

$$\frac{\phi_i^{n+1} \rho_{a,i}^{n+1} s_{a,i}^{n+1} - \phi_i^n \rho_{a,i}^n s_{a,i}^n}{t^{n+1} - t^n} + \sum_{f \in f_i} \rho_{a,f}^{n+1} v_{a,f}^{n+1} - q_{a,i}^{n+1} = 0 \quad (14)$$

Here, t represents time; f_i represents the grid surface set of boundary unit i , $v_{a,f}$ represents the net volume flux of phase α on surface f (here, the outflow is agreed to be

positive). Assuming isothermal conditions, $\rho_{a,i}^n$ is used as a shorthand for $\rho_\alpha(P_i^n)$, and likewise, $\phi_i^n = \phi_i(P_i^n)$.

The surface flux $v_{a,f}^{n+1}$ is the discretized form of the multiphase extension of Darcy’s law (Eq. (14)). This time, a two-point flux approximation scheme is adopted. Denoted the v_α between two faces on the control volume P , assuming that face f represents the common interface between cells k and l , then the flux from cell l to cell k through f can be approximated as:

$$v_{a,f} = -T_f \lambda_{a,f}^{n+1} [p_{a,k}^{n+1} - p_{a,l}^{n+1} - \rho_{a,f}^{n+1} g(z_k - z_l)]. \quad (15)$$

This expression, $\lambda_{a,f}^{n+1} = \lambda_{a,f}(s_f^{n+1}, p_f^{n+1})$ represents the mobility of the α phase, which abbreviates for relative permeability divided by viscosity, i.e., $\lambda_\alpha(s, p) = k_{r,\alpha,f}(s_\alpha) / \mu_\alpha(p_\alpha)$.

In addition, Z_k and Z_l represent the depth values for the centroids of the respective elements, and T_f represents the conductivity associated with the face f . The areal conductivity is a value based on the related element geometry and permeability, and can be expressed as the harmonic mean of the associated half-area conductivities:

$$T_f = (T_{k,f}^{-1} + T_{l,f}^{-1})^{-1} \quad (16)$$

where the half-surface conductivity associated with cell k and face f is given by:

$$T_{k,f} = \frac{C_{k,f}^T K_k N_{k,f}}{\|C_{k,f}\|^2}. \quad (17)$$

In this expression, $\mathbf{K}_k$ represents the permeability tensor of cell k , $\mathbf{C}_{k,f}$ is the vector pointing from the cell centroid of cell k to the face centroid of face f , and $\mathbf{N}_{k,f}$ is the face f outside of cell k .

To close the discretized system, the remaining relations in the continuous case are expressed:

$$\sum_{\alpha} s_{\alpha,i} = 1 \text{ and } p_{n,i} - p_{w,i} = p_c(s_i). \quad (18)$$

In equations (16) and (17), the flux $v_{\alpha,f}$ is associated with the mesh faces, involving additional quantities, namely $\rho_{\alpha,f}$ and $\lambda_{\alpha,f}$.

3 Results and discussion

Effective and secure CO₂ storage necessitates meticulous site selection, with primary considerations focusing on geological stability, reservoir conditions, and physical properties. The geological structure must exhibit stability, reinforced by an impermeable caprock to prevent CO₂ migration upwards and potential leakage into the atmosphere or shallow groundwater. Furthermore, the temperature and pressure state of the reservoir should maintain the CO₂ supercritical state condition to maintain its stability and safety. Finally, the reservoir must have good physical properties, a specific storage capacity scale, and exhibit excellent injectability to ensure practical CO₂ storage [42].

The main geological factors that affect the CO₂ storage capacity are the porosity, permeability, pressure, and temperature of the reservoir. In this study, the constant pressure injection method is used to study the influence of these geological factors on CO₂ storage capacity. The final selected storage location is shown in Figure 3. The chosen site is approximately 100 km from Handan Iron and Steel Group. The selected layers are the Neogene Guantao Formation and the Paleogene Shahejie Formation. The physical properties of these layers meet the specified criteria, as detailed in Table 1.

According to geological data, we built a mechanical model based on the Petrel platform. The porosity of the reservoir is predominantly distributed within the range of 2 – 28%, with an average value of 20%. Likewise, the permeability of the reservoir varies from 0.01 to 260 mD, with an average value of 25 mD. Figure 4 illustrates the established mechanism model's porosity and permeability distribution diagram.

In the CO₂ injection process, it is imperative to ensure that the flow pressure at the well's bottom does not exceed the formation's rupture pressure. Formation rupture pressure is calculated according to the Hubert-Venice empirical formula.

To assess the impact of reservoir factors on CO₂ storage, the model employs a constant pressure injection with the maximum bottom flow pressure. At the same time, the model limits the reservoir rupture pressure, and if any grid reaches this limit, the calculation terminates. The amount of CO₂ stored in the reservoir under these conditions is then calculated upon model completion. Table 2 shows the

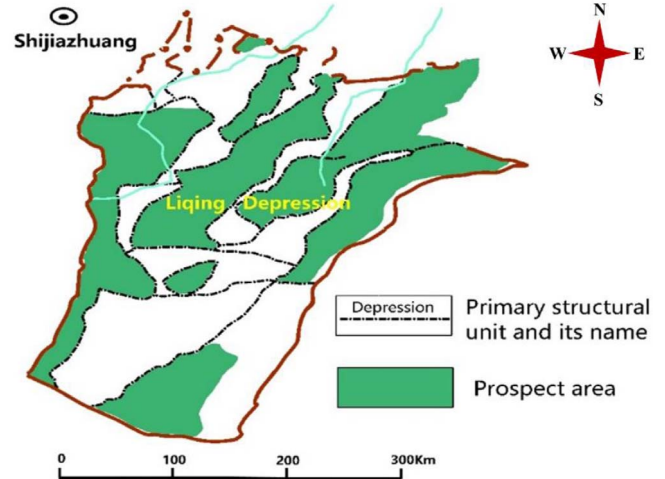


Fig. 3. Select a storage horizon location.

model's relevant parameters, basic reservoir parameters, and fluid properties.

In addition to the mentioned parameters, the simulation sets the boundary pressure to the reservoir pressure, initializing at 15 MPa.

3.1 Simulation results

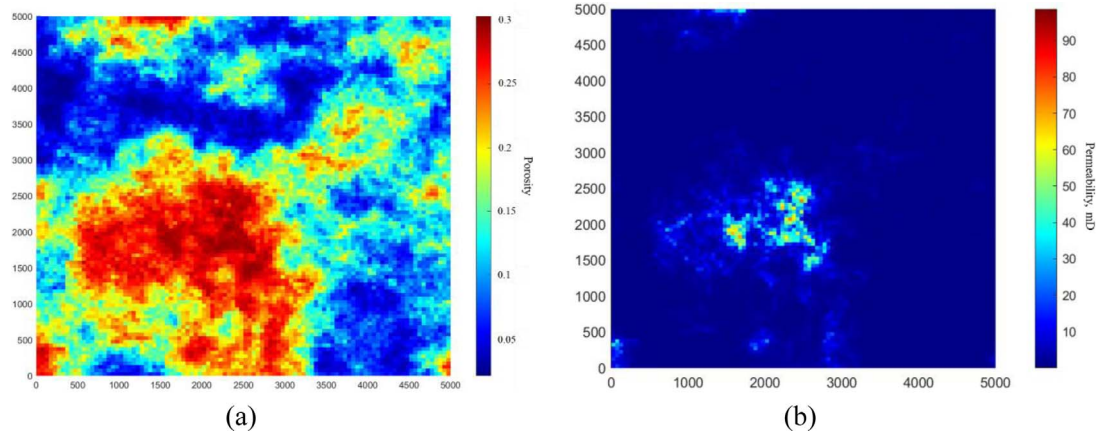
During the CO₂ geological storage process, rapid injection into the reservoir occurs under constant pressure, simulating a 100-year injection process in the preliminary model. The results of the first 20 years of simulation are shown in Figure 5. At the onset of injection, high pressure forces CO₂ from the wellbore into the surrounding pore space. It swiftly traverses the hyperpermeability zone, decelerates upon encountering low-permeability areas, and eventually accumulates at the reservoir's top, forming a spreading CO₂ plume.

Figure 6 shows the pressure changes during the model injection process. Supercritical CO₂ entering the reservoir initiates a drainage process, displacing highly saline brine to a distant location, forming a two-phase displacement flow. Limited mass exchange occurs between the two phases because a small amount of CO₂ dissolves into the brine, and a smaller amount of brine evaporates to CO₂. However, the impact of this mix remains minimal at this stage. Fluid flow is mainly driven by advection, with the high pressure from the wellbore serving as the primary driving force. Considering the pressure change process during the injection process, a reasonable injection rate ensures that formation pressure stays within the prescribed maximum limit. The pressure distribution cloud diffuses from the bottom of the well to the surroundings, and after the 10th year, the pressure distribution remains relatively stable mainly because of the formation's pressure limit.

Figure 7 shows the change in CO₂ saturation distribution during the injection process. Supercritical CO₂, being less dense than the formation brine, experiences buoyancy upward due to the density difference between the two phases causing the CO₂ to rise until the overlying cover

Table 1. Reservoir physical properties of layers.

Stratum	QiaoKou area		BaiMiao area		ShenXian area	
	Porosity (%)	Permeability (mD)	Porosity (%)	Permeability (mD)	Porosity (%)	Permeability (mD)
Es ₁	15~16	10~100	15~22	10~250	20.6	4.1
Es ₂					14.6	1.7
Es _{31~2}	13~20	5~100	13~20	5~150	15.3	2.4
Es ₃₃	8~13	<0.1	8~13	<1		
E ₃₄	6~14	02~6.5	5~11	0.2~0.8		

**Fig. 4.** Reservoir physical property plan. (a) Porosity distribution map. (b) Permeability distribution map.**Table 2.** Basic parameters of the geological model.

Parameter	Value	Unit
Physical model size	$5000 \times 5000 \times 50$	m
Grid size	$100 \times 100 \times 5$	—
Grid size	$50 \times 50 \times 10$	m
Reference reservoir elevation	−1500	m
Reservoir pressure	15	MPa
Maximum bottom injection pressure	30	MPa
Boundary pressure	15	MPa
Reservoir temperature	60	°C
Rock compression coefficient	$4.35e^{-4}$	MPa^{-1}
CO ₂ compression coefficient	8.79×10^{-8}	MPa^{-1}
The viscosity of the saltwater layer	$8e^{-4}$	Pa·s
Water saturation	S_w	—
CO ₂ density	0.604	g/cm^3
CO ₂ viscosity	$2.63e^{-5}$	Pa·s
Maximum water saturation	0.27	—
Maximum CO ₂ saturation	0.20	—

impedes vertical movement. Eventually, the shape of the region containing carbon dioxide develops into an inverted cone. From the following results, we can observe that over time, the upper part of this cone expands outward and gradually thins. Due to the heterogeneity of the reservoir,

the CO₂ transport is mainly in the direction of hyperpermeability Migration.

From the above results, we can obtain that the reservoir pressure distribution after CO₂ injection diffuses from the wellbore to the surroundings. Reservoir heterogeneity

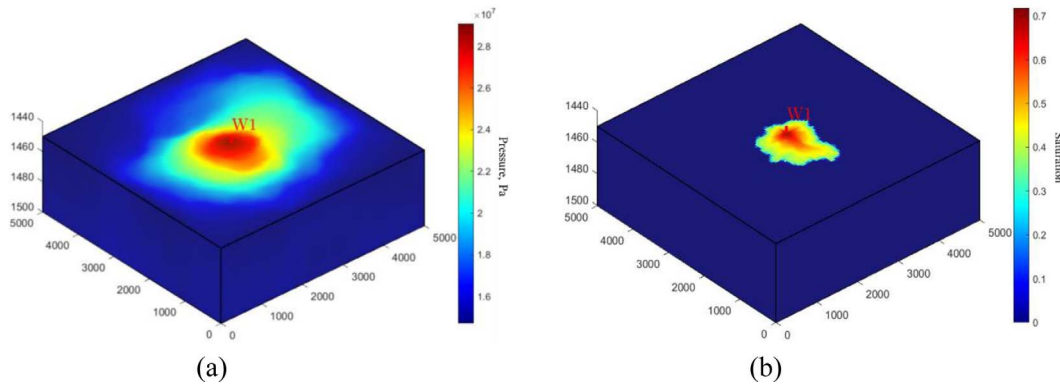


Fig. 5. Simulation results of injection 20 years. (a) Pressure distribution. (b) Saturation distribution.

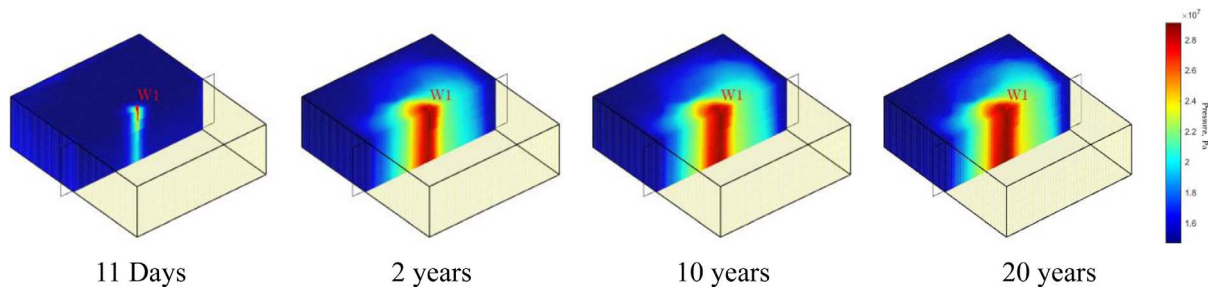


Fig. 6. Pressure change during injection.

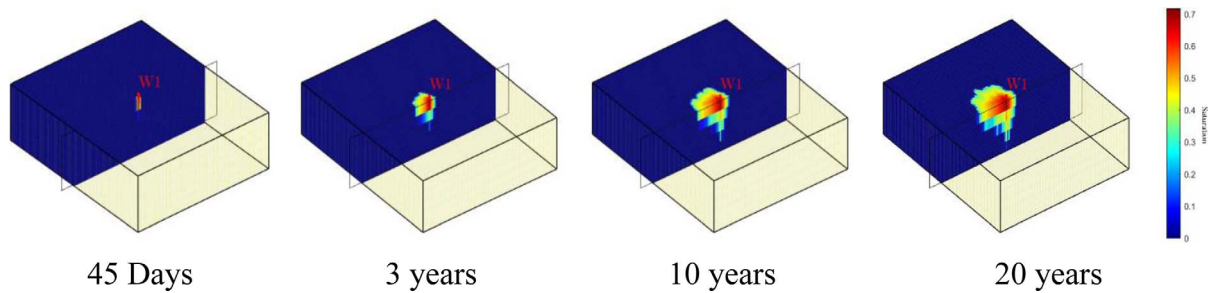


Fig. 7. Change of CO₂ saturation during the injection process.

significantly influences CO₂ transport, with both pressure and CO₂ plume irregularly distributed in the hyperpermeability direction. The reservoir pressure distribution after CO₂ injection shows an overall upward trend, with the pressure around the wellbore being the highest but unevenly distributed.

The uneven distribution of pressure and the CO₂ plume is mainly affected by the reservoir's physical properties. In Figure 8, various points are intercepted at different locations in the model, starting from well W1 and extending one point every 150 m to the left and right. The pressure over time is monitored, and pairs of points (#1 and #5, #2 and #6, #3 and #7, #4 and #8) equidistant from the injection well are compared. Points #5, #6, #7, and #8 exhibit superior physical properties compared to #1, #2, #3, #4.

Figure 9 illustrates the relationship between CO₂ injection time and pressure and saturation at each point. The plot shows a gradual increase in pressure and saturation as injection time increases. At 150 m from the bottom of the well, point 5 exhibits a final saturation of 0.62 and a pressure increase of 28.3 MPa. Similarly, at 600 m from the bottom of the well, point 8 exhibits a saturation of 0.37 and a pressure increase to 26.09 MPa. It indicates that the saturation and pressure increase as the distance from the bottom of the well decreases. Simultaneously, superior physical properties result in faster pressure and saturation rise, accentuating the difference from points with inferior physical properties. In Figure 10, wells #1 and #5, located only 150 m from W1, experience a rapid pressure increase to 28 MPa in just 4 years, representing the fastest rise. In contrast, #4 and #8, situated 600 m from well W1, take

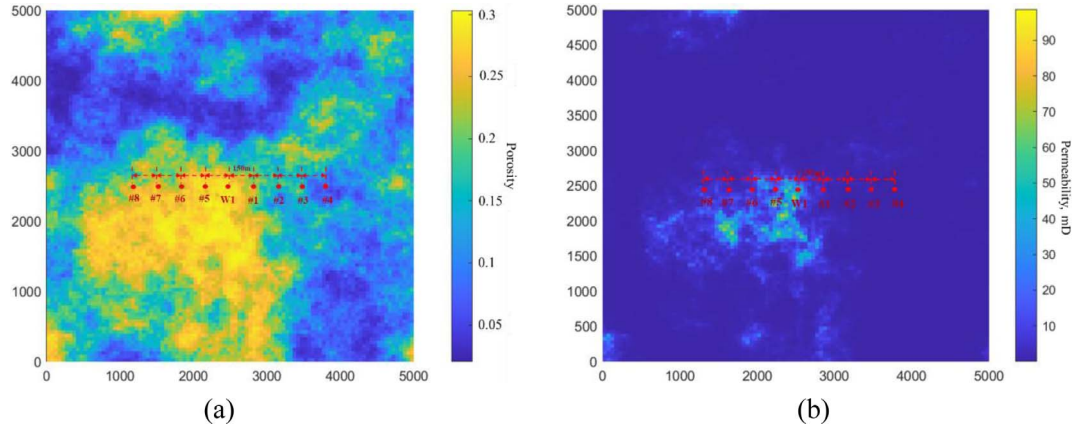


Fig. 8. Distribution of different points of the model. (a) The porosity position distribution at different points of the model. (b) Model permeability location distribution at different points.

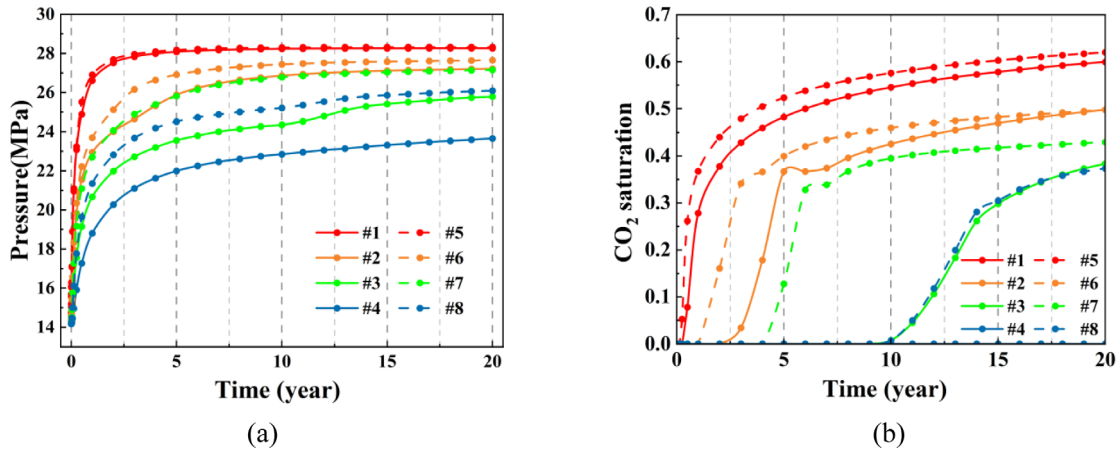


Fig. 9. Relationship between pressure, saturation, and injection age at different points. (a) The relationship between pressure and injection years at different points. (b) Relationship between saturation at different locations and injection years.

18 years to reach a pressure increase to 26 MPa, demonstrating a significantly slower rise than points #1 and #5. Moreover, #2 and #6, #3 and #7, with the same distance, showcase an increasing difference in pressure rise speed characteristics as they move farther from the injection well. The above results show that the physical properties of the reservoir and the distance from the injection well affect changes in reservoir rock pressure and saturation simultaneously. The better the physical properties, the closer the distance from the injection well, and the faster the pressure rises.

CO₂ was injected into the reservoir for 100 years, and the injection velocity curve of the injection well is depicted in Figure 10. The initial CO₂ injection velocity was 582.5 m³/day (under reservoir conditions), after which the injection velocity gradually decreased. It decreases to 424.3 m³/day at 4.6 years, followed by a slow rise to 512 m³/day after 97.4 years. We further analyze this phenomenon based on the saturation distribution cloud of CO₂ at different times.

Initially, CO₂ injection is affected by capillary force, pore wall resistance, etc., maintaining the same flow rate

requires a greater driving force. The bottom pressure must not exceed the maximum injection pressure. As CO₂ is injected, the flow is increasingly affected, leading to higher CO₂ saturation, a larger displacement range, greater flow resistance, increased pressure loss, and a subsequent decrease in displacement pressure, resulting in a reduction in CO₂ flow rate (before 4.6 years). The CO₂ saturation distribution cloud around the trough of the initial velocity indicates the formation and spread of the CO₂ plume from the wellbore to the surroundings, indicating the formation of seepage channels. The CO₂ plume continues to spread around, and the injection rate gradually rises. From Figure 11, for the whole process of CO₂ storage, the amount of CO₂ storage occurs in the slow diffusion period after the 4.6 years, accounting for 96% sequestration in total.

In general, both the physical properties of the reservoir and the distance from the injection well simultaneously impact the changes in reservoir rock pressure and saturation. The reservoir's physical properties and proximity to the injection well play a crucial role in the rate at which pressure and saturation increase, with better physical properties and closer proximity leading to faster increases.

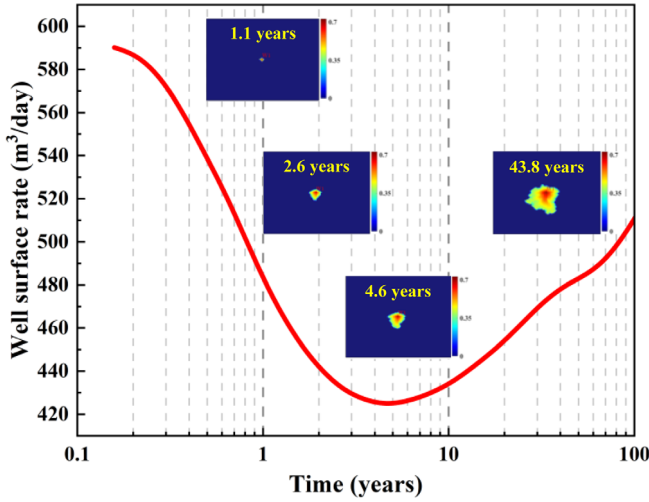


Fig. 10. Injection velocity curve lasting 100 years.

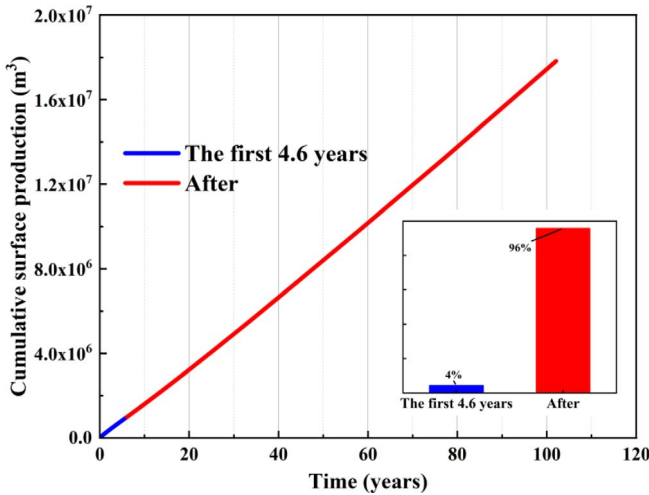


Fig. 11. Cumulative CO₂ sequestration over 100 years.

During the CO₂ injection process, a pressure-holding phenomenon occurs initially, resulting in a reduced injection speed due to the pressure limitations at the well's bottom. Most CO₂ injection occurs after 4.6 years, accompanied by a prolonged period of slow growth in the injection rate.

After the simulation, we compared it with commercial software to verify the accuracy of this model. We chose Eclipse software from Schlumberger for comparison, and the simulation results are shown in Figure 12.

The simulation results show that this model is in good agreement with the simulation results of commercial software, showing that this model has high accuracy.

3.2 Analysis of reservoir susceptibility factors

3.2.1 Reservoir porosity effects

To study the effect of varying porosity on CO₂ storage while considering the reservoir heterogeneity, we used the porosity of the basic scheme as the benchmark. Five

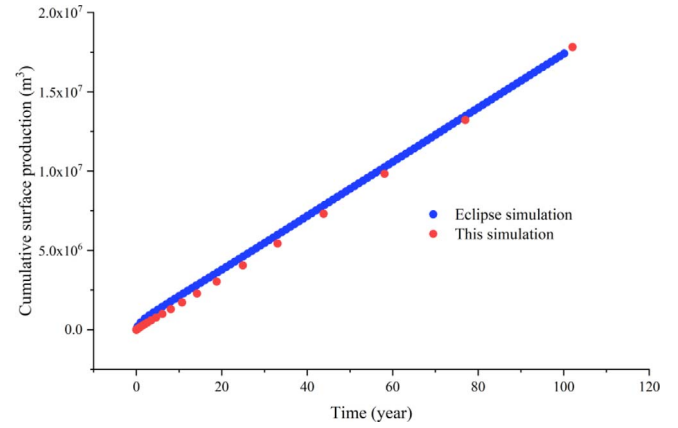


Fig. 12. Compared with commercial software, cumulative injection curve lasts for 100 years.

additional models were established by adjusting the porosity to different multiples: ϕ , 0.9ϕ , 0.8ϕ , 0.7ϕ and 0.65ϕ , respectively. CO₂ was injected at a bottom flow pressure of 30 MPa in the injection well to achieve the maximum injection efficiency, with other parameters held consistent.

The injection velocity curve and cumulative volume curve of the injection well are shown in Figure 13. Before 1000 days, the injection speed gradually decreased from about 560 m³/day to 420 m³/day, after which it gradually increased. The difference in injection speed between different porosities is minimal, indicating that porosity has little effect on CO₂ storage capacity. The cumulative CO₂ storage curve indicated that larger porosities resulted in smaller final cumulative injection amounts. However, the differences in total cumulative injection amounts between different porosities were minimal, suggesting that porosity has a minor influence on CO₂ storage capacity.

Additionally, under different porosities, the injection velocity curve fluctuates, but the maximum and the minimum injection velocities remain the same. According to Darcy's law, the seepage velocity is mainly related to the permeability and pressure difference. As we significantly changed the porosity while keeping reservoir permeability and bottom well pressure constant, the maximum and minimum injection speeds did not change.

3.2.2 Reservoir permeability impact

To investigate the impact of reservoir permeability on CO₂ plume migration, we varied the permeability by a factor of 2 to 0.1 relative to the permeability of the baseline model, while keeping other parameters constant. The injection well was operated at a bottom flow pressure of 30 MPa.

As can be seen from Figure 14, the minimum injection velocity is 683 m³/day, and the maximum injection velocity is 1542 m³/day at a reservoir permeability of 2 K. When the reservoir permeability is 0.1 K, the injection velocity ranges from 35–77 m³/day, indicating that the higher reservoir permeability leads to greater injection speed under constant pressure injection, resulting in a larger final injection volume and suggesting a significant influence of reservoir permeability on CO₂ sequestration.

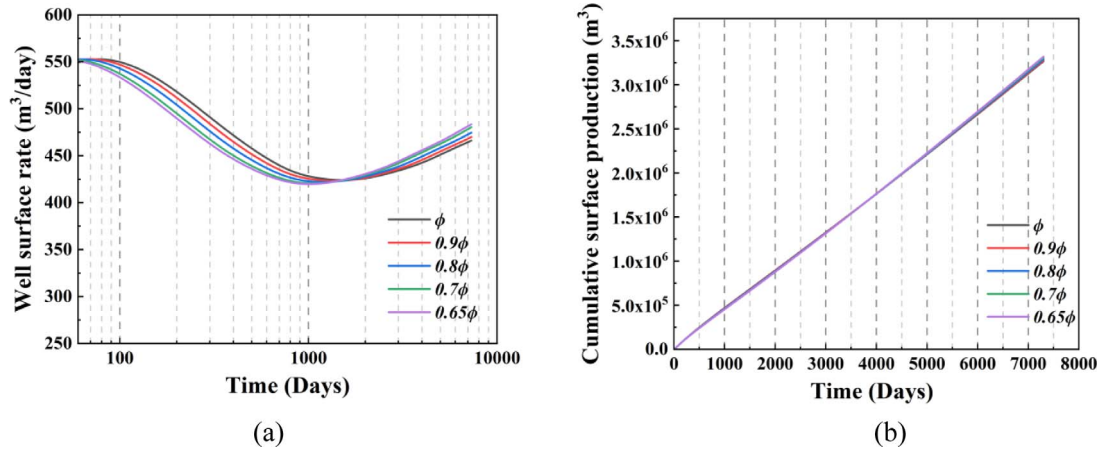


Fig. 13. Injection velocity curve and accumulation volume curve. (a) Injection velocity curve. (b) Cumulative storage curve.

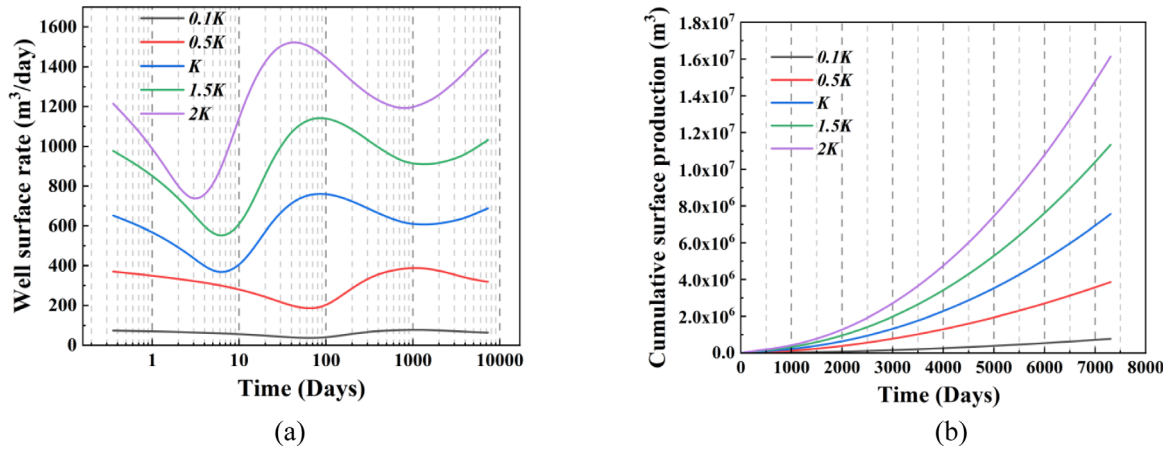


Fig. 14. Injection velocity curves and cumulative storage volume curves for different permeability models. (a) Injection velocity curve. (b) Cumulative storage curve.

Figure 15 illustrates that the CO_2 plume migration range gradually increases with the extended CO_2 injection time. Injecting CO_2 for 20 years at a reservoir permeability of $0.1K$ results in a less extensive CO_2 plume range compared to the 5-year range at K permeability. However, when the reservoir permeability is $2K$, the CO_2 plume migration range becomes more extensive, though still limited. The results indicate that under constant pressure injection conditions, the transmission range of the reservoir CO_2 plume increases with increased permeability. Therefore, when selecting a reservoir for CO_2 storage, it is essential to consider the permeability, as a reservoir with low permeability may hinder CO_2 migration, leading to unsatisfactory storage outcomes.

Figure 16 shows the reservoir pressure distribution of the CO_2 injection model under different reservoir infiltration at various times. Smaller reservoir permeability leads to faster reservoir pressure rise, increasing the risk of reaching rock fracture pressure and generating CO_2 leakage, which is not conducive to CO_2 storage.

In conclusion, CO_2 storage is significantly affected by the physical properties of the reservoir. Better physical

properties lead to increased storage amounts and faster CO_2 injection speeds. However, this comes with a trade-off, as the migration rate of supercritical CO_2 plumes also accelerates, necessitating early consideration of CO_2 leakage risks. Leakage of CO_2 from the reservoir upward to the overlying layer is related to the connectivity of hyper-permeability areas; therefore, we should comprehensively consider the relationship between reservoir physical properties and injection speed in the injection process and appropriately adjust the injection speed under good reservoir physical properties to obtain higher storage capacity while considering the risk of CO_2 leakage.

3.2.3 Reservoir burial depth effects

To study the influence of different reservoir pressures on the migration law of CO_2 plume, considering the positive correlation between reservoir pressure and depth, simulations were conducted at formation depths of 1500 m, 2000 m, 2500 m, 3000 m, and 4000 m. The injection well was still injected using the maximum bottom flow pressure, while other parameters remained unchanged.

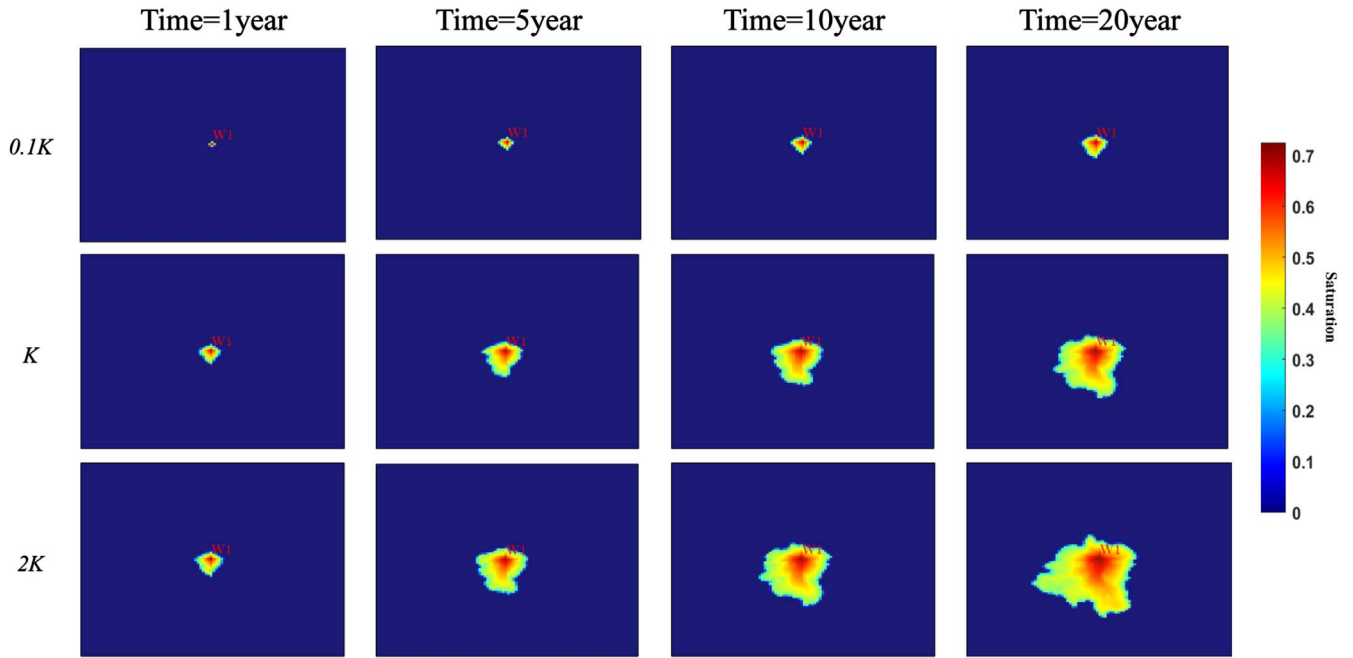


Fig. 15. Pressure distribution of CO₂ injection models with different reservoir permeability at other injection times.

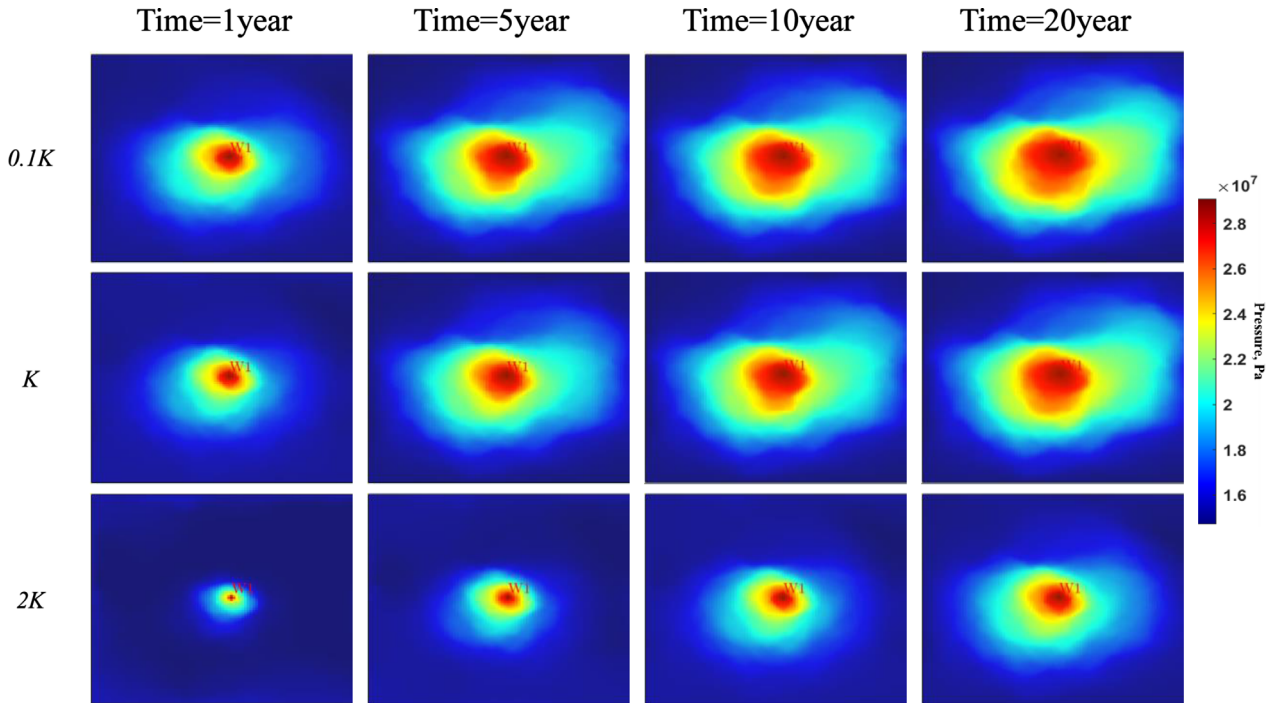


Fig. 16. CO₂ plume distribution of CO₂ injection model at different times under different reservoir infiltration.

Figure 17 displays various models' injection velocity and cumulative storage curves at different formation depths. The results indicate that deeper formations yield higher CO₂ injection velocity and increased cumulative storage.

This phenomenon is because deeper formations have a more significant displacement pressure difference due to the pressure injection at the bottom of the fixed well, resulting in higher displacement efficiency and greater injection

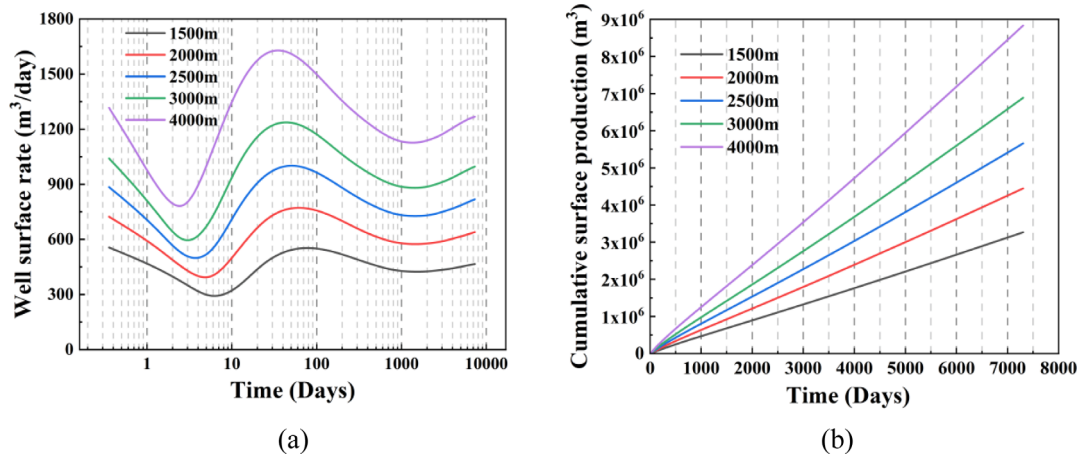


Fig. 17. Injection velocity curves and cumulative storage curves of different models. (a) Injection velocity curve. (b) Cumulative storage curve.

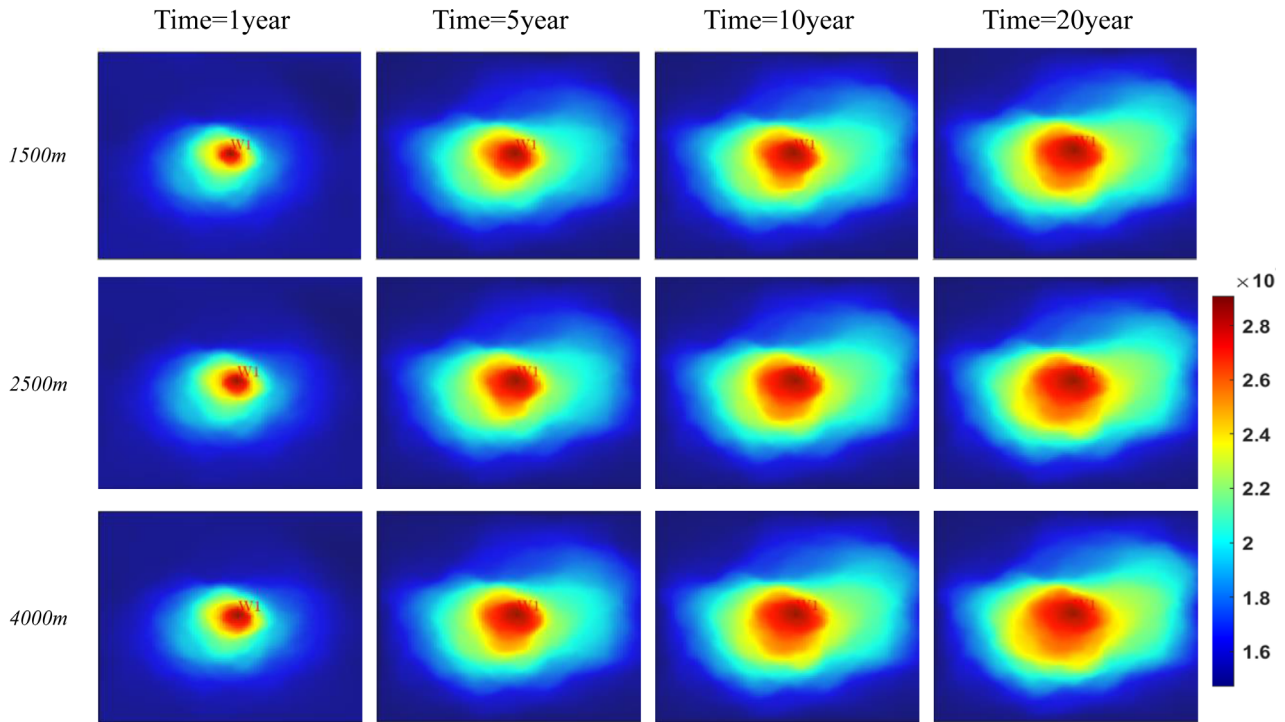


Fig. 18. Pressure distribution at different times under different stratigraphic pressure models.

capacity. Additionally, greater reservoir depth leads to better CO₂ compressibility, which facilitates greater CO₂ trapping underground.

Figure 18 shows the pressure distribution at different times under different stratigraphic pressure models.

Figure 19 shows the distribution range of CO₂ plumes at different injection times under various formation depth models. The deeper the formation depth, the more extensive the distribution range of CO₂ plumes. The underlying reason is that increased formation depth intensifies the

CO₂ displacement pressure difference, resulting in easier movement within the reservoir.

3.2.4 Reservoir temperature influence

To study the influence of different reservoir temperatures on the migration law of CO₂ plume, simulations were conducted at reservoir temperatures of 50 °C, 55 °C, 60 °C, 65 °C, and 70 °C, while the injection well maintained a fixed bottom flow pressure of 30 MPa. The other parameters remain unchanged.

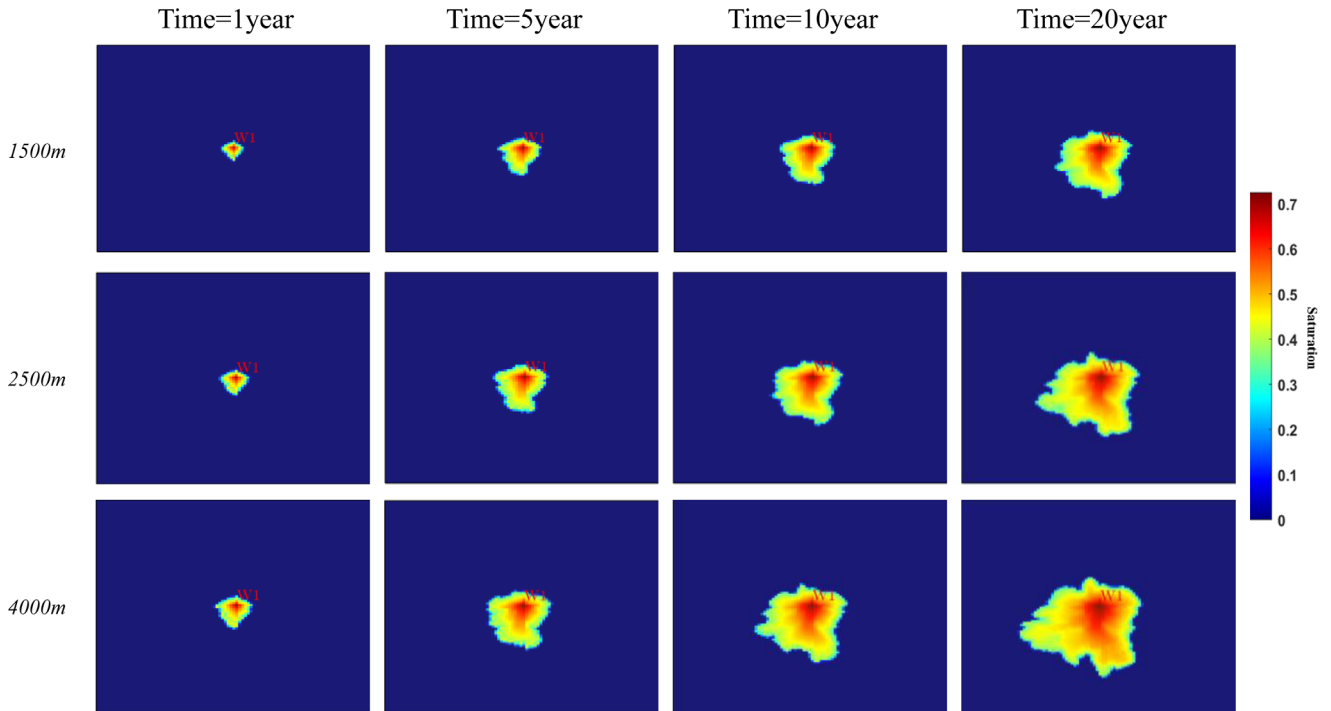


Fig. 19. Distribution range of CO₂ plume at different injection times under other stratigraphic pressure models.

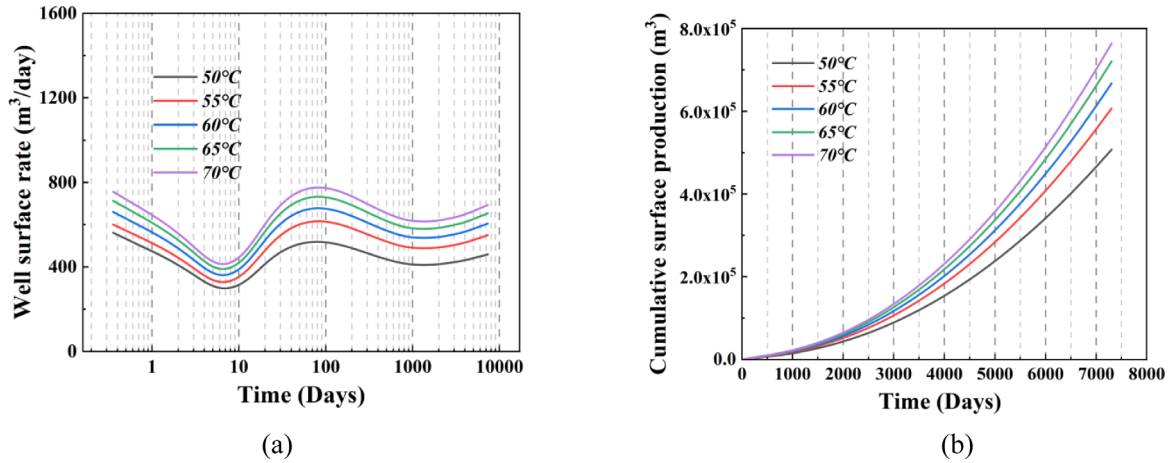


Fig. 20. Injection velocity curves and cumulative storage curves of different models. (a) Injection velocity curve. (b) Cumulative storage curve.

Figure 20 shows the injection velocity curve and cumulative storage curve of different models under different formation temperatures. As the formation temperature rises, the CO₂ injection velocity and cumulative storage capacity also increase.

It is crucial to note that reservoir temperature and pressure mainly affect the physical properties of CO₂. Under different reservoir conditions, the injection pressure and saturation distribution of CO₂ undergo changes. In contrast, the reservoir temperature and pressure simulation results emphasize that reservoir pressure exerts a more profound influence on CO₂ storage, while reservoir temperature has a relatively minor impact.

4 Conclusion

For the storage of CO₂ in deep saline aquifers, numerical simulation is an essential method for early prediction. In this study, we established a numerical model of supercritical CO₂ storage in deep saline aquifers. Our analysis, conducted using the MRST toolbox, focused on understanding the impact of reservoir properties, temperature, depth, and other characteristic factors on CO₂ geological storage capacity. The following conclusions were mainly drawn:

1. After supercritical CO₂ is injected into the reservoir, it is mainly affected by the reservoir heterogeneity,

leading to uneven transport distribution. Rapid transport occurs along hyperpermeability areas. Additionally, a pressure-holding phenomenon is observed initially during CO₂ injection, gradually giving way to increased injection rates as CO₂ seepage channels form over time.

2. The amount of CO₂ storage is mainly affected by the reservoir's physical properties. Enhanced physical properties result in greater storage capacity and faster CO₂ injection rates. However, the swifter migration of supercritical CO₂ plumes necessitates early consideration of CO₂ leakage risks. Therefore, the relationship between the reservoir's physical properties and injection speed should be comprehensively considered in the injection process, and the injection speed should be appropriately adjusted to obtain higher storage capacity while considering the risk of CO₂ leakage when the reservoir's physical properties are suitable.
3. The temperature and depth of the reservoir significantly affect the physical properties of CO₂, thereby affecting the pressure distribution and the migration range of the CO₂ plume under different reservoir conditions. Deeper formation depths and higher formation temperatures correlate with a more extensive distribution range of CO₂ plumes and increased cumulative CO₂ storage. Notably, the impact of temperature is relatively modest.

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Conflict interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Author contributions

Qigui Wang: Methodology, Conceptualization, Writing – Original Draft.

Dongxu Zhang: Review & Editing, Supervision.

Yaqi Li: Investigation, Visualization.

Chengyong Li: Validation, Visualization.

Huiying Tang: Validation, Visualization.

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