Evaluation of carbon dioxide storage in the deep saline layer of the Ordovician Majiagou Formation in the Ordos Basin

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Abstract. Geologic CO₂ storage (GCS) is one of the preferred solutions to reduce greenhouse gas emissions. Comparing with other geological reservoirs, the deep saline aquifers have huge storage potential and currently the most promising one. Since technical and economical viability of geologic CO₂ storage depends highly on the CO₂ storage capacity, this paper mainly uses the storage mechanism method to estimate the CO₂ storage capacity of the Ordovician Majiagou Formation in order to give data support for GCS project in the Ordos Basin. The results show that the total effective CO₂ storage capacity of the deep brine layer of the Ordovician Majiagou Formation in the Ordos Basin is 15.98-109.22Gt. The Majiagou Formation has sufficient storage capacity to accommodate decades of CO₂ emissions generated by multiple coal-fired power plants in the Ordos Basin. For CO₂ geological storage, the structural trapping mechanism contributes the largest amount of CO₂ storage, and the amount of CO₂ storage contributed by the two mechanisms of bound gas trapping and solubility trapping is almost negligible. The above results provide methods and references for CO₂ estimation of GCS project in this region, and provide data support for the site selection and injection of CO₂ sequestration in deep salt layers of the Ordos Basin.

1. Introduction
With the rapid development of industry, the greenhouse gas mainly CO₂ produced by the burning of fossil fuels has been increasing, which have emerged as significant global issues in scientific, environmental, economical, social, and political terms [1-6]. Relevant studies have shown that CO₂ geological storage technology is currently one of the preferred solutions for large-scale low-cost CO₂ emissions reduction in the world [1-3]. For CO₂ geological storage, geological reservoirs such as saline formations (aquifers), hydrocarbon (oil and gas) reservoirs, and coal beds have great storage potential. Among them the deep saline aquifers have huge storage potential and currently the most promising geological reservoirs in CCS projects [3]. CO₂ geological storage mechanisms mainly include structural trapping, irreducible water trapping, solubility trapping and mineral trapping. For deep saline formations, the storage process is the result of the simultaneous effects of different storage mechanisms. In the initial stage of CO₂ injection, structural trapping and irreducible water trapping play a major role. Over time, solubility trapping and mineral trapping has become increasingly prominent.

Technical and economical viability of geologic CO₂ storage (GCS) depends highly on the CO₂ storage capacity, because the CO₂ storage capacity is crucial to project planning, site selection and even
system designing for geologic CO₂ storage [4]. At present, many scholars have proposed a variety of approaches which can be divided into dynamic and static categories to evaluate the theoretical and effective fluid-phase CO₂ storage capacities of saline aquifers by physical trapping [5-7]. The material balance and reservoir simulation approaches belong to the dynamic approaches [8], and the volumetric-based and compressibility-based approaches are among the static approaches [9]. The dynamic approaches require numerous input parameters, and thus they can’t be applied before the site-specific data is acquired. On the other hand, the static approaches rely on only a few parameters (area, thickness and porosity etc.), which are directly related to the geologic formations, and thus they are applicable. As a result, the static approaches have been used more widely than the dynamic approaches [10-12].

The Ordos Basin, which is the subject of this study, is a large-scale energy and chemical base in China. Energy chemical companies are densely populated with high-concentration CO₂ emissions. This provides excellent conditions for the nearby capture and geological storage of CO₂, which is of great significance to achieving CO₂ emission reduction targets in the Ordos Basin.

Up to now, domestic and foreign scholars have done some research work on CO₂ geological storage in deep saline aquifers in the Ordos Basin, mainly focusing on storage mechanism research, experimental research, area selection research. In view of the fact that there are few studies on the carbon dioxide storage potential of the Majiagou Formation in the Ordos Basin by static approach, this paper mainly uses storage mechanism approach (static approach) to evaluate the CO₂ storage potential of the Ordovician Majiagou Formation in the Ordos Basin, in order to give data support for technical and economical viability of GCS in the Ordos Basin.

2. Study area

2.1. Geologic settings
The Ordos Basin has a vast area, spanning the five provinces (regions) of Shaanxi, Gansu, Ningxia, Mongolia and Shanxi. It is the second largest sedimentary basin in China with an area of about 3.7×10⁵ km² [13]. It is not only famous at home and abroad for its rich mineral resources such as oil, natural gas, and coal (Figure 1), but also for its stable internal geological structure, well-developed peripheral outcrops, and complete stratum exposure.

2.2. Roles of geologic formation in geologic CO₂ storage
This paper mainly selects the deep saline layer of the Ordovician Majiagou Formation in the Ordos Basin as the target reservoir for the estimation of CO₂ storage capacity. The carbonate reservoir is more than 800 meters thick, and the temperature and pressure conditions at its depth have reached the CO₂ supercritical state (31°C and 7.4MPa) [11-16]. The target reservoir contains high-salinity brines (20,000-50,000 ppm), which are not suitable for human consumption and currently have little economic value.

From the collected logging data, it can be seen that the Majiagou Formation is a continuous reservoir and the Ordovician in the Ordos Basin has developed weathering crust, dolomite, karst fracture-cavity and other types of reservoirs collectives. The rock porosity of the Majiagou Formation ranges from 1% to 11% with an average porosity of 5%, and the permeability ranges from 1 to 35mD. In addition, the excellent performance of the caprock of the Majiagou Formation can make long-term and safe storage of CO₂. Research shows that the deep saline layer of the Ordovician Majiagou Formation in the Ordos Basin is a favorable reservoir for CO₂ geological storage [16].
3. Estimation of CO2 storage capacity using the storage mechanism method

In view of the long time required for mineral trapping and the insufficient experimental research on the mineralization storage mechanism and the degree of related chemical reactions, this study only considers three storage mechanisms for CO2 injection in the short-term, namely structural trapping, bound gas trapping, and solubility trapping. In this study, the formulas used are as follows [12]:

a. Calculation formula for CO2 capacity by structural trapping:

\[ M_{CO2}^{\text{str}} = \rho \times A \times H \times \Phi \times (1 - S_{\text{wi}}) \times E \] (1)

b. Calculation formula for CO2 capacity by bound gas trapping:

\[ M_{CO2}^{\text{bgt}} = f_{\text{cog}} \times \Phi \times \rho_{f1} \times 10^{-3} \times E \] (2)

c. Calculation formula for CO2 capacity by solubility trapping:

\[ M_{CO2}^{\text{sol}} = A \times H \times \Phi \times (\rho \times X_{S}^{\text{CO2}} - \rho_{f1} X_{f1}^{\text{CO2}}) \times 10^{-3} \times E \]

\[ \approx A \times H \times \Phi \times \rho_{f1} \times R_{CO2} \times M_{CO2} \times E \times 10^{-3} \] (3)

Where, A represents the deep brine layer area (m²); H represents the depth of deep brine layer (m); \( \Phi \) represents the porosity of the deep brine layer (%); \( \rho \) represents the density of CO2 under corresponding stratigraphic conditions (kg/m³); \( S_{\text{wi}} \) represents residual water saturation (%); \( \rho_{f1} \) represents the average density of the formation water (kg/m³); \( X_{S}^{\text{CO2}} \) represents the solubility of CO2 in formation water (mol/kg). \( f_{\text{cog}} \) is the CO2 saturation trapped after the reverse flow (%); \( X_{f1}^{\text{CO2}} \) represents the fraction of CO2 in formation water when it is saturated by CO2 (%); \( X_{S}^{\text{CO2}} \) represents the fraction of raw CO2 in formation water, (%); \( \rho_{f1} \) represents the average density of formation water when saturated with CO2 (kg/m³); E stands for effective storage factor (dimensionless).

Before using the storage mechanism method to estimate the amount of CO2 stored in deep saline aquifers, some important parameters in the above formula need to be obtained. The calculation of the storage capacity of saline aquifer mainly depends on the volume of the saline aquifer in the trap. To estimate the CO2 storage capacity of structural/stratigraphic trapping, the average thickness, the density

Figure 1. Geological structure map of the Ordos Basin [17].
of supercritical CO$_2$ in saline reservoirs and effective storage factor must be determined. Before estimating the CO$_2$ capacity of residual trapping, it is necessary to determine the CO$_2$ density, porosity, and residual CO$_2$ saturation. To estimate the CO$_2$ capacity of solubility trapping, it is necessary to determine the average density of the original formation water, the CO$_2$ solubility of the formation water and the molar mass of CO$_2$.

3.1. Parameter acquisition

3.1.1. Area estimation. The thickness of the formation referred to in the formula is generally the average thickness, and the thickness of the deep saline layer varies in different layers and positions. According to the actual drilling data of thousands of wells in the Ordos Basin we have obtained, it is known that the average thickness of the Ordovician Majiagou Formation in the Ordos Basin is 550m, and the thickness map of the Majiagou Formation is shown in Figure 2.

![Figure 2. Thickness map of Ordovician Majiagou Formation in the Ordos Basin.](image)

According to the study of the structural conditions of the Ordos Basin, the suitable areas for CO$_2$ geological storage in the Ordos Basin are located in the distribution area of Majiagou Formation in the Tianhuan Depression except for the missing area of the central paleo-uplift in the east of the Baiyanjing-Shajingzi fault, the north of the northern margin of the Weibei uplift, the west of the Yellow River fault, and the south of the Yimeng uplift (Figure 3). The area suitable for CO$_2$ geological storage is calculated to be approximately 141,000km$^2$. 
3.1.2. Formation temperature and pressure. According to the measured ground temperature and ground pressure distribution data of the Majiagou Formation in the Ordos Basin, the relationship between temperature and burial depth can be obtained as $T=0.0285\times D+9.4282$ (T is Temperature, °C; H is buried depth, m), and the relationship between pressure and burial depth can be obtained as $P=0.0049H+14.684$ (P is pressure, MPa; H is buried depth, m). The Figure 4 and Figure 5 are drawn according to the relation between temperature and pressure and buried depth. Figure 4 shows that the top surface temperature of the Majiagou Formation gradually increased from 65-75°C in the east to 130-140°C in the west. Figure 5 shows that the top surface pressure of the Majiagou Formation gradually increased from 20 MPa in the east to 40 MPa in the west. The CO2 stored in the Majiagou Formation is in a supercritical state ($T>31.1\, ^\circ\text{C}$ and $P>7.38\, \text{MPa}$) which provides suitable geothermal and geopressure conditions for the effective injection and storage of CO2 [1-5,7,16-19].

**Figure 3.** The Ordovician Majiagou Formation suitable for CO\textsubscript{2} storage in the Ordos Basin.
3.1.3. The solubility of CO₂ in the formation water. The solubility of CO₂ and CO₂ density in the formation water are functions of temperature, pressure and sodium chloride concentration. At present, the models proposed by many international scholars all use the formation pressure, temperature and average concentration of sodium chloride. According to a calculation model for the solubility of CO₂ in pure water and sodium chloride aqueous solution [20], the solubility of CO₂ in the formation water is 0.96 mol/kg.

3.1.4. CO₂ density. Density (ρ) is the mass (m) of a substance per unit volume (V). The number of moles of gas (n) is the ratio of mass (m) to relative molecular mass (M), as (Equation 4):

\[ n = \frac{m}{M} \]  

Then put (Equation 4) into the state equation \( PV = n \cdot R \cdot T \), we get:

\[ PV = \frac{m}{M} \cdot R \cdot T \]  

(5)

Where P is the pressure (MPa); R is the ideal gas constant; T is the temperature (°C).

Considering that the deviation coefficient will affect the real gas, the compression coefficient is introduced, and then the equation of state can be written as:

\[ P = \frac{m}{V} \cdot \frac{R \cdot T \cdot Z}{M} \]

Therefore, the density of CO₂ can be calculated by (Equation 6):

\[ \rho_{CO₂} = \frac{m}{V} = \frac{P \cdot M}{Z \cdot R \cdot T} \]

(6)

Where M refers to the relative molecular mass of CO₂ gas, which is 44; R is the ideal gas constant, in the legal unit of measurement R is 8.314 J·mol⁻¹·K⁻¹. Z is the compressibility. According to the new fitting equation made by Fu Chang et al. [21] on the experimental data of supercritical CO₂
compressibility, Z is 0.4996, so the CO₂ density mainly depends on temperature and pressure, which are related to the buried depth respectively. According to the statistical formula of temperature and buried depth and the statistical formula of pressure and buried depth, the relationship between carbon dioxide density and buried depth can be obtained as ρ = -7×10⁻⁶H² + 0.1248H + 537.09, (ρ is CO₂ density, kg/m³; H is buried depth, m).

From the carbon dioxide density distribution map of the Ordovician in northern Shaanxi (Figure 6), it can be seen that the average CO₂ density is 880kg/m³ in the saline layer with the buried depth ranging from 1000m to 4000m.

3.1.5. Porosity. The Ordovician in the Ordos Basin has developed several types of reservoirs, such as weathering crust, dolomite and karst fracture cave. The porosity range of rocks in the Majiagou Formation is 1%-10%, and the average porosity is 5% [22].

![Figure 6. CO₂ density diagram of Majiagou Formation in the Ordos Basin.](image)

3.1.6. Density of original formation water. The total solubility of solid in the formation water in the study area is about 30-40g/L and the density of water is 1000kg/m³. By using these parameters, the density of the original formation water was calculated to be 1030kg/m³.

3.1.7. CO₂ saturation of bound gas storage. Residual CO₂ saturation is related to porosity, which is calculated by equation (7).

\[
S_{gr} = -0.3136 \times \ln \varnothing - 0.1334
\]  

(7)
Where $S_g$ is the CO$_2$ saturation for bound gas storage (%), and $\varnothing$ is porosity (%). When the average porosity value used in the calculation is 5%, the CO$_2$ saturation of the bound gas storage is 13.34% [23].

3.1.8. Effective storage factor. The United States Department of Energy (USDOE) uses Monte Carlo simulation to obtain the statistical distribution of the effective storage factor (E), which ranges from 0.0117 to 0.04 [24].

3.1.9. Irreducible water saturation. Studies have shown that the irreducible water saturation of the saline layer is 0.2-0.6 [25-28].

3.2. Estimation results of CO$_2$ storage capacity

In fact, there are two main parameters that are difficult to obtain when calculating the amount of CO$_2$ structural storage. One is the effective storage coefficient and the other is the average density of CO$_2$. According to the research conducted by Kopp. A [25] on the effective storage factor of CO$_2$ in the salt water layer, the range is 0.0117-0.04, the average density of CO$_2$ is 880 kg/m$^3$.

Incorporating the above parameters into (Equation 1), (Equation 2) and (Equation 3), the calculation results are as follows:

1. The CO$_2$ capacity of structural trapping is 15.97-109.19 Gt;
2. The CO$_2$ capacity of bound gas trapping is 0.005-0.018 Gt;
3. The CO$_2$ capacity of solubility trapping is 0.002-0.007 Gt;

Therefore, the total capacity of CO$_2$ trapped in the deep saline layer of the Ordovician Majiagou Formation in the Ordos Basin is 15.98-109.22 Gt.

4. Conclusion

(1) The biggest difficulty in using the static storage potential evaluation method is that it is difficult to measure the density of carbon dioxide in the supercritical state. This paper proposes a method to determine the density of carbon dioxide in the supercritical state.

(2) The total effective CO$_2$ storage capacity of the Majiagou Formation of Ordovician in the Ordos Basin is 15.98-109.22 Gt estimated by the storage mechanism method, which can provide data support for the site selection of CCS project in the Ordos Basin.

(3) During the implementation period of carbon dioxide injection, the structural trapping contributes the largest amount of CO$_2$ storage(15.97-109.19 Gt), and the amount of CO$_2$ storage contributed by the two mechanisms of bound gas trapping and solubility trapping is almost negligible(0.005-0.018 Gt, 0.002-0.007 Gt, respectively).

(4) The Majiagou Formation has sufficient storage capacity to accommodate decades of CO$_2$ emissions generated by multiple coal-fired power plants and/or commercial coal to chemical plants in the Ordos Basin.

5. Discuss

(1) In this paper, the author did not consider the dynamic changes of the reservoir during CO$_2$ solubility trapping and the amount of CO$_2$ stored by mineral trapping. During the CO$_2$ geological storage process, CO$_2$ chemically reacts with minerals such as calcite, dolomite, limestone and quartz in carbonate reservoirs. Whether the dissolution reaction has a positive or negative effect on the porosity and permeability of the reservoir needs further experimental study.

With the injection of CO$_2$ in carbonate reservoirs, the balance of the system is altered, where once CO$_2$ is dissolved in the formation fluid, two processes (the solubility trapping and the mineral trapping) can be developed. Carbonate reservoir heterogeneity and flow velocity have a great influence on dissolution kinetics and reaction rate [28-30]. The geochemical reaction of supercritical CO$_2$-brine-reservoir system under reservoir pressure and temperature is the only way to study solubility trapping and mineral trapping, which is the author's next focus research object.
Although solubility trapping and mineral trapping takes an extensive time to occur, it is the safest mechanism to permanently trap CO₂ over long time-scales. Until recently, it was assumed that temperature, pressure, salinity and the mineral composition of the formation rock are the key parameters that affect the mineral trapping process. Recent research has shown that excepting these parameters, aquifer thickness, tilt angle and anisotropy also have significant influences on solubility and mineral trapping [31]. The author intends to combine these factors to conduct the experimental study of CO₂ mineralization and sequestration in carbonate reservoir over long-term time-scales at low temperatures to represent actual reservoir conditions.

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