



Understanding and application of CO₂ adsorption capacity estimation models for coal types



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HIGHLIGHTS

- Characteristics of CO₂ adsorption capacity in various coal types are described.
- Methodologies for estimating CO₂ adsorption capacity in various coal type are presented.
- Effect of adsorbed phase density is presented.
- Adsorption capacity estimation in terms of fugacity and pressure is explained.
- Correlation models and EOS models under highly dense phase conditions are compared.

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ABSTRACT

Geosequestration is an attractive mechanism to store CO₂ for geologically significant time periods in order to minimise climate changing impacts on the environment. Reservoirs such as coal seams are used as storage reservoirs. However, it is very important to estimate the quantity of CO₂ that can be stored in a coal reservoir. In this study, existing storage models such as correlation models and Equations of State (EOSs) in the context of different coal types are compared, together with the experimentally-observed isotherms. Under highly dense phase non-ideal conditions, CO₂ storage potential will be maximised. Therefore, the use of fugacity in place of pressure is suggested to estimate CO₂ storage capacity under highly dense phase conditions. Further, four new modified correlation type models are suggested and found to be of good agreement with existing correlation-type adsorption models such as the DR and Toth models. By using various adsorbed phase density values, it was found that use of value as 1.028 g/cm³ gave the most consistent results across all the proposed isotherm equations. Fugacity did not improve the results for the correlation models, nor did it worsen them. The correlation models were clearly less accurate than the EOS adsorption models, especially under highly dense phase conditions. For less dense phase conditions, all the isotherm models gave comparable results to the experimental adsorption isotherms, while for highly dense phase conditions there were varying results.

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1. Introduction

The concentration of greenhouse gases in the atmosphere has increased extensively due to anthropogenic emissions. The atmospheric concentration of carbon dioxide (CO₂) has increased from approximately 280 ppm (ppm) 200 years ago to around 380 ppm, and these emissions are believed to be leading to significant climate change, which will become more substantial over time [1]. Climate change is mostly associated with the burning of fossil fuels, and the two largest contributors to the emissions of greenhouse gases are transportation and power generation. As these activities provide the basis of modern life, they are unlikely to

cease in the short term. Therefore, the solutions to climate change must be a combination of better efficiency and technology that produces power with little or no CO₂ emissions [2]. One technology that has the potential to reduce CO₂ emissions is carbon capture and storage (CCS), also known as CO₂ sequestration. This involves capturing the carbon dioxide that is produced by large sources such as power stations, transporting it to a storage site and ensuring it remains cut off from the atmosphere for geologically significant periods of time, up to millennia [3,4]. One of the options that exist to help complete this process is storing the carbon dioxide in deep, unminable coal seams.

2. Carbon dioxide sequestration

Though a number of forms of CO₂ sequestration exist, the storage in deep geological media is considered as immediately

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potential and has large capacity for a very long retention time [5]. The geological media that can be used for CO₂ storage are oil and gas reservoirs, deep saline aquifers and coal seams [6]. For coal seams, the identification of a site suitable for storage is a significant challenge. This is because coal beds that are uneconomic to mine at present may become economic in the future. However, thin seams of coal at medium depths are likely to be uneconomic indefinitely and so are likely candidates [3]. One advantage of injection into coal seams is that power stations are situated in major coal basins, increasing the likelihood of suitable sites being available, while there are not necessarily suitable saline aquifers or oil and gas reservoirs nearby [7]. Deep coal seams generally contain considerable quantities of methane, and as carbon dioxide has a higher affinity to the coal, it will replace the methane when injected. Methane is less carbon-intensive than CO₂, and its recovery and use as a fuel can therefore be used to offset the sequestration costs. As coal also has a microporous structure, it has a large surface area and can adsorb large amounts of CO₂ [7–9].

2.1. Carbon dioxide sequestration in coal

The predominant form of storage of gas in coal is adsorption, the adhesion of molecules of the gas to the surface of the coal. According to White et al. ([12], P. 689) “gas stored by adsorption in the coal matrix accounts for 95–98% of the gas in the coal seam”. The characteristics of the coal will clearly influence its storage capacity. Coal varies based on a number of factors, including water content, carbon content and organic matter content. One important factor that distinguishes a coal type is its temperature history, which can be ascertained by looking at its vitrinite reflectance. Vitrinite is a type of organic matter in coal, and its reflectivity is related to the temperature ranges that correspond to hydrocarbon generation. Vitrinite reflectance (V_r) can therefore be used to classify the thermal maturity, or rank, of the coal [10]. Coal can be divided into categories based on V_r values, as is shown in Table 1.

3. Carbon dioxide

Carbon dioxide is a chemical compound composed of a carbon atom bonded with two oxygen atoms. At standard temperature and pressure it exists as a gas, and is a trace element within the Earth's atmosphere [12]. Some of the relevant properties are as shown in Table 2.

As with all gases, the state of carbon dioxide depends on both temperature and pressure. The temperatures and pressures at which carbon dioxide exists in these different states are shown diagrammatically in Fig. 1.

In order to estimate the adsorption capacity, an important factor to be considered is the adsorbed phase density of the carbon dioxide. This is not readily available through experimental measurement, and therefore is usually estimated [13]. Sudibandriyo used regressed estimates from various models, while Arri [14] used the common approximation of the triple point liquid density. These two options gave densities of 0.996 g/cm³ and 1.18 g/cm³

Table 1
Coal types based on vitrinite reflectance [11].

V_r	Category
0.0–0.3	Lignite
0.3–0.7	Sub-bituminous coal
0.7–1.1	High volatile bituminous coal
1.1–1.5	Medium volatile bituminous coal
1.5–1.9	Low volatile bituminous coal
>1.9	Anthracite

Table 2
Carbon dioxide properties.

Property	Value
Molecular weight	44 g/mol
Liquid density (at –20 °C, 19.7 bar)	1.032 g/cm ³
Solid density	1.562 g/cm ³
Gas density (at 15 °C, 1.013 bar)	.002814 g/cm ³
Compressibility factor (Z , at 15 °C, 1.013 bar)	0.9942
Specific gravity (with air = 1)	1.521
Specific volume (at 21 °C, 1.013 bar)	547 cm ³ /g
<i>Critical point</i>	
Critical temperature (T_c)	31 °C
Critical pressure (P_c)	73.825 bar
Critical density (ρ_c)	0.464 g/cm ³
<i>Triple point</i>	
Triple point temperature	–56.6 °C
Triple point pressure	5.185 bar

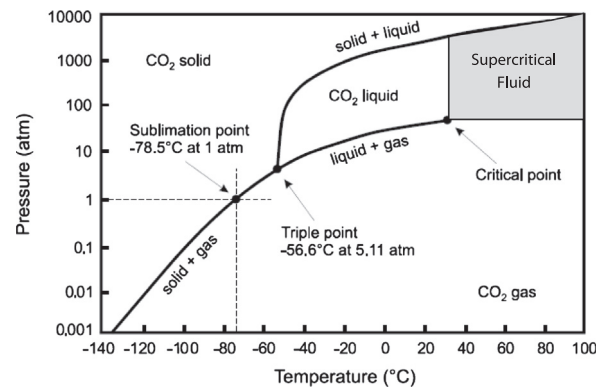


Fig. 1. Phase diagram for carbon dioxide.

respectively. As the adsorbed phase density will clearly influence the accuracy of the models, and it is not well defined, the values which give the most accurate results for various types of coal require investigation.

As can be seen in Fig. 1, at very high temperatures and pressures carbon dioxide is a supercritical fluid. In a supercritical state, a substance such as carbon dioxide can behave as either a gas or a liquid, depending on the conditions, and small changes in temperature or pressure can result in large changes in density [15]. As adsorption into coal will often take place near or above the critical point, the differences in behaviour in this state must be taken into account.

3.1. Fugacity

To correct for the non-ideality of gases at high pressures, pressure should be replaced by fugacity (f), which shows better agreement with reality [16]. This quantity also has units of pressure (P), and can be determined either experimentally or by using various models. Fugacity is related to pressure by the fugacity coefficient, ϕ , as shown in Eq. (1).

$$f = \phi P \quad (1)$$

There are a number of different models that can be used to find the fugacity at a certain pressure. One of the most common models is the Peng Robinson Equation of State (EOS), and the fugacity expression is shown below [17].

$$\ln(\phi) = z_i - 1 - \ln(z_i - B_i) - \frac{A_i}{2.8284B_i} \ln \left(\frac{z_i + 2.4142B_i}{z_i - 2.4142B_i} \right) \quad (2)$$

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