



Molecular simulation of displacement of shale gas by carbon dioxide at different geological depths



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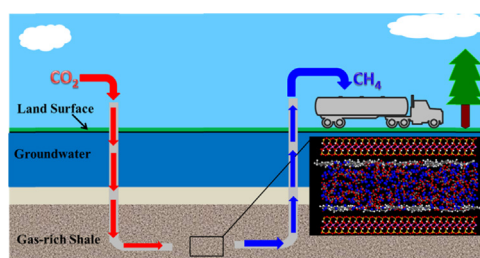
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HIGHLIGHTS

- We investigate the displacement of shale gas by carbon dioxide at different conditions.
- The increase of pore size is beneficial for the displacement of shale gas.
- The optimum operating conditions of carbon dioxide displacing shale gas are recommended.

GRAPHICAL ABSTRACT



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ABSTRACT

The rising worldwide energy demand has greatly stimulated the exploitation of shale gas. Meantime, global warming mainly caused by CO₂ emission is a significant concern. As a new scenario, injecting CO₂ to displace shale gas is proposed to improve the exploitation efficiency of shale gas and reduce the amount of CO₂ emission. In this work, we use a grand canonical Monte Carlo simulation to investigate the displacement of shale gas by CO₂ and the sequestration of CO₂ simultaneously in a modeled shale matrix at different geological depths from 1 to 4 km, where the shale is modeled by inorganic clay mineral and organic matter. We find that both the displacement amount of CH₄ and the sequestration amount of CO₂ increase with the pore size of the shale at a fixed CO₂ injection pressure, which suggests that the hydro-fracturing technology would be very beneficial for displacement exploitation of shale gas. Moreover, we also find that the optimum operating condition for CO₂ displacing shale gas is at the depth of 1 km, which provides a guidance and reference for displacement exploitation of shale gas by CO₂.

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1. Introduction

Recently, the exploration and development of shale gas have received extensive attention worldwide because of its numerous advantages such as low pollution, wide distribution, and abundant resource (Howarth et al., 2011). Shale gas, as an unconventional gas source, refers to a kind of natural gas that exists in shale reservoirs (Shaikh and Ji, 2016; Youinou, 2016), and is now

increasingly deemed as a low carbon and an environmentally friendly energy option. The United States of America (USA) is the earliest country to apply the horizontal drilling and hydro-fracturing into the exploration and development of shale gas (Arora and Cai, 2014; Connor et al., 2015). The output of shale gas has reached 13.78 billion cubic meters per year in USA, with an average annual growth rate of 47.7% (Zhai et al., 2014), while, the natural gas from shale formations is about 23% in 2010. And, it is anticipated to contribute 49% of gas production by 2035 (Ashmoore et al., 2016). In order to reduce pollution and meet a surge in energy demand, China aims to produce 30 billion cubic meters of shale gas per year by 2020, from the current level of 1.3 billion

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cubic meters (Wang et al., 2016). Therefore, considerable efforts are undertaken by Chinese enterprises through the development of research programs in industry to make this resource successfully and economically available (Gasparik et al., 2012).

Currently, the ultralow porosity of shale and ultralow permeability of gas reservoirs are still a great challenge in the exploration of shale gas (Clarkson et al., 2016). Hydro-fracturing is a commonly used method to enhance matrix permeability of unconventional reservoirs and enable the economic production of shale gas from the shale reservoirs (Chen and Carter, 2016; Clark et al., 2012; Clarkson et al., 2016). However, the hydro-fracturing would cause severe environment impacts, e.g. huge water consumption, potential contamination of water and so on (Clark et al., 2012; Connor et al., 2015; Krogulec and Sawicka, 2015; Krupnick and Gordon, 2015). Alternatively, the new scenario, the injection of CO₂ gas to displace the adsorbed CH₄, has been proposed by some researchers (Kowalczyk et al., 2012; Shi and Durucan, 2003; Wang et al., 2015b; Wu et al., 2015; Yu et al., 2008). It arouses extensive interests from scientists, because it can improve the shale gas recovery and sequesterate CO₂ simultaneously.

Most studies on the displacement of CH₄ adsorbed in shale matrix by CO₂ have been carried out by the experiment and computation at present. Wu (Wu et al., 2015) studied the displacement of CH₄ in carbon nanochannels by molecular dynamics (MD) simulations. And they drew a conclusion that CO₂ can displace the adsorbed CH₄ directly. Yuan (Yuan et al., 2015) also explored the displacement of CH₄ by injecting CO₂ on graphene, and found that CO₂ can be adsorbed on graphene more easily than CH₄, which may be a good candidate for displacement of CH₄. Pathak (Pathak et al., 2015) performed MD simulations on the kerogen-methane-carbon dioxide system to understand the absorption-adsorption-desorption phenomena of the super critical CO₂ fluid, and found that CO₂ can sweep the adsorbed CH₄ from the kerogen matrix in the shales. Kowalczyk (Kowalczyk et al., 2012) investigated displacement of CH₄ by Monte Carlo simulations, and proposed two-stage mechanism for the displacement of CH₄ from carbon nanopores by coadsorbed CO₂. Wang (Wang et al., 2015a) conducted experiments to study the coal-bed CH₄ displacement by CO₂ injection, and found that the adsorption capacity of CO₂ is stronger than that of CH₄ under the same condition in the process of displacement.

A large proportion of pores within the gas shale matrix are nanosized, and most of these pores are associated with the constituents of the shale matrix and the contents of each components (Cui et al., 2009). In addition, the shale matrix often contains some free gases in relatively large pores and adsorbed gas on the organic matter and inorganic minerals (Zhang et al., 2012). To deal with the complex situation, it is necessary to simplify the complicated structure of shale matrix to gain some basic insights into its adsorption behavior. There are two ways to address this topic in the literatures. One is to assume the clay-rich shale as the crystal

structure of montmorillonite with the basal spacing and number of ions changing (Zhai et al., 2014). The disadvantage of this method does not include the organic matter. In fact, the organic matter is an indispensable factor on the CH₄ adsorption in shale matrix. The other method is to model the complex natural matrixes as a collection of independent, on-interconnected slit pores with perfect graphitic walls without consideration of inorganic minerals (Hu et al., 2011). As a result, it is important to construct an all-atom shale model including inorganic minerals and organic matter to investigate the adsorption and displacement of CH₄ in gas shale matrix.

In this work, we proposed a modified and generalized shale matrix model including inorganic minerals and organic matter. Then, the mechanism of the displacement of CH₄ by CO₂ in shale matrix model was investigated through molecular simulations. Finally, some discussion was also addressed.

2. Computational details

2.1. Models and potentials

Since CH₄ is the major component of shale gas, we use it to represent the shale gas. The components of gas shale matrix include organic matter, inorganic clay minerals, quartz, carbonate, calcite, pyrite, and the others (Tan et al., 2014). The main ingredients in the gas shale matrix from different places are nearly the same, but their contents of the components are different. Here, we mainly consider the case of CH₄ in shale matrix, which contains organic matter and inorganic clay minerals. To construct the shale matrix model containing inorganic clay mineral and organic matter, we used two perfect montmorillonite sheets to represent the inorganic clay mineral. Montmorillonite is a typical 2:1 inorganic clay mineral, and the unit cell consists of an Al–O octahedral sheet and two Si–O tetrahedral sheets, while the Al–O sheet is sandwiched between Si–O sheets. Generally, it is believed that the polycyclic aromatic hydrocarbon is a major organic component of shale matrix, especially for shale gas reservoirs. Therefore, we used methylnaphthalene to represent the organic matter in the shale matrix here.

We constructed a simulation box (31.1 × 35.9 × c Å) that contains two inorganic layers and two organic layers (see Fig. 1). As mentioned above, the perfect montmorillonite sheets were used to represent the inorganic layers. The structure of the montmorillonite sheets was obtained from the Cambridge Crystallographic Data Centre (CCDC) database. First, two perfect montmorillonite sheets were stacked each other in such a way as shown in Fig. 1. Then, a set of methylnaphthalene molecules were adsorbed into the interlayer space, where the pore size of our model was adjustable through the basal spacing. The methylnaphthalene molecules adsorbed into the interlayer space were fixed, as the

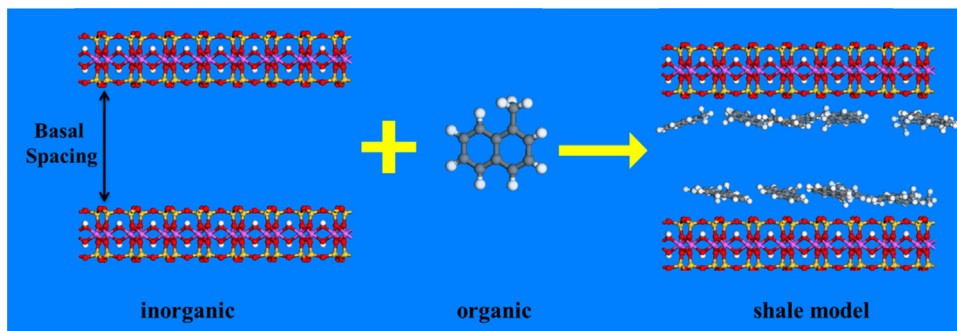


Fig. 1. The scheme of modeled shale matrix. Color scheme: red, oxygen; yellow, silicon; pink, aluminum; white, hydrogen; and black, carbon.

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