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# مدلسازی مولکولی در انتقال CO2 در مونتموریونیت: انتشار و نفوذ

چکیده

ذخیره کردن CO2 در سفره‌های زیرزمینی شور برای کاهش انتشار CO2 در جو مفید است، جایی که انتشار گاز/ مایع و نفوذ در مواد معدنی کان رس نقشی اساسی در نشت CO2 و مهاجرت زیرزمینی دارد. نفوذ پذیری CO2 و نفوذ پذیری مایعات مختلف در لایه‌های کانی رس (مونتموریونیت، Mt) با استفاده از پویایی مولکولی (MD) بررسی می‌شود. نفوذ پذیری CO2 و H2O با غلظت آب و دما افزایش می‌یابد اما بیشینه غلظت CO2 را به صورت غیرمعمولی ۲ مولکول/واحد-سلول نشان می‌دهند. حجم آزاد کسری Mt با غلظت CO2 افزایش می‌یابد اما اگر غلظت CO2 از ۲ بیشتر شود شروع به کاهش می‌کند، بنابراین دلیل تغییر غیر خود نفوذی ( خود پخشی) CO2 به صورت غیرهادی همین است. قابلیت‌های پخش (M-S) و فیک (Fick) رابطه مستقیمی با غلظت و دمای CO2 دارند. در اینجا قابلیت خود نفوذی CO2 برای نخستین بار با روش دینامیکی مولکولی اندازه گیری می‌شود. با این توضیح که قابلیت نفوذ CO2 با فشار CO2 و غلظت H2O افزایش می‌یابد، در صورتی که به علت قابلیت حلالیت پایین CO2 در دمای زیاد، نقطه برگشت را پایین می‌برد.

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Research paper

# Molecular modeling on transportation of $CO_2$ in montmorillonite: Diffusion and permeation

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ABSTRACT

$CO_2$ storage in underground saline aquifers is helpful to reduce $CO_2$ emission in the atmosphere, where gas/fluid diffusion and permeation in clay mineral plays a key role in $CO_2$ leakage and underground migration. $CO_2$ Permeability and different fluid diffusivities in clay mineral (montmorillonite, Mt) interlayers are investigated by molecular dynamics (MD). Both $CO_2$ and $H_2O$ self-diffusivities increase with water concentration and temperature but show a maximum at the $CO_2$ concentration of 2 molecule/unit-cell unconventionally. The fractional free volume of Mt increases with $CO_2$ concentration but begins to decrease if $CO_2$ concentration exceeds 2, thus giving the reason for the above unusual $CO_2$ self-diffusivity variation. Displacement distribution of $CO_2$ molecules is found to be characterized by logarithmic normal distribution. The mean value of such distribution further supports the self-diffusivity dependence on $CO_2$ concentration. M-S and Fick diffusivities of $CO_2$ are positively related to $CO_2$, $H_2O$ concentration and temperature. $CO_2$ permeability is calculated by MD for the first time, which increases with $CO_2$ pressure and $H_2O$ concentration but exhibits a turning point at temperature 360 K due to low $CO_2$ solubility at high temperature.

## 1. Introduction

$CO_2$ storage in underground saline aquifers provides long-term and large-scale storage of $CO_2$, which is a promising way to reduce $CO_2$ emission in the atmosphere. In this process, clay minerals, such as illite, chlorite, kaolinite, and montmorillonite (Mt) (Josh et al., 2012), are the main components of caprocks. Owing to their porous (layered) structure, the clay minerals have remarkable capacity of adsorbing $CO_2$ (Fu et al., 1990; Khosrokhavar et al., 2014). On the other hand, clay mineral has a low permeability and therefore the clay-enriched caprocks show excellent sealing ability to retain injected $CO_2$ (Abdou and Ahmaed, 2010; Gaus, 2010; Gernot et al., 2013). Gas leakage and environmental impacts are the most concerned problems for risk assessments of $CO_2$ storage, which are closely related to fluid (gas) transportation (diffusion and permeation) in clay mineral.

The interactions of $CO_2$ and clay mineral have been reported by many authors. For example, Giesting et al. investigated impact of $CO_2$ absorption on Ca-exchanged Mt expansion under different $CO_2$ pressure (Giesting et al., 2012). $CO_2$ can migrate the interlayer region of montmorillonite based on the in situ X-ray diffraction (XRD), magic angle spinning nuclear magnetic resonance spectroscopy (NMR) and attenuated total reflection infrared spectroscopy (ATR) (Loring et al., 2014; Loring et al., 2012). In addition, quasi-elastic neutron scattering experiments (QENS) experiments on hydrated clays have shown that hydrated cation diffusion mobility is probably a complex dynamic process and the diffusion coefficients of the exchangeable cations were estimated (Sobolev et al., 2009). Kozaki et al. determined the apparent diffusion coefficients of $Cs^+$ as functions of the temperature (Kozaki et al., 1999). Sánchez et al. discussed that the self-diffusion of water depended on temperature and ionic strength in different kinds of clays (Sánchez et al., 2008). However, there are a few experiments on diffusivity of $CO_2$ in clay although permeation processes in sediments and clay-rich rocks have been investigated experimentally by many authors (Javadpour et al., 2007). For instance, permeability of $CO_2$ declined during shearing while increasing sliding velocity reduced the decline rate (Javadpour, 2009). Permeability of simulated granite is highly related to fracture transmissivity (Tanikawa et al., 2014).

Molecular simulation becomes a powerful tool in many fields and has been used for understanding the molecular-scale structural (Lee et al., 2014; Teich-Mcgoldrick et al., 2015), thermodynamic (Boek et al., 1995), mechanical (Zhang et al., 2015), and dynamic (Botan et al., 2010; Krishnan et al., 2013; Malikova et al., 2004; Yang and Zhang, 2005) properties of clay mineral. Grand canonical Monte Carlo (GCMC) method was applied to simulation the adsorption of $CO_2$ with $H_2O$ (Botan et al., 2010), $CH_4$ (Jin and Firoozabadi, 2013; Kadoura et al., 2016; Yang et al., 2015), and organic molecules (Krishnan et al.,

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