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Experimental and theoretical investigations on kinetic mechanisms of low-pressure CO_2 adsorption onto Malaysian coals

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ABSTRACT

The adsorption mechanism of carbon dioxide (CO_2) in the coal matrix is significant in practical stability and migration process of CO_2 into a coalbed seam. This study presents the kinetic investigation and the main controlling step of CO_2 adsorption capacity onto Malaysian coals. The experimental data of CO_2 adsorption were determined using a volumetric technique at 273, 298, 308, and 318 K and pressures up to 99.3 kPa. The experimental data of CO_2 adsorption was studied using kinetic based thermodynamic models. Fourier Transform Infrared Spectroscopy and X−Ray Diffraction analyses were performed for the coal samples characterization. The major functional group in all coal samples is hydroxyl (−OH) functional group. X−Ray Diffraction analysis has shown that the coal samples possessed one major peak assigned to quartz ($d = 3.348$ Å). The experimental results were correlated using kinetic models, which include pseudo−first−order, pseudo−second−order, Avrami, and Intra-particle diffusion models. The Intra−particle diffusion model was found in the best compliance with the experimental data. Therefore, the pore−diffusion is considered to be the primary limiting step for CO_2 interaction with the coal matrix. This indicated that the molecules of CO_2 transferred rapidly from the bulk to the surface of coal matrix and slowly diffused into pores of the coal matrix. The obtained results demonstrated that the overall CO_2 interaction with the coal matrix is influenced by the diffusion limiting step. The value of activation energies for all studied coal samples is lower than 8 kJ/mol. This showed that CO_2 adsorption onto all investigated coal samples is driven by a physical adsorption process.

1. Introduction

Carbon dioxide (CO_2) is considered as one of the main anthropogenic greenhouse gases having a considerable contribution to global warming and environmental issues (Hou et al., 2020; Mukhtar et al., 2020a). Geological storage of CO_2 in un-minable coal seams has been recognized as one of the promising underground deposits to mitigate the excessive emissions of CO_2 and enhance coalbed methane (ECBM) displacement (Weniger et al., 2012; Kang et al., 2019; Sun et al., 2018; Cho et al., 2019). The capabilities of existing separation and capture technologies of CO_2 from the flue gas are costly and require further research (Harbin et al., 2015; Pennline et al., 2008; D'Alessandro et al., 2010; Ullah et al., 2019a; Ullah et al., 2016). Coal typically has a particular pore configuration with a significant internal surface area for the adsorption of gas and has a high affinity towards CO_2 compare to methane (Yutong and Yu, 2018; Niu et al., 2020). The intact coal matrix comprises micropores that regulate CO_2 diffusion and adsorption, and perform as primary gas sequestration reservoirs (Sampath et al., 2020; Wang et al., 2020a). Gas adsorption triggers considerable changes in the micro−porous configuration and resulting in the decline of gas diffusion coefficient imposes impact on the gas transport (Wei et al., 2019). The International Union of Pure and Applied Chemistry (IUPAC) categorized pores in adsorbent into micropores (<2 nm), mesopores (2–50 nm) and macropores (>50 nm) (Zhao et al., 2016). Coal specific surface area was originally

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