Simulation Study on the Separation of SO_2 from CO_2, H_2 and N_2 using ZIF-1

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Zeolite imidazolate frameworks (ZIFs) have gained more attention in recent years [1]. ZIFs are a new and special class of metal–organic frameworks (MOFs), that potentially have the advantages of both inorganic zeolites (for instance, high stability) and of MOFs (for instance, high porosity, high surface area and organic functionality), which are applied to high performance in separation processes [2]. ZIFs comprised of imidazolate linkers and tetrahedral metal ions (e.g., Zn, Co), with structures similar to conventional aluminosilicate zeolites. Their intrinsic porous characteristics, abundant functionalities as well as exceptional thermal and chemical stabilities [3] have led to a wide range of potential applications for various ZIF porous materials [4]. Their attractive and potential applications in gas sorption, gas separation, and catalysis [5], sensing, electronic devices, and drug delivery in the past years are discussed and reviewed [4]. This study investigates the separation based on adsorption of the binary gas mixture of SO_2 with CO_2, H_2 and N_2. Therefore, Grand canonical Monte Carlo (GCMC) simulation is used to study the adsorption of pure gases using ZIF-1 at 10-10000 kPa and 298 K. In all simulations, 1.5×10^7 of iterations were considered. The first half of iterations are used to set up the equilibrium of the system and the last half of iterations is used to calculate the ensemble average values of the thermodynamic parameters. The adsorption and separation behavior of SO_2-CO_2, SO_2-H_2 and SO_2-N_2 binary mixtures in ZIF-1 were investigated using GCMC, with mixture compositions of 50:50 mol%. The results showed that the selectivity of SO_2 is found to be maximum at a pressure less than 10 kPa and also, the calculated selectivity decreases with increasing pressure upper than 10 kPa. Furthermore, the maximum selectivity of SO_2 over CO_2, N_2 and H_2 are observed 6.8, 41.3 and 187.1, respectively.

Keywords: Separation, Zeolite imidazolite framework, GCMC simulation, Sulfur dioxide

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