

The Influence of the Force Field Used in Simulations in the Adsorption Behavior of Carbon Dioxide

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Chemical or physical adsorption of CO₂ onto a material is possibly one of the most promising areas of research for avoiding the emission of CO₂ concentration in the atmosphere. Adsorbent materials capable of capturing CO₂ are already available and used in a wide variety of processes; examples of these solid materials are alumina, zeolites, activated carbon, silicas and clays. However, for the selection of an optimal adsorbent for a given process it is necessary to be able to know the properties of the adsorbent at the adequate process conditions. An attractive route to obtain this knowledge is by the use of predictive tools such as molecular simulations. We present here Monte Carlo simulations in the grand canonical ensemble of CO₂ adsorption in selected materials. The calculated equilibrium properties are easily related to the main properties for selecting a solid adsorbent, the selectivity, and the capacity. In order to study the influence of the force fields used to simulate CO₂ on the adsorption, we model different model porous materials described by simple geometries using different models for the fluid. Two series of results are presented: (i) adsorption in graphite slit pores using a simple and a more refined model for CO₂, to study the influence of the fluid model on the final results and (ii) adsorption using a simple model of CO₂ in slit and cylindrical pores, to study the influence of the geometry on the adsorption behavior. In all cases the results are compared to the experimental results to serve as a reference of the accuracy of the models, but they are not fitted to reproduce the complex geometry of adsorbent materials (i.e. no PSD was used to fit the data)