A molecular simulation study of competitive adsorption of carbon dioxide, propane and butane in porous silica

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In this work we report molecular simulation results for carbon dioxide, propane and butane adsorption in porous silica. The NVT-ensemble molecular dynamics technique with the melt-quench algorithm was utilized for modeling the structure of amorphous silica. The porosity of the adsorbent was modeled by an array of slit-shaped pores, characterized by a pore-size distribution. The adsorbent surface was supplemented by hydroxyl groups (at a density which is close to the experimental value). Monte-Carlo methods in the isobaric-isothermal Gibbs ensemble were used to calculate the adsorption isotherms. The obtained results for single components as well as binary mixtures were consistent with recent obtained experimental data. Carbon dioxide and butane are less adsorbed in mixtures than as single components. Whereas the adsorbed amount of propane in mixtures with carbon dioxide or with butane can be even larger than for the case of pure propane (at a relatively low surface loading). The possible origins of this behavior are discussed.