

Evaluation of Zeolite LTA-Force Fields for Molecular Dynamics Simulation Purposes

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Natural gas produced from gas reservoirs are commonly accompanied by other, undesirable, components. The operator is often required to remove trace components to meet the transport specifications. A number of methods are currently available for removing trace components and/or drying the produced gas. Zeolite-based molecular sieves are one of the commonly used technologies for natural gas drying, but the actual mechanism and details of adsorption/trapping process at a molecular level are still not properly understood. Since most experimental work in this area operates on a rather large scale, when compared to the molecular level, it is hard to gain insights into the steps involved from free gas to adsorbed state. The bulk of the research in the atomic/molecular scale has mainly used Monte Carlo techniques since they lend themselves readily to computation of chemical potentials and Langmuir adsorption constants. Nevertheless, Monte Carlo methods are not designed for either obtaining process kinetics or following its time evolution. Molecular dynamics simulations offer an investigation tool much better suited for these purposes. The majority of previously published and tested Zeolite force fields have been constructed with only Monte Carlo simulations in mind. To determine whether they were suitable for molecular dynamics simulations, several simulations with different force fields have been carried out, with the results evaluated for their agreement with experiments like X-ray diffraction data. Lattice energies and behavior of sodium ions have also been compared to those from previous published works of other groups. Two force fields, both based on Jackson and Catlow's work, have emerged as clear favorites in our study.