ABSTRACT TITLE: DISLOCATION OF HYDROCARBONS USING CO_2

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ABSTRACT

A significant approach that has been employed which has enhanced the rate of production of confined hydrocarbon is the use of carbon dioxide as an additive. Carbon dioxide, when captured could be injected into the reservoir and sequestered due to the interaction between the carbon dioxide and the representative rock. The aim of this paper is to investigate the systems carbon dioxide and octane confined in calcite (1014) pore width of 3 nm using Molecular Dynamics Simulations. Analysis of the structural and dynamic properties of the confined fluids, including density profiles, mean square displacement and diffusion coefficients were carried out. The result obtained also suggested that the carbon dioxide which adsorbed on the calcite (1014) displaced the octane towards the pore centre. Strong multiple peaks were observed in octane density profile which is attributable to multiple layer adsorptions. To quantify the selfdiffusion coefficients of carbondioxide and octane, the mean square displacement with respect to time was plotted. The self-diffusion coefficient of octane was found to decrease with increasing carbon dioxide loading. The 300 K simulation also gave a reduced diffusion coefficient when compared to silica system from a prior research. The computed values of the diffusion coefficient obtained in this work are similar to results in literature.