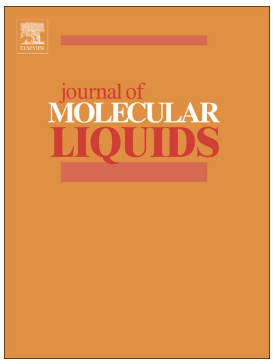

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Molecular Dynamics Simulation of Methane Hydrate Formation in Presence and Absence of Amino acid Inhibitors

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Abstract

In the present work, the methane hydrate growth kinetics is investigated by molecular dynamics simulation (MD) in the presence of different amino acids as inhibitors. The selected amino acids are glycine, alanine, proline, and serine with different concentrations (less than 1.5 wt%). The molecular dynamics simulation of the structure I hydrate is performed under the isobaric-isothermal (NPT) ensemble for both pure water and amino acid solution. Different parameters are determined to characterize the kinetics of methane hydrate formation such as the four-body structural order parameter ($F_{4\varphi}$), radial distribution function (RDF), mean square displacement (MSD), potential energy, density, and hydrogen bond formation. Our obtained MD results are in agreement with results from previous simulation studies and experimental observations. Analyzed MD data indicate that all studied amino acids act as inhibitors of methane hydrate. According to potential energy, van der Waals and electrostatic interactions between the amino acid and the solution lead to instability in the hydrate structure. $F_{4\varphi}$ evaluates the hydrate formation kinetics and the structural variation of hydrate in the presence of amino acids. Analysis of hydrogen bond formation indicates that the solubility of amino acids is an important factor in hydrate inhibition. The disruption of the hydrogen bond network also displays that an amino acid breaks the water hydrogen bond. According to the consequences of our study, the ranking of the inhibitory effect of the amino acids is as follows: serine > glycine > alanine ≈ proline. Serine and glycine are more effective hydrate inhibitors than other amino acids because of their chemical structures, solubilities, hydrogen bond formation, and low hydrophobicity.

Key words: Methane hydrate; Molecular dynamic simulation; Amino acid; Inhibitor; Kinetics.