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Molecular dynamics simulations of methane intercalation in hydrated na-montmorillonite

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In this study, Molecular dynamics simulations were performed to determine the behavior of methane intercalation into hydrated Na-montmorillonite (Na-Mt) with different water contents under two different temperature and pressure conditions (277 K/50 atm and 300 K/10 atm), typical of the marine sediment environments in which methane hydrates can form and decompose in bulk water. The simulation results showed that methane molecules are hydrated by interlayer water molecules and clay surface's oxygen atoms, forming complexes with water molecules and clay surface through the hydrogen-bonded network in the interlayer via coordination to six oxygen atoms of the clay surface. The interlayer cations influenced the construction of the hydrate's network by destroying the balance of hydrogen bonds formed between water molecules causing the distortion of hydrate's cage formed into Na-Mt. The mobility and the distribution of interlayer species influenced the stability of the methane hydrate complexes. Methane molecules are able to inhibit the hydration of Na-Mt by reducing the basal spacing. Analysis of the intercalation of methane molecules into Na-Mt under the simulation conditions revealed that the most stable state of methane hydrate complexes is obtained under 277 K/50 atm compared with 300 K/10 atm.

Biography

Moussa Camara is well-known author in the field of Clay and Clay Minerals, Clay Polymer Nanocomposites and Drilling and Completion Fluids Chemistry for over 6 years in the department of Oil & Gas Well Engineering at China University of Petroleum (East China). He is working now on the rheological properties of thermosensitive polymers in water based drilling fluids, and clay swelling inhibitors using Molecular Dynamics Simulation methods.

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