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Molecular Dynamics Simulation Study of the Influence of Potassium Salts on the Adsorption and Surface Hydration Inhibition Performance of Hexane, 1,6 - Diamine Clay Mineral Inhibitor onto Sodium Montmorillonite

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Abstract : The world's demand for energy is increasing rapidly due to population growth and a reduction in shallow conventional oil and gas reservoirs, resorting to deeper and mostly unconventional reserves like shale oil and gas. Most shale formations contain a large amount of expansive sodium montmorillonite (Na-Mnt), due to high water adsorption, hydration, and when the drilling fluid filtrate enters the formation with high Mnt content, the wellbore wall can be unstable due to hydration and swelling, resulting to shrinkage, sticking, balling, time wasting etc., and well collapse in extreme cases causing complex downhole accidents and high well costs. Recently, polyamines like 1, 6 – hexane diamine (HEDA) have been used as typical drilling fluid shale inhibitors to minimize and/or cab clay mineral swelling and maintain the wellbore stability. However, their application is limited to shallow drilling due to their sensitivity to elevated temperature and pressure. Inorganic potassium salts i.e., KCl, have long been applied for restriction of shale formation hydration expansion in deep wells, but their use is limited due to toxicity. Understanding the adsorption behaviour of HEDA on Na-Mnt surfaces in present of organo-salts, organic K-salts e.g., HCO_2K - main component of organo-salt drilling fluid, is of great significance in explaining the inhibitory performance of polyamine inhibitors. Molecular dynamic simulations (MD) were applied to investigate the influence of HCO_2K and KCl on the adsorption mechanism of HEDA on the Na-Mnt surface. Simulation results showed that adsorption configurations of HEDA are mainly by terminal amine groups with a flat-lying alkyl hydrophobic chain. Its interaction with the clay surface decreased the H-bond number between H_2O-clay and neutralized the negative charge of the Mnt surface, thus weakening the surface hydration ability of Na-Mnt. The introduction of HCO_2K greatly improved inhibition ability, coordination of interlayer ions with H_2O as they were replaced by K+, and H_2O-HCOO- coordination reduced H_2O-Mnt interactions, mobility and transport capability of H_2O molecules were more decreased. While KCl showed little ability and also caused more hydration with time, HCO_2K can be used as an alternative for offshore drilling instead of toxic KCl, with a maximum concentration noted in this study as 1.65 wt%. This study provides a theoretical elucidation for the inhibition mechanism and adsorption characteristics of HEDA inhibitor on Na-Mnt surfaces in the presence of K+-salts and may provide more insight into the evaluation, selection, and molecular design of new clay-swelling high-performance WBDF systems used in oil and gas complex offshore drilling well sections.

Keywords : shale, hydration, inhibition, polyamines, organo-salts, simulation
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