Performance of Surfactants Used as Anti-Agglomerants for Hydrate Management: Insights from Molecular Dynamics Simulations

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Gas hydrates are solid-like inclusion compounds formed by hydrogen-bonded water cages stabilized by guest molecules. Gas hydrates in the oil and gas industry have attracted great scientific attention in particular because gas hydrates can block pipelines, affecting oil and gas production and causing safety and environmental consequences. Surfactants are commonly used as anti-agglomerants to prevent the agglomeration of hydrate particles and their coalescence with water droplets. Employing molecular dynamics, we examine here the performance of various anti-agglomerants in preventing the aggregation of sII methane/ethane hydrate particles immersed in hydrocarbon phase. The anti-agglomerants considered were surface-active compounds with three hydrophobic tails and a complex hydrophilic head that contains both amide and tertiary ammonium cation groups. We conducted umbrella sampling and Weighted Histogram Analysis Method to quantify the interactions of two hydrate particles covered by thin water films and anti-agglomerants. The simulation results are compared against experimental data obtained with the modified high-pressure micromechanical force and rocking cell apparatus. The results show that the length and rigidity of the surfactant molecules and the strength of binding of its molecules to the hydrate surface are the key factors in inhibiting the hydrate particle aggregation in oil phase. This study provides molecular insights into the guidance for the molecular design of effective hydrate anti-agglomerants.