

Rapid Screening and Evaluation of Potential Kinetic Hydrate Inhibitors with Combined Experimental and Computational Methods

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Pipeline plugging in the oil and gas industries is a severe issue due to its potential toward the malfunction or severe disaster in the subsea architectures. Therefore, finding an effective gas hydrate inhibitor is essential. We adapted screening techniques known as COSMO-RS (COnductor like Screening MOdel for Real Solvents) to find active molecules. As a result, three organic molecules were chosen as latent candidates. To scrutinize their performance in real condition, stainless-steel autoclave and micro-differential scanning calorimeter (μ -DSC) were used. The apparatus temperature was slowly decreased to discern the kinetic effect of inserted chemicals. By observing abrupt pressure decrement in the autoclave, and sudden heat flow rise in μ -DSC, onset temperatures of each substance were measured in both apparatuses. Furthermore, the performance principle of chemicals was probed with Density Functional Theory (DFT) and Quantum Theory of Atoms-In-Molecules (QTAIM) methods. This combined pre-screening and post-evaluation of computational methods with experimental methods will enlighten the convenient and tenable way to discover effective and environmentally benign inhibitors.