

An investigation of water-soluble monomers as CH₄ hydrate inhibitors using both experimental and quantum chemistry-based approaches

고우진, 이동영, 서용원[†]

울산과학기술원

(ywseo@unist.ac.kr[†])

The gas hydrate formation in oil and gas pipelines is a significant issue due to the rupture of facilities and high possibilities of vital disasters. Injection of gas hydrate inhibitors is one of the well-known methods to prevent hydrate formation. Kinetic hydrate inhibitors (KHIs) can require only a tiny dosage (~ 1 wt%) for prevention of gas hydrates, so various types of KHIs have been discovered and tested in the literature. In this work, three different water-soluble monomeric compounds (urea, acetamide, and glycine) were suggested as KHIs and their performance as KHIs were evaluated through both a HP autoclave and a HP μ -DSC. All substances showed effective inhibition toward CH₄ hydrate and showed synergism when they were dosed together. Furthermore, a quantum chemistry-based approach including COSMO-RS and QTAIM was also applied to validate the availability of given substances and compare the calculation results with the experimental results. The results obtained in this study provide insights into the exact role of environmentally benign new KHIs and another way of examining particular interactions between hydrate cages and inhibitors.