Selecting effective kinetic hydrate inhibitors (KHIs) for CH₄ hydrates using COSMO-RS

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Avoiding gas hydrate formation is indispensable to safe operation in oil and gas industries. Injecting gas hydrate inhibitors is a well-known method to solve it. In these days, using kinetic hydrate inhibitors is getting more attention from researchers due to their sustainability and economic impacts. Molecules like polymers, organic compounds substituted with other functional groups are good examples of them. However, there are no specific pathways to sift competent inhibitor candidates. Here, we obtained sigma profiles of several molecules using COSMO-RS to see their polarity, which is an essential factor for estimating interactions between molecules. After that, we selected four representative molecules, which showed well-matched trends with a water molecule. With a high-pressure micro differential scanning calorimeter and a high-pressure autoclave, we identified that all those four candidates showed inhibition effects on CH₄ hydrate. The onset temperatures of CH₄ hydrate in the presence of inhibitors were effectively used for the performance evaluation of the selected inhibitors. We can expect that the results of this study will suggest an optimized way to find potential KHIs.