Interactions of Hydrate Promoters Sodium Dodecyl Sulfate and Tetrahydrofuran near Hydrate Forming Conditions

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Thermodynamic hydrate promoters (THP) and kinetic hydrate promoters (KHP) can be used to reduce the environmental conditions for hydrate nucleation to reduce the hydrate induction time, while increasing growth rates. Two commonly used promoters for CCUS research are tetrahydrofuran (THF) and sodium dodecyl sulfate (SDS), which can increase overall promotion when used in tandem as compared to individually. There are several molecular theories regarding how SDS promotes growth: (1) micellular theory, which depends on surfactant aggregates called micelles at a critical micelle concentration (CMC) to increase interfacial surface area, (2) capillary theory, in which hydrates have been observed to "creep" up hydrophobic surfaces in the presence of SDS, and (3) surface adsorption where SDS adsorbs to hydrate surfaces inducing water molecule reorganization to increase growth. The micellular theory is the most investigated and criticized surfactant promotion theory. The thermodynamic promoter, THF, is known to reduce the CMC of SDS at room temperature. This diffusion nuclear magnetic resonance (NMR) study endeavors to confirm formation of SDS micelles in the presence of THF below the Krafft point and at hydrate forming conditions. Gas hydrates are crystalline clathrate networks composed of hydrogen-bonded water molecules, which form cage-like structures stabilized by gas or "guest" molecules, which in this case is sII hydrate former THF and formers that are stable in the presence of THF.

To observe such interactions, two experimental techniques are utilized in this study, H^1 diffusion NMR and C^{13} magic angle spinning NMR. Diffusion NMR provides two data sets, a chemical shift for component identification and the diffusion coefficient of each component with a varied pulse gradient. MAS NMR may be used to identify chemical deshielding of carbon atoms along the SDS hydrophobic chain, which can be related to THF associations with SDS.