Role of Sodium Dodecyl Sulfate Surfactant at the Interface of the Decane + Brine System in the Presence of CO₂, CH₄, and Their Mixture

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Introduction

The emission of anthropogenic CO₂ is one of the major causes of global climatic changes. Carbon capture and storage technology might be beneficial for mitigating these emissions. Various adsorbents (e.g., carbon nanotubes and clays) have been extensively utilized for carbon dioxide capture. In enhanced oil recovery (EOR) operations, the oil recovery could also be combined with carbon dioxide storage. The water-alternating-gas (WAG) approach has been utilized for mobility control during CO₂-EOR operations. The WAG cycles consist of injecting water (or surfactant) and CO₂ alternatively into the reservoirs. Lowering the interfacial tension (IFT) of the oil + water system leads to an increase in the capillary number which may help to recover more oil. In general, the presence of surfactant/CO₂ decreased this IFT. In addition, the captured CO₂ contains impurities (e.g., CH₄) that may have an important influence on the EOR operations.

Simulation Method

MD simulations of Decane + water + surfactant and Decane + brine + surfactant two-phase systems in the presence of CH₄ and CO₂ at 323 and 443 K, and pressure up to 100 MPa were carried out using the GROMACS package. The salt (NaCl) concentration is 2.7 mol/kg and the amount of surfactant adsorbed at the interface are 0.008 and 0.016 SDSÅ². Each system was equilibrated for 5 ns in the NPT ensemble (only Lᵥ varied) and we ran a 5 ns production under NVE conditions.

Results

Figure 2: IFT dependence on the surface concentration of surfactant for the (a) water + surfactant system at 298 K and (b) water + surfactant + CH₄ system at 273.2 K and 7.2 MPa.

Figure 3: IFTs of (a) Decane + brine + surfactant, (b) Decane + brine + surfactant + CH₄ (x CH₄ = 0.5), (c) Decane + brine + surfactant + CO₂ (x CO₂ = 0.5), and (d) Decane + brine + surfactant + CH₄ + CO₂ (x CH₄ = x CO₂ = 0.25) systems at 443 K.

Figure 4: Atomic density profiles for the Decane + brine + surfactant + CH₄ + CO₂ (x CH₄ = x CO₂ = 0.25) system at 443 K and 20 MPa:

Figure 5: RDFs between the S-atom of SDS and different species in the Decane + brine + surfactant + CH₄ + CO₂ (x CH₄ = x CO₂ = 0.25) system at 443 K and 20 MPa. The NaCl concentration is 2.7 mol/kg and the amount of surfactant adsorbed at the interface is 0.016 SDSÅ².

Conclusions

- The addition of CH₄, CO₂, and the presence of SDS surfactant at the interface reduced the IFTs of the Decane + water and Decane + brine (NaCl) systems.
- The effect of CO₂ is more because the interface was highly enriched with CO₂ molecules than with CH₄ molecules.
- The interfacial thickness between water and Decane/CH₄/CO₂ molecules increases with increasing surfactant concentration and decreases with salt.

References


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