Molecular Dynamics Study on the Stability of CO_2 Foam Film

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Abstract: CO_2 foam flooding technology can be used for geological storage of greenhouse gas CO_2 while enhancing oil recovery. The stability issue of foam film is a major challenge of the application in the oilfields. Surfactants have surface and interfacial activity due to the amphiphilic structure. They can reduce the interfacial tension (IFT) between the CO_2 bubble and liquid film, lowering the interfacial Gibbs energy. Thus, they have been widely employed at the CO_2-water interface in order to stabilize CO_2 foam system. Capillary suction and Marangoni effect are crucial to the static and dynamic stability of CO_2 foam film, which can be reflected by the change of IFT and interfacial elasticity of the surfactant formed monolayers at the interface. By using molecular dynamics (MD) simulations, the effect of surfactant concentration, temperature and pressure on the IFT were studied. Subsequently, the influence of different molecular structure (i.e. headgroups/linking groups) on the morphology of surfactant monolayers and the corresponding interfacial properties were investigated. The MD results showed that high interfacial concentration, low temperature and high pressure are beneficial to the stability of foam film. The adsorption of CO_2 molecules at the interface, the interfacial width and solvent accessible surface area of the surfactant to the CO_2 phase are affected by the density of CO_2 bulk phase. Besides, the surfactant monolayers with stronger hydrophilic headgroups and more flexible linking groups have better interfacial elasticity, they can enable the surfactant molecules rapidly recover to the equilibrium state under external disturbance. Finally, the synergistic effects of surfactants and polymer/nanoparticles are briefly discussed on the basis of MD simulations. The simulation results are in good agreement with the experimental works. The microscopic insights delivered here are of great significance to the improvement of CO_2 foam performance in the industrial applications.