

Molecular dynamics simulation of the synergistic effect of a compound surfactant on the stability of CO₂ oil-based foam

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Abstract

It is of great significance to study the stability of foams in the petroleum industry. Therefore, the stability mechanism of Span 20, the fluorinated surfactant FCO-80 and their compound system FS in a CO₂ oil-based foam system was studied by molecular simulation. The sandwich model of CO₂ oil-based foam was constructed to reveal the stability of the foam system from the microscopic perspective. The result shows that the oil-CO₂ distance of the FS foam system is 16.087 Å, and the coordination number of oil molecules is 2.65. The diffusion coefficient of CO₂ in the FS foam system is 3.94×10^{-6} cm²/s. This shows that under the synergistic effect of Span 20 and FCO-80, the diffusion coefficients of CO₂ molecules are small, and the surface tension is reduced, which can improve the stability of foam. The results can supplement previous experimental results on the stability of oil-based foam.