Structural and interfacial properties of the CO2-in-water foams prepared with sodium dodecyl sulfate (SDS): A molecular dynamics simulation study

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Structural characteristics, interfacial distribution and molecular interactions of the components of the CO2(gas)/SDS/water/SDS/CO2(gas) systems as a function of the CO2(gas)/water interface coverage by the SDS surfactant to different amounts of the CO2 were studied with molecular dynamics simulations and the NVT ensemble. Initially, the repulsive nonbonding parameter between the water oxygen and CO2 oxygen was adjusted to improve the prediction of the solvation free energy, solubility of the CO2 gas in water and the behavior of the CO2(gas)/SDS/water/SDS/CO2(gas) systems at molecular level. Our results show that the stability of the studied foams can be improved incrementing of the vapor/water interface coverage with the SDS surfactant and the amount of CO2 in the system. With the highest interface coverage, the sulfate group has a molecular array more compact at the interface. Furthermore, CO2 gas have a reduction of the diffusion across of the hydrocarbon chains to the water layer with an increment of the number of CO2 molecules in the system, indicating a behavior more hydrophobic of the CO2 gas. The tendencies obtained of the simulations are consistent with the reported experimental results.

Foams

Interface coverage

Molecular interaction

Surfactants

Carbon dioxide

Foams

Free energy

Molecular dynamics

Molecular interactions

Molecular oxygen

Molecular structure

Sodium dodecyl sulfate

Sulfur compounds

Surface active agents

Hydrocarbon chains

Interfacial distribution

Interfacial property

Molecular arrays

Molecular dynamics simulations

Molecular levels

Solvation free energies

Structural characteristics

Phase interfaces

carbon dioxide

dodecyl sulfate sodium

oxygen

sulfate

surfactant

water

Article

chemical structure

foam

molecular dynamics

molecular interaction

priority journal

solubility

solvation

vapor