Behavior of the SDS/1-butanol and SDS/2-butanol mixtures at the water/n-octane interface through molecular dynamics simulations

Parra J.G.

Aray Y.R.

Iza P.

Zarate X.

Schott E.

Interfacial properties of water/SDS+1-butanol/n-octane and water/SDS+2-butanol/n-octane systems have been determined using MD simulations with the aim of studying the molecular interactions between alcohols and SDS when are located at the water/n-octane interface. Also, interfacial properties of water/1-butanol/n-octane, water/2-butanol/n-octane and water/SDS/n-octane systems were determined to validate the used force fields. The relations of SDS/alcohol equal to 16:25, 4:5, 1:1 and 6:5 were used. The g(r)s were evaluated to determine effective interaction between the SDS and alcohol molecules at the interface. The g(r)s demonstrate that ?OSO 3 ? group present an effective interaction with the hydroxyl group of the alcohols. This indicate that hydroxyl groups can be located in the gap that exist between the ?OSO 3 ? groups of the SDS molecules. Therefore, interfacial activity of the SDS/alcohol monolayer is better, favoring the stability of the protective film and the reduction of the interfacial tension. This help to the formation and stability of the microemulsion.

Co-surfactants

Emulsions

Interface

Molecular dynamics

Surfactants