# Effect of Triton X-100 surfactant on the interfacial activity of ionic surfactants SDS, CTAB and SDBS at the air/water interface: A study using molecular dynamic simulations

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Molecular dynamics simulations were carried out to investigate the effect of TX-100 surfactant on the interfacial activity of ionic surfactants SDS, CTAB and SDBS at the air/water interface. Here, interfacial properties, molecular orientation of hydrocarbon chains of ionic surfactant and radial distribution functions between hydrophilic headgroups and water molecules at the air/water interface was evaluated by means of MD simulations. Particularly, TX-100 surfactant produces a reduction of the interfacial film thickness obtained using the water layer and increases the hydrophobic film thickness of the systems. In this investigation, we found that TX-100 surfactant present in mixed monolayers and distributed randomly on the water surface can modify the hydrophilic-lipophilic balance of the monolayer increasing the hydrophobic film thickness and reducing the adsorption of ionic surfactants at the air/water interface. Furthermore, the molecular array of these mixed monolayers obtained by the TX-100 surfactant improve the elasticity of the liquid film, which avoid the rupture of foams reducing the liquid drainage velocity of these systems. Finally, the results suggest that hydrophobic film thickness of the mixed monolayers produce by the TX-100 surfactant can reduce the diffusion of gas molecules from air phase toward the water phase, which increase the stability of foams. 

Hydrophobic film

Interfacial thickness

Molecular dynamics

TX-100 surfactant

Distribution functions

Film thickness

Hydrophilicity

Hydrophobicity

Liquid films

Molecular dynamics

Molecular orientation

Molecules

Monolayers

Surface active agents

Air/Water Interfaces

Hydrophilic headgroups

Hydrophilic lipophilic balance

Interfacial activity

Interfacial film thickness

Interfacial property

Molecular dynamics simulations

Radial distribution functions

Phase interfaces

alkylbenzenesulfonic acid

cetrimide

dodecyl sulfate sodium

hydrocarbon

ionic surfactant

surface water

triton x 100

water

air

Article

density

film thickness

foam

gas

hydrophobicity

lipophilicity

liquid

molecular dynamics

priority journal

simulation

structure analysis

surface tension