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论文

油/水界面表面活性剂的复配协同机制

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摘要:

采用耗散颗粒动力学(DPD)方法模拟了椰油酸二乙醇酰胺(6501)分别与十二烷基- $\alpha$ -烯烃磺酸钠(DAOS)、椰油酰胺丙基二甲基甜菜碱(CAB)和十二烷基苯磺酸钠(SDBS)复配体系中表面活性剂在油/水界面的排布行为, 探讨了盐度及分子结构对单一和复配表面活性剂界面活性的影响, 从界面效率、界面密度和分子排布等角度讨论了油水界面表面活性剂混合体系的复配协同增效机制。

关键词: 耗散颗粒动力学模拟 界面密度 界面效率 超低界面张力 复配增效

Investigate of Synergistic Effects Mechanism of Mixed Surfactants at the Oil/Water Interface

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Abstract:

The method of dissipative particle dynamics was adopted to simulate the interfacial orientation of mixed systems between coconut diethanol amide(6501) and dodecyl alpha olefin sulfonate(DAOS), cocoanut amide propyl betaine(CAB), sodium dodecyl benzene sulfonate(SDBS) respectively at the oil/water interface. The effect of salt and molecular structure on the interfacial activity of pure and mixed surfactant systems were investigated. The mechanism of synergistic effects of mixed surfactants is analyzed from the aspects of interfacial efficiency, interfacial density, the array shape of molecules and so on. It was observed that nonionic surfactants have high absorption tendency but low interfacial efficiency, while ionic surfactants have high interfacial efficiency which can be increased with the increase of salinity but low absorption tendency. In the case that ionic or zwitterionic surfactants with higher interface adsorption tendency coexisting with nonionic surfactants, the cavities at the interface layer formed by ionic or zwitterionic surfactants are filled with nonionic surfactant clusters, synergistic effects could be introduced and interface tension could be decreased to ultra low value at low surfactant concentration because of high interfacial efficiency caused by high interfacial density and high interfacial effectiveness of the mixed surfactants.

Keywords: Dissipative particle dynamics Interfacial density Interfacial efficiency Ultra low interfacial tension Synergistic effect

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