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**Modeling Micellization and Interfacial Tension of Nonionic Surfactants using Dissipative Particle Dynamics** LEELA RAKESH, Central Michigan University, VALERIY GINZBURG, PRASANNA JOG, Dow Chemical Company — We use Dissipative Particle Dynamics (DPD) to simulate thermodynamic behavior of nonionic surfactants. In particular, we study the micellization of linear alkylethoxylates ( $\text{CH}_3\text{-}[\text{CH}_2]_{n-1}\text{-O-}[\text{CH}_2\text{-CH}_2\text{-O}]_m\text{H}$  or  $\text{C}_n\text{E}_m$ ) in water, as well as the influence of these surfactants on the oil-water interfacial tension. We demonstrate that for surfactants with  $n = 6$ , the onset of micellization in water occurs when the total surfactant concentration is on the order of 1%, in agreement with experimental data and Quantitative Structure-Property Relationship (QSPR) models. We also simulate the dependence of dynamic and equilibrium interfacial tension in water/hexadecane/surfactant ternary mixture on the surfactant concentration and investigate the influence of micelle formation on the interfacial tension.

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