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 \( \text{CH}_3[-\text{CH}_2]_{n-1}-\text{O}-[\text{CH}_2-\text{CH}_2-\text{O}]_m\text{H} \) 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.