

Abstract Submitted
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Modeling Thermodynamic Behavior of Nonionic Surfactants in Water VALERIY GINZBURG, PIERRE VARINEAU, Dow Chemical Company — Aqueous solutions of nonionic surfactants exhibit a non-trivial phase behavior known as lower critical solution temperature (UCST), where solutions are homogeneous at lower temperatures but become cloudy (two-phase) at higher temperatures. Conventional Flory-Huggins¹ theory of polymer solutions fails to describe such phase behavior. We utilize the approach suggested by Dormidontova² and modify Flory-Huggins theory by explicitly accounting for water-water and water-alkylene oxide hydrogen bonding. While the Dormidontova model was restricted to aqueous solutions of polyethylene oxide (PEO), we extend it to include other monomers and their copolymers. With the new approach, we can semi-quantitatively predict cloud points of various nonionic surfactants (TergitolTM L and EcosurfTM series) as functions of their molecular structures. We also discuss extensions of this model to calculate micellar phase behavior and oil/water/surfactant interfacial tensions. TM Trademark of The Dow Chemical Company

¹M. L. Huggins, *J. Chem. Phys.* **9**, 440 (1941); P. J. Flory, *J. Chem. Phys.* **9**, 660 (1941).

²E. E. Dormidontova, *Macromolecules* **35**, 987 (2002).

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