Polyol-Controlled Self-Assembly and Removal of Hydrophobic oil Films in Nonionic Surfactant/Polyol/Water Systems

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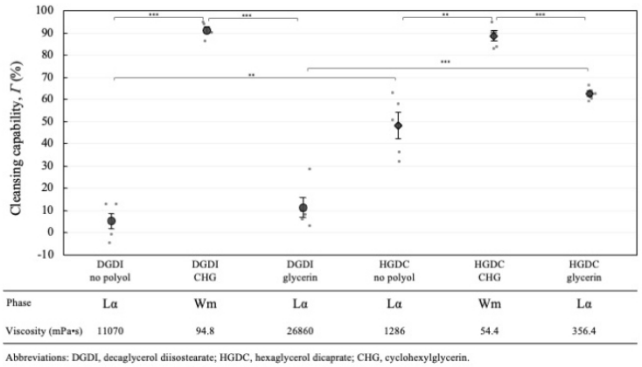
The cleansing capability of aqueous surfactant formulations against hydrophobic oil films depends not only on surfactant concentration and molecular architecture but also on aggregate phase behavior and mesoscale organization [1]. Polyols can tune solvent polarity, hydration, and partitioning between water and surfactant assemblies, but how these effects regulate aggregate packing and hydrophobic oil-film removal remains insufficiently understood [2,3]. Here, we examine nonionic surfactant/polyol/water systems based on decaglycerol diisostearate, hexaglycerol dicaprate, and their mixture. Polyol-free, cyclohexylglycerin-containing, and glycerin-containing formulations were characterized in terms of viscosity, pH, and cleansing capability against hydrophobic oil films. Visual observations together with small-angle X-ray scattering (SAXS) were used to assess phase behavior, while structural parameters, including micelle size, lamellar multilamellarity, interlamellar spacing, and bilayer flexibility, were estimated from the SAXS profiles. In parallel, dissipative particle dynamics (DPD) simulations have been initiated to examine how polyol identity modulates self-assembled structures and associated nanoscale and nanosecond-timescale processes, thereby complementing the experimental characterization [4].

In the absence of polyol, all three surfactant systems predominantly exhibited lamellar organization and showed limited cleansing capability. Cyclohexylglycerin markedly lowered viscosity and promoted lamellar-to-micellar transitions in most formulations; even where lamellar structures persisted, the degree of multilamellarity was reduced. These changes in colloidal organization were accompanied by a pronounced enhancement in cleansing capability across all systems. By contrast, glycerin largely preserved lamellar phases while altering their internal structure. Interlamellar spacing increased substantially, whereas changes in multilamellarity depended on surfactant composition. The corresponding improvement in cleansing capability was modest for decaglycerol diisostearate formulations but more evident for hexaglycerol dicaprate and mixed formulations.

Overall, these results show that hydrophobic oil-film removal is controlled not simply by phase identity but by polyol-dependent changes in aggregate curvature, lamellar packing, and mesoscale organization. This work provides a colloid-based structure-property framework for designing aqueous cleansing formulations.

Keywords:
polyol partitioning, nonionic surfactant, self-assembly, cleansing capability, SAXS, dissipative particle dynamics.



Effect of polyol condition and surfactant type on aggregate phase and cleansing capability (Γ, %) at 30 wt% surfactant.

References:

[1] C. A. Miller, K. H. Raney, Colloids Surf. A 1993, 74, 169–215.
[2] H. Sagitani, Y. Ikeda, Y. Ogo, J. Oleo Sci. 1984, 33, 156–161.
[3] G. D'Errico, D. Ciccarelli, O. G. Ortona, J. Colloid Interface Sci. 2005, 286, 747–754.
[4] E. Schneck, J. Reed, T. Seki, Y. Nagata, M. Kanduč, Adv. Colloid Interface Sci. 2024, 331, 103237.

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