

Doing the dishes with neutrons: milli-flow SANS-DLS of fat removal

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Understanding the mechanisms and kinetics of the removal of fat components such as triacyl glycerides (TAGs) from surfaces is of importance for the design of novel surfactant-based formulations for enhanced performance. Pairing of the physico-chemical properties of surfactants,¹ fat components,² and substrates³ dictates the macro-scale removal/cleaning mechanism and kinetics,⁴ with simulations reporting a number of nano-to-molecular scale pathways for these mechanisms.⁵ Here, we present a coupled in-line milli-fluidic SANS- microfluidic DLS approach to probe both substrate (glass and PDMS) supported TAG structures and nano-to-microscale dynamic solution structures under constant surfactant solution flow (Fig. 1a), using a model ‘dish-washing’ interesterified TAG and surfactant solution of 3:1 mol sodium dodecylsulfate and N,N-dimethyldodecylamine-N-oxide.

From scattering profiles and correlograms, we obtain a plethora of structural and interaction insights into the range of resulting solution structures and an estimation of surfactant partitioning between them (non-interacting micelles, loaded micelles, nano- and micro-scale emulsions), and we thus infer a ‘monomer economy’, %ME, for both dissolution-emulsification and delamination TAG removal mechanisms. Furthermore, the time-dependence of I_0 acts as a probe for the ingress kinetics of the surfactant solution into the TAG by the increase in the volume fraction of fractal interfaces, and we discover a concentration-time superposition for the dissolution-emulsification mechanism. Overall, we show two limiting cases for TAG removal (concentration-limited and mechanism-limited, Fig. 1b), and thus the balance between removal kinetics and molecule economy, these being valuable insights for the bottom-up development of the next generation of surfactant formulations, either through their synthesis or by leveraging synergistic interactions.

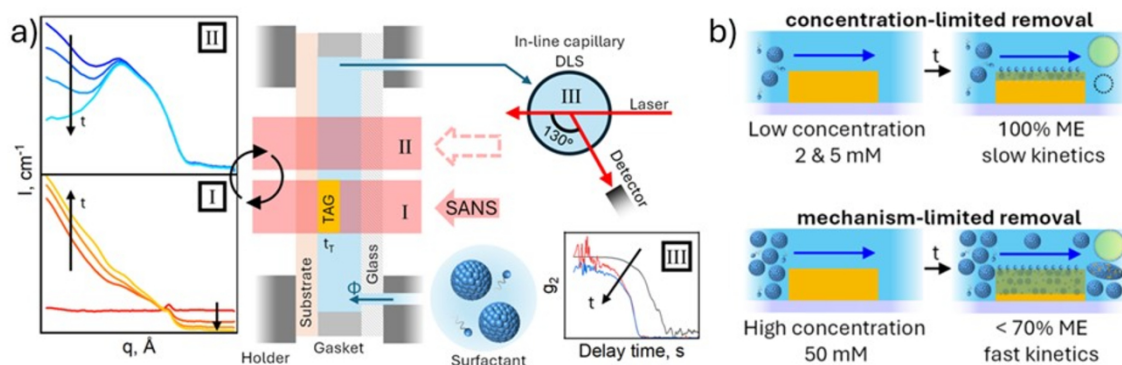


Figure 1: a) SANS-DLS experimental setup. SANS measurements alternate between regions I and II and DLS measurements taken at III. b) The two removal-limiting conditions, with corresponding solutions structures formed, surfactant ingress, and balance between monomer efficiency and kinetics.

References:

- [1] Luis MG Torquato, Gunjan Tyagi, William N Sharratt, Zain Ahmad, Najet Mahmoudi, Jérémie Gummel, Eric SJ Robles, and João T. Cabral. *Langmuir*, 2024, 40, 14, 7433-7443.
- [2] Gunjan Tyagi, Luis MG Torquato, Zain Ahmad, Rebecca Fong, and João T. Cabral. *Journal of Colloid and Interface Science*, 2024, 670, 540-549.
- [3] Gunjan Tyagi, Zain Ahmad, Luca Pellegrino, Luis MG Torquato, Eric SJ Robles, and João T. Cabral, *Surfaces and Interfaces*, 2023, 39, 102992.
- [4] B. A Scott, *Journal of applied Chemistry*, 1963, 13, 3, 133-144.
- [5] Shumeng Wang, Zhi Li, Bei Liua, Xianren Zhang, Qingyuan Yang, *Applied Surface Science*, 2015, 359, 98-105.