Title: Rheology of thread-like micelles and colloid/polymer mixtures for applications in personal care products and latex paints.
PI: Ron Larson
Number of Graduate Students/Post Docs: 1 GS
Time span: Two years
Budget: $200,000

Abstract Paragraph:
Surfactants form reversible threadlike micelles whose properties, such as micelle length and breakage times control their rheology, and rheology needs to be tuned for application. We have developed multi-scale software tools that allow us to connect micelle properties to rheology, and can apply these tools to commercial formulations, with many components. We have similar tools for analyzing colloid-polymer mixtures used in latex paints.

Summary of Project: We will run molecular dynamics simulations to access properties such as micelle breakage time (see Fig. 1) that can be fed into a coarse-grained simulation package (see Fig. 2) called the "pointer algorithm," which allows us to account for micelle breakage, rejoining, and diffusion to predict rheological properties as illustrated in Fig. 3. Alternatively, we can simulate the rheology of colloid/polymer interactions, such as those present in latex paint formulations, where polymers link latex particles into a network for control of rheological properties. The coarse-grained simulation method is illustrated in Fig. 4.

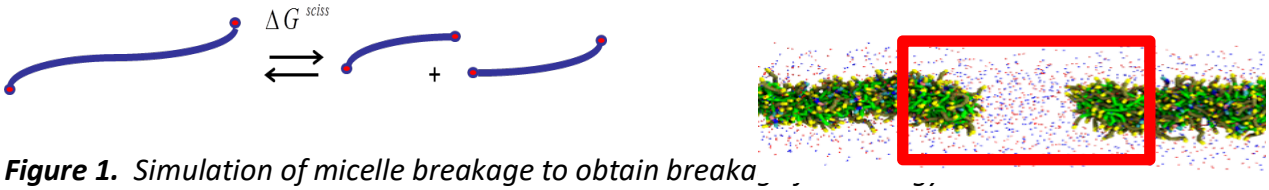

Figure 1. *Simulation of micelle breakage to obtain breaka*

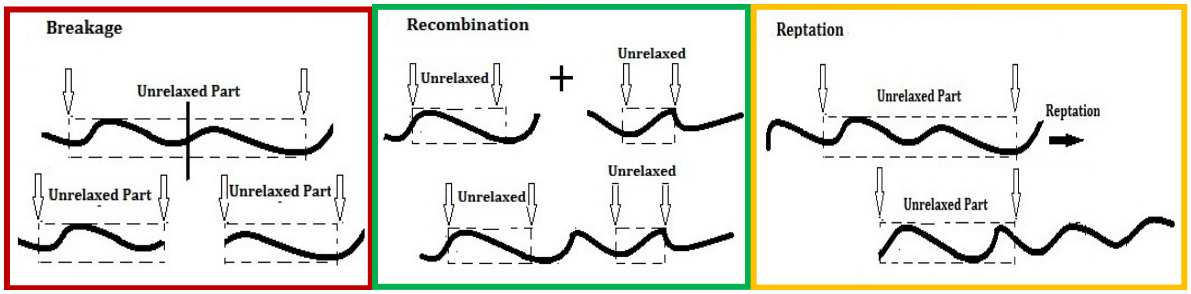

Figure 2. Coarse-grained simulation of micelle breakage, recombination, and reptation.

Aims of Project:

1) Analyze rheological data for commercial surfactant micellar solution to determine micellar properties using the pointer algorithm.
2) Connect micellar properties, such as micelle length and breakage time to molecular composition using molecular dynamics simulations.

3) Apply methods to mixtures of colloids and surfactants, as needed.
3) Develop design tools to map composition to properties.

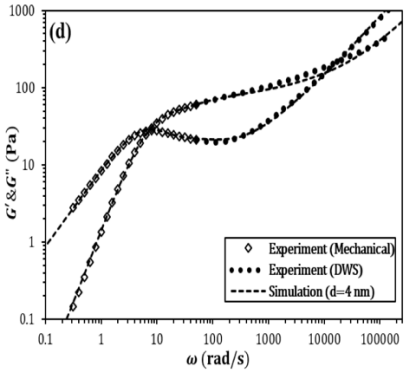

Fig. 3. Fitting of predictions of pointer algorithm (lines) to experimental linear rheology data for a commercial solution of threadlike micelles.

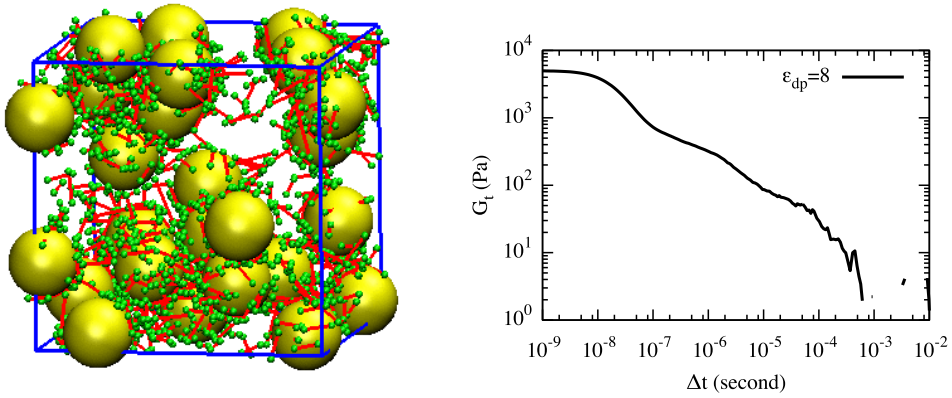

Fig. 4 Simulations of colloid/polymer interactions for prediction of relaxation modulus and rheology.

Outcomes of Work:
The project will result in the ability to design properties of surfactant micellar solutions using advanced software tools. This will impact body wash and shampoos, industrial surfactants, latex paints, aqueous inks, biomedical applications.

References:
1. H. Wang, X. Tang, D.M. Eike, R.G. Larson, and P.H. Koenig, *Langmuir* 34:1564-1573 **2018** "Scission Free Energies for Wormlike Surfactant Micelles: Development of a Scission Protocol, Application, and Validation for Personal Care Formulations."

2. E. Hajizadeh, S. Yu, S. Wang, and R.G. Larson, *J. Rheol.*, 62:235-247 **2018** "A Novel Hybrid Population Balance-Brownian Dynamics Method for Simulating the Dynamics of Polymer-Bridged Colloidal Latex Suspensions.