Project Summary

Collaborative Research: Predictive modeling and measurements of non-Newtonian interfacial hydrodynamics

Overview:

Interfacial hydrodynamics can drastically alter the transfer of mass, momentum, and energy across the interface due to the coupling to the bulk hydrodynamics. The importance of interfacial hydrodynamics is evident everywhere in nature, ranging from small scale systems such as the alveoli in the lungs to CO_2 exchange between the atmosphere and the oceans. In manufacturing, interfacial hydrodynamics impacts everything from micro-electronics to the production of polyurethane foam. Other man-made systems dominated by interfacial phenomena include ink-jet printers, emulsifiers in food processing, and interfacial processing in the pharmaceutical industry. Yet, little is understood about interfacial hydrodynamics, how to predict it, and ultimately, how to control it.

One of the most widely studied systems is DPPC on water, the main constituent of lung surfactant and of the bilayers making up mammalian cell membranes. Even for DPPC, our understanding of its interfacial hydrodynamics is limited. Literature results are confusing and often contradictory. For example, surface shear viscosity values have been reported that differ by several orders of magnitude. One of the stumbling blocks responsible for the inconsistencies has been not accounting correctly for the viscous coupling between the interface and the fluid on which it lies. We have previously developed a method that can calculate the coupled bulk and interfacial flows when both are Newtonian. This led to consistent results between systems over various length scales provided that the surface packing of the film is not very large. However, DPPC, proteins, and other surfactants are non-Newtonian at high surface packing. Even accounting for the coupling, a Newtonian model cannot match with experiments.

Intellectual Merit:

These observations motivate the need for models incorporating both a non-Newtonian constitutive equation for the interface and coupling of the interfacial and bulk stresses. Such models are necessary for interpreting experiments to measure the intrinsic properties of non-Newtonian interfaces, and to then predict their behavior under different conditions. The coupled problem is intrinsically nonlinear and there is a need to develop numerical techniques to solve it. The intellectual merit of the proposed work is the development of such constitutive models, their numerical solutions, and the connection of the model results with experimental observations. This will enable the measurement of intrinsic properties of non-Newtonian interfaces and the prediction of the response under different conditions. Knowledge of intrinsic properties is essential. Apparent properties measured at a given thermodynamic state cannot be used to make predictions at the same thermodynamic state under different flow conditions. The lack of such a capability is hindering scientific progress in understanding nature and in making technological advances.

Broader Impacts:

Interfacial hydrodynamics is vital in many established and emerging fields. The current practice of measuring apparent interfacial properties without a clear way to extract intrinsic properties produces data that is of limited use. Transformational advances in these fields will require a reduced reliance on *ad hoc* experimentation and greater use of synergistic combinations of theory, experiments, and predictive simulations. The multidisciplinary team (from mechanical, chemical, and biological engineering and mathematics), with its proven track record of productive collaboration, is well-suited to bring this project to fruition. Furthermore, the team will continue to provide excellent opportunities for graduate and undergraduate students, including under-represented groups, and motivate their pursuit of careers in science and engineering.