Theoretical and *In-Silico* Insights for Engineering Flow Mediated Phase Transitions

Phase transitions are ubiquitous in nature, and many occur in the presence of fluid flow, such as asphaltene precipitation in oil transport, continuous crystallization in pharmaceutical processing, and clotting in blood. The primary objective of this work is to uncover many of the complex dynamics associated with flow-mediated transformations by using computational techniques. While very broad, the dissertation is split into two sections, one industrial and one biological application.

The specific contexts are for Perovskite solar cell processing and blood flow but can be generalized to crystallization and dense suspension flows. Industrially, the primary focus is studying the effects of shear-flow on crystallization, dynamics that are encountered in Perovskite solar cell production. In doing so, a new model, the Hydrodynamic Structural Phase Field Crystal (HXPFC) method was developed to isolate the hydrodynamic effects on crystallization. The HXPFC is a grid-based model, derived from the particle based Langevin-equations, that consistently couples the Navier-Stokes and Structural Phase Field Crystal equations. The strengths of the HXPFC are that the free energy and chemical potential are directly accessible, thereby unlocking thermodynamic insights. In addition, the disordered liquid phase is not explicitly modeled, leading to computational speed-up by removing unnecessary degrees of freedom. The HXPFC, being a grid-based technique, allows for accelerated numerical techniques to be exploited for computational speed-up. Using the HXPFC, it was found that fluid flow impacts crystallization dynamics.

Biologically, the focus will be on studying shear-driven red blood cell (RBC) migration using the Suspension Balance Model (SBM). Suspensions, defined as particles being $> 2\mu m$, are different than colloidal dispersions in that they are affected by gravity and settle out of solution. Furthermore, suspensions exhibit unique behavior in flow by migrating along the shear-stress gradient in the direction normal to flow. However, migration in RBCs is more significant than in hard particle suspensions due to the particle deformability. In RBCs, the particle deformability creates a cell free layer near the wall, in a phenomenon known as shear-induced migration. In addition, the RBC deformability means the flow behavior is a function of both volume-fraction and shear-rate. Viscosity models as a function of volume fraction have been studied since the time of Albert Einstein. However, successfully modeling suspension viscosities as a function of shear rate, volume-fraction, and particle deformability has not been achieved. To capture the RBC suspension deformability, a novel viscosity model was developed to include the effects of shear-rate and particle deformability on flow-resistance. The novel deformable particle viscosity model is shown to give excellent agreement with experimental data.