Structured fluids, such as polymer solutions and melts, colloidal suspensions, micellar solutions, and liquid foams, are extensively used in the food, personal care, and pharmaceutical industries. These materials exhibit unique rheological behaviors based on their internal microstructures, which has generated significant commercial and scientific interest. A notable class of amphiphilic materials, known commercially as Pluronics, has gained increased attention in recent years due to its extensive range of over fifty polymer-based polymorphic materials. Pluronics are tri-block copolymers, consisting of two hydrophilic polyethylene oxide (PEO) chains and a central hydrophobic polypropylene oxide (PPO) chain. Their customizable molecular characteristics, including PPO/PEO ratio, block lengths, and molecular weight, enable the creation of tailored macromolecules for specific applications. Depending on factors such as concentration, temperature, and shear stresses, these materials can exist in aqueous solutions as individual macromolecules (unimers) or self-assemble into various microstructures, which influence their ultimate properties. Predicting and controlling these properties is crucial for optimizing performance across diverse applications and for designing and scaling up processing equipment. Computational tools, particularly Dissipative Particle Dynamics (DPD), offer an efficient alternative to labor-intensive experimental methods, enabling rapid and cost-effective exploration of structural changes and their effects. DPD, a mesoscopic technique, bridges the gap between micro-scale and macro-scale models, operating at time and length scales inaccessible to molecular-level methods.

This dissertation explores the use of DPD simulation techniques for studying both static and dynamic properties in simple and structured fluids. The primary goal is to enhance the effectiveness of these techniques for reliable virtual experiments on technologically significant materials, including both simple and structured fluids. Two main systems are considered: liquid water and binary mixtures of Pluronics and water.

The standard DPD model, originally designed for simulating molecular liquids, requires extensions and variations for specific applications. Key challenges include improving accuracy in predicting fluid transport properties and rheology, and developing robust parameterization strategies.

The work is divided into methodological development and application sections.

The first section addresses challenges in simulating high Schmidt number fluids and improving the reliability and computational feasibility of predicting transport properties. An "extended" DPD model suitable for high Schmidt number fluids was implemented into the open-source LAMMPS code and extensively tested. This model has been shown to convert gas-like dynamics, described by the standard DPD model, to liquid-like dynamics. The time step size dependency of dynamic properties and the effectiveness of different time integration schemes were investigated. The Shardlow-splitting algorithm, newly applied to the "extended" DPD model, demonstrated superior performance compared to the modified velocity-Verlet algorithm for high Schmidt number fluids. An automated method to compute transport properties from DPD equilibrium simulations was developed, focusing on the reliability and feasibility of the Green-Kubo approach for a wide range of simple DPD systems with varying Schmidt numbers. These findings facilitated a multi-parametric study to systematically explore the relationship between Schmidt number and model parameters.

The second section focuses on parameterization challenges in simulating real systems. The initial case study involves modeling liquid water at various temperatures using a new temperature-dependent version of the extended DPD model. This model improves upon the standard version, accurately predicting both equilibrium and dynamic transport properties, and was validated against experimental data across the entire liquid temperature range. The study also examines DPD-based virtual experiments on Pluronic systems in water, comparing results with real-world data to understand the relationship between morphology and properties. Two distinct applications are proposed, each

involving a different type of Pluronic. Additionally, a data-driven approach for parameterizing Pluronic systems under various conditions is introduced.