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Multiscale Modelling of Complex Fluids

By

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Declaration

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Multiscale Modelling of Complex Fluids

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This thesis develops and assesses a multiscale strategy to predict the flow of complex fluids in mixing equipment by linking microstructure-dependent rheology to process-scale performance. The framework combines Dissipative Particle Dynamics (DPD) as a microscale computational rheometer, Computational Fluid Dynamics (CFD) as the equipment-scale solver, and Gaussian Process Regression (GPR) as a surrogate layer between scales. An automated coupling loop is proposed in which an initial CFD solution identifies the rate-of-strain window explored in the device. DPD simulations are then selected adaptively, and the GPR viscosity model is refined by launching new microscale simulations only where the surrogate predictive uncertainty is highest, until a prescribed uncertainty threshold is reached.

The workflow is demonstrated on an industrial surfactant blend, Miraspec UB75, flowing through a Sulzer SMX static mixer. A DPD model for SLES/water is adopted from the literature and extended to include CMEA through a parameterisation based on water–octanol partition coefficients. The model qualitatively reproduces microstructures consistent with reported SLES/water phase behaviour, including micellar, hexagonal, and lamellar regions, and predicts a lamellar morphology for the UB75 formulation. Non-equilibrium DPD rheometry is used to obtain a shear-thinning viscosity curve, which is then used to train a GPR model embedded in OpenFOAM. This enables process-scale predictions over heterogeneous strain-rate fields and gives realistic pressure-drop levels when compared with similar blends in the same type of mixing device.

To address the poor signal-to-noise ratio of standard non-equilibrium DPD rheometry at low imposed shear rates, the thesis adapts the Transient Time Correlation Function (TTCF) formalism to DPD. It is shown that standard TTCF mappings are not compatible with DPD, because dissipative and random forces break the symmetry required to enforce zero initial dissipation. A covariance-corrected TTCF expression, combined with bootstrap-based uncertainty estimation, provides a practical workflow for DPD without mappings. For the simple DPD fluid investigated here, this approach enables viscosity estimation down to very low shear rates without loss of precision as the shear rate decreases, unlike direct averaging.

Finally, CFD models of unbaffled stirred tanks operating with Newtonian and non-Newtonian Pluronic L64/water mixtures are developed and compared with power-consumption and PIV measurements. A steady laminar Multiple Reference Frame workflow reproduces power-number trends and the main flow structures well at low and intermediate Reynolds numbers, while deviations at higher Reynolds numbers highlight transitional effects and the limits of laminar modelling. A composition-dependent GPR viscosity model is also coupled to CFD for transient mixing simulations. This demonstrates the feasibility of producing spatially varying viscosity fields driven by local composition and shear rate, while revealing the additional challenge of locally changing flow regimes as composition evolves.