Toward a multiscale CFD-DPD model for structured fluids under shear stress.

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Highlights

- Multiscale Modelling
- Dissipative Particle Dynamics – Computational Fluid Dynamics
- Shear Viscosity of Structured Fluids
- Coupled CFD – DPD solver

1. Introduction

Structured fluids are involved in many processes in the personal-care, household cleaner, pharmaceutical and food industries. They are obtained by mixing aqueous and organic solutions with surfactants, resulting in “phases” characterized by different molecular structures (i.e. spherical/cylindrical micelle, hexagonal, lamellar) each corresponding to different rheological behaviors. The way in which the components are mixed together and the local fluid shear affect the molecular structure. In addition, the structure itself influences the rheology of the system. In this work, we studied the modifications in the microstructure of a fluid composed by water and surfactant when shear is applied. We focused our attention on a system composed by water and polyethylene oxide (PEO)-polypropylene oxide (PPO)-polyethilene oxide (PEO), commercially known as Pluronic by BASF. The choice of this system lies in its relative simplicity and in the variety of peculiar different microstructures that can be obtained by varying the concentration of the components. We tested possible equilibrium configurations using mesoscale tools. We also wanted to highlight how information collected at the microscale, such as non-Newtonian behavior, can be transferred to industrial scale and overcome CFD approximations.

2. Methods

Computational Fluid Dynamics (CFD) for the description of the macroscale, was coupled to Dissipative Particle Dynamics (DPD), used for the prediction of microstructures. The latter consists in a mesoscale technique, in which the interactions, described by conservative, dissipative and stochastic forces, between beads that are representative of clusters of atoms or molecules are evaluated. Coarse-grained polymeric chains interact with beads representing water and the hydrodynamic interactions are conserved in DPD algorithm. From the microscopical point of view, Lees-Edwards boundary conditions (LEBC) can be used to describe a fluid confined between two moving slabs. Couette flow, in which a portion of fluid is trapped between two rotating cylinders within a small space compared to the height of the cylinder, such that velocity profile is linear, represents the CFD equivalent of LEBC. DPD technique is intrinsically momentum conserving and this means that shear viscosity can be evaluated by dividing the non-diagonal and non-zero pressure tensor components by the imposed shear rate. The computational codes used to describe the two different scales are OpenFOAM, for the CFD level, and LAMMPS for the DPD level. The two codes are coupled in such a way that each computational cell is a DPD domain, where macroscopic shear stress is calculated and sent to the DPD cell. DPD viscosity is computed and rheological curves can be obtained. Each scale was assessed at equilibrium/steady state condition.

3. Results and discussion

Equilibrium simulations have been used to prove that we were able to describe different peculiar phases in of water/Pluronic mixture using DPD as showed in Figure 1

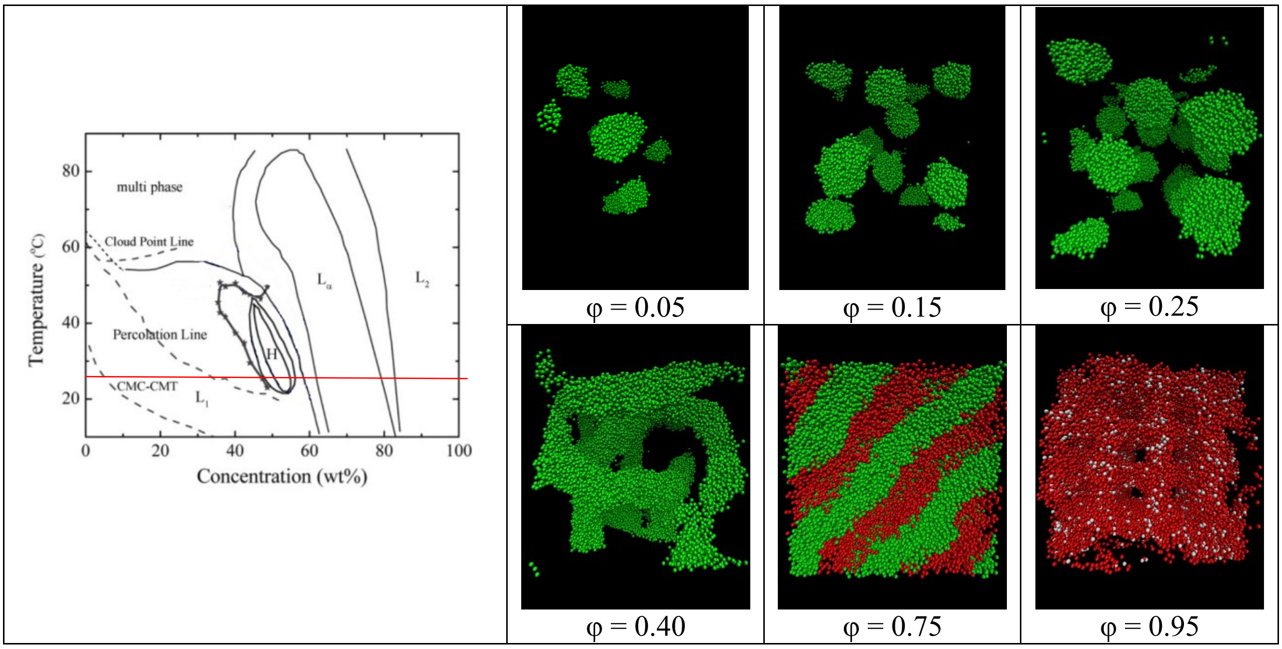

Figure 1. Water/Pluronic L64 phase diagram at equilibrium. Green beads represent PPO, red PEO and white water. Different concentrations have been compared with experimental results [2].

We also performed non-equilibrium simulations and tested how these structures change under shear effect. The variation in the shape of microscopical structure highlighted also a drop in the viscosity of the system. We recorded rheological curves for different concentrations proving the non-Newtonian behavior of the mixture and compared these micro-deformations using clustering analysis, where we focused our attention on how the cluster mass distribution evolves moving from equilibrium to a non-equilibrium condition.

4. Conclusions

The use of mesoscale tools can be helpful in overcoming empirical models implemented in traditional CFD. Especially in complex fluids, where microstructure is affecting macroscopical behavior and the peculiar properties of a final product, the use of this coupled tool could help in fine tuning industrial equipment for manufacturing such complex products by matching their behavior with their microscopical modification.

References

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Keywords

Multiscale Modelling; CFD-DPD; Shear Viscosity, Structured Fluids