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Hybrid quasi-steady thermal lattice Boltzmann model for studying the rheology of surfactants contaminated emulsions

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Thermal conditions determine the outcome of the physical and transport properties of emulsions during their various processing phases. A better understanding of the intricate relationship between thermal, surfactants and hydrodynamics can help in the optimization of these processes during the production of emulsions. To investigate the outcome of coupling thermal, surfactants and hydrodynamics on emulsions behavior, a robust quasi-steady thermal-surfactants numerical scheme is presented and used here. To validate the model, the rheological behavior of oil-in-water system was investigated. The numerical results matched well the experimental results of similar oil-in-water system under steady state thermal conditions. Furthermore, it is shown that, the proposed numerical model can handle cases with transient thermal conditions while maintaining good accuracy.

1. Introduction

Emulsification is the process where oil (dispersed phase)-in-water (continuous phase) emulsions are formed. The boundary between water and oil is identified as the interface. When emulsions compose, both the oil properties and characteristics change dramatically [1]. A framework, which contains oil scattered in a water, is called an oil-in-water emulsion (O/W). A framework comprising of water scattered in an oil is known as a water-in-oil emulsion (W/O) [2]. Water-in-oil emulsions are common in the production and operations of petroleum industry, where the emulsion can contain up to 60% water in volume [3].

Adding surfactants, which are chemical compositions, dilute interfacial tension and reduce the effect of viscosity [4,5]. Development of surfactants-covered droplet is important for many industries. Several experimental and numerical studies with focus on surfactant-covered droplets based emulsions, were presented by many research groups [6–17].

Partal et al. [18] explored the influence of temperature and stabilizer concentration on emulsions' viscosity. The test emulsions were stabilized by a sucrose ester (SE) of high hydrophilic-lipophilic balance (HLB). Emulsions showed shear thinning at intermediate shear rates, metastable behavior at low shear rates and a limiting viscosity at high shear rates. As emulsion temperature increased, the emulsion viscosity decreased. On the other hand, phase separation and coalescence for high oil concentration took place at low temperature.

Kundu and Mishra [2] investigated the removal of oil from oil-in-water emulsion using a packed bed of an ion-exchange resin, which was acting as a coalescing agent for the oil existing in the oil-in-water emulsion system. They evaluated the operating parameters through performing introductory experimental studies to evaluate the operating parameters. These parameters were used for the determination of the oil removal efficiency. The effect of pH, oil concentration, bed height, and flow velocity on the removal efficiency of the resin bed were studied simultaneously. The results indicated that the responses were well predicted and they were satisfactorily within the limits of the input parameters being used.

Gustavo et al. [19] executed experiments on the flow characteristics of concentrated emulsions for Venezuelan bitumen in water with the presence of surfactants. These emulsions were studied between rotating cylinders, in a colloid mill and in pipes. The authors examined the local inversion of an emulsion due to local increases of the bitumen fraction induced by flow. They also observed the conditions that lead to slip flow, in which the drag was reduced by the formation of a lubricating layer of water at the wall. The results revealed the mechanisms that took place in the pumping and pipelining of oil-in-water emulsions.

Kundu et al. [20] studied the rheological behavior of oil-in-water emulsions with several oil concentrations (10–80%), at different temperatures (25–50 C) and with shear strain rates ranging

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from 1 to 100 s-1. Surfactants with varying concentration from 0.5 to 2 w/v % were used in this study. These emulsions exhibited a typical shear thinning behavior. The power law, as a relation between the shear stress and the shear strain rate, described well this rheological behavior. The authors used several viscosity models and the linear regression to curve fit the experimental rheological data. The experiment showed that by increasing the oil concentration, emulsions' viscosity and pseudoplasticity increased. Furthermore, emulsions' viscosity and pseudoplasticity decreased with the increase in temperature. The measurements of surface tension and droplet size distribution showed that they decrease with the increase in oil concentration.

Feigl et al. [21] used simulations and experiments to study the orientation and deformation of three dimensional viscous droplets with and without the presence of surfactants in simple shear flow. The numerical method couples the boundary integral method for interfacial velocity, a second-order Runge–Kutta method for the interface evolution, and a finite element method for surfactants concentration. The simulation results showed a good agreement when compared with another numerical results. The experimental work was done in a parallel-band system with full optical analysis of the droplet. The experimental results showed that the surfactants effects on the droplets shape with smaller viscosity ratios is higher than the droplets with high viscosity ratios. In addition, surfactants forced the droplet to align with the direction of the flow.

Milliken et al. [22] studied the effect of dilute, insoluble surfactants on the deformation and breakup of a viscous drop. The deformation and stretching of a drop was examined. The authors reported that the effects of surfactants were the most influential for small viscosity ratios, where Marangoni stresses substantially impeded the interfacial velocity and caused the drop to behave as more viscous. The authors reported that surfactants facilitated the formation of pointed ends during drop stretching, and this may expound the presence of tip streaming in experiments using viscoelastic droplets.

Drumright and Renardy [23] applied direct numerical simulations with a volume-of-fluid continuous surface stress algorithm to study the effects of insoluble surfactants at low concentration on a drop in strong shear. They used same viscosity and density for the droplet and the surrounding. The movement of the surfactants produces a Marangoni force that acts toward the drop center. For low inertia, viscous force opposes the Marangoni force. This force leads to that a stationary surfactants-covered droplet is more elongated than the one without surfactant. Breakup chances increase with the addition of surfactants through reducing the critical capillary number. The produced daughter droplets for this case are smaller compared to the case of uncontaminated droplets.

Ghanaei and Mowla [24] developed a model based on a combination of the Richardson and Herschel–Bulkley models, with a simplified Eyring equation. The parameters of the model were obtained as functions of wax content in the crude oil, API, and temperature. The authors validated their model by using experimental data, which was extracted from several North Sea oils. The new model was able to predict the trend of viscosity variation against temperature, shear rate, and wax content.

Dan and Jing [25] developed a viscosity model for studying non-Newtonian emulsions. Empirical and theoretical relationships were proposed to describe the apparent viscosity versus water cut behavior of the water-in-crude oil emulsions. Their model was able to predict the relative viscosity of water-in-crude oil emulsions over the range of the maximum and minimum water cut.

Zhi and Jin [26] presented a three-dimensional (3D) numerical study using a uniform staggered Cartesian grid. They explored the deformation and breakup of a droplet suspended in immiscible viscous fluid under shear flow. They treated the surface tension as a modified stress. Their results were in good agreement with the experimental measurements.

Farhat et al. [27] proposed a hybrid model for the study of the droplet flow behavior in an immiscible medium with insoluble nonionic surfactants adhered to the O/W interface. The surfactants concentration distribution on the interface was modeled by using the time-dependent surfactants convection-diffusion equation. A finite difference scheme was used in the solution. The fluid velocity field, the pressure and the interface curvature were calculated using the lattice Boltzmann method (LBM) for binary fluid mixtures. The coupling between the LBM and the finite difference scheme was achieved through the LBM variables and the surfactants equation of state. The Gunstensen LBM was used in their study because it provided local and independent application of a distinct interfacial tension on the individual nodes of the droplet interface. The hybrid model was developed and successfully applied to droplet deformations under a variety of flow conditions.

Taghilou and Rahimian [28] utilized a thermal lattice Boltzmann model to simulate the behavior of a droplet deposited on a solid surface. The simulation took into consideration the contact angle between gas, solid and liquid phases. For this thermal lattice Boltzmann simulation Lee's model [29] was used to track the droplet interface. Boussinesq approximation was implemented to couple energy and momentum equations. Numerical results for the simulation boundary conditions of constant wall temperature and constant heat flux on the wall, were in agreement with previous numerical results.

Inamuro et al. [30] used a lattice Boltzmann method (LBM) for multi-component immiscible fluids for different values of viscosity and capillary numbers under shear flow. In their simulations they used three different values for Reynolds number. The authors utilized the technique to study the deformation and break-up of a droplet in shear flows. The simulation results demonstrated that increasing the Reynolds number makes the deformation and break-up easier.

Among other factors such as shear stress and surfactants, temperature has the most influential role on the composition, rheological and transport characteristics of emulsions characterized by high viscosity ratio. Previous numerical models investigated the role of surfactants and their influence on the behavior of emulsions, with focus on droplets shape orientation and breakup. In this work a LBM based model, which couples the energy equation with the flow hydrodynamics and surfactants-interfacial physics is introduced, presented and used for studying the effects of temperature on the rheology of surfactants-contaminated emulsions in simple shear and in Couette flows. A quasi-steady thermal module characterized by updating the fluid transport properties as a function of the calculated fluid average temperature at each simulation time step is introduced. The calculated average temperature is furthermore used for updating the surfactants elasticity and eventually correcting the emulsion's interfacial tension. The model is capable of reproducing the rheological behavior of emulsions from several experimental cases with the effects of temperature and surfactants. A transient thermal problem is also presented for exploring the potential of using the model in realistic engineering problems, thus providing a robust numerical model for simulating complex flow phenomena such as those encountered in the secondary and tertiary extraction processes in the oil industry. The three way coupling of hydrodynamics, surfactants and thermal energy is evaluated by showing its effects on the flow behavior of surfactants laden droplet under Couette flow conditions. The presented model is intended for the study of emulsions, and it is not suitable for simulating cases involving phase change.