Emulsion Design. Analysis of Drop Deformations in Mixed Flows

The work presented in this thesis concerns numerical and experimental studies of flow induced deformation of drops suspended in a second and immiscible liquid. In the numerical part a model is implemented which is based on a Finite Element (FE) Stokes solver coupled with a Volume of Fluid (VOF) tracking procedure. The FE solver is based on Q2PO elements while the VOF procedure is based on PLIC (Piecewise Linear Interface Calculation) interface reconstruction and a split operator Lagrangian advection procedure which CQILSecVes mass rigorously. The model is fully 3D and can be used for simulating the transient behavior of two phase liquid systems with moving interface topologies. In order to include interfacial tension in the flow calculations both the Continuous Surface Stress (CSS) model of Lafaurie, Nardone, Scardovelli, Zaleski & Zanetti (1994) and the Continuous Surface Force (CSF) model of Brackbill, Kothe & Zemach (1992) are implemented. Due to the high interface curvatures associated with highly deformed drops it is necessary to use a high resolution mesh for our calculations. This leads to extensive computation times mainly due to factorization and back substitution of contributions from the VOF mesh. In order to reduce the computational cost a 2-level procedure is implemented where the fluid tracking algorithms are associated with a fine VOF mesh while the flow field variables are associated with a coarser FE mesh. In the 2-level algorithm the calculation of interfacial tension terms is carried out as a summation of contributions from the VOF mesh. This corresponds to letting the curvature vary within elements of the FE mesh. The implemented model is tested in terms of spatial and temporal convergence by simulating the deformation of a single drop in a simple shear flow field. Furthermore wall effects are also investigated by varying the size of the computational domain, which consists of a box with variable mesh size. In the center of the domain, where the drop resides, the mesh consists of a fine region whereas closer to the walls the elements gradually increase in size. Tests show that wall effects are negligible when the distance from a drop with initial radius \( r_0 \) to the domain boundaries is 24\( r_0 \). In the spatial convergence tests the resolution of the fine mesh region is varied and it is found that a VOF mesh with side lengths \( \nu_{VOF} = r_0/18 \) is adequate when the viscosity ratio, \( A \), between the drop and the continuous phase is one. More thorough tests are carried out both in simple shear and planar elongation. These simulations include dependence of steady-state deformations on the capillary number, drop-break and drop merging. Generally the test results agree well with results reported in the literature. However, simulations carried out for \( A \) different from one indicate that the resolution of the FE mesh needs to be increased compared to simulations carried out with \( A = 1 \). This is probably related to the method used for calculating the viscosity in elements which include both liquid phases. In the experimental part of the thesis the deformation of a single drop suspended in liquid undergoing a complex dispersing flow is studied. The experimental setup is based on a rotor-stator device consisting of two concentric cylinders with teethed walls. In order to monitor the drop deformation and drop position a twin camera system is applied. In the subsequent data analysis the recorded movies are analysed using an automated image analysis procedure which leads to the deformation history of the drop and the drop trajectory in the device. However, due to the geometric complexity of the rotor-stator device numerical calculations are necessary in order to obtain the generated flow field. The obtained experimental data is analysed by two different methods. In the first method the recorded drop deformations are time averaged and compared to a defined apparent shear rate which does not rely on numerical flow field calculations. The results from this analysis indicate that there is a relationship between the average drop deformation and the apparent shear rate. In the second method the experimentally obtained particle track is used together with numerical calculations in order to obtain the local flow experienced by the drop along its track. The data from these calculations lead to time-dependent shear and elongation rates which are used for generating time dependent boundary conditions for the FE-VOF simulations. By using this procedure the flow field experienced by the drop in the rotor-stator device is emulated in the computational box used for carrying out drop shape simulations. Comparison of simulated and experimentally obtained deformations show that in general the agreement is acceptable on a qualitative level. However, the simulations predict deformations which are up to 100% larger than experimentally observed. We have also compared our FE-VOF simulations with results from Boundary Integral (BI) simulations and find good agreement between the two numerical methods. A number of the conducted experiments resulted in drop break-up. The break-up behavior in the rotor-stator device is analyzed qualitatively by relating the configuration of the cylinders with the initiation of the break-up sequence. Here we observe that drop break-up is initiated when a drop travels from a region of minimum gap width into a region with maximum gap width where there is a relaxation in the flow field. Furthermore we observe that for small viscosity ratios (\( A < 0.1 \)) tip streaming is predominant while for larger viscosity ratios either binary or capillary break-up is predominant.

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