Modeling multi-scale liquid dispersion phenomena in conjunction with Computational fluid dynamics

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ABSTRACT

Mixing of fluid in different geometric scales dominates variety of real life applications ranging from engineering chemicals, food materials, pharmaceutical products to biological organs. In this presentation we will address coupling of continuum scales in a number of engineering applications viz., geometrically mediated breakup of drops in microfluidic devices, generation of mono-dispersed droplets with confluent laminar flows and droplet deformation due to surfactant migration at liquid-liquid interfaces. Within the framework of traditional CFD modeling, these applications need both resolution of appropriate scales and / or sub-grid-scale modeling of criteria for interface formation including dynamics such as break-up and coalescence. Additionally they involve heterogeneous species transfer across the interface. In the first example, droplet break-up in microfluidic devices is shown to be a function of extension and capillary numbers. The accuracy in predicting the formation of the daughter droplets is demonstrated. In the second example, role of hydrophobic behavior of the fluids in creation of mono-dispersed droplets in water-oil systems is identified. The last example illustrates the dynamic variation of surface tension by resolving the surfactant concentration distribution between the droplet bulk and the interface. The modified surface tension distribution causes the deformation of the dispersed phase.

Keywords: Mono-disperse droplets, surfactant transport, elasticity, break-up, coalescence, surface tension

1 INTRODUCTION

Emulsions are liquid in liquid dispersions and form an important class of materials produced and handled by the chemical, food, pharmaceutical, and the cosmetic industry. These materials derive their properties based on the droplet size distribution (DSD). Being thermodynamically meta-stable, there is a persistent threat that the texture of the emulsion will be altered during the course of preparation, packaging, or on the shelves of the supermarket. The processes that could cause the DSD to change occur due to inhomogenities occurring over a wide range of length scales. On the one hand, while the macroscopic variations in the velocity and turbulent fields generated during flow causes the DSD to change, the propensity of an individual drop to break is affected by the surface diffusion of surfactants while it undergoes deformation. It is therefore imperative that processes occurring over widely varying length scales be understood so that the desirable DSD be maintained until use.

In this continuing series of articles, we study how the techniques of computational fluid dynamics (CFD) may be used to address some of these issues. In an earlier work [1], we showed how the flow field generated in a stirred tank could be coupled with a population balance model to determine the DSD of an emulsion (Figure 1). In this work, we look at processes occurring at the length scale of an individual droplet.

The modeling of a droplet, in the context of CFD, entails the use of the Volume of Fluid (VOF) model. This model has been successfully used to understand the fluid dynamics of separated phases over macroscopic length scales. We illustrate the efficacy of this model to understand flow in and around droplets that are a few hundred microns in length. In this study we use the VOF model available in the finite volume solver, Fluent [2], to solve the following problems:

1. The generation of droplets at a confluent junction [3]
2. The geometrically mediated breakup of droplets in a microfluidic device [4]

The common theme amongst the experiments is that the experiments were carried out in microfluidic devices, and taken together provide a process to generate emulsions with precisely tailored droplet size distribution.

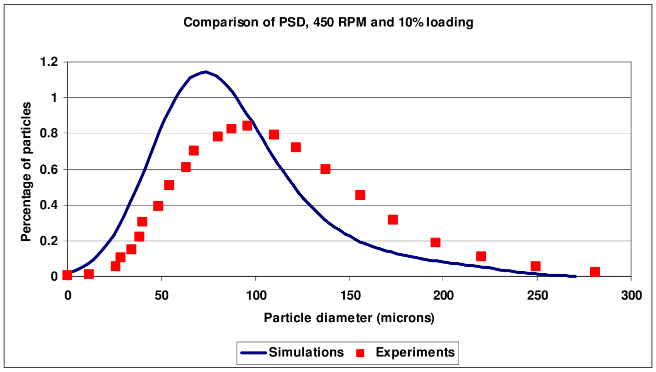

Figure 1. DSD predicted based on the population balance model

2 PRODUCING MONODISPERSE DROPLETS [3]

In [3], streams of two immiscible fluids are injected into separate micro-channels and brought into contact at a junction (Figure 2). Droplets of uniform size are rapidly and reproducibly produced at the junction. The size of the droplets produced is a function of the phasic velocities, surface tension, and the width of the channel.

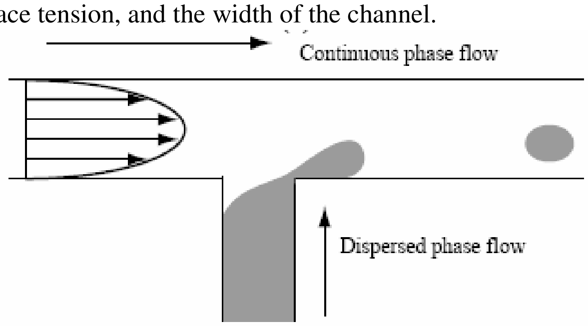

Figure 2. Schematic of experimental setup in [3]

Droplets are formed at the junction as a result of the surface tension and the shearing motion of the fluid flowing in the main channel. As the drop grows in size, it comes into contact with faster moving fluid and is convected along with it. At some point the drop is pinched off at the right side wall of the channel carrying the dispersed phase fluid as shown in Figure 2. The process repeats again.

From the description of the flow in the previous paragraph, it is easy to see that the size of the droplet formed should be a function of the surface tension, velocity of the continuous and dispersed phase. We conducted simulations to ascertain the dependence of the droplet size on the above mentioned parameters.

The simulations carried out confirmed all the qualitative and quantitative features of the experiments as reported in [3]. The major highlights of the simulations are:

- Droplets of uniform size are produced. (Figure3)
- As in the experiments, the successful production of the droplets is strongly dependent on the contact angle; when the dispersed phase is water, hydrophobic surfaces are required to produce droplets. When the wall is hydrophilic the two stream flow parallel to each other as shown in figure 4.

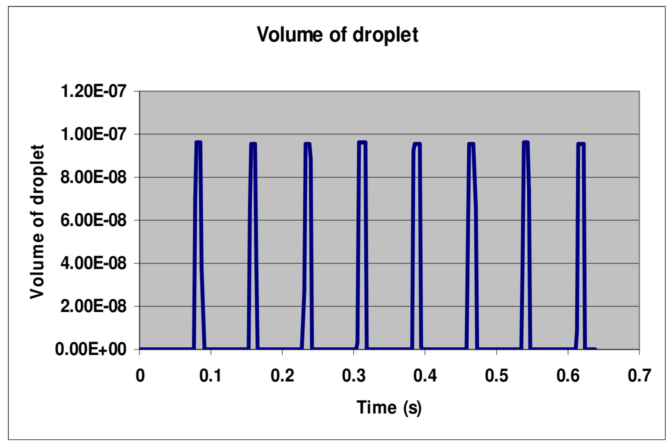

Figure 3 Volume of droplets as measured at the oulet as a function of time.

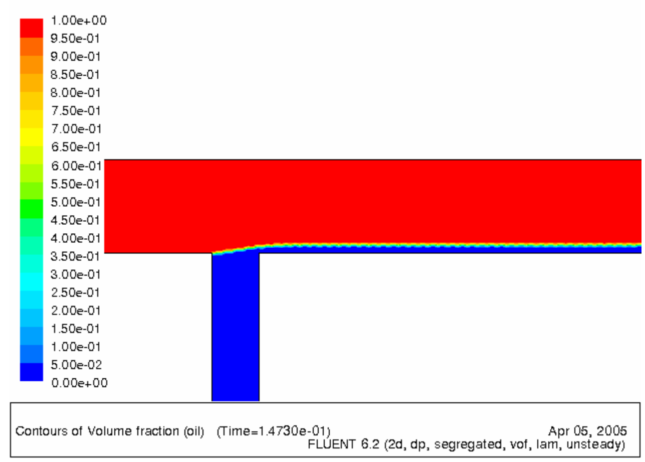

Figure 4. Simulation showing the coflow of the two phases when the wall is hydrophilic. Here the blue region is water while the red region is the oil phase.

The size of the droplets formed was found to increase as a function of the surface tension (figure 5) and decrease as a function of the continuous phase velocity (figure 6). This trend is qualitatively and quantitatively in line with experimental observations.

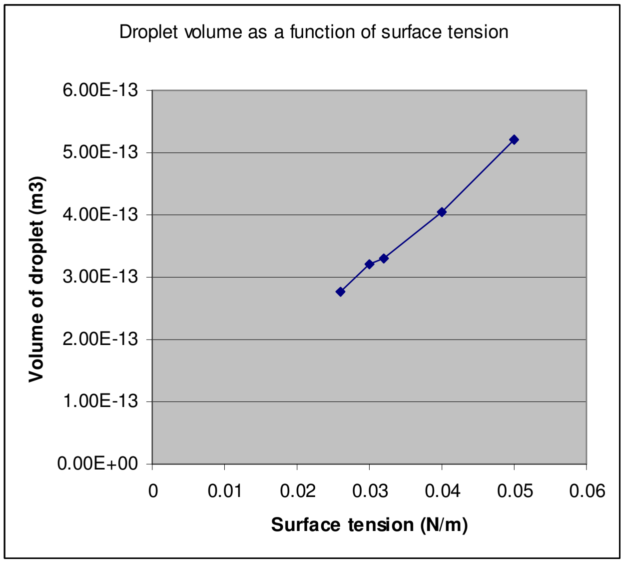

Figure 5 Variation of droplet volume as a function of the surface tension

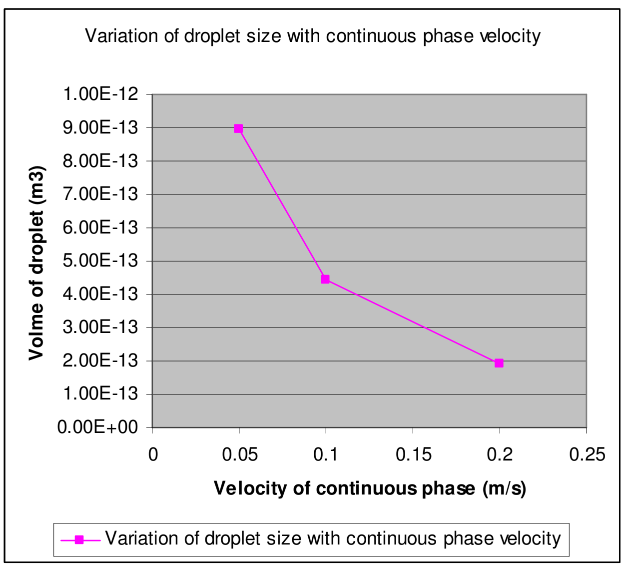

Figure 6 Variation of droplet size with the continuous phase velocity

3 DROPLET BREAK-UP

The problem of producing emulsions of a known Droplet Size Distribution through the use of microfluidic devices was elegantly solved by Link et al. [2]. In their setup, the flow field at a T-junction is used to split droplets. By changing the length of the arms of the T-junctions, the droplet can be broken down to produce daughter droplets of unequal sizes. By using a network of such asymmetric T-junctions, emulsions of a given DSD can be produced.

We conducted both two dimensional and three dimensional simulations to verify the qualitative and quantitative aspects of the experiments. In particular, the simulations are able to reproduce

- The size of the daughter droplets that are produced at the T-junction
- The critical extension number that is required for a droplet to breakup at the T-junction, as a function of the capillary number.

More of these results will be presented during the conference.

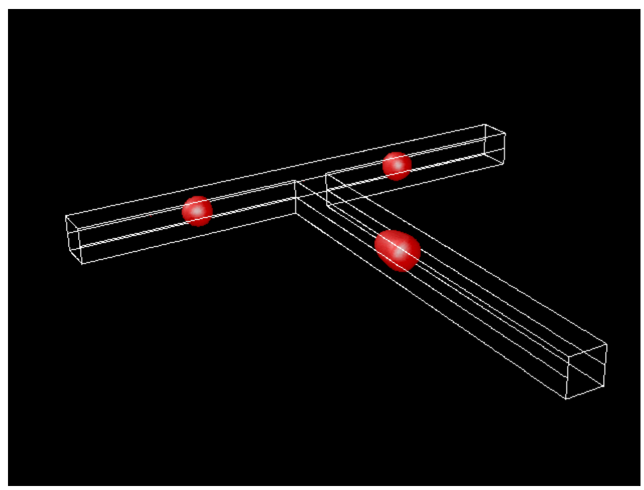

Figure 7 Image showing the splitting of a droplet at a T junction

4 CONCLUSIONS

In this work we have shown how the techniques of CFD can be used to analyze processes occurring in the length scale of a droplet in an emulsion. The ability to understand at least some of the processes occurring at the scale of a droplet also throws open the question of how to integrate information obtained from the microscopic models to macroscopic models so that a truly multi-scale model of emulsions can emerge.

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