A COMSOL Multiphysics® Model of Droplet Formation at a Flow Focusing Device

A. Abrishamkar[1], A.S. Rane[1], K.S. Elvira[1], R.C.R. Wootton[1], T. Sainio[2], A.J. deMello[1]

[1]Swiss Federal Institute of Technology (ETH), Zurich, Switzerland
[2]Lappeenranta University of Technology, Lappeenranta, Finland

Abstract

Introduction
The manipulation of droplets in microfluidic channels is an immensely useful technological platform for applications in many scientific fields such as biology, biomedical studies, chemical synthesis and drug discovery. Therefore a numerical study of microdroplet generation can play a crucial role in providing a model for predicting the effect of different parameters on a droplet generation module. These models may be able to forecast the performance of a module precisely in terms of droplet size and frequency, as well as the functionality of the entire system. Moreover, this will lead to a better understanding of the phenomenon of droplet generation.

Use of COMSOL Multiphysics®
In this work, we numerically investigated the process of droplet generation using water as the dispersed phase and FC-40 oil as the continuous phase in a microfluidic device. We used a two-phase level set method in COMSOL Multiphysics® for our study. The simulations were carried out in a two dimensional domain through a flow-focusing droplet generator which is illustrated in Figure 1 along with the geometric dimensions and the computational mesh. All simulations were fulfilled through the laminar two-phase flow physics module with the channel walls specified as wetted walls with a constant contact angle of 0.349 radian. The effect of the velocity ratio between the aqueous and oil phases on droplet size was studied using two sets of simulations, one with a varying oil velocity at constant water velocity and the other with a constant oil velocity and varying water velocity (the velocity ratios were same in both cases).

For the first set of simulations, the oil inlet velocity was varied between 0.0449 m/s to 0.12 m/s in six steps while the water inlet velocity was kept constant at 0.04 m/s. Figure 2 represents the results of this set of simulations. For the second set of simulations, the oil inlet velocity was held constant at 0.09 m/s and the water inlet velocity was varied between 0.03 m/s and 0.08 m/s in six stages. Figure 3 depicts all the simulations in this set. Droplet size was measured based on 3-4 measurements in each case and the standard deviation was calculated. All the measurements of both sets of simulations were later plotted on one graph representing the effect of the ratio of water to oil input velocities on droplet size (Figure 4).

The results demonstrate that the velocity ratio of the two phases directly determine the size of

the droplets. Both sets of simulations indicate similar droplet sizes for same ratio of input velocities. Additional simulations with different oil and water input velocity ranges are in progress. Moreover, this work could be extended to investigate the polydispersity of droplets and the effect of varying the device geometry, with for example different expansion angles near the nozzle. We will also endeavor to generate experimental results for this nozzle design for comparison with the simulation results.

Reference

1. Kaori Shigeta et al., "Application of a micro-droplet generator for an ICP-sector field mass spectrometer - optimization and analytical characterization," Journal of Analytical Atomic Spectrometry, vol. 28, pp. 646-656, 2013,
2. Tzu-Chun Liao and J. Andrew Yeh, "Microdroplet application in protein sensing," in Optical MEMS and Nanophotonics (OMN), International Conference, 2011, pp. 123-124,
3. Yuehao Li et al., "Numerical Study of Droplet Formation inside a Microfluidic Flow-Focusing Device", COMSOL Conference Proceeding (2012), Boston,
4. Shazia Bashir et al., "Simulations of microfluidic droplet formation using the two-phase level set method", Chemical Engineering Science, 66 (2011) 4733–4741,
5. Ansgar Huebner et al., "Microdroplets: a sea of applications?", Lab Chip., 8 (2008) 1244-54,
6. Petra S. Dittrich and Andreas Manz, "Lab-on-a-chip: microfluidics in drug discovery", Nature Reviews Drug Discovery 5, 210-218 (2006).

Figures used in the abstract

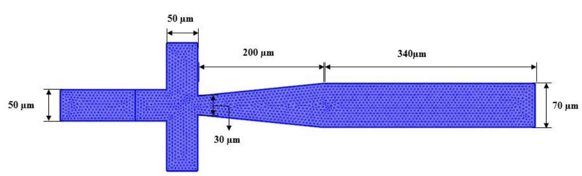

Figure 1: Geometric dimensions and the computational mesh of the flow-focusing droplet generator.

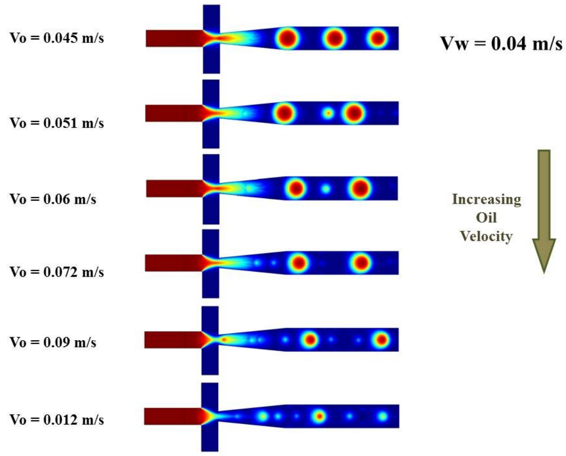

Figure 2: Simulation results for constant water velocity. Vw and Vo denote water and oil input velocities respectively.

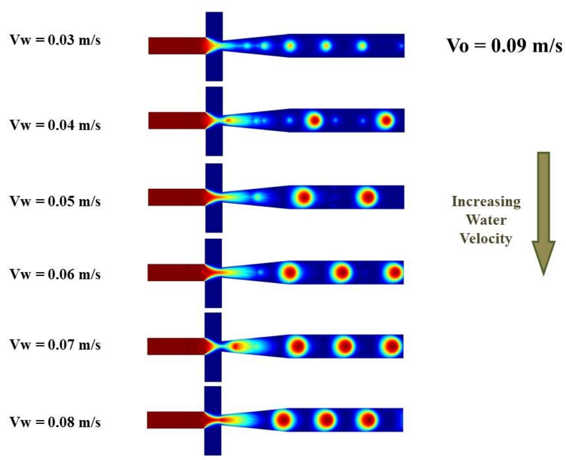

Figure 3: Simulation results for constant oil velocity. Vw and Vo denote water and oil input velocities respectively.

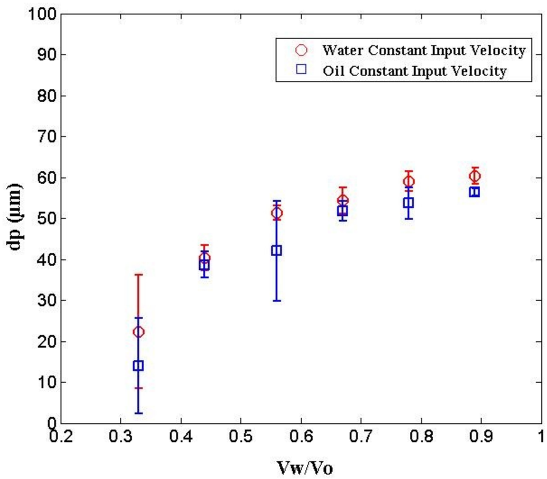

Figure 4: Droplet size (dp) based on the ratio of input velocities.