Simulation of Constant-Volume Droplet Generators for Parallelization Purposes

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Introduction

Droplet microfluidics is revolutionizing the chemical and biological laboratories with assays and reactions not possible in macro scale (e.g. batch)

-Principal problem is their limited volume production (<10ml/h) and they parallelization is challenging (Complex fluid mechanics and coupling)

-To maintain same droplet size across parallel devices, new break-up strategies based on geometry are studied

-When the disperse phase blocks the path of the continuous phase, droplet formation occurs

a) Initial Condition
b) Growth
c) Block
d) Break-up

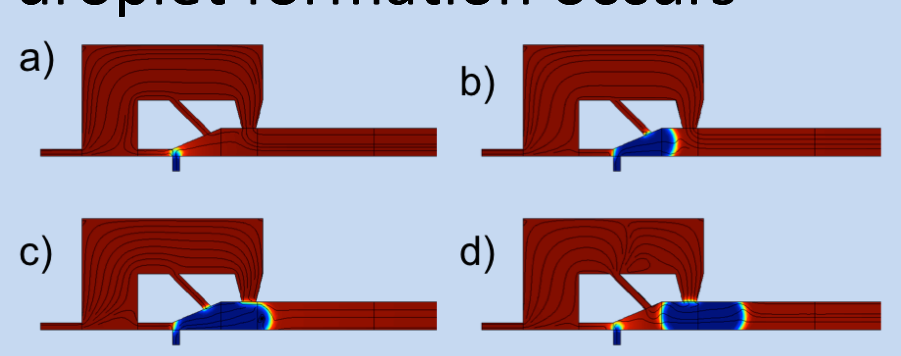

Figure 1. Droplet Break-up Sequence

Computational Methods

We use the computational fluid dynamics (CFD) to simulate the laminar two-phase flow using the phase field method. A continuous phase field variable describes and tracks the interphase between both immiscible fluids in a time dependent study.

Navier – Stockes

$$\rho\frac{\partial \mathbf{u}}{\partial t}+\rho\left(\mathbf{u}\cdot\nabla\right)\mathbf{u}+\nabla p-\nabla\cdot\eta\left(\nabla\mathbf{u}+\left(\nabla\mathbf{u}\right)^{T}\right)=0$$

Continuity – Equation

$$\nabla\cdot\mathbf{u}=0$$

The simulated device is a modification of a classic T-junction generator. The model has to inlets with fixed volumetric flow and an outlet with zero pressure and no viscous stress.

Droplet size is designed by the dimensions of the cavity.

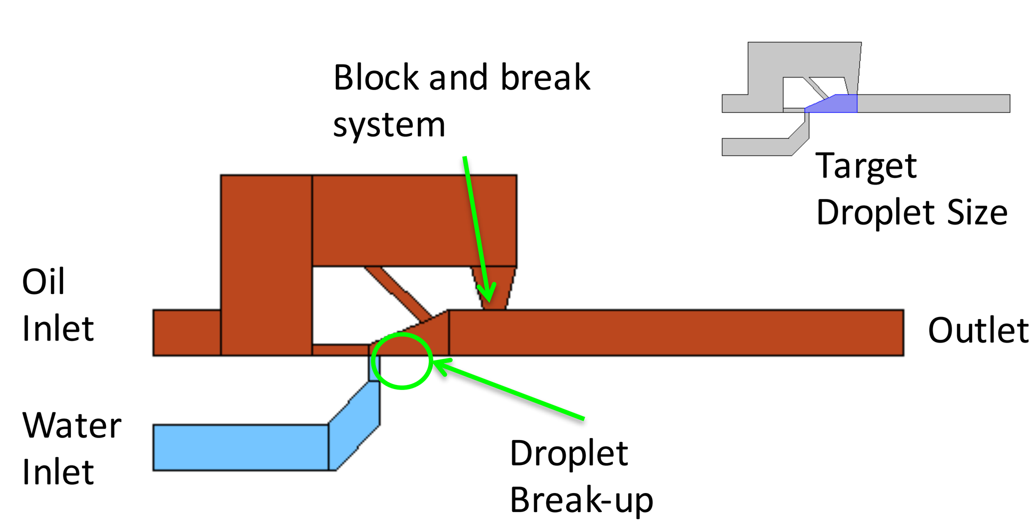

Figure 2. Title of the figure

Results

The simulation was run at several total flow rates and different oil and water flow rate ratios. The volume of the produced droplets remains constant for a wide range of flow conditions

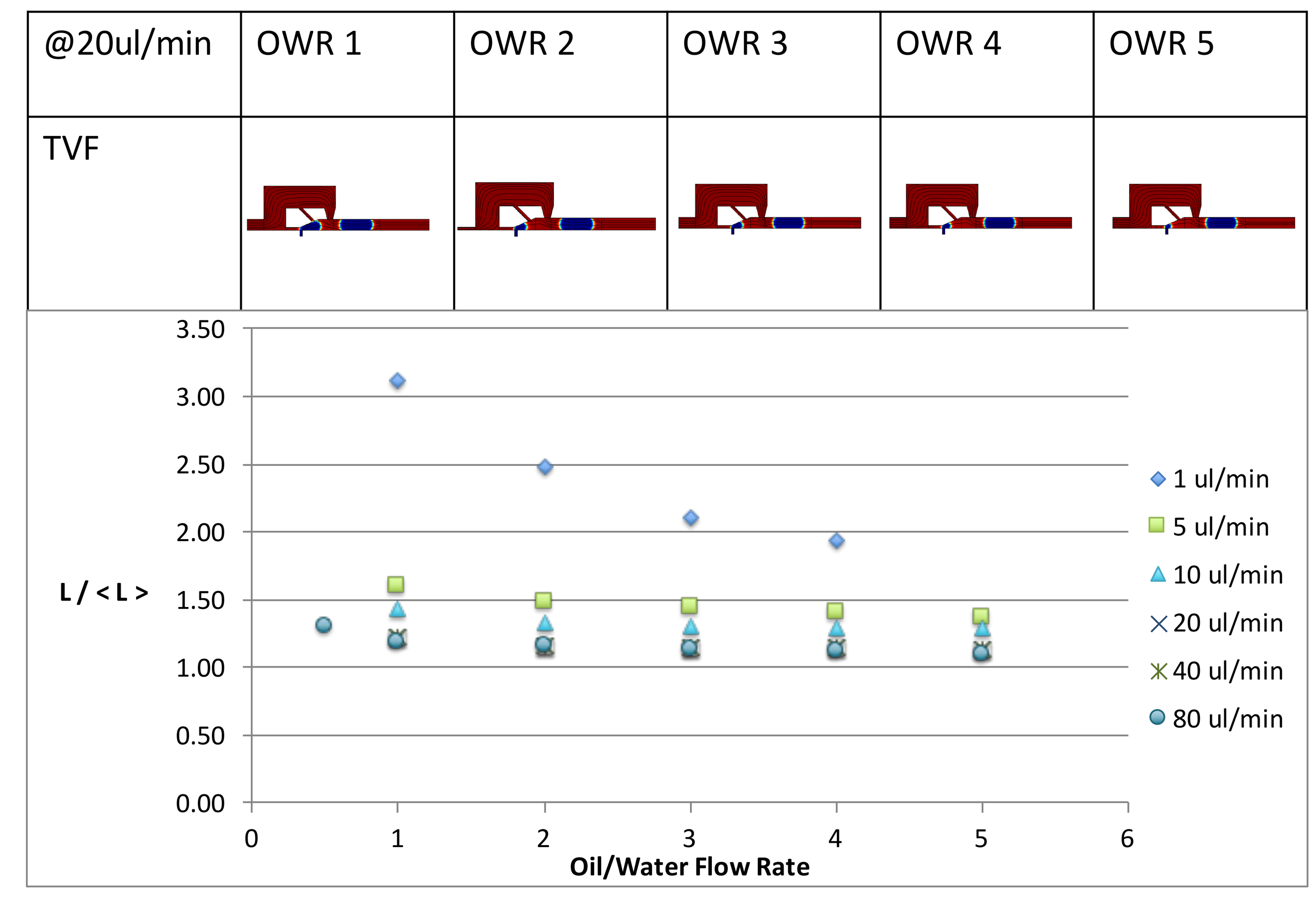

Figure 3. Consistent Droplet Formation

Our simulation also matches the behavior of devices fabricated using soft-lithography
Droplets of larger size were observed at very low total flow rates. At very high flow rates and low oil/water ratios, laminar flow was observed.

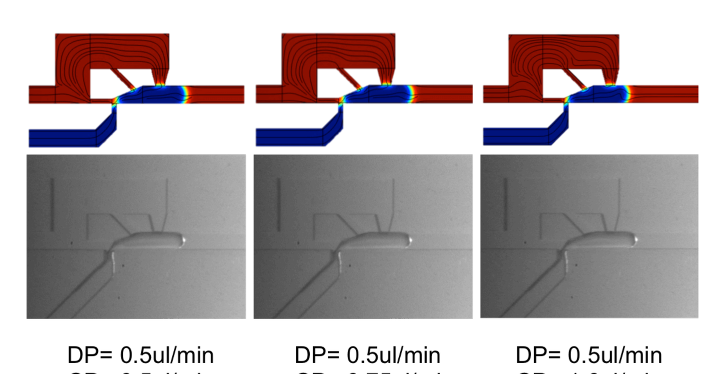

Figure 4. Model vs. Exp.

Table 1. Parameters and liquid properties

Parameter	Value
Oil Density (ρ_o)	$750Kg/m^3$
Water Density (ρ_w)	$1000Kg/m^3$
Oil Dynamic Viscosity (μ_o)	$1.34mPa\cdot s$
Water Dynamic Viscosity (μ_w)	$1mPa\cdot s$
Contact Angle (θ)	$3\pi/4rad$
Interfacial Tension (σ)	$5\times10^{-3}\ N/m$

Conclusions: We successfully simulated a geometrically-set droplet generator. The devices showed consistent droplet formation at different flow rates making it ideal for parallel purposes. Since The simulation match experimental results. We can optimize further the dimensions.

References

1. A B Theberge et al. Microdroplets in Microfluidics: An Evolving Platform for Discoveries in Chemestry and Biology. *Small*, 49:5846–5868 (2010)
2. Volkert van Steijn, et al. Block-and-break generation of microdroplets with fixed volume. *Biomicrofluidics*, 7(2):024108, (2013).
3. D Conchouso, et al. Three-dimensional parallelization of microfluidic droplet generators for a litre per hour volume production of single emulsions. *Lab on a Chip*, 14(16):3011–3020, (2014)

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