Simulation of Constant-Volume Droplet Generators for Parallelization Purposes

D. Conchouso*[1], A. Arevalo[1], D. Castro[1], Y. Yi[1], and I.G. Foulds[1,2]
[1]Computer, Electrical and Mathematical Sciences and Engineering (CEMSE), King Abdullah University of Science and Technology (KAUST)
[2]The University of British Columbia (UBC), School of Engineering, Okanagan Campus
*Corresponding author: 4700 KAUST, Kingdom of Saudi Arabia, david.conchouso@kaust.edu.sa

Abstract: We report on the simulation and characterization of a geometrically-set microfluidic droplet generator that produces droplets of constant volume for a wide range of oil/water flow rate ratios. The simulations were validated with experimental results, and a new design with potentially better reliability is proposed.

Keywords: Droplet Microfluidics, Droplet Generation, Microfluidics, Lab on Chip, Micro-Reaction Technology

1. Introduction

Droplet microfluidics is revolutionizing the level of control and accuracy of assays and reaction technologies in chemical and biological laboratories. As research area, it is growing rapidly and more scientists are adopting these methods in the discovery and development of new materials and better detection systems [1].

The enhanced characteristics of droplet-based microfluidics are just the consequence of the inherent miniaturization and on-chip integration of this technology. Such micro-droplets have large surface area to volume ratio and therefore, surface physics (e.g. thermal conductivity) have greater impact on the system's behavior than volume-based phenomena [1–3]. This allows a whole new level of manipulability and control that was not possible at other scales.

In droplet microfluidics, a set of channels is used to flow and bring together two or more immiscible fluids which by their interaction, droplet formation occurs. The balance between shear stresses, interfacial tension and inertial forces results in a controlled droplet break-up of one fluid into another. The fluid that breaks up into droplets is referred as the disperse phase (DP), whereas the fluid that carries those droplets is known as the continuous phase (CP).

There are several geometries capable of producing these micro-droplets, however most of them have shown that droplet size is strongly dependent on the flowing rates and their ratios. This dependency can be observed specially in flow-focusing geometries in which the DP is hydrodynamically focused into a fine thread prior to droplet formation [2, 3]. Whereas this characteristic could be advantageous in a single device [3]. it also makes their parallelization and consequent scale up a very challenging process [4, 5]. Having generators producing different droplet sizes in a parallel system defeats the purpose of the individual microfluidic system because it is not possible to guarantee the same conditions in each droplet. Therefore, droplet size monodispersity is a crucial characteristic that must be retained in parallelization.

For typical microfluidic droplet generators droplet size depends heavily on the flowing rates (e.g. T-junction, Flow-focusing, Capillary-based generators, etc.). In consequence when these systems are parallelized, the slightest pressure drop or flow fluctuation between one generator to another can result in large droplet size variations. Monitoring sensors based on radio frequency resonators can be used to identify unstable flows in a parallel system [6, 7]. However, robust generators are still needed.

Geometrically-set droplet generators were proposed in order to diminish the influence of the flowing rates in droplet size [8]. In these devices, droplet size can be set by design selecting the dimensions of a cavity and a bypass. Since this generators are less sensitive to flow fluctuations between parallel devices, these geometries are more appropriate for highly parallelizable systems [8].

In this paper, a computational fluid dynamics (CFD) simulation for a geometrically-set microfluidic droplet generator is presented and validated with experimental results. This simulation was then used as a tool in order to expand the understanding of these previously reported geometries [8]. The CFD simulation has also helped us to modify and propose a new geometrically-set generator by mirroring some of the features. Since this new generator is symmetrical, it has the advantage of reducing the probability of unwanted channel wetting that can lead to device failure.

2. Device Description

A geometrically-set microfluidic droplet generator is a device that produces droplets of constant volume that are set by the dimensions of a junction. The device is based on a classic T-junction, that has been modified to include one or more lower resistance paths to the channel transporting the CP. An example of the device's operation is shown in Figure 1.

The bypass system forms a cavity of designed dimensions, in which the DP can grow gradually to form a droplet of constant size. The influence of the shearing forces by the CP is reduced while the bypass channels allow free pass of the carrier fluid through the junction and gets increased when all bypass channels are temporarily blocked by the growing droplet. At this point, the CP cannot flow freely through the junction and therefore, produces droplets. For this reason, this device was referred to as a block-and-break generator and the size of the droplet mainly depends on the size of the cavity that need to be filled prior to droplet break-up [8].

3. Use of COMSOL Multiphysics

To model this phenomenon, we use the CFD module to simulate the laminar two-phase flow using the phase field method. [9, 10]. In this method, a continuous phase field variable describes and tracks the interphase between both immiscible fluids in a time dependent study.

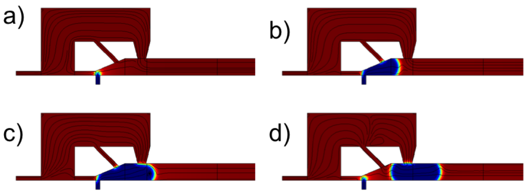


Figure 1: Droplet break-up sequence of a geometrically fixed droplet generator. The disperse phase (blue) grows gradually inside the cavity (a-b) until both bypasses are closed (c) and the built up pressure of the continuous phase (red) induces droplet formation (d).

The COMSOL model solves the motion equations for the two phase system using the Navier-Stokes equations and the continuity equation for the conservation of momentum and mass respectively. Since we are using the phase-field method, the interface is tracked using two additional equations, which describe the phase field variable and the mixing energy density. The motion of the oil-water interface is then determined by minimizing this free energy.

Navier-Stokes:

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{1}{\rho}\nabla p + \gamma \nabla^2 \mathbf{u} + \frac{1}{\rho}\mathbf{F} \qquad (1)$$

Continuity Equation for incompresible flow:

$$\nabla \cdot \mathbf{u} = 0 \qquad (2)$$

Where $\mathbf{u}$ denotes the velocity (m/s), ρ is the density (kg/m^3), μ refers to the dynamic viscosity (Ns/m^2), p is the pressure (Pa) and $\mathbf{F}$ are the external forces.

The transport equations that are solved within the model for the phase field variable are eqs. 3 and 4.

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla = \nabla \cdot \frac{\gamma^{\lambda}}{\varepsilon^2} \nabla \psi \qquad (3)$$

$$\psi = -\nabla \cdot \varepsilon^2 \nabla \phi + (\phi^2 + 1)\phi + \frac{\varepsilon^2}{\lambda}) \frac{\partial \mathbf{F}}{\partial \phi} \qquad (4)$$

Where ϕ is the phase field variable, λ is the mixing energy (N), and ε is the capillary width (m), which is related to the thickness of the multiphase interface.

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)	$5 \times 10^{-3}\ N/m$

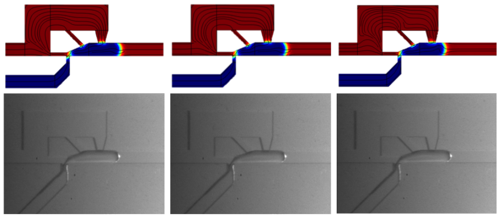
Table 1: Fluids properties used in the two-phase flow model

The chosen the parameters involving the boundary conditions of the model and fluids properties are summarized in Table1.

The oil and water inlet conditions were set to a laminar inflow condition with a constant volumetric flow. The outlet was defined as a zero pressure no stress. The wetting condition at the wall was chosen to have a contact angle of $3\pi/4$.

4. Results and Discussion

The droplet formation was studied at different total flow rates and flow rate ratios in order to evaluate the robustness of the geometrically-set generator. Our simulation matches the behavior of devices fabricated using soft-lithography, Figure 2. The devices showed to be independent of the flowing rates within a wide range of values.



DP= 0.5ul/min
CP= 0.5ul/min

DP= 0.5ul/min
CP= 0.75ul/min

DP= 0.5ul/min
CP= 1.0ul/min

Figure 2: Simulation results vs. Experiments. This figure shows that even at different flow conditions the volume of the produced droplet remains constant, depending only on the size and geometry of the generator

The behavior of the geometrically-set droplet generator under different total flow rates and Oil:Water ratios are shown in Figure 3. The measured length of the droplet ($L_{droplet}$) is shown normalized to its expected length, as determined by the length of the generator's cavity (L_{cavity}). Under very low flow rates ($1-5\mu L/min$) and low Oil:Water ratios, the oil is unable to break the water flow when the bypass is blocked, resulting in droplets 2-3 times longer than expected. In the rest of the cases, the length of the measured droplet becomes very stable, showing a high independence of flow conditions. This characteristic shows their usefulness for parallelization purposes.

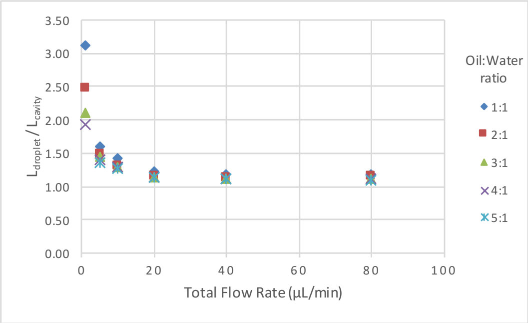
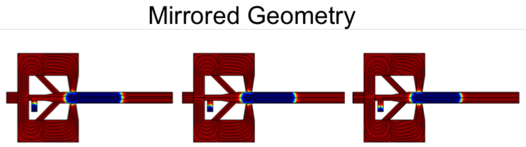


Figure 3: Normalized length vs. total flow rate, for different Oil:Water ratios.

We have also proposed another mirrored geometry (Figure 4), which has the extra advantage of reducing the likelihood of undesirable channel wetting. In T-like junctions, this wetting problem occurs due to the asymmetric droplet pinch off. Every time a droplets forms, the flow of the continuous phases is interrupted in one side of the main channel and the water gets in contact with the channel wall.



DP= 0.33ul/min
CP= 0.66ul/min

DP= 0.25ul/min
CP= 0.75ul/min

DP= 0.166ul/min
CP= 0.833ul/min

Figure 4: Simulation results of proposed mirrored geometry, at different flow conditions.

In a symmetric configuration, this problem is reduced because the flow of oil is not interrupted on either side during droplet formation and there is always a thin film of oil in between the channel wall and the aqueous droplet. This characteristics is especially important for devices in which their substrate is partially hydrophobic or was render hydrophobic using a surface treatment.

The mirrored generator also showed a very uniform and robust droplet formation for a wide range of total flows and flow ratios as shown in Figure 4. A practical problem of this configuration, is the requirement of a more complicated fabrication process. Because the disperse phase flows into the cavity from either the top or the bottom of the channel, a three dimensional network is needed.

5. Conclusions

Simulations of geometrically-set microfluidic droplet generators were done successfully and our model was validated with experimental results.

Flow studies at different total flow rates and oil:water flow ratios show robust and uniform droplet formations for generators with an integrated block and break mechanism. For total flow rates above $20\mu L/min$, the size of the droplet converged to the size of the generator cavity. At lower flow rates (e.g. $\leq 20\mu L/min$), the size of the droplet resulted 2-3 larger than the cavity size because the continuous phase was unable to break the water flow.

A new geometry to avoid undesirable wetting was then proposed. The symmetric configuration allows for an interrupted oil flow that forms a thin layer and protects the channel walls at all times.

The COMSOL model can now be used to design generators that produce droplets of a desire volume and that can be parallelized due to their low sensitivity to flow variations.

6. References

1. A B Theberge, Fabienne Courtois, Yolanda Schaerli, Martin Fischlechner, Chris Abell, Florian Hollfelder, and Wilhelm T S Huck. Microdroplets in Microfluidics: An Evolving Platform for Discoveries in Chemestry and Biology. *Small*, **49**:5846–5868 (2010).
2. G T Vladisavljević, Isao Kobayashi, and Mitsutoshi Nakajima. Production of uniform droplets using membrane, microchannel and microfluidic emulsification devices. *Microfluidics and Nanofluidics*, **13**(1):151–178 (2012).
3. Jing-Tao Wang, Juan Wang, and Jun-Jie Han. Fabrication of Advanced Particles and Particle-Based Materials Assisted by Droplet-Based Microfluidics. *Small*, **7**(13):1728–1754 (2011).
4. Goran T Vladisavljević, Nauman Khalid, Marcos A Neves, Takashi Kuroiwa, Mitsutoshi Nakajima, Kunihiko Uemura, Sosaku Ichikawa, and Isao Kobayashi. Industrial lab-on-a-chip: Design, applications and scale-up for drug discovery and delivery. *Advanced Drug Delivery Reviews*, **65**(11-12):1626–1663 (2013).
5. D. Conchouso, D. Castro, S. A. Khan, and I. G. Foulds. 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).
6. G. McKerricher, D. Conchouso, B. S. Cook, I. G. Foulds, and A. Shamim. Crude oil water-cut sensing with disposable laser ablated and inkjet printed RF microfluidics. In *Microwave Symposium (IMS), 2014 IEEE MTT-S International IS - SN - VO -*, pages 1–3, I, (2014).
7. D. Conchouso, , G. Mckerrichter, D. Castro, A. Arevalo, and I. G. Foulds. Radio Frequency Resonator For Continuous Monitoring Of Parallel Droplet Microfluidic Systems. In *COMSOL Conference, Grenoble, France*, (2015).
8. Volkert van Steijn, Piotr M Korczyk, Ladislav Derzsi, Adam R Abate, David A Weitz, and Piotr Garstecki. Block-and-break generation of microdroplets with fixed volume. *Biomicrofluidics*, **7**(2):024108, (2013).
9. D. Conchouso, E. Rawashdeh, D. Castro, A. Arevalo, and I.G. Foulds. Optimized Channel Geometry of a Flow-Focusing Droplet Generator for Parallelization. In *Proceedings of the 2013 COMSOL Conference*, Rotterdam (2013).
10. D. Conchouso, E. Al Rawashdeh, A. Arevalo, D. Castro, and I. G. Foulds. Simulation of a 3D Flow-Focusing Capillary-Based Droplet Generator. In *COMSOL Conference, Rotterdam, Netherlands.*, (2013).