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Optimization of Shear Driven Droplet Generation in a Microfluidic Device

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ABSTRACT

Hydrophilic and lipophilic interfaces of fluids play an important role in the formation of droplets. A large collection of droplets constitutes emulsions of water dispersive phase into oil continuous phase. Since droplet generation forms the basis of the manufacturing of emulsion, great efforts have been made to understand the science, technological and industrial problems associated with the generation of droplets. This paper presents the optimization of a novel method of droplet generation [1] in a microchannel resulting from the laminar co-flow of water and oil in a T type channel. Water in oil droplets are formed with olive oil (interfacial tension 28mN/m, viscosity 84mPa/s, density 918Kg/m3). At the T-junction, the water stream sent through the middle channel is sheared and cut by the oil stream sent through the outer channel. Competition between interfacial tension and the Laplace pressure at the oil/water interface results in droplets of finite diameter. Fluid properties such as density, viscosity and surface tension and the flow parameters such as pressure, mass flow rate and velocity are varied at the inlets and outlets to optimize size, frequency and periodicity of droplets using CFD-ACE+, a multiphysics modeling tool (CFDRC, Huntsville, AL)

INTRODUCTION

Microdroplets have been generated over the last decades primarily through microporous membrane[1] and jet pinch off[2]. The advancement of microfluidics led to form droplets at the microchannels[3]. Formation of droplets with coflow of oil and water is reported[4]. At the T- junction, the water stream sent through the middle channel is sheared and cut by the oil stream sent through the outer channel. Competition between interfacial tension and the Laplace pressure at the oil/water interface results in droplets of finite diameter. Symmetrically sheared droplets at the T shaped junction are generated and manipulated[5]. The paper is directed towards design and optimization of droplets generated in the microfluidic T channel using CFD simulation.

NOMENCLATURE

F	Liquid volume fraction
T	Time
V	velocity
P	Pressure
ρ	Density
Q1	Flowrate of oil phase
Q2	Flow rate of water phase
σ	Interfacial tension
θ	Contact angle

METHOD

For two immiscible incompressible fluids, the liquid volume fraction, F evolves in the direction of the velocity, v and is determined by solving the following passive transport equation along with the Navier-Stokes Equation.

$$\frac{\partial F}{\partial t} + \nabla \bullet \vec{v} F = 0$$

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla)\vec{v} = -\frac{1}{\rho}\nabla P + \vec{v}\nabla^2 \vec{v}$$

Volume of Fluid method[6] is used for tracking the interface implemented with 'piecewise linear interface calculation' for surface reconstruction using CFD-ACE+, a multiphysics modeling tool[7] (CFDRC, Huntsville, AL). A 2-dimensional flow domain was used in the simulation with orthogonal meshing. The boundary condition is set by fixing mass flow rate at the channel inlets. The outlet is set to a constant pressure same as atmospheric pressure. Water in oil droplets are formed with olive oil (interfacial tension 28 mN/m, viscosity 84 mPa/s, density 918 Kg/m^3). Figure 1 shows the meshes at the junction of inlet and outlet channels. The mesh size is optimized so that the each simulation is completed within 20 hours in a P4 /3.06GHz /1GB DELL computer keeping the good accuracy. 2-d axisymmetric case is considered in the simulation. Optimization of flow rates of oil and water, interfacial surface tension, and geometry of the microfluidic device are considered in this paper.

RESULTS AND DISCUSSION

Droplet generation

Figure 2 shows the simulation of droplets at a volumetric flow rate of 0.1µl/min (mass flow rate=5e-4Kg/sec) of oil in the outer channels and 0.833µl/min (mass flow rate=6e-4Kg/sec) of water in the inner channel. The droplets are periodic and are sensed by measuring the disturbance due to the droplets flow that occurs in the flow rate at the outlet. The flow rate produces a spike as every drop flows as given in Fig. 3a. The peaks are picked and the corresponding time values are replotted for every drop. The plot is a straight line as seen in Fig. 3b and the slope is the time for the generation of a single drop. The radius of the drop can be calculated from this time.

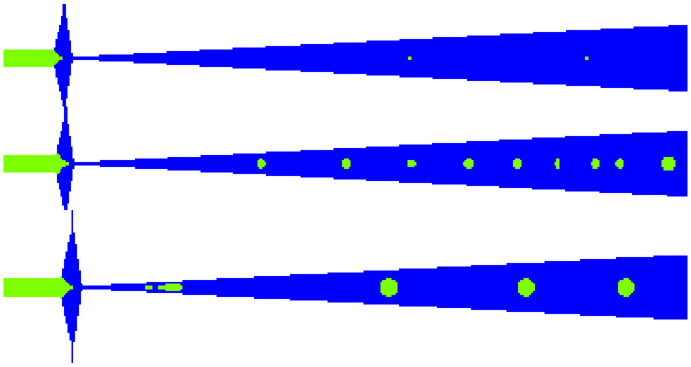


Fig 2. CFD Simulation of Droplets of different sizes generation
(a) Q1=23e-3 kg/s and Q2=6e-4 kg/s
(b) Q1=7e-3 kg/s and Q2=6e-4 kg/s
(c) Q1=5e-3 kg/s and Q2=4e-4

Optimization of Flow Properties

Flow in the outer and inner channels are adjusted with mass flow rates. The flow rate of oil (Q1) in the outer channels are kept constant and the flow rate (Q2) of water in the inner channel is varied in the in the range realized in the experiment. Similarly simulations are carried out with Q2 constant and varying Q1. The time for the generation of a single drop is plotted against the flow rates as given in Fig.4. Figure 4a has a double exponential decay of time as the flow rate of water increases. It is noted that the discontinuity in Fig 4b is due to Raleigh's instability [8]. Very fine droplets with times of the order of microseconds are generated at the discontinuous window. The fine droplets due to Raleigh's instability are observed in Fig 5.

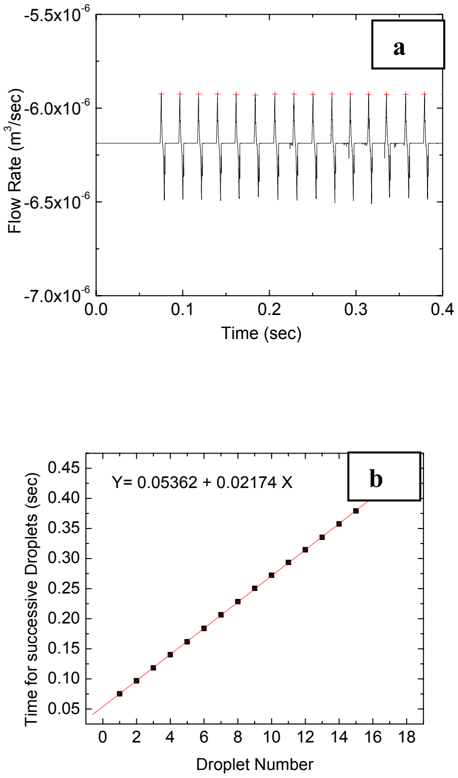
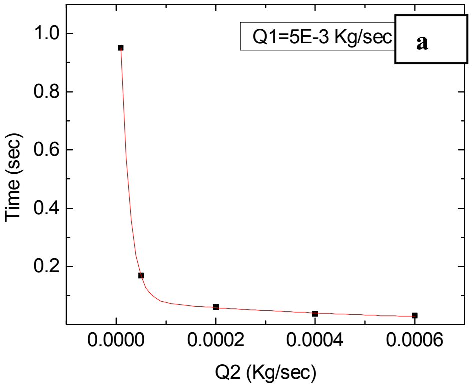


Fig 3. Droplets flow detected and measured from the flow rate at the outlet channel. a) Flow rate calculated from the start of the experiment. b) The corresponding time of the peaks of the flow rate graph is plotted for every drop. The slope of the straight line fit gives the time for generation of a single drop.



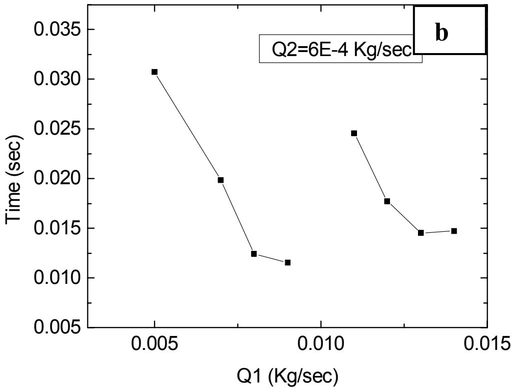


Fig 4. Time of a droplet generation with various flow rates of (a) water and (b) oil

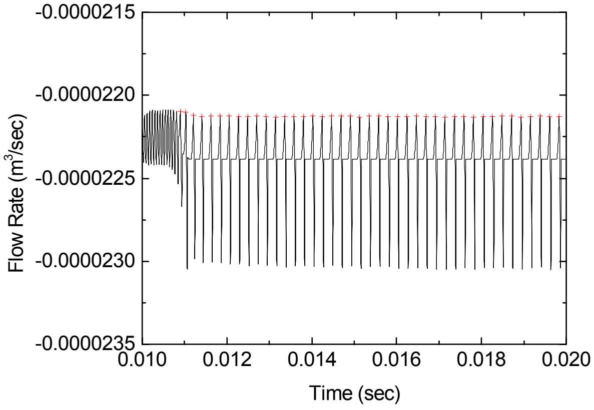


Fig 5. Fine Droplets due to Raleigh's Instability. The droplet generation time is 0.2 msec

Optimization of Fluid Properties

Droplets of fine sizes are generated by adding surfactants to the oil phase and so by reducing the interfacial tension (σ) of oil/water. Simulations predicted that the time per droplet generation exponentially reduces with the decreases of interfacial tension as shown in Fig. 5a. Most of the other simulations are done for olive oil whose interfacial tension with water is 22.8 mN/m and oleic acid (15.6 mN/m). On the other hand, increase of contact angle (θ) of water/oil/wall interface reduces the droplet generation time as presented in Fig. 5b. At high value of contact angle the time goes to saturation. Most of the other simulations are carried out with wall made of PDMS material (the contact angle is ~110° for oil/water/PDMS).

Optimization of Geometry

In order to optimize the geometry, the channel width of the outer channel at the junction and the angle of expansion of the outer channel are varied (See Fig. 7). Figure 6a shows a pair of straight lines with slopes 0.595 and 3.11 sec/mm, (one is 5 times that of the other). Beyond 25 um, fine droplets are generated due to Raleigh's instability. The angle of expansion of the outlet channel shows (Fig 6b) an oscillatory behavior with the droplet generation time. The oscillation has a period of 1.66° and the amplitude of the oscillation decays exponentially as seen in the inserted figure. At larger angles of expansion droplet fusion take place along the length of the channel. However, the droplet generation time changes slightly with the angle of expansion of the channels.

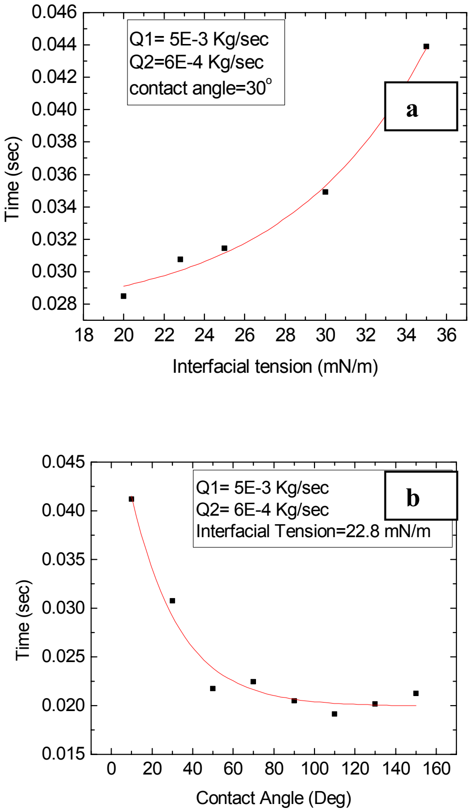
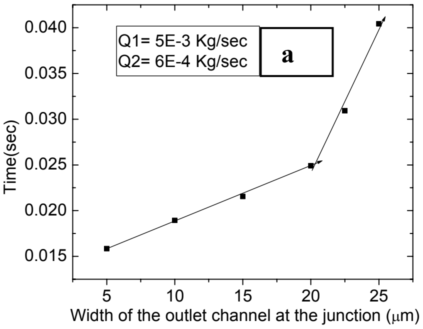


Fig 6. Time of a droplet generation with various (a) interfacial tension of water/oil and contact angle of air/water/wall interface.



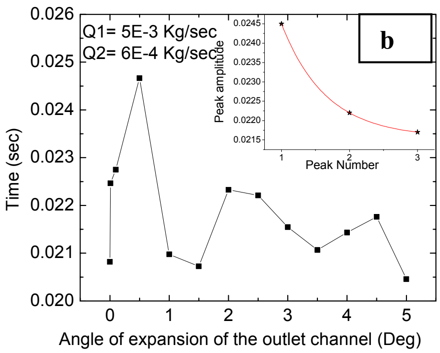


Fig 6. Optimization of the channel width of the outer channel at the junction and the angle of expansion of the outer channel

Experimental Verification

In order to realize the droplet generation, T channel is fabrication in PDMS channel is fabricated using SU-8 molds and is sealed against a microscopic glass slide through oxygen plasma binding [9]. The inlets are attached with plastic tubing connected to syringes loaded with water and oleic acids. The water is dyed with napthol green to indicate the water phase under light microscopy. The syringes inject at constant flow rates controlled by three Picoplus Syringe pumps from Harvard Apparatus. The outlet flow in the PDMS channel is sucked by vacuum at atmospheric pressure. The variation in flow rates of water and oleic acids is changed in steps and the corresponding video microscopic images are recorded at 500 to 10,000 frames/sec using a Photran camera. The radii of the droplets are measured using 'NIH image' software from the recorded images and are showed in Fig. 7. The sizes of droplets generated at various oil flow rates are presented in Fig 8.

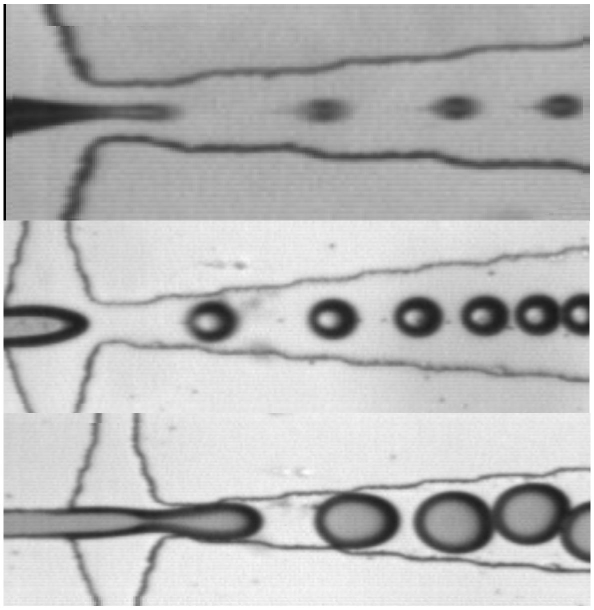


Fig 7. Droplet Generation Experiments
(a) Q1=1μl/min, Q2=15μl/min, camera speed=5000 fps
(b) Q1=1μl/min, Q2=5μl/min, , camera speed 2000 fps
(c) Q1=1μl/min, Q2= 1μl/min, caera speed =2000 fps

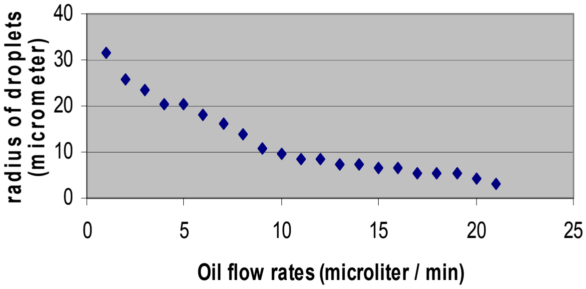


Fig 8. Size of the droplets generated at various oil flow rates

CONCLUSION

These results predict the flow, fluid and geometry parameters for large number of small sized droplets through CFD simulation. The time of a droplet generation is proportional to the radius of the droplets. The size variation of the generated droplets using a particular dimension of the geometry can be found out from this study. The correlation of geometry parameters to the flow and fluid parameters of the microfluidic droplet generator is analyzed. Qualitative and quantitative verification of different sizes of droplets generation is presented with experiment using a microdevice. This study also leads to a wide area of research understanding the Raleigh's instability of the nonlinear fluid dynamics in microsystem.

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