THEORETICAL, COMPUTATIONAL AND EXPERIMENTAL CHARACTERIZATION OF SHEAR-DEPENDENT MICRO-VORTICES IN LIQUID—LIQUID FLOW-FOCUSING GEOMETRY

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ABSTRACT

In this work, we apply theoretical, computational and experimental fluid dynamics to characterize hydrodynamics micro-vortices formation in the dispersed phase at the flow-focusing microfluidic droplet generation junction. This interfacial hydrodynamic method can be exploited to trap cells inside the micro-vortices and later release them in a one-to-one manner to achieve high efficiency single-cell encapsulation inside droplets. This passive trap and release mechanism is controlled by the distance between the closed vortex streamline and the liquid-liquid interface (d_{gap}) and, thus, fundamental understanding of the micro-vortices and parameters affecting their formation, trajectory and magnitude is necessary to achieve effective one-to-one encapsulation.

KEYWORDS: Single-cell encapsulation, Hydrodynamic micro-vortices, Flow-focusing, Droplet microfluidics

INTRODUCTION

Droplet microfluidics has become an integral process for single-cell level studies such as nucleic acid sequencing, 3D single cell culturing and drug cytotoxicity assays. However, droplet based single cell level analysis, requires controlled encapsulation of single particles/cells inside the droplets. In conventional passive microfluidic devices the one-to-one encapsulation efficiency is dictated by Poisson statistics, which limits the amount of droplets containing the preferred number of cells/particles. Therefore, there is a growing need in the field to develop methods that can overcome the hurdle of the random encapsulation process.[1,2] Previously, our group reported a deterministic single cell encapsulation method based on hydrodynamic micro-vortices that can trap and release cells/particles into droplets at >50% encapsulation efficiency. In this technique, a unique flow-focusing design is employed for droplet generation, which gives rise to two symmetric 3D micro-vortices formation in the dispersed phase under the right flow conditions. [1] Herein, we utilize theoretical, computational and experimental fluid dynamics to elucidate the physics behind those micro-vortices and the important parameters affecting them. [2]

THEORY

The occurrence of the micro-vortices depends on the combined effect of interfacial shearing rate (α) and the droplet generation tip oscillation frequency (TOF), which vary with droplet generation regime and are affected by viscosity and flow rate ratio of dispersed to continuous phase, interfacial tension , and channel geometry. Previously, we showed that micro-vortices start to occur at higher values of α and TOF corresponding to dripping and jetting regimes [1]. Upon vortex formation, the dispersed phase enters the control volume through the center channel inlet, recirculates within the vortex, and exits through the d_{gap} out of the orifice as droplets. Based on the assumptions and derivation in our recent work [2], the d_{gap} can be expressed as:

$$d_{gap}=0.3\ C_1\ W_{orifice}\ (Q_d/Q_c)^{0.3} \tag{1}$$

where the constant C_1 is dependent on microchannel geometry and can be derived empirically or numerically, $W_{orifice}$ is the orifice width and Q_d and Q_c are the dispersed and continuous phase flowrates, respectively.

NUMERICAL MODEL

Transient modeling of droplet generation is performed using the commercial CFD package ANSYS Fluent. The explicit coupled level-set and volume of fluid (VOF) model was employed to track the interface between the dispersed and continuous phases. The model is discussed in details in our recent work [2].

EXPERIMENTAL

The polydimethylsiloxane (PDMS) based device features a unique expansion Flow-focusing unit and is fabricated using soft lithography. For the device used in the experiments, the channel height is 75 µm, as measured by a profilometer.

Authors Marked by * contributed equally to this work.

RESULTS AND DISCUSSION

Figure 1a demonstrates the particle dynamics in vortex streamlines. Assuming the particles have radius of R_i, particle trapping occurs if $d_{gap} < R_i$, and release occurs when $d_{gap} \geq R_i$. As such, we can control the number of particles releasing into a droplet by tuning the d_{gap} . Figure 1c-f illustrates the simulation and corresponding experimental results for the selective trap and release of particles. Experimentally, d_{gap} is altered by changing the dispersed to continuous phase flow rate ratio. Next, we evaluated the accuracy of the developed theoretical model in predicting particle trapping and release. Using numerical modelling, the constant C_1 in equation (1) was found to be 0.25. According to figure 1g, there is a relatively good match between experimental and theoretical results.

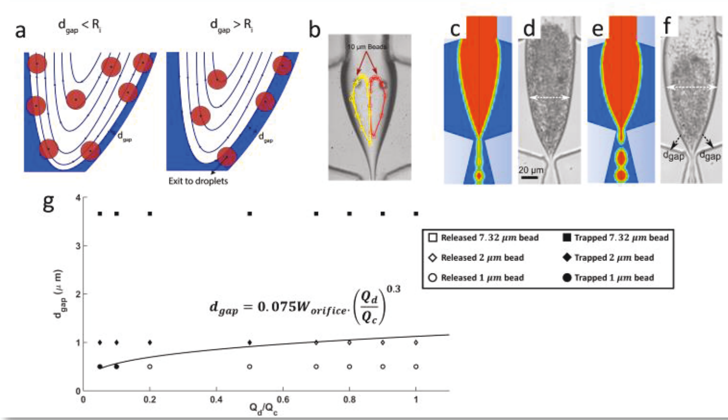

Figure 1: (a) Schematic illustrating trap and release mode. (c & d) CFD model and corresponding experimental image of trapping mode, for 1 µm *particles (e & f) CFD simulation and experimental image of 1 µm particle releasing mode. (g) Theoretical d_{gap} for different flow rate ratios when $W_{orifice} = 15\ \mu m$. The circle, diamond, and square markers correspond to experimental results for the* 1 µm, 2 µm, *and* 7.32 µm *particles*

Figure 2a-b highlights the effect of the PDMS surface treatment and microfluidic channel height on the geometry of micro-vortices. These findings indicate that increasing hydrophobicity and channel height lead to a higher trapping efficiency since the micro-vortices become wider and can hold higher number of cells without significant particle-particle interactions and trajectory shift due to the collisions.

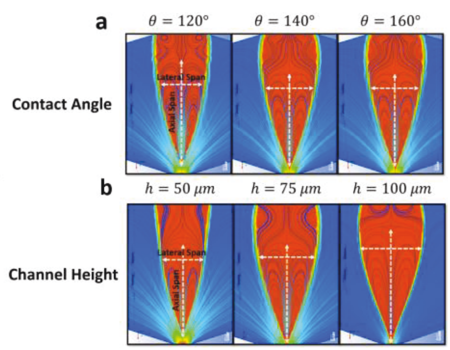

*Figure. 2: (**a**) Comparison of micro-vortices geometry for different contact angles (PDMS surface treatments) (contact angle ↑: Lateral Span ↑, Axial Span ↓) (**b**) Comparison of micro-vortices geometry for different microchannel heights (channel height ↑: Lateral Span ↑, Axial Span ↑).*

CONCLUSION

We utilized theoretical, computational, and experimental fluid dynamics to study formation of shear-dependent micro-vortices and their key controlling parameters. In this study, we introduced d_{gap} as the trapping size threshold and, using theoretical fluid mechanics, correlated it to the orifice width and the flow rates of continuous and dispersed phases (power-law relation). The developed mathematical model matches well with the experimental results in predicting size-based particle trapping inside the micro-vortices. We also evaluated how PDMS hydrophobicity and channel heights affect the micro-vortices geometry. Our results indicates that increasing both hydrophobicity and the channel height facilitates increasing the capacity of the system to trap a larger number of particles/cells and, consequently, improves trapping efficiency.

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REFERENCES

[1] Kamalakshakurup et al, "High-efficiency single cell encapsulation and size selective capture of cells in picoliter droplets based on hydrodynamic micro-vortices." Lab on a Chip 17.24 (2017): 4324-4333.

[2] Kamalakshakurup et al, "Shear-dependent microvortices in liquid–liquid flow-focusing geometry: A theoretical, numerical, and experimental study", Physics of Fluids 33, 032016 (2021)

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