CFD analysis and experimental validation of magnetic droplet generation and deflection across multilaminar flow streams

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ABSTRACT

The use of droplet-based microfluidic systems has increased in the last decade due to the advantages these systems present such as compatibility with many chemical and biological reagents, capability of performing a variety of "digital fluidic" operations that can be rendered programmable and reconfigurable, decreased reaction times and large interfacial areas, repeatability of operations etc. However, with the maturity of this platform technology, sophisticated and delicate control of droplet generation and manipulation is needed to address increasingly complex applications. Magnetic separation has proven a useful and elegant method for manipulating magnetic materials in microfluidic devices. In this work, we present a CFD model to study the continuous processing of droplets by deflecting ferrofluid-based templates through multilaminar flow streams. We introduce different chip designs and an optimization study for the generation and manipulation of droplets by applying magnetic fields generated by a permanent magnet. The numerical method includes the integration of magnetic and fluidic computational models that accurately describe the droplet generation and motion under different magnetic field and flow conditions. The CFD is performed using the volume-of-fluid (VOF) method as implemented in the commercial flow solver ***FLOW-3D***. The flow solver was linked to a FORTRAN subroutine that calculates the magnetic field due to the magnet and the corresponding magnetic force exerted on the droplets. The impact of different process variables and parameters – flow rates, magnet location and chip design – on both droplet size and trajectory, is quantified. Finally, experimental validation of the model is carried out with oil-based ferrofluid droplets and ink aqueous solutions. Theoretical and experimental results are accordingly compared and discussed. Due to the unique advantages of integrating magnetic materials within droplet microfluidics, this technology has the potential to provide novel solutions to different biomedical engineering challenges for advanced diagnostics and therapeutics.

Keywords: magnetic droplets, multilaminar flow microfluidic systems, CFD modeling, droplet generation, droplet deflection

1. INTRODUCTION

The use of droplet-based microfluidics enables the precise handling of minute amounts of fluid. These systems possess high interfacial areas and short diffusion distances which facilitate mass and heat transfer [1]. Thus, recently there has been increased interest in their applications in chemical engineering, biomedical analysis, material synthesis and sensing to name but a few. In order to take advantage of droplet microfluidics, the generation and manipulation of these small volumes should be investigated. Different strategies have been implemented to guide the trajectories of the droplets in continuous flow within the channels, such as acoustophoresis, dielectrophoresis, optical, mechanical methods, etc. However, they require either complex channel configurations or additional expensive peripheral equipment. In this article, we evaluate the use of magnetic technology as one of the most useful and elegant alternatives for manipulating droplets inside continuous-flow systems, provided that the fluid has magnetic properties (ferrofluids) [2,3].

Various authors have addressed the modeling of ferrofluid droplet generation, mostly by passive control (using different flow rates for the continuous and dispersed phases) while active ferrofluid droplet formation and combinations between active and passive methods have been reported as well. Moreover, a significant part of numerical or experimental studies on ferrofluid droplets are devoted to the investigation of motion and deformation of a single droplet under the influence of uniform magnetic fields. Although these studies are important and capture the overall complexity of the problem, i.e. the complex and dynamic interactions among magnetic, surface tension and viscous forces, they are limited to a discrete number of droplets that are located inside microscale structures. In the present study, a computational fluid dynamics approach is implemented to investigate the dynamic behavior of continuous-flow droplet microfluidics in millimeter-scale reaction chambers, by applying non-homogeneous magnetic fields generated by permanent magnets, with the main objective of efficient design for increasingly complex applications where droplets are guided through relatively large chambers/channels.

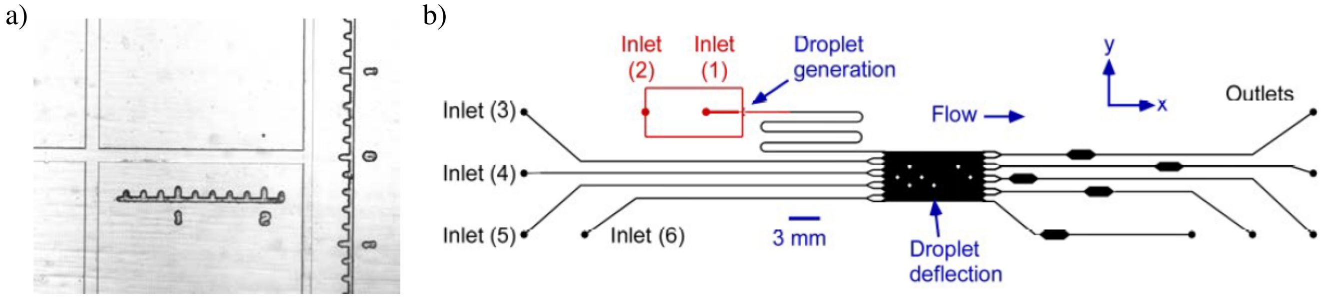

Figure 1. a) Image of the flow-focusing droplet generation device (channel width: 150 μm; length: 2.5 mm). b) Chip design featuring a flow-focusing droplet generation junction and a chamber for the deflection of droplets through multilaminar flow streams. This device is composed of two etched plates: a top layer featuring an interchangeable droplet generation junction (20 µm deep) and a bottom layer featuring a channel structure for the magnetic deflection of droplets through reagent and washing streams (100 µm deep).

2. THEORY

The models for predicting both the ferrofluid droplet generation and deflection through multilaminar flow chambers involve a CFD-based Eulerian-Eulerian and Eulerian-Lagrangian approach. For droplet generation, we modeled the device shown in Fig. 1 a), which consists of a flow-focusing device followed by a straight channel and a T-junction outlet. The numerical model employs the volume of fluid (VOF) method to track the interface between the ferrofluid (dispersed phase) and the aqueous continuous phase. The advantage of the VOF method is that it can model two immiscible fluids with a sharp interface by solving a single set of momentum equations and tracking the volume fraction through the entire flow domain. In the present work, contact angle hysteresis and the effect of magnetic field on the contact angle were not considered. However, the equilibrium contact angle as well as the surface tension coefficient were experimentally measured (140º and 5 mN m^{-1}, respectively) and implemented in the model.

For droplet deflection studies, we modeled the chamber shown in Fig. 1 b). A Lagrangian framework was employed to predict the droplet dynamics under non-uniform magnetic fields. In summary, we considered the droplets as point like particles with fixed hydraulic dimensions (calculated from the droplet generation simulations) and predicted their trajectories across the chamber by applying classical Newtonian dynamics. Only the dominant magnetic and fluidic forces were considered in this work. Expressions for the magnetic and drag forces acting on the droplets can be found in our previously published works [2-4]. A Sm-Co magnet was chosen as the magnetic source, with dimensions of 3 x 4.8 x 7.3 mm^3, and the analytical model developed by E. P. Furlani [5] was adopted for the calculation of the field and force distribution inside the chamber. The fluid velocity field was estimated by the modified Navier-Stokes and continuity equations that account for the interactions between the droplets and the fluids (two-way coupling).

The model was developed by customizing the commercial multiphysics CFD software program, ***FLOW-3D*** from Flow Science Inc. Specifically, custom magnetic field and force algorithms were integrated into the program (through a linked FORTRAN subroutine) to predict the field distribution from various field sources and the corresponding force on magnetic droplets. The simulations were performed on a 24-core workstation with 128 GB of RAM. The runtime for the simulations varied between 10 and 70 hours depending on the specific geometry, number of mesh cells and selected flow rates.

3. EXPERIMENTAL SETUP

For the validation of the CFD models, various experiments were performed. In all cases, an oil-based ferrofluid containing a suspension of 10 nm diameter magnetic nanoparticles at a concentration of 11.8 vol% dissolved in cyclohexane (50% v/v) was used as the dispersed phase. This phase was pumped at the inlet at varying flow rates (depending on the experiment), in order to study the effect of the flow rates on the drop size. Aqueous solutions of poly(vinylpyrrolidone) and Tween 20 (0.05%) were used as continuous phases, which were injected at flow rates ranging from 100 to 500 $\mu L\ h^{-1}$. For the droplet deflection across the multilaminar flow chamber (Fig. 1 b)), ferrofluid droplets were generated at a flow-focusing junction (inlets 1 and 2). Then, they were guided through a serpentine to the main chamber (4.1 x 8 x 0.1 mm^3) and deflected across 5 parallel streams by placing a permanent magnet at the bottom of the chamber. Ink streams were used as coloring agents (injected at inlets 3-6) for visualization. The magnetic deflection was studied by varying the flow rates in the chamber as well as the magnet location with respect to the chamber. Droplet generation and deflection was observed via an inverted fluorescence microscope equipped with a high resolution CCD camera. The ImageJ software was used for the analysis of the experimental images.

4. RESULTS AND DISCUSSION

4.1 Droplet generation

In this subsection, the ferrofluid droplet generation results are presented as a function of the continuous phase flow rate. The volumetric fraction occupied by the dispersed phase (in red color) is presented in Fig. 2 for continuous phase flow rates equal to 100, 200 and 300 μL h^{-1} (Figs. 2 a), b) and c), respectively). For this analysis, the dispersed phase flow rate was fixed at 10 μL h^{-1}. We experimentally observed that droplet size decreases from approximately 240 μm to 135 μm as the continuous phase increases from 100 to 500 μL h^{-1}. Our simulations predict similar droplet shape and size. The simulated results reported droplet sizes between 120 μm and 190 μm as the flow rate of the continuous phase increased in the range under study (the committed error varies between 12% and 20% depending on the specific flow rate). Furthermore, the dispensing rate results are in good agreement with the experimental data.

4.2 Droplet deflection

Regarding the deflection analysis, flow rates between 300-600 μL h^{-1}, for the continuous phase and ink streams, and between 1 and 10 μL h^{-1} for the dispersed phase were tested. Furthermore, different magnet locations and orientations were analyzed. The optimal conditions are presented in Fig. 3. We observed that a flow rate ratio of 1/300 between the dispersed and continuous phases generated droplets of around 50 μm in size. The optimal magnet location was 5.5 mm away from the chamber, generating magnetic forces of around 0.5 nN on the droplets. Under these magnetic conditions, ink streams injected at a 300 μL h^{-1} were used, assuring the parallel co-flow of the 5 streams and inducing a parabolic deflection of the droplets. As it can be perceived from Fig. 3, the simulated droplet trajectory is nearly identical to the experimental one. This agreement between experiments and simulations was obtained for all the tested conditions.

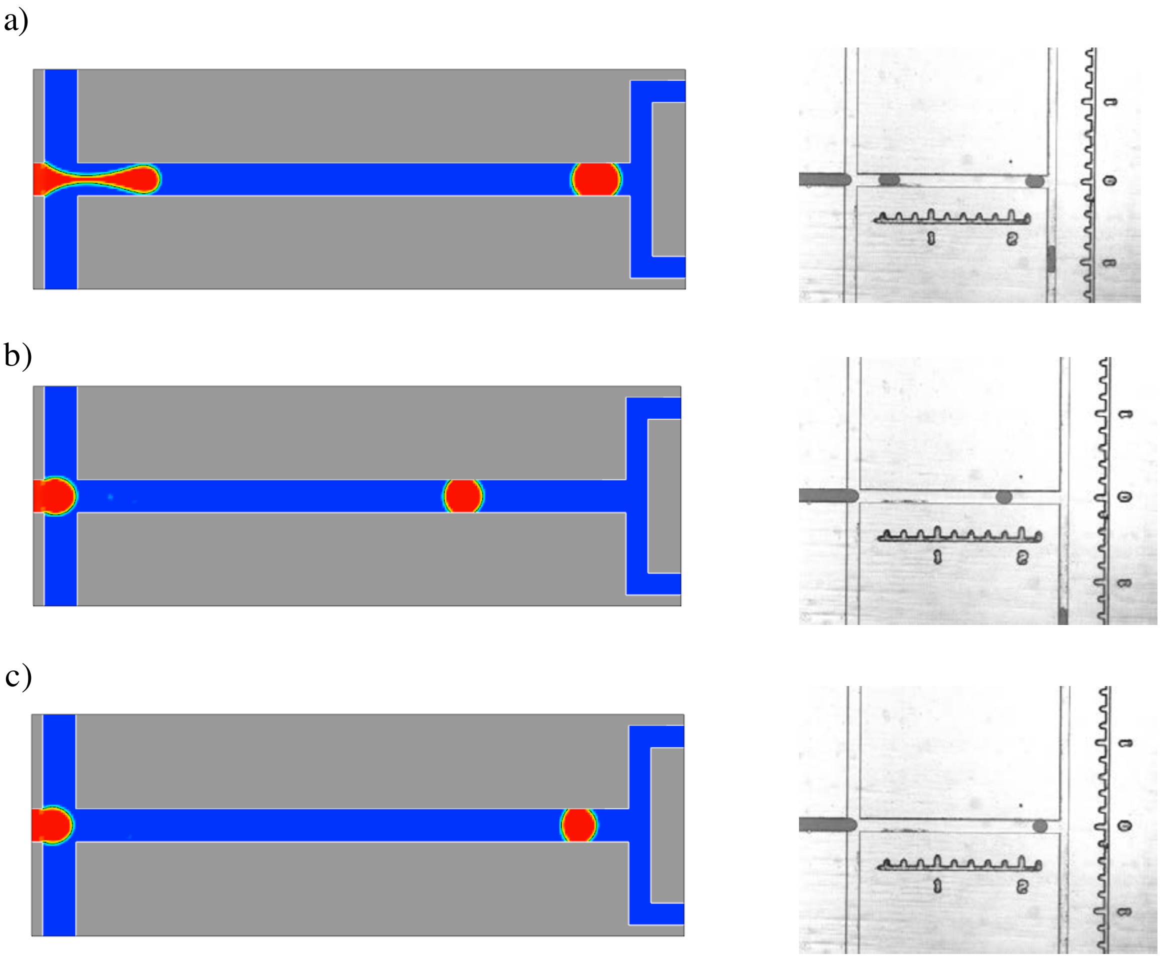

Figure 2. Simulated and experimental results of the flow-focusing droplet generation device (dispersed phase flow rate fixed at 10 μL h^{-1}). Continuous phase flow rates are: a) 100 μL h^{-1}; b) 200 μL h^{-1}; c) 300 μL h^{-1}.

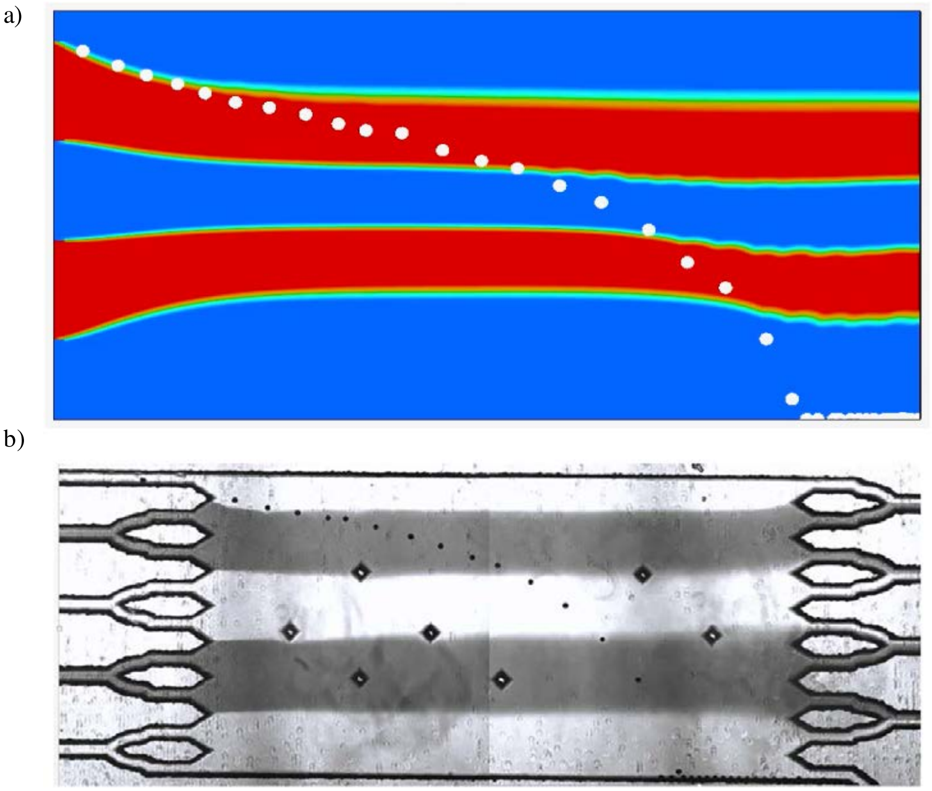

Figure 3. a) Simulated and b) experimental results showing droplet deflection across the multilaminar flow chamber. Continuous and dispersed phase flow rates fixed at 150 and 1 μL h^{-1}, respectively; Ink flow rates of 300 μL h^{-1}; Distance from the top of the magnet to the channel wall equal to 5.5 mm.

5. CONCLUSIONS

We have introduced a novel computational approach for predicting and optimizing the continuous processing of ferrofluid droplets. Our model takes into account the dominant physical phenomena that affect both droplet generation and manipulation with permanent magnets. This modeling effort can be used to study critical details of the process including droplet size and shape, dispensing rate, trajectories of individual droplets, time required for the generation and deflection and the perturbation of the fluid co-flow. The experimental validation of the theoretical model was performed, and the simulated results are in good agreement with the experimental data.

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