CFD Analysis of the Generation and Manipulation of Ferrofluid Droplets

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ABSTRACT

Droplet-based microfluidic systems have attracted significant attention due to their unique advantages and performing several digital fluidics operations in various fields such as chemical and biological microsystems. These operations can be programmed and reconfigured using droplet-based microfluidics. Nonetheless, as demand of using such precise devices rise in different areas, more sophisticated and delicate control of the processes governing droplet generation and manipulation is necessary to address complex applications. Therefore, in this study, we introduced a CFD-based model ferrofluid droplet using the commercial CFD software package ***FLOW-3D*** to further study generation and separation of ferrofluid droplets in microfluidic channels. Different micro-channel designs are examined and an optimization study on the generation and subsequent manipulation of droplets with permanent magnets is performed. The analytical studies were used to model permanent magnet and further combined with CFD analysis using the volume-of-fluid (VOF) method to accurately describe ferrofluid droplet generation and motion under an external magnetic field. For the implementation of magnetic forces, the flow solver was linked to a FORTRAN subroutine that calculates the magnetic field and the corresponding magnetic force exerted on the droplet. We also examine the impact of different process variables such as flow rate, and the application of an external magnetic field during generation, on both droplet size and dispensing rate. The developed model accurately describe the droplet generation, frequency of forming each droplet and motion under different flow conditions. Overall, the model enables better understanding of physical phenomena involved in the continuous droplet processing and serves as an efficient parametric analysis and optimization platform. This magnetic droplet technology has the potential to provide novel solutions to different biomedical engineering challenges for advanced diagnostics and therapeutics.

Keywords: magnetic droplets, CFD modeling, droplet generation, ferrofluids

1. INTRODUCTION

The studies about the concept of droplet-based microfluidic have received a dramatic increase in recent years. This is due to the advantages of such materials, which make them ideal candidates for numerous applications in the chemical, biological and medical fields. Initially, external pressure or electrical forces were used to control the fluid flow in microfluidics. However, due to their disadvantages, such as larger Joule heating effects, manipulating fluid flow via external magnetic forces has taken place for many applications. This process can be done by using colloidal suspensions of single domain magnetic particles in a carrier fluid, so called ferrofluids [1, 2].

During early years after discovery of ferrofluids, they have been used for many traditional applications from electrical, mechanical to optical fields. However, recently, ferrofluids are used to manipulate liquids in microfluidic devices with external magnetic fields, which can have several applications in catalytic reactions, drug delivery, biological analysis, etc. [3-6] For many of these cases, the dispersions are poorly controlled. However, ferrofluid droplet-based microfluidic technology can provide precise control of droplet size at the microscale, and therefore precise control of chemical composition. Ferrofluid droplet-based multiphase microfluidic devices provide several advantages over conventional systems in terms of fast reaction rates due to a large surface to volume ratio compare to surface-based analysis, small sample volumes, high throughput, detection and separation with high sensitivity and resolution, and integration with multiple functionalities. [7] [8].

In this work, we introduce a combination of magnetic and fluidic computational models using the VOF method that describe the ferrofluid droplet trajectory inside microchannel under the influence of an external magnetic field. We present a computational fluid dynamic (CFD) model to investigate the dynamics of oil-based ferrofluid droplets within an aqueous continuous phase under an external inhomogeneous magnetic field. CFD modelling is performed the commercial program and the flow solver was linked to a custom subroutine that analytically calculates the magnetic field due to a rare-earth permanent magnet field source and the corresponding magnetization using a

Langevin function as well as the magnetic force exerted on the droplets. This approach is well-suited for parametric analysis and optimization, thereby facilitating the development of novel micro- magnetofluidic microfluidic systems.

2. COMPUTATIONAL MODEL

The model was developed by customizing a commercial multiphysics CFD software program, ***FLOW-3D*** from Flow Science Inc. (ver11.2, www.flow3d.com). The model for predicting the ferrofluid behavior inside the microchannel shown in **Figure 1(a)** involves a CFD-based VOF approach. The fluid transport is predicted numerically by solving the Navier-Stokes equations and mass transfer between the co-flowing fluids, while magnetic force on ferrofluid droplet is applied using analytical methods. There are two defined phases in this model, dispersed phase (DP) and continuous phase (CP) in which DP is oil-based ferrofluid and water-based is CP.

The model is based on the following assumptions: (a) all fluids are Newtonian and incompressible, (b) interparticle magnetic dipole-dipole coupling is negligible because of a low particle concentration, (c) the field sources are ideal 3D rare-earth permanent magnets, and (d) there are no other magnetic materials present in the computational domain to perturb the magnetic field.

The governing conservation equations for this problem can be divided into three main sections, where it can be solved for continuity equation, momentum equation, and magnetic field analysis based on the assumptions were mentioned for this model. For this case, we consider Maxwell's magnetostatic equations. The magnetic force density acting on droplet was calculated based on volume of droplet as represented in equation (1).

$$\boldsymbol{F_M} = V\mu_0\boldsymbol{M}\cdot\nabla\boldsymbol{H} \tag{1}$$

where V is the volume of the droplet, μ_0 is the permeability of vacuum, $\boldsymbol{M}$ is the magnetization of the ferrofluid droplet, and $\nabla\boldsymbol{H}$ is the gradient of the magnetic field. In another hand, magnetization of a ferrofluid is given by langevin function, where magnetization changes nonlinearly with respect to effective magnetic susceptibility (ξ), as derived in equations (2) and (3):

$$\boldsymbol{M} = M_s\emptyset\left(\coth(\xi) - \frac{1}{\xi}\right)\boldsymbol{H} \tag{2}$$

$$\xi = \frac{\mu_0 V_{np} M_s|\boldsymbol{H}|}{k_B T} \tag{3}$$

Where $\emptyset$ is volume fraction of particles in fluid, M_s is saturation magnetization, V_{np} is volume of magnetic nanoparticles, k_B is Boltzmann constant which is equal to k_B=1.38×10^{-38} $m^2 kg\cdot s^{-2} K^{-1}$, and finally T is temperature in Kelvin (K).

In order to analytically determine the 3D magnetic field from permanent magnet, the model developed by Furlani was employed [9]. Magnetic flux density (**B**) and magnetic field density (**H**) were solved based on position of the permanent magnet with respect to micro-channels as shown in **Figure 1(b)**. The magnitude of magnetic flux density, $\mathbf{B_{t,max}}$ shows the maximum applied magnetic field at the bottom of active fluid domain which is around 65mT.

For the fluid analysis, two fluid phases pumped into two inlets where dispersed phase or DP was composed of oil-based ferrofluid (EMG901, Ferrotec), with magnetic particle concentration of 11.8 vol%, dissolved in cyclohexane (50% v/v). The Continuous Phase (CP) is aqueous water based solution. The simulated generation of ferrofluid droplets is analyzed as a function of the CP flow rate (Q_c) and the channel depths of 25µm, 30µm, and 40µm, under the influence of magnet field. The DP was kept at Q_d=10 µL·h^{-1} for this study. The permanent magnet was located 0.7 mm away from T-shaped outlet in order to obtain the influence of magnetic field on ferrofluid droplets and sort them accordingly at the outlet. The magnet was determined to be magnetized in z-direction analytically. The rare-earth NdFeB magnet was chosen as the magnetic sources, with dimension of 0.5x0.5x0.5 mm^3 .For the sake of a consistent analysis, fully developed boundary conditions are assumed for both cases: with and without permanent magnet.

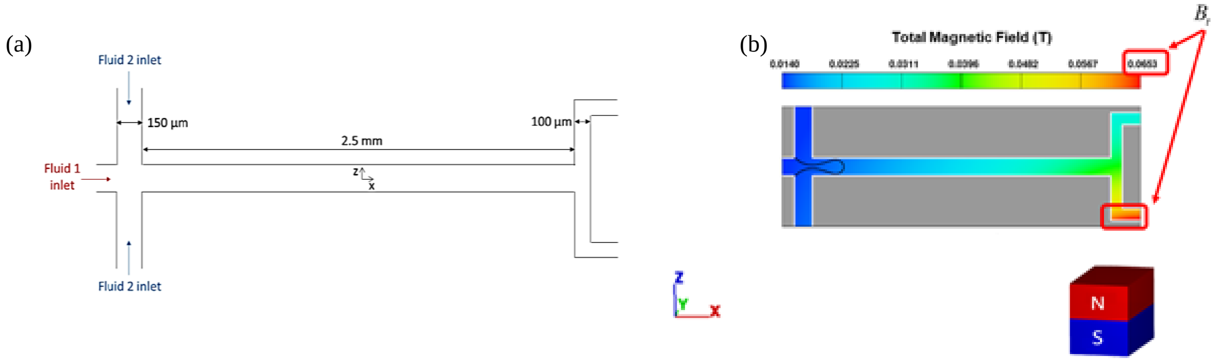

Figure 1. (a) Schematic view of the flow-focusing droplet generation and T-shaped junction outlet (b) Influence of magnetic field on microfluidic device

3. RESULTS AND DISCUSSION

Droplet-based ferrofluids under the influence of a magnetic field hold great potential to enhance generation and manipulation of droplet in microfluidic device. It should be noted that the calculated magnetic field has a spatial gradient, which gives rise to body forces within ferrofluids droplet in both z and x directions and related velocity components that depend on the gradient of the magnetic field.

Figure 2 demonstrates the performance of oil-based ferrofluid droplet sorting at the outlet where (a) and (b) show the times t= 0.7s and t=1.5s with no magnetic field and (c) and (d) show the performance under the applied magnetic field. The fraction of fluid for ferrofluid droplet (indicated with red color) travels through the channel via pressure generated by the flowing CP (indicated with blue color). The behavior of the droplet, when it reaches the outlet shows the droplet deformation due to impact against the T-junction wall. After coupling two commercial programs *FLOW-3D* and Visual-Studio, the magnetic force density was applied in the ferrofluid fraction region of the fluid domain and affected the motion of the ferrofluid droplet, in order to direct the droplet to the bottom outlet of the T-junction. **Figure 2 (c)** and **(d)** indicate how the droplet acts when it reaches to the outlet. In the computational model, the magnetic force successfully redirects all droplets down and there is no splitting of the droplet at the T-junction.

The comparison of droplets diameter, with and without magnetic field, have shown percentage increment under the influence of magnetic field for continuous flow rates (Q_c=100 μL·h^{-1} to 400 μL·h^{-1}). Presence of magnetic field deform the droplet and it elongates from its spherical shape. The magnetic nanoparticles will be aligned under influence of magnetic field and as droplet gets closer to magnetic field and as magnetic field gets stronger with respect to droplet location this elongation is more observable. While comparing three different channel depth of 25μm, 30μm, and 40μm for their droplet size variation under a magnetic field, it can be seen that the deeper the channel gets, the droplet size gets increase due to number of magnetic nanoparticles.

The magnetization of ferrofluid is proportional to position of the permanent magnet. Hence, forces on droplet close to T-junction are larger than those close to the flow focusing channel.

Another study was to investigate the frequency of formation for each droplet. **Figure.3** shows the dispensing rate as a function of CP flow rate for three chip designs. The dispensing rate increases as the CP flow rate increases with and without magnetic field influence on ferrofluid droplet. In the absence of magnetic field, dispensing rate is in the range of 2.1 drop.s^{-1} to 5.3 drop.s^{-1} for 100 μL·h^{-1} to 400 μL·h^{-1}. While under the influence of magnetic field the range changed from 2.2 drop.s^{-1} to 6.2 drop.s^{-1}for the same range of flow rates. By comparing the three chip designs, the greatest dispensing rate is obtained for shallowest channel. This is attributed to relatively fast velocity magnitude. For the same flow rates, the velocity inside 25μm channel depth is almost twice as the value for 40μm depth as the cross sectional area reduced for this design. Though by comparing

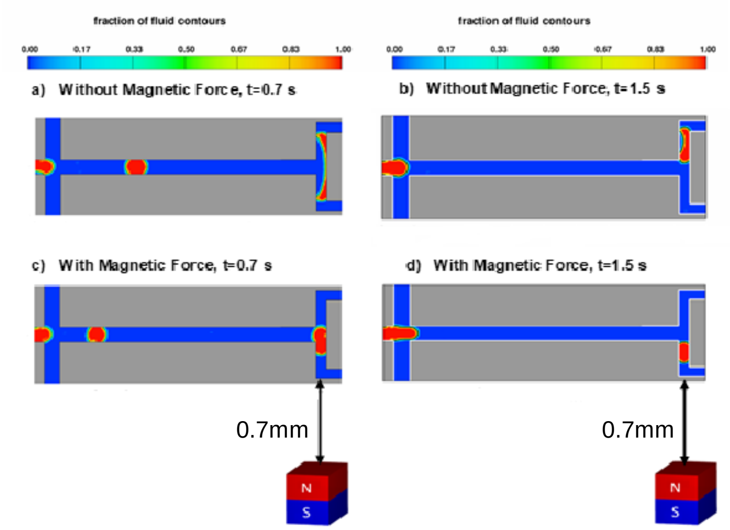

Figure 2. Comparison between sorting of droplets at the outlet (a) and (b) Without magnetic force (c) and (d) With magnetic force, at t =0.7 s and t=1.5 s for channel depth of 25μm at =100 μL·h^{-1} and =10 μL·h^{-1}

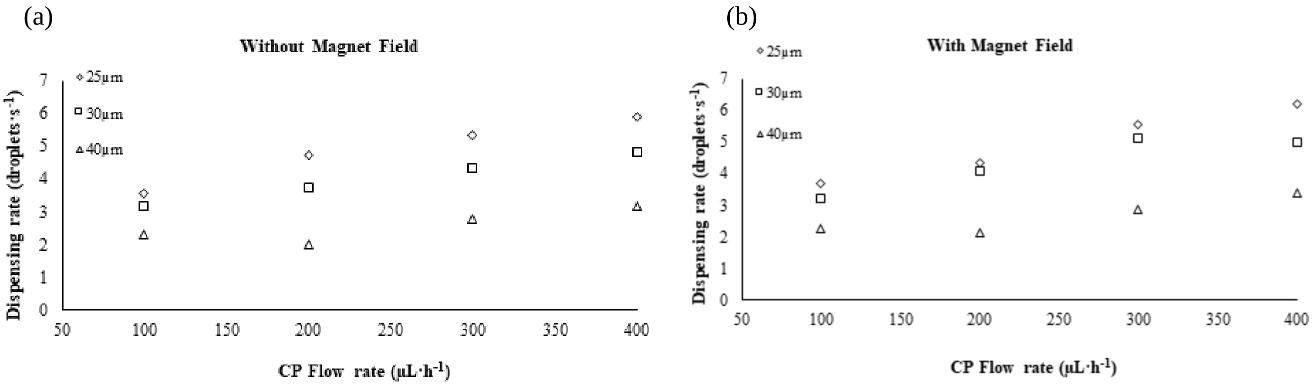

Figure 3 Dispensing rate of droplet formation (a) Without magnetic field (b) Under influence of magnetic field

the influence of magnetic field on increasing formation of ferrofluid droplet the shallowest channel, 25µm have the minimum changes on average of 1.4%, while the greatest increase belongs to 30µm which is about 7.7%, average of all considered CP flow rates. Therefore, for applications where frequency of formation and velocity is more important than volume of droplet, shallow channel depth could be a better option.

4. CONCLUSIONS

We have introduced a novel computational model for predicting and optimizing the process of ferrofluid droplet generation and manipulation in microfluidics device. The model takes into account dominant hydrodynamic and magnetic forces on each droplet. Fluid flow (Navier-Stokes equations) and mass transfer between the co-flowing fluids are solved numerically, while the magnetic force on ferrofluid is programmed using analytical methods. The impact of different process variables and parameters – flow rates, different channel configuration have been studied. We have found that manipulation of ferrofluid droplet in microchannel is mainly due to three effects: volume of ferrofluid which is related to channel configuration and flow rate of fluid, magnet size and strength, distance of permanent magnet form the channel. To conclude, this project donates to the development of precise, computationally inexpensive and useful tools that can be used for the rational design of a high number of applications.

ACKNOWLEDGEMENTS

Financial support from the Spanish Ministry of Economy and Competitiveness under the projects CTQ2015-72364-EXP and CTQ2015-66078-R (MINECO/FEDER) is gratefully acknowledged. Financial support from the U.S. National Science Foundation, through Award CBET-1337860, is also acknowledged.

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