International Journal of Heat and Fluid Flow 56 (2015) 324–334

Contents lists available at ScienceDirect

International Journal of Heat and Fluid Flow

journal homepage: www.elsevier.com/locate/ijheatfluidflow

Seriate microfluidic droplet coalescence under optical forces in a channel flow

Hyunjun Cho, Jin Ho Jung, Hyung Jin Sung*

Department of Mechanical Engineering, KAIST, 291 Daehak-ro, Yuseong-gu, Daejeon 305-701, Republic of Korea

ARTICLE INFO

Article history:
Received 29 May 2015
Revised 2 October 2015
Accepted 2 October 2015

Keywords:
Optofluidics
Droplet coalescence
Optical tweezer
Lattice Boltzmann method

ABSTRACT

The microfluidic holding and coalescence behaviors of droplets subjected to an optical trap within a channel flow were numerically studied by using the lattice Boltzmann method and the dynamic ray tracing. A tightly focused Gaussian laser beam positioned laterally with respect to the channel flow direction was used as the optical trap. In such a system, seriate droplet coalescence was observed between an optically trapped droplet and the subsequent droplet. The numerically predicted droplet coalescence behavior agreed well with the experimental results. A sufficiently high laser power was required to capture an incoming droplet and induce coalescence with the subsequent droplet. The effects of various flow and optical parameters on the coalescence behavior were investigated.

1. Introduction

Droplet microfluidics applications are particularly useful in the fields of chemistry and biology (Churski et al., 2012; Song et al., 2006). Immiscible droplets may be used as reagent carriers to prevent cross-contamination, diffusion, or evaporation, and microdroplets can significantly reduce both the required amount of reagents and the reaction time (Kenig et al., 2013). The use of microdroplet reactors in certain experiments relies on control over the coalescence behaviors between droplets. Microdroplet coalescence may be controlled in a number of ways using the channel geometry (Niu et al., 2008; Tan et al., 2006), thermal effects (Luong et al., 2012), thermo-capillary effects (Baroud et al., 2007), electrical fields (Priest et al., 2006; Thiam et al., 2009), or optical forces (Ashkin, 1970; Dholakia and Čižmár, 2011; Jung et al., 2014). Optical force approaches provide a particularly straightforward, accurate, and non-invasive means for controlling microdroplets (Ashkin, 1970; Jung et al., 2014). Several optical force methods have been developed based on optical vortex traps (Lorenz et al., 2007), laser arrays (Ogura et al., 2011), and optical tweezers (Dholakia and Čižmár, 2011). In situ, seriate, and rapid microdroplet coalescence was obtained using an optical tweezer in conjunction with a low-cost channel geometry (Jung et al., 2015).

Optical tweezers may be realized using lasers. As a droplet enters the focal volume of a laser beam, an optical force is produced due to the change in the photon momentum via refraction and reflection at the droplet interface. When the refractive index of the droplet exceeds that of the medium, an optical gradient force pulls the droplet toward the laser center axis. Jung et al. (2015) examined seriate droplet coalescence in which a sufficiently high optical gradient force was able to trap a flow-driven droplet to induce coalescence with a subsequent droplet driven by the channel flow. A high beam intensity was required to achieve this gradient force, thereby necessitating a high laser power and/or small beam waist. A tightly focused Gaussian laser beam is suitable for this purpose. Kim et al., (2012) derived an analytical expression for the optical gradient and scattering forces produced by a tightly focused Gaussian laser beam acting on a spherical particle. Ellington (2013) provided a theory of the microdroplet deformation by Gaussian laser beam including the scattering patterns for spherical droplets. Unfortunately, due to the nonuniform optical force at the interface, droplets tend to deviate from a spherical shape during the deformations induced by the flow and the optical force, and the analytical expression for a spherical shape may not be the best model for the system. Changes in the optical forces can also affect the shape of the fluid-droplet interface, producing a feedback relationship between the optical forces and the droplet shape. In situ optical force calculations that may be applied to an arbitrary droplet shape are needed. In a transient numerical simulation, the deformed droplet interface as well as the corresponding optical force must be calculated at each time step. The droplet interface may be constructed using the marching cubes algorithm. Originally developed by Lorensen and Cline (1987), the algorithm provides a tool for obtaining the triangulated isosurface of a three-dimensional scalar field. The algorithm has a well-characterized connectivity problem that was resolved in an improved algorithm developed by Masala et al. (2013). The optical forces on a triangulated interface may

* Corresponding author. Tel.: +82 42 350 3027; fax: +82 42 350 5027.
E-mail address: hjsung@kaist.ac.kr (H.J. Sung).

http://dx.doi.org/10.1016/j.ijheatfluidflow.2015.10.002

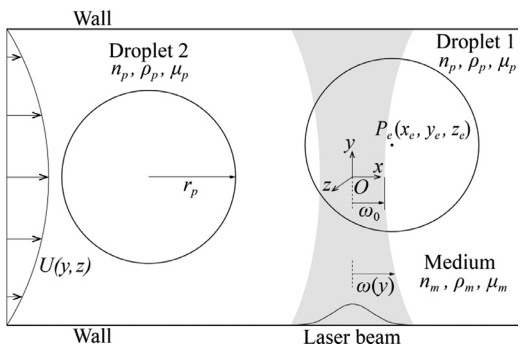

Fig. 1. Schematic diagram showing the optical coalescence simulation system. Two identical droplets 1 and 2 were carried by the channel flow toward a tightly focused Gaussian laser beam. Droplet 1 was fixed at P_e due to the optical gradient force.

be calculated using the dynamic ray tracing (DRT) technique developed by Sraj et al. (2010).

Numerical investigations of the coalescence behaviors of microdroplets were performed using a two-phase flow solver. The lattice Boltzmann method (LBM) is a numerical tool that is capable of modeling a transient flow field in three dimensions, in agreement with the Navier–Stokes equation (Junk et al., 2005). Shan and Chen (1993) developed a multiphase model of the LBM based on an interparticle potential. The model promotes the phase separation by introducing a repulsive force between the phases, rather than tracking the phase interface. As a result, two droplets touching with each other merge without a stable interface, where the effect of the surfactant on the interface drainage or rupture procedure was not taken into account. The model has been used in several microfluidic studies involving topological changes in the interface, such as droplet breakup in a simple shear flow (Xi and Duncan, 1999), water droplet transportation in porous media (Park and Li, 2008; Mukherjee et al., 2009), and mixing behaviors inside microdroplets (Wang et al., 2013). To the best of our knowledge, no studies have examined the seriate optical coalescence of flow-driven microdroplets in a channel.

Three-dimensional transient numerical simulations were conducted here to investigate the holding and coalescence behavior of flow-driven microdroplets in the presence of an optical tweezer. A tightly focused Gaussian beam positioned normal to the channel flow was used as the optical tweezer. The LBM multiphase model of Shan and Chen (1993) was used to obtain an isothermal two-phase flow field. The optical forces that acted on the deforming droplet were calculated using the DRT, whereas the required interface triangulation was accomplished using the improved marching cubes algorithm. The simulation code was verified using the Young–Laplace equation and the analytical solutions for optical forces. The simulation results were then validated by comparison with the experimental data of Jung et al. (2015). Three distinct regimes of droplet coalescence behavior were identified. The effects of various flow and optical parameters were quantitatively investigated by measuring the droplet lagging distance during passing the optical trap.

2. Numerical methods

A schematic diagram showing the optical coalescence simulation system is shown in Fig. 1. Here, $U(y, z)$ denotes the channel flow velocity, r_p the droplet radius, n the refractive index, ρ the density, μ the viscosity, and ω_0 the beam waist. The subscripts p and m represent the droplet and the medium, respectively. The seriate droplets were driven by the channel flow. Under a sufficiently high optical gradient force, the first incoming droplet 1 was captured at the point of equilibrium, P_e. At this position, the optical force applied by the laser beam and the drag force applied by the channel flow were balanced. Coalescence subsequently occurred between droplets 1 and 2, as depicted in Fig. 2. The coalesced droplets exited the optical trap due to the increased viscous drag force from the channel flow. The coalescence phenomenon depicted in Fig. 2 occurred only at moderate laser beam powers. A laser power below a certain threshold was insufficient to allow the optical trap to capture the incoming droplet 1, and the droplets merely passed through the beam. On the other hand, a laser power above a threshold value applied an optical force that captured even the coalesced droplet, and a second coalescence event could occur with a third droplet. Three distinct droplet holding and coalescence behavior regimes were identified: no coalescence, if the droplets merely passed through the optical trap; standard two-droplet coalescence; and coalescences among more than two droplets (multiple coalescences). The simulation results obtained in the three regimes are depicted in Fig. 10 in Section 3.

2.1. Two-phase flow field

A two-phase flow field involving the microchannel and droplet was prepared using the LBM. The multiphase model of Shan and Chen (1993) and the D3Q19 (three-dimensional, nineteen-velocity) lattice velocity set were adopted, as illustrated in Fig. 3. The lattice velocity set endowed each node in the domain mesh with nineteen distributions and their corresponding velocities. The distributions streamed to the neighboring nodes, depending on their velocities, according to

$$\text{Streaming}: f_{\phi,i}(\mathbf{x}+\mathbf{c}_i, t+1) = f^c_{\phi,i}(\mathbf{x}, t), \tag{1}$$

where f represents the distribution, $\mathbf{x}$ the node position vector, $\mathbf{c}$ the lattice velocity vector, and t the time step. The subscripts i and ϕ denote the ith direction in the D3Q19 set and the phase (0 or 1), respectively. After the streaming process, collision occurred among the distributions at a given node according to

$$\mathit{Collision}: f^c_{\phi,i}(\mathbf{x}, t) = f_{\phi,i}(\mathbf{x}, t) - \left[f_{\phi,i}(\mathbf{x}, t) - f^{eq}_{\phi,i}(\mathbf{x}, t)\right]\Big/\tau_\phi, \tag{2}$$

where τ is the relaxation time that determines the fluid viscosity ($\nu = [\tau - 0.5]/3$), f^c the post-collision state of the distribution, and f^{eq} is the equilibrium state of the distribution calculated according to a Taylor series truncation of the Boltzmann distribution equation represented by

$$f^{eq}_{\phi,i}(\mathbf{x}, t) = w_i\rho_\phi(\mathbf{x}, t) \times\left[1 + 3\mathbf{c}_i\cdot\mathbf{u}^{eq}_\phi + 4.5(\mathbf{c}_i\cdot\mathbf{u}^{eq}_\phi)^2 - 1.5(\mathbf{u}^{eq}_\phi)^2\right]_{(\mathbf{x},t)}, \tag{3}$$

where ρ denotes the density, $\mathbf{u}^{eq}$ the equilibrium velocity vector, and w_i the weighting factors, which depend on the velocity:

$$w_0 = 1/3,\ w_{1\sim6} = 1/18,\ w_{7\sim18} = 1/36 \tag{4}$$

Multiphase flow was simulated using a model based on the interparticle potential developed by Shan and Chen (1993). The approach adopted a repulsive force between the two phases, which produced phase separation and a surface tension. The repulsive force on a phase ϕ was defined by

$$\mathbf{F}_\phi(\mathbf{x}, t) = -G\rho_\phi(\mathbf{x}, t)\sum_i w_i\rho_{\bar\phi}(\mathbf{x}+\mathbf{c}_i, t)\mathbf{c}_i, \tag{5}$$

where G is an adjustable coefficient that controls the magnitude of the repulsive force. Here, $\bar\phi$ indicates the parameters corresponding to the other phase. The force was implemented by calculating the equilibrium velocity vector in Eq. (3) according to

$$\mathbf{u}^{eq}_\phi = \mathbf{u} + \tau_\phi F_\phi/\rho_\phi \tag{6}$$

for each phase. Finally, the density and the macroscopic velocity vector were reconstructed from the distribution functions according to