Applied Thermal Engineering 64 (2014) 129–138

Contents lists available at ScienceDirect

Applied Thermal Engineering

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

Simulation on the coalescence of the moving liquid column and droplet in a hydrophilic microchannel by volume of fluid method

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HIGHLIGHTS

- The liquid column coalescing with droplet in hydrophilic microchannel is simulated.
- The coalescence with the droplet can promote the liquid column movement.
- More hydrophilic surface and smaller channel size induce larger acceleration rate.
- Larger droplet size and shorter droplet distance exhibit larger acceleration rate.

ARTICLE INFO

Article history:
Received 6 November 2013
Accepted 8 December 2013
Available online 19 December 2013

Keywords:
Coalescence
Moving liquid column
Droplet
Capillary force
Volume of fluid

ABSTRACT

The dynamic behavior of the moving liquid column coalescing with a sessile droplet in a hydrophilic microchannel is simulated in this work using the volume of fluid (VOF) methodology along with the continuum surface force (CSF) model. Particular attention is paid to the dynamic interfacial phenomena during the coalescence and the effect on advancing the water–air interface. It is interesting to find that the coalescence between the moving liquid column and droplet can accelerate the original liquid column movement due to the formation of the lager-curvature meniscus at the interface induced by the coalescence, which increases the capillary pressure. In addition, effects of the wettability, the sizes of the microchannel and droplet as well as the droplet position on the coalescence behaviors and liquid column movement are also studied. The results show that more hydrophilic surface, smaller channel size and distance between the droplet and inlet, and larger droplet size exhibit a larger acceleration rate as a result of induced higher capillary pressure.

1. Introduction

Microfluidics integrates the functions of mixing, separation, purification and detection together, enabling precise, automated manipulation of tiny volumes of fluid (often nanoliters or even picoliters) [1,2]. Because of a variety of advantages in that they can reduce sample and reagent volumes, shorten reaction times, provide high-throughput, automation and low cost, microfluidic systems are regarded as valuable instrumental platform for chemical and biological applications such as ultrasound contrast agents [3], drug delivery [4], on-line analysis [5], sorting [6] and so on. In microfluidic system, as the geometry shrinks to micrometer or even nanometer, the surface-to-volume ratio dramatically increases. Accordingly, the surface forces become significant, resulting in many interesting interfacial phenomena. In particular for the two-phase flow system, the capillary force will dominate the transport process. As a result, the two-phase flow behaviors in the microfluidic system have received much attention.

Over the past decades, extensive efforts have been directed to the investigation of two-phase flow in microfluidics. Daniel et al. [7] used asymmetric vibration to propel a droplet through a microfluidic and found that the drop velocity depended on the forcing frequency, amplitude, signal shape, and the drop resonance modes. Christopher et al. [8] studied the flow-induced coalescence at a microfluidic T-junction and characterized the response for a wide range of droplet sizes and speeds. Based on thermocapillary stresses locally induced by laser on droplet, Robert de Saint-Vincent et al. [9] performed high velocity droplet switching and sorting in microchannels. More information can be found in the review on the droplet-based microfluidic reaction by Song et al. [10] as well as the

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http://dx.doi.org/10.1016/j.applthermaleng.2013.12.017

flow regimes in two-phase flow system and controlled droplet coalescence by Zhao and Middelberg Anton [11]. Besides, the liquid filling into capillary microchannels or microporous materials have also been explored by many researchers [12–14].

With the advancements in numerical computing power and technique, various numerical methods have been used to study multiphase flows and the interfacial phenomena involved in microfluidic systems [15–20]. Among them, the volume of fluid (VOF) model is one of the most popular approaches to track the interface, because it offers many advantages of easy realization, small computational complexity and high precision, and traces the volume of fluid in the grid but not the motion of fluid particles. Such advantages allow the VOF to be successfully applied to the simulation of the two-phase flow in microchannels. Zhu et al. [21,22] used the VOF model to investigate the water droplet formation from an orifice and shape variation of droplet in a gas microchannel. Rahman et al. [23] also applied the VOF model to simulate numerically the drops generation of ink through a nozzle with the help of electrostatic forces ejection mechanism. The characteristics of Taylor bubble formation in a microchannel T-junction were addressed by Guo and Chen through the implementation of VOF model, in that, numerical results were in good agreement with the experimental measurements [24]. In addition, Zhuan and Wang [25] simulated the behavior of bubble growth and coalescence for boiling flows in microchannel by using VOF method, and the flow patterns predicted by simulation were in agreement with phenomena observed in experiments. The above cases indicate that the VOF model is an effective tool to explore the multiphase flow behaviors in microfluidic systems.

Recently the incorporation of modern optics into microfluidics creates a new area of optofluidics [26]. One of the good examples is a micropump based on photothermal effects of photothermal nanoparticles (PNPs) [27]. During the working process of this new type of micropump, the coalescence between the liquid column and droplet plays an important role in the liquid pumping. Such phenomenon is also encountered in the fluid filling process in case there exist the residual droplets in the microchannel, which affects the performance of the fluid filling. Although Liu et al. [27] believed that the coalescence could assist the advance of the liquid–air interface and previous studies have shown that the coalescence between the droplets can facilitate the droplet movement significantly [28,29], the propulsion mechanism caused by the coalescence of the liquid body and droplets in microchannels on the liquid flow remains unclear. In present paper, therefore, a fundamental aspect of the coalescence of the moving liquid column and a sessile droplet in a hydrophilic microchannel was investigated by employing the VOF model to track interface and the continuum surface force (CSF) model for the surface tension [30]. The entire process including the liquid filling into a microchannel and coalescence with a sessile liquid droplet was simulated to shed light on the underlying mechanism. The effects of the wettability and size of the microchannel, droplet size and position were also discussed in this work.

2. Model description

2.1. Physical model

This paper addresses an isothermal, capillary force driven, dynamic two-phase flow in a rectangular hydrophilic microchannel. The three-dimensional physical model is sketched in Fig. 1. The case conditions in this study correspond to a microchannel with 300 μm in length and square cross section and its side length ranges from 60 μm to 120 μm. The two phase fluids simulated in this research are water and air. Water enters the microchannel spontaneously

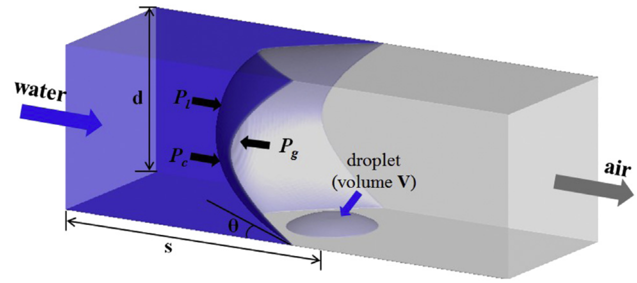

Fig. 1. Schematic diagram of the three-dimensional physical model.

with the assistance of the capillary force and then coalesces with a sessile water droplet. In this regard, the liquid column and the droplet have the same viscosity μ_l and density ρ_l of water, both of which partially wet the surface with a contact angle θ at equilibrium. For all simulation cases, the temperature is set at 293 K, the density ρ_l and viscosity μ_l of water are 998.2 kg/m^3 and 0.001 kg/(m s), respectively. For air, $\rho_g = 1.225$ kg/m^3 and $\mu_g = 1.789 \times 10^{-5}$ kg/(m s). Since the scale of the microchannel is much smaller than the capillary length $l_c = \sqrt{\sigma/\rho_l g}$ (2.7 mm for water) where g is the gravitational acceleration and σ is the surface tension of the water–air interface equal to 0.0728 N/m at 20 °C, the gravitational-potential energy can be neglected in the analysis.

2.2. VOF model

In this study, the VOF method is employed to track the water–air interface between the phases, which have been implemented in many commercial CFD packages. Basically, two fluids simulated by the VOF formulation are not interpenetrating. To identify the phase separately, a volume fraction of liquid phase in each control volume, represented by α, is introduced and defined as

$$\alpha = \frac{\text{Volume of liquid in the control volume}}{\text{Total volume of the control volume}} \tag{1}$$

where α equals to 1 if the cell is filled with liquid, α is 0 if the cell is filled with gas and α is in the range between 0 and 1 if an interface is located in the cell. The determination of α is achieved by solving the following transport equation of the fluid volume fraction to track the interfacial dynamic behaviors,

$$\frac{\partial \alpha}{\partial t} + \mathbf{V} \cdot \nabla \alpha = 0 \tag{2}$$

where $\mathbf{V}$ is the velocity. In addition, the shape of the interface is reconstructed by piecewise linear interface calculation (PLIC) algorithm [31], which can take the transport among adjacent interface fluid into consideration. The reconstruction result is comparatively precise.

In this model, the two-phase flow and the coalescence of the moving liquid column and droplet in a microchannel are simulated with the continuum equation and Navier–Stokes equation as follows.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{V}) = 0 \tag{3}$$

$$\frac{\partial (\rho \mathbf{V})}{\partial t} + \nabla \cdot (\rho \mathbf{V}\mathbf{V}) = -\nabla p + \nabla \cdot \left[\mu\left(\nabla \mathbf{V} + \nabla \mathbf{V}^T\right)\right] + \mathbf{F} \tag{4}$$

where t is time, p is the static pressure, $\mathbf{F}$ is a momentum source term related to surface tension. The properties appearing in these