International Journal of Heat and Mass Transfer 120 (2018) 1085–1100

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

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

# Lattice Boltzmann study of successive droplets impingement on the non-ideal recessed microchannel for high-resolution features

Lei Zhang [a,*], Xiaoding Cheng [a,b], Tao Ku [a], Yan Song [c], Dingyi Zhang [a]

[a] Shenyang Institute of Automation, Chinese Academy of Sciences, Shenyang 110016, China
[b] University of Chinese Academy of Sciences, Beijing 100049, China
[c] Liaoning University, Shenyang 110036, China

ARTICLE INFO

*Article history:*
Received 12 July 2017
Received in revised form 19 December 2017
Accepted 23 December 2017

*Keywords:*
Lattice Boltzmann method
Microchannel
Multiple-relaxation-time
Contact angles hysteresis
Collision modes

ABSTRACT

Successive droplets deposited high-resolution features on the non-ideal recessed microchannel is investigated utilizing a 3D multiple-relaxation-time (MRT) pseudopotential lattice Boltzmann (LB) model with large density ratios and high Reynolds numbers. The non-ideal hydrophilic wettability is modeled by the geometric formulation within the pseudopotential LB framework. Firstly, for single droplet impingement on the square microchannel, three liquid morphologies including quatrefoil-like, quasi-square and quasi-rounded footprints are observed with varying aspect ratios of microchannel. Next, considering two successive droplets impingement on the rectangular microchannel, with the droplet spacings increasing, the liquid morphologies including bulging, uniform and dumbbell footprints are quantitatively identified. With the formation of connecting ridge, the optimal droplet spacing in in-phase collision mode is larger than that in out-of-phase mode. Besides, the deviations between simulations and theoretical values are observed which are attributed to the intensive inertial dominated flows. Finally, as extending to the multi-droplets deposited lines and films, the optimal droplet spacings are adaptive in both collision and placement modes for uniform and high-resolution features.



## 1. Introduction

In recent years, inkjet printing technology has drawn considerable attention due to its direct patterning in various industries such as RFID tags [1], solar cell fine line metallization [2], microfabrication [3,4] and flexible prototyping [5]. During the ink-jetting process, multiple droplets comprised of functional materials are deposited precisely and coalesce on the substrate. To form fineness and uniform printed features, the inkjet parameters including substrate wettability, droplet diameter and velocity need to be well modulated. Nevertheless, a high-resolution printed pattern is of great challenge for inkjet printing particularly on hydrophilic substrates. As inkjet droplets impingement on structured rough substrates [6], the enhanced partial wettability due to the substrate topography results in a large and inhomogeneous spreading region which extremely influences the resolution of printed features.

An obvious way for attaining high resolutions is to reduce the diameter of the print-head's nozzle. However, it gives rise to the difficulties on the inks formulation due to the rheological constraints [7]. A more effective strategy is to modulate the surface energies [8] which guides the inkjet droplets to spread along the pre-patterning bands. However, a drawback of utilizing surface energy pre-patterning is that the patterned regions are not visible and hard to be detected. Furthermore, the additional masks are needed to offer guidance of inkjet droplets for precise deposition. The utilization of masks eliminates the inkjet printing's maskless features and, moreover, the overall manufacturing time is increased and some restraints are placed on up-scaling to roll-to-roll production.

Instead of varying substrate wettability, an alternate approach is to offer an appropriate recessed topography structures to the droplets. The predefined structures effectively align the inkjet features toward the desired dimensions. Hendriks et al. [9] dispensed the droplets into the as-formed grooves formed by hot-embossed technology. The inks filled the grooves were dominated by the capillary forces and the uniform tracks were formed. Besides, the width of tracks could be modulated via different masters. To extend this approach applicable for rigid substrates such as textured silicon wafers, Liu et al. [10] developed an organic sacrificial layer to form geometric confinement features on hydrophilic rough surfaces. The inkjet droplets were physically restricted and a much higher resolution in the range of $\sim 50$ μm was achieved. Mahajan

* Corresponding author.
*E-mail addresses:* leizhang@sia.cn, Leizhang0318@126.com (L. Zhang).

https://doi.org/10.1016/j.ijheatmasstransfer.2017.12.124
0017-9310/

et al. [11] created high-resolution channels in a thermosetting polymer using imprint lithography. The reactive Ag inks were then filled into the channels by capillary forces. This novel approach fabricated high-resolution and high-aspect ratio metal lines for flexible electronics applications.

Although the high-resolution inkjet features have been obtained by predefined physical structures as discussed above, the mechanisms of multi-droplets deposition dynamics with confinement need to be well understood. Numerical simulations have been a crucial alternative to explore the nature of multi-droplets interactive behaviors. Lee and Son [12] investigated droplets impingement and coalescence dynamics numerically in a micro-line patterning process based on the sharp-interface level-set method. The effects of advancing/receding contact angles and droplets spacing on droplets interactions were explored and a uniform droplets coalescence patterning was optimized to be attained. Li et al. [13] and Li et al. [14] performed numerical computations utilizing a volume of fluid (VOF) method to investigate the successive deposition of molten metal droplets on solid substrates. The different stages of fusion process were identified which were crucial to effectively control the process of metal additive manufacturing. However, it is noted that complex dynamics of multi-droplets interactions are of great challenges to be calculated by conventional VOF methods [15]. In recent decades, the lattice Boltzmann (LB) method [16,17] has been successfully employed to solve multiphase and multi-component flow problems in mesoscopic scales. LB model does not require the dynamic contact line to be specified before droplets deposition and offers a powerful capability in simulating complicated physical phenomena. Castrejón-Pita et al. [18] investigated multi-droplets coalescence and mixing dynamics experimentally and numerically. The mixing behaviors of similar-sized and unequal-sized droplets were analyzed based on pseudo-potential LB model. Zhou et al. [19,20] proposed a phase-field based LB model to investigate interface dynamics of multi-droplets impinging on ideal and non-ideal solid substrates. The droplet spacing and receding contact angle played more significant roles in determining the final footprint length to width ratio. More recently, Ashoke Raman et al. [21] performed three-dimensional (3D) computations on two successive droplets impingement on the chemical heterogeneous substrate. The spread factors and mixing dynamics were emphasized and two kinds of interaction modes were identified for different velocity ratios. The droplets impingement behaviors in these modes were significantly influenced by the corresponding advancing and receding contact angles.

However, most investigations by previous researchers focus on the scenarios of two or multi-droplets deposited features on planar surfaces. The morphologies and dynamics of multi-droplets impingement and coalescence on geometric confinement structures for uniform and high-resolution features, to authors' best knowledge, have not been studied. The geometric confinement structures such as recessed rectangular microchannel can effectively modulate the fluids morphology toward desired geometrical precise states, particularly for the hydrophilic substrates. Hence, the objective of the present work is to offer dynamic insights to reveal the nature of complex interactions between droplets and microchannel which are dominated by inertial forces. In addition, we aim to find out the optimal parameters to fabricate uniform and high-resolution features on non-ideal hydrophilic substrates.

To understand the complex interplay between multi-droplets and non-ideal microchannel, a 3D MRT pseudopotential LB model is considered which is effective to simulate complex interfacial phenomenon with large density ratios and high Reynolds numbers. In addition to the capability in modelling multiphase and multi-component flows, LB method is naturally applicable for massively parallel computations. These characteristics make it a significant numerical tool for large-scale calculations and complex fluids simulations in various conditions. The paper is organized as follows. Section 2 outlines the details of 3D MRT pseudopotential LB mathematical model. The wettability of rectangular microchannel with contact angle hysteresis is modeled by the geometric scheme which is validated against the experimental data in the literature. Results and discussion of multi-droplets impingement dynamics on the rectangular microchannel are presented in Section 3. Finally, a summary and conclusion are given is Section 4.

## 2. Mathematical model

### 2.1. 3D MRT pseudopotential LB model

The MRT pseudopotential LB model is employed to handle complex multiphase flows which can improve numerical stability at large density ratios by adjusting relaxation parameters [22]. In the present work, nineteen-velocity (D3Q19) LB model is considered for 3D simulations. The LB equation with the MRT collision operator and the forcing term [23,24] can be given as

$$f_a(\vec{x}+\vec{e}_a\delta_t, t+\delta_t) - f_a(\vec{x},t) = -\sum_\beta \Omega_{\alpha\beta}(f_\beta(\vec{x},t) - f_\beta^{eq}(\vec{x},t)) + S_\alpha(\vec{x},t) - \frac{1}{2}\sum_\beta \Omega_{\alpha\beta}S_\beta(\vec{x},t), \quad (1)$$

where $f_a(\vec{x},t)$ is the density distribution function along the $\alpha th$ direction, $\vec{x}$ is the spatial position, $\delta_t$ is the time step and $\vec{e}_a(\alpha = 0, 1, \ldots, 0.18)$ is the discrete velocity in the $\alpha th$ direction given by

$$\vec{e}_\alpha = \begin{cases} 0,0,0 & \alpha = 0 \\ (\pm1,0,0)c, (0,\pm1,0)c, (0,0,\pm1)c & \alpha = 1\sim6 \\ (\pm1,\pm1,0)c, (\pm1,0\pm1)c, (0,\pm1,\pm1)c & \alpha = 7\sim18 \end{cases}. \quad (2)$$

$S_\alpha(\vec{x},t)$ is the forcing term in the velocity space given by

$$S_\alpha(\vec{x},t) = \omega_\alpha\left[\frac{\vec{e}_\alpha - \vec{u}}{c_s^2} + \frac{\vec{e}_\alpha\cdot\vec{u}}{c_s^4}\vec{e}_\alpha\right]\cdot\vec{F}, \quad (3)$$

where $c_s^2 = c/\sqrt{3}$ is the lattice sound speed and $c = \delta_x/\delta_t$ is the ratio between the lattice spacing $\delta_x$ and time step $\delta_t$ which are set to be unity in this paper. The weighting factors $\omega_\alpha$ are given by

$$\omega_\alpha = \begin{cases} 1/3, & \alpha = 0; \\ 1/18, & \alpha = 1\sim6; \\ 1/36, & \alpha = 7\sim18. \end{cases} \quad (4)$$

In the pseudopotential LB model, $\vec{F}$ is the total force acting on each particle. $\Omega_{\alpha\beta}$ is the collision matrix in the velocity space. The transformation matrix $M$ is used to map Eq. (1) to moment space which is given as

$$f_a(\vec{x}+\vec{e}_a\delta_t, t+\delta_t) - f_a(\vec{x},t) = -M^{-1}\Lambda(m(\vec{x},t) - m^{eq}(\vec{x},t)) + M^{-1}\left(I - \frac{\Lambda}{2}\right)\bar{S}_\alpha(\vec{x},t), \quad (5)$$

where the transformation matrix $M$ for the D3Q19 LB model is given as