Chemical Engineering Science 171 (2017) 534–544

Contents lists available at ScienceDirect

Chemical Engineering Science

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

Numerical investigation of multi-droplets deposited lines morphology with a multiple-relaxation-time lattice Boltzmann model

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HIGHLIGHTS

- Multi-droplets deposited line process is simulated by three dimensional MRT LB model.
- Contact angle hysteresis is modeled by geometric formulations.
- The lines morphologies with different overlap ratios are quantitatively identified.
- An optimal droplet overlap ratio for uniform line is proposed.
- The proposed optimal overlap ratio is valid in the out-of-phase coalescence mode.

ARTICLE INFO

Article history:
Received 14 March 2017
Received in revised form 2 June 2017
Accepted 6 June 2017
Available online 8 June 2017

Keywords:
Multi-droplets
Uniform line formation
Multiple-relaxation-time
Lattice Boltzmann method
Contact angles hysteresis
Coalescence mode

ABSTRACT

The formation and morphology of multi-droplets deposited lines are investigated by employing a 3D MRT pseudopotential LB model with large density ratios and high Reynolds numbers. A geometric formulation is considered to replace the fluid-solid interaction scheme to model the contact angles hysteresis. Of particular interest in this study is to find out the optimal conditions of uniform line formation. The effects of droplet overlap ratios and advancing contact angles on the lines morphology are investigated numerically. With the droplet overlap ratio increasing, the lines morphologies including isolate, scalloped, uniform and bulging formation are quantitatively identified. An optimal droplet overlap ratio is proposed to obtain uniform morphology of lines and validated via varying Ohnesorge numbers. The effects of vertical droplet spacing on the lines morphology at the optimal droplet overlap ratio is investigated and two coalescence modes are identified. Results show that the proposed optimal overlap ratio for uniform line formation is not sufficient condition and is valid in the case of out-of-phase coalescence mode.

1. Introduction

Additive manufacturing process such as inkjet printing (Derby, 2010), micro-fabrication (Fathi and Dickens, 2013; Vaezi et al., 2013), rapid prototyping (O'Neill et al., 2014; Zhang et al., 2003) and aerosol jetting (Mette et al., 2007), characterized with direct patterning, has drawn greater attention in the manufacture of electronic products such as RFID tags (Subramanian et al., 2005), polymer transistor circuits (Sirringhaus et al., 2000) and solar cell fine line metallization (Gizachew et al., 2011). In the process of printed lines formation, multiple droplets made up of functional materials need to be deposited precisely on the substrate and forms a conductive line. The line morphologies, such as fineness and uniformity, are essential to improve the quality of product. Therefore, a good understanding of how uniform morphologies features are formed is of great significance in the process of additive manufacturing. Moreover, dynamical insights can help to find out the optimal manufacturing conditions to modulate the fluid morphology toward desired geometrically precise states.

Printed line is formed through a train of successive droplets at a specified spacing impingement onto solid substrates. Duineveld (2003) investigated the behaviors of inkjet-printed line formation with zero receding contact angle. The instability mechanism was present when a capillary-driven flow along the liquid line was large enough to transport newly printed droplets into the regularly spaced bulges separated with liquid ridges. These bulge instabilities would arise when inkjet-printed droplets impinged the substrate at large overlap and low traverse velocities. The experimental investigation of the formation of inkjet-printed lines was carried out by Soltman and Subramanian (2008). Five kinds of line patterns were observed such as individual droplets, a scalloped

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http://dx.doi.org/10.1016/j.ces.2017.06.014
0009-2509/

line, a uniform line, a bulging line and stacked coins. Moreover, a simple geometric model was proposed to predict the transition among mapped line morphology regimes. Meanwhile, Stringer and Derby (2010) predicted the printed line width based on a volume conservation model and reformulated Duineveld's model. Criteria of lower and upper bounds for inkjet-printed line stability was proposed and agreed well with experiments. However, it was noted that the stable line inkjet-printed experimentally was obtained under the capillary forces due to relative low printing frequency. Recently, Hsiao et al. (2014) investigated the stability of line formation with nonzero receding contact angle experimentally. They found that the Soltman's model underestimated the maximum droplets spreading radius and line width due to not accounting for droplets impact inertia. In addition, destabilizing effect of a receding contact line and reduced capillary-driven flow were illustrated which resulted in different behaviors in contrast to that expected in previous models.

Numerical simulations have been a significant alternative to offer dynamical insights of multi-droplets interaction behaviors. Lee and Son (2011) investigated droplets impingement and coalescence dynamics numerically in a micro-line patterning process by employing the sharp-interface level-set method. Their numerical simulation illustrated that the dynamics of droplets coalescence patterning depended significantly on the advancing and receding contact angles. In addition, the optimal droplet spacing was investigated to find out in manufacturing micro-lines. H. Li et al. (2012), Q. Li et al. (2012), and Li et al. (2015) performed numerical simulations based on a volume of fluid (VOF) method to investigate the successive deposition of molten metal droplets on solid substrates. The different stages of the fusion process were identified which was crucial to effectively control the process of metal additive manufacturing. However, it is very challenging to numerical modeling the complex interface of multi-droplets deposited line formation using a conventional VOF method (Chen and Wang, 2014; Yokoi et al., 2009). In contrary, the pseudopotential lattice Boltzmann (LB) method (Chen and Doolen, 2003; Li-Shi, 2000) has been successfully employed to solve multiphase and multi-component flow problems due to its simplicity and versatility compared with free energy model (Chen and Deng, 2017) and diffuse interface model (Lee and Liu, 2010). LB model does not require the dynamic contact line to be specified before droplets deposition and presents the powerful capability in simulating complicated physical phenomena. Castrejón-Pita et al. (2013) investigated multi-droplets coalescence and mixing dynamics experimentally and numerically. The mixing behaviors of similar-sized and unequal-sized droplets were analyzed based on pseudopotential LB model. Zhou et al. (2014) proposed a phase-field 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. Chen et al. (2015) explored the deformation dynamics of double emulsion droplets under shear. The modes of transient deformation topologies and deformation oscillations of emulsion droplets are identified and analyzed. More recently, Ashoke Raman et al. (2016) performed three-dimensional computations on two successive droplets impingement on a chemical heterogeneous substrate. The spread factors and mixing dynamics were focused on 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.

Although the scenarios of droplets impingement on solid substrates have been investigated numerically, most of the studies focused on the dynamics of two successive or simultaneous droplets impingement and coalescence. A few studies have been performed to investigate the formation and morphology of multi-droplets deposited line process with non-ideal substrates. How to obtain uniform morphology and high resolution of printed line plays a significant role in industrial process including high density polymer electronics (Meier et al., 2009) and fine line metallization of solar cells (Gizachew et al., 2011; Stuwe et al., 2015). The geometric model of uniform line formation proposed by Stringer and Derby (2010) is suitable for the capillary forces driven scenarios with moderate Reynolds numbers. How to obtain uniform morphology of multi-droplets deposited line which is impact inertial driven with high Reynolds numbers, to the authors' best knowledge, have not been studied. In the present work, three dimensional (3D) numerical simulations are performed to investigate the dynamics and morphology of printed line on non-ideal solid substrates. We aim to find out the optimal conditions of uniform line formation by tuning the numerical parameters including droplet overlap ratio, advancing contact angle, droplets viscosity and printing frequency.

To understand the complex interplay between multi-droplets and non-ideal solid substrates, 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 modeling multiphase and multi-component flows, LB method is naturally applicable for massively parallel computation. 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 which validated with two tests. Results and discussion are presented in Section 3. Finally, a summary and conclusion are given is Section 4.

2. Mathematical model

2.1. 3D multi-relaxation-time LB model

The multi-relaxation-time (MRT) method is employed to handle complex multiphase flows which can improve numerical stability at large density ratios by adjusting relaxation parameters (D'Humieres et al., 2002). In the present work, nineteen-velocity (D3Q19) LB model is considered for 3D simulations. The LB equation with MRT collision operator 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 αth direction, $\vec{x}$ is the spatial position, δ_t is the time step and $\vec{e}_a(\alpha = 0,1,\ldots 0.0.18)$ is the discrete velocity in the αth direction given by

$$\vec{e}_\alpha = \begin{cases} 0,0,0 & \alpha = 0 \\ (\pm1,0,0)c, (0,\pm1,0)c, (0,0,\pm1)c & \alpha = 1\text{–}6 \\ (\pm1,\pm1,0)c, (\pm1,0\pm1)c, (0,\pm1,\pm1)c & \alpha = 7\text{–}18 \end{cases} \quad (2)$$

$S_\alpha(\vec{x},t)$ 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 δx and time step δt which are set to be unity in this paper. The weighting factors ω_α are given by