Inkjet droplet deposition dynamics into square microcavities for OLEDs manufacturing

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Abstract
The dynamics of inkjet deposition in square microcavities are investigated utilizing a three-dimensional multi-relaxation-time pseudopotential lattice Boltzmann (LB) model with large density ratios. A geometric scheme is considered within the pseudopotential LBM framework to obtain the desired contact angles. The effects of wettability, density ratios, droplet viscosity and impact velocity are explored to reveal the droplet–microcavity interactions. With the contact angles of microcavity increasing, the physical outcomes including the crown-like shape with a small round dot, circular hollow core, uniform film and convex film are identified and analyzed. At a lower density ratio $\rho_r = 11.6$, the surrounding denser gas resists the droplet recoiling flow resulting in an increasing hollow core. The appropriate higher droplet viscosity and decreasing impact velocity are preferred which could eliminate the hollow core in the recoiling phase and accelerate the inkjet deposition process straightforward. The revelation of droplet-microcavity dynamics is beneficial for optimizing inkjet deposition process and fabricating uniform OLEDs panels.

Keywords Microcavity · Inkjet · OLEDs · Lattice Boltzmann method · Multi-relaxation-time · Density ratios

1 Introduction

As a direct patterning technique without masks, inkjet printing (Derby 2010) has drawn considerable attention in various applications. The organic light-emitting diodes (OLEDs) displays currently on the market are mainly fabricated by the thermal evaporation of organic materials in an ultrahigh-vacuum environment. It has been successful in the mass production of mobile OLEDs. However, the thermal evaporation process has many disadvantages such as materials wastes and low yielding which gives rise to the high cost for large size OLEDs panels (Villani et al. 2009). As an alternate technique, inkjet printing sprays the organic solutions into the microcavities (Gorter et al. 2013) to fabricate the light emissive layer and hole transport layer, respectively. It greatly improves the utilization of organic materials and eliminates the expensive fine metal masks. Therefore, inkjet technology is now considered a promising candidate for mass production of large size OLEDs panels (Shimoda et al. 2003; Zheng et al. 2013).

The performance of mura-free OLEDs depends not only on the organic materials and microcavities properties (Sun et al. 2000), but also on the nature of inkjet-deposited processes. Therefore, a good understanding of dynamic behavior of droplet deposition on microcavities is of great significance in the inkjet manufacturing process. Moreover, dynamical insights could provide beneficial guidance to optimize inkjet deposition conditions and fabricate mura-free OLEDs displays.

For single droplet impingement and its subsequent interaction with the solid substrate, much research has been performed extensively and fruitful progress has been made for couple of years (Rein 1993; Rioboo et al. 2002; Yarin 2006). By contrast, the scenarios of one droplet impingement into microcavity have drawn relatively little attention. Subramani et al. (2007) performed experiments to explore the dynamics of a droplet impact on a rectangular slot. The internal and external splash modes were identified, and phase diagrams were proposed to demonstrate regimes of drop spreading...
and splashing. Ding and Theofanous (2011) carried out numerical calculations based on a diffuse interface solver to investigate the inertial regime of droplet impact on a pore. The unidentified flow phenomena and impact inertial effects which could not be accessible experimentally were revealed and understood intensively. Enriquez and Meer (2014) investigated droplet impingement near closed pits and open-ended pores experimentally. Three distinct phenomena denoted as a splash, a jet and air bubble were observed and analyzed. Liou et al. (2008) and Liou et al. (2009) performed numerical simulations of droplet impact on rectangular and square cavities with an inclined sidewall using the volume of fluid (VOF) method. The effect of impact inertia characterized by Weber number on surface characteristics was explored, and a unified correlation was proposed to obtain uniform film within cavities. For the scenarios of droplet impact onto the outside of cavities, Suh and Son (2010) numerically investigated the droplet self-alignment behavior utilizing the VOF method to overcome placement errors and to improve the accuracy in film formation.

However, for the conventional VOF method, it is very challenging to numerical modeling the complex interface of droplet impact on the microstructured surface (Yokoi et al. 2009). On the contrary, the lattice Boltzmann (LB) method (Chen and Doolen 2003; Luo 2000) has been successfully utilized to handle mesoscopic multi-phase flow problems. Yan and Zu (2007) proposed a hybrid LB model to explore the liquid droplet dynamics on the partial wetting surface. The dynamics of liquid droplets impingement on homogeneous (Lee and Liu 2010) and heterogeneous (Zhang et al. 2017) solid surfaces were investigated with a high-density ratio-based LB model. For cases of textured surfaces, Dupuis and Yeomans (2005) investigated superhydrophobic behavior of droplet impact on an array of micrometer-scale posts. Connington and Lee (2013) performed simulations of a droplet placed on a textured surface to explore the transition between Cassie–Baxter and Wenzel state. More recently, Ju et al. (2017) and Shi et al. (2015) performed 3D LB models to study the coalescence-induced droplet jumping on the superhydrophobic complex textured surfaces. The above studies mainly focus on the dynamics of droplet impingement on the textured surface composed of square or conical pillar-structures. However, the scenario of droplet impingement on the microcavity by using the LB method, to author’s best knowledge, has not been studied. Moreover, in the inkjet-deposited OLEDs process, the shielding gas needs to be injected to completely isolate organic materials from water and oxygen which could influence the density ratio between fluid and gas. The varying viscosities and impact velocities of different organic materials also have an effect on the final outcome of OLEDs pixels. The motivation of the present work is to investigate the effects of wettability of microcavity, density ratios, viscosity and impact velocity of droplets on the resulting droplet-microcavity interaction dynamics which have not been considered in prior studies.

To understand the complex interplay between the droplet and microcavity, a 3D multi-relaxation-time (MRT) pseudo-potential LB model is considered which could be effective to simulate complex interfacial phenomenon with large density ratios and high Reynolds number. The paper is organized as follows. Section 2 outlines the details of 3D MRT pseudo-potential LB mathematical model which validated with theoretical model and numerical results in the literature. Results and discussion are presented in Sect. 3. Finally, concluding remarks are given in Sect. 4.

### 2 Mathematical model

#### 2.1 3D MRT LB model

As a mesoscopic numerical approach, the LB model simulates multi-phase flows by solving the discrete Boltzmann equation with certain collision operators. In the present work, the MRT collision operator is adopted to simulate the droplet impingement dynamics within microcavities which could improve numerical stability at large density ratios by adjusting relaxation parameters. Nineteen-velocity (D3Q19) LB model is employed for 3D simulations. The pseudo-potential LB equation which governs the evolution of the density distribution with MRT collision operator can be written as (Lallemand and Luo 2000)

\[
f_a(\vec{x} + \vec{e}_a \delta_t, t + \delta_t) - f_a(\vec{x}, t) = -M^{-1} A(m(\vec{x}, t) - m^{eq}(\vec{x}, t)) + M^{-1} \left( I - \frac{A}{2} \right) \tilde{S}(\vec{x}, t),
\]

(1)

where \( f_a(\vec{x}, t) \) is the density distribution function, \( \vec{x} \) is the spatial position, \( \delta_t \) is the time step and \( \tilde{S}(\vec{x}, t) \) is the forcing term in the moment space. \( \vec{e}_a(a = 0, 1, \ldots, 18) \) is the discrete velocity along the \( a \)th direction. \( M \) is a transformation matrix for D3Q19 LB model (Krüger et al. 2017).

The density distribution function \( f_a \) and its equilibrium distribution \( f^{eq}_a \) could be mapped to the moment space via \( m = Mf \) and \( m^{eq} = Mf^{eq} \). The equilibrium distribution functions \( m^{eq} \) in the moment space is expressed as

\[
m^{eq} = \left( \rho, -11\rho + \frac{19}{\rho} (J_x^2 + J_y^2 + J_z^2), 3\rho - \frac{11}{2\rho} (J_x^2 + J_y^2 + J_z^2), J_x, \right.
\]

\[
- \frac{2}{3\rho} J_x J_y, - \frac{2}{3\rho} J_x J_z, - \frac{2}{3\rho} J_y J_z, \frac{1}{\rho} (2J_z^2 - (J_x^2 + J_y^2)), \left. - \frac{1}{2\rho} (2J_x^2 - (J_y^2 + J_z^2)), \frac{1}{\rho} (2J_y^2 - (J_x^2 + J_z^2)), \right.
\]

\[
- \frac{1}{2\rho} (J_x^2 - J_y^2), \frac{1}{\rho} J_x J_y, \frac{1}{\rho} J_x J_z, \frac{1}{\rho} J_y J_z, 0, 0, 0 \right)^T.
\]

(2)
where \( j_x = \rho u_x \), \( j_y = \rho u_y \), and \( j_z = \rho u_z \) are components of the momentum fluxes. In Eq. (1) is the density matrix and \( \Lambda \) is a diagonal matrix which is given by

\[
\Lambda = \text{diag}(s_1, s_2, s_3, s_4, s_5, s_6, s_7, s_8, s_9, s_{10}, s_{11},
\quad s_{12}, s_{13}, s_{14}, s_{15}, s_{16}, s_{17}, s_{18}, s_{19})
\]

\[
= \text{diag}(0, s_x, s_y, 0, 0, s_y, 0, s_x, 0, s_{xy}, s_{xy}, s_{xy})
\]

where relaxation rates of 0 are specified for the conserved moments of density and momentum. \( s_x \) and \( s_y \) are connected with shear and bulk viscosities. The others are free parameters to be tuned for numerical stability. The shear viscosity and bulk viscosity can be derived with the elements in Eq. (3) which are given as

\[
b = \frac{1}{3} \left( \frac{1}{s_x} - \frac{1}{2} \right),
\]

(4)

and

\[
\xi = \frac{2}{9} \left( \frac{1}{s_y} - \frac{1}{2} \right).
\]

(5)

Considering the computation efficiency and numerical stability within the MRT framework, we adopt an improved forcing scheme (Li et al. 2012) which could achieve thermodynamic consistency requirement in a wide range of temperature. The forcing scheme for MRT pseudopotential LB model extended to D3Q19 lattice is given by

\[
S = (0.38(a_i F_i + u_i F_i) + \frac{114e \tilde{F}^2}{\psi^2(1/s_2 - 0.3)},
\]

\[
- 11(u_i F_i + u_j F_j + u_k F_k) F_i - \frac{2}{3} F_j F_j - \frac{2}{3} F_k F_k,
\]

\[
- \frac{2}{3} F_j, 2(2u_i F_i - u_j F_j - u_k F_k), -2u_i F_i + u_j F_j + u_k F_k, 2(u_i F_i - u_j F_j),
\]

\[
-u_i F_i + u_j F_j + u_k F_k, u_i F_i, u_j F_j, u_k F_k, 0, 0, 0)^T,
\]

(6)

where \( \tilde{F}^2 = (F_x^2 + F_y^2 + F_z^2) \) and \( e \) is tuned to be \( e = 0.3 \) to improve the mechanical stability.

The macroscopic fluid density and velocity could be calculated as follows

\[
\rho = \sum_{\alpha=0}^{18} f_{\alpha}, \quad \rho \vec{u} = \sum_{\alpha=0}^{18} \vec{v}_{\alpha} f_{\alpha} + \frac{\delta}{2} \tilde{F}.
\]

(7)

The fluid–solid interaction force \( \vec{F} \) is expressed as (Martys and Chen 1996)

\[
\vec{F}(\vec{x}, t) = -G \psi(\vec{x}, t) \sum_{i=0}^{18} \omega_i \psi(\vec{x} + \vec{e}_i, t) \vec{e}_i,
\]

(8)

where \( G \) is the parameter which handle the strength of the interparticle force. \( \psi(\vec{x}, t) \) is the effective mass which can be defined by the equation of state (EOS):

\[
\psi(\vec{x}, t) = \sqrt{\frac{2(\rho - \rho c^2)}{c^2 G}}.
\]

(9)

The choice of the EOS is essential in LB model for obtaining large density ratios and improving numerical stabilities. From the study of Yuan and Schaef (2006), the Carnahan–Starling (C–S) EOS which provides large density ratios and maintains lower spurious currents is adopted and is calculated as follows

\[
p = \rho RT \frac{1 + b\rho/2 + (b\rho/4)^2 - (b\rho/4)^3}{(1 - b\rho/4)^2} - \alpha \rho^2,
\]

(10)

where \( T \) is the temperature, \( p \) is the pressure and \( R \) is the ideal gas constant. The attraction parameter \( a \) and the repulsion parameter \( b \) are defined as \( 0.4963(RT_c)^2/p_c \) and \( 0.1873RT_c/p_c \), respectively, where \( p_c \) and \( T_c \) are the critical pressure and critical temperature. Following Ref. (Li et al. 2013), the parameters in our simulations are set to \( R = 1 \), \( b = 4 \) and \( a = 0.5 \) which provide sufficient interface thickness that significantly improve numerical stability at large density ratios.

### 2.2 Wetting boundary condition

In pseudopotential LB community, wettability can be varied via an artificial fluid–solid interaction force (Benzi et al. 2006). However, it is still an estimated method and plenty of LB simulations are required to determine the values of fluid–solid interaction parameters. In this paper, we employ a geometric scheme proposed by Ding and Spelt (2007) within the pseudopotential LBM framework to obtain the prescribed wettability. The contact angle \( \theta \) can be calculated geometrically in terms of density \( \rho \) as

\[
\tan \left( \frac{\pi}{2} - \theta \right) = \frac{-n \cdot \nabla \rho}{\| \nabla \rho \|},
\]

(11)

Figure 1 shows the faces, edges and corners in the microcavity. On the bottom face, the extra-layer adjacent to the solid boundary is added and corresponding discrete form of the densities on the extra-layer lattices can be expressed as

\[
\rho_{ij,1} = \rho_{ij,3} + \tan \left( \frac{\pi}{2} - \theta \right) \xi_f,
\]

(12)

where \( i \) and \( j \) index denote the two orthogonal directions on the bottom face, respectively. In the normal to the solid boundary, 1 and 3 indicate the extra-layer lattices and liquid phase lattices adjacent to the solid boundary, respectively. The quantity \( \xi_f = \| (t \cdot \nabla \rho) t \| \) is expressed as

\[
\xi_f = \sqrt{(\rho_{i+1,j,2} - \rho_{i-1,j,2})^2 + (\rho_{i,j+1,2} - \rho_{i,j-1,2})^2},
\]

(13)
where third index 2 of density $\rho$ indicates the bottom face lattices. At the contact point and the contact line, in the above way, the values of density $\rho_{i,j,1}$ on the extra-layer directly influence the interaction interparticle force for pseudopotential model. Similarly, the values of densities on extra-layer adjacent to the side walls can also be obtained.

Regarding to the edges and corners within microcavity, special discrete forms are needed to handle these positions. Edges of microcavity are at the intersection of two orthogonal faces (edges 1, 2, 3, 4, 5, 6, 7, 8). The forward difference scheme can be applied along with the diagonal plane of microcavity. Hence, densities on the extra-layer adjacent to edge “1” can be derived as

$$
\rho_{i,j,1} = \rho_{i,j,3} + \sqrt{2} \tan \left( \frac{\pi}{2} - \theta \right) \zeta_e,
$$

where $\zeta_e$ is expressed as

$$
\zeta_e = \sqrt{(-3\rho_{i-1,j,2} + 4\rho_{i-2,j,2} - \rho_{i-3,j,2})^2 + (\rho_{i-1,j+1,2} - \rho_{i-1,j-1,2})^2}.
$$

The other densities adjacent to edges can be obtained in the same way. As for corners on the bottom face (corners A, B, C, D), the forward different schemes along with diagonal line of microcavity are applied. Densities on the extra-layer adjacent to corner “A” can be derived as

$$
\rho_{i,j,1} = \rho_{i-2,j-2,3} + \sqrt{3} \tan \left( \frac{\pi}{2} - \theta \right) \zeta_c,
$$

where $\zeta_c$ is expressed as

$$
\zeta_c = \sqrt{(-3\rho_{i-1,j-1,2} + 4\rho_{i-1,j-2,2} - \rho_{i-1,j-3,2})^2 + (-3\rho_{i-1,j-1,2} + 4\rho_{i-2,j-1,2} - \rho_{i-3,j-1,2})^2}.
$$

From the above discrete forms, the desired contact angle $\theta$ could be simply prescribed before simulations.

### 2.3 Model validation

Initially, the satisfaction of the Laplace’s law is considered to validate the 3D MRT pseudopotential LB model. The Laplace’s law, defined as $\Delta p = 2\sigma/r$, denotes the relationship of the pressure difference $\Delta p$ inside and outside a droplet, surface tension $\sigma$ and droplet radius $r$. To verify the Laplace’s law, the computational domain with $121 \times 121 \times 121$ lattice nodes is adopted and a resting droplet with different radius is initialized at the center of the domain. All sides of the domain employ the periodic boundary conditions. The parameters are fixed at $R = 1$, $a = 0.5$, $b = 4$ and $T/T_c = 0.50$. The function of $\Delta p$ and $1/r$ is plotted in Fig. 2. The pressure difference, droplet radius and surface tensions are all in lattice units. It is observed that the pressure difference $\Delta p$ is inversely proportional to droplet radius $r$. It indicates that 3D MRT LB model agrees well with the Laplace’s law.

To validate the geometric scheme of wetting condition, the equilibrium morphologies of one droplet on a solid surface with varying contact angles are simulated. In the simulations, a resting droplet with radius $r = 20$ is initialized on the solid surface. The halfway bounce-back boundary conditions are applied to the top and bottom sides, and the other sides apply periodic boundary conditions. Figure 3 illustrates the static droplet shapes with varying contact angles, and the differences between prescribed and measured contact angles are plotted as well.
The static contact angles are measured on the contact line using the geometric droplet profile from the simulations. It is observed that simulations based on the geometry scheme are in good agreement with the theoretical values.

### 3 Results and discussion

After the numerical validation, the dynamic behaviors of droplet deposition in a square microcavity with different conditions are investigated numerically utilizing 3D MRT pseudopotential LB model. The scenario that a liquid droplet with diameter $D_0$ and initial impact velocity $v_l$ is placed right above the square microcavity is illustrated in Fig. 4. The square microcavity is formed with vertical side walls and bottom surface. The contact angle of bottom surface is fixed at $\theta_b = 75^\circ$ and the contact angle of side wall is defined as $\theta_s$. The length and height of the microcavity for case of $\theta_s = 40^\circ$ are set to be $L = 60$ and $H = 60$, respectively. Whereas for case of $\theta_s = 70^\circ, 90^\circ$ and $110^\circ$, $L = 60$ and $H = 40$ are considered. The diameter of droplet is fixed at $D_0 = 40$ which is consistent with the validation cases and a large liquid–gas density ratio $\rho_l/\rho_g$ can be achieved as 726 for subsequent calculations. It is noted that, in the pseudopotential LB model, the dynamic liquid–gas viscosity ratio $\mu_l/\mu_g$ is equal to the density ratio due to the same relaxation time used in the whole computational domain. The computational domain is set to be $121 \times 121 \times 121$ lattice units. The dimensionless time is calculated via $T^* = t_v/D_0$, where $t$ is the simulation time in lattice units. Figure 5 illustrates the spreading height $H_c$ at the center of side walls, $H_e$ at the edge between side walls and hollow core width $W_{ho}$ on the bottom surface which are non-dimensionalized by the initial droplet diameter $D_0$ as $H_c^*$, $H_e^*$ and $W_{ho}^*$, respectively. The upper and bottom surface, as well as four vertical side walls apply halfway bounce-back scheme to impose the no-slip boundary conditions. Periodic boundary conditions are applied to the domain above.

![Fig. 3](image1.png) Differences between prescribed contact angles ($\theta_s$) and measured contact angles

![Fig. 4](image2.png) Schematic of droplet deposition on a square microcavity. a Cross-sectional view, b top view

![Fig. 5](image3.png) Schematic of spreading height $H_c$, $H_e$ and hollow core width $W_{ho}$ in a square microcavity
Fig. 6 Snapshots of droplet deposition in a microcavity over time with different contact angles (Re=225, We=31.9, $\theta_b = 75^\circ$): a $\theta_s = 40^\circ$, b $\theta_s = 70^\circ$, c $\theta_s = 90^\circ$, d $\theta_s = 110^\circ$
Fig. 7 Snapshots (cross-sectional view) of droplet deposition in a microcavity over time with different contact angles ($\text{Re} = 225$, $\text{We} = 31.9$, $\theta_b = 75^\circ$): (a) $\theta_s = 40^\circ$, (b) $\theta_s = 70^\circ$, (c) $\theta_s = 90^\circ$, (d) $\theta_s = 110^\circ$
the microcavity. Hereafter, the same boundary conditions are adopted in all cases unless otherwise specified.

3.1 Effect of contact angles of vertical side walls

In this section, the morphology and dynamics of the droplet impingement in the microcavity are numerically explored by varying contact angles of side walls. The Reynolds and Weber numbers are set to be Re = 225 and We = 31.9, respectively, which lie within the conditions of inkjet-printed droplets (Dong et al. 2007). Figures 6 and 7 illustrate the sequences of the droplet deposition in a microcavity with varying wettability of side walls. At the initial stage, the droplet impinges on the bottom surface and spreads outward in the microcavity as seen at $T^* = 0.41$ and 0.62. With high Reynolds numbers, droplet impingement behavior in this stage is dominated by the inertial force. However, upon collision with side walls, different wettability $\theta_s$ greatly influences the dynamics and final outcomes of droplet–microcavity interactions. For case of hydrophilic wettability $\theta_s = 40^\circ$, when the droplet collides with side walls as seen in Fig. 6a at $T^* = 0.83$ and 1.24, it is observed that the rims of droplet are boosted upward along the side walls by the inertial force and the wettability gradient between bottom surface and side walls. As the fluids on the side walls coalesce, a sharp rise of fluids along the edges is observed at $T^* = 1.65$ and 2.68 in Fig. 6a which is attributed to the combined velocities and capillary rise. Meanwhile, however, since more fluids are accumulated along the side walls, the droplet height on the bottom surface is gradually decreased as seen in Fig. 7a at $T^* = 2.68$. Afterward, the surface tension and viscosity of liquids take control of recoiling and relaxation phases. It is observed that a breakage occurs nearby the bottom center at $T^* = 2.68$ and eventually a small round dot is attained at $T^* = 3.09$ in Fig. 6a. The corresponding velocity fields inside the fluids shown in Fig. 8 further elucidate the observations. We notice that a large velocity magnitude around the bottom center pulls the fluids outward to the side walls. Further, an ongoing sharp rise of fluids along the edges, as well as the recoiling trend of fluids on the bottom center stimulates the breakage occurrence along the diagonal directions. As the fluids on the bottom are pulled due to the hydrophilic side walls and attain equilibrium outcomes corresponding to the contact angles, a crown-like shape with a small round dot is formed.

For case of $\theta_s = 70^\circ$, with the moderate rise of fluids along the edges, a circular hollow core appears on the bottom center as seen in Fig. 6b at $T^* = 2.89$ and its diameter gradually increases under the wettability influences until the equilibrium shape is attained at $T^* = 5.78$ in Fig. 7b. Whereas for cases of natural and hydrophobic wettability $\theta_s = 90^\circ$ and $110^\circ$, differing from the above hydrophilic cases, a small hollow core on the bottom center appears transiently at $T^* = 2.48$ in Figs. 6c, d and 7c, d. Afterward, during the recoiling phase, the fluids on the side walls flow downward due to the hydrophobic side walls and fill up the small hollow core. Eventually, the equilibrium liquid film is uniform for $\theta_s = 90^\circ$ as seen in Figs. 6c and 7c at $T^* = 6.19$. However, for case of $\theta_s = 110^\circ$, we notice that the corners are exposed for a while due to the intensive recoiling effects
at $T^* = 5.78$ in Fig. 6d. The droplet height on the bottom surface is increased which results in a convex liquid film eventually at $T^* = 6.70$ in Fig. 7d.

Figure 9 illustrates the temporal evolutions of spreading factors including $H_{c}^*$, $H_{e}^*$ and $W_{ho}^*$ with varying wettability of side walls. It is observed that the values of $H_{c}^*$ undergo spreading, recoiling and equilibrium phases which are similar with the scenario of one droplet impingement on the solid surface. However, the values of $H_{e}^*$ are of large deviations with different wettability of side walls which result in interesting physical outcomes. For case of $\theta_s = 40^\circ$, the curve of $H_{e}^*$ undergoes an ongoing sharp rise due to the impact inertia force and capillary rise. In addition, the values of $H_{e}^*$ which are far above the corresponding $H_{c}^*$ indicate a strong adhesive force on the edges overwhelming the recoiling surface tension. Therefore, a sharp increase in $W_{ho}^*$ is observed during the recoiling phase. For case of $\theta_s = 70^\circ$ which is approximately equal to $\theta_b = 75^\circ$, after an initial rise in $H_{e}^*$, its value attains a constant. The values of $W_{ho}^*$ are lower than the case of $\theta_s = 40^\circ$ which result in a circular hollow core shape as previously discussed. For case of $\theta_s = 90^\circ$, the values of $H_{e}^*$ undergo downflow in the later stages which refill the circular hollow core on the bottom center. Eventually, a uniform film within the microcavity is obtained. Whereas for $\theta_s = 110^\circ$, during the recoiling phase, the values of $H_{e}^*$ decrease to zero due to the hydrophobic wettability of side walls which lead to the exposed corners. Afterward, the second recoiling of $H_{e}^*$ refills the corners of microcavity and

![Figure 9 Temporal evolutions of spreading factors $H_{c}^*$, $H_{e}^*$ and $W_{ho}^*$ with different contact angles of side walls](image-url)
Fig. 10 Snapshots of droplet deposition in a microcavity over time with different density ratios (Re = 225, $\theta_s = 90^\circ$ and $\theta_b = 75^\circ$): a $\rho_r = 11.6$, b $\rho_r = 132$, c $\rho_r = 726$
attains a convex liquid film. In summary, with the contact angles of side walls increasing, four types of droplet shapes are generated which are crown-like shape with a small round dot ($\theta_s = 40^\circ$), circular hollow core ($\theta_s = 70^\circ$), uniform hollow core ($\theta_s = 90^\circ$) and convex film ($\theta_s = 110^\circ$). It is known that the non-uniformities of light emissive layer and hole transport layer of OLEDs deteriorate the performance (color, efficiency and lifetime) of products. Therefore, the wettability $\theta_s = 90^\circ$ of side walls is preferred for mura-free OLEDs manufacturing. In the following sections, the dynamics of droplet–microcavity interactions with different conditions are numerically investigated with the fixed contact angle $\theta_s = 90^\circ$.

### 3.2 Effect of density ratios

In the inkjet deposition OLEDs process, the shielding gases such as the mixture of ultrapure nitrogen, $CF_4$, plasma and helium are essential to isolate organic materials of OLEDs from water and oxygen. Therefore, it is important to explore the effect of varying density ratios resulting from the mixing process on the droplet–microcavity interactions. The contact angles of side walls and bottom surface are fixed as $\theta_s = 90^\circ$ and $\theta_b = 75^\circ$, respectively. The Reynolds number is set as $Re = 225$, and the density ratios are set as $\rho = 11.6, 132$ and 726 in the following computations. Figure 10c illustrates the sequences of droplet deposition in a microcavity with $\rho = 726$ discussed in prior section as a benchmark case. It is observed that the sequences with $\rho = 132$ in Fig. 10b are almost identical with the scenario with $\rho = 726$. However, as the density ratio decreases to $\rho = 11.6$, the breakage occurs after $T^* = 3.30$ in Fig. 10a which is a little later than the scenarios of larger density ratios. Furthermore, upon formation of hollow core, it maintains for a longer time as seen from $T^* = 4.13$ to $T^* = 8.25$. Figure 11 illustrates the temporal evolutions of spreading factors including $H^*_c$, $H^*_e$ and $W^*_{ho}$ with different density ratios. It is noticed that there are the similar tendencies of $H^*_c$ and $H^*_e$ during the impact inertial dominated spreading phases. For cases of $\rho = 132$ and $\rho = 726$, the values of $H^*_c$, $H^*_e$ and $W^*_{ho}$ vary slightly which indicate the influences of gas density on the droplet dynamics could be negligibly with the order of density ratio $O(100)$. However, as the density ratio decreases to $\rho = 11.6$, the larger gas density plays a significant role on the droplet–microcavity interactions particularly in the recoiling and relaxation phases. It is observed that the curves of $H^*_c$ and $H^*_e$ continue to rise in the later spreading phase and begin a slower decline compared with the cases of larger density ratios. Meanwhile, although the occurrence of breakage is delayed obviously, the values of $W^*_{ho}$ increase sharply and maintain for some time in the recoiling and relaxation stages.

The velocity fields inside the microcavity with $\rho = 11.6$ (top row) and $\rho = 132$ (bottom row) are illustrated in Fig. 12.

![Fig. 11 Temporal evolutions of spreading factors $H^*_c$, $H^*_e$ and $W^*_{ho}$ with different density ratios](image)

At a lower $\rho = 11.6$, the inertia of surrounding denser gas is larger. Hence, when the fluids inside the microcavity with $\rho = 132$ start to enter the recoiling phase at $T^* = 2.06$, the fluids of droplet with $\rho = 11.6$ are still under the spreading phase due to the large inertia of surrounding gas. Therefore, the values of $H^*_c$ and $H^*_e$ could continue to increase in the extended spreading phase. Meanwhile, the occurrence of breakage is delayed resulting from the later transition between spreading and recoiling phase. Afterward, the surrounding denser gas fills in the space of breakage and an increased resistance to the recoiling motion of liquids is imposed which could be apparently observed at $T^* = 3.92$ in Fig. 12a. In consequence, the values of $W^*_{ho}$ are larger than those with $\rho = 132$ and decrease gradually. Therefore, for $\rho = 11.6$, the time of obtaining equilibrium outcome is extended compared with those of larger density ratios.

### 3.3 Effect of droplet viscosity and impact velocity

We next investigate the influences of droplet viscosity and impact velocity during the droplet impingement. The Ohnesorge number is considered to characterize the influence of liquid viscosity on the droplet-microcavity dynamics. The
Weber number is fixed at $W_e = 31.9$, and contact angles of side walls and bottom surface are fixed as $\theta_s = 90^\circ$ and $\theta_b = 75^\circ$, respectively. The Ohnesorge numbers $Oh = 0.0952, 0.0547$ and $0.0159$ are varied by changing droplet viscosities corresponding to $Re = 59.3, 103.3$ and $355.2$, respectively. Selected snapshots of droplet deposition sequences with different liquid viscosities are shown in Fig. 13. It is apparent that, with the droplet viscosity increases, the droplet–microcavity interactions are more moderate and the equilibrium shapes could be attained swiftly. In addition, no hollow core is observed with large droplet viscosities. This could be attributed to the fact that the rate of energy dissipation is accelerated during the spreading phase with increased droplet viscosity. Upon impact with the side walls, the viscous stress inside the fluids hinders the droplet movement which is beneficial to shorten the process of droplet-microcavity dynamics and attain the equilibrium outcome swiftly.

Figure 14 illustrates temporal evolutions of spreading factors $H_c^*, H_e^*$ and $W_{ho}^*$ with varying droplet viscosities. For lower liquids viscosity $Oh = 0.0159$, it is observed that the values of $H_e^*$ undergo intense undulation driven by the large impact inertial force. Furthermore, the fluids on the edges are pushed upward which results in a sharp rise of $W_{ho}^*$. For larger liquid viscosity $Oh = 0.0952$, it clearly manifest that the curves of $H_c^*$ and $H_e^*$ get to rapid convergence in the later stage and no hollow core is observed.

Finally, we investigate the effect of impact velocity of droplet on the droplet–microcavity interactions. The Ohnesorge number is fixed as $Oh = 0.0251$. The impact velocities are set as $v_l = 0.085, 0.115$ and $0.140$ corresponding to $We = 8.47, 15.5$ and $23.0$, as well as $Re = 115.9, 156.8$ and $191.1$, respectively. Figure 15 illustrates temporal evolutions of spreading factors $H_c^*, H_e^*$ and $W_{ho}^*$ with varying impact velocities. With the decrease in impact velocity, the collision moment of droplet and microcavity is delayed. Hence, the curves of $H_c^*$ and $H_e^*$ get to rapid convergence in the later stage and no hollow core is observed. Liou et al. (2008) investigated the effect of Weber number on the equilibrium shapes of droplet. In their work, the ratio of droplet diameter and microcavity width was small and Reynolds number was moderate. Hence, the fluids could not refill the hollow core during the recoiling phase. However, as the impact velocity continues to decrease as seen at $W_e = 8.47$, the hollow core does not occur. Liou et al. (2008) investigated the effect of Weber number on the equilibrium shapes of droplet. In their work, the ratio of droplet diameter and microcavity width was small and Reynolds number was moderate. Hence, the fluids could not refill the hollow core during the recoiling phase. Recently, Miers and Zhou (2017) concluded that higher frequencies of droplet formation could be achieved by increasing ejection velocities. Besides, the dimensions of microcavity need to be reduced to meet the requirement of high-definition OLEDs. Consequently, the effects of recoiling flow in the process of inkjet deposition for OLEDs must be considered.
Fig. 13 Snapshots of droplet deposition in a microcavity over time with different droplet viscosities.  

- **a**: Oh = 0.0952
- **b**: Oh = 0.0547
- **c**: Oh = 0.0159 with $\theta_s = 90^\circ$ and $\theta_b = 75^\circ$
In summary, in this section, it is found that an appropriate higher droplet viscosity is preferred which could eliminate the hollow core in the inkjet deposition process and attain the equilibrium outcome swiftly. It is beneficial for the mura-free OLEDs manufacturing. However, higher droplet viscosity increases the risk of inkjet nozzles clog. Alternately, decreasing the impact velocities of droplet is another optimal approach. It is noted that the sufficient kinetic energy should be satisfied (Wijshoff 2010) to overcome the limit imposed by surface tension. Hence, the effects of droplet viscosity and impact velocity are significant on the dynamics of droplet–microcavity interactions. Optimizing those parameters could accelerate the inkjet deposition process straightforward and fabricate the uniform OLEDs displays.

4 Conclusions

The dynamics and final outcome of inkjet deposition in a square microcavity are investigated by utilizing a 3D MRT pseudopotential LB model with large density ratios and high Reynolds numbers. A geometric scheme is considered within the pseudopotential LBM framework to obtain the prescribed wettability. The influence factors including wettability of microcavity, density ratios, droplet viscosity and impact velocity are explored to reveal the interaction dynamics between droplet and microcavity. For case of hydrophilic wettability $\theta_s = 40^\circ$, the curve of $H'_e$ undergoes an ongoing sharp rise due to the impact inertia force and capillary rise which results in a crown-like shape with a small round dot. For case of $\theta_s = 70^\circ$, a circular hollow core is formed on the bottom center. Whereas for case of $\theta_s = 90^\circ$ and $110^\circ$, due to the effect of recoiling flow, fluids refill the hollow core which is not observed in the literature. The uniform and convex liquid film is formed eventually. At a lower density ratio $\rho_s = 11.6$, the surrounding denser gas with larger inertia resists the droplet recoiling flow resulting in an increasing hollow core. Moreover, the time of obtaining equilibrium outcome is extended compared with those of larger density ratios. Additionally, the effects of droplet viscosity and impact velocity are investigated during the droplet impingement. The appropriate higher droplet viscosity is preferred which could eliminate the hollow core in the inkjet deposition process and
accelerate the inkjet deposition process straightforward. Alternately, decreasing the impact velocities of droplet is another optimal approach to obtain no hollow core. In conclusion, the numerical investigation of dynamics and final outcome of droplet–microcavity interactions is beneficial for optimizing inkjet deposition process and fabricating uniform OLEDs displays.

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