

Simulating multicomponent multiphase electrohydrodynamic flows using a hybrid pseudopotential lattice Boltzmann and finite difference model

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Electrohydrodynamics (EHD) are widely utilized to manipulate fluid behaviors in practical applications, such as EHD high-resolution printing and EHD nebulization for producing monodispersed small droplets. In these applications, multicomponent multiphase (MCMP) phenomena with large density contrasts are usually involved. However, previous studies either focused on modeling single-phase multicomponent EHD problems where the densities of different components are the same or multiphase single-component EHD flows with large density contrasts where only one fluid component is considered. Therefore, in this work, a hybrid numerical framework combining MCMP pseudopotential LBM and FDM is implemented and applied to simulate EHD flows, which is capable of simulating MCMP EHD flows with large density ratios and offers tunable surface tension that is independent of viscosity and density ratios. The numerical model is comprehensively validated through benchmarks, including the thermodynamic consistency test, Young-Laplace droplet test, contact angle test, and droplet deformation under an electric field. The results demonstrate the capability of the present model for accurately simulating EHD MCMP flows with high-density ratios, good thermodynamic consistency, low spurious velocity, adjustable surface tension, and wettability. Lastly, the developed model is applied to investigate the effects of fluid electrical properties and electric field strength on the deformation and wettability of a sessile droplet under an external electric field.

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I. INTRODUCTION

Electric field-induced flows, namely, electrohydrodynamics (EHD), involving multiple fluid components and multiple phases have been widely observed in both the science and engineering disciplines and play an important role in various fields, for instance, electrospray [1], droplet evaporation and condensation in the boiler and condenser [2,3], fluid mixing [4,5], and EHD high-resolution printing [6]. The complex interplay between different fluid components, phases, and physical fields makes modeling this problem extremely challenging. This is further complicated by the moving fluid interface existing within these systems.

Some attempts have been made using traditional numerical methods, such as finite element method (FEM), finite volume method (FVM), and finite difference method (FDM). More importantly, additional interface tracking or capturing schemes are required in those methods to handle discontinuities and interactions between phases. For example, volume

of fluid (VOF) has been widely adopted to model various droplet phenomena under an electric field, such as droplet deformation [7], coalescence [8], and emulsification [9]. Another popular approach is the level set (LS) method, which has been widely used to simulate droplet deformation, breakup, and coalescence [10–12], and liquid fuel injection [13]. Other methods, such as the boundary integral method [14,15] and front-tracking method [16,17], have obtained many achievements in simulating multiphase EHD flows. However, these models encounter difficulties in maintaining mass conservation and accurately implementing surface tension forces [18]. Therefore, intermediate algorithmic steps are required to smooth the composition profile across the interface to ensure mass conservation and better implement the surface tension force [19,20], which makes the simulation more complex and may lead to other problems such as spurious currents that need to be solved using additional algorithms [20].

In contrast to the traditional methods mentioned above, the pseudopotential lattice Boltzmann method (LBM), which is rooted in kinetic theory, serves as a mesoscopic approach and has become a promising alternative for simulating multicomponent and/or multiphase fluid flows [21]. It offers some key advantages, such as simplicity, inherent parallelism, and straightforwardness and accuracy in handling complex stationary or moving geometries. Furthermore, explicit front-tracking schemes are not required when managing multifluid dynamical systems. The interface can emerge automatically due to the pseudopotential force between different fluids.

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Furthermore, belonging to diffuse-interface models, LBM shows its strength when modeling multiphase flows by treating the interface as a smoothly diffused layer [22]. An initial study on EHD problems using pseudopotential LBM was presented by Zhang and Kwok [23] in 2005, where a multi-component pseudopotential LBM and a standard LBM were employed to simulate the hydrodynamic and electric field, respectively. The results showed that their model could be an excellent alternative to electrohydrodynamics studies compared to traditional computational fluid dynamics methods. However, the density ratio between different fluid components was 1 due to the limitation of the original pseudopotential LBM [23]. After this, many studies focused on investigating the multiphase EHD flows with large density ratios using single-component multiphase pseudopotential LBM [24–27] and multicomponent EHD flows with a density ratio of 1 using single-phase multicomponent pseudopotential LBM [28–30]. However, to the best of our knowledge, no study has focused on the numerical modeling of multicomponent multiphase (MCMP) EHD flows using LBM.

Therefore, in this study, a hybrid LB and FD numerical framework is proposed, where MCMP LBM is used to simulate the hydrodynamic field, whereas the second-order central FDM is employed to solve the electric field, as FDM demonstrates a faster convergence compared to LBM [31,32]. The coupling between the hydrodynamic and electric fields is realized through the leaky dielectric model. The capability and accuracy of this hybrid method are assessed by the Young-Laplace test, thermodynamic consistency test, and droplet deformation under an electric field. It is then applied to investigate the effect of an electric field on a sessile water droplet, where the droplet wetting behaviors under different conductivity ratios R and permittivity ratios Q are explored.

II. PROBLEM DESCRIPTION AND GOVERNING EQUATIONS

To mathematically describe the MCMP EHD fluid flows, two separate constitutive equations are required to collectively represent the hydrodynamic and electric fields. The hydrodynamic behavior of a fluid mixture with α components ($\rho = \sum_{\alpha} \rho^{\alpha}$) can be described by the incompressible Navier-Stokes equations (NSE):

$$\nabla \cdot \mathbf{u} = 0, \quad (1)$$

$$\rho[\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u}] = -\nabla P + \mu \Delta \mathbf{u} + \gamma \kappa \mathbf{n} \delta + \nabla \cdot \mathbf{S}_M, \quad (2)$$

where ρ , $\mathbf{u}$, P , and μ represent the total density, mixture velocity, local static isotropic pressure, and dynamic viscosity, respectively. γ , κ , $\mathbf{n}$, and δ are the interfacial tension, the local curvature of the interface, the unit vector normal to the interface, and the Dirac-delta function. $\mathbf{S}_M$ corresponds to the Maxwell stress tensor [33–35],

$$\mathbf{S}_M = \varepsilon [\mathbf{E} \mathbf{E} - \frac{1}{2} (\mathbf{E} \cdot \mathbf{E}) \mathbf{I}], \quad (3)$$

where ε and $\mathbf{E}$ are the fluid electric permittivity and electric field strength. By taking the divergence of $\mathbf{S}_M$, the electrical

force can be expressed as

$$\mathbf{F}_e = \nabla \cdot \mathbf{S}_M = \mathbf{E} q_v - \frac{1}{2} (\mathbf{E} \cdot \mathbf{E}) \nabla \varepsilon, \quad (4)$$

where $q_v = \nabla \cdot (\varepsilon \mathbf{E})$ is the free charge density. The first and second terms on the right-hand side of Eq. (4) represent the Coulomb force and dielectric electrophoretic force, respectively. To obtain the electrical force, the governing equation for the electric field, namely the electric charge conservation needs to be solved, which can be written as

$$\frac{\partial q_v}{\partial t} + \nabla \cdot (q_v \mathbf{u} + \sigma \mathbf{E}) = 0, \quad (5)$$

where σ is the electric conductivity.

For the leaky dielectric model, it is assumed that the electric charges accumulate at the interface almost instantly as the electric relaxation timescale is much smaller compared to the time scale of the fluid motion. Therefore, Eq. (5) can be simplified as

$$\nabla \cdot (\sigma \mathbf{E}) = 0. \quad (6)$$

Moreover, as the electric field strength $\mathbf{E}$ is irrotational, namely $\nabla \times \mathbf{E} = 0$, the electric field can be written as the gradient of electric potential U , i.e., $\mathbf{E} = -\nabla U$. As a result, the above equation can be rewritten as,

$$\nabla \cdot (\sigma \nabla U) = 0. \quad (7)$$

III. NUMERICAL METHOD

A. Multicomponent multiphase MRT pseudopotential LBM

MCMP pseudopotential LBM is used to solve the hydrodynamic field. To simulate fluid flows with high-density contrast, the MRT collision operator [36] is adopted, which shows better numerical stability than the Bhatnagar-Gross-Krook (BGK) collision operator [37]. In the present study, the two-dimensional and nine-velocity (D2Q9) lattice structure is utilised. As a result, the evolution equation of the particle density distribution function of each fluid component for the multicomponent multiphase pseudopotential LB model with the MRT collision operator can be expressed as [38,39]

$$\begin{aligned} f_{\alpha,i}(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) \\ = f_{\alpha,i}(\mathbf{x}, t) - (\mathbf{M}^{-1} \mathbf{\Lambda} \mathbf{M})_{ij} [f_{\alpha,i}(\mathbf{x}, t) \\ - f_{\alpha,i}^{\text{eq}}(\mathbf{x}, t)] + \Delta t F'_{\alpha,i}(\mathbf{x}, t), \end{aligned} \quad (8)$$

where $f_{\alpha,i}(\mathbf{x})$ represents the particle distribution function for the α th component along the i direction at time t and position $\mathbf{x}$. Δt denotes the time step and is set to be 1. $F'_{\alpha,i}$ stands for the forcing term in the discrete velocity space for component α . For the D2Q9 lattice structure, the discrete lattice velocity vector $\mathbf{e}_i$ is defined as

$$\begin{aligned} [\mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_4, \mathbf{e}_5, \mathbf{e}_6, \mathbf{e}_7, \mathbf{e}_8, \mathbf{e}_9] \\ = c \begin{bmatrix} 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \end{bmatrix}, \end{aligned} \quad (9)$$

where $c = \Delta x / \Delta t$ is the lattice speed with Δx and Δt representing the lattice spacing and time spacing, respectively. In this study, Δx and Δt are assigned to be 1. $f_{\alpha,i}^{\text{eq}}$ is the

corresponding equilibrium distribution function defined as

$$f_{\alpha,i}^{\text{eq}}(\mathbf{x}, t) = \omega_i \rho_\alpha \left[1 + \frac{\mathbf{e}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_i \cdot \mathbf{u})^2}{2c_s^4} - \frac{(\mathbf{u})^2}{2c_s^2} \right], \quad (10)$$

where ω_i are the weighting coefficients. For the D2Q9 lattice structure considered in this study, ω_i is given by $\omega_0 = 4/9$, $\omega_{1-4} = 1/9$, $\omega_{5-8} = 1/36$. c_s is the speed of sound, which is $c/\sqrt{3}$. The macroscopic variables, such density ρ_α and mixture velocity $\mathbf{u}$ can be calculated by [39–41]

$$\rho_\alpha = \sum_i f_{\alpha,i}, \quad (11)$$

$$\mathbf{u} = \frac{\sum_\alpha (\sum_i f_{\alpha,i} \mathbf{e}_i + 0.5 \Delta t \mathbf{F}_\alpha)}{\sum_\alpha \rho_\alpha}, \quad (12)$$

where $\mathbf{F}_\alpha$ is the total force acting on the component α , including the fluid-fluid interaction force, fluid-solid interaction force, and electrical force.

$\mathbf{M}$ in Eq. (8) is the transformation matrix and $\mathbf{\Lambda}$ is the diagonal relaxation matrix, which for the D2Q9 structure is defined as

$$\mathbf{M} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\ 4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & -2 & 0 & -2 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\ 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \end{bmatrix}, \quad (13)$$

$$\mathbf{\Lambda} = \text{diag}[\tau_\rho^{-1}, \tau_e^{-1}, \tau_\zeta^{-1}, \tau_j^{-1}, \tau_q^{-1}, \tau_j^{-1}, \tau_q^{-1}, \tau_v^{-1}, \tau_v^{-1}], \quad (14)$$

where τ_ρ^{-1} and τ_j^{-1} are set to be 1 to recover the correct NS equations. τ_ζ^{-1} and τ_q^{-1} are adjustable parameters in the MRT-LB model, which are set as $\tau_\zeta^{-1} = \tau_e^{-1} = 0.8$ and $\tau_q^{-1} = 1.1$, respectively [42]. The remaining parameter τ_v^{-1} is related to the fluid viscosity ν by

$$\nu = c_s^2 (\tau_v - 0.5) \Delta t. \quad (15)$$

Using the transformation matrix $\mathbf{M}$, the collision step in Eq. (8) can be transformed to the moment space and rewritten as follows:

$$\mathbf{m}_\alpha^* = \mathbf{m}_\alpha - \mathbf{\Lambda}(\mathbf{m}_\alpha - \mathbf{m}_\alpha^{\text{eq}}) + \Delta t(\mathbf{I} - 0.5\mathbf{\Lambda})\mathbf{S}_\alpha, \quad (16)$$

where $\mathbf{m}_\alpha = \mathbf{M}\mathbf{f}_\alpha$ and $\mathbf{m}_\alpha^{\text{eq}} = \mathbf{M}\mathbf{f}_\alpha^{\text{eq}}$ are the distribution functions at the moment space. $\mathbf{I}$ is the unit tensor. The equilibrium moment $\mathbf{m}_\alpha^{\text{eq}}$ can be expressed as

$$\mathbf{m}_\alpha^{\text{eq}} = \rho_\alpha (1, -2 + 3|\mathbf{u}|^2, 1 - 3|\mathbf{u}|^2, u_x, -u_x, u_y, -u_y, u_x^2 - u_y^2, u_x u_y)^T. \quad (17)$$

Then, the streaming step becomes

$$f_{\alpha,i}(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) = f_{\alpha,i}^*(\mathbf{x}, t) = \mathbf{M}^{-1} \mathbf{m}_\alpha^*. \quad (18)$$

The fluid-fluid interaction force consists of two terms for the multicomponent multiphase LB model, namely, the intra-component interaction force $\mathbf{F}_{\alpha,\alpha}$ and the inter-component interaction force $\mathbf{F}_{\alpha,\bar{\alpha}}$, which are expressed as

$$\mathbf{F}_{\alpha,\alpha}(\mathbf{x}) = -G_{\alpha,\alpha} \psi_\alpha(\mathbf{x}) \sum_i \varpi_i \psi_\alpha(\mathbf{x} + \mathbf{e}_i \Delta t) \mathbf{e}_i \Delta t, \quad (19)$$

$$\mathbf{F}_{\alpha,\bar{\alpha}}(\mathbf{x}) = -G_{\alpha,\bar{\alpha}} \varphi_\alpha(\mathbf{x}) \sum_i \varpi_i \varphi_{\bar{\alpha}}(\mathbf{x} + \mathbf{e}_i \Delta t) \mathbf{e}_i \Delta t, \quad (20)$$

where $G_{\alpha,\alpha}$ and $G_{\alpha,\bar{\alpha}}$ are used to control the interaction strength between the same components (intra) and different components (inter), respectively. In this paper, we focus on MCMP flows with $\alpha = 1$ and $\alpha = 2$ representing the liquid phase and gas phase, respectively. w_i represents the weighting coefficient. For the D2Q9 lattice structure, $\varpi_0 = 4/3$ and $\varpi_{1-4} = 1/3$ for the four nearest lattices, $\varpi_{5-8} = 1/12$ for the four next-nearest lattices. To achieve a high-density ratio, the pseudopotential ψ_α is defined as a function of the local density instead of directly using the component density or its exponent form:

$$\psi_\alpha(\mathbf{x}) = \sqrt{\frac{2(p_{\text{EOS}}^\alpha - \rho_\alpha c_s^2)}{c^2 G_{\alpha,\alpha}}}, \quad (21)$$

where the pressure p_{EOS}^α is obtained from the non-ideal EOS. Utilizing a more realistic EOS can significantly enhance the maximum liquid-gas density ratio and reduce spurious currents near the phase interface [43–46]. For the liquid component, the Peng-Robinson (P-R) EOS is adopted [45],

$$p = \frac{\rho R_g T}{1 - b\rho} - \frac{a\phi(T)\rho^2}{1 + 2b\rho - b^2\rho^2} \quad (22)$$

$$\phi(T) = [1 + (0.37464 + 1.54226w - 0.26992w^2) \times (1 - \sqrt{T/T_c})]^2, \quad (23)$$

where $a = 0.45724R^2T_c^2/p_c$ and $b = 0.0778RT_c/p_c$. T is temperature and R_g denotes the gas constant, which is equal to 1. T_c and p_c correspond to critical temperature and pressure. In this work, the acentric factors w , a , and b are chosen to be 0.344, 1/49, and 2/21, respectively [45]. Furthermore, a dimensionless coefficient k is introduced to the EOS to adjust the interfacial tension independently from the density ratio without influencing the Maxwell construction [47–50]. Thus, the EOS can be modified as

$$p' = kp = k \left(\frac{\rho R_g T}{1 - b\rho} - \frac{a\phi(T)\rho^2}{1 + 2b\rho - b^2\rho^2} \right). \quad (24)$$

For the gas component, the ideal gas equation is adopted:

$$p = \rho R_g T. \quad (25)$$

Also, the interaction strength G_{22} is set to be 0 for the ideal gas, which means that the pseudopotential $\psi_\alpha(\mathbf{x})$ for the gas phase becomes irrelevant. As for the pseudopotential $\varphi_\alpha(\mathbf{x})$ used in the intercomponent interaction force in Eq. (20), $\varphi_\alpha(\mathbf{x}) = \rho_\alpha(\mathbf{x})$ is used to ensure an appropriate distribution of different components [39,51].

The fluid-solid adhesion force relating to the contact angle is implemented by defining a virtual wall density ρ_w [52]:

$$\mathbf{F}_{\text{ads}} = -G_{\alpha,\alpha} \psi(\rho(\mathbf{x}, t)) \sum_i \varpi_i \psi(\rho_w) s(\mathbf{x} + \mathbf{e}_i \Delta t) \mathbf{e}_i, \quad (26)$$

where $s(\mathbf{x} + \mathbf{e}_i \Delta t)$ is an indicator function that is equal to 1 or 0 for a solid or fluid node. The virtual wall density is defined by the geometric formulation approach [53], which is capable of reproducing the prescribed contact angle,

$$\rho_w = \rho_{x,0} = \rho_{x,1} + \tan(\pi/2 - \theta) |\rho_{x+1,1} - \rho_{x-1,1}|, \quad (27)$$

where θ is the analytical prescribed static contact angle, and $\rho_{x,0}$ represents the ghost layer density beneath the solid boundary ($i, 1$). More generally, the second subscript denotes the coordinates in the normal direction.

To maintain thermodynamic consistency, the modified Li's forcing scheme [38] is employed, which in the moment space can be expressed as

$$\mathbf{S} = \begin{bmatrix} 0 \\ 6(u_x F_{\alpha,x} + u_y F_{\alpha,y}) + \frac{12\zeta |\mathbf{F}_\alpha|^2}{\psi_\alpha^2 \Delta t (\tau_e - 0.5)} \\ -6(u_x F_{\alpha,x} + u_y F_{\alpha,y}) - \frac{12\zeta |\mathbf{F}_\alpha|^2}{\psi_\alpha^2 \Delta t (\tau_e - 0.5)} \\ F_{\alpha,x} \\ -F_{\alpha,x} \\ F_{\alpha,y} \\ -F_{\alpha,y} \\ 2(u_x F_{\alpha,x} - u_y F_{\alpha,y}) \\ (u_x F_{\alpha,y} + u_y F_{\alpha,x}) \end{bmatrix}, \quad (28)$$

$$\begin{aligned} & \sigma_{i,j} \left[\frac{U_{i+1,j} - 2U_{i,j} + U_{i-1,j}}{\Delta x^2} + \frac{U_{i,j+1} - 2U_{i,j} + U_{i,j-1}}{\Delta y^2} \right] \\ & + \left[\frac{\sigma_{i+1,j} - \sigma_{i-1,j}}{2\Delta x} \cdot \frac{U_{i+1,j} - U_{i-1,j}}{2\Delta x} + \frac{\sigma_{i,j+1} - \sigma_{i,j-1}}{2\Delta y} \cdot \frac{U_{i,j+1} - U_{i,j-1}}{2\Delta y} \right] = 0. \end{aligned} \quad (31)$$

Then, the discretized equation, i.e., Eq. (31), is solved iteratively by the successive over-relaxation (SOR) method [55] at each time step of LBM to obtain the electric potential distribution in the computational domain. The solution is considered to be converged when

$$\frac{|U^n - U^{n-1}|}{|U^n|} < \delta_U, \quad (32)$$

where δ_U is the tolerance to determine if the calculation converges, which is set to be 10^{-5} by considering the balance between the accuracy and computational cost. n represents the iteration number. Obviously, the development of the hydrodynamic field also impacts the electric field. Therefore, Eq. (7) will be solved at every time step of LBM to get the updated distribution of the electric field. The electric permittivity ε and conductivity σ of the entire computational domain can be redistributed based on the mixed fluid density of the

where ζ is an adjustable parameter to achieve a good thermodynamic consistency. After extensive tests, the parameter ζ is set to 0.1067 for the liquid component and 0 for the gas component.

Linear interpolation for τ_v in Eq. (14) can be used to achieve a high viscosity ratio [54],

$$\tau_v = \tau_l + \frac{\rho - (\rho_{\alpha,\text{in}} + \rho_{\bar{\alpha},\text{in}})}{(\rho_{\alpha,\text{out}} + \rho_{\bar{\alpha},\text{out}}) - (\rho_{\alpha,\text{in}} + \rho_{\bar{\alpha},\text{in}})} (\tau_g - \tau_l), \quad (29)$$

where $\rho = \sum_\alpha \rho_\alpha$ is the density of the mixed fluids. Taking the water droplet surrounded by the gas as an example, $\rho_{\alpha,\text{in}}$ and $\rho_{\alpha,\text{out}}$ are the densities of component α (water) inside and outside the droplet. Whereas, $\rho_{\bar{\alpha},\text{in}}$ and $\rho_{\bar{\alpha},\text{out}}$ represent the density of component $\bar{\alpha}$ (gas) inside and outside the droplet. τ_l and τ_g are the viscosities of the liquid water and gas, respectively.

For simulating the electrohydrodynamic phenomena, the electrical force $\mathbf{F}_e$ represented by Eq. (4) is incorporated into the total force $\mathbf{F}_\alpha$ of the LB model as an external force, which can be obtained by solving Eq. (7) as discussed below. The total electrical force calculated from Eq. (4) is partitioned among the fluid components in proportion to their local densities. Specifically, the electrical force applied to component α is given by

$$\mathbf{F}_e^\alpha = \frac{\rho_\alpha}{\rho} \mathbf{F}_e. \quad (30)$$

B. FDM for the electric field equations

It has been found that the convergence rate to attain a steady electric potential distribution using LBM is slower than using FDM [31]. Therefore, to achieve a better computational efficiency, a second-order central differencing scheme is employed to discretise Eq. (7), which yields

hydrodynamic field ρ as follows:

$$\varepsilon(\mathbf{x}, t) = \varepsilon_l + \frac{\rho(\mathbf{x}, t) - (\rho_{\alpha,\text{in}} + \rho_{\bar{\alpha},\text{in}})}{(\rho_{\alpha,\text{out}} + \rho_{\bar{\alpha},\text{out}}) - (\rho_{\alpha,\text{in}} + \rho_{\bar{\alpha},\text{in}})} (\varepsilon_g - \varepsilon_l), \quad (33)$$

$$\sigma(\mathbf{x}, t) = \sigma_l + \frac{\rho(\mathbf{x}, t) - (\rho_{\alpha,\text{in}} + \rho_{\bar{\alpha},\text{in}})}{(\rho_{\alpha,\text{out}} + \rho_{\bar{\alpha},\text{out}}) - (\rho_{\alpha,\text{in}} + \rho_{\bar{\alpha},\text{in}})} (\sigma_g - \sigma_l), \quad (34)$$

where the superscripts l and g indicate liquid and gas phases, respectively.

IV. RESULTS AND DISCUSSION

In this section, three benchmark cases are first conducted to validate the MCMP LBM, namely, the thermodynamic consistency test, Laplace test, and wettability test. Then, the droplet

deformation in the presence of an electric field is simulated to verify the accuracy of the present numerical framework for simulating electrohydrodynamics of MCMP fluid flows with high-density contrast. Lastly, the validated hybrid numerical framework is applied to study the behavior of a sessile droplet surrounded by air under an electric field. It should be noted that all variables are measured in lattice units (l.u.).

A. Validation of the pseudopotential LBM

1. Thermodynamic consistency

A two-component two-phase flow is considered in the study for the benchmark cases mentioned above, where the liquid component is treated as the nonideal fluid and the gas component is treated as the ideal gas. The intraparticle interaction strength of the nonideal component is chosen to be $G_{\alpha,\alpha} = 1$, as the only function of $G_{\alpha,\alpha}$ is to ensure the positiveness inside the square root of in Eq. (21) [45,56], whereas the intraparticle interaction strength $G_{\bar{\alpha},\bar{\alpha}}$ for the ideal gas is set to be 0. Moreover, the interparticle interaction strengths between the liquid and gas, namely, $G_{\alpha,\bar{\alpha}}$ and $G_{\bar{\alpha},\alpha}$, are chosen as 0.15 to provide a suitable immiscibility and good numerical stability [39,51]. Also, as mentioned in Sec. III A, the adjustable parameter ζ in Eq. (28) is used to achieve a good thermodynamic consistency. In this work, $\zeta = 0.1067$ is chosen based on our previous study [39].

To determine the equilibrium coexisting densities of the vapor and liquid phases, a droplet with an initial radius of $R_0 = 50$ is positioned at the center of a square domain (200×200 l.u.) with periodic boundary conditions applied in all directions. The local density of the computational domain for different fluid components is initialized as follows:

$$\rho_\alpha(x, y) = \frac{\rho_{\alpha,\text{in}} + \rho_{\alpha,\text{out}}}{2} - \frac{\rho_{\alpha,\text{in}} - \rho_{\alpha,\text{out}}}{2} \times \tanh \left[\frac{2(\sqrt{(x-x_0)^2 + (y-y_0)^2}) - R_0}{W} \right], \quad (35)$$

where ρ_α represents the density of component α . $\rho_{\alpha,\text{in}}$ and $\rho_{\alpha,\text{out}}$ denote the densities of component α inside and outside the droplet, respectively. $W = 5$ is the initial thickness of fluid-fluid interface, (x_0, y_0) represents the center of the domain.

Different κ values are used to study the effects of κ on the thermodynamic consistency of the numerical model. Then, the coexisting densities for the liquid phase are simulated and compared with the theoretical results obtained by the Maxwell equal-area construction [56]. As can be seen in Fig. 1, the equilibrium coexisting densities for the liquid component show good agreement with the analytical solution and κ has negligible impact on the thermodynamic consistency. This demonstrates the capability of the present model for simulating MCMP flows having high-density ratios with good thermodynamic consistency over a wide temperature.

2. Laplace test

Based on the coexistence densities obtained from the thermodynamic consistency test, the Laplace test under different

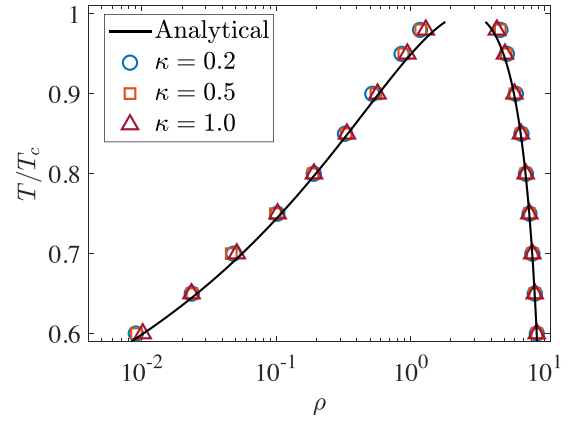


FIG. 1. Comparison of the coexistence curve of density between the numerical results and the analytical solution from Maxwell construction at $\kappa = 0.2, 0.5$, and 1.0 .

κ values is conducted to further validate the numerical model. According to Laplace's law, the pressure difference Δp across the fluid interface at the equilibrium state is proportional to the radius of curvature $1/r$ [57], i.e., $\Delta p = \gamma/r$, where γ is the surface tension. A liquid droplet with an initial radius of R_0 surrounded by gas is positioned at the center of a periodic domain with the grid size of 200×200 in the absence of gravity. In this test, the temperature is $T = 0.85T_c$, which, according to the thermodynamic consistency test, corresponds to the liquid density $\rho_{\alpha,\text{in}} = 6.62$ and vapor density $\rho_{\alpha,\text{in}} = 0.34$. For the gas component, the initial density is set as $\rho_{\bar{\alpha},\text{out}} = 0.0001$. An extremely small density is initialized within the liquid phase, namely, $\rho_{\bar{\alpha},\text{in}}$, to ensure the simulation convergence. Finally, the initialization of the local density for different fluid components is the same as Eq. (35). Figure 2(a) shows the density distribution of the liquid component at $T = 0.85T_c$ and $\kappa = 1$, where a smooth density transition between the liquid and vapor can be observed. Furthermore, Fig. 2(b) presents the spurious velocity distribution with the maximum values distributed near the interface. Simulations are then conducted over different κ values. It can be quantitatively seen from Fig. 2(c) that densities for both liquid (solid lines) and gas (dashed lines) transit smoothly across the interface with the achieved density ratio between the liquid and gas being 1500. Further, the interface thickness increases as the decrease of κ values without influencing the densities for both phases, which means that κ has no impact on the resulting density ratio. The results also indicate that the maximum spurious velocity increases with κ , as shown in Fig. 2(d). However, the maximum spurious velocity obtained in the present numerical model at different κ values is much smaller compared to some previous studies in the literature [41,47,58].

After reaching the equilibrium state, the system pressure is calculated as

$$p_{\text{sys}} = c_s^2 \sum_{\alpha} \rho_{\alpha} + 0.5c^2 \sum_{\alpha} G_{\alpha,\alpha} \psi_{\alpha}^2 + 0.5c^2 \sum_{\alpha \neq \bar{\alpha}} G_{\alpha,\bar{\alpha}} \varphi_{\alpha} \varphi_{\bar{\alpha}}. \quad (36)$$

A linear relationship between the pressure difference Δp and radius of curvature $1/r$ can be obtained for different κ values, as can be seen in Fig. 3, further proving the accuracy of

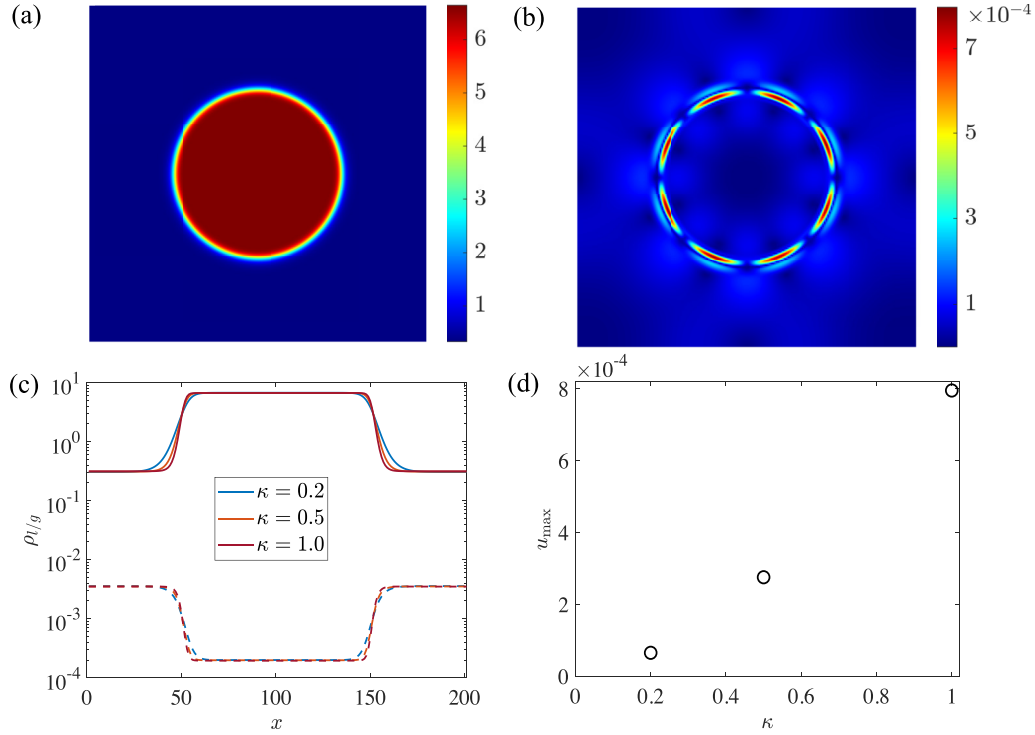


FIG. 2. (a) Density distribution of the liquid component at steady state and (b) contour plot of the spurious velocity. (c) Density distribution along the center line of the droplet at $\kappa = 0.2, 0.5$, and 1.0 and (d) the maximum spurious velocity under different κ values. The temperature T and κ are $T = 0.85T_c$ and $\kappa = 1$.

the present model. Through linear fitting, the surface tensions γ at $\kappa = 0.2, 0.5$, and 1.0 , namely the slopes of fitted lines, are $0.065, 0.087$, and 0.098 , respectively. These results indicate that the interfacial tension can be adjusted independently from the density ratio by simply changing the value of κ in the present model.

3. Contact angle

The present numerical framework is then extended to consider the wettability effects of the solid wall by employing the geometric formation approach [53]. To validate this method, a

droplet surrounded by the ideal gas on a flat surface with a prescribed contact angle ranging from 30° to 150° is simulated. The temperature and initial density are the same as in the Laplace test. The grid size is 200×100 with the initial radius of a semicircular droplet being 30 l.u.. The halfway bounce-back boundary condition is applied at the top and bottom walls and periodic boundary condition is imposed on the left and right boundaries. After the droplet reaches the steady state, the measured contact angles obtained from the numerical simulations are compared with the analytical solution, namely, the prescribed contact angle. As depicted in Fig. 4, the numerical

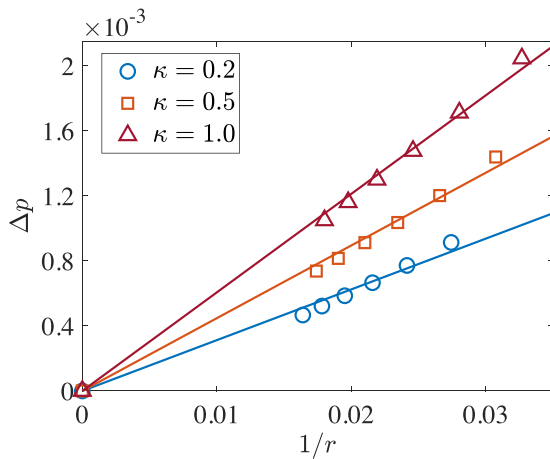


FIG. 3. Young Laplace fitting at $\kappa = 0.2, 0.5$, and 1.0 at $T = 0.85T_c$. The slope of each fitted line represents the surface tension γ .

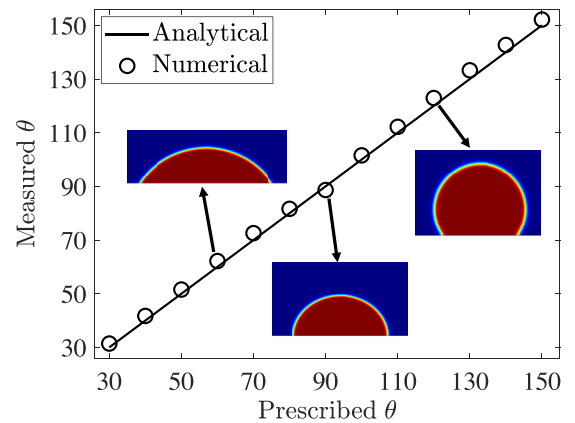


FIG. 4. Contact angle test by comparing the measured contact angle from the simulation with the prescribed contact angle. The insets show the droplet shapes at contact angle $\theta = 60^\circ, 90^\circ$ and 120° .

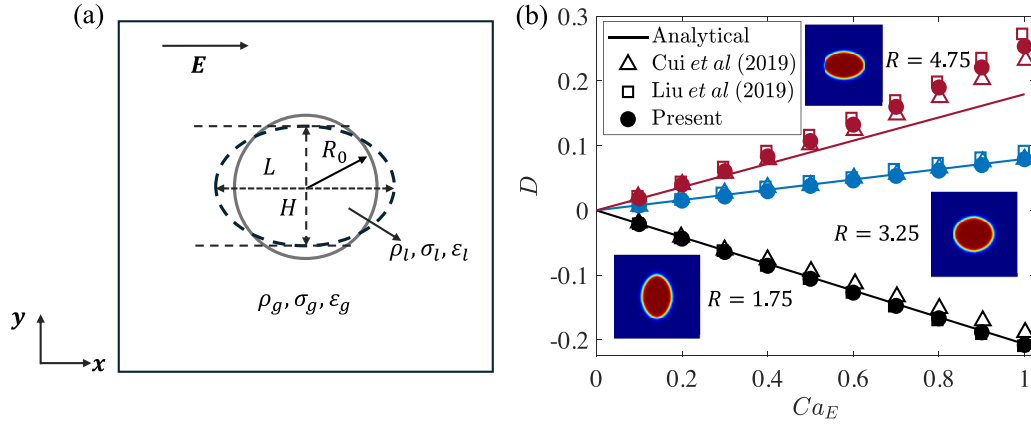


FIG. 5. (a) Configuration of the droplet deformation under an electric field. The droplet with solid lines represents the initial circular droplet, whereas the deformed droplet is denoted by the dashed line. (b) Comparison of the droplet deformation parameter D between the numerical results from the present model (solid circles) and the analytical solution (solid lines) and previous numerical studies (hollow triangles and squares) under different conductivity ratios R and electric field strength Ca_E .

results agree well with the analytical solutions with the biggest difference between them being 1.3%.

The above benchmark tests demonstrate that good thermodynamic consistency can be achieved under different κ values by adjusting the parameter ζ , and the interfacial tension can be adjusted independently by changing κ . Lastly, the geometric formulation approach is employed and validated to realize different contact angles. In summary, the present MCMP LBM is capable of simulating high-density ratio fluid flow problems with good accuracy.

B. Validation of leaky dielectric model

The coupling between the leaky dielectric model solved by the FDM and MCMP LBM is validated by simulating the deformation of a circular droplet with density ρ_l in a gravity-free field surrounded by another immiscible fluid component of density ρ_g under an electric field, as shown in Fig. 5(a). The temperature and density for each component used in this test are the same as in the Laplace test. Both the droplet and the surrounding components are considered leaky dielectric fluids with their corresponding conductivities σ_l and σ_g and permittivities ϵ_l and ϵ_g . Thus, two dimensionless parameters can be defined based on these electrical properties, i.e., conductivity ratio $R = \sigma_l/\sigma_g$ and permittivity ratio $Q = \epsilon_l/\epsilon_g$. Initially, a circular droplet with radius $R_0 = 25$ is suspended at the center of the computational domain of grid size 200×200 . A horizontal electric field E is applied with high electric potential U on the left boundary and zero potential on the right (Dirichlet boundary condition). The Neumann boundary condition is employed along the top and bottom boundaries of the electric field. The temperature and initial densities are chosen to be the same as in previous tests.

In the presence of an electric field, the droplet can be deformed into a prolate or oblate shape depending on the conductivity ratio R and permittivity ratio Q . The deformation is characterized by the deformation parameter D ,

$$D = \frac{L - H}{L + H}, \quad (37)$$

where L and H correspond to the lengths of the deformed droplet in the direction parallel and perpendicular to the applied electric field, respectively. Based on the theoretical work of the leaky dielectric droplet deformation conducted by Taylor [33], an improved analytical solution for the droplet deformation under an electric field is proposed as follows [59]:

$$D = \frac{Ca_E f_d(R, Q)}{3(1 + R)^2} \quad (38)$$

where $Ca_E = \sigma_g E^2 R_0 / \gamma$ is the electric capillary number defined as the ratio of the electric force to the surface tension. $f_d(R, Q) = R^2 + R + 1 - 3Q$ represents the discriminating function, which determines whether the droplet will deform into a prolate ($f_d > 0$) or an oblate shape ($f_d < 0$).

Simulations are conducted for three cases with different electrical properties, namely, $(R, Q) = (1.75, 3.5)$, $(R, Q) = (3.25, 3.5)$, and $(R, Q) = (4.75, 3.5)$ for Ca_E in the range of 0 to 1. After the droplet reaches the steady state, the droplet deformation obtained from the numerical simulations is compared with the analytical solution, i.e., Eq. (38). As shown in Fig. 5(b), both positive and negative deformations, which correspond to prolate and oblate shapes, can be simulated. Furthermore, for all the cases considered, the deformation increases monotonically with the increase of the electric field strength Ca_E . The numerical results show good agreement with the analytical solutions and previous numerical studies when the deformation is small ($D \approx 0.1$). However, the simulated results gradually depart from the analytical solutions for larger deformation, especially for the case $(R, Q) = (4.75, 3.5)$. This is because the analytical solution from Ref. [59] is only applicable to small droplet deformation. Similar phenomena were also observed by Cui *et al.* [60] and Liu *et al.* [61], as denoted by the hollow triangles and squares in Fig. 5(b).

Figure 6 depicts the distributions of the electric potential, electric charge, and electrical force distributions, which demonstrate the capability of the present model for accurately capturing these microscopic variables.

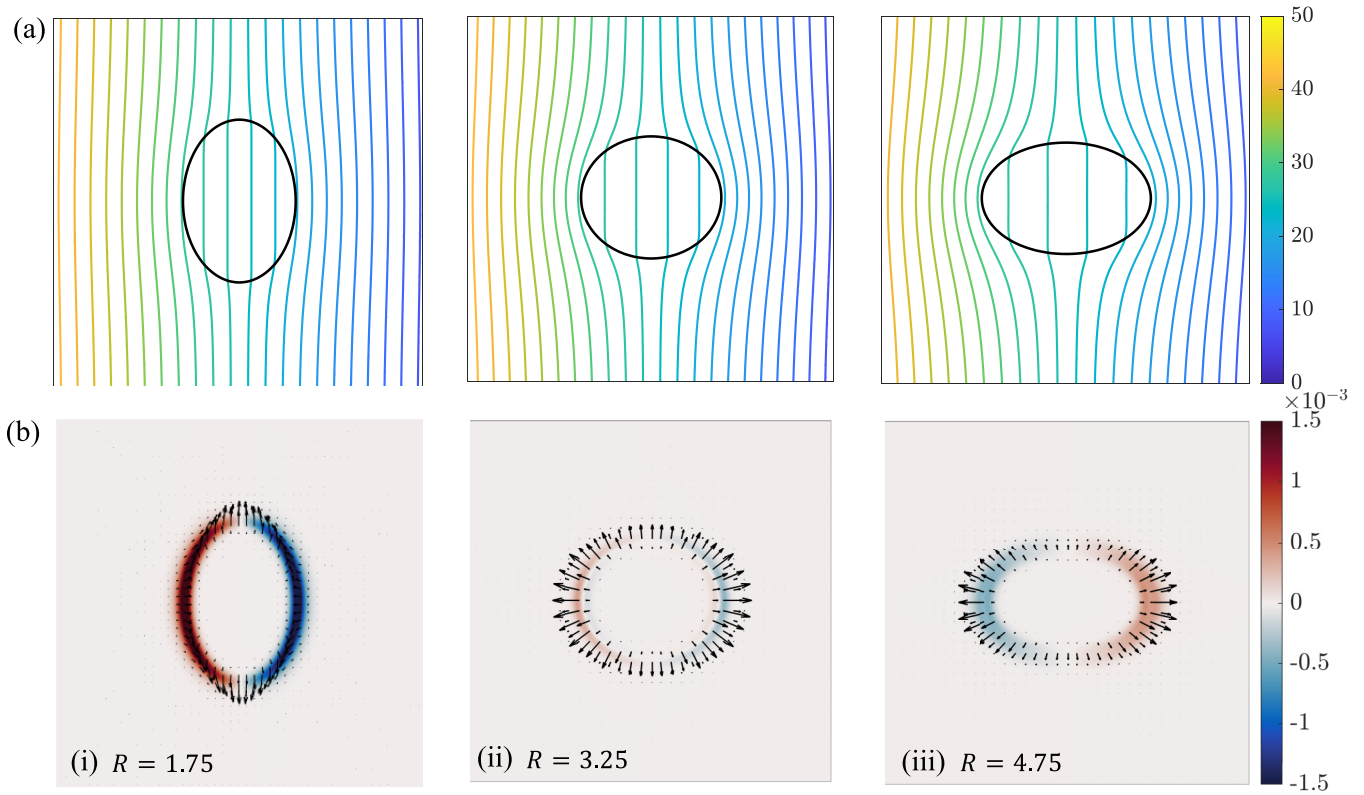


FIG. 6. The distribution of (a) the electric potential, (b) the electric charge, and electrical force, as indicated by the contour and black arrows for (i) $(R, Q) = (1.75, 3.5)$, (ii) $(R, Q) = (3.25, 3.5)$, and (iii) $(R, Q) = (4.75, 3.5)$. The electric field strength Ca_E is 0.8.

C. Application

The validated numerical framework is then applied to investigate the behaviors of a sessile water droplet surrounded by air under an electric field in a coplanar configuration, as depicted in Fig. 7. Manipulating droplets on surfaces is of great importance in various applications, such as medical diagnostics and microelectronics [62]. Extensive studies have been conducted on investigating droplet wetting behaviors in an open needle-electrode configuration (electrowetting) [25,63–66], where a needle inserted into the droplet acts as one electrode and the dielectric substrate serves as another electrode. In these works, the droplet is considered a perfect conductor, and the surrounding phase is a dielectric fluid. However, realistically, most fluids have finite conductivity, as Taylor *et al.* [33] discovered, known as leaky dielectrics. This

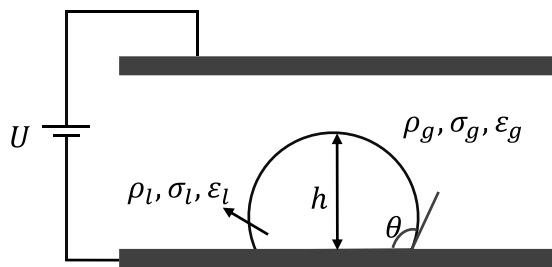


FIG. 7. Problem configuration. A sessile water droplet with $\rho_l, \sigma_l, \epsilon_l$ is surrounded by air with $\rho_g, \sigma_g, \epsilon_g$ under an electric field with high electric potential on the top and zero potential on the bottom.

leaky dielectric model was later validated experimentally by other researchers [35,67], highlighting its broader range of applicability. Further, it has been found that the contact angle saturates at high voltages, which has been a major challenge in electrowetting. Another electrode configuration for manipulating the droplet is the coplanar configuration. However, very few studies have focused on the numerical modeling of droplet deformation under a constant (dc) electric potential for this configuration [68]. Therefore, in the following, the deformation of a sessile water droplet sitting on a solid surface and surrounded by air is investigated in the coplanar

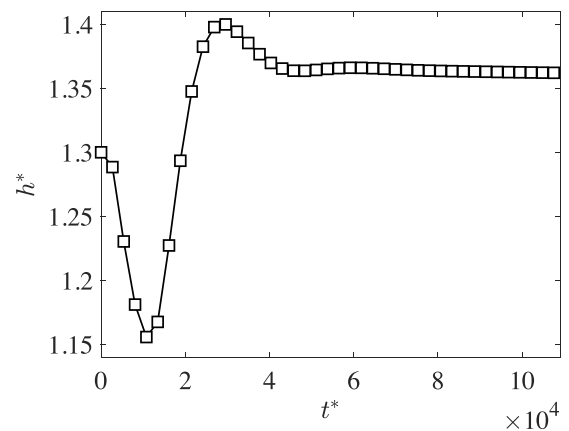


FIG. 8. The temporal variations of the dimensionless droplet height h^* at $R = 10$, $Q = 10$, and $Ca_E = 0.9$.

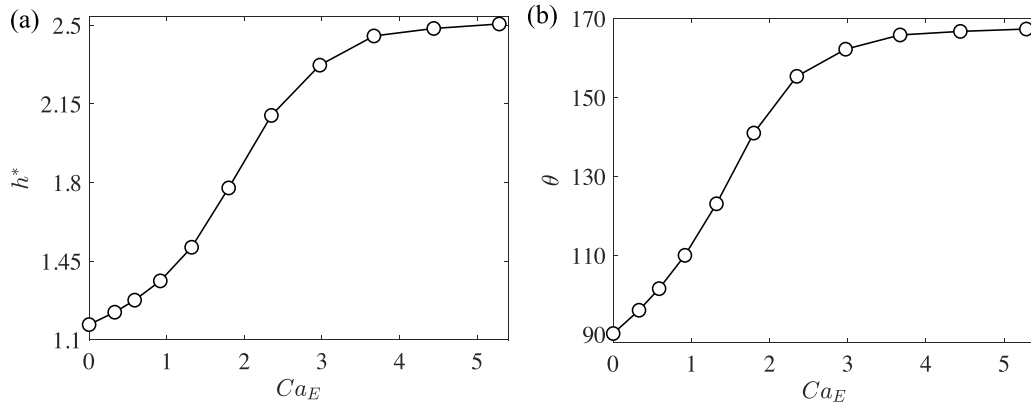


FIG. 9. The variations of (a) dimensionless droplet height h^* and (b) contact angle θ , with the electric capillary number Ca_E . The conductivity and permittivity ratios are $R = 10$ and $Q = 10$.

configuration using the hybrid numerical framework. Both the droplet and air are considered to be leaky dielectric fluids. The temperature and density for each component are the same as in previous benchmarks. The dimensionless droplet height $h^* = h/R_0$ and contact angle θ are used to characterize the droplet behaviors under an electric field. For the water-air system considered in this work, the conductivity and permittivity ratios are $R \approx 10^{10}$ and $Q \approx 10^{-8}$. However, due to the numerical instability of the numerical model for fluids having large contrasts in electrical properties, both the conductivity and permittivity ratios for the water-air system are taken to be $R = Q = 10$ [69], which has similar electrohydrodynamic behaviors as that of large ratios. This is because the normal and tangential electric stress at the droplet interface for the case of an immiscible droplet suspended in another liquid can be expressed as

$$\mathbf{F}_{E,r} = \frac{9E_0^2\epsilon_g}{8\pi(2+R)^2}[Q-1+(R^2+1-2Q)\cos^2\theta], \quad (39)$$

$$\mathbf{F}_{E,\theta} = -\frac{9E_0^2\epsilon_g}{4\pi(2+R)^2}(R-Q)\cos\theta\sin\theta, \quad (40)$$

where E_0 is the electric field strength and the subscript g means the surrounding phase. As indicated in Eq. (40), it is obvious that the tangential electric stress $\mathbf{F}_{E,\theta}$ is negligible when $R \gg 1$. In this case, the deformation of the droplet is

only due to the normal electric stress $\mathbf{F}_{E,r}$. The same condition can be obtained when $R = Q$, in which Eq. (40) becomes zero. Furthermore, Eq. (39) clearly shows that the magnitude of normal electric stress at $R = 10$ and $Q = 10$ is similar to that with large conductivity and permittivity contrast. This is due to the fact that, when $R = 10$ or greater, the normal stress $\mathbf{F}_{E,r}$ on the dispersed phase approaches the asymptotic limit as $R \gg 1$. Based on the above analysis, $R = Q = 10$ will be chosen to represent the electrical properties in the water-air system.

The temporal variation of the dimensionless centerline height of the droplet h^* at a given electric capillary number $Ca_E = 0.9$ is first presented to show the transient droplet evolution in the presence of an electric field. The droplet is assumed to be neutral with a contact angle of 90° . The electric field starts to take effect when the contact angle becomes 90° , which corresponds to the lowest point in Fig. 8. In the presence of an electric field, h^* first reaches the maximum value within a relatively short period of time and starts to oscillate due to the competition between the surface tension and electric force, after which the droplet achieves the equilibrium state. The increased dimensionless height h^* means that the electric field stretches the droplet in the vertical direction, reducing its wettability on the surface.

We then investigate the effects of the electric field strength on the droplet deformation at the steady state. As shown in

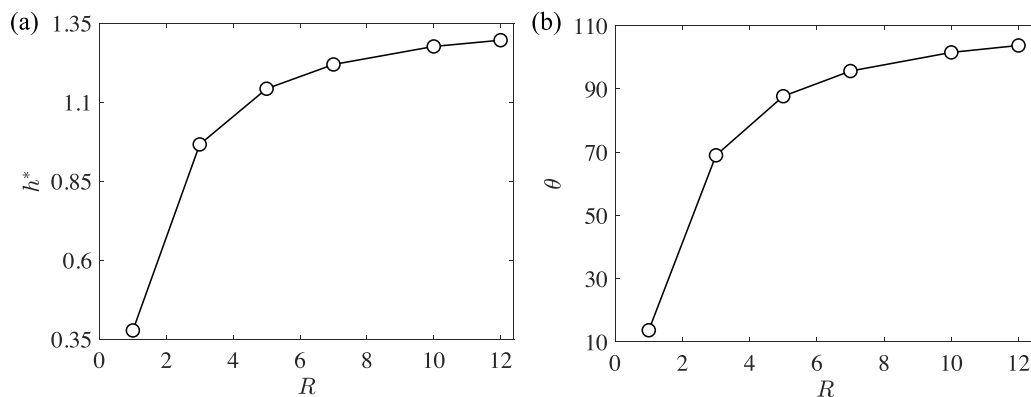


FIG. 10. The variations of (a) dimensionless droplet height h^* and (b) contact angle θ , with the conductivity ratio R . The permittivity ratio and electric capillary number are $Q = 10$ and $Ca_E = 0.6$, respectively.

Fig. 9, both the dimensionless height h^* and contact angle θ increase with the electric capillary number Ca_E , indicating the enhanced dewetting effects. However, this increase becomes less pronounced when $Ca_E > 3.7$ and the droplet deformation reaches the saturation regime. This is due to the competing effects between the increased surface tension force resulting from the large deformation and the electrical force. With the further increase of the electric field strength, the droplet will detach from the bottom electrode, which is not the scope of the current study.

Furthermore, the effects of the conductivity ratio R on the dimensionless droplet height h^* and contact angle θ are studied for a constant $Q = 10$ at $Ca_E = 0.6$. As shown in Fig. 10, completely different droplet behaviors can be observed under different R values. When $R = 5$, namely, the green point in Fig. 10(b), the contact angle $\theta \approx 90^\circ$, which means that the external electric field imposes no effects on the droplet due to the counterbalance between the normal component of the electrical force and surface tension force [33,70]. For $R < 5$, the dimensionless height h^* decreases under the influence of the electric field, resulting in increased droplet spreading along the surface and a corresponding reduction in the contact angle θ . In contrast, the applied electric field tends to pull the droplet upward, resulting in reduced wettability for $R > 5$.

Lastly, extensive and systematic simulations are conducted across a wide range of conductivity ratios R and permittivity ratios Q . A $R - Q$ phase diagram is established based on the results to characterize the distinct droplet deformation behaviors under an electric field. Overall, it has been found that three distinct modes, namely, wetting, neutral (no effects), and dewetting, can occur depending on the values of R and Q . The solid black line in Fig. 11 represents the analytical solutions where the electric field has no effect on droplet deformation, corresponding to the condition where the discrimination function $f_d = 0$ [33]. The numerical results show good agreement with this analytical solution, as evidenced by the two points lying on the solid black line in Fig. 11. These two points correspond to $(R, Q) = (1, 1)$ and $(5, 10)$ with the contact angles θ being 90.2° and 89.6° , respectively. Deviating from this line, the droplets exhibit entirely different behaviors under the influence of electric fields, with wetting occurring on the top left and dewetting on the bottom right regions of Fig. 11, respectively. Furthermore, the values of the contact angle for different R and Q are represented by the color bar. It can be observed that the closer a data point is to the black line, the weaker the electric field's effect on the droplet. This work has also found that changing the direction of the electric field from vertical to horizontal reverses the trend in droplet deformation. This occurs because the direction of the electrical force changes accordingly when the orientation of the applied electric field is altered. However, this also indicates that various droplet behaviors can be achieved by simply modifying the electrode configuration.

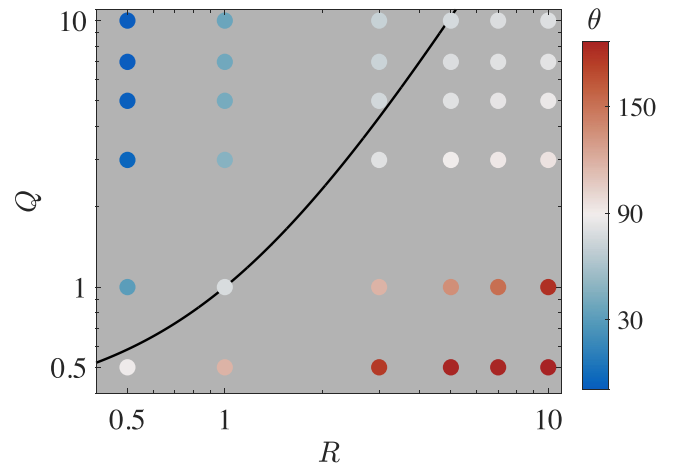


FIG. 11. R - Q phase diagram for the droplet wetting behaviors with the color bar representing the contact angle values θ . The solid black line represents the analytical solution, where the applied electric field does not affect the droplet deformation.

V. CONCLUSION

In this work, a hybrid LBM and FDM numerical framework for simulating MCMP electrohydrodynamic phenomena with high-density contrast was proposed and validated. The results highlight the model's capability to achieve high-density ratios, maintain good thermodynamic consistency, adjust surface tension, and accurately capture the microscopic effects of the electric field. Subsequently, the deformation of a water droplet suspended in air under the influence of an electric field was investigated in a coplanar configuration. The results reveal a dewetting effect induced by the electric field in this fluid system, which becomes more pronounced as the electric field strength increases. Moreover, it was demonstrated that both wetting and dewetting effects can occur at different values of R at $Q = 10$. Therefore, a phase diagram based on extensive simulations was constructed in the $R - Q$ space, with the corresponding contact angles represented by the color bar. This diagram reveals three distinct modes of droplet deformation, determined by the varying values of R and Q , providing a valuable guide for controlling droplet behavior in electrohydrodynamic applications.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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