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2018

Zhang, L., Yang, S., Zeng, Z., & Chew, J. W. (2018). Consistent second-order boundary implementations for convection-diffusion lattice Boltzmann method. *Physical Review E*, 97(2), 23302-.

<https://hdl.handle.net/10356/85187>

<https://doi.org/10.1103/PhysRevE.97.023302>

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Consistent second-order boundary implementations for convection-diffusion lattice Boltzmann method

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(Received 7 August 2017; revised manuscript received 21 December 2017; published 8 February 2018)

In this study, an alternative second-order boundary scheme is proposed under the framework of the convection-diffusion lattice Boltzmann (LB) method for both straight and curved geometries. With the proposed scheme, boundary implementations are developed for the Dirichlet, Neumann and linear Robin conditions in a consistent way. The Chapman-Enskog analysis and the Hermite polynomial expansion technique are first applied to derive the explicit expression for the general distribution function with second-order accuracy. Then, the macroscopic variables involved in the expression for the distribution function is determined by the prescribed macroscopic constraints and the known distribution functions after streaming [see the paragraph after Eq. (29) for the discussions of the “streaming step” in LB method]. After that, the unknown distribution functions are obtained from the derived macroscopic information at the boundary nodes. For straight boundaries, boundary nodes are directly placed at the physical boundary surface, and the present scheme is applied directly. When extending the present scheme to curved geometries, a local curvilinear coordinate system and first-order Taylor expansion are introduced to relate the macroscopic variables at the boundary nodes to the physical constraints at the curved boundary surface. In essence, the unknown distribution functions at the boundary node are derived from the known distribution functions at the same node in accordance with the macroscopic boundary conditions at the surface. Therefore, the advantages of the present boundary implementations are (i) the locality, i.e., no information from neighboring fluid nodes is required; (ii) the consistency, i.e., the physical boundary constraints are directly applied when determining the macroscopic variables at the boundary nodes, thus the three kinds of conditions are realized in a consistent way. It should be noted that the present focus is on two-dimensional cases, and theoretical derivations as well as the numerical validations are performed in the framework of the two-dimensional five-velocity lattice model.

DOI: [10.1103/PhysRevE.97.023302](https://doi.org/10.1103/PhysRevE.97.023302)

I. INTRODUCTION

As a convenient alternative for the traditional computational fluid dynamics (CFD) method, the lattice Boltzmann (LB) method has achieved widespread applications for hydrodynamic systems, such as the multiphase flows [1–6], porous media flows [7–11], and nonequilibrium gas flows [12–19]. Many efforts have been devoted to extending the LB method to include heat and mass transfer, and correspondingly LB models for the convection-diffusion equation (CDE) were developed [20–32]. Under the framework of the standard LB method, the internal energy model [31] and the total energy model [30] were successively proposed as thermal LB models by introducing additional sets of distribution functions coupled with the hydrodynamic distribution functions. Subsequently, the temperature distribution function or concentration distribution function was directly defined for recovering the macroscopic CDE [21–24,26,28], and additional modifications were then

implemented to remove the deviation term in the recovered macroscopic equation [21,22]. Furthermore, CDE LB models were also proposed for nonlinear CDE [23,26] and anisotropic diffusion [21,24,32,33] processes, and thus the applications of the LB method in heat and mass transfer systems are significantly extended.

In addition to the CDE coupled with the Navier-Stokes (NS) equation, boundary conditions are necessary for completing the mathematical description of a system involving heat and mass transfer. In particular, complicated boundary conditions are widely encountered in heat and mass transfer systems, such as the Neumann condition at the adiabatic boundary [34] and conjugate interfaces [35–41], the linear and nonlinear Robin conditions for surface reactions [42,43], adsorption kinetics [44], and radiative heat transfer process [45]. Therefore, boundary implementations in accordance with the macroscopic boundary constraints are crucially important for the accuracy and efficiency of the CDE LB simulations. It should be noted that some hydrodynamic LB boundary schemes have been effectively applied to the temperature and concentration boundary conditions: the thermal boundary scheme by

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He *et al.* [31] was developed based on the bounce-back rule of the nonequilibrium distribution functions by He *et al.* [46]; the nonequilibrium extrapolation scheme by Guo [47,48] was also extended to CDE LB simulations [49]; following the idea of the regularized scheme [50], a regularized CDE boundary scheme was developed by Huang *et al.* [49]; the “multireflection” approach by Ginzburg [51] was also extended to the Dirichlet and Neumann condition for CDE [52]; the classical halfway bounce-back scheme by Ladd for particulate flows [53,54] was also applied for temperature and concentration boundary conditions by Zhang *et al.* [55,56], and then improved by Chen *et al.* [57] with a midpoint bounce-back scheme. The above-mentioned bounce-back rule based boundary schemes were built for the Dirichlet condition, and the implementations of the Neumann and Robin conditions were realized by reducing the boundary constraints to the Dirichlet condition with an additional finite difference approximation of the normal derivative [55–57]. Besides, the halfway bounce-back scheme was alternatively applied to Dirichlet and Neumann conditions by Yoshida *et al.* [24] with their proposed multiple-relaxation-time (MRT) CDE LB model, and the normal derivative at the discrete lattice velocity direction was directly applied to determine the unknown distribution functions at the boundary nodes. Although asymptotic analysis demonstrated that their boundary implementations were second-order accurate, their implementation of the Neumann condition at a curved boundary led to considerable discrepancies which were then removed by a modified scheme. Furthermore, based on the halfway bounce-back rule by Yoshida *et al.* [24] and the interpolation of the distribution functions at the neighboring fluid nodes, second-order accurate boundary schemes were proposed for the Dirichlet and Neumann conditions on straight boundaries by Li *et al.* [58]. The proposed Dirichlet boundary scheme was directly applicable to curved geometries, but the extension of the Neumann boundary scheme to curved boundaries required determining the projection of the normal derivative at the discrete lattice velocity directions by a Cartesian decomposition method (CDM) in which complicated interpolation involving distribution functions from four neighboring nodes was introduced. It was indicated by Li *et al.* [58] that (i) the second-order accuracy of their Dirichlet boundary scheme was confirmed by the numerical validations for both straight and curved geometries; (ii) the curved Neumann boundary scheme was first-order accurate in the numerical tests; (iii) implementation of the Robin condition was carried out by reducing the mixed condition to the Neumann constraints. Recently, a single-node boundary scheme for the general Robin condition was proposed by Huang *et al.* [59], and the unknown distribution functions were represented as a linear combination of the known postcollision distribution functions at the same node. Numerical validations demonstrated that the Huang *et al.* scheme [59] was second-order accurate for straight boundaries but only first-order accurate for curved geometries. In order to further improve the accuracy of the curved boundary treatments, Huang *et al.* developed a second-order curved boundary scheme [60] by deriving second-order approximation of the boundary value and its normal derivative at the computational boundary nodes, and thus a second-order bounce-back scheme was obtained. It was noted that the derivations of the normal derivative for the Neumann

condition requires the finite difference approximation for the second-order derivatives, and macroscopic information at a previous time step was also introduced. Besides, similar to the scheme by Li *et al.* [58], the second-order implementation of the Robin condition with the Huang *et al.* scheme [60] was also indirect in that the Robin condition had to be first reduced to the Neumann condition.

Additionally, there are some other boundary schemes derived directly for the CDE LB method that do not have hydrodynamic counterparts, such as the Robin scheme based on the moment equations for linear heterogeneous surface reaction [42], the mass conservative scheme by Gebäck *et al.* [61], and the direct extrapolation scheme for the Neumann condition with zero flux by Huang *et al.* [49]. Conclusions are drawn from the existing CDE LB boundary schemes that the second-order accurate implementation for the Dirichlet condition is relatively easy to be realized for both straight and curved boundaries, and the single-node scheme by Huang *et al.* [59] and the local scheme by Meng *et al.* [42] also provide efficient second-order Robin condition treatments at straight boundaries. However, second-order Neumann and Robin condition schemes for curved geometries are not easy to implement since the second-order bounce-back scheme by Huang *et al.* [60] requires macroscopic information from four neighboring nodes and the finite difference approximation for second-order derivatives is introduced. Moreover, the implementation of the Robin condition by the Huang *et al.* scheme [60] is always indirect since the Robin condition is first transformed into the Neumann condition by introducing an approximated temperature or concentration value. Therefore, second-order boundary schemes, applicable for Dirichlet, Neumann, and Robin conditions at both straight and curved boundaries with simple and efficient implementations, are still highly desired.

Moreover, as alternative implementations of the hydrodynamic boundary conditions, boundary schemes were proposed based on the explicit expression of the distribution functions derived from the Chapman-Enskog (CE) analysis [50,62–65]. A local second-order boundary method (LSOBM) for the LB FCHC model was proposed by Ginzbourg and D’Humières for arbitrarily inclined flat walls, in which the second-order CE analysis was applied to derive the distribution function expression and also second-order Taylor expansions were adopted to transfer the macroscopic information at the boundary surface to the computational boundary nodes [62]. Therefore, the LSOBM was actually third-order accurate since all the truncation terms resulting from the theoretical derivations were third order. Despite the rigorous theoretical treatment, the LSOBM did not attract much attention due to its cumbersome formulas. Subsequently, as a direct extension of the LSOBM, a second-order curved boundary scheme for the nonslip velocity condition was developed in our recent work by degrading the accuracy from third order to second order with first-order CE and Taylor expansions, and thus the practical implementations were greatly simplified [65]. In this work, the idea of the our second-order curved boundary scheme is first applied to the CDE LB method with the Bhatnagar-Gross-Krook (BGK) collision model [66], and then the extension of the proposed boundary scheme for the MRT LB method [24,67] is carried out in the Appendix. Based on the explicit expression of the distribution function derived from the

CE analysis and the Hermite expansions technique [68,69], a second-order boundary scheme is proposed for consistent and local implementations of the Dirichlet, Neumann, and linear Robin conditions for both straight and curved boundaries. The macroscopic constraints are directly introduced to the expression of the distribution functions at the boundary nodes for the straight boundary, and then all the macroscopic information necessary for the distribution function is determined by the known distribution functions at the same nodes. After that, the unknown distribution functions are obtained by the macroscopic information at the boundary nodes, and the present boundary implementations are local and consistent for all the three kinds of macroscopic boundary conditions. Furthermore, by applying the local curvilinear coordinate system, the present scheme is extended to the curved boundaries by preserving its locality and consistency and without affecting the overall accuracy. Numerical validations of the proposed boundary implementations are performed for five test cases, and the second-order accuracy of the present boundary scheme for various boundary conditions is confirmed. Note that only two-dimensional (2D) cases are considered in this work, and both the theoretical derivations and the numerical validations are performed based on the 2D five-velocity (D2Q5) lattice model.

II. FORMULATIONS

In this part, the theoretical basis of the present boundary scheme for the CDE LB method with BGK collision model is described, and the extended application for the MRT LB method is given in the Appendix. The CE analysis and the Hermite expansion technique are first applied to derive the expression of the distribution function, then the boundary implementations of Dirichlet, Neumann, and linear Robin conditions are introduced for both straight and curved geometries. The second-order accuracy of the present boundary scheme is well demonstrated by the theoretical derivations.

A. CDE LB model with BGK collision model

For simplicity, the present boundary scheme is developed under the framework of the D2Q5 CDE LB model with BGK collision operator [66], with the LB equation given as

$$f_\alpha(\mathbf{x} + \boldsymbol{\xi}_\alpha \delta t, t + \delta t) - f_\alpha(\mathbf{x}, t) = -\frac{1}{\tau}(f_\alpha - f_\alpha^{(eq)}), \quad (1)$$

where $f_\alpha(\mathbf{x}, t)$ and $f_\alpha^{(eq)}(\mathbf{x}, t)$ are respectively the distribution function and its equilibrium form at the position $\mathbf{x}$ and time t for the macroscopic scalar ϕ (temperature, concentration, etc.). $\boldsymbol{\xi}_\alpha$ is the discrete lattice velocity of the D2Q5 lattice model with the following definition:

$$\boldsymbol{\xi}_\alpha = \begin{cases} (0, 0) & \alpha = 0 \\ c(\cos[(\alpha - 1)\pi/2], \sin[(\alpha - 1)\pi/2]) & \alpha = 1, 2, 3, 4 \end{cases}, \quad (2)$$

where c is the lattice speed and relates to the discrete spatial step δx and the time step δt as $c = \delta x / \delta t$, and $w_0 = 1/3$, $w_{1,2,3,4} = 1/6$ are the weight coefficients prescribed in the D2Q5 lattice

model. Besides, τ is the single relaxation parameter for the BGK collision operator, and relates to the diffusion coefficient D as follows, which will be used in the macroscopic equation in Eq. (17):

$$D = \left(\tau - \frac{1}{2}\right)RT'\delta t. \quad (3)$$

Additionally, the equilibrium distribution function $f_\alpha^{(eq)}$ is determined as

$$f_\alpha^{(eq)} = \phi w_\alpha \left(1 + \frac{\mathbf{u} \cdot \boldsymbol{\xi}_\alpha}{RT'}\right), \quad (4)$$

with $\mathbf{u}$ the fluid velocity, R and T' the ideal gas constant and reference temperature, respectively, and $RT' = 1/3$. Last, the present D2Q5 BGK model is completed by the following computing formula for the macroscopic scalar ϕ :

$$\phi = \sum_\alpha f_\alpha. \quad (5)$$

Besides, a local calculation of the scalar gradients is obtained in the literature [24,60] as

$$\nabla \phi = \frac{3}{\tau} \left(\frac{\delta t}{\delta x^2} \mathbf{u} \phi - \frac{1}{\delta x} \sum_\alpha f_\alpha \boldsymbol{\xi}_\alpha \right). \quad (6)$$

B. Expression of the distribution function f_α

The CE expansion analysis is first introduced with the expansion parameter ε ,

$$\frac{\partial}{\partial t} = \varepsilon \frac{\partial}{\partial t_0} + \varepsilon^2 \frac{\partial}{\partial t_1} + O(\varepsilon^3), \quad (7a)$$

$$\frac{\partial}{\partial \mathbf{x}} = \varepsilon \frac{\partial}{\partial \mathbf{x}_0} + O(\varepsilon^2), \quad (7b)$$

$$f_\alpha = f_\alpha^{(0)} + \varepsilon f_\alpha^{(1)} + \varepsilon^2 f_\alpha^{(2)} + O(\varepsilon^3). \quad (7c)$$

Then, the second-order Taylor expansion of Eq. (1) is obtained:

$$\begin{aligned} \delta t \left(\frac{\partial}{\partial t} + \xi_{\alpha i} \frac{\partial}{\partial x_i} \right) f_\alpha + \frac{\delta t^2}{2} \left(\frac{\partial}{\partial t} + \xi_{\alpha i} \frac{\partial}{\partial x_i} \right)^2 f_\alpha + O(\delta t^3) \\ = -\frac{1}{\tau} (f_\alpha - f_\alpha^{(eq)}). \end{aligned} \quad (8)$$

Substituting the expansions in Eq. (7) into Eq. (8) leads to

$$\varepsilon^0 : f_\alpha^{(0)} = f_\alpha^{(eq)}, \quad (9a)$$

$$\varepsilon^1 : \left(\frac{\partial}{\partial t_0} + \xi_{\alpha i} \frac{\partial}{\partial x_{0i}} \right) f_\alpha^{(0)} = -\frac{1}{\tau \delta t} f_\alpha^{(1)}, \quad (9b)$$

$$\varepsilon^2 : \frac{\partial}{\partial t_1} f_\alpha^{(0)} + \left(1 - \frac{1}{2\tau}\right) \left(\frac{\partial}{\partial t_0} + \xi_{\alpha i} \frac{\partial}{\partial x_{0i}} \right) f_\alpha^{(1)} = -\frac{1}{\tau \delta t} f_\alpha^{(2)}. \quad (9c)$$

Moments of Eq. (9) are obtained as

$$\frac{\partial}{\partial t_0} \sum_{\alpha} f_{\alpha}^{(0)} + \frac{\partial}{\partial x_{0j}} \sum_{\alpha} f_{\alpha}^{(0)} \xi_{\alpha j} = 0, \quad (10a)$$

$$\frac{\partial}{\partial t_0} \sum_{\alpha} f_{\alpha}^{(0)} \xi_{\alpha i} + \frac{\partial}{\partial x_{0j}} \sum_{\alpha} f_{\alpha}^{(0)} \xi_{\alpha i} \xi_{\alpha j} = -\frac{1}{\tau \delta t} \sum_{\alpha} f_{\alpha}^{(1)} \xi_{\alpha i}, \quad (10b)$$

$$\frac{\partial}{\partial t_1} \sum_{\alpha} f_{\alpha}^{(0)} + \left(1 - \frac{1}{2\tau}\right) \frac{\partial}{\partial x_{0j}} \sum_{\alpha} f_{\alpha}^{(1)} \xi_{\alpha j} = 0. \quad (10c)$$

Applying the given moments of $f_{\alpha}^{(eq)}$

$$\begin{aligned} \sum_{\alpha} f_{\alpha}^{(0)} &= \phi, \quad \sum_{\alpha} f_{\alpha}^{(0)} \xi_{\alpha j} = \phi u_j, \\ \sum_{\alpha} f_{\alpha}^{(0)} \xi_{\alpha i} \xi_{\alpha j} &= \phi RT' \delta_{ij}, \end{aligned} \quad (11)$$

the macroscopic equations at various scales are derived from Eqs. (10),

$$\frac{\partial}{\partial t_0} \phi + \frac{\partial}{\partial x_{0j}} (\phi u_j) = 0, \quad (12a)$$

$$\frac{\partial}{\partial t_0} (\phi u_i) + \frac{\partial}{\partial x_{0j}} (\phi RT' \delta_{ij}) = -\frac{1}{\tau \delta t} \sum_{\alpha} f_{\alpha}^{(1)} \xi_{\alpha i}, \quad (12b)$$

$$\frac{\partial}{\partial t_1} \phi + \left(1 - \frac{1}{2\tau}\right) \frac{\partial}{\partial x_{0j}} \sum_{\alpha} f_{\alpha}^{(1)} \xi_{\alpha j} = 0, \quad (12c)$$

and the first-order moment of $f_{\alpha}^{(1)}$ is obtained from Eq. (12b),

$$\sum_{\alpha} f_{\alpha}^{(1)} \xi_{\alpha i} = -\tau \delta t \left(RT' \frac{\partial \phi}{\partial x_{0i}} + \frac{\partial}{\partial t_0} (\phi u_i) \right), \quad (13)$$

where the second term in Eq. (13) is viewed as the error term and would lead to incorrect macroscopic CDE. Hence, excluding the effects from the external force term, the error term is further expressed as follows:

$$\frac{\partial}{\partial t_0} (\phi u_i) = \phi \frac{\partial u_i}{\partial t_0} + u_i \frac{\partial \phi}{\partial t_0}, \quad (14)$$

where $\frac{\partial u_i}{\partial t_0}$ is obtained from the CE analysis for the standard hydrodynamic LB model [70–72], while $\frac{\partial \phi}{\partial t_0}$ is directly derived from Eq. (12a), thus Eq. (14) is further transformed as

$$\frac{\partial}{\partial t_0} (\phi u_i) = -\phi \frac{\partial}{\partial x_{0j}} (u_i u_j + p \delta_{ij}) - u_i \frac{\partial}{\partial x_{0j}} (\phi u_j), \quad (15)$$

which demonstrates that the error term $-\tau \delta t \frac{\partial}{\partial t_0} (\phi u_i)$ in Eq. (13) is of the order $O(\delta t Ma^2)$, where Ma is the Mach number, which can be neglected for low Ma flows. Therefore, without affecting the overall accuracy of the present analysis, Eq. (13) is simplified as

$$\sum_{\alpha} f_{\alpha}^{(1)} \xi_{\alpha i} = -\tau \delta t RT' \frac{\partial \phi}{\partial x_{0i}}, \quad (16)$$

and then the macroscopic equation recovered from the present CDE LB model is obtained,

$$\frac{\partial}{\partial t} \phi + \frac{\partial}{\partial x_j} (\phi u_j) = \frac{\partial}{\partial x_j} \left(D \frac{\partial \phi}{\partial x_j} \right), \quad (17)$$

with D the diffusion coefficient defined in Eq. (3).

After that, the expression of the distribution function f_{α} is derived from the results obtained from the above CE analysis in Eq. (16), i.e., the first-order moment of the nonequilibrium part of f_{α} ,

$$\sum_{\alpha} f_{\alpha}^{(neq)} \xi_{\alpha i} = -\tau \delta t RT' \frac{\partial \phi}{\partial x_i}, \quad (18)$$

with $f_{\alpha}^{(neq)} = f_{\alpha} - f_{\alpha}^{(eq)} = \varepsilon f_{\alpha}^{(1)} + O(\varepsilon^2)$ denoting the nonequilibrium part of the distribution function, and Eq. (18) is second-order accurate since the higher order terms $\varepsilon^2 f_{\alpha}^{(2)}$ are neglected. Thus, the moments of the distribution function f_{α} necessary for recovering the accurate macroscopic equation in Eq. (17) are obtained:

$$\sum_{\alpha} f_{\alpha} = \phi, \quad \sum_{\alpha} f_{\alpha} \xi_{\alpha i} = \phi u_i - \tau \delta t RT' \frac{\partial \phi}{\partial x_i}. \quad (19)$$

Subsequently, the Hermite expansion technique is applied to derive the expressions of f_{α} from the moment constraints in Eq. (19). The dimensionless distribution function $\hat{f}$ and particle velocity $\hat{\xi}$ are defined as

$$\hat{f} = \frac{RT'}{\rho_0} f, \quad \hat{\xi} = \xi / \sqrt{RT'}, \quad (20)$$

with $\rho_0 = 1$ as the constant density. The leading order Hermite tensorial polynomials $H_i^{(n)}(\hat{\xi})$ are provided as

$$H^{(0)}(\hat{\xi}) = 1, \quad (21a)$$

$$H_i^{(1)}(\hat{\xi}) = \hat{\xi}_i. \quad (21b)$$

The dimensionless equilibrium distribution function $\hat{f}$ is expanded as

$$\hat{f}(\hat{\xi}, \mathbf{x}, t) = \omega(\hat{\xi}) \sum_{n=0}^{\infty} \frac{1}{n!} a_i^{(n)}(\mathbf{x}, t) H_i^{(n)}(\hat{\xi}), \quad (22)$$

where $\omega(\hat{\xi}) = \frac{1}{2\pi} e^{-\hat{\xi}^2/2}$ is the weight function and the expansion coefficient $a_i^{(n)}(\mathbf{x}, t)$ determined as

$$a_i^{(n)}(\mathbf{x}, t) = \int \hat{f} H_i^{(n)}(\hat{\xi}) d\hat{\xi} = \frac{1}{\rho_0} \int f H_i^{(n)}(\hat{\xi}) d\hat{\xi}, \quad (23)$$

and the continuous expression of the distribution function f is then obtained by applying the moments in Eq. (19),

$$a^{(0)} = \phi, \quad a_i^{(1)} = \frac{1}{\sqrt{RT'}} \left(\phi u_i - \tau \delta t RT' \frac{\partial \phi}{\partial x_i} \right), \quad (24)$$

$$f(\xi, \mathbf{x}, t) = \frac{1}{2\pi RT'} e^{-\xi^2/2RT'} \left(\phi + \phi \frac{\xi_i u_i}{RT'} - \tau \delta t \frac{\partial \phi}{\partial x_i} \xi_i \right). \quad (25)$$

Equation (25) is then discretized in the phase space by the D2Q5 lattice model following the work by He and Luo [73],

$$f_\alpha(\mathbf{x}, t) = w_\alpha \left(\phi + \phi \frac{\xi_{\alpha i} u_i}{RT'} - \tau \delta t \frac{\partial \phi}{\partial x_i} \xi_{\alpha i} \right), \quad (26)$$

which is the basis of the present boundary implementations.

C. Present boundary scheme for straight boundaries

For the straight boundary treatments, the physical boundary surface, on which the macroscopic constraints are prescribed, is placed directly on the last layer of the lattice nodes. And the macroscopic information necessary for the determination of f_α in Eq. (26) is

$$\phi, \frac{\partial \phi}{\partial n}, \frac{\partial \phi}{\partial \tau'}, \quad (27)$$

where $\frac{\partial \phi}{\partial n}$ and $\frac{\partial \phi}{\partial \tau'}$ are respectively the normal (n) and tangential (τ') projections of the scalar gradients $\nabla \phi$, and the normal and tangential directions are directly the x and y directions of the adopted Cartesian coordinate system for straight boundaries. Thus, the expression for f_α is further transformed into a linear combination of the macroscopic variables in Eq. (27),

$$\begin{aligned} f_\alpha(\mathbf{x}, t) &= w_\alpha \left(1 + \frac{\xi_{\alpha i} u_i}{RT'} \right) \phi - w_\alpha \tau \delta t \left(\frac{\partial \phi}{\partial n} \xi_{\alpha n} + \frac{\partial \phi}{\partial \tau'} \xi_{\alpha \tau'} \right) \\ &= A_\alpha \phi + B_\alpha \frac{\partial \phi}{\partial n} + C_\alpha \frac{\partial \phi}{\partial \tau'}, \end{aligned} \quad (28)$$

with $\xi_{\alpha n} = \xi_\alpha \cdot \mathbf{n} = \xi_{\alpha i} n_i$ and $\xi_{\alpha \tau'} = \xi_\alpha \cdot \boldsymbol{\tau}' = \xi_{\alpha i} \tau'_i$ respectively representing the normal and tangential projections of the discrete lattice velocity at the boundary nodes, and n_i, τ'_i are the components of the normal and tangential unit vectors $\mathbf{n}$ and $\boldsymbol{\tau}'$, respectively. The coefficients in Eq. (28) are defined as

$$A_\alpha = w_\alpha \left(1 + \frac{\xi_{\alpha i} u_i}{RT'} \right), \quad (29a)$$

$$B_\alpha = -w_\alpha \tau \delta t \xi_{\alpha n}, \quad (29b)$$

$$C_\alpha = -w_\alpha \tau \delta t \xi_{\alpha \tau'}. \quad (29c)$$

It should be noted that the LB equation in Eq. (1) is solved by two steps, namely, the collision step $f_\alpha^+(\mathbf{x}, t) = f_\alpha(\mathbf{x}, t) - \frac{1}{\tau}(f_\alpha - f_\alpha^{(eq)})$ and the streaming step $f_\alpha(\mathbf{x} + \xi_\alpha \delta t, t + \delta t) = f_\alpha^+(\mathbf{x}, t)$. In particular, the streaming step is executed by shifting the distribution functions from $(\mathbf{x}, t)$ to $(\mathbf{x} + \xi_\alpha \delta t, t + \delta t)$ in accordance with their corresponding discrete lattice velocity ξ_α . After the streaming step, the distribution functions at the boundary nodes are readily classified into two subsets, I^{loc} for the known distribution functions f_α^{loc} and I^{in} for the unknown ones f_α^{in} , with N^{loc} and N^{in} denoting the subsets for their corresponding discrete lattice directions, respectively. In particular, under the framework of the D2Q5 lattice model, only the distribution function along the inner normal direction is unknown at the boundary nodes for the present straight geometry, and thus the tangential derivative $\frac{\partial \phi}{\partial \tau'}$ has no direct contribution to the unknown distribution function. Hereafter, a consistent way for determining the unknown distribution function f_α^{in} at the boundary nodes is developed in accordance

with various macroscopic boundary constraints by applying the distribution function expression in Eq. (28).

1. Dirichlet condition

The physical constraints at the boundary surface prescribed by the Dirichlet condition are given as

$$\phi = \phi^s, \quad \frac{\partial \phi}{\partial \tau'} = \frac{\partial \phi^s}{\partial \tau'}, \quad (30)$$

where ϕ^s is the known macroscopic scalar at the boundary surface. Thus, under the Dirichlet condition, the normal derivative $\frac{\partial \phi}{\partial n}$ is the only remaining unknown macroscopic variable at the boundary nodes, which can be determined by the known distribution function at the outer normal direction,

$$\frac{\partial \phi}{\partial n} = (f_\alpha^{\text{loc}} - A_\alpha \phi^s) / B_\alpha \quad \text{with } \xi_\alpha \parallel \mathbf{n} \text{ and } \alpha \in N^{\text{loc}}. \quad (31)$$

And then, the unknown distribution functions f_α^{in} in I^{in} are determined with the obtained macroscopic information in Eqs. (30) and (31). Furthermore, since the discrete lattice velocity of the only unknown distribution function f_α^{in} is parallel to the normal direction, the constraint for tangential derivative $\frac{\partial \phi}{\partial \tau'} = \frac{\partial \phi^s}{\partial \tau'}$ cannot be reflected in the present implementation under the framework of the D2Q5 lattice model.

2. Neumann condition

The macroscopic constraint for the normal derivative is imposed by the Neumann condition $\frac{\partial \phi}{\partial n} = \phi_n^s$ at the boundary surface, and the macroscopic scalar at the boundary surface ϕ^s is necessary for the unknown distribution function. Here, the known distribution function at the outer normal direction is used for ϕ^s ,

$$\phi^s = (f_\alpha^{\text{loc}} - B_\alpha \phi_n^s) / A_\alpha, \quad \text{with } \xi_\alpha \parallel \mathbf{n} \text{ and } \alpha \in N^{\text{loc}}. \quad (32)$$

And then, the unknown distribution function f_α^{in} is obtained as

$$f_\alpha^{\text{in}} = A_\alpha \phi^s + B_\alpha \phi_n^s, \quad \text{with } \alpha \in N^{\text{in}}. \quad (33)$$

3. Linear Robin condition

First, the definition for the linear Robin condition is provided as

$$\beta_1 \phi^s + \beta_2 \frac{\partial \phi^s}{\partial n} = \beta_3, \quad (34)$$

where β_1, β_2 , and β_3 are given coefficient functions. Equation (34) is directly substituted into the expression of the known distribution function along the outer normal direction,

$$f_\alpha^{\text{loc}} = A_\alpha \phi^s + B_\alpha \frac{\partial \phi^s}{\partial n}, \quad \text{with } \xi_\alpha \parallel \mathbf{n} \text{ and } \alpha \in N^{\text{loc}}, \quad (35)$$

which leads to

$$\begin{aligned} \phi^s &= \left(f_\alpha^{\text{loc}} - \frac{B_\alpha \beta_3}{\beta_2} \right) / \left(A_\alpha - \frac{B_\alpha \beta_1}{\beta_2} \right), \\ &\text{with } \xi_\alpha \parallel \mathbf{n} \text{ and } \alpha \in N^{\text{loc}}, \end{aligned} \quad (36)$$

FIG. 1. Schematic description of boundary nodes around a curved boundary.

and

$$\frac{\partial \phi^s}{\partial n} = (\beta_3 - \beta_1 \phi^s) / \beta_2. \quad (37)$$

Thus, the unknown distribution function is determined as

$$f_\alpha^{\text{in}} = A_\alpha \phi^s + B_\alpha \frac{\partial \phi^s}{\partial n}, \quad \text{with } \alpha \in N^{\text{in}}. \quad (38)$$

D. Present boundary scheme for curved boundaries

As schematically demonstrated in Fig. 1, P and P^s denote the computational boundary node around the curved boundary surface and its normal projection at the boundary surface, respectively, and the computational boundary nodes are defined as inner fluid nodes with at least one lattice link intersected by the physical boundary surface. The origin of the main differences between the boundary implementations for the straight and curved boundaries lie in that the computational boundary nodes are always not on the physical boundary surface, and the macroscopic boundary constraints cannot be directly applied to the distribution function expression as in the above straight boundary treatments. For an accurate evaluation of the effects by the curved geometry, a local curvilinear coordinate system is introduced to transfer the macroscopic information from the boundary surface to the computational boundary nodes.

First, the local polar coordinate system is applied for representing the circular boundaries and the associated tensor calculus is applied for the vector calculations at different coordinate systems. The coordinate variables in the present polar coordinate system are $x^1 = r$ and $x^2 = \theta$, with r and θ respectively the local radius and azimuth, which are naturally the normal and tangential directions for the curved boundaries. Under the framework of the present polar coordinate system, the covariant local basis $\mathbf{g}_i$ is defined by the differential of the position vector $\mathbf{r} = r \cos \theta \mathbf{e}_x + r \sin \theta \mathbf{e}_y$,

$$\mathbf{g}_i = \frac{\partial \mathbf{r}}{\partial x^i}, \quad (39)$$

$$\mathbf{g}_1 = \cos \theta \mathbf{e}_x + \sin \theta \mathbf{e}_y, \quad (40a)$$

$$\mathbf{g}_2 = -r \sin \theta \mathbf{e}_x + r \cos \theta \mathbf{e}_y, \quad (40b)$$

where $\mathbf{e}_x$ and $\mathbf{e}_y$ are unit basis vectors in the Cartesian coordinates. Then, the contravariant basis $\mathbf{g}^i$ is derived from the orthogonality rule $\mathbf{g}^i \cdot \mathbf{g}_j = \delta_j^i$ with δ_j^i being the Kronecker

delta:

$$\mathbf{g}^1 = \cos \theta \mathbf{e}_x + \sin \theta \mathbf{e}_y, \quad (41a)$$

$$\mathbf{g}^2 = \frac{-\sin \theta}{r} \mathbf{e}_x + \frac{\cos \theta}{r} \mathbf{e}_y. \quad (41b)$$

The gradients of the macroscopic scalar $\nabla \phi$ is represented in the local polar coordinates as

$$\nabla \phi = \frac{\partial \phi}{\partial x^i} \mathbf{g}^i, \quad (42)$$

and then the vector dot product between $\nabla \phi$ and the discrete lattice velocity ξ_α is obtained as

$$\nabla \phi \cdot \xi_\alpha = \left(\frac{\partial \phi}{\partial x^i} \mathbf{g}^i \right) \cdot (\xi_\alpha^j \mathbf{g}_j) = \frac{\partial \phi}{\partial x^i} \xi_\alpha^i, \quad (43)$$

where $\xi_\alpha^i = \xi_\alpha \cdot \mathbf{g}^i$ and $\xi_{\alpha i} = \xi_\alpha \cdot \mathbf{g}_i$ are respectively the contravariant and covariant components of the discrete lattice velocity ξ_α in the present curvilinear coordinates. Thus, the expression of the distribution function in Eq. (26) is further extended to the present polar coordinate system as

$$f_\alpha = w_\alpha \left(\phi + \phi \frac{\xi_{\alpha i} u^i}{RT'} - \tau \delta t \frac{\partial \phi}{\partial x^i} \xi_\alpha^i \right), \quad (44)$$

where the Einstein summation convention of summing up repeated indices is applied.

Next, the first-order Taylor expansion is introduced for connecting the macroscopic information at the boundary surface to the boundary node P in Fig. 1,

$$\phi(P) = \phi(P^s) + \frac{\partial \phi}{\partial r}(P^s) \delta_n + O(\delta_n^2), \quad (45)$$

where δ_n is the normal distance from P to the boundary surface with $\delta_n = r(P) - r(P^s)$, as depicted in Fig. 1. Moreover, the scalar gradients at the boundary node P is derived by a first-order approximation as

$$\nabla \phi(P) = \nabla \phi(P^s) + O(\delta_n), \quad (46a)$$

which would markedly simplify the present curved boundary implementations by avoiding the second-order derivatives, and its effects on the overall accuracy of the present boundary scheme are evaluated by directly substituting Eq. (46a) to the expression of the distribution function in Eq. (44):

$$\begin{aligned} f_\alpha(P) &= w_\alpha \left(\phi(P) + \phi(P) \frac{\xi_\alpha \cdot \mathbf{u}}{RT'} - \tau \delta t \nabla \phi(P) \cdot \xi_\alpha \right) \\ &= w_\alpha \left(\phi(P) + \phi(P) \frac{\xi_\alpha \cdot \mathbf{u}}{RT'} - \tau \delta t \nabla \phi(P^s) \cdot \xi_\alpha \right) \\ &\quad + O(\delta t \delta_n). \end{aligned} \quad (46b)$$

By applying the definition of the constant lattice speed $c = \delta x / \delta t$, and considering that the normal distance δ_n scale per $\delta_n \propto \delta x$, we obtain

$$\begin{aligned} f_\alpha(P) &= w_\alpha \left(\phi(P) + \phi(P) \frac{\xi_\alpha \cdot \mathbf{u}}{RT'} - \tau \delta t \nabla \phi(P^s) \cdot \xi_\alpha \right) \\ &\quad + O\left(\frac{\delta x}{c} \delta x\right) = w_\alpha \left(\phi(P) + \phi(P) \frac{\xi_\alpha \cdot \mathbf{u}}{RT'} \right. \\ &\quad \left. - \tau \delta t \nabla \phi(P^s) \cdot \xi_\alpha \right) + O(\delta x^2), \end{aligned} \quad (46c)$$

which demonstrates that the overall accuracy would not be affected by the first-order approximation in Eq. (46a).

Finally, the theoretical preparations for the present curved boundary scheme are completed by combining Eqs. (44)–(46) to give

$$\begin{aligned} f_\alpha(P) &= w_\alpha \left\{ \left(\phi^s + \frac{\partial \phi^s}{\partial r} \delta_n \right) \left(1 + \frac{\xi_{\alpha i} u^i}{RT'} \right) - \tau \delta t \frac{\partial \phi^s}{\partial x^i} \xi_\alpha^i \right\} \\ &= A'_\alpha \phi^s + B'_\alpha \frac{\partial \phi^s}{\partial r} + C'_\alpha \frac{\partial \phi^s}{\partial \theta}, \end{aligned} \quad (47)$$

where ϕ^s and $\frac{\partial \phi^s}{\partial x^i}$ are respectively the macroscopic scalar and the corresponding gradient at the projection node P^s on the physical boundary surface, and the linear combination coefficients in Eq. (47) are defined as

$$A'_\alpha = w_\alpha \left(1 + \frac{\xi_{\alpha i} u^i}{RT'} \right), \quad (48a)$$

$$B'_\alpha = w_\alpha \left[\left(1 + \frac{\xi_{\alpha i} u^i}{RT'} \right) \delta_n - \tau \delta t \xi_\alpha^1 \right], \quad (48b)$$

$$C'_\alpha = -\tau \delta t w_\alpha \xi_\alpha^2. \quad (48c)$$

It is noted that with Eqs. (47) and (48), the distribution functions at the computational boundary nodes directly relate to the macroscopic information at the physical boundary surface, and thus the macroscopic constraints from various boundary conditions can be consistently applied to determine the unknown distribution functions at P . However, compared with the implementation for straight boundaries, more unknown distribution functions f_α^{in} are included in the subset I^{in} , and their lattice velocity directions in N^{in} do not have to be parallel to the normal directions. Therefore, a more general way of determining the known distribution function f_α^{in} is developed in the following.

1. Dirichlet condition

Applying the macroscopic constraints for the Dirichlet condition, $\phi = \phi^s$ and $\frac{\partial \phi}{\partial \theta} = \frac{\partial \phi^s}{\partial \theta}$, to Eq. (47), and the normal derivative at the boundary surface $\frac{\partial \phi^s}{\partial r}$ is determined by a known distribution function f_α^{loc} in I^{loc} with nonzero coefficient B'_α :

$$\begin{aligned} \frac{\partial \phi^s}{\partial r} &= \left(f_\alpha^{\text{loc}} - A'_\alpha \phi^s - C'_\alpha \frac{\partial \phi^s}{\partial \theta} \right) / B'_\alpha, \\ \text{with } \alpha \in N^{\text{loc}} \text{ and } B'_\alpha \neq 0. \end{aligned} \quad (49)$$

2. Neumann condition

With the Neumann condition $\frac{\partial \phi^s}{\partial r} = \phi_n^s$, the macroscopic scalar ϕ^s and its tangential derivative $\frac{\partial \phi^s}{\partial \theta}$ at the boundary surface are obtained as

$$\phi^s = \frac{f_0^{\text{loc}}}{w_0} - \frac{\partial \phi^s}{\partial r} \delta_n, \quad (50)$$

$$\begin{aligned} \frac{\partial \phi^s}{\partial \theta} &= \left(f_\alpha^{\text{loc}} - A'_\alpha \phi^s - B'_\alpha \frac{\partial \phi^s}{\partial r} \right) / C'_\alpha, \\ \text{with } \alpha \in N^{\text{loc}} \text{ and } C'_\alpha \neq 0. \end{aligned} \quad (51)$$

3. Linear Robin condition

With the definition for the linear Robin condition, $\beta_1 \phi^s + \beta_2 \frac{\partial \phi^s}{\partial r} = \beta_3$, the macroscopic information at the boundary surface is determined as follows:

$$\phi^s = \left(\frac{f_0^{\text{loc}}}{w_0} - \frac{\delta_n \beta_3}{\beta_2} \right) / \left(1 - \frac{\delta_n \beta_1}{\beta_2} \right), \quad (52)$$

$$\frac{\partial \phi^s}{\partial r} = (\beta_3 - \beta_1 \phi^s) / \beta_2, \quad (53)$$

and then, Eq. (51) is applied for $\frac{\partial \phi^s}{\partial \theta}$.

It is concluded from the above theoretical derivations of the present boundary scheme that (i) for the straight boundaries, the macroscopic constraints are directly substituted into the expression of the distribution function, and the second-order accuracy for all the boundary conditions considered is well demonstrated; (ii) the first-order Taylor expansion for the scalar ϕ and first-order approximation for the corresponding gradient $\nabla \phi$ are applied for the macroscopic information transfer from the curved boundary surfaces to the computational boundary nodes, which would not affect the overall accuracy of the boundary scheme; (iii) all the three kinds of boundary conditions are consistently implemented by directly substituting the prescribed macroscopic constraints to f_α^{loc} for determining the unknown macroscopic information necessary for f_α^{in} ; (iv) most importantly, the proposed boundary scheme is local for both straight and curved geometries, and no higher-order derivatives are required. Therefore, efficient boundary implementations are developed for various physical and geometric boundary conditions, and second-order accuracy is preserved. Moreover, extended application of the above boundary scheme for the CDE LB method with the MRT collision model can be directly realized by deriving the corresponding second-order expression of the distribution functions as in the Appendix, and then the practical implementations follow the formulations in Secs. IIC and IID.

III. NUMERICAL RESULTS

In this section, numerical validations for the proposed boundary scheme are performed using five tests with various physical constraints and boundary geometries. Note that the analytical solutions for the first four tests are applied to evaluate the order of the numerical accuracy, while the remaining test is also introduced for investigating the accuracy of the developed boundary implementations in more practical applications. Particularly, the present boundary scheme for the LB method with BGK model is first applied for all the tests, and then the effects of the collision model on the present boundary implementations are investigated based on the tests in Secs. IIIB–IIID.

A. One-dimensional transient convection diffusion

The mathematical model for the one-dimensional (1D) unsteady-state CDE test is defined as follows:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2}, \quad 0 < x < L, t > 0, \quad (54a)$$

$$C(x, t)|_{t=0} = 0, \quad 0 < x < L, \quad (54b)$$

FIG. 2. Concentration distribution at various times obtained from the BGK model based boundary scheme for cases of (a) $Pe = 1$; (b) $Pe = 10$.

$$\left(uC - D \frac{\partial C}{\partial x} \right) \Big|_{x=0} = uC_f, \quad t > 0, \quad (54c)$$

$$\frac{\partial C}{\partial x} \Big|_{x=L} = 0, \quad t > 0, \quad (54d)$$

where $D = 0.01$ and $C_f = 50$ are constants for all the test cases. The dimensionless Peclet number $Pe = uL/D$ is introduced for reference when determining the convection velocity u at various mesh resolution conditions $L = (N_x - 1)\delta x$, with δx and N_x denoting respectively the spatial lattice step and the number of the lattice nodes in the x direction. The spatial lattice step δx and the time step δt are set as 1 for all the tests

throughout this work. In particular, the following boundary condition is adopted in the y direction so that the 1D test can be described by the present 2D CDE LB model:

$$f_\alpha(i, 1) = f_\alpha(i, 2), \quad \alpha = 0 - 4, \quad (55a)$$

$$f_\alpha(i, N_y) = f_\alpha(i, N_y - 1), \quad \alpha = 0 - 4. \quad (55b)$$

With the present boundary scheme for the straight wall in Sec. II C and the CDE LB model in Sec. II A, transient results at different times are first obtained with $N_x = 41$ and the resulting concentration distributions are plotted in Fig. 2 together with the analytical solution

$$C(x, t) = C_f \left[\frac{1}{2} \text{erfc} \left(\frac{x - ut}{2\sqrt{Dt}} \right) + \sqrt{\frac{u^2 t}{\pi D}} \exp \left(-\frac{(x - ut)^2}{4Dt} \right) - \frac{1}{2} \left(1 + \frac{ux}{D} + \frac{u^2 t}{D} \right) \exp \left(\frac{ux}{D} \right) \text{erfc} \left(\frac{x + ut}{2\sqrt{Dt}} \right) \right] \quad \text{for } 0 < L < 1, \quad t < 5, \quad (56)$$

which is reported to be valid for the prescribed D and C_f . Exact agreements between the numerical results from the present straight boundary implementations and the analytical solutions are well demonstrated in Fig. 2, except for a few points at $x/L \sim 1$ for $t = 5$ and $Pe = 10$ in Fig. 2(b). These slight discrepancies are acceptable particularly since the analytical solution in Eq. (56) is only valid for $t < 5$. Furthermore, the convergence rate of the L_2 normal errors at various mesh resolutions are investigated with the following error definition:

$$E_2(C) = \frac{\sqrt{\sum_{i,j} |C^{\text{numerical}} - C^{\text{analytical}}|^2}}{\sqrt{\sum_{i,j} |C^{\text{analytical}}|^2}}. \quad (57)$$

The convergence of the L_2 normal errors for mesh resolutions $L = (N_x - 1)\delta x$ corresponding to $N_x = 21, 41, 61, 81, 101$, and 121 are exhibited in Fig. 3 for $Pe = 1$ and 10 , which shows that the relative errors decrease with L in both cases and the errors are relatively greater for the lower Pe . Notably, the convergence rates of the error trends for the two cases,

directly estimated by the slope of the best fit line, are -1.92 and -1.98 , respectively as in Fig. 3, which are both close to -2 . And thus the second-order accuracy of the present straight boundary scheme is well affirmed by the present test.

B. Heat transfer in a 2D channel flow

Consider the heat transfer in a 2D channel flow with uniform velocity u to investigate the numerical accuracy of the present scheme for the Dirichlet and Neumann conditions. The governing equation is given as

$$u \frac{\partial T}{\partial x} = D \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right), \quad (58)$$

and the constant velocity u relates to the diffusion coefficient D by the Peclet number $Pe = uH/D$ with $H = (N_y - 1)\delta x$ denoting the height of the channel. In the present LB simulations, the dimensionless parameter Pe is fixed at 20. With periodic conditions in the x direction, and two kinds of boundary condition definitions at the top and bottom walls, different

FIG. 3. Relative error at different Pe for the concentration versus mesh resolution $L = (N_x - 1)\delta x$ for the unsteady 1D tests obtained from the BGK model based boundary scheme. The blue dashed reference line has a slope of -2 , which reflects the second-order accuracy of the results. The calculated slopes of the best fit line for the error trends, as well as a blue dashed reference line with a slope of -2 , are provided.

analytical solutions result. The Dirichlet condition and the resulting exact solution are first defined as

$$T(x, 0) = T(x, H) = \cos(kx), \quad \text{with } k = 2\pi/L, \quad (59a)$$

$$T_D(x, y) = \text{Re} \left[\exp(ikx) \left(\frac{\exp(\lambda y) + \exp[\lambda(H - y)]}{\exp(\lambda H) + 1} \right) \right], \quad (59b)$$

with $\lambda = k\sqrt{1 + \frac{iU}{Dk}}$. Similarly, the Neumann condition and its derived analytical solution are provided as

$$\left. \frac{\partial T}{\partial y} \right|_{y=0} = \left. \frac{\partial T}{\partial y} \right|_{y=H} = \cos(kx)/H, \quad (60a)$$

$$T_N(x, y) = \text{Re} \left[\exp(ikx) \left(\frac{\exp(\lambda y) + \exp[\lambda(H - y)]}{\lambda H [\exp(\lambda H) - 1]} \right) \right]. \quad (60b)$$

Three notes pertaining to the present implementation are highlighted here. First, besides the relative error for the temperature or concentration distribution of the entire computational domain in Eq. (57), another error definition for the scalar gradients is introduced for the interior nodes (i.e., excluding the boundary nodes) to further evaluate the numerical accuracy of the present boundary implementations,

$$E_2^I(\nabla T) = \frac{\sqrt{\sum_{\text{interior nodes}} |(\nabla T)^{\text{numerical}} - (\nabla T)^{\text{analytical}}|^2}}{\sqrt{\sum_{\text{interior nodes}} |(\nabla T)^{\text{analytical}}|^2}}, \quad (61)$$

where the scalar gradients from the present LB simulations are locally determined by Eq. (6). Second, as in the Li *et al.* work [58], the present test was applied for investigating the numerical stability of the boundary scheme by demonstrating the results from a small relaxation parameter ($\tau = 0.505$ was studied here, which is smaller than the $\tau = 0.51$ by Li *et al.* [58]), and the resulting errors with various mesh resolutions are demonstrated. Third, because the solution for the case of the Neumann condition is nonunique [$T_N(x, y) + T_c$ with T_c denoting an arbitrary constant leads to various alternatives], additional treatments are adopted in the present simulations by fixing a few reference nodes at the boundary surface to the analytical solution in Eq. (60b), and thereby all the boundary nodes are also excluded when calculating the relative error for the temperature distribution in Eq. (57) for the present case.

The convergence of the relative error for both the temperatures and the interior temperature gradients are demonstrated for various τ values in Fig. 4 for the Dirichlet condition case and Fig. 5 for the Neumann condition case, and the slope of the best fit line for the error trends is provided. It is clear that the second-order accuracy of the present scheme for both kinds of boundary conditions is well confirmed since the convergence rates of the relative errors for both the scalar and its gradients are all close to -2 .

Moreover, comparisons of the present boundary schemes developed within the framework of the BGK collision operator in Sec. II and the MRT collision operator in the Appendix are performed based on the present test. The relative errors for the temperature distribution obtained from the two boundary

FIG. 4. Relative error at various τ values for the temperature (a) and the interior temperature gradient (b) vs mesh resolution $H = (N_y - 1)\delta x$ for heat transfer in a 2D channel flow with the Dirichlet condition obtained from the BGK model based boundary scheme. The calculated slopes of the best fit line for the error trends, as well as a pink dashed reference line with a slope of -2 , are provided.

FIG. 5. Relative error at various τ values for the temperature (a) and the interior temperature gradient (b) vs mesh resolution H for heat transfer in a 2D channel flow with the Neumann condition obtained from the BGK model based boundary scheme. The calculated slopes of the best fit line for the error trends, as well as a pink dashed reference line with a slope of -2 , are provided.

schemes are first compared for the Dirichlet condition case in Fig. 6(a) and the Neumann condition case in Fig. 6(b). It is demonstrated that (i) the convergence rates of the error trends are all around -2 , and thus the present boundary scheme for the MRT LB method is also second-order accurate; (ii) for a relatively larger relaxation parameter value ($1/s_1 = 1.5$), the MRT collision operator has the advantage of increasing the accuracy of the present boundary scheme. Additionally, the effect of the relaxation parameter (i.e., τ for the BGK model and $1/s_1$ for the MRT model) on the accuracy of the present boundary scheme is evaluated in Fig. 7(a) for the Dirichlet condition case and Fig. 7(b) for the Neumann condition case. For both cases, the present boundary scheme for the MRT LB method is more accurate than the BGK model based scheme for relatively large relaxation parameters. However, different error trends with respect to the relaxation parameter are demonstrated for the two test cases. On one hand, for the Dirichlet condition case, the relative errors for both boundary schemes grow with the increase of the relaxation parameter. On the other hand, for the Neumann condition case, the relative errors from the boundary scheme for the MRT model decrease with the increase of the relaxation parameter, while the errors for the BGK model based

scheme first decrease for $0.5 < \tau < 0.8$ and then increase for $\tau > 0.8$, which leads to a relaxation parameter value of around 0.8 that minimizes the relative errors.

As for the numerical stability of the present boundary scheme, convergent results for the two test cases are obtained from the proposed boundary schemes based on both collision models for relaxation parameter $\tau - 0.5 = 1/s_1 - 0.5 = 10^{-7}$ with mesh resolution of $H = 10$. Namely, the improvements in numerical stability caused by the MRT collision operator may lead to differences in minimum relaxation parameters for convergent results around 10^{-8} , which is on the order of the round-off error. Therefore, the effects of the collision model on the numerical stability of the proposed boundary scheme are not discussed here.

C. Helmholtz equation in a square domain

Here, the accuracy of the present boundary scheme for the linear Robin condition is validated by the following test:

$$\nabla^2 C = (\lambda^2 + \mu^2)C, \quad 0 < x < 1, \quad 0 < y < 1, \quad (62a)$$

$$C(x, 0) = \exp(-\lambda x), \quad (62b)$$

$$C(x, 1) = 0, \quad (62c)$$

FIG. 6. Relative error comparisons between the BGK collision operator and the MRT collision operator based on the tests of heat transfer in a 2D channel flow with the Dirichlet condition (a) and Neumann condition (b). The calculated slopes of the best fit line for the error trends, as well as a pink dashed reference line with a slope of -2 , are provided.

FIG. 7. Relative error for the temperature vs relaxation parameter values (i.e., τ for the BGK model and $1/s_1$ for the MRT model) for the tests of heat transfer in a 2D channel flow with the Dirichlet condition (a) and Neumann condition (b) obtained from the BGK collision operator and the MRT collision operator, respectively.

$$C(0, y) = \sinh[\mu(1 - y)]/\sinh(\mu), \quad (62d)$$

$$\lambda C(1, y) + \frac{\partial C(1, y)}{\partial x} = 0, \quad (62e)$$

with $\lambda = \mu = 1$, and the derived exact solution is given as

$$C(x, y) = \exp(-\lambda x) \sinh[\mu(1 - y)]/\sinh(\mu). \quad (62f)$$

By regarding the right-hand side of Eq. (62a) as a source term, convergent results are obtained by the present boundary scheme for the Dirichlet condition and the Robin condition, and the relative errors for the entire concentration distribution as well as the interior gradients, from cases with various mesh resolution and relaxation parameters, are demonstrated in Fig. 8, and again, the second-order accuracy of the present scheme is confirmed by the present test. Moreover, at a fixed relaxation parameter of $\tau = 0.75$, comparisons of the relative errors with the second-order scheme by Huang *et al.* [60], with the boundary surface being a half lattice spacing away from the last lattice layer, are performed in Fig. 9. It is clear that whereas the present scheme is more accurate for concentrations, the Huang *et al.* scheme [60] is more accurate

for the interior concentration gradients. However, it should be noted that the implementation of the Huang *et al.* scheme [60] is more complicated since the second-order derivatives are involved and information from the neighboring fluid nodes is also necessary for the adopted interpolations.

Furthermore, the effects of the collision model on the accuracy of the present boundary scheme are investigated based on the present test and demonstrated in Fig. 10, which demonstrates that the boundary scheme for the MRT LB method is of second-order accuracy and more accurate than the BGK model based boundary scheme for all the relaxation parameters assessed. Additionally, the relative errors from the boundary schemes based on both collision models versus relaxation parameters are exhibited in Fig. 11. It is clear that there is a relaxation parameter value around 0.52 for both schemes which minimizes the relative error. For the interval $0.5 < \tau < 0.52$, the relative errors from both schemes agree exactly with each other; and for $\tau > 0.52$, the relative errors from both schemes grow with the increase of the relaxation parameter and the boundary scheme for the MRT model becomes more accurate.

FIG. 8. Relative error at various τ values for the concentration (a) and the interior concentration gradients (b) vs mesh resolution L for the Helmholtz equation in a square domain obtained from the BGK model based boundary scheme. The calculated slopes of the best fit line for the error trends, as well as a pink dashed reference line with a slope of -2 , are provided.

FIG. 9. Relative error comparisons between the present scheme for BGK model and the Huang *et al.* [60] scheme based on the test of the Helmholtz equation in a square domain: (a) concentration; and (b) error interior concentration gradients.

D. Steady-state heat conduction inside a circle

In the present test, the performance of the present boundary scheme for curved boundary condition treatments is investigated and compared with the second-order scheme by Huang *et al.* [60]. The governing equation is given as

$$\nabla^2 T = 0, \quad 0 \leq r < r_0, \quad 0 \leq \theta < 2\pi, \quad (63)$$

and various test cases are studied by the adopted boundary conditions at $r = r_0$:

(i) Dirichlet condition,

$$T = \cos(k\theta), \quad (64)$$

(ii) Neumann condition,

$$\frac{\partial T}{\partial r} = \frac{k}{r_0} \cos(k\theta), \quad (65)$$

(iii) linear Robin condition,

$$T + \frac{\partial T}{\partial r} = \left(1 + \frac{k}{r_0}\right) \cos(k\theta), \quad (66)$$

with the constant $k = 4$. And the following analytical solution is applicable for all the three test cases:

$$T(r, \theta) = \left(\frac{r}{r_0}\right)^k \cos(k\theta). \quad (67)$$

In addition to the relative errors defined in Eqs. (57) and (61), error definitions for the computational boundary nodes are introduced as

$$E_2^B(T) = \frac{\sqrt{\sum_{\text{boundary nodes}} |T^{\text{numerical}} - T^{\text{analytical}}|^2}}{\sqrt{\sum_{\text{boundary nodes}} |T^{\text{analytical}}|^2}}, \quad (68a)$$

$$E_2^B(T_n) = \frac{\sqrt{\sum_{\text{boundary nodes}} |T_n^{\text{numerical}} - T_n^{\text{analytical}}|^2}}{\sqrt{\sum_{\text{boundary nodes}} |T_n^{\text{analytical}}|^2}}, \quad (68b)$$

to investigate the numerical accuracy of the present scheme at the boundary nodes near the curved boundary surface. Again, due to the nonuniqueness of the solutions for the Neumann

FIG. 10. Relative error comparisons between the BGK collision operator and the MRT collision operator based on the test of the Helmholtz equation in a square domain. The calculated slopes of the best fit line for the error trends, as well as a pink dashed reference line with a slope of -2 , are provided.

FIG. 11. Relative error for the concentration vs relaxation parameter values (i.e., τ for the BGK model and $1/s_1$ for the MRT model) for test of the Helmholtz equation in a square domain obtained from the BGK collision operator and the MRT collision operator, respectively.

FIG. 12. Relative error at various τ values for the temperature (a), interior temperature gradients (b), boundary value (c), and the boundary flux (d) vs mesh resolution $r_0 = (N_r - 1)\delta x$ for the heat conduction inside a circle with Dirichlet condition obtained from the BGK model based boundary scheme. The calculated slopes of the best fit line for the error trends are provided.

condition case, the temperature at some boundary points are fixed based on the analytical solution in Eq. (67). Therefore, the boundary nodes are excluded when determining the relative errors for temperature distribution in the Neumann condition case. The convergence of the relative errors with respect to mesh resolution $r_0 = (N_r - 1)\delta x$ for (a) the entire temperature distribution in Eq. (57), (b) interior temperature gradient in

Eq. (61), (c) boundary value in Eq. (68a), and (d) boundary flux Eq. (68b) are demonstrated for the Dirichlet condition case in Fig. 12, the Neumann condition case in Fig. 13, and linear Robin condition case in Fig. 14. Two observations are clear from Figs. 12–14. First, the convergence order with respect to r_0 of the relative errors for the entire temperature distribution and the boundary values are of second order, and

FIG. 13. Relative error at various τ values for the temperature (a), interior temperature gradients (b), and the boundary flux (c) vs mesh resolution r_0 for the heat conduction inside a circle with Neumann condition obtained from the BGK model based boundary scheme. The calculated slopes of the best fit line for the error trends are provided. Note: the relative errors for the boundary value are not presented here due to the additional treatments of the boundary nodes needed for the present case.

FIG. 14. Relative error at various τ values for the temperature (a), interior temperature gradients (b), boundary value (c), and the boundary flux (d) vs mesh resolution r_0 for the heat conduction inside a circle with linear Robin condition obtained from the BGK model based boundary scheme. The calculated slopes of the best fit line for the error trends are provided.

thus the second-order accuracy of the present scheme for curved boundary treatments is confirmed. Second, due to the first-order approximation for the scalar gradients in Eq. (46a) in the present curved boundary implementations, the convergence orders for the interior gradient errors and the boundary flux errors are between 1.0 and 1.5, but this would not affect the overall accuracy for the entire temperature distribution.

Furthermore, accuracy comparisons between the present curved boundary condition with the second-order scheme by Huang *et al.* [60] are also carried out in Figs. 15 and 16 for the Dirichlet condition case and the Robin condition case, respectively. Despite the lower-order accuracy for the scalar gradients, the present curved boundary implementations are demonstrated to be more accurate than the Huang *et al.* scheme [60] for the temperature distribution for both cases. Comparisons based on the Neumann condition case are not included here, since additional treatments are needed in the present simulation for the Neumann condition case to restrict the numerical results to the analytical one in Eq. (67) and thus the relative error values may be affected.

Moreover, the effects of the collision model on the accuracy of the present boundary scheme are also discussed for the present curved boundary treatments. As demonstrated in Fig. 17, the boundary scheme for the MRT LB method is more accurate than the BGK model based scheme for the relatively larger relaxation parameters (i.e., $1/s_1 = 1.5$ and 3.0), and the convergence rates for the error trends for all the test cases are

around -2 , which thereby confirms the second-order accuracy of the present boundary scheme for the MRT LB method.

FIG. 15. Relative error comparisons at $\tau = 0.75$ for the temperature distribution between the present scheme for BGK model and the Huang *et al.* [60] scheme based on the test of the heat conduction inside a circle with Dirichlet condition. Note: comparisons for the boundary value are not presented here because the reference data are not provided in Huang *et al.* [60].

FIG. 16. Relative error comparisons at $\tau = 0.75$ between the present scheme for BGK model and the Huang *et al.* scheme [60] based on the test of the heat conduction inside a circle with linear Robin condition: (a) error for the temperature distribution; (b) error for the boundary values.

E. 2D natural convection in a square enclosure with a circular cylinder in the center

Last, a more practical test is considered for further validating the performance of the present boundary implementations when coupling with the hydrodynamic boundary schemes. The stationary nonslip condition is applied at both the four outer straight boundaries and the inner circular surface, and the Dirichlet condition with a higher temperature T_h at the inner surface and lower temperature T_c at the outer straight walls are adopted. A body force term $\rho a_z = -\rho g \beta (T - T_m)$ is introduced to the momentum equation by invoking the Boussinesq approximation, where $T_m = (T_h + T_c)/2$ is the reference temperature, g is the gravitational acceleration, and β is the thermal-expansion coefficient. The flow structures and temperature distributions depend on two dimensionless parameters: the Prandtl Number $Pr = \nu/D$ and the Rayleigh number $Ra = g \beta (T_h - T_c) L^3 / (D \nu)$, with ν denoting the kinematic viscosity of the flow, $L = 5r_0$ the length of the outer boundary, and r_0 the radius of the inside circular cylinder. In addition to the present boundary scheme for the Dirichlet temperature condition for both the straight wall and the inner

curved wall, our earlier second-order hydrodynamic boundary scheme [65] is applied for the nonslip velocity condition at the inner curved boundary and the outer straight walls.

With a fixed $Pr = 0.71$, steady-state results from the present LB simulations are obtained for test cases of $Ra = 10^3, 10^4, 10^5$, and 10^6 with the mesh resolution of $N_x = 201$. The temperature distributions and the flow structures are respectively demonstrated in Figs. 18 and 19 for a range of Ra values in terms of the isotherms and streamlines, which accord well with the published results in the literature [74–76]. Moreover, the surface-averaged Nusselt number $\overline{Nu}$ with the following definition is then applied for further quantitative validations of the present boundary scheme:

$$\overline{Nu} = \frac{1}{L} \int_0^L Nu \, ds, \quad \text{with } Nu = \left. \frac{\partial T}{\partial n} \right|_{\text{wall}}. \quad (69)$$

The obtained surface-averaged Nusselt number value $\overline{Nu}$ for all the test cases are tabulated in Table I, and quantitative agreement with the reference results reported in the literature

FIG. 17. Relative error comparisons between the BGK collision operator and the MRT collision operator based on the tests of heat conduction inside a circle with Dirichlet condition (a), Neumann condition (b), and linear Robin condition (c). The calculated slopes of the best fit line for the error trends, as well as a pink dashed reference line with a slope of -2 , are provided.

FIG. 18. Isotherms in the region between the circular cylinder and the cavity walls for Ra values of (a) 10^3 ; (b) 10^4 ; (c) 10^5 ; and (d) 10^6 obtained from the BGK model based boundary scheme.

[74–76] is demonstrated, which again confirm the accuracy of the present boundary scheme in practical applications.

IV. CONCLUSION

In this work, a second-order boundary scheme for CDE LB method is proposed by applying the expression for the distribution function derived from the CE analysis and the Hermite expansion technique. Then consistent boundary implementations for the Dirichlet condition, Neumann condition, and linear Robin condition are developed for both straight and curved boundaries under the framework of the BGK collision model in Sec. II and the MRT collision model in the Appendix. For the straight boundary treatments, the boundary nodes are placed at the physical boundary surface and macroscopic information necessary for the unknown distribution function is directly determined by substituting macroscopic boundary constraints into the known distribution functions at the boundary nodes. On the other hand, for the curved geometries, the Taylor expansions under the framework of the local polar coordinate system are first introduced to transfer the macroscopic boundary constraints at the curved boundary surface to the computational boundary nodes, and then the unknown macroscopic information is derived from the local known distribution functions at the boundary nodes. Then, the unknown distribution functions are determined by the

derived macroscopic information, and thus the essence of the present boundary scheme is that the unknown distribution functions are represented by the known ones at the same boundary nodes in accordance with the macroscopic boundary condition. Two highlights of the present scheme are noted here. First, the present boundary scheme is local for both straight and curved boundary implementations and no information from the neighboring fluid nodes is required. Second, the developed boundary implementations are consistent since all the boundary conditions considered are directly applied to the expression for the distribution function in Eqs. (28) and (47). Both of these features are attractive advantages of the present scheme over the existing second-order boundary schemes for the CDE LB method.

The accuracy of the present scheme is validated by numerical tests with analytical solutions and the demonstrated convergence order for the relative errors confirms the second-order accuracy of the proposed boundary implementations for both straight and curved boundaries. In particular, due to the first-order approximation for the scalar gradients in the present curved boundary treatments, the relative errors for the interior temperature gradients and boundary flux converge at less than second order, while the accuracy for the temperature and concentration distribution are second order. Moreover, comparisons with the second-order scheme by Huang *et al.* [60] are performed for a straight boundary and the present

FIG. 19. Streamlines in the region between the circular cylinder and the cavity walls for Ra values of (a) 10^3 ; (b) 10^4 ; (c) 10^5 ; and (d) 10^6 obtained from the BGK model based boundary scheme.

scheme is demonstrated to be more accurate for the scalar distribution but less accurate for the interior gradients. However, for curved boundary treatments, although the convergence order for the scalar gradient errors for the present scheme is lower than that of the Huang *et al.* scheme [60], the present boundary scheme provides more accurate results for the scalar distribution. Additionally, detailed comparisons between the boundary schemes for different collision models demonstrated that the MRT model has the advantage of improving the accuracy of the proposed boundary scheme for relatively large relaxation parameters.

TABLE I. The surface-averaged Nusselt number $\overline{Nu}$ for various Ra values.

Ra	$\overline{Nu}$			
	Present scheme	Li <i>et al.</i> [74]	Peng <i>et al.</i> [75]	Kim <i>et al.</i> [76]
10^3	3.168	3.167		3.396
10^4	3.226	3.226	3.24	3.414
10^5	4.904	4.912	4.84	5.138
10^6	8.860	8.966	8.75	9.390

ACKNOWLEDGMENTS

We would like to thank for financial support the National Research Foundation (NRF), Prime Minister's Office, Singapore under its Campus for Research Excellence and Technological Enterprise (CREATE) program, and the Joint Singapore-Germany Research Project Fund (SGP-PROG3-019). This work was also financially supported by the National Natural Science Foundation of China (Grants No. 11572062 and No. 41672292) and the Program for Changjiang Scholars and Innovative Research Team in University (Grant No. IRT13043).

APPENDIX: EXTENSION OF THE PRESENT BOUNDARY SCHEME FOR MULTIPLE-RELAXATION-TIME (MRT) LB METHOD

In this Appendix, the extended application of the present boundary scheme for the MRT CDE LB method is directly realized by deriving the second-order expression of the distribution functions, and the practical implementations similarly follow the formulations in Secs. II C and II D.

Under the framework of the D2Q5 lattice model, the LB equation for the MRT CDE LB method is given as

$$f_\alpha(\mathbf{x} + \mathbf{e}_\alpha \delta t, t + \delta t) - f_\alpha(\mathbf{x}, t) = -\Lambda_{\alpha\beta} (f_\beta - f_\beta^{(eq)}), \quad (\text{A1})$$

where $\mathbf{e}_\alpha$ is the discrete lattice velocity with lattice speed $c = 1$ (for all the tests in Sec. III, the discrete spatial step δx and the time step δt are both assumed to be constant 1, which results $c = \delta x / \delta t = 1$). $\Lambda_{\alpha\beta}$ is the collision matrix and can be further simplified as $\mathbf{\Lambda} = \mathbf{M}^{-1} \mathbf{S} \mathbf{M}$ with a transformation matrix $\mathbf{M}$,

$$\mathbf{M} = \begin{pmatrix} \langle \mathbf{e}_\alpha^0 | \\ \langle e_{\alpha x} | \\ \langle e_{\alpha y} | \\ \langle 4\mathbf{e}_\alpha^0 - 5\mathbf{e}_\alpha^2 | \\ \langle e_{\alpha x}^2 - e_{\alpha y}^2 | \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 \\ 4 & -1 & -1 & -1 & -1 \\ 0 & 1 & 1 & -1 & -1 \end{pmatrix}, \quad (\text{A2})$$

and a diagonal relaxation matrix $\mathbf{S}$,

$$\mathbf{S} = \text{diag}(s_0, s_1, s_2, s_3, s_4). \quad (\text{A3})$$

Additionally, the distribution function vector $|f\rangle = (f_0, f_1 \dots f_4)^\dagger$ can be transformed into the moment space by

the transformation matrix $\mathbf{M}$ as

$$|\mathbf{m}\rangle = \mathbf{M}|f\rangle = (m_0, m_1, \dots, m_4)^\dagger, \quad (\text{A4})$$

where † denotes the transpose operator, and m_i is the component of the moment vector $|\mathbf{m}\rangle$. Applying the definition of the equilibrium distribution function in Eq. (4), the equilibrium moment vector is derived as

$$|\mathbf{m}^{(0)}\rangle = \mathbf{M}|f^{(0)}\rangle = (m_0^{(0)}, m_1^{(0)}, \dots, m_4^{(0)})^\dagger \\ = \phi(1, u_x, u_y, \frac{2}{3}, 0)^\dagger, \quad (\text{A5})$$

with u_x and u_y the macroscopic fluid velocity components at the x and y directions, respectively. Applying the CE analysis to Eq. (A1), we obtain

$$\varepsilon^0 : f_\alpha^{(0)} = f_\alpha^{(eq)}, \quad (\text{A6a})$$

$$\varepsilon^1 : \left(\frac{\partial}{\partial t_0} + e_{\alpha i} \frac{\partial}{\partial x_{0i}} \right) f_\alpha^{(0)} = -\frac{\Lambda_{\alpha\beta}}{\delta t} f_\beta^{(1)}, \quad (\text{A6b})$$

$$\varepsilon^2 : \frac{\partial}{\partial t_1} f_\alpha^{(0)} + \left(\frac{\partial}{\partial t_0} + e_{\alpha i} \frac{\partial}{\partial x_{0i}} \right) f_\alpha^{(1)} + \frac{\delta t}{2} \left(\frac{\partial}{\partial t_0} + e_{\alpha i} \frac{\partial}{\partial x_{0i}} \right)^2 f_\alpha^{(0)} = -\frac{\Lambda_{\alpha\beta}}{\delta t} f_\beta^{(2)}, \quad (\text{A6c})$$

and moments of Eq. (A6b) are

$$\frac{\partial}{\partial t_0} m_0^{(0)} + \frac{\partial}{\partial x_0} m_1^{(0)} + \frac{\partial}{\partial y_0} m_2^{(0)} = 0, \quad (\text{A7a})$$

$$\frac{\partial}{\partial t_0} m_1^{(0)} + \frac{\partial}{\partial x_0} \left[\frac{1}{10} (5m_4^{(0)} - m_3^{(0)} + 4m_0^{(0)}) \right] = -\frac{s_1 m_1^{(1)}}{\delta t}, \quad (\text{A7b})$$

$$\frac{\partial}{\partial t_0} m_2^{(0)} + \frac{\partial}{\partial y_0} \left[-\frac{1}{10} (5m_4^{(0)} + m_3^{(0)} - 4m_0^{(0)}) \right] = -\frac{s_2 m_2^{(1)}}{\delta t}. \quad (\text{A7c})$$

Substituting the equilibrium moment vector defined in Eq. (A5) into Eq. (A7) leads to

$$m_1^{(1)} = -\frac{\delta t}{3s_1} \frac{\partial \phi}{\partial x_0}, \quad (\text{A8a})$$

$$m_2^{(1)} = -\frac{\delta t}{3s_2} \frac{\partial \phi}{\partial y_0}. \quad (\text{A8b})$$

Thus, the first-order moment of $f_\alpha^{(1)}$ is obtained by assuming $s_1 = s_2$,

$$\sum_\alpha f_\alpha^{(1)} e_{\alpha i} = -\frac{\delta t}{3s_1} \frac{\partial \phi}{\partial x_{0i}}. \quad (\text{A9})$$

Moreover, the zeroth-order moment of Eq. (A6c) is derived as

$$\frac{\partial}{\partial t_1} m_0^{(0)} + \frac{\partial}{\partial x_0} m_1^{(1)} + \frac{\partial}{\partial y_0} m_2^{(1)} + \frac{\delta t}{2} \frac{\partial}{\partial x_0} \left(\frac{1}{3} \frac{\partial \phi}{\partial x_0} \right) \\ + \frac{\delta t}{2} \frac{\partial}{\partial y_0} \left(\frac{1}{3} \frac{\partial \phi}{\partial y_0} \right) = 0, \quad (\text{A10})$$

and combining Eqs. (A10) and (A7) leads to the macroscopic CDE in Eq. (17) with the following definition for the diffusion coefficient D :

$$D = \frac{\delta t}{3} \left(\frac{1}{s_1} - \frac{1}{2} \right). \quad (\text{A11})$$

Besides, the second-order expression of the distribution function is derived from its moments as

$$\sum_\alpha f_\alpha = \phi, \quad \sum_\alpha f_\alpha \xi_{\alpha i} = \phi u_i - \frac{\delta t}{3s_1} \frac{\partial \phi}{\partial x_i}, \quad (\text{A12})$$

$$f_\alpha(\mathbf{x}, t) = w_\alpha \left(\phi + 3\phi e_{\alpha i} u_i - \frac{\delta t}{s_1} \frac{\partial \phi}{\partial x_i} e_{\alpha i} \right). \quad (\text{A13})$$

Implementing the formulations in Secs. IIC and IID in accordance with Eq. (A13), the proposed boundary scheme developed under the framework of the BGK collision operator is extended to the MRT LB method. We note that the relaxation parameters in Eq. (A3) are given as

$$s_0 = 1.0, \quad s_1 = s_2 = 1/\tau, \quad s_3 = s_4 = 1.8, \quad (\text{A14})$$

for all the tests when evaluating the effects of the collision model on the present boundary scheme. The numerical accuracy and stability of the boundary implementations for the

MRT LB method may be further improved by adjusting the relaxation parameters s_3 and s_4 , but the relevant discussions are not included here.

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