

A lattice Boltzmann method for electric field-space charge coupled problems

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Abstract— A lattice Boltzmann method (LBM) is developed to solve the electric field-space charge coupled problems. Instead of solving the macroscopic current continuity equation and the Poisson's equation, two discrete lattice Boltzmann equations are formulated and solved to obtain the distributions of charge density and electric potential. The non-equilibrium extrapolation scheme is used to treat the boundary conditions with complex geometry. Our technique is verified with several test cases for which analytical solution and/or numerical results exists. A key feature of this methodology lies in its natural coupling with the LBM for fluid flow. As a demonstration, the injection induced electroconvection of dielectric liquids in a concentric-cylinder configuration is considered.

I. INTRODUCTION

Electrohydrodynamics (EHD) is an interdisciplinary science dealing with the interaction of fluid with electric field [1]. The complex physics involved in electroconvective phenomena together with some promising applications draw a wide attention to this very active field. Some representative applications include EHD pumps, electronic cooling, heat transfer augmentation, active flow control with electric field, charge injection atomizers, electro-spinning, etc [2]. In general, EHD flows possess strong nonlinearity, which encourages the use of direct numerical simulation approach to gain deeper insights into such physical phenomena.

During the last three decades, the lattice Boltzmann method (LBM), which is a mesoscopic modelling approach, has experienced rapid development and has become an established alternative for complex flows [3,4]. However, only until recent years, LBM has been introduced into the EHD field [5], which is in contrast to the fact that LBM has long been applied to magnetohydrodynamic (MHD) flows since the early 1990s. Indeed EHD and MHD can be viewed as two special subjects due to the interaction between the electromagnetic field and flow motion [1]. However, as far as we know, the LBM has not been well established for EHD problems yet.

The material presented here represents the first results of a broader research project aimed at extending the application of the LBM in simulating EHD flows of single-phase dielectric liquids. In a recent study [6], we have developed a unified LBM based on three

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consistent lattice Boltzmann equations (LBEs) to calculate the fluid flow, electrical potential and charge density distribution. The Chapman-Enskog multi-scale analysis has also been performed to link the mesoscopic LBEs with the macroscopic governing equations. By this way, we provide a solid theoretical basis for our LBM. However, only a simple geometry problem, i.e., the unipolar injection induced electroconvection in a plate-plate configuration, was considered to validate the method in [6]. The objective of this study is to extend the LBM to EHD flows with complex geometries. The first and crucial step is test the feasibility of the LBM with the electric field-space charge coupled problems with complex geometries. Later a natural coupling with the LB model for flow motion can be achieved.

The reminder of this paper is organized as follow. In section II the macroscopic governing equations are described. Then in section III we present the LBEs for electric potential and charge density equations. In particular, the method for boundary condition treatment is explained in details. After that, in section IV the method is verified with several test cases. As an application, the results with the injection induced electro-convection of dielectric liquids in a concentric-cylinder configuration are also presented. Finally a conclusion is drawn up in the last section.

II. MATHEMATICAL FORMULATION

A. Governing equations

For electric field-space charge coupled problems, the governing equations include the potential and charge conservation equations. In this study, we consider the simplest case with only one charge species, and thus the current continuity equation reads:

$$\frac{\partial q}{\partial t} + \nabla \cdot \mathbf{J} = 0, \quad (1)$$

where q is the volume charge density and \mathbf{J} is the current density. There are three basic transport mechanisms for free charges in the electric and flow fields: drift under the action of the electric field, convection along with the flow field and charge diffusion,

$$\mathbf{J} = qK\mathbf{E} + q\mathbf{u} - D\nabla q, \quad (2)$$

where the vectors \mathbf{E} and \mathbf{u} are the electric field and the fluid velocity field; the scalars K and D are the ion mobility and the diffusion coefficient. For turbulence flows, besides the molecular diffusion, D also includes an extra contribution due to turbulent transport.

The space charges are related to the electrical potential by the Poisson's equation,

$$\nabla^2 V = -q / \varepsilon \quad (3)$$

where V is the electrical potential and ε is the dielectric permittivity. For vacuum, $\varepsilon = \varepsilon_0 = 8.854 \times 10^{-12} \text{ F / m}$. The electric field is defined as,

$$\mathbf{E} = -\nabla V. \quad (4)$$

As shown through Eqns. (1-4), the electric field and charge density distribution are nonlinearly coupled, as the charge distribution influences the electric field which in turn, modifies the space charge distribution by the ion drift mechanism. Another characteristic of the electric field-space charge coupled problems lies in the typical smallness of the charge diffusion coefficient. That is, Eqn. (1) is a strongly convection-dominating equation.

For conventional methods based on the partial differential equations (PDEs), special discretization schemes or methods (such as the particle in cell method, the method of characteristic, the flux corrected transport and total variation diminishing schemes and so on) are unusually required to solve this equation to obtain low numerical diffusion and oscillation-free solutions [7,8].

B. Boundary conditions

For the test cases presented in Section 4, there are two types of boundary conditions with the two independent variables q and V : Dirichlet and Neumann conditions. The electric potentials on the electrodes are either specified with a given value or set to be zero to represent the grounded case: $V_{\text{electrode}} = V_{\text{applied}}$ or 0. Depending on the physical problems modelled, the value of charge densities on the electrodes can either be prescribed or show a zero gradient: $q_{\text{electrode}} = q_{\text{applied}}$ or $\partial q_{\text{electrode}}/\partial n = 0$, with n denotes the normal to the electrode surface. In addition, on the symmetry planes, all dependent variables are assumed to have a zero gradient in the direction normal the plane (i.e., Neumann condition).

III. 3. THE LATTICE BOLTZMANN METHOD

The LBM is a mesoscopic method and it is most frequently used to compute solutions of the Navier-Stokes equations. However, the idea of mesoscopic modelling can also be applied to other macroscopic systems. In this study, a LBM approach is formulated for the Poisson's equation and the current continuity equation. The basic idea of LBM is to solve a set of discrete equations for the mesoscopic distribution functions in a domain discretized by the Cartesian grid. Then the macroscopic quantities (i.e., the fluid density and velocity, electrical potential and charge density) can be determined from their corresponding distribution functions [9].

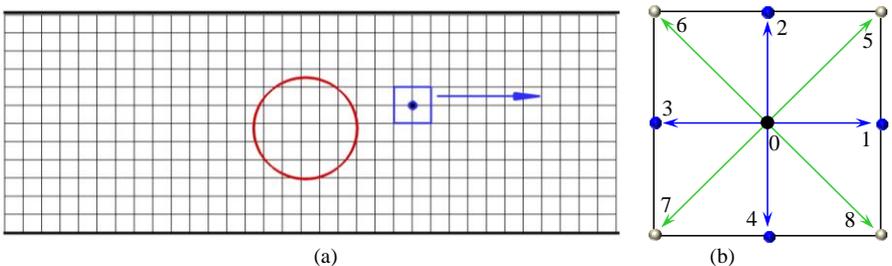


Fig. 1. (a) Lattice Boltzmann discretization of a domain containing a circle and (b) the D2D9 model.

Since the discrete equations are first order PDEs, they are much easier to solve than the macroscopic governing equations. In addition, the solution procedure of these discrete equations can be vividly understood by the collision-streaming process of some pseudo particles. An example of the discretization grid for the domain containing a circular is shown in Fig. 1a. For 2D problems, the D2Q9 velocity discretization scheme is commonly used. In other words, during one time step, the pseudo particles can either stay at the original place or stream to the eight neighboring locations in certain directions; see Fig. 1b. For D2Q9 model, the nine velocity vectors are given by

$$\mathbf{c}_j = \begin{cases} (0,0) & j=0 \\ c(\cos[(j-1)\frac{\pi}{2}], \sin[(j-1)\frac{\pi}{2}]) & j=1-4, \\ \sqrt{2}c(\cos[(2j-1)\frac{\pi}{4}], \sin[(2j-1)\frac{\pi}{4}]) & j=5-8 \end{cases} \quad (5)$$

where the streaming speed c is defined as $c = \Delta x / \Delta t$, Δx and Δt being the size of lattice cell and the lattice time step, respectively. The weight function ω_j for the j th velocity direction is given as

$$\omega_j = \begin{cases} 4/9 & j=0 \\ 1/9 & j=1-4. \\ 1/36 & j=5-8 \end{cases} \quad (6)$$

Based on the above D2Q9 model, we have developed two LBEs for electrical potential and the charge density in [6]. In addition, the two LBEs are coupled to another LBE with a body force for flow motion. In the following, we first make a brief description of the LBEs. Then we focus on the treatment of curved boundary.

A. Lattice Boltzmann method for electric potential and electric field

The LBM is a method that intrinsically deals with parabolic equations with temporal terms. However, the Poisson's equation is an elliptical equation, thus it is necessary to introduce an artificial time dependent term into Eq. (3) [10]:

$$\frac{\partial V}{\partial t} = \gamma \nabla^2 V + \frac{\gamma q}{\varepsilon}. \quad (7)$$

A nonzero coefficient γ ($\gamma > 0$) is also introduced to control the evolution speed. Note that a steady solution of Eqn. (7) will also satisfy Eqn. (3) for any γ . The value of γ will affect the numerical stability and also the computational cost of the solution procedure. Its optimal value depends on the specific problems under consideration. For the test cases presented later, an optimal value 0.3 is chosen based on some preliminary tests.

The LBE for Eqn. (7) can be formulated as

$$g_j(\mathbf{x} + \mathbf{c}_j \Delta t, t + \Delta t) - g_j(\mathbf{x}, t) = -\frac{1}{\tau_\phi} [g_j(\mathbf{x}, t) - g_j^{eq}(\mathbf{x}, t)] + \Delta t S_j \quad (8)$$

where g_j is the distribution function of electric potential and its equilibrium distribution g_j^{eq} is given by $g_j^{eq}(\mathbf{x}, t) = \omega_j V$. The source term is defined as $S_j = \gamma \omega_j q / \varepsilon$.

The relaxation time τ_ϕ in Eq. (8) is computed from,

$$\tau_\phi = \frac{3\gamma}{c^2 \Delta t} + \frac{1}{2}. \quad (9)$$

The electric potential is related to its corresponding distribution functions by

$$V = \sum_j g_j. \quad (10)$$

The electric field can also be directly determined from the distribution functions [11],

denoted as \mathbf{x}_b . The small circles on the curved boundary, \mathbf{x}_w , denote the intersection position of the solid wall with other lattice links. The fraction Δ is defined as $\Delta = |\mathbf{x}_f - \mathbf{x}_w| / |\mathbf{x}_f - \mathbf{x}_b|$, $0 \leq \Delta \leq 1$.

The post-collision distribution functions $\tilde{g}_{\bar{j}}(\mathbf{x}_b, t)$ and $\tilde{h}_{\bar{j}}(\mathbf{x}_b, t)$ from the node \mathbf{x}_b to the node \mathbf{x}_f are unknown. Their values are determined by idea of non-equilibrium extrapolation scheme [13]. Taking $\tilde{g}_{\bar{j}}(\mathbf{x}_b, t)$ as the example, the unknown distribution function can be separated into an equilibrium component and a non-equilibrium one,

$$\tilde{g}_{\bar{j}}(\mathbf{x}_b, t) = \tilde{g}_{\bar{j}}^{eq}(\mathbf{x}_b, t) + \tilde{g}_{\bar{j}}^{neq}(\mathbf{x}_b, t). \quad (16)$$

The equilibrium part can be calculated as,

$$\tilde{g}_{\bar{j}}^{eq}(\mathbf{x}_b, t) = w_{\bar{j}} V_b, \quad (17)$$

where V_b is determined by the following extrapolation [13],

$$V_b = \begin{cases} [V_w + (\Delta - 1)V_f] / \Delta & \Delta \geq 0.75 \\ [V_w + (\Delta - 1)V_f] + (1 - \Delta)[2V_w + (\Delta - 1)V_{ff}] / (1 + \Delta) & \Delta < 0.75 \end{cases}. \quad (18)$$

For the Dirichlet condition, the value of V_w is directly known. For the Neumann condition, its value should be determined by extrapolation with the known values of outer nodes. In this study a simple second order scheme $V_w = (4V_f - V_{ff}) / 3$ is used [14], and the more accurate schemes can be found in [15].

The next task is to determine the non-equilibrium component $\tilde{g}_{\bar{j}}^{neq}(\mathbf{x}_b, t)$. We consider the following second-order approximation [13],

$$\begin{cases} \tilde{g}_{\bar{j}}^{neq}(\mathbf{x}_b, t) = g_{\bar{j}}(\mathbf{x}_f, t) - g_{\bar{j}}^{eq}(\mathbf{x}_f, t) & \Delta \geq 0.75 \\ \tilde{g}_{\bar{j}}^{neq}(\mathbf{x}_b, t) = \Delta [g_{\bar{j}}(\mathbf{x}_f, t) - g_{\bar{j}}^{eq}(\mathbf{x}_f, t)] + (1 - \Delta) [g_{\bar{j}}(\mathbf{x}_{ff}, t) - g_{\bar{j}}^{eq}(\mathbf{x}_{ff}, t)] & \Delta < 0.75 \end{cases}. \quad (19)$$

Note that for this component, there is no difference between Dirichlet and Neumann conditions.

D. Calculation algorithm

The initialization is done by setting all distribution functions with the equilibrium values computed with the given macroscopic initial conditions. Then a successive iteration in time is performed. At each time step, the LBE (8) is first solved, and then the electric field is obtained with Eqn. (11). After that, the LBE (12) is solved with the latest electric field to obtain the charge density distribution. If we also consider the flow motion, the LBE with a body force model should then be solved to obtain the flow velocity field, which will be used to determine the charge density distribution at the next time step.

IV. NUMERICAL TESTS

In [6], our LBM for the coupled Poisson's equation and the charge transport equation has been verified with the hydrostatic regime of the injection induced electroconvection problem in a plate-plate configuration. For this simple geometry case, our LBM for the

potential and charge density shows second order accuracy in space, which is consistent with the accuracy order predicted by the Chapman-Enskog analysis. Here three test cases with a more complex geometry are considered to verify the proposed method. The first two cases only solve the potential equation: one without any space charge and the other one with constant space charge. In the third case, the electric field and space charge distribution are fully coupled with each other.

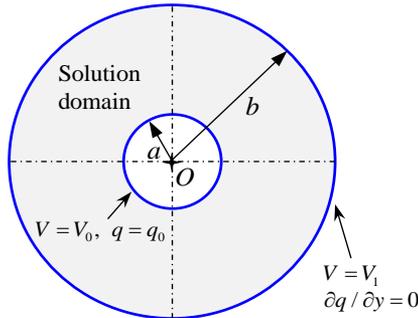


Fig. 3. Modal geometry, solution domain and boundary conditions for the concentric cylinder configuration.

A concentric cylinder configuration is shown in Fig. 3. The geometry of this problem is defined by the radii of the inner and outer cylinders, a and b . A high DC voltage ($V_0 > 0$) is applied to the inner electrode while the outer electrode is grounded ($V_1 = 0$). For the following case A, there is no free charge from the electrode and the charge density in the solution domain is set to be zero or a constant value. For case B, charges are generated at the inner electrode and then enter into the solution domain, thus Eqns. (1-4) are required to be solved simultaneously.

A. Poisson's equation with a wire-cylinder configuration

For the concentric cylinder configuration, the analytical solutions of Eq. (3) are available for both zero and constant space charge cases [16]:

$$V(r) = \frac{q_c}{4\epsilon_0} (b^2 - r^2) + \left[V_0 - \frac{q_c}{4\epsilon_0} (b^2 - a^2) \right] \frac{\ln r - \ln b}{\ln a - \ln b}, \quad (20)$$

Where r is radial distance from the inner cylinder center. For no space charge $q_c = 0$ and constant space charge $q_c = 20\mu\text{C}/\text{m}^3$, with the geometry $2a = 2.77$ mm, $2b = 203.2$ mm, the applied voltage $V_0 = 50$ KV and $\epsilon = \epsilon_0 = 8.854 \times 10^{-12}$ F/m, the analytical and numerical results are shown in Fig. 4. A very good agreement for both cases is readily seen. The numerical results are obtained with a 301×301 lattice nodes. In this case, since the radius ratio between the inner and outer cylinders is fairly small and at least 10 lattice cells are required to represent the inner cylinder, a large number of lattice nodes is required. However, the LBM shows its advantage of using Cartesian grids, easy boundary condition treatment and computational efficiency. To reduce the number of lattice nodes, the non-uniform LBM [17] or the multi-block technique [18] may be considered in the future study.

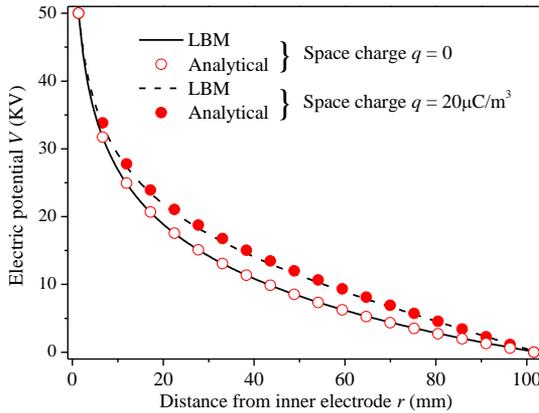


Fig. 4. Comparison between numerical and analytical solutions with the zero or constant space charge cases.

B. Hydrodynamic solutions between two concentric cylinder

In the second case, we consider a uniform distribution of constant charge density q_0 enters into the solution domain from the inner cylinder. Such a process can represent the charge injection at the dielectric liquid/electrode interface and the corona discharge of air close to the electrode. Here we consider the former case with dielectric liquids. The Coulomb force due to the electric field exerting on the injected space charges tends to destabilize the system and to induce flow motion (named the annular electroconvection). Because of the symmetrical characteristic of the configuration and the uniform injection, the problem is characterized by a linear instability bifurcation. In other words, flow motion arises only when the Coulomb force is sufficiently strong and overcomes the damping action of the viscous force. Otherwise, there is no flow motion and system is at the hydrostatic state. The linear stability analysis with this problem was analyzed in [19]. In a recent study [20], we have performed a numerical study with this problem with FVM. The purpose here is to verify our LBM with the hydrodynamic regime solution.

Taking $(b-a)$, V_0 and $\varepsilon V_0/a^2$ as the scales for length, electric potential and charge density, Eqs. (1) and (3) can be transformed into the following dimensionless form (for clarity, the same symbols are used for dimensionless variables),

$$\frac{\partial q}{\partial t} + \nabla \cdot (q\vec{E}) = D\nabla^2 q \quad (21)$$

$$\nabla^2 V = -q \quad (22)$$

where D is the dimensionless diffusion coefficient. The non-dimensional boundary conditions for this problem are: $V_{\text{injector}} = 1$, $q_{\text{injector}} = C$ for inner cylinder and $V_{\text{collector}} = 0$, $\partial q/\partial n = 0$ for outer cylinder. The injection strength parameter C is defined as $C = q_0(b-a)/\varepsilon V_0$. The analytical solution of hydrostatic state with the case of $D = 0$ is:

$$q(r) = A_e [r^2 + B_e]^{-1/2} \quad \text{and} \quad E_r(r) = \frac{A_e}{r} [r^2 + B_e]^{1/2}, \quad (23)$$

where A_e and B_e are two constants depending on the ratio between the radii of cylinders $\Gamma = a/b$ and the injection strength C . For $C = 10$ and various value of Γ , the values of A_e

and B_e can be found in Table 1 of [20].

On Fig. 5 we have displayed the profiles of charge density and the electric field strength in the radial direction versus the modified distance $r^* = (r - a)$ for three radius ratios $\Gamma = 0.1, 0.3$ and 0.5 . For all cases, the computational domain is discretized with 301×301 lattice nodes. A very good agreement between our numerical solutions and the analytical ones is obtained. In particular, the sharp variation of charge density in the region close to the inner electrode is accurately captured; see Fig.5 (a). On Fig. 6 we have presented the charge density iso-contours, and no unphysical-oscillation is observed.

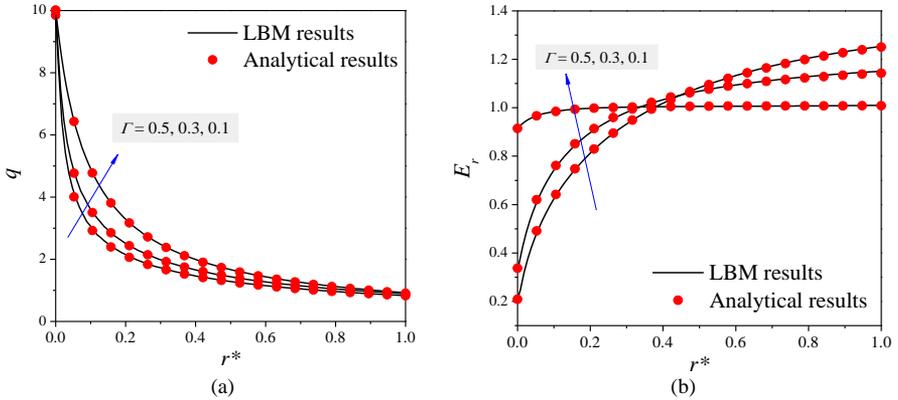


Fig. 5. Comparison between numerical and analytical solutions of the hydrostatic regime with three radius ratios Γ : (a) charge density, and (b) the electric field in the radial direction.

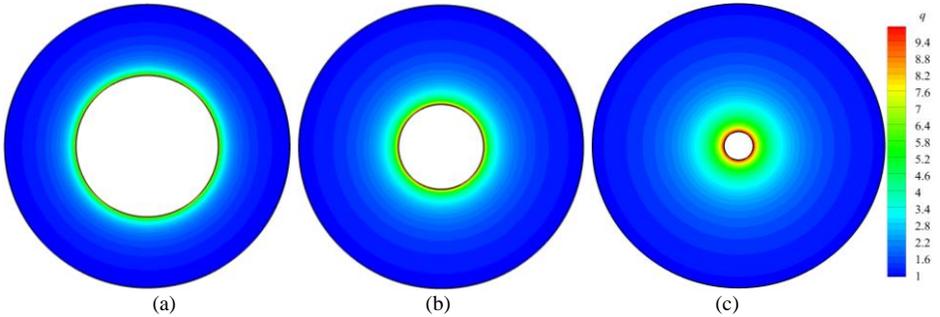


Fig. 6. Iso-contours of the numerical solutions of charge density with three radius ratios Γ : (a) $\Gamma = 0.5$, (b) $\Gamma = 0.3$ and (c) $\Gamma = 0.1$.

C. Annular electroconvection between two concentric cylinders

An attractive advantage of the proposed LBM for electric field-space charge coupled problems is its natural coupling with the LBM for flow motion. An illustration example is provided in this subsection. In [22], we have coupled the LBMs for energy equation and flow motion based on the split-forcing model [23] and investigated the natural convection heat transfer problem with concentric and eccentric cylinders. The same coupling idea is adopted in [6]. We consider the annular electroconvection induced by unipolar injection from the inner electrode. This problem has been carefully investigated by the FVM in [20,

24]. When the Coulomb force is sufficiently strong, the hydrostatic state described by Eqns. (23) is no longer stable and annular electroconvection arises. In the dimensionless form, the Coulomb force is controlled by the electric Rayleigh number T and the ion mobility is expressed through the mobility number M . As shown in Fig. 7b, for the set of parameters ($C = 10$, $T = 210$, $M = 10$, $D = 10^{-4}$ and $\Gamma = 0.5$), the flow shows a steady motion with 8 pairs of counter-rotating vortices, which is the same number as predicted by FVM [20]. The results are computed with 401×401 lattice nodes. We have also compared the amplitude of the fluid velocities, and the maximum difference with the solutions obtained by FVM and LBM is less than 1%. In Fig. 7a, we observe eight regions, which are almost free of charges. This kind of charge void region is a very characteristic feature of Coulomb-driven flows with symmetrically placed electrodes. Our LBM have accurately captured the transition from the charge covered region to the charge void region.

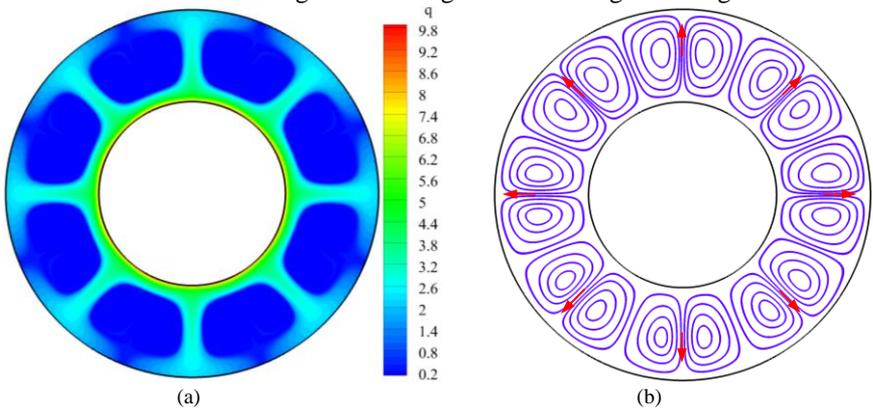


Fig. 7. (a) Charge density distribution and (b) stream function for an injection induced annular electro-convection case. Parameters: $C = 10$, $T = 210$, $M = 10$, $D = 10^{-4}$ and $\Gamma = 0.5$.

V. CONCLUSION

In this paper, we present a lattice Boltzmann model to solve the electric field-space charge coupled problems in complex geometries. Instead of solving the macroscopic equations, two consistent lattice Boltzmann equations are formulated for charge density and electric potential. The curved boundaries are treated by a non-equilibrium extrapolation idea. An attractive advantage of the proposed LBM lies in its direct coupling with the LBM for flow motion. Three test cases with available analytical solutions were used to verify our method. The good agreement between numerical and analytical results demonstrates that LBM is a promising alternative for electric field-space charge coupled problems and EHD flows in simple and complex geometries.

In a future work, we plan to extend the physical model to take into account multi-species ions and non-isothermal field.

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