# Use of the Lattice Boltzmann Equation Method to Simulate Charge Transfer and Electrohydrodynamic Phenomena in Dielectric Liquids

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***Abstract*** - *The Lattice Boltzmann Equation (LBE) method was used to simulate a liquid flow with space electric charge. New approaches to describing the charge transfer due to conduction currenst and convective charge transfer were proposed. Diffusive and mean mass velocity models of convective charge transfer were realized. Electrohydrodynamic flow regimes with prevalence of the conducive or convective mechanisms of charge transport were simulated.*

## 1 Introduction

The Lattice Boltzmann Equation (LBE) method is a relatively new approach in the computational fluid dynamics. Unlike traditional finite-difference methods, in the LBE method a liquid flow is simulated based on a mesoscopic kinetic equation [1]. Major advantages of the method are improved numerical stability and easy in handling of complicated boundary conditions. Different modifications of this method were developed to simulate flows with variable temperature and multiphase flows [2,3]. In the present work, computer simulations of charge transfer and electrohydrodynamics of dielectric liquids were performed by the LBE method specially modified to simulate an electrohydrodynamic flows.

## 2 Lattice Boltzmann Equation method

The LBE method is based on solving the kinetic equation for a certain model system in which special particles can move along the links of a fixed lattice. The evolution equations have form

$$N_i(\vec{x}+\vec{c}_i, t+\tau) = N_i(\vec{x}, t) + \Omega_i(N(\vec{x}, t)).$$

We used a collision operator in the BGK form [4], which means relaxation to the local equilibrium $\Omega_i(N) = -(N_i - N_i^{eq})/\tau_*$. The equilibrium distribution functions $N_i^{eq}$ depend on the local density $\rho = \sum N_i$, flow velocity at a node $\vec{u} = (\sum \vec{c}_i N_i)/\rho$, and temperature, so that the conservation laws for mass, momentum, and energy are satisfied in collisions. In the BGK model, the relaxation time $\tau_*$ governs the transport coefficients: viscosity, heat conductivity, and diffusivity ($1/2 \le \tau_* < \infty$).

In computations we used a one-dimensional model with three values of particle velocity $c_i = -1$, 0, and +1, a two-dimensional model on a square lattice with three velocity values $|\vec{c}_i| =$ 0, 1, and $\sqrt{2}$ (9 possible velocity vectors) [3], and a two-dimensional model with four velocity values $|\vec{c}_i| =$ 0, 1, $\sqrt{2}$, and 2 (13 possible velocity vectors) [2,3]. The basic value of velocity of the particles in the one-dimensional LBE method is $c_{+1} = h/\tau$, where $\tau$ is the time step, $h$ is the length of lattice bond. Hereinafter all values will be in some arbitrary units, in which, for example, $\tau = 1$ and $h = 1$.

## 3 Modeling of liquid flow with impurities of conductive phase

To simulate a liquid flow with a space electric charge, the LBE method was modified to take into account the charge transfer and the change in momentum due to the action of electrodynamic forces.

The charge transfer was calculated in two stages. At the first stage, the charge was passively transported by moving particles of continuous medium (convective transfer and diffusion of the charge). At the second stage, charges move due to the currents in conductive phase of matter.

The diffusive and the mean velocity models of the convective charge transfer were proposed. In the first model, the part of node charge $q(\vec{x})N_i(\vec{x})/\rho(\vec{x})$ is passively transported to the neighboring node together with particles that move in the direction $\vec{c}_i$ and have total mass $N_i$.

The second model is based on the finite-difference method. Electric charge is transferred from one node to another in accordance to the mean mass velocity $u$. For the one-dimensional case, the finite-difference equations have the form

$$\frac{q_j^{n+1} - q_j^n}{\tau} =$$

$$q_{j-1}^n(|u_{j-1/2}| + u_{j-1/2})/2h + q_{j+1}^n(|u_{j+1/2}| - u_{j+1/2})/2h$$

$$-q_j^n(|u_{j-1/2}| - u_{j-1/2})/2h - q_j^n(|u_{j+1/2}| + u_{j+1/2})/2h.$$

In both models there is some diffusion of electric charge, but the charge conservation law is satisfied exactly. As an example, motion of electric charge that is initially distributed as $q(x) = q_0$ at $x_1<x<x_2$ together with a uniform flow of an "incompressible" liquid is shown in Figure 1. The mass velocity of the liquid was constant $u = u_0$ and is equal to 0.1 .

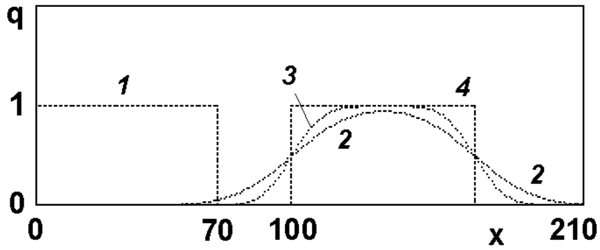


**Figure. 1.** Transformation of charge distribution in a one-dimensional liquid flow in the case of zero electrical conductivity. Initial distribution of charge at time $t = 0$ (curve *1*), diffusive model (curve *2*), mean velocity model (curve *3*), and ideal distribution of charge (curve *4*) after $t = 1000$.

In the first model, the diffusivity is $D_1 = c_s^2\tau/2$, where $c_s$ is the sound velocity. For one-dimensional LBE method described here $c_s = h/\sqrt{3}\tau$ and $D_1 = h^2/6\tau$ . The second model yields a lower value of the diffusivity, which is equal $D_2 = \frac{h^2}{2\tau}\left(1 - \frac{u}{c_{+1}}\right)\frac{u}{c_{+1}}$. For $u = 0$, the diffusivity is absent ($D_2 = 0$) and its maximum value is $D_2\big|_{MAX} = h^2/8\tau$ at $u/c_{+1} = 0.5$.

These formulae for diffusivity of both models were tested for the case of a one-dimensional liquid flow with constant velocity $u_0$ by comparison of numerical results with the well-known exact solution for the diffusion equation

$$q(x) = \frac{Q}{\sqrt{4\pi Dt}}\exp\left(-\frac{(x-u_0t)^2}{4Dt}\right)$$

with the charge $Q$ initially located at the point $x = 0$.

At the second stage of calculations, in the case of conductive liquid Poisson's equation for the electric field potential was solved at every time step together with the equation of electric charge transfer by conduction currents. The system of finite-difference equations was solved by new time-implicit finite-difference method of [5].

The resistance of each bond was calculated using the expression $G = l_{jk}\Big/\sigma_0\sqrt{\rho_j^*\rho_k^*}$ , where $\sigma_0$ is a constant value, $l_{jk}$ is the length of the bond, and $\rho_j^*$ and $\rho_k^*$ are the concentrations of the conductive phase at the edges of the bond.

This expression ensures electric charge transfer by current only inside the region occupied by the conductive phase.

The electrodynamic forces acting on the electric charge at each node are calculated using the distributions of the charge and the electric field potential

$$\vec{F} = q\vec{E} = -q\nabla\varphi.$$

Thus, the local equilibrium state in the collision operator of the LBE method was modified to add the necessary momentum at the lattice site in which the electric charge is in the electric field

$$\rho(\vec{x})\,\Delta\vec{u}(\vec{x}) = \vec{F}(\vec{x})\tau\,.$$

## 4 **Calculations**

An example of purely convective charge transfer and diffusion in compressible liquid is shown in Figure 2. The diffusive model of charge transfer was used. In this case, there are initial discontinuities of density and hence, pressure. The initial charge distribution $q(\vec{x})=q_0\,\rho(\vec{x})$ is proportional to the density. Here $\rho(\vec{x})$ is the liquid density at the node $\vec{x}$, and $q(\vec{x})$ is the electric charge at this node.

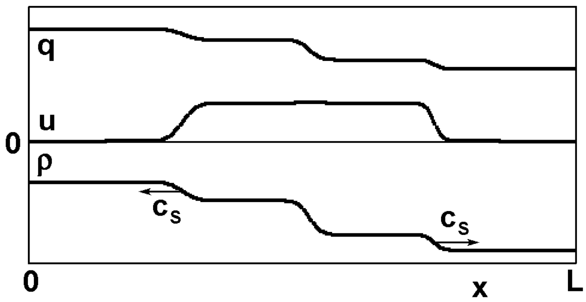


**Figure. 2.** The liquid flow and charge distribution in the case of zero electrical conductivity and electrodynamic forces. Here $L$ is the width of calculation region.

In the calculations, the charge distribution practically coincides with the density distribution (charge is frozen into the liquid). Shock wave propagated approximately with the sound velocity to the right direction from the initial discontinuity. Rarefaction wave propagated in the left direction.

An example of one-dimensional electrohydrodynamic flow in compressible liquid is shown in Fig. 3. Electrical conductivity was zero. Hereinafter the mean mass velocity model of the convective charge transfer was used. At the beginning, the density distribution was uniform $\rho = \rho_0$. The initial mass velocity $u$ was equal to 0. Negative electric charge was initially distributed as $q(x) = -q_0$ at $x_1<x<x_2$.

Solid walls ($u = 0$) were placed at the boundaries $x = 0$ and $x = L$ . The boundary conditions for Poisson's equation were $\varphi = 0$ at $x = 0$ and $\varphi = \varphi_0$ at $x = L$.

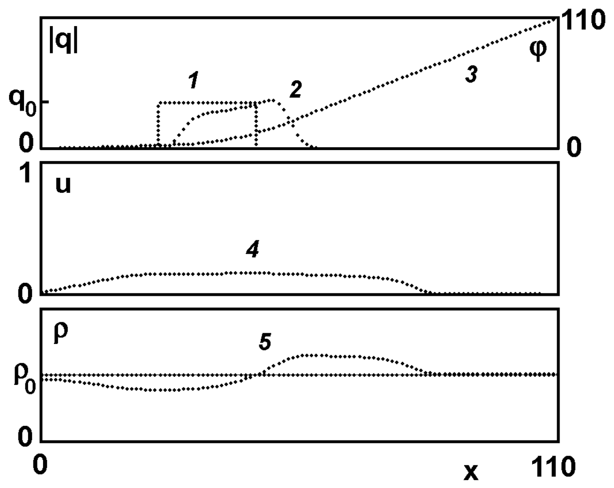


**Figure. 3**. The liquid flow and charge distribution in compressible liquid. Distributions of charge (curve *1* is the initial distribution of charge at time $t = 0$ and curve *2* at $t = 60$). Distributions of electric potential (curve *3*), velocity (curve *4*), and density (curve *5*) at time $t = 60$. $\rho_0 = 1$, $\varphi_0 = 110$, $q_0 = 5.6 \cdot 10^{-3}$, $x_1 = 26$, $x_2 = 46$.

The charge began to move under the action of electrodynamic forces and waves arose in the liquid. A compression wave (shock wave) and a rarefaction wave propagated to the right and left, respectively, from the piece of charge with the velocity of sound (Fig. 3). After some time the charge distribution acquires a certain slope (the charge density becomes higher on the right side of charge distribution). As a whole, the charge moves to the right in the electric field. As mentioned above, there is some diffusion of the electric charge.

It is interesting, that the pressure in the rarefaction wave can become low enough for boiling of liquid at fixed temperature. At later stages of simulations, the shock wave reflected from the right wall and the rarefaction wave reflected from the left one, respectively. Later these waves after many reflections from the walls decayed due to the viscosity of the material.

The similar results were obtained in two-dimensional numerical simulations of the liquid flow by the 13-velocity model [2,3]. The calculations were performed in a rectangular area with periodic boundary conditions in the $y$ direction.

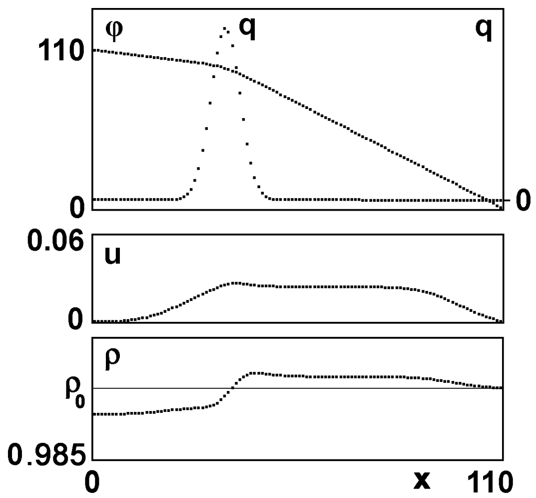


**Figure. 4**. The liquid flow and charge distribution in compressible liquid. $\rho_0 = 1.0$, $\varphi_0 = 110$, $Q = 0.08$, $x_0 = 36$, $t = 70$.

A simulation of the one-dimensional liquid flow is presented in Fig. 4. The positive charge $Q$ was initially distributed in the left side of computation area

$$q(x) = \frac{Q}{\sqrt{2\pi\sigma^2}} \exp\left( -\frac{(x - x_0)^2}{2\sigma^2} \right),$$

so that charge density was constant along $y$ direction. Boundary conditions for Poisson's equation were $\varphi = \varphi_0$ at $x = 0$ and $\varphi = 0$ at $x = L$. As in the previous case, waves arose. At the stage of simulation shown in Fig. 4 the rarefaction wave has already reflected from the left wall.

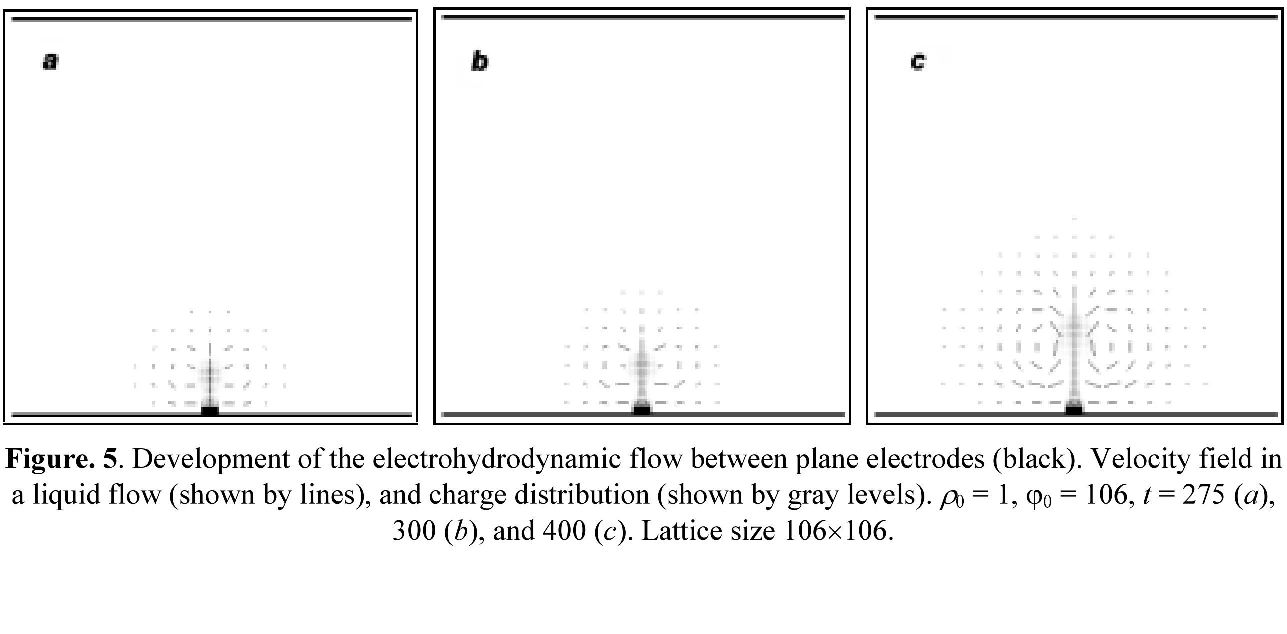


**Figure. 5**. Development of the electrohydrodynamic flow between plane electrodes (black). Velocity field in a liquid flow (shown by lines), and charge distribution (shown by gray levels). $\rho_0 = 1$, $\varphi_0 = 106$, $t = 275$ (*a*), 300 (*b*), and 400 (*c*). Lattice size 106×106.

An example of two-dimensional electrohydrodynamic flow with an electric charge injection is presented in Fig. 5. A liquid flow was computed using the 2D 9-velocity model of [3].

Computations were performed in the rectangular region between two horizontal plane electrodes. Periodic boundary conditions in the $x$ direction were used. Electric potential of the upper electrode was $\varphi=0$, of the lower electrode $\varphi=\varphi_0=106$, so the mean electric field between electrodes was 1. There was a small protrusion 5×2 lattice sites in the middle of the lower electrode. The sites, which are contiguous to this protrusion, were slightly conductive (the conductivity was $\sigma = 2\cdot10^{-4}$).

After the moment of voltage applied, a charge injection began from the protrusion. Then the charged liquid began to move upwards under the action of electrodynamic forces. A viscous flow in the form of a plane vortical dipole moving to the upper electrode was clearly observed. The velocity field and charge distribution at some moments of time are shown in Fig. 5. One can see a charged "drop" moving upwards. The size of region involved in the movement and the magnitude of velocity increased with time. The maximum velocity of liquid was about 0.05. As the head part of injected charge jet increased, electric field at the tip of protrusion decreased. So the new charge injection became more difficult.

## 5 Conclusions

The LBE method allows one to simulate different electric phenomena in liquids including the dynamics of conductive and charged inclusions and also charge injection.

Regimes of electrohydrodynamic flows with prevalence of conductive or convective charge transport mechanisms were investigated.

This method is very promising for application in stochastic models of breakdown in dielectric liquids.

## References


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