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Lattice Boltzmann Equation Method in Electrohydrodynamic Problems

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Abstract *- A consistent LBE model for simulating the electrohydrodynamic (EHD) phenomena is developed. The model includes fluid dynamics, electric charge transport via advection and conduction currents, and action of electric forces upon space charges in liquid. Problems with different thermodynamic phases (liquid and gaseous) and with inhomogeneous electric permittivity and conductivity can also be simulated, as well as charge injection and recombination.*

1 Introduction

In simulations of EHD problems, following physical phenomena should be consistently modeled: hydrodynamics, transport of electric charge carriers, evolution of electric potential distribution, action of electric field on charged liquid.

The Lattice Boltzmann equation (LBE) methods [1-3] are widely used for solving the hydrodynamic Navier–Stokes equations. Because of their kinetic nature, these methods possess high numerical stability, and complex boundary conditions are easy to implement. Multiphase and multicomponent flows can also be simulated with moderate computation cost.

Finite-difference methods was previously used for calculation of charge transfer. In these methods, the value of charge diffusivity is large enough [4,5]. Moreover, it is not constant and depends on velocity of fluid $\mathbf{u}$ as $D = 3\Delta t|\mathbf{u}|\left(h/\Delta t - |\mathbf{u}|\right)$ [5]. In [5], we proposed another method to calculate convective and diffusive charge transport in that charge diffusivity is velocity-independent and can be adjusted.

In present work we used the Lattice Boltzmann equation methods for solving the equations for concentrations of carriers of electric charge.

2 Equations

Hydrodynamic equations are the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \mathbf{u}) = 0, \qquad (1)$$

and the Navier-Stokes equation

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \Pi^{(0)}_{\alpha\beta} = \mathbf{F} + \eta \nabla^2 \mathbf{u} + (\zeta + \frac{\eta}{3})\mathrm{grad}\,\mathrm{div}\,\mathbf{u}. \qquad (2)$$

Here, ρ is the density of liquid, $\mathbf{u}$ is the velocity of fluid flow, $\Pi^{(0)}_{\alpha\beta} = p\delta_{\alpha\beta} + \rho u_\alpha u_\beta$ is the non-viscous part of the momentum flux tensor.

Equations for concentrations n_i of carriers of electric chargé are

$$\frac{\partial n_i}{\partial t} + \nabla(n_i \mathbf{u}) = D_i \Delta n_i - \mathrm{div}(\frac{q_i}{|q_i|} b_i n_i \mathbf{E}) + w_i - r_i. \qquad (3)$$

Here, D_i are the diffusivities, b_i are the macroscopic effective mobilities of charges carriers q_i; w_i, r_i are the rates of ionization and recombination of charge carriers.

The Poisson's equation for potential of electric field φ is

$$\mathrm{div}(\varepsilon \nabla \varphi) = -4\pi q, \qquad \mathbf{E} = -\nabla \varphi, \qquad (4)$$

The electric force acting on the space charge $q = \sum q_i n_i$ in a liquid is

$$\mathbf{F} = q\mathbf{E} = -q\nabla\varphi. \qquad (5)$$

The electric current could be expressed as

$$\mathbf{j} = \sum (q_i n_i \mathbf{u} - D_i q_i \nabla n_i + b_i |q_i| n_i \mathbf{E}) = q\mathbf{u} - \sum D_i q_i \nabla n_i + \sigma \mathbf{E}, \qquad (6)$$

Here, the local conductivity $\sigma = \sum b_i |q_i| n_i$ depends on local concentrations of charge carriers and can be not constant in space and in time.

3 Method of splitting

To solve the system of equations (1)–(5), the method of splitting on physical processes [6] is used. The whole time step is divided into several stages implemented sequentially. These stages are

1. Modeling of hydrodynamic flows.
2. Simulation of convective transport and diffusion of charge carriers.
3. Calculation of electric potential and charge transfer due to mobility of charge carriers.
4. Calculation of electrostatic forces acting on space charges in liquid.
5. Simulation of phase transition or interaction between immiscible liquids.

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3.1. Modeling of hydrodynamic flows

For simulation of hydrodynamic flows, the LBE method [1-3] was used. The evolution equations for single-particle distribution functions $N_k(\mathbf{x},t)$ have the form

$$N_k(\mathbf{x}+\mathbf{c}_k\Delta t, t+\Delta t) = N_k(\mathbf{x},t) + \\ + (N_k^{eq}(\rho,\mathbf{u}(\mathbf{x},t)) - N_k(\mathbf{x},t))/\tau + \Delta N_k, \quad (7)$$

where $\mathbf{c}_k$ are the particle velocities, Δt is the time step (lattice vectors are $\mathbf{e}_k = \mathbf{c}_k\Delta t$), ΔN_k are the changes of distribution functions due to action of volume forces.

Equilibrium distribution functions are

$$N_k^{eq}(\rho,\mathbf{u}) = \rho w_k\left(1+3\mathbf{c}_k\mathbf{u}+\frac{9(\mathbf{c}_k\mathbf{u})^2}{2}-\frac{3\mathbf{u}^2}{2}\right). \quad (8)$$

Here, $\rho = \sum_k N_k$ and $\rho\mathbf{u} = \sum_k \mathbf{c}_k N_k$. For the two-dimensional nine-velocity D2Q9 model [3] ($|\mathbf{c}_k| = 0$, 1 or $\sqrt{2}$) on a square lattice (Fig. 1), the weight coefficients are $w_0 = 4/9$, $w_{1-4} = 1/9$, and $w_{5-8} = 1/36$. The reduced relaxation time τ determines the kinematic viscosity $\nu = \frac{h^2}{3\Delta t}(\tau - 1/2)$.

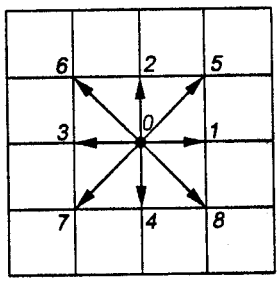

Fig. 1.

The exact difference method (EDM) was specially developed for LBE [7] to take into account the action of electric forces on space charges in a liquid

$$\Delta N_k = N_k^{eq}(\rho,\mathbf{u}+\Delta\mathbf{u}) - N_k^{eq}(\rho,\mathbf{u}). \quad (9)$$

Here $\Delta\mathbf{u} = \mathbf{F}/\rho\cdot\Delta t$ is the velocity change due to body force $\mathbf{F}$ during time step Δt.

3.2. Convective transport and diffusion of charge carriers

Equations of convective transport of every type of charge carriers and their diffusion, ionization and recombination

$$\frac{\partial n_i}{\partial t} + \nabla(n_i\mathbf{u}) = D_i\Delta n_i + w_i - r_i \quad (10)$$

are solved using the method of additional LBE components with zero mass (passive scalar) [5] similar to one used in [8].

The evolution equations for distribution functions $Q_{ki}(\mathbf{x},t)$ for every type of charge carriers q_i are

$$Q_{ki}(\mathbf{x}+\mathbf{c}_k\Delta t, t+\Delta t) = Q_{ki}(\mathbf{x},t) - \\ - (Q_{ki}(\mathbf{x},t) - Q_{ki}^{eq})/\tau_i. \quad (11)$$

Equilibrium distribution functions $Q_{ki}^{eq}(q,\mathbf{u})$ depend on concentrations of every type of charge carriers $n_i q_i = \sum_k Q_{ki}$ and on fluid velocity $\mathbf{u}$

$$Q_{ki}^{eq}(q,\mathbf{u}) = n_i q_i w_k\left(1+3\mathbf{c}_k\mathbf{u}+\frac{9(\mathbf{c}_k\mathbf{u})^2}{2}-\frac{3\mathbf{u}^2}{2}\right). \quad (12)$$

Diffusivities $D_i = \frac{3h^2}{\Delta t}(\tau_i - 1/2)$ can be adjusted independently changing the relaxation times τ_i.

The exact values of rates of ionization w_i and recombination r_i of charge carriers in liquids are unknown, but some discussion and approximate laws for weakly conductive liquids could be found in [9].

3.3. Calculation of electric potential and charge transport due to mobility of charge carriers (conductivity)

A finite-difference method is used to calculate the electric potential φ with charge transfer due to mobility of charges carriers in electric field. Transport of electric charge via mobility of charges carriers is computed simultaneously with the solution of Poisson equation for potential of electric field. The time-implicit finite-difference equations for the concentrations of charge carriers were substituted into the Poisson equation as it was done in [10]. The resulting equations for all concentrations of charge carriers n_i^{n+1} and values of potential φ^{n+1} at the next time step $n+1$

$$n_i^{n+1} = n_i^n + \tau\,\mathrm{div}\left(\frac{q_i}{|q_i|}b_i n_i^{n+1}\nabla\varphi^{n+1}\right), \\ \mathrm{div}(\varepsilon\nabla\varphi^{n+1}) = -4\pi\sum q_i n_i^{n+1}, \quad (13)$$

were solved by the method of iterations.

Charge injection from the surface of electrodes can be modeled introducing certain electric conductivity near electrodes.

3.4. Action of electrostatic forces on space charges in liquid

The total charge density in the node q was calculated from equation

$$\Delta\varphi = -4\pi q. \quad (14)$$

It takes into account both free space charge density and charge density due to non-uniform polarization of dielectrics. Electric field $\mathbf{E}$ acting on this charge was calculated as numerical derivative of electric potential. In finite-difference form we have

$$F_x = -q_{i,j}(\varphi_{i+1,j} - \varphi_{i-1,j})/2h, \qquad F_y = -q_{i,j}(\varphi_{i,j+1} - \varphi_{i,j-1})/2h. \tag{15}$$

Use of the central differences excludes the contribution of charge density in given site to the electric field there, hence, the self-action of charge is avoided.

3.5. Phase transitions

Phase transitions are simulated in LBE method using the method of Shan and Chen [11]. To describe the phase transition in this model, the attractive forces were introduced between every neighbor nodes. For two-dimensional case we have

$$\mathbf{F}(\mathbf{x}) = \psi(\rho(\mathbf{x}))\sum_k G_k \psi(\rho(\mathbf{x}+\mathbf{e}_k))\mathbf{e}_k . \tag{16}$$

Here $G_k > 0$ are the coefficients that are different for basic and diagonal directions, $\psi(\rho)$ is an increasing function of density (effective mass). We used the following function as suggested in [11]

$$\psi(\rho) = \rho_0(1-\exp(-\rho/\rho_0)). \tag{17}$$

To ensure the isotropy of space, coefficients for the force must satisfy the equation $G_1 = G_0/4$. Here, G_0 is the coefficient for basic directions, and G_1 is the coefficient for diagonal directions. In this case, the equation of state for isothermal model is

$$P = \rho\theta - \frac{3}{2}G_0\psi^2(\rho), \tag{18}$$

where $\theta = 1/3$. The critical point is $G_{0*} = 4/9$ and $\rho_* = \rho_0 \ln 2$. For the values of $G_0 > G_{0*}$, coexistence of dense (liquid) and rarefied (gaseous) phases is possible.

3.6. Simulation of immiscible liquids

For simulations with two immiscible liquids, we used the method of Shan and Chen [11]. In the simplest case, the interactions between every neighbor nodes were introduced in form

$$\mathbf{F}_s(\mathbf{x}) = \psi(\rho_s(\mathbf{x}))\sum_\lambda\sum_k G_{ks\lambda}\psi(\rho_\lambda(\mathbf{x}+\mathbf{e}_k))\mathbf{e}_k , \tag{19}$$

Here, we denote the components by the indexes s and λ. In the case of two liquids, every index can take values 1 or 2. ρ_s are the densities of components at the nodes.

The total fluid density at a node depends on densities of components as $\rho = \sum_s \rho_s$, where $\rho_s = \sum_s N_{sk}$. Here, N_{ks} are the single-particle distribution functions for each component. The total momentum at a node is $\rho\mathbf{u} = \sum_s \rho_s \mathbf{u}_s$, where $\mathbf{u}$ is the mean velocity, $\rho_s\mathbf{u}_s = \sum N_{sk}\mathbf{c}_k$ are the momenta of components. The interaction forces change the velocity of each component at the node $\Delta\mathbf{u}_s = \mathbf{F}_s\Delta t/\rho_s$, that should be taken into account in the collision operator for every component $\Omega_{ks}(\rho_s, \mathbf{u}_s)$. In our simulations, we used the same relaxation time τ for different liquids. It means that the viscosities of these liquids were equal.

In simulations with two immiscible liquids without phase transition, we used $G_{kss} = 0$, $G_{ks\lambda} = G_{k\lambda s} > 0$, $G_{1s\lambda} = G_{0s\lambda}/4$ and the following simplest function $\psi(\rho) = \rho$.

4 Results

We investigated deformation and fragmentation of conductive gas bubbles in electric field, the dynamics of gas bubbles caused by electrostriction, and deformation of liquid drops with electric permittivity different from this of main liquid.

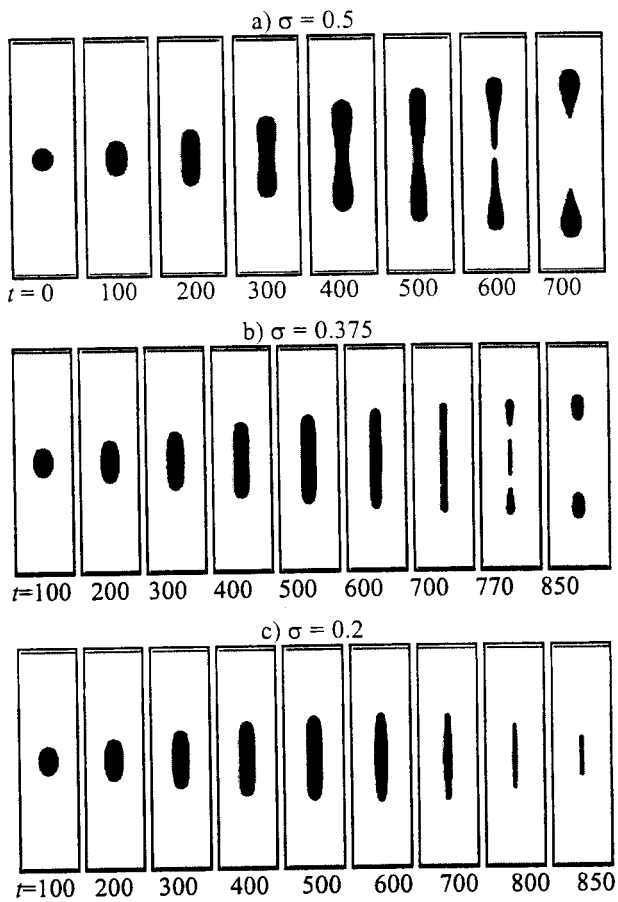

Fig. 2. Deformation and breakup of vapor bubble in electric field at different conductivity inside the bubble. Lattice size 250×65.

The electric strength of gases is much lower than that of liquids. Hence, the electric breakdown occurs when vapor bubbles grow to a certain critical size. After breakdown, the bubble becomes conductive, and it is deformed under the action of electric field. The dynamics of bubble deformation is shown in Fig. 2. Dark color corresponds to lower density.

At comparatively high conductivity, bubble grows and elongates (see Fig. 2,a). Then, a neck arises at the equator, and bubble breaks into two smaller ones.

At lower conductivity inside the bubble, the deformation proceeds slower, and two necks can appear resulting in the emission of two bubbles from the poles of the original one (Fig. 2,b). The central bubble has practically no charge and, hence, it collapses rapidly.

Finally, in the case of even lower conductivity, the external pressure prevails, and the bubble first elongates and then collapses (Fig. 2,c).

Similar processes are observed at the breakdown of dielectric liquids [12]. At the incomplete breakdown, the streamer channel decays to the chain of bubbles, which then disappears rapidly.

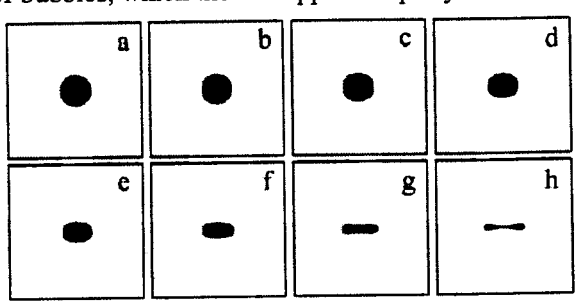

Fig. 3. Deformation of vapor bubble due to electrostriction. $t =$ 60 (a), 100 (b), 140 (c), 180 (d), 220 (e), 260 (f), 300 (g), 340 (h).

Usually, electric permittivity of substances depends on density. This leads to deformation of samples in electric field (electrostriction). We simulated the evolution of a bubble in dielectric liquid with permittivity $\varepsilon = 1 + \rho/\rho_e$.

Results are shown in Fig. 3. Dark color corresponds to lower density. Electrodes were placed at the top and bottom boundaries of computation area, with periodic boundary conditions at the side boundaries. When the voltage was applied, the bubble gradually flattened and later broke into two smaller ones. The total volume of the bubble also decreased due to the compression by electrostriction forces.

The dynamics of liquid drops with electric permittivity ε_1 different from permittivity of main dielectric liquid ($\varepsilon = 1$) in external electric field was studied (Fig. 4 and Fig. 5).

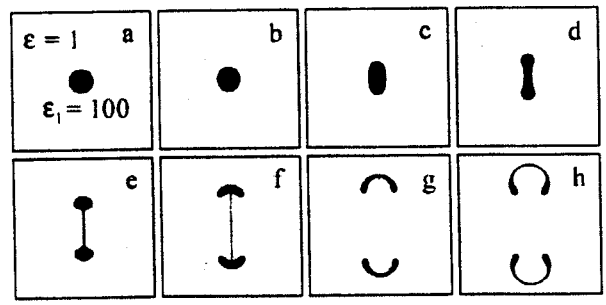

Fig. 4. Liquid drop with electric permittivity different from one of main liquid dielectric in external electric field. $\varepsilon_1 = 100$, $E_a = 0.035$. $t =$ 0 (a), 100 (b), 200 (c), 300 (d), 400 (e), 500 (f), 600 (g), 700 (h).

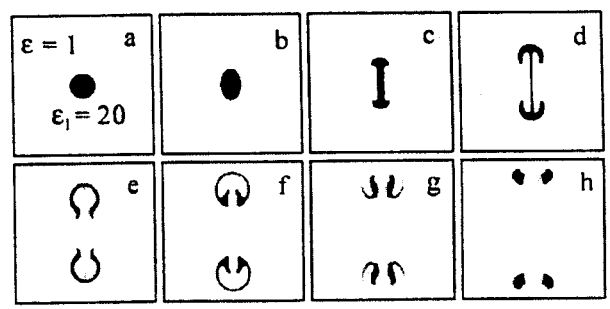

Fig. 5. Liquid drop with electric permittivity different from one of main liquid dielectric in external electric field. $\varepsilon_1 = 20$, $E_a = 0.1$. $t =$ 0 (a), 100 (b), 200 (c), 300 (d), 400 (e), 500 (f), 600 (g), 700 (h).

In the case shown in Fig. 5, the vortices are more pronounced than for simulation shown in Fig. 4 despite the lower value of ε_1. The reason of this is the higher value of external electric field E_a resulting in higher electric forces that are proportional to $\varepsilon E_a^2(\varepsilon_1 - \varepsilon)/\varepsilon_1$.

5 Discussion and conclusions

A new method for simulating the EHD phenomena is developed. It provides the consistent model of all physical processes involved. Hydrodynamic flows and convective and diffusive transport of charge carriers are simulated by the LBE scheme, as well as interaction of liquid components and phase transitions and action of electric forces on a charged liquid. Evolution of potential distribution and conductive charge transport are calculated using the finite difference method.

Simulations show the great potential of the method especially for problems with free boundaries (systems with vapor bubbles and multiple components with different electric properties).

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