Study of Microstructure of Dielectric Liquid in High Electric Field

Molecular Dynamic Simulation

D. I. Karpov A. L. Kupershtokh

Lavrentyev Institute of Hydrodynamics
Novosibirsk, Russia
karpov@hydro.nsc.ru

Abstract*—The method of molecular dynamics (MD) was applied to study the processes in liquid and dense gas under the action of an extremely high electric field. Two following model for a dielectric was used. A substance consisted of the molecules with a constant electrical dipole moment. The parallel code was specially developed using the CUDA technology in order to produce the computations of large ensembles of the molecules with the MD method using the high-performance graphic cards. The correlation function of the orientation of the dipole molecules was calculated for various densities of the substance. The density dependence was studied of the radius of the region in which the ion influences on the molecules with the constant dipole moment. The density dependency of the electric potential well depth near the ion placed in a polar dielectric was obtained. The formation of vapour channels in a liquid dielectric under the action of extremely high electric field (anisotropic spinodal decomposition) was also simulated. It was shown that channels are formed approximately along the electric force lines and the process looks like the formation of cracks in solid body due to mechanical stresses. The results obtained are important for understanding the microprocesses preceding a streamer formation during the process of discharge development in dielectric liquids.

Keywords — ion in dense media; breakdown of dielectric liquids; molecular dynamics; phase transitions; electrostriction.

I. INTRODUCTION

The processes of conduction and breakdown in dense fluids are closely related to the development of various electrohydrodynamic (EHD) flows. The EHD study is important both for fundamental scientific researches and also for industrial applications (such as designing microdosage devices, EHD-pumps and so on). The electric-field forces produce flows in electrolytes and in dielectrics by different mechanism. The movement of an ion involving the part of the fluid causes flows in electrolyte. For the dielectric, the body forces acting on dipole molecules in non-uniform electric field. Both mechanisms are operative in real fluids containing both polar molecules and ions.

The mean free path of the electron is very small in liquids, therefore the electrical breakdown inception in dielectric liquids can not be explained with the mechanisms of impact ionization or electronic avalanches development. Another mechanism is based on the idea of the electrical discharges in cavities that exist on the electrode surfaces or in the volume or arise after the high voltage application. The three basic mechanisms of breakdown in liquids are discussed. The first one is the heating of the liquid with ionic electric currents. The second one is the phase transition because of the local pressure decrease near the electrodes under the action of electric forces on the injected electric charges (the so called electrodynamic cavitation). The third mechanism is the anisotropic instability with the decay into the system of the vapour channels in a liquid due to electrostriction forces [1,2].

The conventional methods of continuum mechanics do not allow studying such processes at micro- and mesoscales. The most appropriate tool for the study of these microprocesses and revealing new processes is the molecular-dynamic method. There are only several works that are devoted to the studies of EHD microflows with this MD method [3] or with the combination of the MD method with conventional finite-difference methods (so called hybrid methods) [4]. The main obstacle for applying the MD method to the problems of fluid flows is the limited capability of the modern computing systems. Ten years ago the simulations of the MD ensemble of the order of 10^6 particles was possible only using computer cluster. The number of the particle was by a several order of magnitude less if the electric interaction was taken into account. The evolution of the ensemble could be calculated up to time intervals about 1 ns. At present, high performance computations with use of the graphic processing units (GPU) allow performing physical properties of significantly larger ensembles than earlier and for longer periods of time.

The MD method was applied to study the anisotropic spinodal decomposition under the action of a high electric field in [5] for the ensemble of 1000 particles. This number of particle is insufficient for understanding the decay dynamics. In this work, we realized the MD method taking into account the electrical forces in a polar dielectric with the action of high electric fields on GPU. The CUDA technology of programming was used. This allows us increasing the number of the particles in an ensemble more than by the order. Using a simple model of a dielectric substance, we studied the region of influence of a “free” ion on the molecules around it.

978-1-4799-2063-1 $31.00 ©2014 IEEE

Fig. 1. Spinodal decay of a polar dielectric liquid in a high electric field. The MD ensemble consists of 11000 particles.

II. PARALLEL COMPUTATIONS

Graphic processing units have a possibility of massive parallel computations using hundreds calculating cores. For GPU programming we use the CUDA technology. The significant acceleration of the computations using GPU is due to 1) a large number of cores, 2) the fact that up to 80 percent of the electronic components inside GPU are specialized on only arithmetic calculations, 3) the data exchange rate between GPU and inner memory is very high, and others.

The graphic accelerator NVIDIA GeForce GTX-580 having 512 CUDA cores was used in our work. All the cores have an access to the fast enough internal GPU memory of the size of 3GB. The parallel programming implies run of hundreds million calculating threads performing relatively simple calculations for each pair of the particles or each particle.

The calculations of the particle pair interactions take up to 98 percent of the simulation time. The time of calculation of pair interaction increases proportionally to $N(N-1)/2$ (here N is the total number of the molecules). At parallel algorithm of computations, long interacting pair forces are calculated in separate thread for each particle. Thus, the double cycle of the calculations for all pairs of particles in linear program becomes a single cycle for each particle in parallel case. Thus, instead of the square-law dependence of the computation time on the value of N, we have only linear dependence.

It is sufficient to parallelize the force calculations that were performed for the first time in [6]. There are specially designed software packages for MD simulations with GPU (e.g. [7]) but it takes special adaptation of the packages for the purposes of this work that are comparable with the efforts of designing the original software. Thus, we developed the computer program for the MD simulations in the presence of high electric field. The use of the GPU increases the calculation rate from 40 to 50 times.

III. ANISOTROPIC SPINODAL DECAY

Molecules were modeled with spherical particles interacting in accordance with the Lennard-Jones potential. The electrical interactions were calculated using the Coulomb law. Two point charges (positive and negative) of the same absolute quantity were placed symmetrically in each molecule. The molecules were placed into the rectangular region. The upper and lower borders of the region were considered as the electrodes. The uniform external electric field was applied to this region after thermalization of this ensemble (approximately 100000 time steps). The molecules rotated orienting in average along the electric force lines. At the microscopic level, the molecules formed structures looked like chains such that the positive charge of one molecule attracted to the negative charge of another one. This effect led to the local increase of the density near the chain and to the density decrease far from it. Thus, the conditions arose for the formation of the cavity in which the density was smaller.

Figure 1 shows the snapshot of the ensemble after high voltage application. Small cavities extended along electric force lines are formed in the liquids due to the action of tensile stresses. Then, several cavities combined with the formation of large elongated cavity. We saw in our simulations that the formation and the growth of the channels resembled the formation of mechanical cracks in solids. The estimations showed that the time of the cavity formation is in sub nanosecond range. The growth of the cavity causes a compression wave that is observed indirectly as subsequent change of local densities of substance around the cavity.

The extremely high electric field of the order of 10 MV/cm was in the cavity as in the liquid phase. This field is not sufficient for a liquid breakdown but it is more than by the order higher than the breakdown strength of the vapour in the cavity. The results of simulations as well as experimental results do not allow to predict the vapour density, the electric field strength and the time corresponding to the discharge of the vapour cavity. Nevertheless, a rough enough extrapolation from the low fields and densities showed that the time of discharge does not exceed 1 nanosecond. The mechanism of the anisotropic spinodal decomposition can explain formation of very fast filamentary streamers with the tip velocity more than 100 km/s in dielectric liquids at the application of extremely high voltage.

IV. SIMULATION OF AN ION IN DENSE DIELECTRIC MEDIA

Slow discharge structures looked like non-transparent formations with strongly irregular boundary near the electrode develop under at the local electric field strengths of the order of 1 MV/cm. They velocities of their expansion are from 100 m/s up to about 1 km/s. The simulation of the growth of gas cavities in the electric field was performed in [8]. It was shown that the growth dynamics and the development of the EHD flows are governed with the electric field acting on injected ions near the vapour-liquid interface. Therefore, the question about the ion movement in a dielectric liquid is of special interest.

The size of the ion influence zone on the neighbor polar molecules of the liquid dielectric and microstructure of the ion environment were studied at various densities of the liquid.

978-1-4799-2063-1 $31.00 ©2014 IEEE

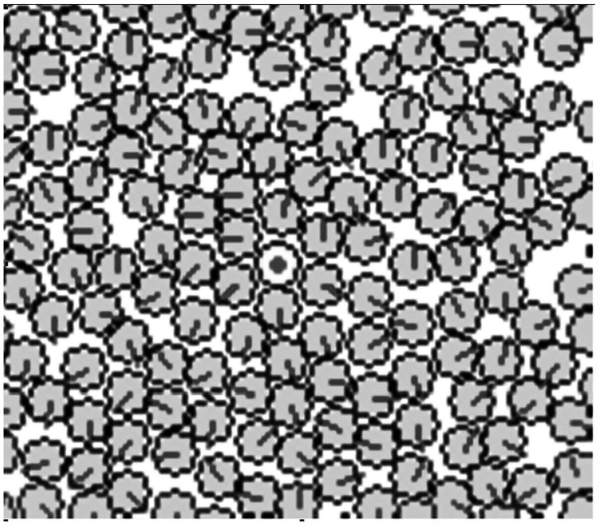

Fig. 2. Dipole orientations (circles with arrows) in dense media near the ion (the circle with the point).

A positive ion was placed to the substance of polar molecules after initial thermalization of the ensemble. The dipole orientations depend on the strength and the local direction of the radial electric field of the ion and on the dipole-dipole interaction with the neighbor molecules. The dipole moments are oriented in average radially from the ion. It is most evident in the nearest neighborhood of the ion (fig. 2).

A correlation function $\gamma(r)$ between dipole moment orientations of a molecule and the direction from the molecule to the ion was calculated according to

$$\gamma(r) = \frac{1}{2\pi\, r\, n(r)} \sum_{i=0}^{n(r)} (p_i \cdot r_i), \qquad (1)$$

here r is the distance from the ion, r_i is the distance from the ion to the particle with the number i, p_i is the dipole moment of the i-th particle. The summation is performed over all the dipoles in a thin layer at the distance from r to $(r + \Delta r)$ from the ion.

The values of the correlation function are strongly fluctuating during simulations. Therefore, the calculated values of (1) were averaged for time intervals of duration of 400000 time steps.

The plot of the correlation function is a decaying curve having maximum at the ion position. This curve is well approximated by the exponent of the form

$$f(r) = A\exp(-r / \Delta_r) + B. \qquad (2)$$

The parameter Δ_r is the characteristic radius of the region of the ion influence on the dipoles. In this region, the orientation of the dipole molecules depends primarily on the ion electric field.

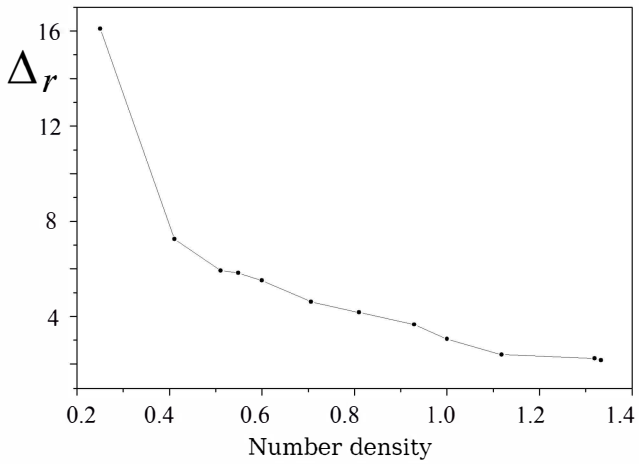

Fig. 3. The density dependence of the characteristic radius Δ_r.

For example, the ion influence decays at the distance of 3 - 4 molecular diameter (from 30 to 50 molecules in the sphere of radius of Δ_r) at the relative density $\rho = 0.549$. One can expect that the ion mobility decreases because of the collective movement of this shell together with the ion.

We performed the MD simulations for series values of the substance density and calculated the dependence of the size of the ion influence region of dipole orientations on the density. The results were averaged over 3-4 runs for each value of the density. Then, the correlation function for each ρ was approximated with the formula (2) and the parameter Δ_r was calculated.

The density dependence of Δ_r is shown in the fig. 3. The results show that the size of the region of the ion influence decreases when the density increases. The reason is that the rotation of the polar molecule is hindered in more dense media due to the stronger dipole-dipole interaction.

The dependence of the electric field potential on the distance from the ion $\varphi(r)$ in dense polar dielectric was calculated. The electric field fluctuates very greatly with the local density fluctuations near the ion. Therefore, we calculated the averaged values of the electric potential in dependence of the distance from the ion for fixed distances. The averaging over the angle was performed at each time step. The averaging in time was performed also for each distance for a period of 400000 time steps.

Fig. 4 shows the radial dependence of the electric field potential $\varphi(r)$. The more the density of the substance the more the depth of the potential well. Global and local minima of the function $\varphi(r)$ (fig. 4) correspond to the local excess of the negative charge. The maxima correspond to the local excess of the positive charges.

Thus, the potential well around the ion in dense dielectric media was simulated in the two-dimensional model with the MD method.

978-1-4799-2063-1 $31.00 ©2014 IEEE

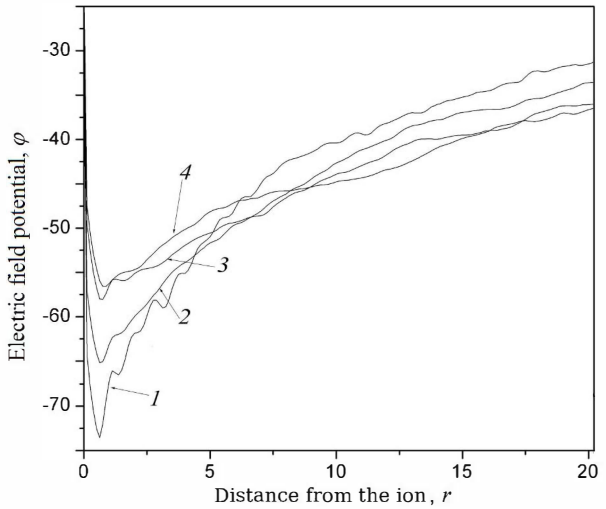

Fig. 4. The dependence of the electric field potential on the distance from the ion. $\rho = 1.1$ (1), $\rho = 0.929$ (2), $\rho = 0.705$ (3), $\rho = 0.52$ (4).

V. CONCLUSION

The MD method was applied to simulations of dielectric liquids and dense gases. We considered ensembles of polar molecules and molecules with possible polarization of them in the electric fields. The microstructure of dielectric liquids was studied in external electric field and in the field of an ion imbedded into the medium. It was shown that the decay of initially uniform liquid into the system of channels of lower density in a liquid can occur under the action of strong electric field. This new phase of lower density forms the condition for electric breakdown inception.

The ion imbedded into the liquid or gaseous dielectric creates the local strong electric field in which the neighbor dipoles of molecules are oriented in average radially from the ion. This layer of electric dipoles screens partially the electric field of the ion.

ACKNOWLEDGMENT

This work was supported by the grant of the Russian Foundation for Basic Researches (No. 13-08-00763).

REFERENCES

1. A.L. Kupershtokh and D.A. Medvedev “Anisotropic instability of a dielectric liquid in a strong uniform electric field: Decay into a two-phase system of vapor filaments in a liquid,” Physical Review E, vol. 74, no. 2, 2006, pp. 021505(1-5).
2. Kupershtokh A.L. Three-dimensional LBE simulations of a decay of liquid dielectrics with a solute gas into the system of gas–vapor channels under the action of strong electric fields. Computers and Mathematics with Applications, 2014, vol. 67, no. 2, pp. 340-349.
3. W.D. Luedtke, Jianping Gao, and Uzi Landman “Dielectric nanodroplets: structure, stability, thermodynamics, shape transitions and electrocrystallization in applied electric fields,” J. Phys. Chem. C, vol. 115, 2011, pp. 20343-20358.
4. Jie Sun, Ya-Ling He, and Wen-Quan Tao “Molecular dynamics–continuum hybrid simulation for condensation of gas flow in a microchannel,” Microfluidics and Nanofluidics, vol. 7, no. 3, 2012, pp. 407-422.
5. D.I. Karpov and A.L. Kupershtokh “Anisotropic spinodal decay of polar dielectric in strong electric field: method of molecular dynamics,” Technical Physics Letters, vol. 35, no. 5, 2009, pp. 479-482.
6. I. Buck, V. Rangasayee, E. Darve, V. Pande, and P. Hanrahan, “Accelerating molecular dynamics with GPUs,” Proceedings of ACM Workshop on General Purpose Computing on Graphics Processors, (http://www.cs.unc.edu/Events/Conferences/GP2/proc.pdf)
7. J.A. Anderson, C.D. Lorenz, and A. Travesset “General purpose molecular dynamics simulations fully implemented on graphics processing units,” Journal of Computational Physics, V. 227, no.10, 2008, pp. 5342-5359.
8. A.L. Kupershtokh, D.I. Karpov, D.A. Medvedev, C.P. Stamatelatos, V.P. Charalambakos, E.C. Pyrgioti, and D.P. Agoris “Stochastic models of partial discharge activity in solid and liquid dielectrics,” IET Sci. Meas. Technol., vol. 1, no. 6, 2007, pp. 303-311.

978-1-4799-2063-1 $31.00 ©2014 IEEE