The pre-breakdown characteristics of weakly ionized media in the high non-uniform electric field using calculations with refined grid cells

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Abstract. The theoretical model of a pre-breakdown ions formation in a liquid dielectric and their flows, caused by high non-uniform electric field is represented. The 3D system of the macroscopic pre-breakdown electrohydrodynamic equations is written. Influence of the electric field on the molecule dissociation rate is taken into account. The system includes the Poisson equation for electric field potential, the equation of ions formation and the Navier-Stokes equations with electric force. In addition, results of modelling using refined mesh are presented.

1. Introduction

Deviations from the Ohm’s law for weakly ionized solid media in pre-breakdown uniform electric fields experimentally discovered by Poole about 100 years ago [1]. In a weakly conductive liquid media the same experimental effect was obtained by Wien about 100 years ago also [2]. Deviations from the Ohms law for gaseous were also obtained in high electric field many years ago.

Theoretically exponential effect for significant number of media was explained by Frenkel for solid dielectrics. This effect was also explained by Onsager [2] for liquid weak electrolytes and for weakly conductive liquid dielectrics. Forming of hydrodynamic flows and space charge had been observed in these dielectrics at a pre-breakdown conditions [3].

Formation of space charge occurs in a pre-breakdown field while establishing of all electrohydrodynamic characteristics, according to [4]. Stable conductivity can be unipolar (type of corona discharge) or quasi-neutral (type of plasma or electrolyte). Theoretical and experimental pre-breakdown current-voltage characteristics of considered media in non-uniform electric fields had been described in [5]. The goal of present work is to study the electrohydrodynamic flows, caused by high non-uniform electric field, mostly in numerical way. These flows of rather high intensity are observed in fluids such as transformer oil [6, 7] of in fluids with complex molecular structure [8]. Transfer of space charge, which is created under the influence of electric field, was described in [9]. Influence of surface effects of high voltage electrode on pre-breakdown electrohydrodynamic flows was researched in the review [7]. This influence should be considered when designing high voltage electrodes. Influence of volume effects on the considerable flows is dominated, when applied high voltage electric field is non-uniform.
2. Theoretical model

The following inequalities are valid for the space charge concentration \( n_\pm \), concentration of impurities \( n_p \) and concentration of neutrals \( n_a \) in a low-conducting medium

\[
\begin{align*}
    n_\pm & \ll n_a, \\
    n_p & \ll n_a.
\end{align*}
\]

(1)

First relation can be considered as the condition of weak ionization (dissociation) or low conductivity in a medium. The rates of ionization (or dissociation) and recombination in a volume are supposed to be known as thermodynamics functions of the above mentioned concentrations, electric field intensity \( E \) and temperature. They can be represented as follows:

\[
W_i = W_i(n_a, n_p, T, |E|) = W_i(n_a, n_p, T, 0)f(|E|).
\]

(2)

Here \( W_i \) is the rate of ionization (dissociation) in a volume, \( W_r \) is the volume rate of ion recombination, \( b \) is the mobility of ions, \( e \) is the elementary charge and \( T \) is the absolute temperature.

The expression for recombination constant \( K_r \) was obtained by Langevin in 1903 and by Onsager in 1934 for particular case of weak electrolytes. This is two-particle ion-ion recombination. In this case the excess of energy is absorbed by the medium. Onsager had shown the weak influence of sub-breakdown electrical fields on \( K_r \) as well. Here the direct process is the ionization, and the reverse process is the recombination. But the influence of \( E \) on \( K_r \) can not be disregarded in a case when these processes are the dissociation and reverse dissociation. The Langevin ratio is valid for dense gases with chemical reactions, besides weak electrolytes. In this case ionic conductivity is much greater than electronic one.

We have used known the Einstein-Nernst relation for the ion diffusion coefficient:

\[
Z D_\pm = \frac{k_B T b_\pm}{|e|},
\]

(4)

where \( Z \) is the ion valence, \( D \) is the diffusion coefficient of ions, \( k_B \) is the Boltzmann constant.

Function \( f(|E|) \) describes the dependence of the ionization (or dissociation) rate on the electric field intensity. This expression was obtained by Frenkel for the solid dielectrics. Further it had been generalized by Ostroumov for the case of weakly conductive liquid dielectrics (\( Z > 1 \)), having ion chemical bonds in their molecules [3]. This expression is used in the present research and has the form:

\[
f(E) = \exp(\beta |E|^{1/2}), \quad \beta = \frac{|Ze|^{3/2}}{\sqrt{\pi \epsilon_0 k_B T}}.
\]

(5)

Equations, which describes creation and annihilation of the space charge, conductivity in a presence of high voltage electric field and the electric field distribution itself, can be written as:

\[
\frac{\partial q}{\partial t} + (V, \nabla q) - \frac{k_B T b}{|e|} \Delta q + (E, V \sigma) = -\frac{q \sigma}{\epsilon \epsilon_0}, \quad \Delta \phi = -\frac{q}{\epsilon \epsilon_0}
\]

(6a)

\[
\frac{\partial \sigma}{\partial t} + (V, \nabla \sigma) + b^2 (E, V \sigma) - \frac{k_B T b \Delta \sigma}{Z} - \frac{\sigma^2}{\epsilon \epsilon_0} \exp(\beta |E|^{1/2}) + \frac{\sigma^2}{\epsilon \epsilon_0} = 0,
\]

(6b)

where \( V \) is the velocity vector, \( q \) is the space charge, \( \sigma \) is the conductivity, \( \phi \) is the potential of the electric field.

Valence of liquid ions \( Z \) may be determined via chemical analyses and other theoretical or experimental methods (for example, using molecular dynamic method). In our works we suppose, that \( Z = \text{const} \). The low-voltage conductivity of significant number of liquids depends on \( Z \). In this case high-voltage conductivity may be obtained from equation (6b) with initial and boundary conditions.
These equations were obtained in [4] from continuity equations for volume concentrations of liquid ions. Formula (5) for pre-breakdown volume dissociation (ionization) rate of neutral particles is taken into account.

3. Improvement of the software algorithm for the numerical simulation of the liquid dielectrics flow in an inhomogeneous electric field

We continue our numerical research and modification of the numerical algorithm. A three-dimensional version of the algorithm is being developed. At the moment, debugging the construction of the computational grid and test calculations are carried out. On the figure 1 one can see an example of a three-dimensional grid, which will be used in future calculations.

In addition, a two-dimensional version of the algorithm has been developed that uses an adaptive computational grid. It is planned that this grid is finer in the calculation regions with velocity gradients greater than certain values. This will make it possible to use fewer calculated cells, and therefore less time, to achieve the same “detail” of the flow as when applying more cells that are used at the current stage of work. To achieve this, the structure of storing information in settlement cells was completely redone. This has been achieved using linked lists. As an example, on the figure 2 it can be seen computational cells that initially had the same size, several of which were divided and contains 4 cell descendants.
Let’s take a look at one of test calculations and see how this approach actually works. The algorithm itself is based on the MacCormack method and was described in more detail earlier [10].

Well-known hydrodynamics equations should be added to equations (6a,b) to get the closed system of equations. The first of them is the continuity equation for incompressible media:

$$ \frac{\partial V}{\partial t} = 0 $$

(7)

In addition to the continuity equation (7) the momentum conservation equation in such a form is being solved:

$$ \rho \left( \frac{\partial V}{\partial t} + (VV)V \right) = -\nabla p + \eta \Delta V + qE, $$

(8)

where \( \rho \) is the pressure, \( \eta \) is the dynamic viscosity of the fluid. This equation does not take into account the ponderomotive force, acting on polarized molecules, since it is small compared to the Coulomb force. The corresponding estimates were given by one of the author earlier in his work [11].

The initial conditions for the equations (7) and (8) are

$$ q(t = 0) = V(t = 0) = 0, \quad \sigma(t = 0) = \sigma_0. $$

Consider the boundary conditions. Condition of adhesion \( (V = 0) \) are observed on the surfaces of the wire-electrode and the counter-electrode. On the other boundaries there are free outflow conditions and \( q = 0 \). The other parameters are represented as:

- \( Z = 2 \),
- \( \varepsilon = 2.5 \),
- \( T = 300 \) K,
- \( \rho = 800 \) kg/m\(^3\),
- \( \eta = 0.00016 \) Pa s,
- \( \mu = 10^{-9} \) m\(^2\)/(V s) is the mobility of the ions.

Voltage between the electrodes equals to 500 V. Inter-electrode distance equals to 2 cm. Size of the square computational domain equals to 5 cm x 5 cm along Ox and Oy axes correspondently. Wire electrode presented as square in cross section and its size equals to 4 mm x 4 mm (approximation of
round electrode with the radius equals to 2 mm). The whole domain is considered to be divided on 250 x 250 cells (see figure 3). But cells in nearest neighborhood of the wire electrode are divided on 4 part, so this neighborhood has more fine grid in its representation. Amount of these cells under refinement equals to 50 x 50. This domain of fine grid is designated via white square on the figure 4.

![Figure 3. Scheme of computational domain. The wire-electrode is depicted as a black square. The counter-electrode (plane) lies on the Ox axe from 0 to 250 cell.](image)

![Figure 4. Magnitude of the velocity for a weakly conducting liquid in an electric field near the wire square electrode with cells refinement. Inner square is for wire-electrode border. Outer square is for refinement region border.](image)

Earlier it was shown [12] that the finer grid we use, the greater maximum velocity will be at the line connecting two electrodes. In the 250 x 250 grid the velocity maximum ≈ 1.1 mm/s. In the 500 x 500 grid the velocity maximum ≈ 2.1 mm/s. In our test calculation with refine grid near the wire electrode the velocity maximum ≈ 1.7 mm/s. At the same time, the calculation time was 3.2 times less
than when using fine grid, and the gained value of maximum velocity is already much closer to that calculated for fine mesh.

Conclusion
The approach with refinement of the computational grid is not new, of course, but after carrying out the first test calculations, we are convinced that it works and reduces the computation time with obtaining acceptable results. Of course, it is necessary to select the degree of cell fragmentation and the conditions under which this must be done. This approach will be especially useful for computations on a 3D mesh.

Acknowledgments
This work was supported by the Russian Foundation for Basic Research (project No. 18-08-00136).

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