SIMULATION OF ELECTRON INTERACTION WITH LIQUID WATER AND PROCESSES RELATED TO SUB-NANOSECOND ELECTRICAL BREAKDOWN

Petr BÍLEK, Zdeněk BONAVENTURA

Department of Physical Electronics, Faculty of Science,
Masaryk University, Brno, Czech Republic, EU,
petrbilek248@gmail.com

Abstract

Sub-nanosecond electrical breakdown in dielectric liquids is of vital interest for applications, e.g. in high-voltage insulation, high-current switching and electric field-cell interactions. Liquid dielectrics in strong nonuniform electric fields are under influence of electrostrictive force that tends to move the fluid into the regions with higher electric field. If the voltage rise is fast enough(nanoseconds), the liquid does not have enough time to be set into motion in order to reduce the internal stress. In this case the electrostrictive force induces significant stress in the bulk of the liquid which is manifested as a negative pressure. At certain threshold, the negative pressure causes cavitation ruptures of the fluid. Subsequently, free electrons can be produced by emission from the surface inside the cavity and accelerated to energies exceeding the energy for ionization of water and thus, contribute to electrical breakdown of water.

We present numerical model, which gives us basic ingredients necessary to study interaction of accelerated electrons with liquid water during sub-nanosecond electrical breakdown. We aim to determine geometrical conditions in electrode vicinity needed for electron multiplication and subsequent build up of space charge, for which we propose to use Monte Carlo software Geant4-DNA. Using of proper simulation techniques could enable us to explain some experimentally observed properties of sub-nanosecond electrical breakdown in liquid water.

Keywords: Liquid water, sub-nanosecond electrical breakdown, cavitation, negative pressure, Geant4-DNA

1.   INTRODUCTION

While electrical breakdown in gases seems to be already well explained [1], the challenge stays to set light to electrical breakdown in dielectric fluids such as deionized water. The breakdown in liquids depends on the rise time of the applied high voltage pulse and for „long" high-voltage pulse (~0.1 - 100 µs) occurs through gas bubbles. In this case it is not very different from the usual electrical breakdown in gases, and it has been well studied [2]. Gas bubbles creation in sub-nanoseconds is impossible, since the Joule heating has not enough time to provide energy for evaporation and the expansion of the bubbles, as was pointed out in [3]. Experiments [4, 5, 6, 7] performed in liquid water in presence of nanosecond voltage in a point to plane geometry have measured formation of streamer-like branching and were able to associate characteristic emission spectra with the most important phases of the discharge. The emission spectra showed a broad-band continuum evolving during the first expansion of the discharge and collapse, followed by H/O atomic lines occurring together with continuum emission during the second expansion and collapse [4]. Detailed study of discharge emission dynamics has been performed by [7].

The following text will be devoted to liquid water breakdown with nanosecond rise time, which can be used for wide range of applications, e.g. in high-voltage insulation, high-current switching [8] and sub-nanosecond electric pulse - cell interactions [9].

2.   MOTIVATION

Nowadays, accepted scenario of nanosecond electrical breakdown in dielectric liquids was described by [3] and consists of the following steps (see **Figure 1**):

1)   At the beginning, the strong inhomogeneous electric field in the vicinity of the needle electrode creates a region saturated by cavitation nanopores.
2)   In the nanopores of sufficient sizes, the primary electrons are accelerated by electric field to energies exceeding the ionization potential of water molecule.
3)   Many ionization collisions form electron avalanche and build-up of space charge.
4)   After neutralization of electrons at the electrode, positive charged liquid forms a virtual needle electrode, and electrostrictive conditions for the appearance of the next set of nanocavities are fulfilled.
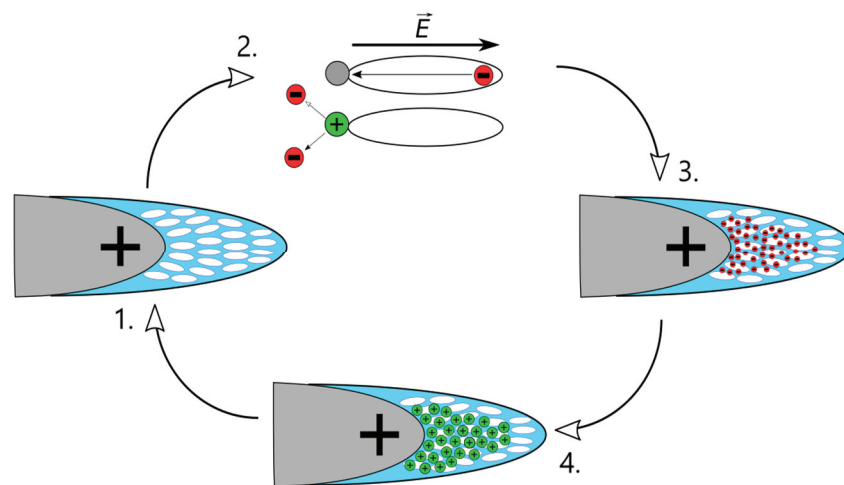

Figure 1 Accepted scenario of nanosecond electrical breakdown in dielectric liquids

The aim of our work is to formulate and develop complex numerical model to study nanosecond electrical breakdown in deionized liquid water. We believe that the model could explain experimentally observed features of the phenomenon such as spatio-temporal characteristics of the discharge and emission spectra. Presented model can be divided into three main stages(submodels):

A)   Model of dielectric liquid under influence of electrostrictive forces.
B)   Model of cavitation ruptures grow.
C)   Model of electron interaction with liquid water containing nanopores.

3.   RESULTS

Each of the previous submodels has different spatio-temporal scale and thus requires different physical approach. In what follows, we give short description of each of the submodels (A-C).

3.1.   Model of dielectric liquid under influence of electrostrictive forces

Liquid dielectric in strong inhomogeneous electric field is under influence of electrostrictive force, which can cause negative pressure acting on the fluid and initiate discontinuity in the fluid. Experimental data show that the critical negative pressure for water rupture and start of nanometer size cavitation is about 30 MPa.

We have developed hydrodynamic model to study the dynamics of water in a pulsed strongly inhomogeneous electric field in the approximation of compressible flow described by equation of continuity for mass and momentum [10,11]. The hydrodynamic model allows us to find time dependence for pressure and velocity in

the liquid for given electrode radius and voltage pulse. In the **Figure 2** we present results of our hydrodynamic model for electrode radius 100 μm and voltage amplitude 54 kV. We have pointed out that in case of long rise time of voltage pulse(left part of the **Figure 2**), the hydrodynamic pressure compensates the electrostrictive pressure and the total pressure (red curve) does not exceed critical negative pressure for the water rupture. When we shorten rise time up to few nanoseconds(right part of the **Figure 2**), electrostrictive pressure prevails the hydrodynamic and the total pressure exceeds the critical pressure, which is necessary for start of nanometer-size cavitation. This model enables us to identify conditions favourable for nanocavitation generation [12].
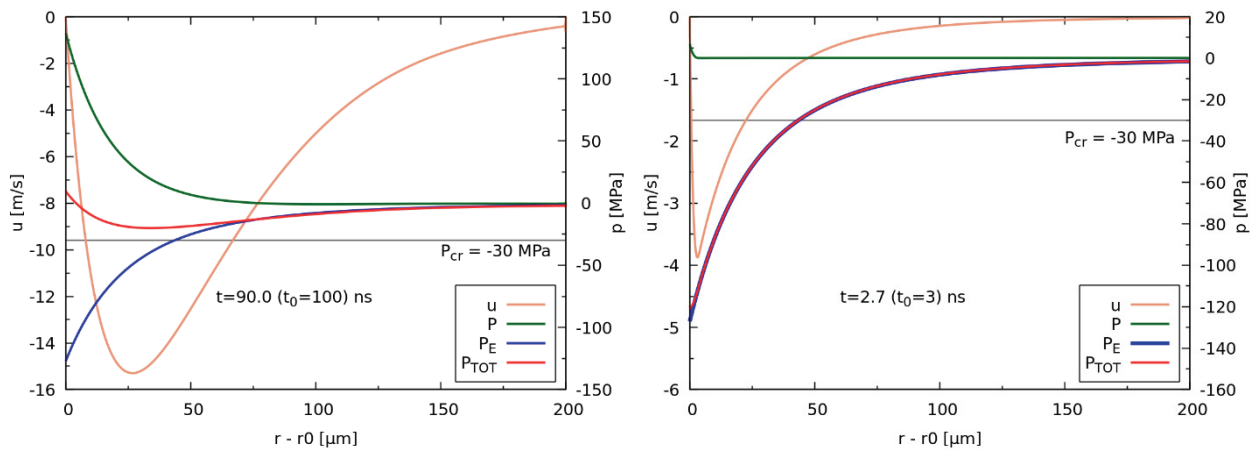

Figure 2 Hydrostatic pressure P, electrostrictive pressure P_E, total pressure P_{tot}, and velocity of fluid u as a function of distance from the electrode at: t_0 = 100 ns (on the left), t_0 = 3 ns (on the right). Horizontal line indicates critical pressure P_{cr} = −30 MPa. Negative values of the velocity corresponds to the motion of the fluid towards the electrode.

3.2. MODEL OF CAVITATION RUPTURES GROW

The previous model confirmed existence of nanopores in the presence of very steep high voltage pulse. Model of cavitation ruptures grow presented in this section aims to reveal grow of these nanocavities. Forces averaged over the surface of the nanocavity give rise to pressure which consists of electrostrictive pressure, surface tension and hydrodynamics pressure:

$$P_{av} = (3/4)(\alpha - 1)\varepsilon_0\varepsilon E^2 - k_\sigma\sigma/R - p,$$

Nanocavities will collapse if the pressure is negative, on the other hand they will expand if the pressure is positive. Dynamics of the expanding nanocavity is driven by the balance for the kinetic energy of expanding fluid and by the work of pressure forces [4, 13]. Radius of the microcavity as a function of time can be described by the following equation:

$$\frac{d}{dt}\left(R^3\left(\frac{dR}{dt}\right)^2\right) = \frac{4}{\rho}R\frac{dR}{dt}\left(\frac{3}{8}R(\alpha-1)\varepsilon_0\varepsilon E^2 - \frac{pR}{2} - k_\sigma\sigma\right).$$

Solution of this equation allows us to find time dependence of cavity radius at the end of the pulse rise time and determine energy that electron gains inside the cavity. This is important, in order to identify volume in the vicinity of the electrode where ionization of water is possible [3]. To illustrate this, we present **Figure 3** with a numerical solution of the previous equation for these parameters: electrode radius (r_0= 100 μm), water permittivity (ε = 81), α = 1.5, voltage pulse amplitude (U_0 = 54 kV), rise time (t_0 = 3 ns), water surface tension (σ = 0.072N/m) and iniatial nanocavity radius (R_0 = 2 nm).
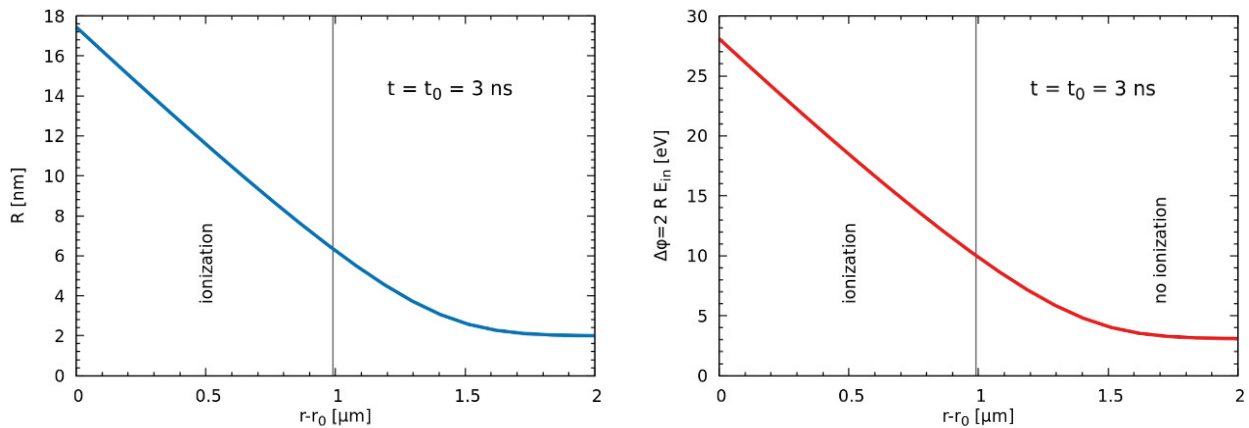
(a) Radius of expanded micropore as a function of distance from the electrode at the end of the voltage rise time. Vertical line separates regions where ionization of water is and is not possible.

(b) Energy gained by an electron when crossing a cavity as a function of distance from the electrode at the end of the voltage rise time.

Figure 3 Development of nanopores in inhomogeneous pulsed electric field

3.3. MODEL OF ELECTRON INTERACTION WITH LIQUID WATER CONTAINING NANOPORES

Having geometrical parameters (ionization region and cavity radius as a function of distance from electrode) enables us to investigate electron propagation on the nanoscopic scale. For this reason we decided to use Geant4 toolkit (GEometry ANd Tracking) [15,16]. Geant4 is a toolkit for the simulation of the passage of particles through matter and it is developed since 1994. Its areas of application include high energy, nuclear and accelerator physics, as well as studies in medical and space science. Recent release contains a new set of physics models - Geant4-DNA extension for modelling of low-energy electron transport in liquid water (for energies lower than 10keV) [15,16].
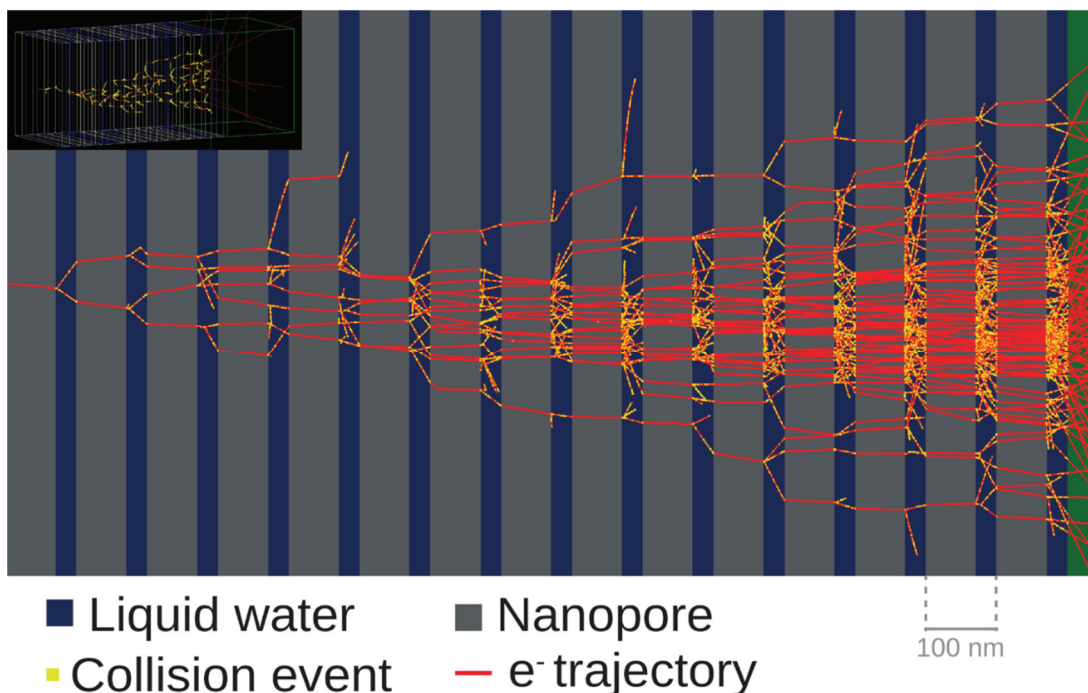

Figure 4 Electron avalanche on the set of nanocavity/liquid layers simulated using Geant4-DNA

Within Geant4-DNA we had to define: geometry as a set of liquid/nanocavity layers, source of primary electrons, electric field based on applied electric pulse and finally, we chose physical models (processes and cross sections). We are able to simulate development of electron avalanche originating from one seed electron accelerated on the set of layers composed from cavities and liquid-water layers as it is shown in the **Figure 4**. It seems that the main source of electron energy loss comes from vibrational excitations of water molecules. Geant4-DNA gives us way how to compute electron energy distribution function after avalanche formation, with which is connected light emission during the sub-nanosecond electrical breakdown.

4. OPEN PROBLEMS AND CONCLUSION

Within the conclusion we should mention some open problems which we have to face: Implementation of scattering distribution for vibrational excitations of electron on water molecule in Geant4-DNA is still missing and the collision has currently only forward scattering. Further, we should try to answer questions as: What is the origin of primary electrons during the electric breakdown? and What exactly happens after electron avalanche formation? With the aim to quantitatively describe build-up of space charge after the electron avalanche formation.

Fluid dynamics with electrostrictive forces(model A), nanopore-grow model(model B) and Geant4-DNA Monte Carlo code with appropriate processes and cross sections(model C) could enable us to describe whole scenario of the electrical breakdown in liquid water. The presented conjunction of models gives us basic tools necessary to study sub-nanosecond electrical breakdown in liquid water. Microscopic view on the electron population could help us to explain experimentally observed emission spectra.

ACKNOWLEDGEMENTS

REFERENCES

[1]   RAIZER, Yuri P. *Gas Discharge Physics.* Springer-Verlag Berlin Heidelberg, 1991. p. 449.

[2]   USHAKOV, Vasily Y., KLIMKIN, V. F. and KOROBEYNIKOV S. M. *Impulse Breakdown of Liquids.* Springer-Verlag Berlin Heidelberg*, 2007.* p. 398.

[3]   SHNEIDER, Mikhail N, PEKKER, Mikhail. Liquid Dielectrics in an Inhomogeneous Pulsed Electric Field. *IOP Publishing,* 2016.

[4]   ŠIMEK, Milan, PONGRÁC, Branislav, BABICKÝ, Václav, ČLUPEK, Martin and LUKEŠ, Petr. Luminous phase of nanosecond discharge in deionized water: morfology, propagation velocity and optical emission. *Plasma Sources Science and Technology.* 2017. vol. 26, no. 7, pp. 9.

[5]   MARINOV, Ilya L., GUAITELLA Olivier, ROUSSEAU, Antoine, STARIKOVSKAIA Svetlana M. Succesive Nanosecond Discharge in Water. *IEEE Transactions on Plasma Science.* 2011. 392672.

[6]   SEEPERSAD Y., PEKKER Mikhail, SHNEIDER Mikhail N., FRIDMAN A. And DOBRYNIN D. Investigation of positive and negative modes of nanosecond pulsed discharge in water and electrostriction model of initiation. *J. Phys. D.: Appl. Phys.* 2013. 48424012.

[7]   STARIKOVSKIY, A., YANG A., CHO Y. I., FRIDMAN A. Non-equlibrium plasma in liquid water: dynamics of generation and quenching. *Plasma Sources Science and Technology.* 2011. 20024003.

[8]   JOSHI, Ravindra P., KOLB, Jurgen F., XIAO Shu, SCHOENBACH Karl H. Aspects of Plasma in Water: Streamer Physics and Applications. *Plasma Processes and Polymers.* 2009. vol. 6, no. 11, pp. 763-777.

[9]   SCHOENBACH, K. H. et al. Biological Effects of Intense Subnanosecond Electrical pulses. *IEEE Transactions on Plasma Science.* 2006. 1-4244-0019-8, pp. 573-576.

[10]   SHNEIDER, Mikhail N, PEKKER, Mikhail. Liquid Dielectrics in an Inhomogeneous Pulsed Electric Field. *Physical Review E.* 2013. vol. 87, no. 4, 043004.

[11]   SHNEIDER, Mikhail N, PEKKER, Mikhail. Cavitation in dielectric fluid in inhomogeneous pulsed electric field. *Journal of Applied Physics.* 2013. vol. 114, 214906.

[12]   ŠLAPANSKÁ, M., BÍLEK, P., HNILICA, J., BONAVENTURA, Z. Study of cavitation in liquid water under the action of inhomogeneous pulsed electric fields: application to sub-nanosecond electrical breakdown. *45th Conference on Plasma Physics.* Žofín Palace, Prague.

[13]   BÍLEK, P., ŠLAPANSKÁ, M., HODER, T., ŠIMEK, M., BONAVENTURA, Z. Simulation of electron interactions with liquid water and processes related to sub-nanosecond electrical breakdown. *45th Conference on Plasma Physics.* Žofín Palace, Prague.

[14]   SHNEIDER, Mikhail N, PEKKER, Mikhail. Pre-breakdown processes in a dielectric fluid in inhomogeneous pulsed electric fields. *Journal of Applied Physics.* 2015. vol. 117, 224902.

[15]   BERNAL M.A. et al. Track structure modeling in liquid water: A review of the Geant4-DNA very low energy extension of the Geant4 Monte Carlo simulation toolkit. *Physica Medica.* 2015, vol. 31, no. 8, pp. 861 - 874.

[16]   INCERTI, S. et al. GEANT4 very low energy cross section models with experimental data in water. *Medical Physics.* 2010. vol. 37, no. 9.