

# MODEL ANALYSIS OF BREAKDOWN IN HIGH-VOLTAGE, WATER-BASED SWITCHES

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## *Abstract*

A time-dependent model containing several new features has been developed for treating the breakdown of water under nanosecond pulsed conditions. It is argued that the traditional mechanisms such as bubble formation and thermal heating no longer apply. Instead, the mechanism of breakdown will be dictated by the surface electric field behavior and subsequent injection of electrons at the interface. Thus, the interface layer and electrode conditions will begin to be far more important than the bulk liquid properties in determining breakdown and hold-off voltage levels. It is shown that very strong electric field enhancements can occur due to the collective orientation of dipoles near the interface. Under high voltage conditions, the injected electrons are assumed to have relatively long lifetimes due to a continuous replenishment of energy from the external field. The simulations show a breakdown within about 200 ns for an applied pulse of 20 kV for a 200  $\mu\text{m}$  water-filled switch. The predictions are in keeping with recent experimental observations by our group.

## I. INTRODUCTION

There is considerable interest in the study of electrical breakdown in water (and other liquids) for a variety of reasons [1]. Practical applications of dielectric liquids include water-filled gaps for the design of acoustic equipment, the insulation of high-voltage devices, as the medium in spark erosion machines, and use in energy storage and switching elements for pulsed power systems. Generally, for high voltage pulsed power generators, solids or vacuum have been used as the dielectric material, and gases at high pressure for high power switches. However, the use of polar liquids seems to have advantages for both energy storage and as switch media, particularly for nanosecond pulse generators. Polar liquids not only have a high dielectric constant, but also have a higher breakdown strength than compressed gases. Water, for example, with a dielectric constant of 81 up to frequencies of 2 GHz, has been found to hold off electrical fields up to 1 MV/cm for durations up to hundreds of ns [2]. In comparison to solids, their ability to circulate leads to better thermal management, easier removal of debris after breakdown, and homogeneity. Liquid dielectrics are also better suited for applications involving complex geometries.

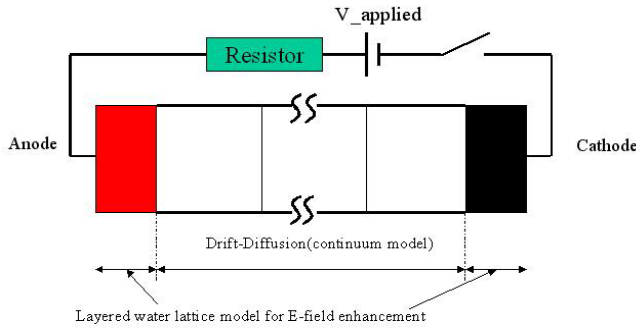
The mechanisms responsible for the breakdown in dielectric liquids have long been studied. The observed influence of hydrostatic pressure on the breakdown strength, results of chromatographic analyses, and application of optical techniques, have collectively led researchers to believe that liquid electrical breakdown involves the creation and propagation of streamers [3]. The role of thermal processes and the possible occurrence of discharges within thin vapor bubbles has been advanced since electron avalanche processes in liquids (e.g. water) are known to be nearly negligible [4]. Hence, the hypothesis is that the vapor phase plays a role in the overall breakdown process. However, this requires internal heating, and can only be possible if the duration of the applied voltage is sufficiently long, i.e., at least in 10-100 microsecond range or larger. In recent experiments, breakdown of water filled switches has been observed with 200 ns voltage pulses [5]. This time duration is too small for any significant heating, and as shown through simulations in the next section, only a modest temperature increase of  $\sim 7$   $^{\circ}\text{C}$  can occur. The lack of heating rules out the possibility of vapor bubble formation. Moreover, a simple application of the electrostatic image method reveals that charged particles immersed in the high dielectric water medium cannot penetrate any naturally occurring micro-bubbles due to electrostatic Coulomb repulsion. Instead, a separate mechanism, differing from the traditional viewpoint has to be considered, and is discussed in this contribution.

## II. SIMULATION APPROACH

A one-dimensional, time-dependent simulation model was developed and implemented as shown in Fig. 1. A 50 Ohm external resistor,  $R$ , along with a supply voltage  $V_{\text{app}}$  was placed in series with the simulation volume representing the water-filled switch device. The entire device simulation region was divided into a central region consisting of "N" boxes of equal size, and characterized by ion transport on the basis of the drift-diffusion theory. Current continuity was used to update the internal electric field  $E(x,t)$  and the potential at grid points within the center of each box, through the relation:  $J_{\text{cct}}(t) = V_{\text{app}}(t)/R = \epsilon dE(x,t)/dt + \sigma E(x,t)$ . The interface region, on the other hand, requires more careful modeling given the existence of an electrical double layer, the large charge densities, possible dipole re-alignment effects, and the breakdown of traditional Gouy-Chapman theory [6]. Here, it is

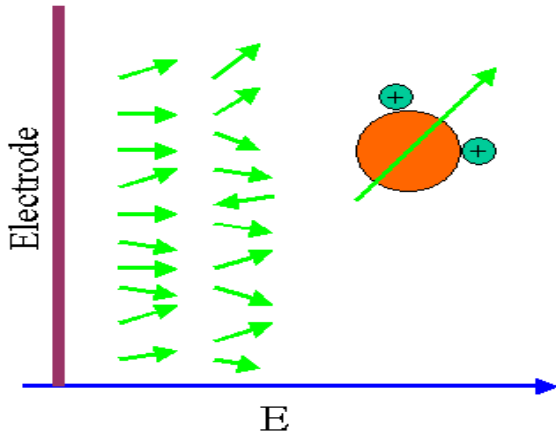
# Preprint

assumed that an appropriate representation of the interface layer physics can best be achieved by considering a few monolayers of water molecules adjacent to the electrodes through an effective “lattice model” for the liquid. The existence of high-electric fields localized at the interface arising from strong clustering of mobile ions at the electrode surface, forms the basis of this approach. Conceivably, the presence of such high electric fields will lead to an ordering and re-alignment of the strongly polar water molecules due to the electrostatic interactions with the molecular dipoles. Energy minimization will then lead to the possible formation of an ordered molecular lattice over a few molecular mono-layers of the interface. Fig. 2 shows a possible scenario, with the electric field forcing the water dipoles at the molecular level to orient over a region a few monolayers thick near the electrode. The effective polarization would then increase because of such collective, field-dependent ordering. Obviously, the



**Fig. 1.** One-dimensional simulation model schematic.

usual Langevin equation would govern the polarization magnitude [6]. From the equilibrium density of water, the mono-layer thickness is roughly 0.31nm. Recently, experimental evidence for such ordering at high fields in water has been forthcoming [7].

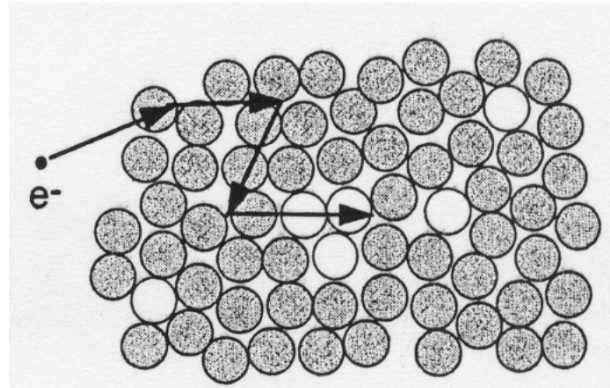


**Fig. 2.** Schematic showing possible orientation of the water dipoles adjacent to the electrode due to high fields.

Microscopic treatment of the double layer adjacent to the electrodes, in our model, facilitated precise calculations of the surface electric field, with the inclusion

of field enhancements due to the collective dipole orientation. As shown through our results in the next section, such field enhancements strongly increase the possibility for electron injection from the cathode contact. We believe, it is the onset of such injection at the interface that modulates the device conductivity, and drives the device towards electrical breakdown. The usual Fowler-Nordheim mechanism of tunneling from the metal into the conduction band of water is assumed to hold.

Another feature of our breakdown model is the inclusion of a field dependent lifetime for the injected electrons. These charges are assumed to be in the quasi-free state within the conduction band of water. Qualitatively, the electrons are assumed to enter the liquid through initial high-field injection at the cathode. These particles lose energy due to atomic/molecular collisions, as shown in Fig. 3, but can also gain energy from the electric field. Thus, at low electric fields, the net result would be a continuous slowing down and eventual localization of injected electrons. However, with increasing field, the effective lifetime  $\tau$  can be expected to increase due to energy gain from the external field. Here, a field dependent lifetime  $\tau(E)$  given by:  $\tau(E) = \{\tau_1 \exp[-E_{thr}/E] + \tau_2\}$  was assumed, with  $\tau_1 = 0.1\mu s$ ,  $\tau_2 = 0.1ns$ , and  $E_{thr} = 2 \times 10^7$  V/m.



**Fig. 3.** Picture of electron movement in water [After 8].

Our microscopic treatment of the double layer on either side was based on a four-slice lattice model as shown in Fig. 4. The dotted lines represent ions in the form of line charges of density  $\sigma_i$ , while the associated dipole layer consisting of equal and opposite line charges  $\sigma_{id}$  and  $\sigma_{di}$ , are placed on either side of  $\sigma_i$ , at a separation “d”. In keeping with the density of water at room temperature,  $d \sim 0.31$  nm. The associated electric fields  $E_{id}$ ,  $E_{di}$  and  $E_{i-1,i}$  were computed for each layer starting from the known value at the bulk side of the lattice region. A self-consistent analysis is necessary, since the polarization and charge densities at the layers depend on the electric field and potential values. Thus, for example, the relevant equations linking the electric field and potentials are :

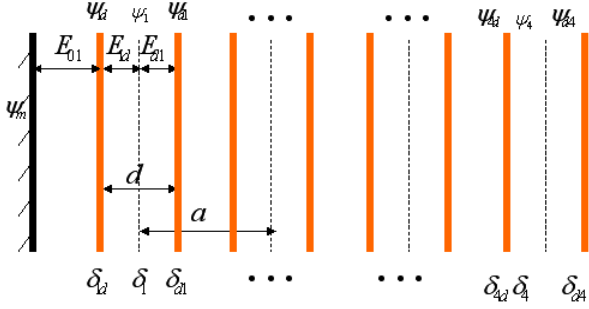


Fig. 4. A four-slice lattice model of the double layer.

$$\psi_{d,i-1} - \psi_{id} = bE_{i-1,i}, \quad (1a)$$

$$\psi_{i,d} - \psi_i = (d/2)E_{id}, \quad (1b)$$

$$\psi_i - \psi_{di} = (d/2)E_{d,i}, \quad (1c)$$

$$\psi_{di} - \psi_{i+1,d} = bE_{i,i+1}. \quad (1d)$$

The relationship between the field and various charge densities is:

$$E_{i,i-1} - E_{id} = -\delta_{id} / \epsilon_a, \quad (2a)$$

$$E_{id} - E_{di} = -\delta_i / \epsilon_a, \quad (2b)$$

$$E_{di} - E_{i,i+1} = -\delta_{di} / \epsilon_a, \quad (2c)$$

$$E_i \equiv \frac{1}{2}(E_{id} + E_{di}). \quad (2d)$$

Finally, the polarization and ion densities are assumed to depend on the potentials through the usual equilibrium relations:

$$\delta_{di} = -\delta_{id} = P_i, \quad (3a)$$

$$\delta_m = -\sum_{i=1}^{\infty} \delta_i, \quad (3b)$$

$$\delta_i = -2qaN_v \delta \sinh(\phi_i) / Z_i, \quad (3c)$$

$$P_i = N_v(1-2\delta)p[y_i \cosh(y_i) - \sinh(y_i)] / (y_i^2 Z_i), \quad (3d)$$

$$\text{and, } Z_i = 2\delta \cosh(\phi_i) + (1-2\delta) \sinh(y_i) / y_i. \quad (3e)$$

In the above,  $\delta=10^{-4}$ ,  $\phi_i = q\psi_i / kT$ ,  $y_i = pE_i / kT$ , “p” is the dipole moment equal to  $6.2 \times 10^{-30}$  Cm for water, “a” the molecular size  $\sim 0.31$  nm, and  $d \sim 0.25$  nm, in keeping with Ref. 6.

### III. RESULTS AND DISCUSSION

Results of the surface electric field at the electrode, based on the four-layer water lattice model, are shown in Fig. 5. The x-axis represents the field at the lattice-bulk interface, while the y-axis shows the enhancement factor of the field at the electrode-lattice interface. Values as large as 70 are seen, and imply that electric fields well in excess of  $2 \times 10^9$  V/m can easily be reached at the metallic electrodes, despite much lower values in the bulk. The increased surface field arises from the orientation and

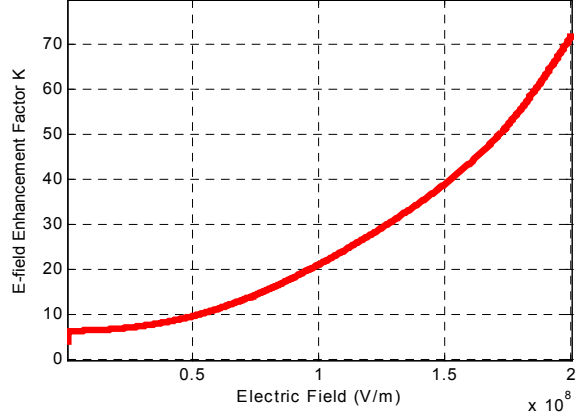


Fig. 5. Surface field enhancement from lattice model.

alignment of the dipoles. This enhancement makes it possible for electron (or even hole) injections to occur from the contact into the water. The eventual breakdown is the manifestation of strong electron injection and resulting conductivity modulation.

For completeness, simulation results of the internal temperature profile are presented for a 200  $\mu\text{m}$  point-plane geometry to a 200 ns, 0.98 MV/cm electric pulse. The intent is to demonstrate the near non-thermal conditions for the short, nanosecond pulses. The magnitude and duration was chosen to be in accordance with actual experiments conducted at Old Dominion University. The temperature profile is shown in Fig. 6. The calculations predict that the maximum temperature rise would be on the order of 7  $^\circ\text{C}$ . This value is in very good agreement with the experimental measurement, and clearly demonstrates that internal heating leading to bubble formation would not be possible for the nanosecond-type short pulsed experiments. Hence, a separate mechanism for electric breakdown must be operative under these short pulse conditions.

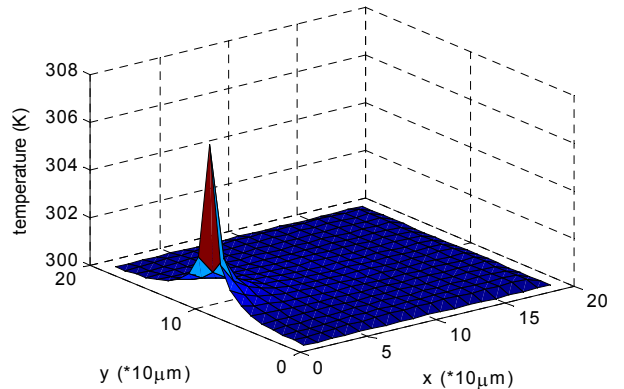


Fig. 6. Temperature profile for 200ns voltage pulse.

Finally, simulation results obtained for the temporal development of device currents and surface electric fields in response to a 200 ns, 20-kV applied pulse, are discussed. In keeping with actual experiments, the length

and cross-sectional area of a water switch was taken to be  $200\ \mu\text{m}$  and  $10^{-7}\ \text{m}^2$ , respectively. Fig. 7 shows a semi-logarithmic plots of the total circuit current and the injected current, along with the surface electric field. Several important features are evident. The circuit current has an initial spike due to the displacement current component in the sub-nanosecond regime. The injection current remains almost negligible until about 75 ns following the initiation of the voltage pulse. The electric field at the surface quickly builds up and reaches a fairly large value of about  $10^9\ \text{V/m}$ . The high magnitude is the direct result of enhancement produced by the dipole orientation near the interface. Despite being rather high, the surface field is still not large enough to facilitate electron injection via Fowler-Nordheim tunneling at the cathode. In the absence of carrier injection, the circuit current remains larger than the internal conduction current within the device, and hence, a slow and continuous build-up of the internal electric field continues. Eventually, beyond 75 ns, the injection current begins to increase, until it roughly reaches the external circuit current value. Within about 200 ns of the voltage initiation, a sharp increase in the currents is predicted. Thus, a breakdown regime is effectively reached. This simulation result predicting a breakdown time of about 200 ns and a net circuit current of about 1-5 A, is in keeping with the actual experimental observations at ODU.

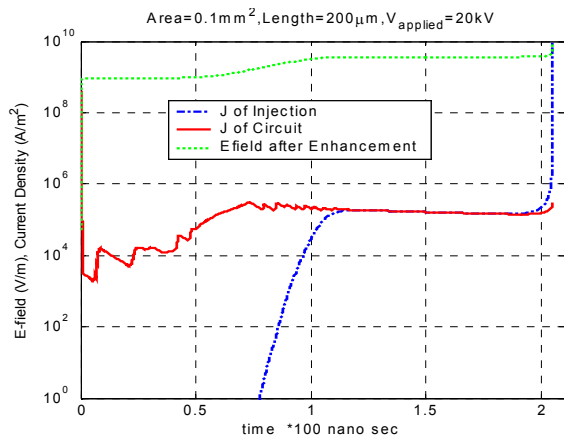


Fig. 7. Results showing temporal development of injected and circuit currents, and surface electric field.

#### IV. CONCLUSIONS

A model containing several new features has been developed for treating the breakdown of water under nanosecond pulsed conditions. It is argued that bubble formation and thermal heating will no longer apply. Instead, the mechanism of breakdown will be dictated by the electric field behavior and subsequent injection of electrons at the interface. Thus, the interface layer and the condition of electrodes will begin to be far more important than the bulk liquid properties in determining breakdown and hold-off voltages. This prediction is in keeping with our recent experimental observations [5]. Efforts at improving the electrode surface through polishing or

changing the effective work function are predicted to have a significant impact on the breakdown characteristics. It has been shown that strong electric field enhancements can occur due to the collective orientation of dipoles near the interface. Such enhancement can lead to electron injection at the cathode. Under high voltage conditions, the injected electrons are assumed to have relatively long lifetimes due to a continuous replenishment of energy from the external field.

The time-dependent simulations show that a fast breakdown on the nanosecond time scale can occur. Furthermore, in actual practice, the breakdown can be expected to initiate stochastically at different locations of the cathode due to local fluctuation in the ion density and surface roughness. This would lead to streamers and the “treeing” structures, as has been observed experimentally. Finally, since electron injection is seen to play a role, we predict that optical triggering through the injection of photo-electrons should also be possible.

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#### VI. ACKNOWLEDGMENTS

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