https://doi.org/10.46813/2025-158-092

NUMERICAL INVESTIGATION OF THE ELECTROPHYSICAL AND PLASMA-CHEMICAL MECHANISMS OF FORMATION OF A NEGATIVE STREAMER OF AN IMPULSE HIGH-VOLTAGE DISCHARGE IN AN AIR BUBBLE IN WATER

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The article presents the results of numerical modeling of the formation of a negative streamer of an impulse high-voltage discharge in an air bubble inside the water. The distributions of the electric field intensity, potential, current density, electron temperature, and concentrations of charged and excited particles are shown. The calculations indicate that the streamer evolves into a highly conductive channel, causing a sharp increase in the electric field strength in the water. The process of development of the conduction current in an air bubble and the displacement current in water is demonstrated, taking into account the "air (plasma) − water interface". The obtained results provide a basis for optimizing the parameters of nanosecond discharges in air bubbles in water and justify significant interest for further experimental and theoretical investigations.

PACS: 52.65.-y, 52.80.-s

INTRODUCTION

In today's reality, the search for effective energy-efficient alternatives for water purification and disinfection is a priority task for the global community. The most widespread methods of water disinfection and purification, such as chlorination, ozonation, and ultraviolet irradiation, have their drawbacks. Among these are the undesirable formation of toxic by-products during chlorination [1] and the existence of chlorine-resistant microorganisms [2]. When ozonation is used, not all the advantages of electrical discharges are realized; in addition, the formation of toxic compounds (for example, bromates) is observed, and the incomplete oxidation of complex organic pollutants leads to the formation of intermediate transformation products with potentially increased toxicity [3]. On the other hand, for the effective operation of ultraviolet systems, there are strict requirements regarding water turbidity [4]; suspensions, colloids, and organic substances in the water can reduce the penetration of UV radiation, thus diminishing the disinfection effect.

Over the past decade, advanced oxidation processes have been rapidly evolving − innovative water treatment methods that involve the introduction of energy (chemical, electrical, radiative) into the reaction zone to generate particles, such as hydroxyl radicals (OH) with an oxidation potential of 2.8 V [5]. Technologies based on electrical discharges allow the use of a wide range of active agents for water treatment: strong electric fields, ultraviolet radiation, and the formation of highly reactive oxidizers that effectively remove organic impurities and inactivate pathogens [5 - 9]. This determines the significant interest in using electrical discharges for water treatment.

Among the various types of discharges (corona, barrier, spark, arc), high-voltage nanosecond impulse discharges in gas bubbles in water [10 - 12] deserve special attention. The generation of discharges in gas bubbles within the water layer enables the concentration of all active factors directly in the treated water. This approach is innovative and has the potential for the effective treatment of process water and liquid waste from nuclear power plants.

The aim of this work is to use a mathematical model of the formation of a negative streamer of an impulse high-voltage discharge in an air bubble in water to determine the dynamics of the distribution of electric field intensity, conduction current density and displacement currents, generation of ions and excited atomic states, and the distribution of electron temperature, for further optimization of discharge processes in the two-phase medium "air bubble (plasma) – water".

CALCULATION RESULTS AND THEIR DISCUSSION

For the modeling, a mathematical model of negative-streamer formation during a pulsed high-voltage discharge inside an air bubble in water was used, together with the corresponding boundary and initial conditions presented in the previous study [13].

The Fig. 1 illustrates the potential distribution in the reactor.

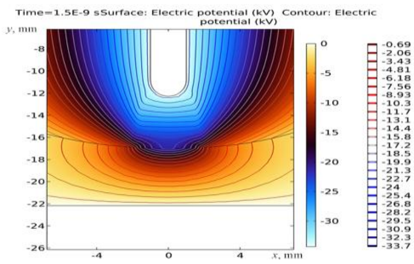

Fig. 1. Potential distribution in the reactor

Until 1.5 ns, the voltage in the reactor reaches a maximum of 34 kV, and according to the modeling calculations, as the conductivity of the gas bubble increases due to the formation of a streamer channel, a significant portion of this voltage is applied to the water. The streamer acts as an extension of the high-voltage electrode, ensuring electrical contact with the water. Thus, rather than a complete potential drop occurring within the gas bubble at the initial stages of streamer development, the majority of the potential drop occurs in the water at the moment when the maximum (in absolute value) potential is reached. The conductive streamer channel is an additional link in the discharge circuit and forms a strong electric field in the water.

The Fig. 2 illustrates the spatial distribution of electron temperature in the gas bubble.

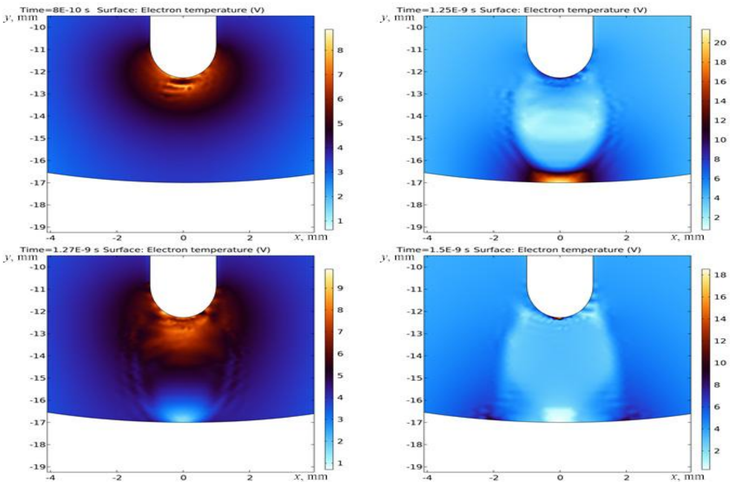

Fig. 2. Spatial distribution of electron temperature

During the formation of the streamer (0.8…1.5 ns), the temperature of most electrons is 4…5 eV. However, within the air bubble, there are localized regions where the temperatures are several times higher, and these regions are responsible for the primary shock ionization. The highest temperatures are recorded in areas with maximum electric field amplitudes, particularly near the tip of the high-voltage electrode and in the streamer head region. At 0.8 ns, the maximum electron temperature is observed near the electrode tip in the area where the initial streamer is forming. Here, the temperature reaches approximately 8 eV, which is characteristic of an active ionization process. In the streamer head, the electron temperature increases to 21 eV in regions of the most intense electron movement and where the electric field amplitude reaches up to 300 kV/cm. By 1.5 ns, the electron temperature becomes more uniform along the streamer, reaching a maximum of about 18 eV near the tip in a submillimeter zone and decreasing closer to the gas (plasma) – water interface.

The Fig. 3 shows the distribution of the electric field intensity.

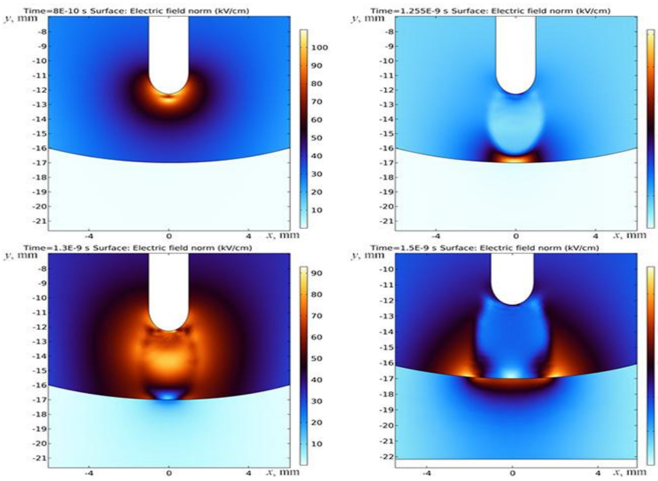

Fig. 3. Distribution of electric field intensity

Outlined the main stages of the distribution of electric field intensity during the formation of a negative streamer in an air bubble. Initial stage (up to t = 0.8 ns): the highest electric field intensity is concentrated near the tip of the high-voltage electrode, forming a zone with a maximum intensity of ~107 kV/cm, this is due to the high curvature of the tip that promotes local field enhancement. At this moment, local accumulation of electrons is observed near the tip, which triggers the streamer formation process. It is known that the streamer begins to form from an avalanche provided that the field of its space charge reaches a magnitude on the order of the external field [14]. Stage of streamer formation (from t = 0.8 ns to t = 1.255 ns): in the head of the streamer, a local increase in field intensity occurs up to ~300 kV/cm in a narrow zone between its front and the gas volume. Such a potential gradient is caused by intense ionization in this zone, which accelerates the development of the streamer toward the boundary of the gas bubble. This process corresponds to the classical streamer model, where the discharge front advances due to locally high electric field intensity in the streamer head. Stage of transition into a well-conducting channel (from t = 1.255 ns to t = 1.3 ns): when the streamer completes formation and reaches the phase boundary "air bubble (plasma) – water", the electric field intensity rapidly drops to approximately 90 kV/cm due to screening by the charge accumulated on the surface of the gas bubble and due to the increase in specific electrical conductivity within the streamer channel thanks to a sufficiently high concentration of electrons and ions. Charge distribution over the surface (t = 1.5 ns): at the moment when the voltage (potential) reaches the amplitude value of the discharge pulse, additional charge redistribution occurs across the bubble surface, and part of the potential drop propagates into the water, causing a sharp increase in the electric field strength in the water. Similar results for the electric field distribution in a reactor with an air bubble in water were obtained and demonstrated using a mathematical model described in detail in the study, where the conductivity of the air bubble was defined as a function of time [15]. At the same time, the field intensity inside the formed conductive channel is significantly reduced, while near the "air (plasma) – water" boundary and in the water its elevated level up to 115 kV/cm is maintained, reflecting the interaction between the gas plasma and the liquid phase. On the "bubble – water" surface, branching of the streamer discharge and its spreading over the surface is observed, which may explain the electric field intensity in the lateral regions.

Fig. 4 shows the distribution of displacement current density and electron current density (conductivity current).

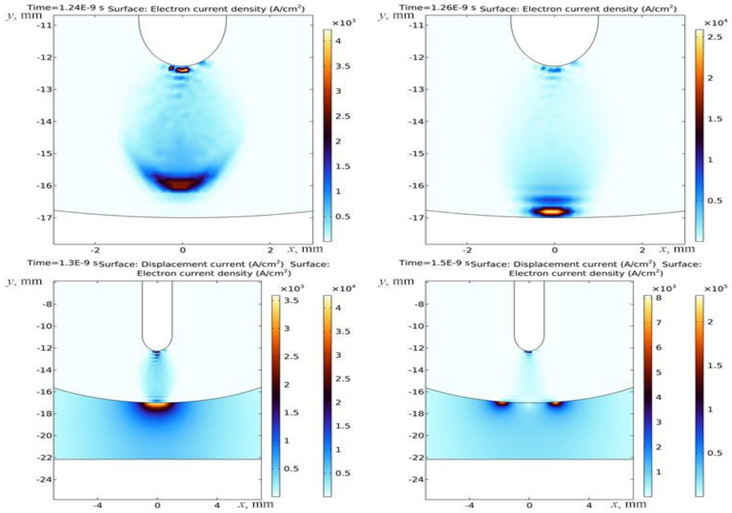

Fig. 4. Displacement current density and conductivity current density

The total current in the model, which is the sum of conduction current, displacement current, and ionic currents, always remains continuous in accordance with the law of charge conservation, and, once the streamer is fully formed, conduction current flows predominantly inside the gas bubble, whereas the surrounding water carries mainly displacement current. The displacement current arises from the rapid variation of the electric field ahead of the streamer head, whereas the electron current results from charge transport inside the plasma channel. Modeling results indicate that until the moment of 7 ns, the displacement current dominated over the conduction current in the system. The transition during which the conduction current begins to prevail over the displacement current occurs approximately in the time interval between 7 and 7.1 ns. At the moment when the streamer reaches the phase boundary "air bubble (plasma) – water", the density of both conduction and displacement currents sharply increases, rising by a factor of 6.3 within 0.02 ns. This sharp increase in currents after the completion of streamer formation is explained by the fact that the streamer (with its high density of electrons and ions) transforms into a well-conducting channel, and the resistance of this channel significantly drops. At 1.3 ns, the process of developing conduction current in the air bubble and displacement current in water is illustrated, taking into account the boundary separating the media "air (plasma) – water", where current continuity is maintained − a key feature of the physical processes of plasma-water contact during discharges in a gas bubble. At 1.5 ns, the branching of the streamer at the phase boundary "air (plasma) – water" is demonstrated, which is accompanied by a local increase in conduction current density in a submillimeter zone near the electrode tip, where its magnitude exceeds the average values along the streamer by an order of magnitude.

Fig. 5 shows the final distribution of negative and positive ions.

On Fig. 5 at the time of 1.5 ns, the calculated maximum concentrations for each ion type in the streamer are obtained: positive nitrogen ions (N_2^+) reach ~$2.2{\cdot}10^{16}$ cm^{-3}, oxygen ions (O_2^+) ~$7.2{\cdot}10^{15}$ cm^{-3}, negative atomic oxygen ions (O^-) have a concentration of ~$13{\cdot}10^{14}$ cm^{-3}, and nitrogen ions (N_2^-) up to ~$2.1{\cdot}10^{14}$ cm^{-3}. The main zone of positive ion formation (O_2^+, N_2^+) during streamer formation is located in its frontal part, where the most intense ionization is observed under the influence of a strong electric field. After the streamer formation is completed, the maximum ion concentrations are localized near the tip. Negative oxygen ions (O^-) are formed as a result of electron attachment by O_2 molecules. The concentration of nitrogen ions (N_2^-) is expected to be significantly lower, especially compared to the electron concentration that dominates the structure of the negative streamer. This can be explained by the fact that for the formation of a stable negative ion, it is necessary that the molecule have an energy level at which the additional electron is in a bound state with an energy lower than that of a free electron (taken as zero). This ensures the stability of the attached electron. For example, in oxygen (O_2) there exists a state that meets this condition, whereas in the case of nitrogen (N_2) a similar energy state is either absent or very unstable, so N_2^- quickly decomposes.

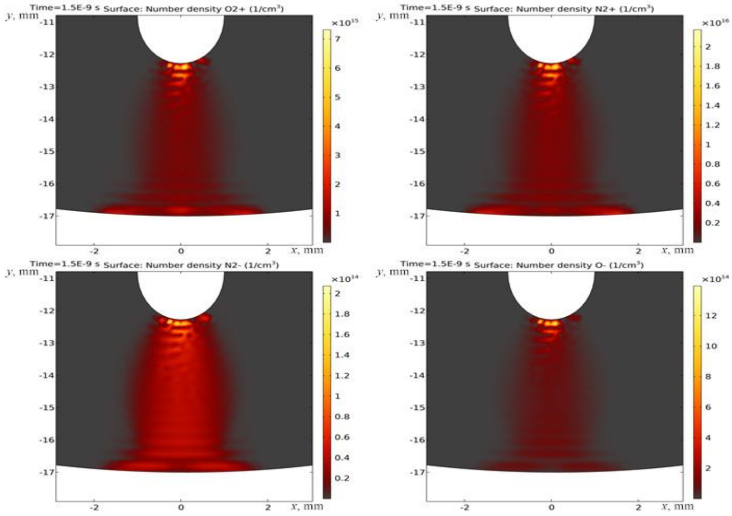

Fig. 5. Distribution of negative and positive ions

Calculations showed that in a submillimeter region near the tip of the electrode and the streamer head during its formation, a local violation of plasma quasi-neutrality is observed. Due to the high speed of ionization processes in regions with the highest electric field amplitudes, intense production of electrons and ions occurs, while transport processes (drift, diffusion, recombination) are unable to instantly level and compensate for the local excess or deficit of charged particles. Meanwhile, in larger regions of the streamer, quasi-neutrality is maintained.

Fig. 6 shows the spatial distribution of excited oxygen atoms $O(^1D)$, typical for all excited plasma particles.

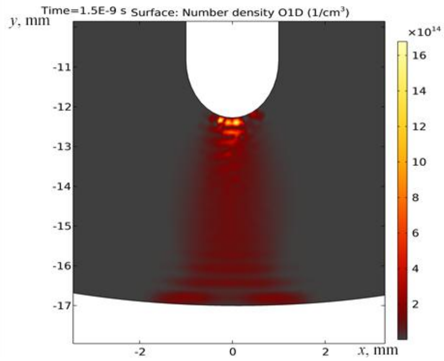

Fig. 6. Distribution of excited oxygen atoms $O(^1D)$

In Fig. 6, the maximum concentrations are observed in the immediate vicinity of the electrode tip and the streamer head during its formation, where the most intense particle excitation processes occur, driven by high electric field intensity and significant ionization. As the distance from the tip increases, the concentration of all plasma particles gradually decreases.

Maximum calculated concentrations of the main plasma particles at the time moment 1.5 ns: $O(^3P) \sim 4.5\cdot10^{16}$ cm⁻³, $O(^1S) \sim 15\cdot10^{14}$ cm⁻³, $O_2(A^3) \sim 14\cdot10^{14}$ cm⁻³, $O_2(b_1) \sim 5\cdot10^{15}$ cm⁻³, $O_2(a^1) \sim 2.2\cdot10^{16}$ cm⁻³, $O \sim 15\cdot10^{16}$ cm⁻³, $N_2(A^3) \sim 5\cdot10^{16}$ cm⁻³, $N_2(B^3) \sim 5.5\cdot10^{16}$ cm⁻³, $N_2(W^3) \sim 5.5\cdot10^{16}$ cm⁻³, $N_2(A'^3) \sim 3\cdot10^{16}$ cm⁻³, $N_2(a''^1) \sim 3\cdot10^{16}$ cm⁻³, $N_2(C^3) \sim 2.1\cdot10^{16}$ cm⁻³, $N_2(E^3) \sim 8.1\cdot10^{16}$ cm⁻³, $N_2(G^3) \sim 16\cdot10^{14}$ cm⁻³. It should be added that for O_2 and N_2 there is a reverse distribution of concentrations, meaning that in zones where the concentrations of other plasma particles reach their maxima, the concentrations of nitrogen molecules (N_2) and oxygen molecules (O_2) will be at their minima: $O_2 \sim 4.1\cdot10^{18}$ cm⁻³, $N_2 \sim 1.72\cdot10^{19}$ cm⁻³.

The comparison of concentrations of ions, microparticles in excited states, and electrons indicates that a high level of ionization and excitation occurs in a limited region of the streamer. It is precisely here that the maximum electric field intensity causes avalanche ionization and the formation of numerous electron-ion pairs, while in the formed conductive channel the electric field is significantly shielded.

Among the particles formed in the streamer, special attention should be given to the atomic states of oxygen $O(^1D)$, O, which can participate in subsequent reactions leading to the formation of radicals OH, HO_2, as well as ozone (O_3) and hydrogen peroxide (H_2O_2). These micro-particles, upon entering the water, additionally contribute to its disinfection and purification together with the intensity of the strong pulsed electric field, ultraviolet radiation in the water. In addition to oxygen compounds, excited nitrogen molecules N_2^* also play a role in further chemical reactions, as they can interact with oxygen to form nitrogen oxides (NO, NO_2). These compounds, upon entering the water, promote the formation of nitrates (NO_3^-) and nitrites (NO_2^-), which participate in oxidation reactions. During the relaxation of ions, excited atoms, and molecules, radiation across a wide spectrum − from infrared to ultraviolet and even shorter wavelengths.

CONCLUSIONS

Computer modeling of the spatiotemporal distribution of electric field intensity, potential, current densities, electron temperature, and the concentrations of charged and excited particles was carried out using a reactor model with an interelectrode gap corresponding to the reactor in which nanosecond discharges in air bubbles were experimentally obtained during water treatment. The results indicate that the streamer transitions into a well-conducting channel, as a result of which a strong electric field penetrates the water medium. The process of development of the conduction current in an air bubble and the displacement current in water is demonstrated, taking into account the “air (plasma) − water interface”.

Ionization, excitation, and recombination of particles in the discharge plasma in gas bubbles play a key role in the formation of a wide spectrum of active particles, excited molecules, and ions, which is characteristic of non-equilibrium nanosecond discharges in atmospheric air.

The results obtained lay the groundwork for optimizing the parameters of nanosecond discharges in gas bubbles in water and substantiate strong interest in further experimental and theoretical studies, opening up prospects for using such discharges in technologies for the purification and disinfection of drinking, pool, and process water, as well as the treatment of liquid radioactive waste from nuclear power plants.

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Article received 25.07.2025

ЧИСЕЛЬНЕ ДОСЛІДЖЕННЯ ЕЛЕКТРОФІЗИЧНИХ ТА ПЛАЗМОХІМІЧНИХ МЕХАНІЗМІВ ФОРМУВАННЯ НЕГАТИВНОГО СТРИМЕРА ІМПУЛЬСНОГО ВИСОКОВОЛЬТНОГО РОЗРЯДУ В ПОВІТРЯНІЙ БУЛЬЦІ У ВОДІ

М.І. Бойко, А.В. Макогон

Представлено результати чисельного моделювання формування негативного стримера імпульсного високовольтного розряду в повітряній бульці у воді. Показано розподіл напруженості електричного поля, потенціалу, густини струмів, температури електронів, концентрацій заряджених і збуджених частинок. З розрахунків випливає, що стример переходить у добре провідний канал, забезпечуючи різке зростання напруженості електричного поля у воді. Розглянуто процес розвитку струму провідності у повітряної бульці і струму зміщення у воді з урахуванням наявності границі розділу «повітря (плазма) − вода». Отримані результати створюють основу для оптимізації параметрів наносекундних розрядів у повітряних бульках у воді та обґрунтовують значний інтерес для подальших експериментальних і теоретичних досліджень.