Capacity calculation of the electrotechnical scheme of discharge gap replacement of the ozonizer in the COMSOL environment

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Abstract. The investigation of electrostatic field distribution of ozonator electrode gap caused by inhomogeneous permittivity has been done. The paper presents calculation of electrostatic field energy of ozonator electrode gap. From the energy of electrostatic field distribution the information about electrode system capacity has been extracted. For calculation of the electrostatic field and capacity of electrode system the software integrated environment COMSOL has been used.

1. Introduction
The application and physical phenomenon of barrier discharge is one of the most interesting and important direction for the fields like gas discharge of modern physics, gas electronics, physical chemistry and ozone synthesis. Currently, the barrier discharge is considered as discharge caused by electrodes voltage drop which takes place in a gas, where at least one of electrodes must be covered with dielectric.

The fields of technical application of barrier discharge have stimulated an interest in this type of discharge and physical phenomena of corresponding processes. These include application of barrier discharge for water purification, plasma technology, etching, semi-conducting materials processing, integrated circuits growing.

The successful ozone formation reaction in the barrier discharge is one of the few plasma-chemical processes utilize an industrial scale. The application of powerful ozonized installations is gradually growing and even 1MW capacity devices have been made.

However, strong spatial inhomogeneity and short duration of the physical processes which take place in the barrier discharge are causing difficulties for investigation of this phenomenon. Most recently, through the use of modern physical methods of research, modern methods of mathematical modeling and the growing capabilities of computer technology, we have been able to get a certain idea of the nature and sequence of the processes which take place in the discharge gap, but the full picture of the phenomenon still remains incomplete.

It is necessary to study in detail the development dynamics of the gas electrical breakdown in the barrier discharge in order to solve the optimization problem of plasma technologies and electrosynthesis of ozone technology.
The existing methods of mathematical modeling and interpretation of the electrical phenomena are mainly directed to the study of the processes which take place in the AC circuit. This is due to the fact that the alternating current can use well-developed mathematical technique of electrical engineering. However, the shape of the applied voltage in the circuit significantly affects the physical phenomenon of the processes occurring in the discharge gap, and as a consequence increases the energy contribution to the process. In some cases it is preferable and economical to use a pulse voltage. The processes which take place under the influence of a pulsed voltage include piecewise constant voltage areas. Within these areas, the voltage drop can be considered as a constant value, and the field in the electrode gap is considered as the electrostatic field.

Many authors suggest that the most successful way of barrier discharge description is an electrical equivalent circuit. The equivalent circuit diagram is a circuit diagram that has circuit elements which are chosen so that the current and voltage of the circuit have the same values as a discharge gap of the ozonizer. Thus, the information about the capacity of the equivalent circuit is extracted from the calculation of the electrostatic field of the discharge gap. Therefore, the aim of the article is the calculation of the electrostatic field of the discharge gap, followed by extraction of information about the capacity of the energy gap of the electrostatic field [1-6].

2. An Experimental Setup
The experimental setup that utilizes the method of water purification and disinfection is considered in various papers [5].

In the process of treatment the water droplets about 1-3 mm in diameter are falling on the electrode system which is illustrated in Figure 1. The discharge is generated between cylindrical electrodes, which are isolated from each other by dielectric barriers. Barriers are used to limit the discharge current through the gap and volume combustion of the discharge, when the uniform processing of the gap volume takes place.

In the case of a low permittivity of a barrier (a tube of quartz glass has permittivity \( \varepsilon = 4 \)) the discharge exists in a form of a large number of low-voltage micro sparks, nonequilibrium plasma of which is an effective source of active species which are involved in the oxidation processes and degradation of contaminants in the treated water. The discharge is powered by a high-voltage pulse generator. The pulse duration is about 300–500 ns, and the amplitude of the voltage is \(-20–30\) kV.

![Figure 1. The electrode system of barrier discharge for the treatment of the water (arrows show the direction of the water flow).](image)

3. Calculation of the Electrostatic Field
As a study of the system, let us consider the configuration of an electrode used for water purification as the group of round, equidistant metal cylinders with the diameter of 5 mm. These cylinders are arranged in parallel between the grounded planes (Figure 1, the sizes are given in millimeters). The geometry of the electrodes adopted in the calculations reproduces the real electrode system. The metal cylinders are inserted in 1 mm thick tightly fitting glass flasks (quartz glass barriers \( \varepsilon = 4 \), Figure 2). Each cylinder is supplied with voltage \( U = 10 \div 15 \) kV with the alternating sign while the electrode
potential difference is about $U = 20 \pm 30$ kV. The electrodes are fed by voltage in the form of a pulse with the duration of about 0.6 microseconds. In the vertical direction, the various fractions of water droplets are passed through the electrode system. The size of each water droplet does not exceed the size of the air gap.
Since the electrode system has a complex form, the field of which is not uniform in the presence of barriers, the media between electrodes have boundaries and each separate part of media has different values of permittivity $\varepsilon$. The electrode system is not closed and the field distribution calculation for this electrode system is a challenging task [5].

The paper describes a method of electric field calculation of the electrode system with complex geometry by using software integrated environment COMSOL. The method simplifies the calculation of the complex system of electrodes. Calculation was done by using Electrostatics interface AC / DC module. After the geometry model is defined and assigned values of material properties, it is assumed that the conductor is an equipotential surface. The modeling domain is surrounded by a region of infinite elements, which is a way to truncate a domain which stretches to infinity. Although the thickness of the infinite element domain is finite, it can be thought of as a domain of infinite extent [8-10]. Then the physical parameters have been defined. On the first pair of electrodes positive voltage has been set $U$ and on other pair of electrode negative voltage has been set $-U$.

The capacity calculation of the system was carried due to the calculation of the electric field on the assumption that the voltage supplied to each cylinder $U = 0.5$ V. In this case, the electrode potential difference was $U = 1$ V. The capacity of the electrode system is defined by a known ratio:

$$W = C \frac{U^2}{2} \rightarrow C = 2W.$$  

From the simulation results, the information about the density of the energy distribution of the electrostatic field has been extracted. Then the calculation of the energy of the entire system as a volume integral has been done. In this case, it is necessary to take into account the geometrical dimensions of the system. The last stage was the calculation of full energy of the field as a value proportional to the capacity.

In the COMSOL environment, these actions were carried out in the following order: Surface Integration / Energy and power / Energy density.

The value of the capacitance obtained due to the simulation is a good estimation of its analytical counterpart obtained in [4] by the hybrid technique which involved the method of the integral equation and the method of Green function $C = 1.74 \times 10^{-10}$ F/m. Let us note that the symmetric distribution of the electrostatic field allows us to determine the local capacities. To determine the local capacitance between two nearest electrodes, it is necessary to use the following ratio:

![Figure 2. The picture of electrostatic field distribution of the electrode system which is presented in Figure 1](image)
Knowing the capacity of one section, we can determine the capacity of the gap filled with glass and the capacity of the gap filled with air.

4. Conclusion
The result of simulation presented above allows us identify the most intense areas of the electrostatic field. These areas are the boundaries between glasses and air (Figure 2). Thus, a strong field on the surface of conductive electrodes is pushed to the boundaries of the glass - air areas. Consequently, in the barrier discharge, the most intense impact of discharge on the water droplets will occur near the glass-air boundaries.

The calculation of the electrostatic field allowed us to determine the field energy, and the field energy is proportional to the value of capacitance of the electrode system. The symmetrical configuration of the electrostatic field helped us to determine the resulting capacitance of the electrode system as well as the local capacitance between two nearest electrodes.

The obtained capacitances can be used in the equivalent circuit of the barrier discharge.

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