NUMERICAL INVESTIGATION OF THE FORMATION OF CHEMICALLY ACTIVE COMPONENTS IN THE SPARK DISCHARGE IN WATER VAPORS

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The numerical investigation of the formation of chemically active components and a change in the thermodynamic parameters of the spark discharge at the values of the initial pressure of water vapors 10^5 and $0.4\cdot10^5$ Pa was carried out. The formation domains of *OH, O, H, H_2O_2, HO_2, H_2O* components have been determined. It is established that the initial pressure of water vapors produces certain influence on the formation of chemically active components in the spark discharge.

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INTRODUCTION

The electrohydraulic discharge found a wide application for different technological processes [1, 2]. Presently, the electrohydraulic technology is intensively developed in the field of pulse electrochemistry. Such a development is related to the search of new energy-efficient methods used for the media treatment that are alternative to the chemical methods. Special attention is paid to the production of chemically active components that can be used for the disinfection and treatment of the drinking water and waste water and for the textile bleaching and can change the acidity of the treated media.

Therefore, the search of energy-efficient methods of the impact on liquids for the purpose of the formation of chemically active components in the spark discharge is of great interest. It is known [1, 3, 4] that a change in the initial pressure of the liquid results in a change of the development dynamics of the gas-vapor cavity that results from the electrohydraulic discharge. However, the issue of influence of the initial pressure on the formation of chemically active components in the electrohydraulic discharge requires additional studies. The underwater spark discharge is actually developed in the water vapor; therefore it is enough to carry out the investigation of the formation process of chemically active components in the spark discharge in the first approximation in the vapor-filled area.

The purpose of this paper is to carry out the numerical investigation of the influence produced by the initial pressure of water vapors on the formation of chemically active components in the spark discharge.

1. NUMERICAL MODEL OF THE DEVELOPMENT OF THE SPARK CHANNEL IN WATER VAPORS

The model described in [5, 6] was used for computations. We assumed that a local thermodynamic equilibrium was established in the area of the current-conducting channel. Outside the current-conducting channel the computations were done using the equations of nonequilibrium chemical kinetics [7].

The spark channel expansion process is described by the following equation system:

$$\frac{\partial\rho}{\partial t}+\frac{\partial(r\rho u)}{r\partial r}=0; \quad (1)$$

$$\frac{\partial\rho u}{\partial t}+\frac{\partial(r(p+\rho u^2))}{r\partial r}=\frac{p}{r}; \quad (2)$$

$$\frac{\partial(\rho\varepsilon+\frac{\rho u^2}{2})}{\partial t}+$$

$$+\frac{\partial(r(u(\rho\varepsilon+\frac{\rho u^2}{2}+p)+k_T\frac{dT}{dr}))}{r\partial r}=\sigma E^2-Q_{em}; \quad (3)$$

$$\frac{\partial y_i}{\partial t}+\frac{\partial(ruy_i)}{r\partial r}=\dot{\omega}_i, \quad (4)$$

where ρ is the gas density, u is the velocity, p is the pressure, ε is the internal gas energy per the mass unit of gas, k_T is the heat conduction coefficient, E is the electric field intensity in the current channel gap, σ is the channel plasma conductivity, Q_{em} is the radian loss of the discharge energy, r is the radius coordinate, T is the gas temperature, y_i is the molar concentration of the *i-th* component (H_2O, H, O, OH, H_2O_2, HO_2); $\dot{\omega}_i$ is the rate of change in the concentration of the *i-th* component of the mixture due to chemical reactions.

Electrical processes in the discharge circuit and in the current channel were described by the following equations:

$$L\frac{di}{dt}+\left[R_c+R_s(t)\right]\cdot i+\frac{1}{C}\int_0^t i dt=U_0;$$

$$R_s=l_s\left(\int_0^{r_s}2\pi r\sigma dr\right)^{-1};$$

$$E=\frac{R_s i}{l_s}, \quad (5)$$

where L is the equivalent induction of the discharge circuit, i is the discharge current, R_c is the equivalent active resistance of the discharge circuit, R_s is the current channel resistance, C is the electric capacitance of the capacitor, U_0 is the initial voltage of the capacitor charge, l_s is the current channel length; r_s is the current channel radius.

For initial conditions the following distribution of thermogas dynamic parameters in the computation area was prescribed:

$$p(r)\big|_{t=0} = p_0;\ T(r)\big|_{t=0} = T_0;\ u(r)\big|_{t=0} = 0.$$

Numerical investigations were carried out for two values of the initial pressure in water vapors, in particular $p_{01} = 10^5$ Pa and $p_{02} = 0.4\cdot10^5$ Pa. To provide vaporous state of water under considered pressure values in the computation area the temperature at the zero time was taken equal to $T_0 = 473$ K for both cases. The parameters of the discharge circuit were equal to $C = 2$ μF, $U_0 = 25$ kV, $L = 3$ μH, $R_c = 0.1$ Ohm. The discharge channel length was equal to 5 mm ($l = 5$ mm).

2. SIMULATION RESULTS AND THEIR DISCUSSION

Fig. 1,a,b give the distributions of the molar concentration of the components *H*, *O* and *OH* and the thermodynamic radius parameters of the spark channel that are obtained after 2 μs from the beginning of the spark expansion at different initial pressures of water vapors: $p_{01} = 10^5$ Pa and $p_{02} = 0.4\cdot10^5$ Pa. It should be noted that the three regions are available, in particular the region of the current-conducting channel, the region between the channel and the shock wave front and the region before the shock wave front. Independently of the initial pressure of water vapors the region of the current-conducting channel shows the prevalence of atomic hydrogen and oxygen. As the initial pressure of water vapors is increased an increased concentration of atoms is observed in this region at the same time from the beginning of the discharge development. It results from a decrease in the spark expansion velocity as the initial pressure of water vapors is increased and the gas density drop velocity is decelerated. When the gas temperature reaches $T \sim 16000\ldots13000$ K, dissociation reactions prevail in this region. Therefore, atomic oxygen and hydrogen cannot be used at such temperatures for the purpose of changing the acidity of the gas discharge medium.

In the region between the current conducting channel and the shock wave front the gas temperature is reduced to the ambient temperature. In this region chemically active components *H, O, OH, H_2O_2, HO_2*, are formed that can affect a change in the chemical composition when reacting admixtures are present in water vapors. As the initial pressure rises the maximum concentrations of chemically active components are also increased.

As for the computations the reduction in pressure by 2.5 times results in a decrease of the maximum concentrations of the *OH* component by a factor of 1.4 to 2 (Fig. 2). As the initial pressure is decreased the radial width of the region between the current-conducting channel and the shock wave front remains actually invariable by the same time from the beginning of the channel expansion. However, due to an increase in the radial coordinate the region volume in which a change in the chemical composition of the medium can occur is increased.

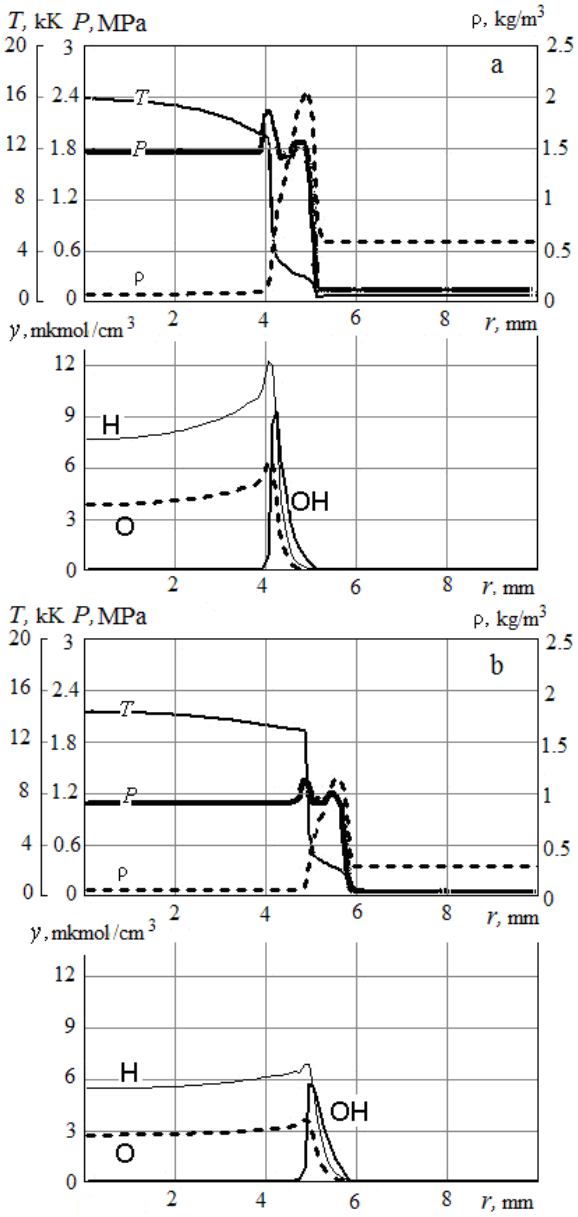

Fig. 1. Distribution of the molar concentrations of H, O, OH components taking into consideration the changes in thermodynamic parameters in the computation region at a time point of 2 μs: a – at initial pressure of vapors $p_1 = 10^5$ Pa; b – at initial pressure of vapors $p_2 = 0.4\cdot10^5$ Pa

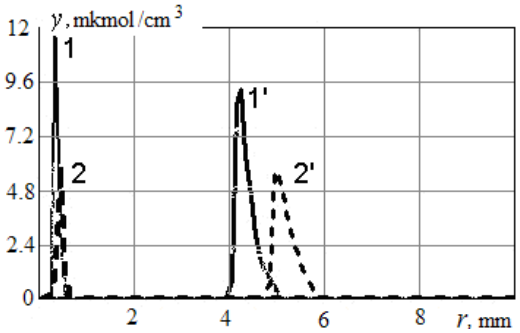

Fig. 2. The distribution of the molar concentrations of the OH radical in the computation region: 1, 2 at a time t = 0.1 μs; 1′, 2′ at a time t = 2 μs. The solid line gives the relationship at initial vapor pressure $p_1 = 10^5$ Pa; and the dashed line corresponds to the initial vapor pressure $p_2 = 0.4\cdot10^5$ Pa

Fig. 3,a,b gives the formation of chemical components *H, O, OH, H_2O_2, HO_2* at a time t = 2 μs from the beginning of the spark channel expansion.

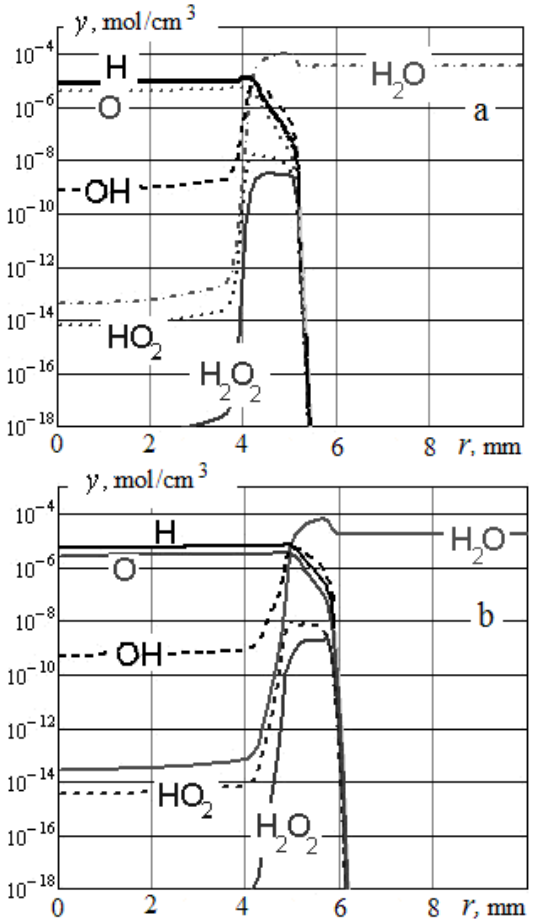

Fig. 3. Distribution of the molar concentrations of H_2O, H, O, OH, H_2O_2, HO_2 components in the computation region at a time t = 2 μs: a – at initial vapor pressure of $p_1 = 10^5$ Pa; b – at initial vapor pressure of $p_2 = 0.4 \cdot 10^5$ Pa

The obtained distribution shows that in the case of the availability of admixtures a change in the chemical composition of the medium can mainly be provided by chemically active components *H, O, OH*, because their concentration exceeds that *of H_2O_2, HO_2* components by a factor of 1 or 2.

An efficiency of the use of the spark channel energy to change the chemical composition of the medium is an important issue. As the spark channel progresses a portion of the discharge energy is lost in the discharge channel, in particular connecting wires, and the internal resistance of the capacitor. To have a prevailing portion of the discharge energy released in the spark channel we must use the discharge circuit with the active resistance, which is much less than the spark resistance. The computation data of the spark channel obtained at a different initial pressure of water vapors are given in Fig. 4,a. It follows from the obtained data that the calculated active resistance of the discharge circuit must not exceed 5…10 mOhm.

The revealed interrelation between the electric field intensity in the spark channel gap and the formation of chemically active components in the spark channel is of great interest. A decay of initial pressure results in a decrease of the electric field intensity that occurs at the same time after the beginning of the discharge development (see Fig. 4,b). For the computation option the difference in the electric field intensity is within one order (Fig. 5). We assume that the regularity of a decrease in the maximum concentrations of chemically active components with a drop of the initial pressure in water vapors is mainly caused by thermal gas dynamic processes that exert influence on nonequilibrium chemical processes and the field intensity affects this process through a change in the quantity of energy released into the spark channel.

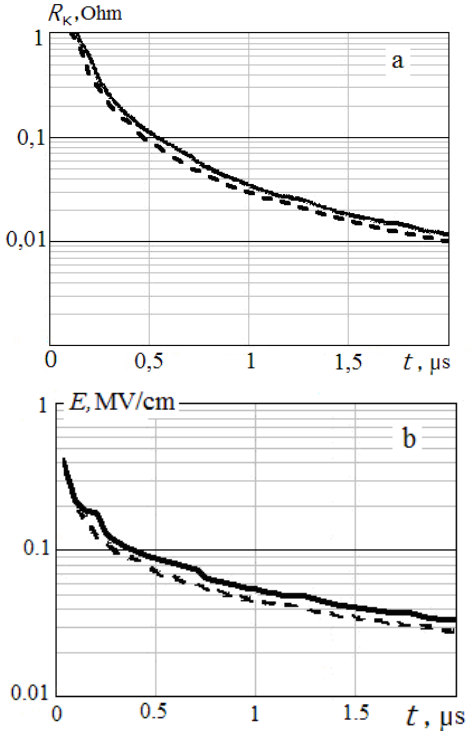

Fig. 4. Spark channel resistance (a) and electric field intensity in the spark channel gap (b) at different initial water vapor pressures: solid line –10^5 Pa, and dashed line – $0.4 \cdot 10^5$ Pa

Treatment of the medium by the irradiation is one of the most useful applications of the underwater spark discharge. This paper delves into the investigation of the influence produced by the initial water vapor pressure on the quantity of energy radiated by the spark discharge.

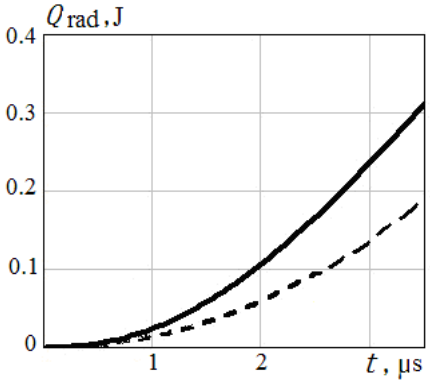

Fig. 5. The quantity of energy radiated by the spark discharge at a different time from the beginning of the discharge development: at initial pressures of water vapors 10^5 Pa (solid line),and $0.4 \cdot 10^5$ Pa (dashed line)

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CONCLUSIONS

The numerical investigation of the formation of chemically active components in water vapors for two pressure values of water vapor $p_1 = 10^5$ Pa and $p_2 = 0.4 \cdot 10^5$ Pa has been carried out. It has been established that the formation of chemically active components occurs in the region of the current conducting channel and in the region between the channel and the shock wave front. The availability of admixtures shows that a change in the chemical composition of the medium can mainly be provided by chemically active components *H, O, OH*. It is shown that the drop in pressure by 2.5 times for the computation option results in the decrease of the maximum concentration of the *OH* component by 1.42 times. A volume of the region in which a change in the chemical composition of the medium can occur is increased at lower pressures. It has been established that the quantity of energy radiated by the spark discharge is decreased with the pressure drop.

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ЧИСЛЕННОЕ ИССЛЕДОВАНИЕ НАРАБОТКИ ХИМИЧЕСКИ АКТИВНЫХ КОМПОНЕНТОВ В ИСКРОВОМ РАЗРЯДЕ В ПАРАХ ВОДЫ

Д.В. Винников, К.В. Корытченко, А.В. Сакун

Проведено численное исследование наработки химически активных компонентов и изменения термодинамических параметров искрового разряда при значениях начального давления паров воды 10^5 и $0{,}4 \cdot 10^5$ Па. Определены области образования компонентов *OH, O, H, H_2O_2, HO_2, H_2O*. Выявлено влияние начального давления паров воды на наработку химически активных компонентов в искровом разряде.

ЧИСЕЛЬНЕ ДОСЛІДЖЕННЯ НАПРАЦЮВАННЯ ХІМІЧНО АКТИВНИХ КОМПОНЕНТІВ В ІСКРОВОМУ РОЗРЯДІ У ВОДЯНІЙ ПАРІ

Д.В. Вінніков, К.В. Коритченко, А.В. Сакун

Проведено чисельне дослідження напрацювання хімічно активних компонентів і зміни термодинамічних параметрів іскрового розряду при значеннях початкового тиску водяної пари 10^5 та $0{,}4 \cdot 10^5$ Па. Визначено області утворення компонентів *OH, O, H, H_2O_2, HO_2, H_2O*. Виявлено вплив початкового тиску водяної пари на напрацювання хімічно активних компонентів в іскровому розряді.