NUMERICAL SIMULATION OF A MICROWAVE DISCHARGE IN A MIXTURE OF ETHANOL AND WATER [[1]](#footnote-1)\*)

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In recent decades great attention of researchers is attracted by discharges in liquids and in contact with them, due to the possibilities of solving various applied problems. In particular, discharges in a mixture of ethanol and water are used to produce hydrogen. Various types of electrical discharges are used, but the least investigated are microwave discharges. This work continues our cycle of works on simulating a microwave discharge in liquids and is devoted to the study of kinetic processes in a gas mixture of decomposition products of a mixture of ethanol with water. The calculations are carried out for atmospheric pressure in the zero-dimensional approximation.

The model contains the balance equations for neutral and charged gas components of the plasma, the Boltzmann equation for free plasma electrons, the equation for the average microwave field in a small volume filled with plasma [1] and the equation for the temperature of the gas mixture. The San Diego Mechanism set of reactions is used to describe thermal processes [2]. Reactions with charged particles are added. When calculating the gas temperature, it is assumed that the energy required to carry out processes under electron impact is taken from electrons. The electron energy distribution function (EEDF) is found from the Boltzmann equation, written in the two-term approximation of the EEDF expansion in spherical harmonics. The rate constants of reactions of electronic processes, being functions of the values of the reduced field E/N, are calculated by means of a set of corresponding cross sections for reactions and EEDF. In this work, the EEDF is calculated using the BOLSIG+ program [3] and a set of cross sections for collisions of electrons with mixture molecules. The kinetic model for ethanol included the processes of direct ionization, dissociation, dissociative attachment and associative detachment. The model includes positively and negatively charged ions: H2O+, H3O+, H5O2+, H3O+(H2O), H3O+(H2O)2, H3O+(H2O)3, O2+, СH3O+, C2H5O+, C2H5OH+, CH3+, C2H3+, H-, O-, OH- , C2H5OH-, CO-.

Our calculations allow analyzing the role of various reactions in the dissociation of a mixture, the formation of neutral products, in particular hydrogen, and in the formation and loss of negatively and positively charged particles for various E/N values and gas temperature. The main decomposition products of the mixture are hydrogen, carbon monoxide and acetylene. The concentrations of hydrogen and carbon monoxide obtained in the calculations coincide with the experimental data [4].

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References

1. V.B. Gil’denburg, V.E. Semenov Sov. J. Plasma Phys. (1980) **6** 244
2. <https://web.eng.ucsd.edu/mae/groups/combustion/mechanism.html>
3. <https://fr.lxcat.net/solvers/BolsigPlus/index.php.__>
4. Tonghui Zhu , Bing Sun \*, Xiaomei Zhu , Liru Wang , Yanbin Xin , Jinglin Liu Journal of Analytical and Applied Pyrolysis (2021) **156** 105111

1. \*) [abstracts of this report in Russian](http://www.fpl.gpi.ru/Zvenigorod/XLIX/Lt/ru/EN-Tatarinov.docx) [↑](#footnote-ref-1)