2D SIMULATION OF CHEMICAL PROCESSES IN A MicroWave DISCHARGE IN LIQUID HEAVY HYDROCARBONS [[1]](#footnote-1)\*)

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Nonequilibrium microwave discharges in various liquids have been the subject of intensive research in recent decades [1,2]. A microwave discharge is an effective means of carrying out plasma-chemical reactions in liquid heavy hydrocarbons; n-heptane (being the main component of various fuels) can serve as a model hydrocarbon for them. The present work builds on the results of experiments in the microwave discharge in liquid n-heptane [3,4] and the data, obtained by numerical zero-, one- and two-dimensional simulations [5-7]. For solid particles, we developed a model, where the surface growth of solid particles was carried out in the reactions of addition of acetylene to active centers on a solid surface. The size distribution function of soot particles has been obtained [6]. Charging of heavy particles leads to a change in the distribution function for their sizes. The maximum of the distribution function shifts from the region of light particles to the region of particles of medium size [7]. Two-dimensional calculations [5] made it possible to determine the details of the formation and detachment of a plasma bubble from the electrode surface, the characteristic size of the bubble, and the rate of its ascent. This paper presents the results of a two-dimensional simulation that includes the main kinetic processes of n-heptane pyrolysis in a plasma bubble.

The two-dimensional model includes the hydrodynamic equations for an incompressible liquid and a compressible gas, the heat equation, the Maxwell equation for the microwave field, and the balance equations for the electron concentration and the main components of n-heptane decomposition. The simulation takes into account the diffusion of gas particles to the boundaries of the discharge chamber and the influx of n-heptane into the plasma bubble due to evaporation.

The calculations made it possible to trace the evolution of the gaseous products of n-heptane pyrolysis reactions up to 0.1 second for two values of the power applied to the discharge. It is shown that the amount of generated hydrogen increases with the increase in the input power. A qualitative analysis of the evolution of the formation of the main components of the gas discharge has been carried out. The results of calculation and experiment are compared.

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References

1. Bruggeman P. *et al* Plasma Sources Science & Techn., 2016, V. 25, 053002.
2. Lebedev Yu.A., Plasma Phys. Rep. 2017, V. 43, P. 577-588
3. Averin K.A., Lebedev Yu.A., Shchegolikhin, A. N., and Yablokov, M. Yu.  Plasma Processes and Polymers 2017, 14, Issue 9, DOI 10.1002/ppap.20160022
4. Lebedev Yu.A., Averin K.A., Tatarinov A.V., Epstein I.L., EPJ Web of Conferences, 2017, V. 149, 02002
5. Lebedev Yu.A., Tatarinov A.V., Epstein I.L., Averin K.A. Plasma Chem. Plasma Process. 2016, V. 36, P. 535-552
6. Lebedev Yu.A., Tatarinov A.V., Epstein I.L., Plasma Chem. and Plasma Process., 2019, V. 39, P. 787–808
7. Lebedev Yu.A., Tatarinov A.V., Epstein I.L., Plasma Sources Sci. Technol. V. **29,** 2020, 065013
1. \*) [abstracts of this report in Russian](http://www.fpl.gpi.ru/Zvenigorod/L/Lt/ru/FR-Lebedev.docx) [↑](#footnote-ref-1)