COMPARISON OF THE SMALLEST SQUARES AND SMALLEST MODULES METHODS IN MODELING PROCESSING OF MATERIALS BY PLASMA OF A GAS-VAPOR DISCHARGE WITH LIQUID ELECTRODES

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Abstract. This paper describes the application of the least squares and least modulus methods to obtain the values of the power parameters of the central Lennard-Jones potential when modeling processes in the technology of processing materials with vapor-gas discharge plasma with a liquid electrode.

1. Introduction.
The mathematical apparatus is a universal tool for describing technical problems [1-5]. Therefore, the progress of engineering and technology (technical sciences, engineering practice) is closely connected with the development of mathematics. The emergence and improvement of a large number of numerical methods of mathematics is associated with applied needs. The paper compares the possibilities of using two mathematical methods - the method of least squares (MLS) [6] and the method of least modules (MLM) [7] - for processing the results of a technical experiment to study the characteristics of one of the modifications of the electric discharge. As in other areas of engineering and technology [8], the experimental study of processes in low-temperature plasma may be accompanied by the need to solve problems based on the extremal principle associated with one of the areas of mathematics - the theory of optimal control. The possibilities of obtaining low-temperature plasma by igniting an electric discharge between solid metallic and liquid non-metallic (electrolytes with the addition of inorganic and organic impurities) electrodes are interesting from the point of view of developing technologies for improving the performance properties of materials with different physical and mechanical properties. A large number of statistical data that appear during the experiments described in this paper require generalization [9–10]. Most often, MLS is used to process experimental statistical information. MLM is used less often, but its statistical properties are more often better [1, 6–7]. When using the least squares, the conditions are determined for which the values of the square of the known function are the smallest. In this general form, the method is widely used for the mathematical description of scientific and technical problems (in physics, mechanics, mathematical statistics, in the theory of errors in the processing of experimental data, in solving problems of numerical analysis). The method makes it possible to use others, simpler and more convenient in research, for an approximate representation of the given functions. The described
advantages of the method determined its choice for processing the results of a technical experiment to
study the characteristics of the investigated modifications of the electric discharge [11-14].
Among a large number of factors affecting the results of the technological process of processing
surfaces of products by a vapor-gas discharge between solid metal and liquid non-metal electrodes,
there are the electric current in the discharge and the voltage drop in the interelectrode gap [6-7, 9-14].
MLS and MLM, just optimal for consideration in the processing of experimental information with a
combination of several factors of influence. As in all types and varieties of chemical technology and
electrical technology, the use of various modifications of the vapor-gas discharge between solid metal
(or liquid non-metal) and liquid electrodes is associated with a large number of complex, time-
consuming experiments. It is for this reason that the involvement of the mathematical apparatus in
describing the results of experiments is a useful tool in the research work in this area, and the
mathematical methods we have chosen for comparison allow us to build probabilistic-statistical
models that allow us to make predictions in complex studies [1-14].

2. The relevance of research.
The work is devoted to the study of two mathematical methods (MLS and MLM) for describing the
process of processing substances using an electric discharge in a vapor-air environment and the
possibility of generalizing the results of the study for the technological description of various
modifications of a vapor-gas discharge between solid metal (or liquid non-metallic) and liquid
electrodes. At the same time, the degree of correspondence between calculated and experimental data
depends on the selection of constants that determine the intensity of physical and chemical processes.

3. Research methods.
The scheme of the technological experiment is shown in fig. 1, where it is indicated: 1. Electrochemical cell; 2. Electrolyte (liquid electrode); 3. Solid state metal electrode; 4. Metal plate. The material processing technology involves the simultaneous action of both an electric discharge and electrochemical processes on it [6-7, 9-14].

Figure 1. Scheme of technological experiment.

When a part is exposed to low-temperature plasma in the interelectrode gap in the pre-breakdown
mode and during breakdown, hydrogen and oxygen are released on the metal electrode. This process is
accompanied by the release of heat, the transition of the gas-liquid state into a vapor-gas state with the
formation of a layer of gas and liquid. The need to take into account a large number of processes
greatly complicates the mathematical modeling of the considered physical system [6-7, 9-14].
The coefficients of diffusion and viscosity of gas mixtures were obtained on the basis of a strict
kinetic theory of gases using the central potential of Lennard-Jones (8-6) [6-7, 15-17]. MLS and MLM
made it possible to obtain the force parameters of some real gases. For comparison, we used the values
of binary collision integrals obtained in experiments on the scattering of molecular beams in the temperature range 20000–50000 K [17].

4. Results. The obtained values of power parameters for some real gases are presented in Table 1:

| Substance | MLS | MLM |
|-----------|-----|-----|
|           | $\sigma$, Å | $\varepsilon / \kappa, K$ | $\sigma$, Å | $\varepsilon / \kappa, K$ |
| H$_2$     | 2.786 | 34  | 2.812 | 36  |
| O         | 2.695 | 117 | 2.578 | 112 |
| N$_2$     | 3.586 | 96  | 3.593 | 86  |
| O$_2$     | 3.619 | 117 | 3.683 | 119 |
| NO        | 3.324 | 124 | 3.154 | 129 |
| CO        | 3.435 | 101 | 3.412 | 105 |

Below, in fig. 2 shows potential curves for molecular hydrogen. Here, the number 1 denotes the curve corresponding to the Lennard–Jones potential (8–6) with the parameters obtained using the MLM (Table 1); the number 2 is the classical Lennard-Jones potential (12–6) with the parameters taken from the handbook [17]; 3 – potential of Lennard- Jones type (8–6) with parameters obtained using MLS (Table 1); 4 – experimental data on molecular beam scattering [17]. It can be seen that the potential of the Lennard-Jones type (8–6) is in better agreement with the potential curve obtained from the data on molecular beam scattering. At the same time, the data obtained using the MLS are in better agreement with the experiment at high temperatures, and those obtained using the MLM are at low temperatures.
5. Conclusions.
The choice of algorithm for solving the problem of interpolation, curve approximation or smoothing depends on the nature of the data being processed and on the desired output result. When choosing an algorithm to use on a computer, the limitations of that device must be taken into account. Often there is a contradiction between the accuracy and time of computing on a computer, on the one hand, and the required amount of memory, on the other. MLS and MLM require the solution of a system of linear algebraic equations. As the order of least squares approximation increases, the number of equations in the system increases. In the MLS problem, the number of equations increases with the increase in the considered points. This increase in the size of the system leads to an extension of the execution time and a significant increase in the amount of memory for arrays required when obtaining a solution [1, 6-7]. Taking into account these features of the two mathematical methods and comparing the data on the power parameters of the proposed central potential of the Lennard-Jones type (8–6) (Fig. 2) allows us to choose the most appropriate model for an adequate description of the technological process associated with the use of a vapor-gas discharge.

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