On the issue of modeling the processing of materials by plasma of a vapor-gas discharge with liquid electrodes

R R Takseitov¹, R K Galimova¹ and Z Y Yakupov¹

¹KNR TU-KAI named after A N Tupolev, Kazan, Russia

E-mail: RRTakseitov@kai.ru, RKGalimova@kai.ru, zymat@bk.ru

Abstract. This work describes a method for using the power parameters of the Lennard-Jones central potential to simulate phenomena in the technology of material processing by a vapor-gas discharge plasma with a liquid electrode.

1. Introduction
Mathematical modeling of the processes of processing materials with low-temperature plasma leads to a system of semi-empirical equations containing a certain set of constants, the values of which are determined by the technology used. Both the composition of the electrolyte and the composition of the gas in which the discharge combustion process takes place is of great importance. In this case, various types of effects (plasma-chemical, electrolytic, etc.) appear on the coatings. When a vapor-gas discharge with a liquid electrode burns, gas mixtures are released. One of the assumptions in this case is the use of the transfer characteristics of gas mixtures obtained by the methods of the rigorous kinetic theory of gases. This, in turn, allows obtaining high-quality results when developing models of an engineering experiment.

2. The relevance of research
The process of processing materials by low-temperature plasma is a certain set of stochastic processes (physicochemical, chemical-technological), therefore, when describing it, it becomes necessary to make a number of assumptions. In this case, a satisfactory agreement between the calculated and experimental data is largely determined by the successful selection of constants that depend on the experimental conditions.

3. Research Methods
The configuration of technological elements used in the study during processing of a substance (liquid or solid) 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 method proposed in this work assumes a combined effect on the material of an electric discharge and electrochemical processes [1-5].

When processing a part with low-temperature plasma in the interelectrode gap in the pre-breakdown mode and during the breakdown at the metal electrode, hydrogen and oxygen are released, accompanied by the processes of heat release, the transition of the gas-liquid state to the vapor-gas state with the formation of a layer of gas and liquid, and ionization. In addition, there is an effect on the...
result of uncontrolled input variables. All this greatly complicates the mathematical description of complex physical systems [3]. The mutual influence of a large number of processes becomes the main problem in modeling technical processes [1-9].

![Figure 1. Configuration of technological objects](image)

To calculate the diffusion coefficients and viscosity of gas mixtures, the Lennard-Jones central potential was used (8-6). Its dependence on the intermolecular distance \( r \) is determined by the formula:

\[
\phi(r) = \frac{256}{27} \varepsilon \left( \frac{\sigma}{r} \right)^8 - \left( \frac{\sigma}{r} \right)^6,
\]

where \( \varepsilon, \sigma \) - are the parameters of the potential (power parameters).

The rigorous kinetic theory of gases makes it possible to relate the transport characteristics of gas mixtures with the intermolecular potential through binary collision integrals (or \( \Omega \)-integrals).

The numerical techniques used to calculate the reduced binary collision integrals are described in [6]. To obtain the values of the parameters \( \sigma \) and \( \varepsilon/k \), where \( k \) is the Boltzmann constant, the method of least moduli (MLM) was used [7]. In this case, the calculated values were compared with the values of the binary collision integrals obtained from experiments on the scattering of a molecular beam [8]. As an initial approximation for starting the iterative process, we used the values of \( \sigma \) and \( \varepsilon/k \) from [9]. The summation was carried out in the temperature range of \( 2000^0-5000^0 K \).

4. Results

The obtained values of the power parameters for some real gases are presented in table 1:

| Substance | \( \sigma, \si \) | \( \varepsilon/k, K \) |
|-----------|----------------|-----------------------|
| H\(_2\)   | 2.812          | 36                    |
| O         | 2.578          | 112                   |
| N\(_2\)   | 3.593          | 86                    |
| O\(_2\)   | 3.683          | 119                   |
| NO        | 3.154          | 129                   |
| CO        | 3.412          | 105                   |


Below, in Fig. 2 shows potential curves for molecular nitrogen obtained in accordance with the data for various model potentials most frequently used in practice. In this case, the number 1 denotes the curve corresponding to the Buckingham potential with the parameters taken from [9]; number 2 - the Lennard – Jones potential (12–6) with parameters taken from [9]; 3 - the considered potential of the Lennard – Jones type (8–6) with the obtained values of the force parameters (Table 1); 4 - experimental data on molecular beam scattering. It can be seen from the figure that of the three types of potentials under consideration, it is the Lennard – Jones type potential (8–6) that is in better agreement with the potential curve obtained on the basis of data on the scattering of a molecular beam.

![Figure 2. Potential curves for molecular nitrogen](image)

5. The discussion of the results
When designing a technological process associated with the use of a vapor-gas discharge, it is necessary to take into account the entire complex of physicochemical processes occurring in the volume of the electrolyte and in the inter-electrode gap. Adequate construction of a mathematical model requires reliable information on transport processes at high temperatures. In this case, the choice of the potential and the correspondence of the power parameters to the considered temperature range are of great importance.

6. Findings
The results obtained using the method of least moduli for the power parameters of the Lennard-Jones type potential make it possible to adequately describe the transport properties of gas mixtures released during the combustion of a vapor-gas discharge with a liquid electrode.

References
[1] Pavlova A. A., Iutin R. V., Yakupov Z. Ya. Averaging the surface roughness during the treatment of the part using the least square method. VIII Intern. scientific youth school-seminar *Math. Simulation, number methods and complexes of programs*. Saransk: SVMO, 2018. 78-81. Access Mode: [http://conf.svmo.ru/files/2018/ThesesSaransk2018.pdf](http://conf.svmo.ru/files/2018/ThesesSaransk2018.pdf)

[2] Pavlova A. A., Shakirov A. Sh., Galimova R. K. Estimation of the acidity of the solution in the process of obtaining sols by the method of least moduli. VIII Intern. scientific youth school-seminar *Math. Simulation, number methods and complexes of programs*. Saransk: SVMO, 2018. 82-85. Access Mode: [http://conf.svmo.ru/files/2018/ThesesSaransk2018.pdf](http://conf.svmo.ru/files/2018/ThesesSaransk2018.pdf)
[3] Yakupov Z. Y., Abdulasis Abrahem H., Bogomolov V. A., Plohotnikov S. P. Algorithm for Constructing Modified Relative Phase Permeability for the Average Model of Three-Phase Filtration in A Multilayered Layer. 2020 IOP Conference Series: Material Science and Engineering. 765 (1), 012003.

[4] Shakirov A. Sh., Galimova R. K., Yakupov Z. Ya. Problems of forecasting in sol-gel technologies. XIII Intern. scientific and technical conf. young specialists, graduate students and students Math. and computer modeling of natural-scientific and social problems. Penza: Publishing house of PSU, 2019. 184-188.

[5] Pavlova A. A., Galimova R. K., Yakupov Z. Ya. Development of technology for producing sols for the production of nanocoatings in aviation. Innovation Promotion Fund “UMNIK – AERONET 2018”. Access Mode: https://umnik.fasie.ru/aeronet

[6] Ignat’ev V.N., Takseitov R. R. High-temperature coefficients of viscosity and diffusion of some gases and gas mixtures calculated on the basis of central potential. Izvestiya Vysshikh Uchebnykh Zavedenij. Aviatsionnaya Tekhnika, 2004 (4). 20-22.

[7] Yakupov Z. Ya., Galimova R. K. Methods of least squares and least moduli in scientific and technical calculations. Kazan: KNRTU-KAI, 2017. 140 p.

[8] Alemasov V.E., Dregalin A.F., Tishin A.P., Khudyakov V. A. Thermodinamic and thermophysical properties of combustion products. Handbook in five volumes. Vol. 1. Moscow: VINITI, 1972. 267 p.

[9] Takseitov R. R., Galimova R. K., Yakupov Z. Ya. Calculation of portable properties of some real gas mixtures at high temperatures. 2020 Journal of Physics: Conference Series. 1588 (1), 01265.