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Transport and thermodynamic properties of equilibrium arc discharge in a mixture of air with hydrogen, argon with hydrogen

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The calculation of transport and thermodynamic properties of equilibrium arc discharge in mixtures of air and hydrogen, as well as argon and hydrogen in the temperature range from 300 to 25000 K is performed. The calculation methodology used for determination of electrical conductivity, thermal conductivity, viscosity, heat capacity and density is given. The results of calculations are given and analysed, taking into account the application in plasma technologies.

Keywords: transport properties, thermodynamic properties, equilibrium arc discharge, plasma torch.

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The study of the use of low-temperature plasma is necessary for many areas of technology and industry: plasma thermal coating, plasma cutting, testing of chemical composition, plasma welding, development of new types of switching devices, etc. [1–3]. Various plasma-forming mixtures are used depending on the application. For example, plasma-forming mixtures of gases Ar, H_2 or He are used in plasma welding or cutting: Ar/H_2, Ar/He, Ar/H_2/He. SF_6, CO_2 or air mixed with materials of nozzle ablation and erosion of electrodes (contacts) are used as an arc extinguishing medium in gas-filled switches: C_2F_4, Cu, W, Ag, Al [4]. Therefore, determination of the properties of gas mixtures is one of the key tasks for designing and modernization of existing devices with an equilibrium gas discharge.

One of the directions of plasma technologies is plasma sputtering, which has now received an additional impetus for the development of - because of the possibilities of application in additive technologies [5]. Traditionally, argon and air are used in plasma thermal coating technology, however, plasma-forming mixtures of argon with hydrogen (or with helium) or air with hydrogen can be used to increase the enthalpy of the plasma flow. Various powders are fed into the plasma stream (Al_2O_3, MgO, TiO_2, Cr_2O_3, ZrO_2, etc., etc.), which are melted in a plasma jet and then applied to the surface. The optimization of such a technological process requires experiments and numerical modeling. The flow velocity is hundreds of m/s since the core temperature of the arc exceeds 12,000K. Numerical modeling can become an auxiliary tool for a researcher to make informed decisions in real applied plasma spraying problems. The purpose of this work is to establish the transport and thermodynamic properties of an equilibrium arc discharge in a mixture of air with hydrogen, argon with hydrogen.

Computer-aided engineering (CAE) is used for development of the technological process and for reduction of the cost of experimental studies. SAE is one of the central and most high-tech technologies of modern industry that ensures the competitiveness of new generation products and allows taking into account all the material properties of mixtures, such as thermodynamic functions, transfer coefficients, specific radiation power, etc. It is necessary to use spatially and temporarily resolved numerical models for such systems for taking into account the complexity of plasma processes in time and space, for a more accurate description and behavior prediction. This approach will allow conducting a detailed analysis, taking into account nonlinear phenomena, and studying the dynamics of processes in case of theoretical studies in addition to the experiment.

The literature often provides data on thermodynamic equilibrium in systems, which allows calculations of high-temperature processes [6]. The establishment of equilibrium at high temperatures occurs quickly, so such data are quite accurate. They are more accurate than the kinetic parameters and information about the mechanism of the process, which are also given in the literature [7]. In many cases, the theoretical results are in good agreement with the experimental data.

The main technological parameters of the process, such as the degree of transformation, energy consumption for obtaining the product, as well as the thermodynamic properties of the final products (heat capacity, total enthalpy of the mixture, etc.) can be determined using thermodynamic calculations of equilibrium compositions of multicomponent systems.

The calculation of plasma composition is the basis for calculating its thermodynamic and transport properties. Four plasma-forming mixtures with different mass ratios are considered. The calculation parameters are given in the table. The following composition of air was considered

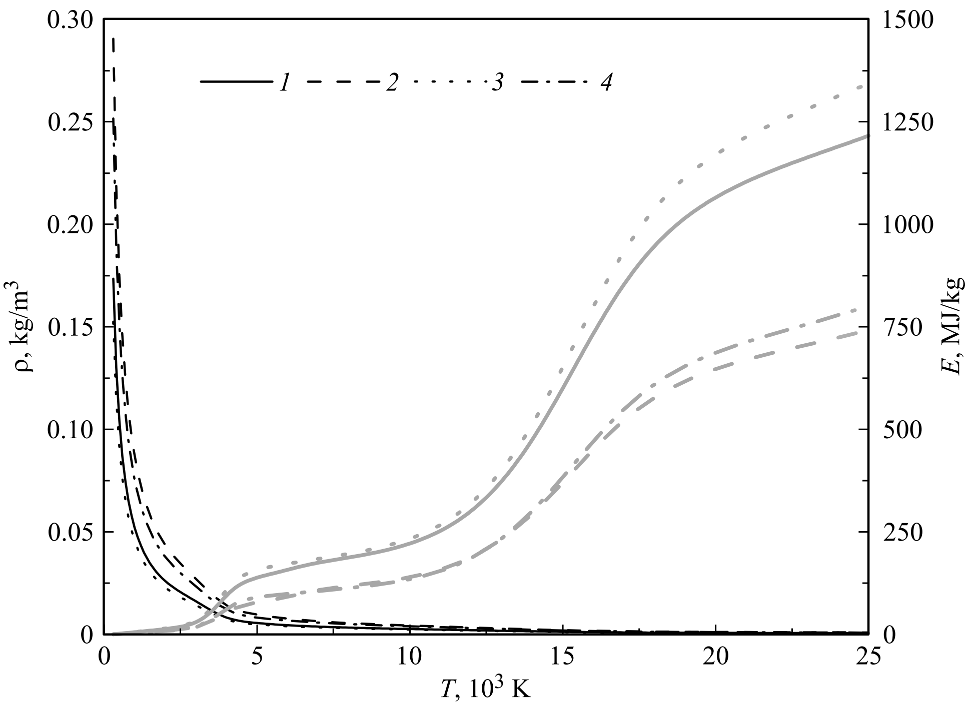

Figure 1. Dependences of density (black lines) and enthalpy (gray lines) on temperature. The curves are numbered in accordance with the calculation number in the table.

(by weight): Ar — 1.3%, O_2 — 23.15%, N_2 — 75.55%. Determining the number of components that should be taken into account in the calculation is the first step for thermodynamic calculations. This choice is based on the analysis of the literature data on the process and the analysis of the equilibrium constants [8,9].

The following components were considered for a mixture of air with hydrogen: e, H, H^-, H^+, H_2, H_2^+, Ar, Ar^+, Ar^{2+}, Ar^{3+}, Ar^{4+}, Ar^{5+}, Ar^{6+}, O, O_2, O^-, O_2^-, O^+, O^{2+}, O^{3+}, O^{4+}, O^{5+}, O^{6+}, O_2^+, N, N^+, N_2, N_2^+, N_2^{2+}, N_2^{3+}, N_2^{4+}, N_2^{5+}, N_2^{6+}, OH^-, NH, NH^+, OH, OH^+, NO, NO^+.

The following components were considered for a mixture of argon and hydrogen: e, H, H^-, H^+, H_2, H_2^+, Ar, Ar^+, Ar^{2+}, Ar^{3+}, Ar^{4+}, Ar^{5+}, Ar^{6+}.

The KintechDB database which contains all the necessary interpolation coefficients, data on substances for calculating thermodynamic properties was used for calculation of the properties of plasma-forming mixtures. The transport properties of plasma depend on the collision integrals $\Omega^{(L,s)}$ according to the molecular kinetic theory, which constitute cross sections of collisions of pairs of particles averaged using the Maxwellian particle velocity distribution. The thermodynamic calculation of the plasma composition is performed using the assumption that the plasma is in a thermodynamic equilibrium state at a constant temperature in the range from 300 to 25 000 K and a pressure of 1 atm.

The density of the mixture was calculated using the ideal gas equation $\rho = (P\mu)/(RT)$, where ρ — the density, μ — the molecular weight of the mixture, R — the gas constant, T — the temperature. The heat capacity of the mixture was determined as the sum of the heat capacities of the components, which were determined using the interpolation function

$$C_p(T) = \phi_2 + 2\phi_3 x^{-2} + 2\phi_5 x + 6\phi_6 x^2 + 12\phi_7 x^3,$$

where ϕ — the interpolation coefficient, $x = 10^{-4}T$.

The calculation of transport properties, including electrical conductivity, viscosity and thermal conductivity, is based on the solution of the integral and differential Boltzmann equation using the Chapman and Enskog method [10]. Thermal conductivity is defined as the sum of four components: the contact thermal conductivity of heavy particles, the contact thermal conductivity of electrons, the internal thermal conductivity in the second approximation, and the reactive thermal conductivity calculated in accordance with Mason–Monchik theory [11]. The viscosity, which is the viscosity of heavy particles, is calculated in the second approximation.

The distributions of density and enthalpy (Fig. 1), heat capacity and thermal conductivity (Fig. 2), viscosity and electrical conductivity (Fig. 3) were obtained as a result of the conducted studies. The dependences of the parameters (Fig. 1–3) are given in accordance with the table: calculation № 1 — 95% air, 5% hydrogen; calculation № 2 — 98% air, 2% hydrogen; calculation № 3 — 95% argon, 5% hydrogen; calculation № 4 — 98% argon, 2% hydrogen.

It can be seen from the dependence of density on temperature (Fig. 1) that the density of the mixture slightly differs for the various considered compositions at temperatures above 2500 K. Hydrogen is broadly used in

Calculation parameters

Calculation number	Components	Mass ratios
1	Air (95%)+H_2 (5%)	0.017 Ar/0.3 O_2/0.98 N_2/H_2
2	Air (98%)+H_2 (2%)	0.044 Ar/0.78 O_2/2.55 N_2/H_2
3	Ar (95%)+H_2 (5%)	0.95 Ar/H_2
4	Ar (98%)+H_2 (2%)	2.45 Ar/H_2

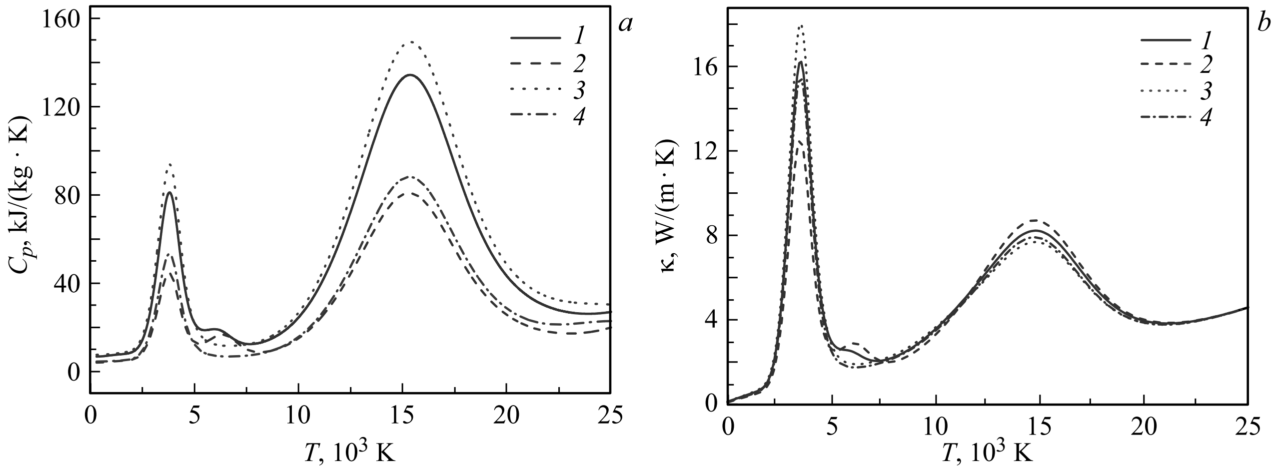

Figure 2. Dependences of heat capacity (*a*) and thermal conductivity (*b*) on the temperature. The curves are numbered in accordance with the calculation number in the table.

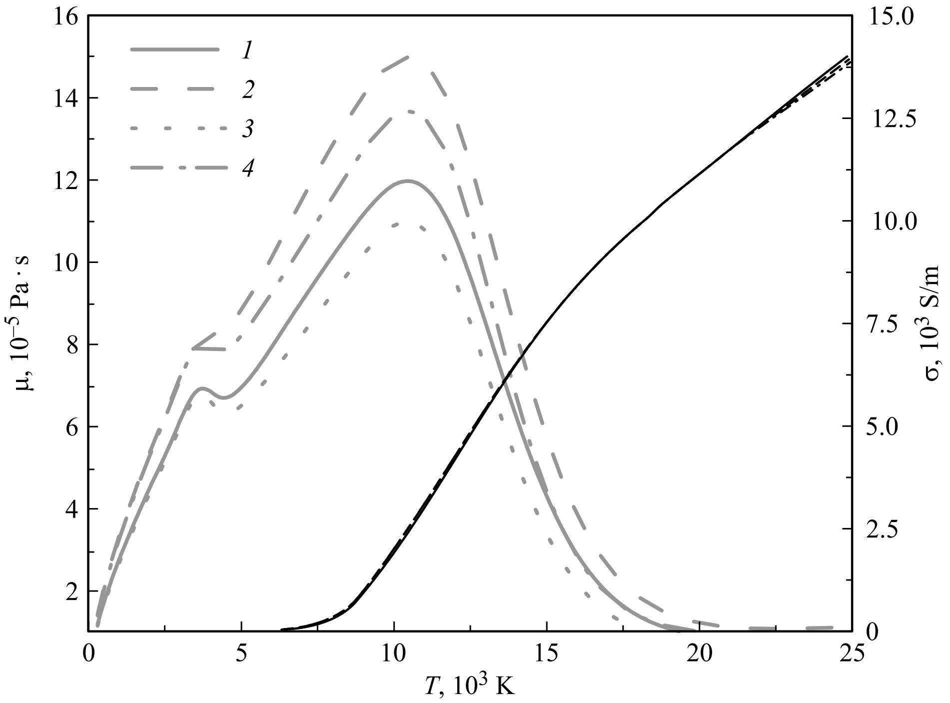

Figure 3. Dependences of viscosity (gray lines) and electrical conductivity (black lines) on temperature. The curves are numbered in accordance with the calculation number in the table.

industrial arc and plasma processes: for example, hydrogen is added to argon for increasing heat transfer to the product in case of gas arc welding of aluminum and for increasing the enthalpy of plasma jets in case of plasma sputtering. It can be seen from the calculation (Fig. 1) that an increase in enthalpy will occur in the core of the plasma torch arc at temperatures above 15,000 K with equal percentages of the components of the plasma-forming mixture of air with hydrogen and argon with hydrogen.

The addition of hydrogen had an effect on the heat capacity and thermal conductivity (Fig. 2) in the range from 3000 to 5000 K: the heat capacity of pure argon increased 180 times and the heat capacity of air increased 23 times.

Thus, the paper presents the thermophysical properties of mixtures of air with hydrogen, argon with hydrogen in thermal plasma at various ratios. The addition of hydrogen made it possible to increase the enthalpy and heat capacity of plasma mixtures. The results obtained will later be used of creating numerical models of a DC plasma torch for sputtering.

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Conflict of interest

The authors declare that they have no conflict of interest.

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