Calculation of a plasma composition and its thermophysical properties in cases of maintaining or quenching of electric arcs

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Abstract. The paper presents a technique for calculating a composition as well as thermodynamic and transport properties of plasma which is used both in plasma technologies and in arc chambers of electrical apparatuses. Examples of calculations are given.

1. Introduction
Modern plasma technologies are implemented with using of various gases depending on the technological task. Typical plasma-forming gases are argon, helium, nitrogen, oxygen, hydrogen, carbon dioxide etc. as well as mixtures of these gases (air, argon-hydrogen etc.). A quenching of electric arcs in electrical apparatuses is carried out in the medium of SF6 gas, air etc. In this case plasma processes are accompanied by erosion of electrodes and ablation of the chamber walls that greatly influences the thermophysical properties of the plasma.

Currently not only experimental methods but also methods of mathematical modeling are used during the development of modern plasma processes. To perform mathematical modeling of plasma processes it is necessary to know thermophysical properties of plasma which depend on the composition of plasma, its temperature and pressure. Dependences of those properties on temperature are given in the scientific literature [1, 2] for some gases used in plasma technologies. However, in a number of cases (for example, in case of using a mixture of gases or in case when a pressure is different from atmospheric pressure) the data available in the literature are insufficient, and the properties of plasma need to be calculated. The procedure for calculating the thermophysical properties of plasma is given below.

2. Calculation of plasma composition
Calculation of the plasma thermophysical properties starts with the calculation of the plasma composition as a result of which the number densities of plasma species are determined.

If the number of individual species considered in the calculation (including electrons) is \( m \) and the number of chemical elements forming the system is \( n \) then to determine the equilibrium composition it is possible to write \((m-n-1)\) equations of the mass action law. For neutral components it is convenient to write these equations for the dissociation of molecules into atoms [3-5]:

\[
K_j(T, p) = \prod_{i=1}^{n} \frac{p_i^{n_{i,j}}}{p_j},
\]

(1)
where \( K_j(T, p) \) is the constant of the reaction; \( p_i \) is partial pressure of elements (atoms); \( p_j \) is partial pressure of complex components (molecules); \( a_{i,j} \) are stoichiometric coefficients of reaction of dissociation of molecules onto atoms.

For electrically charged components of plasma (ions) the mass action law is expressed by the well-known Saha equation:

\[
\frac{n_i \cdot n_e}{n_a} = \frac{Z_i(T) \cdot g_e}{Z_a(T)} \cdot \left( \frac{2\pi m_e k T}{\hbar^2} \right)^{3/2} \cdot \exp \left( -\frac{E_{\text{ion}}}{kT} \right),
\]

(2)

where \( n_i \), \( n_e \), \( n_a \) are number densities of ions, electrons, atoms respectively; \( Z_i(T) \), \( Z_a(T) \) are partition functions of the ion and atom; \( g_e = 2 \) is the statistical weight of the electron; \( m_e \) is the electron mass; \( k \) is the Boltzmann constant; \( h \) is Planck's constant; \( E_{\text{ion}} \) is the ionization energy.

Dalton’s law on the sum of the partial pressures also needs to be included to the system of equations of thermodynamic equilibrium:

\[
\sum_{j=1}^{m} p_j = p.
\]

(3)

Another equation that is necessary for calculating the plasma composition is the quasi-neutrality equation:

\[
\sum_{i} a_i \cdot n_{i^+} = \sum_{j} a_j \cdot n_{j^-},
\]

(4)

where \( a_i \) and \( n_{i^+} \) are the charge and the number density of positively charged ions; \( a_j \) and \( n_{j^-} \) are the charge and the number density of negatively charged ions (and electrons).

To close the system of equations it is necessary to include \((n-1)\) equations of material balances:

\[
\sum_{i=1}^{m} a_{g_i} \cdot p_i = \sum_{i=1}^{m} a_{k_i} \cdot p_i = G/K,
\]

(5)

where \( a_{g_i} \) and \( a_{k_i} \) are the quantities of atoms of the kind \( g \) and \( k \) respectively in the molecule of the \( i \)-th specie, \( G \) and \( K \) are the total numbers of atoms of the kind \( g \) and \( k \) in the plasma.

It is convenient to solve the obtained system of equations of thermodynamic equilibrium of the form (1) – (5) by the modified Newton method for increments of logarithms of unknown values [4].

As an example let us consider the plasma that appears in the discharge chamber of a multi-chamber arrester used for lightning protection of power lines [6]. The walls of the chamber are made of silicone rubber; the electrodes are made of copper. The following relationship between chemical elements is considered:

\[
\text{Si}: \text{O}: \text{C}: \text{H} = 1: 1: 2: 6, \text{Cu}: \text{O} = 1: 10.
\]

The composition of such a plasma at a pressure of 2 atm is shown in Fig. 1.

![Figure 1](image_url)

**Figure 1.** Composition of the plasma of silicone rubber vapor in the presence of copper vapor at a pressure of 2 atm: a – monoatomic species, b – diatomic species, c – polyatomic species
3. Calculation of thermodynamic properties

Knowing the plasma composition one can calculate its thermodynamic properties [4]:

1) Plasma mass density $\rho$:

$$\rho = \sum_i m_i n_i,$$

where $m_i$ is the mass of the atom (ion, molecule) of the $i$-th specie of plasma, $n_i$ is its number density.

2) The total enthalpy of the plasma (measured in J/kg):

$$h = \frac{\sum_i n_i H_i}{M_{\text{mix}}},$$

where $n_i$ is the number density of the $i$-th specie; $H_i$ is the enthalpy of the $i$-th specie (measured in J/mol, the temperature dependence can be found in the reference books [7, 8]); $M_{\text{mix}}$ is the molar mass of the gas mixture (plasma), $M_{\text{mix}} = \rho \cdot N_A / n_e$; $N_A$ is Avogadro's number; $n_e$ is the total number density of all plasma species.

3) Specific heat of the plasma at constant pressure:

$$c_p = \frac{dh}{dT}.$$

An example of the calculated thermodynamic properties is shown in Fig. 2.

Figure 2. Mass density (a) and specific heat (b) of the plasma of silicone rubber vapor in the presence of copper vapor at different pressures: 1 – 1 atm; 2 – 2 atm; 3 – 5 atm; 4 – 10 atm; 5 – 20 atm

4. Calculation of transport properties

The main difficulty in the calculation of transport properties is their dependence on the cross sections of collisions. Knowing the reduced collision integrals for each pair of plasma species one can calculate the transport properties of the plasma:

1) The electrical conductivity of plasma can be calculated in the fourth approximation of the Chapman-Enskog theory by the following formula [9]:

$$\sigma = 3e^2 n_e^2 \left( \frac{\pi}{2kT_m} \right)^{\frac{1}{2}} \left[ 1 q_1^{01} q_1^{02} q_1^{11} q_1^{12} q_1^{21} q_1^{22} \right],$$

where the coefficients $q$ depend on the number densities and reduced collision integrals; formulas for calculating $q$ can be found in [5].

2) The viscosity of plasma can be calculated in the first approximation of the Chapman-Enskog theory by the formula [10, 11]:

$$\nu = \frac{1}{3} \frac{\tau}{\rho},$$

where $\tau$ is the relaxation time and $\rho$ is the mass density of the plasma.
\[ \mu = -\frac{5}{2} \left( 2\pi kT \right)^{\frac{1}{2}} \left[ \begin{array}{c} q_0^0 \frac{n_i}{n_j} \left( m_j \right)^{\frac{1}{2}} \end{array} \right] \left[ \begin{array}{c} q_0^0 \end{array} \right], \]  

(10)

where \( q_0^0 \) is a square matrix consisting of elements \( q_{ij}^0 \) that depend on number densities and reduced collision integrals, formulas for calculation can be found in [5].

3) A total thermal conductivity \( \lambda \) of the plasma is composed of four parts: a thermal conductivity \( \lambda_h \) of heavy species, a thermal conductivity \( \lambda_e \) of electrons, a reaction heat conductivity \( \lambda_R \) and an internal thermal conductivity \( \lambda_{int} \):

\[ \lambda = \lambda_h + \lambda_e + \lambda_R + \lambda_{int}. \]  

(11)

In the second approximation of the Chapman-Enskog theory the thermal conductivity of heavy species is determined by the formula [10, 11]:

\[ \lambda_h = -\frac{75k}{8} \left( 2\pi kT \right)^{\frac{1}{2}} \left[ n_i / \left( m_j \right)^{\frac{1}{2}} \right] \left[ \begin{array}{c} q_{ij}^{00} \end{array} \right] \left[ \begin{array}{c} n_i \end{array} \right], \]  

(12)

where \( q_{ij}^{00} \) is a square matrix consisting of elements \( q_{ij}^{00} \) that depend on number densities and reduced collision integrals, formulas for calculation can be found in [5].

In the second approximation of the Chapman-Enskog theory the thermal conductivity of electrons is determined by the formula [12, 13]:

\[ \lambda_e = \frac{75}{8} n_e^2 k \left( \frac{2\pi kT}{m_e} \right)^{\frac{1}{2}} \left[ \begin{array}{c} q_{ij}^{12} \end{array} \right] \left[ \begin{array}{c} 1 \end{array} \right] \left[ \begin{array}{c} 0 \end{array} \right] \left[ \begin{array}{c} q_{ij}^{11} \\ q_{ij}^{22} \\ q_{ij}^{22} \\ q_{ij}^{22} \end{array} \right], \]  

(13)

where the values of \( q_{ij}^{11} \), \( q_{ij}^{12} \) etc. are determined by the same formulas as for the electrical conductivity.

The reaction heat conductivity can be found by the method given in [14, 15]. The internal thermal conductivity is calculated using the Eiken approximation [16].

An example of calculated transport properties is shown in Fig. 3.

![Figure 3. Electrical conductivity (a) and thermal conductivity (b) of the plasma of silicone rubber vapor in the presence of copper vapor at different pressures: 1 – 1 atm; 2 – 2 atm; 3 – 5 atm; 4 – 10 atm; 5 – 20 atm](image)

5. Conclusions

The above described technique allows to calculate the thermophysical properties of both simple gases and their mixtures which can be used in cases of maintaining as well quenching of electric arcs taking into account erosion of electrodes and ablation of the chamber walls. The obtained distributions are
necessary for the modeling of plasma processes. They can also be used to compare the properties of various gases in the development of plasma technologies.

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