CALCULATION OF THERMODYNAMIC AND TRANSPORT PROPERTIES OF A TWO-TEMPERATURE ARGON PLASMA

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ABSTRACT

Thermodynamic and transport properties such as plasma composition, enthalpy, specific heat at constant pressure, electrical conductivity, thermal conductivity, and viscosity have been computed for a two-temperature argon plasma at atmospheric pressure. Results are presented in graphical form and compared with equilibrium calculations ($T_e=T_h$) which show excellent agreement; but there are substantial disagreements for $\theta > 1$ with data available in the literature. Possible reasons for these discrepancies are discussed.

1. INTRODUCTION

There is increasing evidence that deviations from kinetic equilibrium in thermal arc plasmas are rather common, in particular in the arc fringes and close to confining walls and/or electrodes (1). Since thermodynamic and transport properties are a pre-requisite for arc modeling, there is a growing need for calculating non-equilibrium properties.

Although some computations of thermodynamic and transport properties for a thermal argon plasma are available in the literature, e.g. (2-4), there are relatively few papers concerned with the calculation of two-temperature properties (5-7). Unfortunately, the usefulness of the data based on a two-temperature model is limited due to uncertainties and the lack of completeness of these data.

In this paper the electron gas and the heavy species are treated as two different perfect gases. A Maxwell-Boltzmann distribution shall prevail among electrons as well as among heavy particles, but with different temperatures. The particle number densities are determined from a generalized mass action law. Thermodynamic and transport properties are computed for a two-temperature argon plasma at atmospheric pressure with the electron temperature T_e varing from 1,000 K to 25,000 K and the ratio T_e/T_h from 1 to 10.

2. PLASMA COMPOSITION AND THERMODYNAMIC PROPERTIES

For the case of various ionization stages of a monatomic gas in which the excitation temperature (governed by electron collisions) equals the electron temperature, the generalized mass action may be written as (8)

$$n_e \left(\frac{n_{r+1}}{n_r}\right)^{T_h/T_e} = \frac{2Z_{r+1}(T_e)}{Z_r(T_e)} \left(\frac{2\pi m_e kT_e}{h^2}\right)^{3/2} \exp\left(-\frac{E_{r+1}-\Delta E_{r+1}}{kT_e}\right) \qquad (1)$$

where m_e is the electron mass, h is Planck's constant, k is the Boltzmann constant, n_e is the number density of electrons, n_r and Z_r are the number density and the excitational partition function of atoms (r=0) or ions (r>1), respectively. (E_{r+1}-ΔE_{r+1}) is the lowered ionization potential at the rth ionization state. According to Griem (9), lowering of the ionization potential due to Coulomb interaction may be evaluated from

$$\Delta E_{r+1} = \frac{(r+1)e^2}{4\pi\varepsilon_o\lambda_D} \qquad (2)$$

where ε_o is the dielectric constant, and e is the elementary charge. The Debye shielding length λ_D for the case under consideration is

$$\lambda_D = \left[\frac{\varepsilon_o kT_e}{e^2 n_e (1+\frac{T_e}{T_h})}\right]^{1/2} \qquad (3)$$

If the temperature is below 25,000 K, ionization beyond r=3 (Ar^{+++}) is negligible. The modified Saha equations for this temperature range are

$$n_e \left(\frac{n_1}{n_o}\right)^{T_h/T_e} = \frac{2Z_1(T_e)}{Z_o(T_e)} \left(\frac{2\pi m_e kT_e}{h^2}\right)^{3/2} \exp\left(-\frac{E_1-\Delta E_1}{kT_e}\right) \qquad (4)$$

$$n_e \left(\frac{n_2}{n_1}\right)^{T_h/T_e} = \frac{2Z_2(T_e)}{Z_1(T_e)} \left(\frac{2\pi m_e kT_e}{h^2}\right)^{3/2} \exp\left(-\frac{E_2-\Delta E_2}{kT_e}\right) \qquad (5)$$

Since the correction term for the ideal gas pressure considering Coulomb interactions is very small, Dalton's law becomes

$$P = n_e kT_e + (n_o+n_1+n_2)kT_h \qquad (6)$$

where P is the total pressure of the mixture. Quasi-neutrality requires that

$$n_e = n_1+2n_2 \qquad (7)$$

Therefore, the composition of a four-component, two-temperature plasma can be determined from equations (4), (5), (6), and (7).

With the calculated plasma composition, thermodynamic properties of this plasma can be determined. The mass density is obtained from

$$\rho = n_e m_e + (n_o+n_1+n_2)m_{Ar} \tag{8}$$

By using the methods of statistical mechanics, the total enthalpy of the mixture (h_T) may be divided into there components

$$h_T = h_h+h_i+h_e \tag{9}$$

where

$$h_h=\frac{1}{\rho}\left[\frac{5}{2}kT_h(n_o+n_1+n_2)+kT_e{}^2(n_o\frac{\partial \ln Z_o}{\partial T_e}+n_1\frac{\partial \ln Z_1}{\partial T_e}+n_2\frac{\partial \ln Z_2}{\partial T_e})\right] \tag{10}$$

$$h_i = \frac{1}{\rho}\left[n_1(E_1-\Delta E_1)+n_2(E_2+E_1-\Delta E_1-\Delta E_2)\right] \tag{11}$$

$$h_e = \frac{1}{\rho}\left[\frac{5}{2}kT_e n_e\right] \tag{12}$$

The enthalpy of the heavy species h_h, includes the translational energy and the excitational energy, h_i respresents the chemical energy (ionization), and h_e is the electron enthalpy. Taking T_e as an independent variable and θ (T_e/T_h) as a parameter the average specific heat and its components at constant pressure may be defined as

$$C_p^T = C_p^h + C_p^i + C_p^e \tag{13}$$

$$C_p^j = \left.\frac{h_j(T_e+\Delta T_e)-h_j(T_e)}{\Delta T_e}\right|_\theta \quad , \quad j=h,i,e \tag{14}$$

3. TRANSPORT PROPERTIES

Computations of non-equilibrium transport properties of plasmas are based on the solutions of the Boltzmann integro-differential equation. For local thermodynamic equilibrium, the distribution function is nearly Maxwellian, assuming the form

$$f_i = f_i^o\,(1+\Phi_i)$$

where f_i^o represents the Maxwellian distribution function and Φ_i represents a small deviation. Because of the relatively small mass of the electrons, the electrons may be decoupled from the Boltzmann equation of the heavy-species. By applying the Chapman-Enskog approach (10), the transport coefficients of electrons and heavy species can be computed independently (11). As a first step in this approach Φ_i is expanded as a function of the temperature gradient, the mass velocity gradient and other driving forces. By substituting the corresponding equations into the simplified Boltzmann equations and by comparing the coefficients of corresponding gradients, a set of integral equations can be derived for the unknown coefficients. These equations are then solved by expansion, using finite Sonine's polynominals in velocity space. The solutions in terms of these coefficients provide then the desired transport coefficients. The resulting expressions which contain many collision cross sections are rather complex defying a simple physical interpretation.

If the interaction potentials between any combination of two different species are known, the collision cross sections may usually be computed and, therefore, the transport coefficients can be determined. Because of uncertainties and incomplete information about collision cross section and/or interaction potential data, the calculated transport coefficients will also suffer from these problems.

In this paper, the collision cross sections or interaction potentials of argon plasmas are taken from (4). For calculating the heavy particle transport properties, the first approximation is used and the third approximation is applied for calculating the electron transport properties. It is assumed that viscosity is entirely due to the heavy particles and only the electrons contribute to the electrical conductivity.

4. RESULTS AND DISCUSSION

Figure 1 shows the electron mole fraction ($f_e = n_e/(n_e + n_o + n_1 + n_2)$ with the electron temperature T_e varying from 1,000 K to 25,000 K and the ratio $\theta = T_e/T_h$ from 1 to 10. The curves show a crossover point at a temperature of approximately 15,000K ($n_e = n_1 = n_o$) and beyond this the electron mole fraction remains essentially independent of θ. At the crossover point itself n_e does not depend on T_h (Eq. 4) and the electron mole fraction assumes a value of 1/3. The mass density is illustrated in Fig. 2. The curves for $\theta > 1$ reveal higher densities because there are more heavy particles involved.

The total enthalpy and its components h_h, h_i, h_e for thermodynamic equilibrium are shown in Fig. 3. As expected, the heavy species dominate at low temperatures and the contribution by chemical reactions becomes important at high temperatures. The corresponding components of the specific heat at constant pressure are plotted in Fig. 4, indicating that C_p^i is the main contribution to the total specific heat at constant pressure for $T > 10^4$K (large number density of ions). The total enthalpy and the total specific heat for different θ are illustrated in Fig. 5 and 6. The relatively sharp peaks are associated with the rapid change of the ionization rates around 15,000 K.

The viscosity shown in Fig. 7 reveals at low temperature the classical behavior (proportional to the square root of the heavy particle temperature). Therefore, the curves for $\theta > 1$ are shifted downward in the low temperature region. When the temperature rises, the number density of ions increases and the mechanism of momentum transport is dominated by ion-ion interactions. Because of the very large collision cross section of charged particles, the viscosity drops sharply above 12,000K.

The curves in Fig. 8 represent the electrical conductivity for different θ. By comparing Fig. 8 with Fig. 1, it is obvious that the relative position and the trend of all the curves in these two figures are similar. This finding suggests that the number density of electrons determines primarily the electrical conductivity. The electrical conductivity for different θ shows a substantial spread at low T_e and becomes almost independent of θ for T_e>15,000K. Because of the big change of the electrical conductivity in non-equilibrium situations, the current density distribution in low temperature regimes as, for example, in the fringes of thermal arcs will be strongly affected by this variation.

The electron thermal conductivity and the total thermal conductivity (heavy species + electrons + reaction) are shown in Figs. 9 and 10. At low T_e, the mixture is essentially composed of heavy species and the energy transport is due to collisions of the heavy species. As soon as chemical reactions become important, the energy transfer due to ionization begins to dominate. This effect is enhanced as θ increases because of rapid change of ionization rates near T_e = 15,000 K. At high T_e, the thermal conductivity is dominated by the electrons because of their high mobility.

The results of this work for $\theta=1$ compare favorably with equilibrium calculations available in the literature. The work reported in (5) shows higher viscosities in the high temperature region even for $\theta=1$. One possible reason for this discrepancy is the choice of the ion-ion collision cross sections in (5). The fact that the results of this work are in excellent agreement with equilibrium calculations reported in the literature (3,4) supports the reliability of the data presented in this paper.

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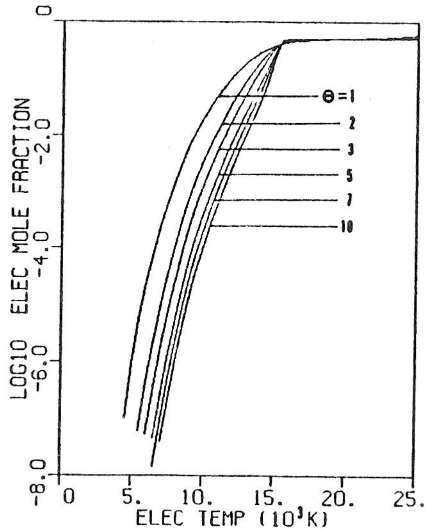

Fig. 1: Electron mole fraction of a two-temperature argon plasma at p=1 atm; $\theta=T_e/T_h$.

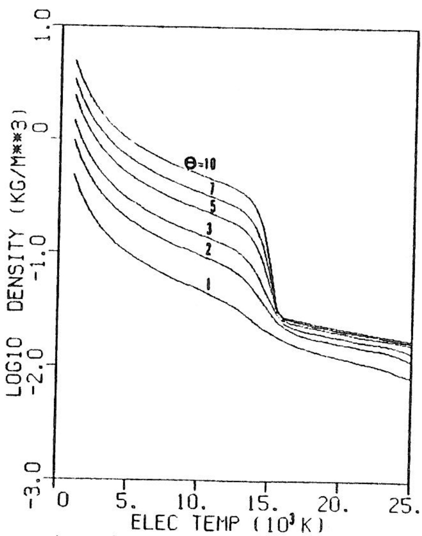

Fig. 2: Mass density of a two-temperature argon plasma at p=1 atm; $\theta=T_e/T_h$.

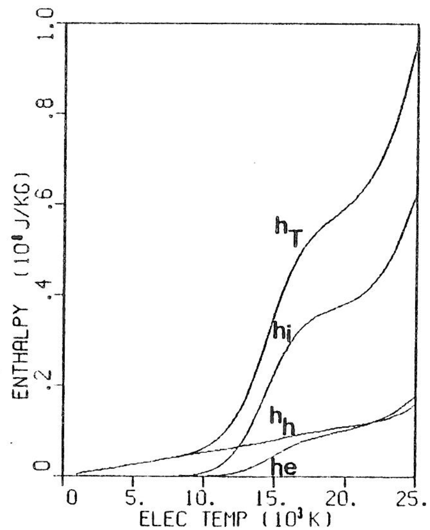

Fig. 3: Total enthalpy and its components for thermodynamic equilibrium (θ=1) argon plasma at p=1 atm.

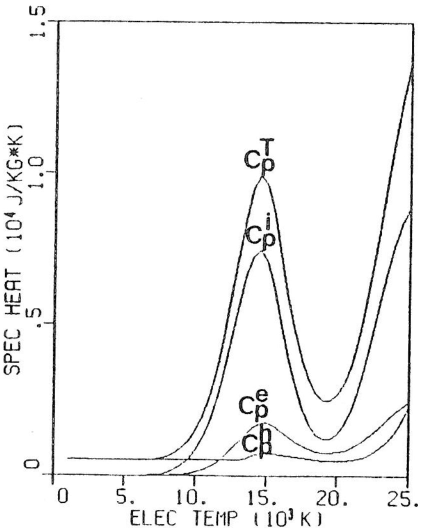

Fig. 4: Total average specific heat at constant pressure and its components for thermodynamic equilibrium (θ=1) argon plasma at p=1 atm.

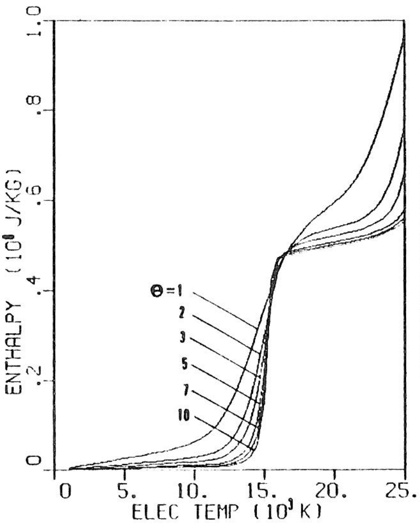

Fig. 5: Total enthalpy of a two-temperature argon plasma at p=1 atm; $\Theta=T_e/T_h$.

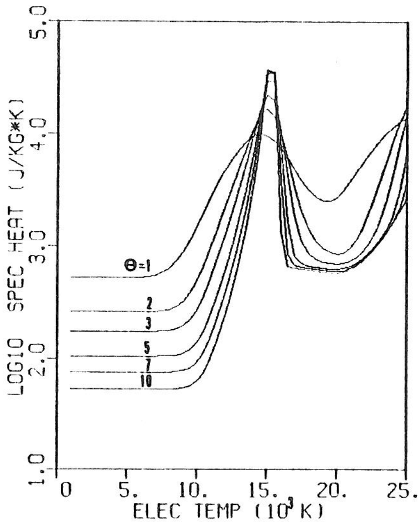

Fig. 6: Total average specific heat at constant pressure of a two-temperature argon plasma at p=1 atm; $\theta=T_e/T_h$.

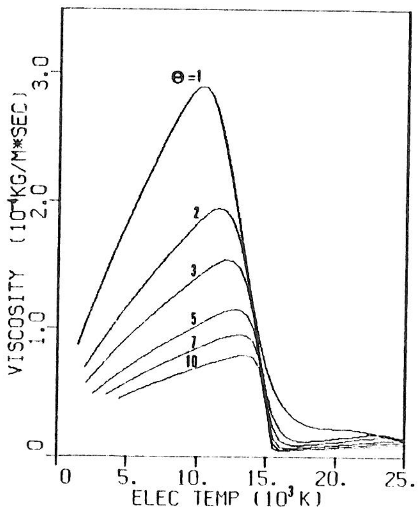

Fig. 7: Viscosity of a two-temperature argon plasma at p=1 atm; $\theta=T_e/T_h$.

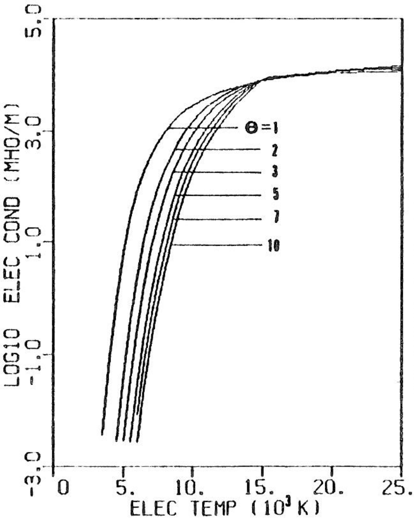

Fig. 8: Electrical conductivity of a two-temperature argon plasma at p=1 atm, $\theta=T_e/T_h$,

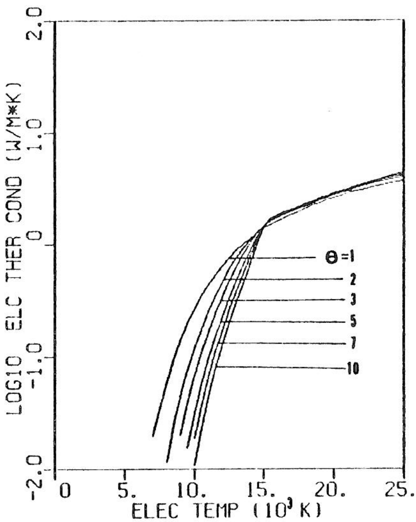

Fig. 9: Electron thermal conductivity of a two-temperature argon plasma at p=1 atm; $\theta=T_e/T_h$.

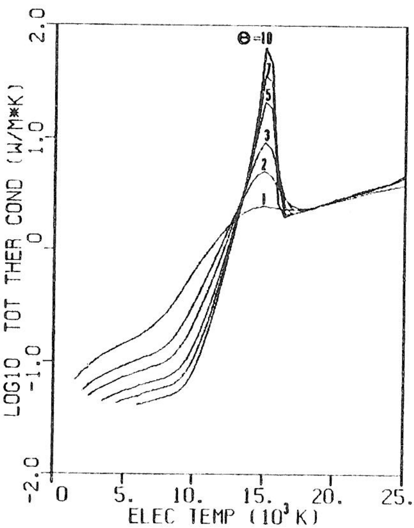

Fig. 10: Total thermal conductivity (heavy species+electrons+reaction) of a two-temperature argon plasma at p=1 atm; $\theta=T_e/T_h$.