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# New method to derive transport properties including diffusion in a two-temperature plasma

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## Abstract

A new derivation of transport properties in a two-temperature plasma has been performed. The electron kinetic temperature  $T_e$  is supposed to be different from that of heavy species  $T_h$ . The resolution of the Boltzmann's equation, thanks to the Chapman-Enskog method, is used to calculate transport coefficients and it allows to the generalisation of bracket integrals out of thermal equilibrium. Two-temperature diffusion coefficients are defined and the obtained results are presented for an atmospheric two-temperature argon plasma.

## 1. Introduction

Recent works [1] have shown that the simplified theory of transport properties out of thermal equilibrium introduced by Devoto [2] and Bonnefoi [3] neglecting the coupling between electrons and heavy species, and very often used in modeling, leads to unphysical results. Thus, two-temperature transport coefficients have been derived [4] without the Bonnefoi's assumptions starting from the Boltzmann's equation. The electron temperature  $T_e$  is supposed to be different from that of heavy species  $T_h$ . Only elastic processes are considered in a collision dominated plasma. Firstly, is presented the principle of the resolution of the Boltzmann's equation in a two-temperature model. Secondly, the modifications of this resolution, with respect to equilibrium, give rise to a generalisation of bracket integrals giving transport coefficients. The differences with thermal equilibrium are then highlighted. Lastly, two-temperature diffusion coefficients resulting of this derivation are displayed as function of the non-equilibrium parameter  $\theta=T_e/T_h$ .

## 2. Resolution of the Boltzmann equation

The distribution function  $f_i$  of the  $i$ th species is the solution of the integro-differential equation of Boltzmann [5]:

$$\frac{Df_i}{Dt} = \sum_{j=1}^N \iiint (f'_i f'_j - f_i f_j) g b d b d \epsilon d \bar{v}_j \quad (1)$$

$f'_i$  is the distribution function after the elastic collision of the  $i$ th species,  $g$  is the relative velocity of the species  $i$  and  $j$ ,  $b$  and  $\epsilon$  are respectively the impact parameter and the incidence azimuthal angle.

It has been assumed that the zero-order approximation function is Maxwellian at  $T_e$  for electrons and  $T_h$  for heavy species. The distribution function of the  $i$ th species, solution of (1), is approximated by a Maxwellian distribution function  $f_i^{(0)}$  perturbed by a slowly time and space dependent first-order perturbation function  $\Phi_i$  of the  $i$ th species with the temperature  $T_i$ :

$$f_i = f_i^{(0)}(1 + \Phi_i) \quad (2)$$

Inserting (2) into (1), it can be shown that:

$$\frac{Df_i^{(0)}}{Dt} = I_i^{(0)} + \sum_{j=1}^N \iiint f_i^{(0)} f_j^{(0)} ((\Phi_i' + \Phi_j') K_i - \Phi_i - \Phi_j) \mathcal{E} b db d\epsilon d\bar{v}_j \quad (3)$$

$I_i^{(0)}$  represents the zero-order approximation of the Chapman-Enskog's expansion and does not vanish for two colliding particles with different temperatures:

$$I_i^{(0)} = \sum_{j=1}^N \iiint (f_i^{(0)} f_j^{(0)} - f_i^{(0)} f_j^{(0)}) \mathcal{E} b db d\epsilon d\bar{v}_j \quad (4)$$

A term  $K_i(W_i, \theta_{ij})$ , taking into account the thermal non-equilibrium when electrons and heavy species collide, has been introduced as follows:

$$f_i^{(0)} f_j^{(0)} = f_i^{(0)} f_j^{(0)} K_i(W_i, \theta_{ij}) \quad \forall i, j \in [1; N] \quad (5)$$

where 
$$K_i(W_i, \theta_{ij}) = \exp(-(W_i'^2 - W_i^2)(1 - \theta_{ij})) \quad (6)$$

with 
$$\theta_{ij} = \frac{T_i}{T_j} \quad (7)$$

and  $W_i'$  is the reduced velocity after collision such as  $\bar{W}_i = \left(\frac{m_i}{2kT_i}\right)^{1/2} \bar{V}_i$  where  $\bar{V}_i = \bar{v}_i - \bar{v}_0$ .  $\bar{v}_i$  and  $\bar{v}_0$  are respectively the velocity of the  $i$ th species and flow velocity.

The introduction of  $K_i$  allows the definition of bracket integrals to be generalised out of thermal equilibrium.

The calculation of  $\frac{Df_i^{(0)}}{Dt}$  and  $\frac{Df_i^{(0)}}{Dt}$  ( $i \geq 2$ ) is obtained using the equations of change

[4]. The transport terms in equations (3), show that transport phenomena are due to a new gradient  $\bar{V} \ln \theta$ , which characterizes the temperature difference between electrons and heavy species, the heavy species temperature gradient, the velocity gradient, external forces (forced diffusion), the concentration and pressure gradients and a term acting on the hydrostatic pressure to the first-order approximation of Sonine polynomials.

Following the linear form of transport terms, it can be supposed that the first-order perturbation function can be written as:

$$\Phi_i = -\bar{A}_i \cdot \bar{\nabla} \ln T_h - \bar{B}_i : \bar{\nabla} \bar{v}_0 + \sum_{j=1}^N \bar{C}_i^j \cdot \bar{d}_j + D_i Q_i^{(0)} + \sum_{j=1}^N \bar{E}_i^j \cdot g_j \bar{\nabla} \ln \theta - \bar{F}_i \cdot \bar{\nabla} \ln \theta \quad (8)$$

The diffusion forces are written as follows for *electrons*:

$$\bar{d}_1 = \frac{\rho_1}{\rho} \sum_{j=1}^N n_j \bar{F}_j - n_1 \bar{F}_1 + \left( \frac{x_1 \theta}{D} - \frac{\rho_1}{\rho} \right) \bar{\nabla} p + \frac{\theta p}{D^2} \bar{\nabla} x_1 \quad (9)$$

and 
$$g_1 = \frac{x_1 p (1 - x_1)}{D^2} \quad (10)$$

For *heavy species*, it is written:

$$\bar{d}_i = \frac{\rho_i}{\rho} \sum_{j=1}^N n_j \bar{F}_j - n_i \bar{F}_i + \left( \frac{x_i}{D} - \frac{\rho_i}{\rho} \right) \bar{\nabla} p + \frac{p}{D} \bar{\nabla} x_i - \frac{x_i (\theta - 1) p}{D^2} \bar{\nabla} x_i \quad (11)$$

and 
$$g_i = -\frac{x_i x_1 p}{D^2} \quad (12)$$

$\rho_i$ ,  $\bar{F}_i$ ,  $x_i$  and  $p$  are respectively the density, an external force and the molar fraction of the  $i$ th species and the total pressure.

$Q_i^{(0)}$  corresponds to the exchanged kinetic energy between electrons and heavy species during collisions. It can be shown:

$$Q_i^{(0)} = 4k_B n_1 (T_h - T_c) \left( \frac{8k_B T_c}{\pi m_1} \right)^{1/2} \sum_{j=2}^N n_j \frac{m_1}{m_j} \bar{Q}_{ij}^{(1,1)} \quad (13)$$

$k_B$  being the Boltzmann constant.

The unknowns  $\bar{A}_i$ ,  $\bar{B}_i$ ,  $\bar{C}_i^j$ ,  $D_i$ ,  $\bar{E}_i^j$  and  $\bar{F}_i$  are determined by assuming that they can be splitted on the Sonine polynomial basis [5] which allows the introduction of systems of linear equations following the approximation order.

The introduction of  $\bar{\nabla} \ln \theta$  prevents from considering the uncoupling between electrons and heavy species in the resolution of systems of linear equations which gives the transport coefficients. As a result, two-temperature diffusion coefficients not only include ordinary and thermal diffusion but also new diffusion coefficients due to the temperature difference ( $\bar{\nabla} \ln \theta$ ) between electrons and heavy species [4].

### 3. Bracket integrals

Transport coefficients results in the resolution of systems of linear equations. Each element  $q_{ij}^{mp}$  ( $m$  and  $p$  represents the order of approximation of Sonine polynomials) of the considered matrix depends on bracket integrals. The latter are expressed as a linear combination of collision integrals which account for the interaction between the colliding species.

For example, in the first-order approximation of Sonine polynomials, the following bracket integral can be written:

$$\left[ \bar{W}_i S_{3/2}^1(w_i^2) \bar{W}_j S_{3/2}^1(w_j^2) \right]_{ij} = C \sum_{r\ell} A_{11r\ell} \Omega_{ij}^{(r,\ell)} \quad (14)$$

where  $C$  depends on  $m_i$ ,  $m_j$ ,  $T_i$  and  $T_j$ .

$\Omega_{ij}^{(r,\ell)}$ ,  $i$  and  $j$  being the colliding species, is the integral of the transport cross section over a Maxwellian distribution function. Table 1 gives the values of the coefficients  $A_{11r\ell}$  at equilibrium ( $\theta=1.0$ ) and for different values of  $\theta$  calculated for a collision between an electron and a heavy species, that is for a mass ratio of  $10^{-5}$ .

Table 1: Calculation of  $A_{11r\ell}$  for different values of  $\theta$  and with a mass ratio  $m_j/m_i=10^{-5}$ .

$\theta$	1.00	1.25	1.50	2.00	3.00
$A_{1111}$	-13.75	-8.50	-5.00	-0.63	-3.75
$A_{1121}$	5.00	3.30	3.00	4.50	11.00
$A_{1122}$	2.00	0.75	-0.50	-3.00	-8.00
$A_{1131}$	-1.00	-1.40	-2.00	-3.50	-7.00
$A_{1132}$	0.00	0.50	1.00	2.00	4.00

Firstly, it is shown that our results strictly lead to those of Hirschfelder et al [5]. Secondly, the coefficients  $A_{11r\ell}$  are drastically changed following the applied thermal non-equilibrium. Lastly, coefficients such as  $A_{1132}$  do not vanish when the non-equilibrium parameter  $\theta$  is different from unity. As a result, collision integrals  $\Omega_{ij}^{(r,\ell)}$  with indexes  $(r,\ell)$  higher than at thermal equilibrium should be taken into account out of thermal equilibrium.

#### 4. Two-temperature diffusion coefficients

Two-temperature diffusion coefficients are displayed for a two-temperature argon plasma. Calculations are performed at atmospheric pressure and the two-temperature plasma composition is obtained using the Saha equation for ionization of Van de Sanden et al [6].

Electrons, Ar and  $\text{Ar}^+$  species have been considered.

First, it has to be noted that the rate of convergence of diffusion coefficients are similar to that of thermal equilibrium that is the second-order approximation is sufficient for diffusion coefficients implying electrons. However, for argon, around 5000 K (the electron temperature) the third-order approximation is required because of the Ramsauer effect of the momentum cross section.

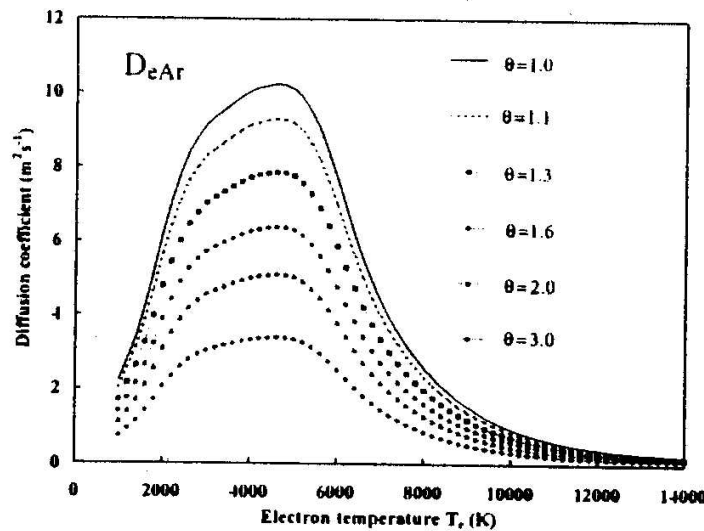
The two-temperature diffusion coefficients  $D_{e\text{Ar}}$  and  $D_{\text{Ar}^+e}$  are respectively displayed in figure 1(a) and 1(b) as a function the electron temperature from 1000 up to 20000 for different values of  $\theta$  (between 1 and 3). The calculation have been performed to the third-order approximation. When ionisation is weak, namely below 6000 K, two-temperature ordinary diffusion coefficients increase with temperature.

For  $D_{e\text{Ar}}$ , the effect of temperature is dominant with respect to the collision integral  $\bar{Q}_{e\text{Ar}}^{(1,1)}$  which increases slowly with  $T_e$ . However, between 4500 and about 6000 K, the effect of the collision integral  $\bar{Q}_{e\text{Ar}}^{(1,1)}$  overcomes the effect of temperature but, at these temperatures the binary approximation is not valid anymore. As a result, the  $\text{Ar}^+$  species has to be taken into account and the effect of the charge transfer collision integral  $\bar{Q}_{\text{ArAr}^+}^{(1,1)}$  contributes to increase

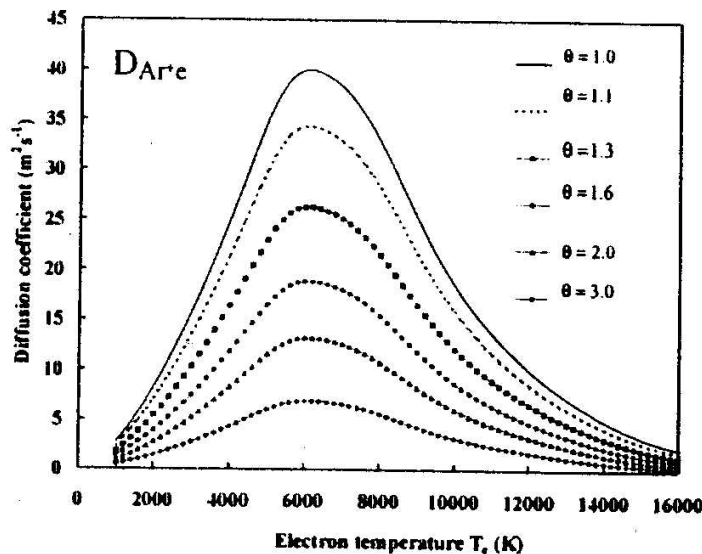
ordinary diffusion coefficients since it decreases with temperature faster than  $\bar{Q}_{eAr}^{(1,1)}$  increases (for example,  $\bar{Q}_{ArAr^+}^{(1,1)} / \bar{Q}_{eAr}^{(1,1)}$  is about 55 at 5000 K). The same evolution for  $D_{Ar^+e}$  is observed, the charge transfer collision integral being dominant at low temperature.

When ionization becomes significant around 6000 K,  $D_{eAr}$  and  $D_{Ar^+e}$  decreases with temperature because the charged-charged collision integral  $\bar{Q}_{eAr^+}^{(1,1)}$  counterbalances the effect of temperature.

Besides, it is observed in figure 1(a) and 1(b) that two-temperature diffusion coefficients decrease with the non-equilibrium parameter  $\theta$ . Figure 2 depicts the influence of the non equilibrium parameter  $\theta$  on diffusion coefficients and that it can be written that at low temperature  $D_{eAr} = \theta D_{Ar^+e}$ .



(a)



(b)

Figure 1: Two-temperature diffusion coefficient  $D_{eAr}$  (a) and  $D_{Ar^+e}$  (b) as function of electron temperature  $T_e$  and  $\theta$ .

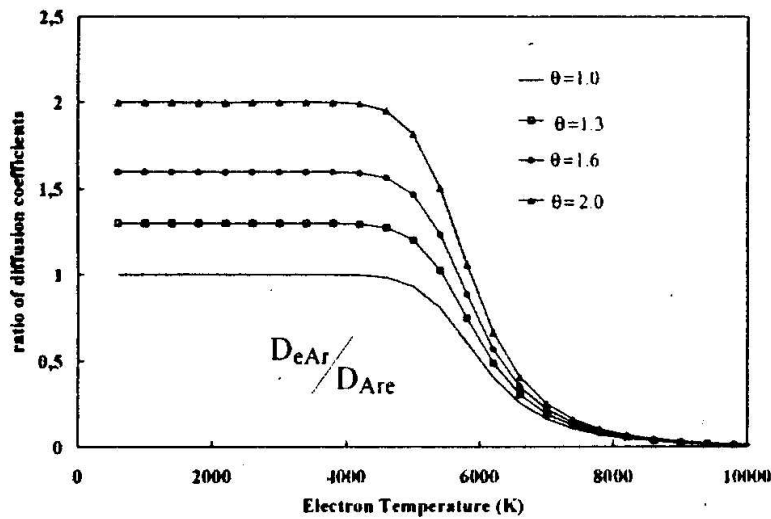


Figure 2: Ratio  $D_{eAr}/D_{Are}$  as function of electron temperature  $T_e$  and  $\theta$ .

## 5. Conclusion

A new method of derivation of transport properties in a two-temperature plasma has been performed. Two-temperature transport coefficients have been derived starting from the Boltzmann's equation. The latter is solved by using the well-known Chapman-Enskog method which has been adapted to thermal non-equilibrium plasmas. It has been assumed that the distribution function of species, solution of the Boltzmann's equation, is a Maxwellian, at  $T_e$  for electrons and  $T_h$  for heavy species, perturbed by a slowly time and space dependent first-order perturbation function. The introduction of the gradient  $\bar{\nabla}\theta$  allows to maintain the coupling between electrons and heavy species in the calculation of two-temperature transport coefficients. Two-temperature diffusion coefficients in an atmospheric argon plasma were calculated between electrons and heavy species, contrarily to what happens when using the simplified theory of transport coefficients of Devoto[2] and Bonnefoi [3].

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