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Vincent Rat, Pascal André, Jacques Aubreton, Marie-Françoise Elchinger, Pierre Fauchais, et al..
New method to derive transport properties including diffusion in a two-temperature plasma. 15
International Symposium on Plasma Chemistry, 2001, France. pp.819-824. hal-00019934

HAL Id: hal-00019934

<https://hal.science/hal-00019934v1>

Submitted on 2 Mar 2006

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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]:

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

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

ρ_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 θ 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 θ and with a mass ratio $m_j/m_i=10^{-5}$.

θ	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 θ is different from unity. As a result, collision integrals $\Omega_{ij}^{(r,\ell)}$ with indexes (r, ℓ) 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 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.

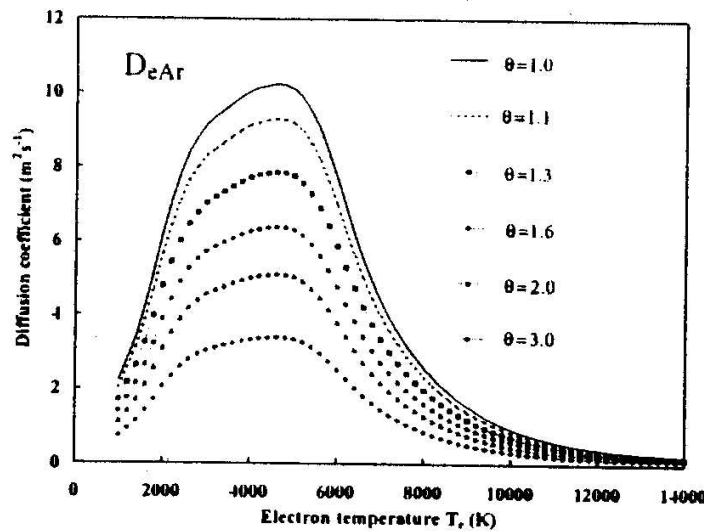
The two-temperature diffusion coefficients $D_{e\text{Ar}}$ and D_{Ar^+e} are respectively displayed in figure 1(a) and 1(b) as a function the electron temperature from 1000 up to 20000 for different values of θ (between 1 and 3). The calculation have been performed to the third-order approximation. 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 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

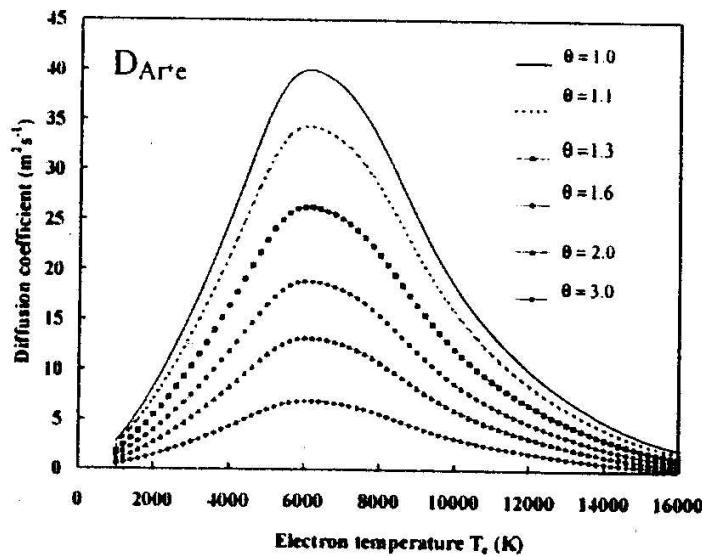
ordinary diffusion coefficients since it decreases with temperature faster than $\bar{Q}_{eAr}^{(1,1)}$ increases (for example, $\bar{Q}_{ArAr^+}^{(1,1)} / \bar{Q}_{eAr}^{(1,1)}$ is about 55 at 5000 K). The same evolution for D_{Ar^+e} is observed, the charge transfer collision integral being dominant 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 θ . Figure 2 depicts the influence of the non equilibrium parameter θ 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 θ .

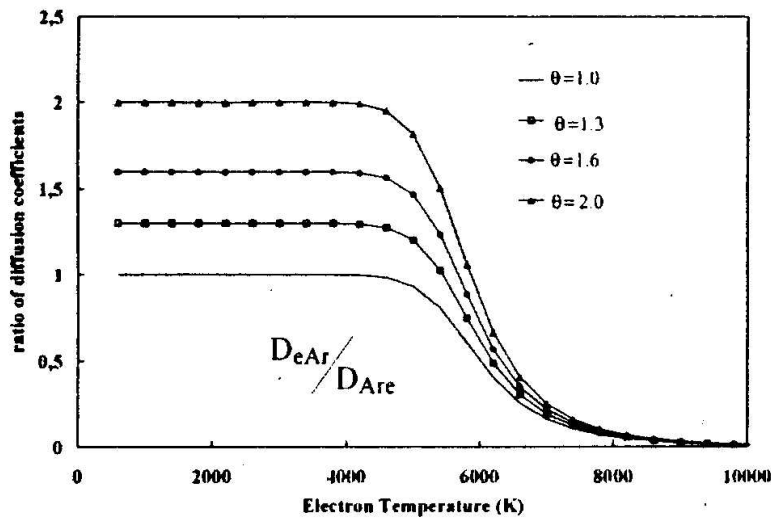


Figure 2: Ratio D_{eAr}/D_{Ar} as function of electron temperature T_e and θ .

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].

References

- [1] V. Rat, J. Aubreton, M.F. Elchinger, and P. Fauchais, *Plasma Chem. Plasma Process.* **21** (2001), 355-364.
- [2] R.S. Devoto, *Phys. Fluids* **10** (1967), 2105-2112.
- [3] C. Bonnefoi, State Thesis, University of Limoges, France (1983).
- [4] V. Rat, P. André, J. Aubreton, M.F. Elchinger, P. Fauchais, and A. Lefort, to be published, *Phys. Rev. E*.
- [5] J.O. Hirschfelder, C.F. Curtis, and R.B. Bird, *Molecular Theory of Gases and Liquids*, 2nd ed., Wiley, New York (1964).
- [6] M.C.M. Van de Sanden, P.P.J.M. Schram, A.G. Peeters, J.A.M. van der Mullen and G.M. Kroesen, *Physical Review A*, **40** (1989), 5273-5276.