

Calculation method of electrical conductivity, thermal conductivity and viscosity of a partially ionized gas

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ABSTRACT

The calculation method of the transport properties (electrical conductivity, thermal conductivity and viscosity) of a partially ionized gas is described in this paper. The calculation method is based on the Chapman-Enskog method and on the knowledge of the collision integrals for each pair of species of a partially ionized gas. The generally methods of the collision integral calculation are introduced.

Keywords: Electrical conductivity, thermal conductivity, viscosity, partially ionized gas, Chapman-Enskog method

1 INTRODUCTION

The knowledge of the transport properties of the gas mixture is very important because the operating properties of some technical devices are determined by the transport processes in the gas mixture. The thermal plasma created by the electrical arc gives the important advantages for technological applications, the plasma high temperatures in the interval of 5-50 kK, the high density and the high degree of the energy transport, the high speed of the chemical reactions in the plasma. These properties are essential for some technical applications. The chief characteristics of these applications are the using of the different gas mixtures of the different transport properties.

2 CHAPMAN-ENSKOG METHOD AND COLLISION INTEGRAL

The kinetic gas theory is the base for the determination of the gas transport properties [1], [2] and it is based on the knowledge of the distribution function. This equilibrium distribution function is determined for every particle in the gas on terms of the same temperature for all particles in the gas and of the same speed of the all particles. The equilibrium distribution function formulates the equilibrium of the every species and the equilibrium between species in the gas system too. When the gas system is not in the equilibrium, the distribution function agrees with the Boltzmann integral-differential equation.

function agrees with the Boltzmann integral-differential equation.

The Chapman-Enskog method [1] of the solution of the Boltzmann equation is the theoretical base for the transport properties calculation of the partially ionized gases. This method was extended for the multicomponent gas system by Hirschfelder, Curtis a Bird [2]. For the every species in the gas system is formulated one Boltzmann equation and therefore the multicomponent gas system is described by the system of the integrodifferential equations. The Chapman-Enskog method makes over these equations to the linear equation system and gives several approximations of the distribution function. If the multicomponent gas system contains N species and it is used ζ -th approximation, the linear equation system for $N\zeta$ variables is solved.

Chapman and Enskog introduce the new variable called the collision integral Ω_{ij} and formulated for a pair of particles i, j . The determination of these collision integrals is the important part of the calculation of the transport properties. The collision integral is defined by the equation

$$\Omega_{ij}^{(l,s)}(T) = \sqrt{\frac{kT}{2\pi\mu_{ij}}} \int_0^{\infty} \exp(-\gamma_{ij}^2) \gamma_{ij}^{2s+3} Q_{ij}^{(l)}(g_{ij}) d\gamma_{ij} \quad (1)$$

where

$$Q_{ij}^{(l)}(g_{ij}) = 2\pi \int_0^{\infty} (1 - \cos^l \chi_{ij}) b db \quad (2)$$

is the total transport cross section of two colliding particles i and j . In the equations (1) and (2) k is the Boltzmann constant, T is the temperature, μ_{ij} is the reduced mass ($1/\mu_{ij} = 1/\mu_i + 1/\mu_j$) and γ_{ij} is the reduced initial relative speed of i th and j th species

$$\gamma_{ij} = \sqrt{\frac{\mu_{ij}}{2kT}} g_{ij} \quad (3)$$

g_{ij} is the initial relative speed, χ_{ij} is the angle of deflection between i th and j th species

$$\chi_{ij}(g_{ij}, b) = \pi - 2\Theta_m = \pi - 2b \int_{r_m}^{\infty} \frac{dr/r^2}{\sqrt{1 - \frac{b^2}{r^2} - \frac{\varphi(r)}{1/2 \mu_{ij} g_{ij}^2}}} \quad (4)$$

b is the impact parameter and l, s are the parameters defining the order of the collision integral and $s \geq l$. The collision integrals are calculated not only for a pair of colliding particles but also for the given combination of the parameters l and s . These combinations result from the used degree of approximation.

The determination of the collision integrals is possible by using three solution ways. The tables of collision integrals are published for some pairs of colliding particles. In the most cases the collision integrals are calculated from the potential energy between two molecules $\varphi(r)$ and by using (1), (2). The integration of experimental values of the momentum transfer cross section and the using of (1), (2) can be calculated for some interaction including collisions between electron and neutrals.

The simplest way of the collision integral calculation is the model of rigid spheres [2] and it can be used for all types of collisions except the Coulomb interaction and it is equal to

$$\begin{aligned} [Q_{ij}^{(l)}]_{rs} &= \left[1 - \frac{1 + (-1)^l}{2(1+l)} \right] \pi \left(\frac{\tilde{\sigma}_i + \tilde{\sigma}_j}{2} \right)^2, \\ [Q_{ij}^{(l,s)}]_{rs} &= \sqrt{\frac{kT}{2\pi\mu_{ij}}} \frac{(s+1)!}{2} [Q_{ij}^{(l)}]_{rs}, \end{aligned} \quad (5)$$

where $\tilde{\sigma}_i, \tilde{\sigma}_j$ are the diameters of the particles i and j . The method of the Lennard-Jones potential can be used for a pair of neutral particles but the Lennard-Jones parameters of both particles must be known. The simple approximation method of the Lennard-Jones potential is described in [3] and it is based on the approximation $Q^{(l)*}(g^*)$

$$Q_{ap}^{(l)*}(g^*) = A^{(l)*}/g^{*2} + B^{(l)*}/g^{*2} + C^{(l)*} + D^{(l)*} g^* \quad (6)$$

and on the expression of the collision integral in the form

$$\begin{aligned} \Omega_{ap}^{(l)*} &= \frac{A^{(l)*}}{(s+1)T^{*s}} + \\ &+ \frac{B^{(l)*}\Gamma(s+3/2)}{\sqrt{T^{*s}}(s+1)!} + C^{(l)*} + D^{(l)*}\sqrt{T^*} \frac{\Gamma(s+5/2)}{(s+1)!} \end{aligned} \quad (7)$$

The values of $A^{(l)*}, B^{(l)*}, C^{(l)*}, D^{(l)*}$ are given in the Tab. 1 [3].

Tab. 1 The coefficient values of polynom $Q^{(l)*}(g^*)$

l	$A^{(l)*}$	$B^{(l)*}$	$C^{(l)*}$	$D^{(l)*}$
1	-1,209905	1,625491	0,481139	-0,003985
2	-0,555427	1,551493	0,604085	-0,005300
3	-0,464707	1,474890	0,566188	-0,004980
4	0,245314	1,345058	0,651817	-0,005958

For the collisions of neutral-ion the polarisability method can be used [4]

$$\bar{Q}^{(l,s)} = \left(\frac{Z^2 e^2 \xi}{2\pi \varepsilon_0 k T} \right)^{1/2} \frac{\Gamma\left(s + \frac{3}{2}\right) A_{(4)}^{(l)}}{(s+1)! \left(1 - \frac{1 + (-1)^l}{2(1+l)} \right)}, \quad (8)$$

where e is the electron charge, ε_0 is the permittivity of the vacuum, $A_{(4)}^{(l)}$ are the numerical constants, $A_{(4)}^{(1)} = 0,65466$, $A_{(4)}^{(2)} = 0,38521$. The method is based on the knowledge of the polarisability ξ of the neutral.

For the some collisions the experimental data of the momentum transfer cross section can be used. These data are in the literature in the form of the graphs or in the tables. The experimental data can be approximated by the function in the form

$$Q_{ij} = A\sqrt{\varepsilon} + B\varepsilon + C\varepsilon\sqrt{\varepsilon} + D\varepsilon^2 \quad (9)$$

and the collision integral is calculated from the relation

$$\begin{aligned} \Omega_{ij}^{(l,s)} &= \frac{1}{2} \sqrt{\frac{kT}{2\pi\mu_{ij}}} \left[A\sqrt{\varepsilon}\Gamma(s+5/2) + B\varepsilon(s+2)! + \right. \\ &\left. C\varepsilon\sqrt{\varepsilon}\Gamma(s+7/2) + D\varepsilon^2(s+3)! \right] \end{aligned} \quad (10)$$

In the equations (9), (10) $\varepsilon = kT/e$.

3 CALCULATION METHOD OF ELECTRICAL CONDUCTIVITY

The relation for the electrical conductivity calculation of a partially ionized gas is in the form [5]

$$\sigma = \frac{e^2 n^2}{p\rho^2} \sum_i Z_i \sum_j n_j m_j^2 D_{ij} \left(\sum_{k=1}^N n_k Z_k - \frac{\rho Z_j}{m_j} \right) \quad (11)$$

where the charge of a particle is marked eZ_i ($Z_e = -1$) and if the condition $\sum_k n_k Z_k = 0$ is satisfied the equation (11) is

modified

$$\sigma = -\frac{e^2 n^2}{p\rho} \sum_{i=1}^N Z_i \sum_{j=1}^N Z_j n_j m_j D_{ij} \quad (12)$$

In the given equation (12) n_j or m_j is the number density or the mass of the j th species, n is the total number density, p is the pressure, ρ is the mass density. In the sums only the charge particles are included, because Z is not zero only for these particles. D_{ij} is the diffusion coefficient defined by the equation

$$D_{ij} = \frac{\rho n_i}{2nm_j} \sqrt{\frac{2kT}{m_i}} c_{iji}^{(0)} \quad (13)$$

where $c_{iji}^{(0)}$ is one solution of linear equation system

$$\begin{aligned} &-(\delta_{ih} - \delta_{ik})\delta_{0m} \frac{3}{2} \sqrt{\frac{2kT}{m_i}} = \\ &= \sum_{j=1}^N \sum_{m'=0}^{\zeta-1} \left(\tilde{W}_{ij}^{(m,m')} - \frac{n_j}{n_i} \sqrt{\frac{m_j}{m_i}} \tilde{W}_{ii}^{(m,m')} \delta_{0m} \delta_{0m'} \right) c_{jhm}^{(m')} \end{aligned} \quad (14)$$

In this equation $\delta_{ih}, \delta_{ik}, \delta_{0m}, \delta_{0m'}$ are Cronecker delta, $i = 1, 2, \dots, N, m = 0, 1, \dots, \zeta-1$. For the electrical conductivity calculation of a gas system third approximation was chosen

($\zeta = 3$), therefore the system of $3N$ equations must be solved and m, m' can have values 0, 1 or 2. Only for $m = 0$ the left side of equation (14) can be different from zero. Relations for calculation of coefficients $\tilde{W}_{ij}^{(m,m')}$ are functions of the colli-

sion integrals $\Omega_{ij}^{(l,s)}$ and for the third approximation they are given in the relations (15) [5].

$$\begin{aligned}
\tilde{W}_{ij}^{(0,0)} &= 8 \sum_{l=1}^N \frac{n_l m_l}{(m_i + m_l) \sqrt{m_i m_j}} [n_i m_i (\delta_{ij} - \delta_{jl}) - n_j m_j (1 - \delta_{il})] \Omega_{il}^{(1,1)}, \\
\tilde{W}_{ij}^{(0,1)} &= -8 \left(\frac{m_i}{m_j} \right)^{3/2} \sum_{l=1}^N \frac{n_i n_l m_l^2}{(m_i + m_l)^2} (\delta_{ij} - \delta_{jl}) \left[\Omega_{il}^{(1,2)} - \frac{5}{2} \Omega_{il}^{(1,1)} \right], \quad \tilde{W}_{ij}^{(1,0)} = \frac{m_j}{m_i} \tilde{W}_{ij}^{(0,1)}, \\
\tilde{W}_{ij}^{(0,2)} &= 8 \left(\frac{m_i}{m_j} \right)^{5/2} \sum_{l=1}^N \frac{n_i n_l m_l^3}{(m_i + m_l)^3} (\delta_{ij} - \delta_{jl}) \left[\frac{35}{8} \Omega_{il}^{(1,1)} - \frac{7}{2} \Omega_{il}^{(1,2)} + \frac{1}{2} \Omega_{il}^{(1,3)} \right], \quad \tilde{W}_{ij}^{(2,0)} = \left(\frac{m_j}{m_i} \right)^2 \tilde{W}_{ij}^{(0,2)}, \\
\tilde{W}_{ij}^{(1,2)} &= 8 \left(\frac{m_i}{m_j} \right)^{5/2} \sum_{l=1}^N \frac{n_i n_l m_l^2}{(m_i + m_l)^4} \left\{ (\delta_{ij} - \delta_{jl}) \left[\frac{35}{16} (12m_j^2 + 5m_l^2) \Omega_{il}^{(1,1)} - \frac{21}{8} (4m_j^2 + 5m_l^2) \Omega_{il}^{(1,2)} + \right. \right. \\
&\quad \left. \left. \frac{19}{4} m_l^2 \Omega_{il}^{(1,3)} - \frac{1}{2} m_l^2 \Omega_{il}^{(1,4)} \right] + (\delta_{ij} + \delta_{jl}) \left[7m_j m_l \Omega_{il}^{(2,2)} - 2m_j m_l \Omega_{il}^{(2,3)} \right] \right\}, \quad \tilde{W}_{ij}^{(2,1)} = \frac{m_j}{m_i} \tilde{W}_{ij}^{(1,2)}, \\
\tilde{W}_{ij}^{(2,2)} &= 8 \left(\frac{m_i}{m_j} \right)^{5/2} \sum_{l=1}^N \frac{n_i n_l m_l}{(m_i + m_l)^5} \left\{ (\delta_{ij} - \delta_{jl}) \left[\frac{35}{64} (40m_j^4 + 168m_j^2 m_l^2 + 35m_l^4) \Omega_{il}^{(1,1)} - \frac{7}{8} m_l^2 (84m_j^2 + 35m_l^2) \Omega_{il}^{(1,2)} + \right. \right. \\
&\quad \left. \left. + \frac{1}{8} m_l^2 (108m_j^2 + 133m_l^2) \Omega_{il}^{(1,3)} - \frac{7}{2} m_l^4 \Omega_{il}^{(1,4)} + \frac{1}{4} m_l^4 \Omega_{il}^{(1,5)} + 2m_j^2 m_l^2 \Omega_{il}^{(3,3)} \right] + \right. \\
&\quad \left. + (\delta_{ij} + \delta_{jl}) \left[\frac{7}{2} m_j m_l (4m_j^2 + 7m_l^2) \Omega_{il}^{(2,2)} - 14m_j m_l^3 \Omega_{il}^{(2,3)} + 2m_j m_l^3 \Omega_{il}^{(2,4)} \right] \right\}, \\
W_{ij}^{(0,0)} &= \frac{16}{3} \frac{m_i}{m_j} \sum_{l=1}^N \frac{n_i n_l m_l}{(m_i + m_l)^2} \left\{ (\delta_{ij} - \delta_{jl}) 5m_j \Omega_{il}^{(1,1)} + (\delta_{ij} + \delta_{jl}) \frac{3}{2} m_l \Omega_{il}^{(2,2)} \right\}, \\
W_{ij}^{(0,1)} &= \frac{16}{3} \left(\frac{m_i}{m_j} \right)^2 \sum_{l=1}^N \frac{n_i n_l m_l^2}{(m_i + m_l)^3} \left\{ (\delta_{ij} - \delta_{jl}) \left[\frac{35}{2} m_j \Omega_{il}^{(1,1)} - 7m_j \Omega_{il}^{(1,2)} \right] + (\delta_{ij} + \delta_{jl}) \left[\frac{21}{4} m_l \Omega_{il}^{(2,2)} - \frac{3}{2} m_l \Omega_{il}^{(2,3)} \right] \right\}, \\
W_{ij}^{(1,0)} &= \frac{m_j}{m_i} W_{ij}^{(0,1)}, \\
W_{ij}^{(1,1)} &= \frac{16}{3} \left(\frac{m_i}{m_j} \right)^2 \sum_{l=1}^N \frac{n_i n_l m_l}{(m_i + m_l)^4} \left\{ (\delta_{ij} - \delta_{jl}) \left[\left(35m_j^3 + \frac{245}{4} m_j m_l^2 \right) \Omega_{il}^{(1,1)} - 49m_j m_l^2 \Omega_{il}^{(1,2)} + 8m_j m_l^2 \Omega_{il}^{(1,3)} + \right. \right. \\
&\quad \left. \left. + 3m_j m_l^2 \Omega_{il}^{(3,3)} \right] + (\delta_{ij} + \delta_{jl}) \left[\left(\frac{77}{4} m_j^2 m_l + \frac{147}{8} m_l^3 \right) \Omega_{il}^{(2,2)} - \frac{21}{2} m_l^3 \Omega_{il}^{(2,3)} + \frac{3}{2} m_l^3 \Omega_{il}^{(2,4)} \right] \right\}.
\end{aligned} \tag{15}$$

4 CALCULATION METHOD OF THERMAL CONDUCTIVITY

Thermal conductivity can be calculated as the sum of three components [5]

$$\lambda = \lambda_{tr} + \lambda_{int} + \lambda_r \tag{16}$$

where λ_{tr} is the translation thermal conductivity, λ_{int} is the internal thermal conductivity and λ_r is the reaction thermal conductivity.

The first component λ_{tr} of the thermal conductivity is the translation thermal conductivity due to the heavy particles and it can be written in the form

$$\lambda_{tr} = -\frac{5}{4}k \sum_{j=1}^N \left(n_j \sqrt{\frac{2kT}{m_j}} a_j^{(1)} \right) + nk \left\| \mathcal{D}_i^T \right\| \cdot \left\| \mathcal{D}_{ij} \right\|^{-1} \cdot \left\| \mathcal{D}_j^T \right\| \quad (17)$$

where the coefficient $a_j^{(1)}$ is one solution of the following equation system

$$-\frac{15}{4}n_i \sqrt{\frac{2kT}{m_i}} \delta_{1,m} = \sum_{j=1}^N \sum_{m'=0}^{\zeta-1} \left(\tilde{W}_{ij}^{(m,m')} - \frac{n_j}{n_i} \sqrt{\frac{m_j}{m_i}} \tilde{W}_{ii}^{(m,m')} \delta_{om} \delta_{om'} \right) a_j^{(m')} \quad (18)$$

where $i = 1, 2, \dots, N$, $m = 0, 1, \dots, \zeta-1$ ($\zeta = 3$). The coefficients $\tilde{W}_{ij}^{(m,m')}$ are the functions of the collision integrals (15).

In the equation (17) the notation $\left\| \mathcal{D}_i^T \right\| \cdot \left\| \mathcal{D}_{ij} \right\|^{-1} \cdot \left\| \mathcal{D}_j^T \right\|$ is the product of three matrixes formed from the binary diffusion coefficients \mathcal{D}_{ij} and from the binary thermal diffusion coefficients \mathcal{D}_{ij}^T

$$\mathcal{D}_{ij} = \frac{n^2 m_j}{n_i \rho} D_{ij}, \quad \mathcal{D}_i^T = \frac{1}{n_i m_i} D_i^T, \quad (19)$$

where D_{ij} is given in the equation (13) and D_i^T is calculated by the equation

$$D_i^T = \frac{n_i m_i}{2} \sqrt{\frac{2kT}{m_i}} a_i^{(0)}, \quad (20)$$

where $a_i^{(0)}$ is the one solution of equation system (18).

The second component of thermal conductivity λ_{int} is the internal thermal conductivity, sometimes is termed as the Eucken thermal conductivity λ_{Eucken} . It is given by the equation

$$\lambda_{int} = \frac{5\sqrt{k}}{16\sqrt{\pi} N_A} \sqrt{T} \sum_i x_i \frac{(c_{pi} - 2.5R)}{\sum_j x_j \frac{\sigma_{ij}^2}{\sqrt{\frac{M_i + M_j}{2M_i M_j}}}} \quad (21)$$

In this equation N_A is Avogadro constant, R is the perfect gas constant, x_i or x_j , respectively M_i or M_j , is the molar fraction, respectively the molar mass, of i th or j th species, c_{pi} is the specific heat at the constant pressure of i th species and σ_{ij} is the radius of particles i and j , $(\sigma_i + \sigma_j)/2$.

The third component of the thermal conductivity λ_r is the reaction thermal conductivity arising like a consequence of chemical reactions in gas system and it is defined by the expression [6]

$$\lambda_r = -\frac{1}{RT^2} \begin{vmatrix} A_{11} & \dots & A_{1N'} & \Delta H_{N'} \\ \vdots & & \vdots & \vdots \\ A_{1N'} & \dots & A_{N'N'} & \Delta H_{N'} \\ \Delta H_1 & \dots & \Delta H_{N'} & 0 \end{vmatrix} \quad (22)$$

where

$$A_{ij} = \sum_{k=1}^{N-1} \sum_{l=k+1}^N \frac{RT}{\mathcal{D}_{kl} P} x_k x_l \left(\frac{v_{ik}}{x_k} - \frac{v_{il}}{x_l} \right) \left(\frac{v_{jk}}{x_k} - \frac{v_{jl}}{x_l} \right), \quad (23)$$

$$A_{ij} = A_{ji}, \quad \Delta H_i = \sum_{k=1}^N v_{ik} H_k.$$

In the equations (22), (23) N' is the number of the independent chemical reactions, $i, j = 1, 2, \dots, N'$, ΔH_i is the heat of the independent chemical reaction, v_{ik} , v_{il} , v_{jk} , v_{jl} are the stoichiometric coefficients for species k (l) in reaction i (j).

5 CALCULATION METHOD OF VISCOSITY

The viscosity can be calculated by the using of the relation [5]

$$\eta = \frac{1}{2} kT \sum_{j=1}^N n_j b_j^{(0)} \quad (23)$$

where $b_j^{(0)}$ is one solution of the equation system

$$5n_i \delta_{om} = \sum_{j=1}^N \sum_{m'=0}^{\zeta-1} W_{ij}^{(m,m')} b_j^{(m')} \quad (24)$$

The values of the coefficients $W_{ij}^{(m,m')}$ are calculated only for $m \leq 1$ and $m' \leq 1$ and the relations are in (15).

6 CONCLUSION

In this paper the calculation method of the electrical conductivity, the thermal conductivity and viscosity is described. The important part of calculation of these properties is the knowledge of the composition of the gas system. In the paper the generally calculation ways of the collision integrals are showed. For some pairs of particles, which have dominant concentration in the gas system, it is better to use the experimental values of momentum transfer cross section (for electron-neutral) or to use the table values.

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