Heat flux and stress tensor in plasma flow with electronic excitation

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Abstract

The aim of this work is to describe the influence of electronic excitation on the heat flux and stress tensor in chemically non-equilibrium weakly ionized gas mixtures. The modified Chapman-Enskog method is applied to derive the closed set of governing equations. Transport coefficients of diffusion, thermal diffusion, relaxation pressure and bulk viscosity are evaluated as functions of temperature and mixture composition in the temperature range 500–25000K. Prandtl and Schmidt numbers are calculated and compared with commonly used values.

1. Introduction

For the correct predictions of the drag and heat flux in the strongly non-equilibrium plasma flows, it is necessary to develop a transport processes theory under highly non-equilibrium conditions. At the moment, there is a large number of works devoted to the study of the mass, momentum and energy transport. However systematic evaluations of the relaxation pressure and bulk viscosity were not carried out and still represent a challenging task. The influence of electronic excitation on the transport phenomena was found to be important in few recent papers [1,2,3,4]. In the most simulations of strong non-equilibrium plasma flows quantities of bulk viscosity and relaxation pressure are neglected, although this assumption is often intuitive. In this paper, based on the method proposed in [5], the influence of non-equilibrium chemical reactions on the diagonal terms of the stress tensor is investigated in the case of fast translational and electronic energy exchanges. The novelty of this study is in taking into account the electronic excitation of nitrogen atoms in the calculation of the relaxation pressure and bulk viscosity. Using the modified Chapman-Enskog method we derive the transport linear systems for the calculation of the bulk viscosity, relaxation pressure, heat conductivity, diffusion and thermal diffusion coefficients. The transport coefficients are calculated in the temperature range 500-25000 K; the influence of the chemical composition of the mixture on the relaxation pressure and bulk viscosity is studied. Prandtl and Schmidt numbers are calculated and compared with commonly used values. The results of this paper can be useful for improving the accuracy of modeling for the spacecraft reentry.

2. Governing equations

In the present paper, chemically non-equilibrium weakly ionized nitrogen $N/N^+/e^-$ mixture is considered. Weakly-ionized means that a number density of electrons and ions is much smaller than the number density of neutral atoms. The ionized atomic species and electrons are supposed to be structure-less particles, whereas neutral atoms have a manifold of electronic states. The following relation between characteristic times of processes holds: the exchange of translational and electronic energy as well as charge transfer are assumed to be rapid processes, and ionization is supposed to be slow process:

$$\tau_{tr} < \tau_{el} \ll \tau_{ioniz} \sim \theta, \qquad (1)$$

here τ_{tr} is the characteristic time of the translational energy exchange, τ_{el} is the characteristic time of the exchange of electronic energy, τ_{ioniz} is the characteristic time of ionization, θ is the time of variation of gas-dynamic parameters.

This case corresponds to the one-temperature model. Under such assumptions the gas mixture flow can be considered on the basis of the generalized Chapman-Enskog method described in [5].

A closed description of the flow in the one-temperature approximation is given by following set of macro-parameters: $n_N(\boldsymbol{r},t), n_{N^+}(\boldsymbol{r},t)$, $n_{e^-}(\boldsymbol{r},t)$ are the number densities of nitrogen atoms, ions and electrons, respectively; $v(\boldsymbol{r},t)$ is the gas velocity; $T(\boldsymbol{r},t)$ is the gas temperature.

The governing equations for macroscopic parameters have the following form:

$$\rho\frac{dv}{dt} + \nabla\cdot\boldsymbol{P} = 0, \tag{2}$$

$$\rho\frac{dU}{dt} + \nabla\cdot\boldsymbol{q} + \boldsymbol{P}:\nabla\boldsymbol{v} = 0, \tag{3}$$

$$\frac{dn_c}{dt} + n_c\nabla\cdot\boldsymbol{v} + \nabla\cdot(n_c\boldsymbol{V}_c) = R_c^{ioniz},\ \ c = N, N^+, e^-, \tag{4}$$

here U is total specific energy including electronic degrees of freedom, $\boldsymbol{V}_c$ is diffusion velocity, ρ is the mixture density, $\boldsymbol{P}$ is the pressure tensor, $\boldsymbol{q}$ is the heat flux, R_c^{ioniz} is the production term due to ionization,

$$R_N^{ioniz} = \sum_n \int J_{Nn}^{sl} du_N = \sum_d n_d\left(k_{rec}^d n_{N^+} n_{e^-} - k_{ion}^d n_N\right), \quad R_{N^+}^{ioniz} = R_{e^-}^{ioniz} = -R_N^{ioniz} \tag{5}$$

J_{cn}^{sl} is the collision operator for slow processes, $\boldsymbol{u}_c$ is the particle velocity, k_{rec}^d, k_{ion}^d are the rate coefficients of recombination and ionization at the collision with a partner d.

Charged particles have only translational degrees of freedom, and neutral atoms have also electronic energy:

$$\begin{aligned} U_N &= E_{tr} + E_{el}, \\ U_{N^+} &= E_{tr}, \\ U_{e^-} &= E_{tr}, \end{aligned} \tag{6}$$

here E_{tr}, E_{el} are the specific translational and electronic energy.

System (2)-(4) describes non-equilibrium chemical kinetics in a one temperature gas flow.

3. Zero and first-order approaches

Macroparameters that characterize mass, momentum, and energy transfer are specified by the distribution function. In the zero-order approach of the Chapman-Enskog method the distribution function has the form of Maxwell-Boltzmann distribution:

$$f_{cn}^{(0)} = \left(\frac{m_c}{2\pi kT}\right)^{\frac{3}{2}} \frac{n}{Z_{el,c}(T)} g_{cn}\left(-\frac{m_c \boldsymbol{c}_c^2}{2kT} - \frac{\varepsilon_{cn}}{kT}\right), \tag{7}$$

where m_c is the mass of the particle, T is the temperature, k is Boltzmann constant, g_{cn} is the statistical weight, $Z_{el,c}(T)$ is the equilibrium internal partition function. For charged particles the distribution function has the form of Maxwell distribution over reduced peculiar velocity.

In the first-order approximation the distribution function is obtained in the following form:

$$f_{cn} = f_{cn}^{(0)}(1 + \varphi_{cn}), \tag{8}$$

$$\varphi_{cn} = -\frac{1}{n}\boldsymbol{A}_{cn}\cdot\nabla lnT - \frac{1}{n}\sum_d \boldsymbol{D}_{cn}^d\cdot\boldsymbol{d}_d - \frac{1}{n}\boldsymbol{B}_{cn}:\nabla v - \frac{1}{n}F_{cn}\nabla\cdot v - \frac{1}{n}G_{cn}, \tag{9}$$

here φ_{cn} is the first-order correction, $\boldsymbol{d}_d$ is the diffusion driving force, $\boldsymbol{A}_{cn}$, $\boldsymbol{D}_{cn}^d$, $\boldsymbol{B}_{cn}$, F_{cn}, G_{cn} are the unknown functions, which are found from linear integral equations.

Substituting the first-order distribution function to the definition of heat flux, pressure tensor, diffusion velocity we obtain the following expressions:

$$\boldsymbol{q} = -\lambda'\nabla T - \rho \sum_c D_{T_c} \boldsymbol{d}_c + \sum_c \rho_c h_c \boldsymbol{V}_c, \tag{10}$$

$$\boldsymbol{P} = (p - p_{rel})\boldsymbol{I} - 2\eta \boldsymbol{S} - \zeta \nabla \cdot \boldsymbol{v} \boldsymbol{I}, \tag{11}$$

$$\boldsymbol{V}_c = -\sum_d D_{cd} \boldsymbol{d}_c - D_{T_c} \nabla lnT, \tag{12}$$

here h_c is the specific enthalpy of chemical species c, η and ζ are shear and bulk viscosity coefficients, p_{rel} is the relaxation pressure, D_{cd} and D_{T_c} are diffusion and thermal diffusion coefficients, $\boldsymbol{S}$ is the deformation rate tensor, $\lambda' = \lambda_{tr} + \lambda_{el}$ is the thermal conductivity coefficient including contributions of translational and electronic degrees of freedom.

One can see that the stress tensor contains additional contributions to the normal mean stress. Relaxation pressure appears as a result of the rapid inelastic exchanges of electronic and translation energy and of the slow ionization process. If all rapid exchanges are elastic or resonant, relaxation pressure is equal to zero. Also, p_{rel}=0, if slow processes don't occur in the system.

The coefficient of bulk viscosity appears if in the rapid process, the non-resonant exchange between the translational and internal energy occurs. Bulk viscosity is equal to zero if all internal energy exchanges proceed slowly or if the systems of translational and internal degrees of freedom are isolated.

4. Transport coefficients

Transport coefficients are determined by the functions $\boldsymbol{A}_{cn}$, $\boldsymbol{D}^d_{cn}$, $\boldsymbol{B}_{cn}$, F_{cn}, G_{cn} by following equations:

$$\begin{gathered} \eta = \frac{kT}{10}[\boldsymbol{B},\boldsymbol{B}], \\ \zeta = kT[F,F], \\ p_{rel} = kT[F,G], \\ D_{cd} = \frac{1}{3n}[\boldsymbol{D}^c,\boldsymbol{D}^d], \\ D_{T_c} = \frac{1}{3n}[\boldsymbol{D}^c,\boldsymbol{A}], \\ \lambda' = \frac{k}{3}[\boldsymbol{A},\boldsymbol{A}], \end{gathered} \tag{13}$$

here $[F,G] = \frac{1}{4n^2}\int\int\int\int f_c f_d (F + F_1 - F' - F'_1)(G + G_1 - G' - G'_1) d\boldsymbol{g}\, db\, d\varepsilon\, d^3\boldsymbol{c}\, d^3\boldsymbol{c}_1$ is the integral bracket, g is relative velocity, b is the impact parameter, ε is the angle between the planes of vector $\boldsymbol{c}$ and $\boldsymbol{c}_1$, $\boldsymbol{c}$, $\boldsymbol{c}_1$ are the peculiar velocities.

For the solution of integral equations, the unknown functions are expanded into the series of Sonine and Waldmann-Trübenbacher orthogonal polynomials over reduced peculiar velocity and internal energy. The functions $\boldsymbol{A}_{cn}$, F_{cn}, G_{cn} are expanded into the double polynomial systems. In the case of ionized gas due to the slow convergence of Sonine polynomials the expansion should necessarily contain not only first non-vanishing terms, but high-order expansion terms.

Substituting the current expansion in the integral equations we obtain the linear algebraic equations system for expansion coefficients $a_{c,rp}$, $d^d_{c,r}$, $b_{c,r}$, $f_{c,rp}$, $g_{c,rp}$. These equations contain bracket integrals as the coefficients. The bracket integrals are simplified using the Mason and Monchick assumptions [6]. Expansion coefficients are expressed as solutions of linear equations, which are solved by the Gauss method. The transport coefficients come out from the expansion coefficients. All transport coefficients are expressed via reduced collision integrals and integrals depending on the energy variation in the inelastic collision.

Reduced collision integrals are calculated for all types of interactions: neutral-neutral, neutral-charged, charged-charged particles. Thus the reduced collision integral for atom-ion interactions is given by [7]:

$$\Omega^{(l,r)*} = \sqrt{\Omega_{el}^{(l,r)*} + \Omega_{ch-ex}^{(l,r)*}}\text{ , } l \text{ - odd}, \tag{14}$$

$$\sigma^2\Omega_{ch-ex}^{(l,r)*} = d_1 + d_2 lnT + d_3 (lnT)^2, \tag{15}$$

here $\Omega_{el}^{(l,r)*}$ is the contribution of elastic interactions, $\Omega_{ch-ex}^{(l,r)*}$ is the contribution of charge transfer cross–section, d_1, d_2, d_3 are the coefficients. For atom-electron interactions the following equation is proposed:

$$\sigma^2\Omega^{(l,r)*} = \frac{g_3 (lnT)^{g_6} \exp\left(\frac{lnT - g_1}{g_2}\right)}{\exp\left(\frac{lnT-g_1}{g_2}\right) + \exp\left(-\frac{lnT-g_1}{g_2}\right)} + g_7 \exp\left(-\left(\frac{lnT-g_1}{g_2}\right)^2\right) + g_4 + g_{10}(lnT)^{g_5}, \tag{16}$$

Coefficients d_i, g_i are given in [7].
Integral brackets which specify bulk viscosity and relaxation pressure are reduced to the following formulas [4]:

$$\beta_{1100}^{cd} = -5kT \frac{x_c x_d}{A_{cd}\eta_{cd}} \frac{m_c m_d}{(m_c+m_d)^2} + \frac{4T}{\pi} \frac{x_c x_d}{\eta_{cd}} \frac{m_c m_d}{(m_c+m_d)^2} \left(\frac{m_c c_{int,c}}{\varsigma_c^{int}} + \frac{m_d c_{int,d}}{\varsigma_d^{int}}\right), \forall d \neq c, \tag{17}$$

$$\beta_{1100}^{cc} = \sum\nolimits_{b\neq c} \left[5kT \frac{x_c x_b}{A_{cb}\eta_{cb}} \frac{4T}{\pi} \frac{x_c x_b}{\eta_{cb}} + \frac{4T}{\pi} \frac{x_c x_b}{\eta_{cb}} \frac{m_c m_b}{(m_c+m_b)^2} \left(\frac{m_c c_{int,c}}{\varsigma_c^{int}} + \frac{m_b c_{int,b}}{\varsigma_b^{int}}\right)\right] + \frac{4T}{\pi} \frac{x_c x_c}{\eta_{cc}} \frac{m_c c_{int,c}}{\varsigma_c^{int}}, \tag{18}$$

$$\beta_{0110}^{cd} = -\frac{4T}{\pi} \frac{x_c x_d}{\eta_{cd}} \frac{m_c}{(m_c+m_d)} \frac{m_c c_{int,c}}{\varsigma_c^{int}}, \tag{19}$$

$$\beta_{0110}^{cc} = -\frac{4T}{\pi} \sum\nolimits_{b\neq c} \frac{x_c x_b}{\eta_{cb}} \frac{m_b}{(m_c+m_b)} \frac{m_c c_{int,c}}{\varsigma_c^{int}} - \frac{4T}{\pi} \frac{x_c x_c}{\eta_{cc}} \frac{m_c c_{int,c}}{\varsigma_c^{int}}, \tag{20}$$

$$\beta_{0011}^{cd} = 0, \tag{21}$$

$$\beta_{0011}^{cc} = \frac{4T}{\pi} \sum\nolimits_{b\neq c} \frac{x_c x_b}{\eta_{cb}} \frac{m_c c_{int,c}}{\varsigma_c^{int}} + \frac{4T}{\pi} \frac{x_c x_c}{\eta_{cc}} \frac{m_c c_{int,c}}{\varsigma_c^{int}}, \tag{22}$$

here x_c is the molar fraction of particles, $A_{cd} = \frac{\Omega_{cd}^{(2,2)*}}{\Omega_{cd}^{(1,1)*}}$, $\eta_{cb} = \frac{5}{8} \frac{kT}{\Omega_{cd}^{(2,2)}}$, $\varsigma_c^{int} = \frac{4}{\pi} \frac{p\tau_{cd}^{int}}{\eta_{cd}}$ is the number of collisions, $c_{int,c}$ is the contribution of internal degrees of freedom to the specific heat.
The right hand side of algebraic equations system for expansion coefficient $g_{c,rp}$ contains the integral depending on the ionization reaction cross sections $\sum_n \int S_{1/2}^{(r)} P_n^{(p)} J_{cn}^{sl(0)} d\boldsymbol{u}_c$, here r, $p = 0$, 1. Provided that the cross section σ is independent on the electronic levels n, we obtain $\sum \int P_n^{(1)} J_{cn}^{sl(0)}\, d\boldsymbol{u}_c = 0$. Thus we are interested in calculation of the integrals $\sum_n \int S_{1/2}^{(1)} P_n^{(0)} J_{cn}^{sl(0)} d\boldsymbol{u}_c + \sum_n \int S_{1/2}^{(0)} P_n^{(0)} J_{cn}^{sl(0)} d\boldsymbol{u}_c$, here.
Evaluation of the zero-order collision integral gives [8]: $J_{cn}^{sl(0)} = \omega_r \sum \int f_{cn}^{(0)} f_{dm}^{(0)}\, \boldsymbol{g}\, \sigma_{f,r}\ d^2\Omega d\boldsymbol{u}_d$, here $\sigma_{f,r}$ is the differential collision cross section, $d^2\Omega$ is the solid angle, $\omega_r = 1 - \exp(\frac{A_{r,ion}}{R_G T})$, $A_{r,ion}$ is the affinity of ionization reaction, R_G is the gas constant.
Let us use the following notations: $\boldsymbol{c}_c = \boldsymbol{u}_c - \boldsymbol{v}$ is the peculiar velocity, $\boldsymbol{G} = \mu_c \boldsymbol{u}_c - \mu_d \boldsymbol{u}_d$, $\boldsymbol{g} = \boldsymbol{u}_c - \boldsymbol{u}_d$ are the velocities of the center of mass and relative velocity, respectively. The corresponding dimensionless velocities are

$$\boldsymbol{C}_c = \left(\frac{m_c}{2kT}\right)^{1/2} \boldsymbol{c}_c,\quad \boldsymbol{G}_0 = \left(\frac{m_c+m_d}{2kT}\right)^{\frac{1}{2}} (\boldsymbol{G} - \boldsymbol{g}),\quad \boldsymbol{g}_0 = \left(\frac{m_{cd}}{2kT}\right)^{1/2} (\boldsymbol{G} - \boldsymbol{g}).$$

Then, using the kinematic relations for a binary collision [3], we find the expression for the integral:

$$\sum_n \int S_{\frac{1}{2}}^{(1)} P_n^{(0)} J_{cn}^{sl(0)} d\boldsymbol{C}_c = \omega_r \sum_n \sum_m \int \pi^{-3}\, n_c n_d \exp(-\boldsymbol{G}_0 - \boldsymbol{g}_0) \times$$

$$\left(\frac{3}{2} - \mu_c \boldsymbol{G}_0^2 + 2(\mu_c\mu_d)^2 \boldsymbol{g}_0 \cdot \boldsymbol{G}_0 - \mu_d \boldsymbol{g}_0^2\right) \left(\frac{m_{cd}}{2kT}\right)^{-0.5} \boldsymbol{g}_0 \sigma_{f,r} d^2\Omega d^3\boldsymbol{G}_0 d^3\boldsymbol{g}_0 \tag{23}$$

here $\mu_c = \frac{m_c}{m_c+m_d}$, $m_{cd}^{-1} = m_c^{-1} + m_d^{-1}$.

Finally, after some transformations, we obtain

$$\sum_n \int S_{\frac{1}{2}}^{(1)} P_n^{(0)} J_{cn}^{sl(0)} dC_c = 2\omega_r n_c n_d \left(\frac{3}{2}\mu_d \Omega_{cd}^{(1,0)} - \mu_d \Omega_{cd}^{(0,1)}\right). \qquad (24)$$

Integrals in (24) are evaluated numerically.

4. Results

The transport coefficients were calculated for N/N$^+$/e$^-$ mixture in the temperature range 500-25000K. 170 electronic states of N atoms are taken into account.

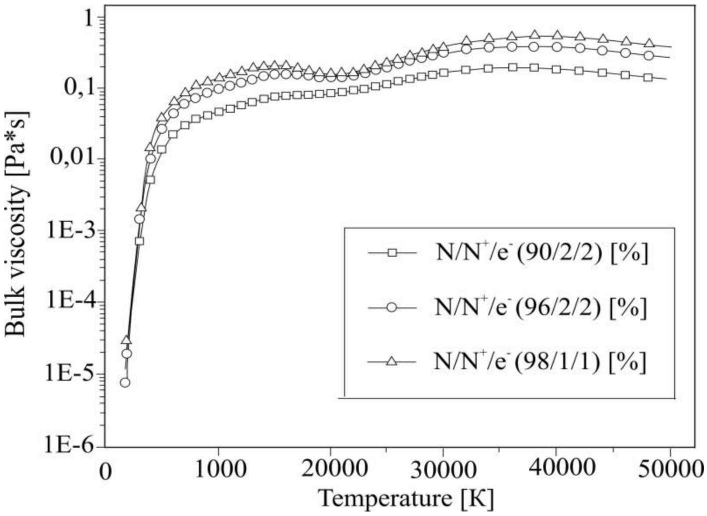

Figure 1: Bulk viscosity coefficients as a function of temperature

In Fig.1 the coefficient of bulk viscosity is shown as a function of temperature in the temperature range 500-25000K. The bulk viscosity coefficient increases strongly with temperature. One can notice non-monotonic behavior in the temperature range from 15000 to 25000 K. At high concentrations of atoms the value of bulk viscosity increases sharply in the temperature range 3000-5000K. For N/N$^+$/e$^-$ mixture, the bulk viscosity coefficient increases with the rise of fraction of neutral atoms in the mixture. Increasing of the molar fraction of structure-less particles leads to the decrease of the bulk viscosity coefficient.

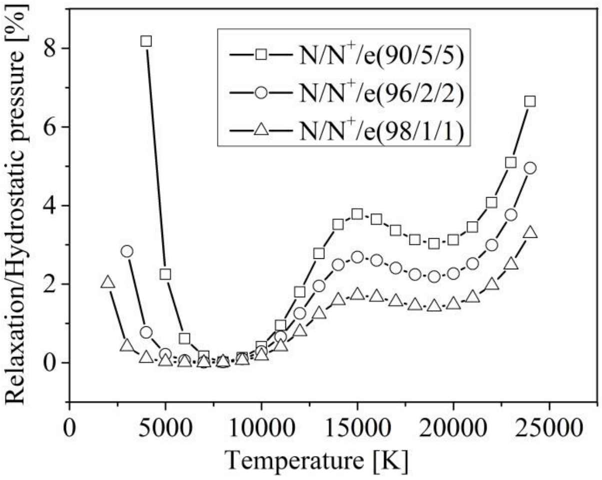

Figure 2: Ratio of the relaxation pressure to the hydrostatic pressure as a function of temperature

Contribution of the relaxation pressure into the stress tensor as a function of temperature is presented in Fig.2. When we take into account the electronic excitation, the contribution of the relaxation pressure can reach 9%. On the other hand, in the temperature range 5000-10000K the contribution of the relaxation pressure is negligibly small. Also it should be noted that the sign of the relaxation pressure changes, and the relaxation pressure of approximately zero corresponds to the chemical equilibrium: $\boldsymbol{R}_{\boldsymbol{N}}^{\boldsymbol{ioniz}} = 0$. Sign of the relaxation pressure determined by the direction of the chemical reaction.

Since the bulk viscosity is independent of pressure, its contribution to the stress tensor remains unchanged with pressure variation. Thus at low pressures, the main contribution to the stress tensor is given by the bulk viscosity, even for low values of the velocity divergence.

In Fig.3 and Fig.4 the thermal diffusion coefficients as functions of temperature are presented for different mixture compositions. As we can see, thermal diffusion of electrons is significantly higher than thermal diffusion of ions and neutral atoms.

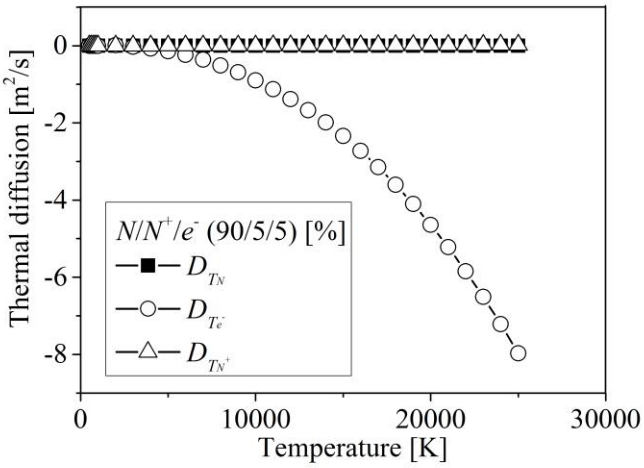

Figure 3: Thermal diffusion coefficients as functions of temperature

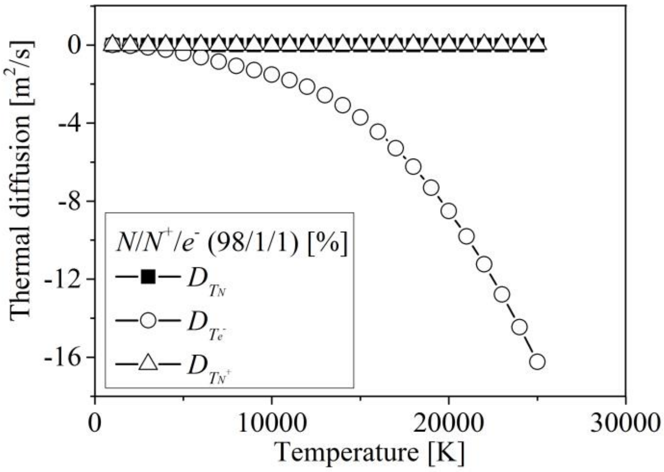

Figure 4: Thermal diffusion coefficients as functions of temperature

The Prandtl number characterizes the ratio of momentum and heat transfer in the gas:

$$\boldsymbol{Pr} = \frac{c_p\eta}{\lambda} \qquad (25)$$

For monatomic gases the Prandtl number is usually assumed to be a constant. If we take into account the electronic excitation of atoms, the Prandtl number becomes a non-monotonic function of the temperature. The Prandtl number as a function of temperature is shown in Fig.5. It is shown, that ionization process leads to the decrease of the Prandtl number in the temperature range 4000 – 20000 K.

The Schmidt number is the similarity criterion for the gas flows with diffusion processes and viscous effects:

$$\boldsymbol{Sc} = \frac{\boldsymbol{\eta}}{\boldsymbol{\rho D_{cd}}}\,. \tag{26}$$

The Schmidt number as function of temperature is shown in Fig.6. As we can see, Schmidt number for a plasma flow is a non-monotonic function of the temperature. The contribution of structure-less particles leads to the Schmidt number decrease.

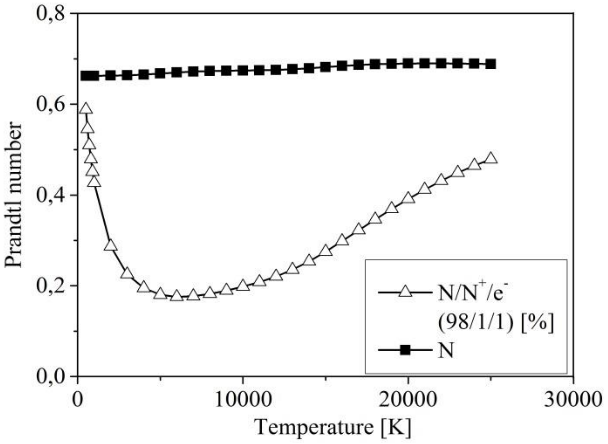

Figure 5: Prandtl number as a function of temperature

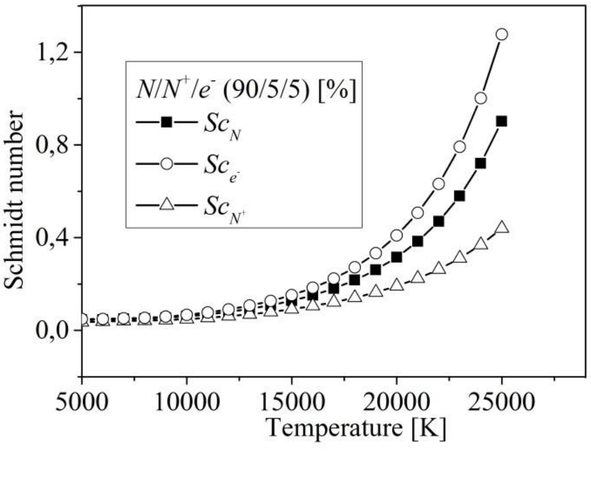

Figure 6: Schmidt numbers as functions of temperature

6. Conclusions

Mathematical model for the calculation of transport coefficients in strongly non-equilibrium plasma flows with electronic excitation of neutral atoms is developed. The relaxation pressure and bulk viscosity coefficients in chemically non-equilibrium weakly ionized gas mixture in the temperature range 500-25000 K are calculated. The contribution of electronic excitation is estimated. Rise of the concentration of structure-less particles leads to the increase of the relaxation pressure coefficient. The main contribution to the stress tensor is given by the relaxation pressure at atmospheric pressure and by the bulk viscosity at low pressures.

The Prandtl and Schmidt numbers are evaluated, and they are found to be essentially non-constant. In the temperature range 5000 – 18000 K for the plasma flow the Schmidt number is much less that constant value 0.5.

7. Acknowledgements

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