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Diffusion velocity and reactive thermal conductivity for shock waves propagating in the hydrogen gas

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Abstract. Large gradients of the temperature and ionization degree in shock waves lead to diffusion of ions with respect to neutral atoms. In order to take into account this phenomenon, we modify the fluid dynamics equations of the shock wave model described by Fadeyev & Gillet (2000). The principal goal of our study was to determine the reactive thermal conductivity. We obtained the non-LTE equation for the reactive thermal conductivity for the nonequilibrium two–temperature gas consisting of heavy particles (ions and neutral atoms) and free electrons. For the single temperature gas in LTE our expressions become the same as those given by Devoto (1967) and Nowak & Ulmschneider (1977). Finally, we discuss the importance of the heat flux induced by the reactive conductivity for shock waves propagating through hydrogen gas with typical properties for atmospheres of pulsating stars (10^{-7} gm cm^{-3} $\le \rho \le 10^{-10}$ gm cm^{-3} and 3000 K $\le T \le$ 8000 K). The reactive conductivity could be efficient behind the shock front, at the end of the thermalization zone when ionization process brutally occurs. When the gas is very dense, the reactive heat flux is of the same order of magnitude as the classical electronic heat flux.

Key words. conduction – shock waves – hydrodynamics – stars: atmospheres

1. Introduction

In our previous paper (Fadeyev et al. 2002) we considered effects of electron thermal conduction in the structure of steady–state radiative shock waves propagating through the partially ionized hydrogen gas. In particular, we have shown that though the electron heat conduction substantially affects the electron temperature in the close vicinity of the viscous jump, the whole structure of the radiative shock wave does not undergo perceptible changes at shock velocities less than ≈70 km s^{-1}. It should be noted, however, that in Fadeyev et al. (2002) we took into account effects of the translational electron thermal conduction, whereas the effective heat flux can contain also the reactive component (see, for example, Hirschfelder et al. 1954; Chapman & Cowling 1970). In the partially ionized gas the reactive thermal conduction is due to diffusion velocity of neutral atoms, ions and electrons. The ion velocity is not equal to the neutral atom velocity ($U_{\mathrm{H}^+} \neq U_{\mathrm{H}}$) and at the same time the electron velocity is nearly the same as that of ions ($U_{\mathrm{e}} = U_{\mathrm{H}^+}$).

The difference between diffusion velocities of ions and neutral atoms is due to the existence of the ionization gradient but can be influenced also by the temperature and pressure gradients. Thus, of great importance is to evaluate effects of the both diffusion phenomena and reactive conductivity in regions with steep gradients of radiative shock waves.

Expressions for the reactive thermal conductivity for partially ionized gases in chemical equilibrium were obtained by Devoto (1967). Nowak & Ulmschneider (1977) developed these expressions for the mixture of hydrogen and helium with arbitrary degree of ionization. Unfortunately, the studies of both Devoto (1967) and Nowak & Ulmschneider (1977) were done for the thermally equilibrium gas at constant pressure with ionization obeying the Saha–Boltzmann equation. Furthermore, in his analysis Devoto (1967) followed the approach of Hirschfelder et al. (1954) and assumed that all species are characterized by the same temperature. Thus, the expression for the diffusion velocity given by Hirschfelder et al. (1954) cannot be applied for the post-shock region where the temperature of heavy particles substantially exceeds the electron temperature. Appropriate expressions were obtained by Conrad & Schunk (1979) in their study of the high–latitude topside ionosphere with large temperature differences of interacting species. They obtained the multi–temperature expression for the ambipolar diffusion velocity which follows from the system of transport equations derived by Grad (1949, 1958) and from the collision terms given by Burger (1969).

In Sect. 2 we give the fluid dynamics and statistical equilibrium equations which take into account the difference in diffusion velocity between ions and neutral atoms. Then we compute the reactive conductivity of a hydrogen gas undergoing the nonequilibrium ionization and characterized by different temperatures of heavy particles and electrons. Here we show that in LTE our expressions are transformed to those given

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by Devoto (1967). In Sect. 3 we study the role of the reactive conductive flux in shock waves propagating in cool stellar atmospheres. Final conclusions are given in Sect. 4.

2. Equations of fluid dynamics and reactive thermal conduction

In this study we consider the one-dimensional steady–state gas flow in planar geometry. The system of fluid dynamics and rate equations for the shock wave where all particles have the same hydrodynamic velocity is given in Fadeyev & Gillet (1998, 2000). In general, the multi–velocity behavior of the fluid is described in terms of the continuity, momentum and energy equations for each species. In such an approach the reactive heat conductive flux is considered implicitly and in order to obtain the explicit expression for the reactive thermal conductivity we introduce the mass center velocity

$$\boldsymbol{U} = \frac{1}{\rho} \sum_j n_j m_j \boldsymbol{U}_j, \tag{1}$$

where $\boldsymbol{U}_j$ is the velocity of the j species and ρ is the gas density.

By definition the diffusion velocity is $\boldsymbol{u}_j \equiv \boldsymbol{U}_j - \boldsymbol{U}$. On the other hand, if we neglect the electron inertial velocity, we find that $n_{\mathrm{H}^+}\boldsymbol{u}_{\mathrm{H}^+} = -n_{\mathrm{H}}\boldsymbol{u}_{\mathrm{H}}$, where n_{H^+} is the ion density and $n_{\mathrm{H}} \equiv \sum n_i$ is the total number density of neutral atoms.

In order to obtain the fluid dynamics equations we applied the approach developed by Braginskii (1965) and Fontenla et al. (1990). As well known, the equations of continuity, momentum and energy conservation for one species are found from multiplication of the Boltzmann's equation of this species by 1, $m\boldsymbol{v}$, and $mv^2/2$, respectively, and consequent integration of the resulting equations with respect to velocity. Summation of momentum equations for each species (electrons, ions, neutral and excited atoms) gives us the plasma momentum equation. In this equation we replace the velocity of each species $\boldsymbol{U}_j$ by $\boldsymbol{U}_j = \boldsymbol{u}_j + \boldsymbol{U}$. Here, we neglect the electron inertia and second order terms because u_j is small in comparison with velocities of other species.

The same procedure is employed in order to obtain the plasma equations for mass and energy conservation. It should be noted, however, that we consider two energy equations because there are two distinct temperatures: the temperature heavy particles (ions and neutral atoms) and the temperature of electrons. We also assume that the heat generated in the gas as a consequence of the change of momentum between electrons and neutral atoms can be neglected due to the smallness of m_{e}, $u_{\mathrm{e}} - u_{\mathrm{H}}$ and the cross section of collision between electrons and neutral atoms. It should be noted that for each species we neglect the viscosity.

Thus, the equation of mass conservation is

$$\frac{\mathrm{d}}{\mathrm{d}x}(\rho U) = 0, \tag{2}$$

where $\rho U = \dot{m}$ is constant in a planar geometry. The momentum conservation equation is

$$\dot{m}\frac{\mathrm{d}U}{\mathrm{d}x} = -\frac{\mathrm{d}P_{\mathrm{g}}}{\mathrm{d}x}, \tag{3}$$

where $P_{\mathrm{g}} = n_{\mathrm{a}}kT_{\mathrm{a}} + n_{\mathrm{e}}kT_{\mathrm{e}}$ is the total gas pressure and n_{a} is the number of heavy particles (ions and neutral atoms) per unit volume. The equation of energy conservation of the electron gas is written as

$$\begin{aligned} U\frac{\mathrm{d}E'_{\mathrm{e}}}{\mathrm{d}x} &= -P_{\mathrm{e}}U\frac{\mathrm{d}V}{\mathrm{d}x} + Q_{\mathrm{elc}} + Q_{\mathrm{inc}} - \frac{1}{\rho}\nabla\cdot\boldsymbol{F}_{\mathrm{e}} \\ &\quad -\frac{1}{\rho}\nabla\left(\frac{5}{2}kT_{\mathrm{e}}\, n_{\mathrm{e}}\boldsymbol{u}_{\mathrm{e}}\right) + \frac{u_{\mathrm{e}}}{\rho}\frac{\mathrm{d}P_{\mathrm{e}}}{\mathrm{d}x}, \end{aligned} \tag{4}$$

where Q_{elc} and Q_{inc} are the rates of energy gain by electron gas in elastic and inelastic collisions (Fadeyev & Gillet 2000). The rate of energy gain in inelastic collisions is (Murty 1971)

$$\begin{aligned} Q_{\mathrm{inc}} &= -\frac{\nabla\cdot\boldsymbol{F}_{\mathrm{R}}}{\rho} - \frac{e_{\mathrm{H}^+}}{\rho}\nabla\left[n_{\mathrm{H}^+}(\boldsymbol{u}_{\mathrm{H}^+} + \boldsymbol{U})\right] \\ &\quad -\sum_{i=1}^{L}\frac{e_{\mathrm{H}^+\left(1-\frac{1}{i^2}\right)}}{\rho}\nabla\left[n_i\ (\boldsymbol{u}_{\mathrm{H}} + \boldsymbol{U})\right]. \end{aligned} \tag{5}$$

The energy equation for heavy particles is

$$U\frac{\mathrm{d}E'_{\mathrm{a}}}{\mathrm{d}x} = -P_{\mathrm{a}}\,U\frac{\mathrm{d}V}{\mathrm{d}x} - Q_{\mathrm{elc}} - \frac{u_{\mathrm{H}^+}}{\rho}\frac{\mathrm{d}P_{\mathrm{e}}}{\mathrm{d}x} \tag{6}$$

where $E'_{\mathrm{e}} = \frac{3}{2}\frac{n_{\mathrm{e}}kT_{\mathrm{e}}}{\rho}$, $E'_{\mathrm{a}} = \frac{3}{2}\frac{n_{\mathrm{a}}kT_{\mathrm{a}}}{\rho}$ and the specific volume is $V \equiv \frac{1}{\rho}$. $e_{\mathrm{H}^+} = 13.6$ eV, L is the number of bound atomic levels, $\nabla\cdot\boldsymbol{F}_{\mathrm{R}}$ is the divergence of radiative flux and $\nabla\cdot\boldsymbol{F}_{\mathrm{e}}$ is the divergence of the electron heat conductive flux.

The last terms in energy Eqs. (4) and (6) describe polarization electrostatic field that appears because of the tendency of electrons and ions to separate. The polarization electrostatic field can be expressed in the form (Zel'dovich & Raizer 1967; Conrad & Schunk 1979)

$$\frac{\mathrm{d}P_{\mathrm{e}}}{\mathrm{d}x} = -en_{\mathrm{e}}E, \tag{7}$$

where we neglect the influence of thermal diffusion. In more detail the system of conservation Eqs. (2–6) is discussed in Appendix A.

Thus, in order to solve this system of equations it is necessary to determine the diffusion velocity and the statistical equilibrium equation. Equations of statistical equilibrium for ions and neutral atoms are

$$\nabla\cdot\left[n_{\mathrm{H}^+}\ (\boldsymbol{u}_{\mathrm{H}^+} + \boldsymbol{U})\right] = \sum_{i=1}^{L}\left(n_i\,P_{ik} - n_{\mathrm{e}}\,P_{ki}\right), \tag{8}$$

$$\nabla\cdot\left[n_i\ (\boldsymbol{u}_{\mathrm{H}} + \boldsymbol{U})\right] = n_{\mathrm{e}}\,P_{ki} - n_i\,P_{ik} + \sum_{\substack{j=1 \\ j\neq i}}^{L}\left(n_j\,P_{ji} - n_i\,P_{ij}\right), \tag{9}$$

where u_{H} is the diffusion velocity of neutral hydrogen atoms, P_{ij} and P_{ji} are the total (collisional plus radiative) rates of bound-bound upward and downward transitions between the ith and jth atomic levels, respectively, and P_{ik} and P_{ki} are the total rates of ionization and recombination for the ith atomic level. These coefficients are described by Fadeyev & Gillet (2000).

The diffusion velocities are determined according to Conrad & Schunk (1979). Indeed, with general system of transport equations derived by Schunk (1975, 1977) the ambipolar diffusion velocity is

$$\boldsymbol{V}_\mathrm{A} = \boldsymbol{u}_\mathrm{H} - \boldsymbol{u}_{\mathrm{H}^+} = D_\mathrm{a}\left[\frac{\nabla n_{\mathrm{H}^+}}{n_{\mathrm{H}^+}} + \frac{\nabla(T_\mathrm{a}+T_\mathrm{e})}{T_\mathrm{a}+T_\mathrm{e}}\right] + 2D_\mathrm{a}\,(w+w^\star)\frac{\nabla T_\mathrm{a}}{T_\mathrm{a}+T_\mathrm{e}}, \tag{10}$$

where

$$D_\mathrm{a} = \frac{k\,(T_\mathrm{e}+T_\mathrm{a})}{m_\mathrm{H}\,\nu_{\mathrm{H}^+\mathrm{H}}}\frac{1}{(1-\Delta_{\mathrm{H}^+\mathrm{H}})} \tag{11}$$

and $\nu_{\mathrm{H}^+\mathrm{H}}$ is the frequency of momentum transfer in collisions between ions and neutral atoms. The first term in the right–hand–side of Eq. (10) is the diffusion velocity describing effects of ionization and the pressure gradient. The second term is due to the thermal diffusion. Expressions for w, $w^\star$, $\nu_{\mathrm{H}^+\mathrm{H}}$ and $\Delta_{\mathrm{H}^+\mathrm{H}}$ are given in Appendix A. For $T_\mathrm{H} = T_\mathrm{H}^+ = T_\mathrm{a}$ we have $\Delta_{\mathrm{H}^+\mathrm{H}} \simeq 0.01$. As was noted above Conrad & Schunk (1979) did not take into account effects of the radiative flux on the diffusion velocity. As is shown below in the next section the ambipolar diffusion velocity is efficient within a small region of the shock structure where the gas is practically transparent to the radiative flux (see Figs. 3 and 4). Thus, we assumed that the radiative flux does not affect perceptibly the diffusion velocity.

The diffusion velocity was computed under assumption that collisions between species are elastic, that is excitation and ionization can be ignored. This assumption is corroborated by the fact that in the shock wave region with steep gradient of ionization the elastic collisions are more important in comparison with inelastic ones. Thus, writing $n_{\mathrm{H}^+}\boldsymbol{u}_{\mathrm{H}^+} = -n_\mathrm{H}\boldsymbol{u}_\mathrm{H}$ we derive the diffusion velocities of ions and neutral heavy particles as

$$\boldsymbol{u}_{\mathrm{H}^+} = \boldsymbol{u}_\mathrm{e} = -\frac{n_\mathrm{H}}{(n_\mathrm{H}+n_{\mathrm{H}^+})}\boldsymbol{V}_\mathrm{A} \tag{12}$$

and

$$\boldsymbol{u}_\mathrm{H} = \frac{n_{\mathrm{H}^+}}{(n_\mathrm{H}+n_{\mathrm{H}^+})}\boldsymbol{V}_\mathrm{A}, \tag{13}$$

respectively.

Now we can solve the fluid dynamics Eqs. (2)–(9) together with Eqs. (12)–(13). It should be noted that this system of equations is similar to that given by Fadeyev & Gillet (2000) but now the gas flow velocity $\boldsymbol{U}$ is replaced by the center of mass velocity derived by Eq. (1) and the inelastic collision term Q_inc is modified due to the new equations of statistical equilibrium. Moreover, a new divergence term ($\frac{5}{2}kT_\mathrm{e}\,n_\mathrm{e}\boldsymbol{u}_\mathrm{e}$) appears in the right–hand–side of the electron energy Eq. (4). This term represents the electron enthalpy flux which is a part of the reactive thermal conductivity. In fact, there is a similar term in the heavy particles energy equation which is written as $\frac{5}{2}kT_\mathrm{a}(n_\mathrm{H}\boldsymbol{u}_\mathrm{H} + n_{\mathrm{H}^+}\boldsymbol{u}_{\mathrm{H}^+})$. This term, however, vanishes due to the fact that $n_{\mathrm{H}^+}\boldsymbol{u}_{\mathrm{H}^+} = -n_\mathrm{H}\boldsymbol{u}_\mathrm{H}$. Diffusion of neutral hydrogen atoms and hydrogen ions in the opposite direction leads to cancelation of the enthalpy flux terms and there is no enthalpy flux connected with the diffusion velocity in the heavy particles energy equation (Eq. (6)).

2.1. A non-LTE equation of the reactive thermal conductivity

In this section we obtain the reactive thermal conductivity following formalism developed by Devoto (1967) but without LTE simplifying assumption and using the ambipolar diffusion velocity given by Conrad & Schunk (1979). The divergence of reactive thermal conductivity is obtained from summation of all diffusion terms in the energy equations. If we write this equation in a vector form and if we neglect the small number of excited states of the hydrogen atom (last term in Eq. (5)), the reactive conductivity becomes

$$\boldsymbol{Q}_\mathrm{r} = n_\mathrm{e}\boldsymbol{u}_\mathrm{e}\,\Delta h, \tag{14}$$

where $\Delta h = h_\mathrm{e} + h_{\mathrm{H}^+} - h_\mathrm{H} = \frac{5}{2}kT_\mathrm{e} + e_{\mathrm{H}^+}$. This equation takes into account diffusion of electrons and ions with respect to neutral atoms as well as the recombination of atoms which leads to the liberation of the ionization energy and electron enthalpy. Substituting Eq. (12) into Eq. (14) we obtain the reactive heat flux

$$\boldsymbol{Q}_\mathrm{r} = -n_\mathrm{H}\Delta h\,D_\mathrm{a}\times\frac{\nabla\alpha}{(1+\alpha)} - \alpha\,n_\mathrm{H}\Delta h\,D_\mathrm{a} \times\left[\frac{\nabla n}{n} + \frac{\nabla(T_\mathrm{a}+T_\mathrm{e})}{T_\mathrm{a}+T_\mathrm{e}}\right] - \alpha\,n_\mathrm{H}\Delta h\,D_\mathrm{a}(w+w^\star)\times\frac{2\,\nabla T_\mathrm{a}}{T_\mathrm{a}+T_\mathrm{e}}, \tag{15}$$

where

$$\alpha \equiv \frac{n_\mathrm{e}}{n_\mathrm{H}+n_{\mathrm{H}^+}} \tag{16}$$

is the ionization degree. This relation will be used below in Sect. 3 in order to evaluate the intensity of the reactive thermal conductivity in the shock wave.

There are no simplifying assumptions on LTE ionization. The contribution of thermal diffusion into $\boldsymbol{Q}_\mathrm{r}$ (last term in Eq. (15)) is generally small (Devoto 1967). Moreover, in shock wave the pressure gradient (the second term in Eq. (15)) is small enough in comparison with the term of the ionization gradient $\nabla\alpha$ (the first term in Eq. (15)).

Thus, the thermal reactive conductivity can be considered as diffusion of ions and electrons in the presence of the ionization gradient toward the layers with deficiency of these particles, whereas neutral atoms move in the opposite direction. During this motion the particles carry the ionization energy as well as the translational enthalpy. For the zero ionization gradient (e.g. the neutral or fully ionized gas) $\nabla\alpha = 0$ and therefore $\boldsymbol{Q}_\mathrm{r}$ vanishes.

2.2. The temperature dependence of reactive thermal conductivity

Expressions for reactive conductivity in LTE were obtained by Devoto (1967) but, unfortunately, his formalism was not described in detail. First, various authors give different definitions of the ambipolar diffusion coefficient. Comparing the electron diffusion velocity of Eq. (12) with that of Schunk & Walker (1970, Eq. (18)) we find that for the single temperature $D_\mathrm{A} = \frac{n_\mathrm{H}}{n}D_\mathrm{a}$ and $\frac{D_\mathrm{A}^\mathrm{T}}{m_{\mathrm{H}^+}} = D_\mathrm{a}\,(w+w^\star)\,\frac{n_\mathrm{H}\,n_\mathrm{e}}{n_\mathrm{H}+n_\mathrm{e}}$ where D_A and D_A^T are

Devoto's (1966) ordinary and thermal ambipolar diffusion coefficients. It should be noted that these coefficients arise from the theory of Hirschfelder et al. (1954), whereas D_a, w and $w^\star$ are found from the 13–moment system of transport equations. Nevertheless, the above expressions are only approximate (see Conrad & Schunk 1979). Thus, at constant pressure and single temperature Eq. (15) becomes

$$\boldsymbol{Q}_r = -\frac{n^2 m_H}{\rho}\Delta h D_A \nabla x_e - \Delta h \frac{D_A^T}{m_{H^+}} \nabla \ln T \tag{17}$$

where $n = n_H + 2n_{H^+}$ and $x_e = \frac{n_e}{n}$. Furthermore, considering a quasi-neutral ($n_e = n_{H^+}$) and constant pressure (P_g = const.) gas, we easily find (Meador & Station 1965) that

$$\nabla x_e = \frac{n_e n_H}{2n(n_e + n_H)} \frac{\partial \ln K_P}{\partial T} \nabla T \tag{18}$$

where $K_p \equiv \frac{P_{H^+} P_e}{P_H P_0}$ is the pressure–standardized equilibrium constant. P_{H^+}, P_H and P_e are respectively the ion, neutral hydrogen and electron pressures in local thermal and chemical equilibrium, P_0 is the standard pressure which is independent of space coordinates. Differentiation of $\ln K_P$ relates the enthalpy change due to Van't Hoff's expression:

$$\frac{\partial \ln K_p}{\partial T} = \frac{\Delta h}{kT^2} \tag{19}$$

where $\Delta h = h_e + h_{H^+} - h_H = \frac{5}{2}kT + e_{H^+}$. Here it should be noted that Van't Hoff's relation can be deduced directly from the Saha equation. Finally, substituting Eqs. (18) and (19) into Eq. (17) we obtain the relation similar to that of Devoto (1967, 1968) at constant pressure:

$$\boldsymbol{Q}_r = -\Delta h \left[\frac{n m_H}{2\rho k T^2} \frac{n_e n_H}{n_e + n_H} \Delta h D_A + \frac{D_A^T}{m_H T} \right] \nabla T \tag{20}$$

where D_A is about equal to $2\mathcal{D}_{H^+H}$ (see Devoto 1966) and $\mathcal{D}_{H^+H}$ is the first approximation of the binary diffusion coefficient computed by Hirschfelder et al. (1954, p. 508) in the case of rigid spheres. For the hydrogen this coefficient is given by (Ulmschneider 1970)

$$\mathcal{D}_{H^+H} = \frac{3}{16n} \left(\frac{4\pi k T}{m_H} \right)^{\frac{1}{2}} \times \frac{1}{Q_{H^+H}}, \tag{21}$$

where the cross section between ions and neutral atoms was given by (Nowak & Ulmschneider 1977):

$$\begin{aligned} Q_{H,H^+} &= 2.5585 \times 10^{-14} - 2.0315 \times 10^{-15} \ln T \\ &\quad +4.0371 \times 10^{-17} (\ln T)^2. \end{aligned} \tag{22}$$

Using $\Delta h = \frac{5}{2}kT + e_{H^+}$ and Eq. (21), we finally return, by neglecting D_A^T, to the relation for pure hydrogen gas given by Nowak & Ulmschneider (1977):

$$\begin{aligned} \boldsymbol{Q}_r &= -\lambda_r \nabla T \\ &= -5.208 \times 10^{-12}\, T^{-\frac{3}{2}} X_H X_{H^+} \frac{(63\,114 + T)^2}{Q_{H,H^+}} \nabla T, \end{aligned} \tag{23}$$

where $X_{H^+} \equiv \frac{n_{H^+}}{n_{H^+} + n_H}$, and $X_H \equiv \frac{n_H}{n_{H^+} + n_H}$.

In our analysis we expressed ∇x_e as a function of ∇T using the Van't Hoff's equation. Thus, the reactive conductivity depends only on the temperature gradient provided that the Saha ionization law is valid. This is not true for the solar transition region (Fontenla et al. 1990) as well as for the shock waves.

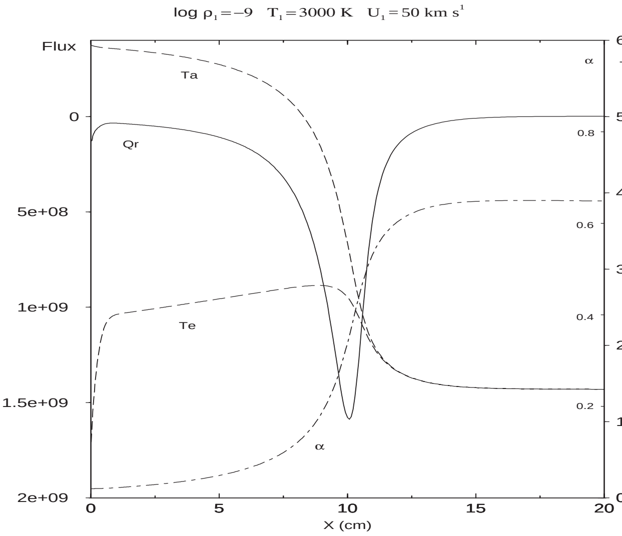

Fig. 1. Shock wake structure behind the discontinuous jump for the case $\rho_1 = 10^{-9}$ gm cm^{-3}, T_1 = 3000 K and U_1 = 50 km s^{-1}. In dot–dashed, solid and dashed lines are represented the ionization rate α, reactive conductivity Q_r and temperatures (electronic T_e and heavy particles T_a), respectively.

3. Reactive conductivity in shock waves

In this section we use Eq. (15) to study the reactive thermal conductivity in steady–state radiative shock waves propagating in the partially ionized hydrogen gas. It should be emphasized that we do not take into account the reactive conductivity self–consistently because this is beyond the scope of our approach. Thus, we determine the reactive conductivity for thermodynamic quantities of the shock wave previously computed without heat conduction (Fadeyev & Gillet 2000). The input parameters for models are the shock velocity, the temperature and the density of the unperturbed gas. We consider the strength of the reactive thermal conductivity as a function of these quantities. Our study is restricted to the range of parameters typical for shocks propagating in atmospheres of pulsating stars (10^{-10} gm cm^{-3} $\le \rho_1 \le$ 10^{-7} gm cm^{-3}, 40 km s^{-1} $\le U_1 \le$ 80 km s^{-1}, and 3000 K $\le T_1 \le$ 8000 K).

In Fig. 1 we plot the reactive thermal conductivity (Eq. (15)) in the post-shock region for the model with $\rho_1 = 10^{-9}$ gm cm^{-3}, T_1 = 6000 K, and U_1 = 50 km s^{-1}. In this figure we give also the plots of the ionization degree α as well as the temperatures of heavy particles and electrons. As is seen, the reactive conductivity is efficient within the narrow interval at the tail of the thermalization region where ionization degree rapidly increases and the temperature of heavy particles becomes nearly equal to that of electrons. Because the ionization degree increases with decreasing temperature, the reactive thermal conductivity, which is a function of the temperature gradient (Eq. (20)), has the opposite sign with respect to the reactive flux of $\nabla\alpha$ (Eq. (15)). Thus, we understand that a reactive heat flux function of a temperature gradient such as Eq. (20) assuming LTE, would not be relevant in the case of a shock wave.

For large enough shock velocities ($U_1 \gtrsim$ 85 km s^{-1}) the Lyman continuum flux emerging from the postshock region into the radiative precursor completely ionizes the preshock

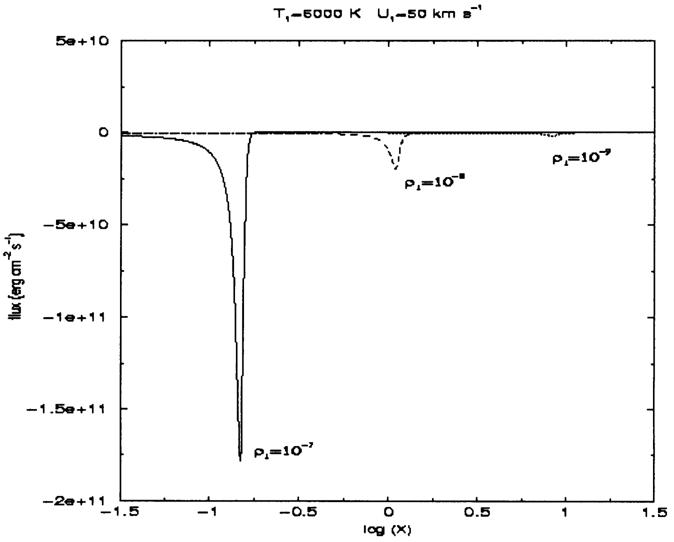

Fig. 2. The postshock reactive conductivity in the vicinity of the discontinuous jump for three densities of the unperturbed gas: $\rho_1 = 10^{-7}$ (solid line), 10^{-8} (dashed line), and 10^{-9} gm cm^{-3} (dotted line).

gas so that $\nabla\alpha$ as well as the reactive conductivity become very small throughout the whole shock wave. Thus, only for the partially ionized radiative precursor the reactive conductivity flux increases with increasing shock velocity. Nevertheless, the reactive flux increase with the velocity about in the same manner than others fluxes. Thus, if the reactive conductivity is smaller or equal (in absolute value) than the Lyman flux and the translational electronic flux, it would stay smaller even with an increasing shock velocity (Fig. 3).

It should be noted that the temperature of the ambient unperturbed gas does not affect perceptibly the reactive conductivity strength and only at high temperatures ($T_1 \gtrsim 10^4$ K) the reactive conductivity becomes negligible because of the full ionization.

In Fig. 2, we give the plots of the reactive thermal conductivity in the post–shock zone for shocks propagating at speed $U_1 = 50\,\mathrm{km\,s^{-1}}$ with $T_1 = 6000\,\mathrm{K}$ and for three densities of the unperturbed gas. The strength of the reactive conductivity strongly increases with density and the higher the density of the ambient gas the faster thermalisation occurs behind the shock front. This is due to the fact that the mean free paths of both electrons and heavy particles decrease with increasing gas density. Changes of the ionization degree and of the reactive conductivity are much stronger at higher densities.

In Fig. 4 are shown the reactive conductivity, the Lyman continuum flux and the translational electronic heat flux for $\rho \simeq 10^{-10}$ gm cm^{-3} and $\rho \simeq 10^{-7}$ gm cm^{-3}. At low density ($\rho \simeq 10^{-10}$ gm cm^{-3}) the reactive conductivity flux is small in comparison with other fluxes, whereas at high density ($\rho \simeq 10^{-7}$ gm cm^{-3}) the reactive conductivity flux is stronger than the Lyman flux and is of the same order of magnitude as the translational electronic heat flux. It should be noted that in the ionization zone the temperature decreases with increasing distance from the discontinuous jump, whereas the ionization degree increases. That is why the electronic heat flux is directed upstream, whereas the reactive thermal conductivity is directed downstream (see Fig. 4). Thus, in the hydrogen ionization zone the reactive heat flux tends to diminish the role of the translational electronic conductivity.

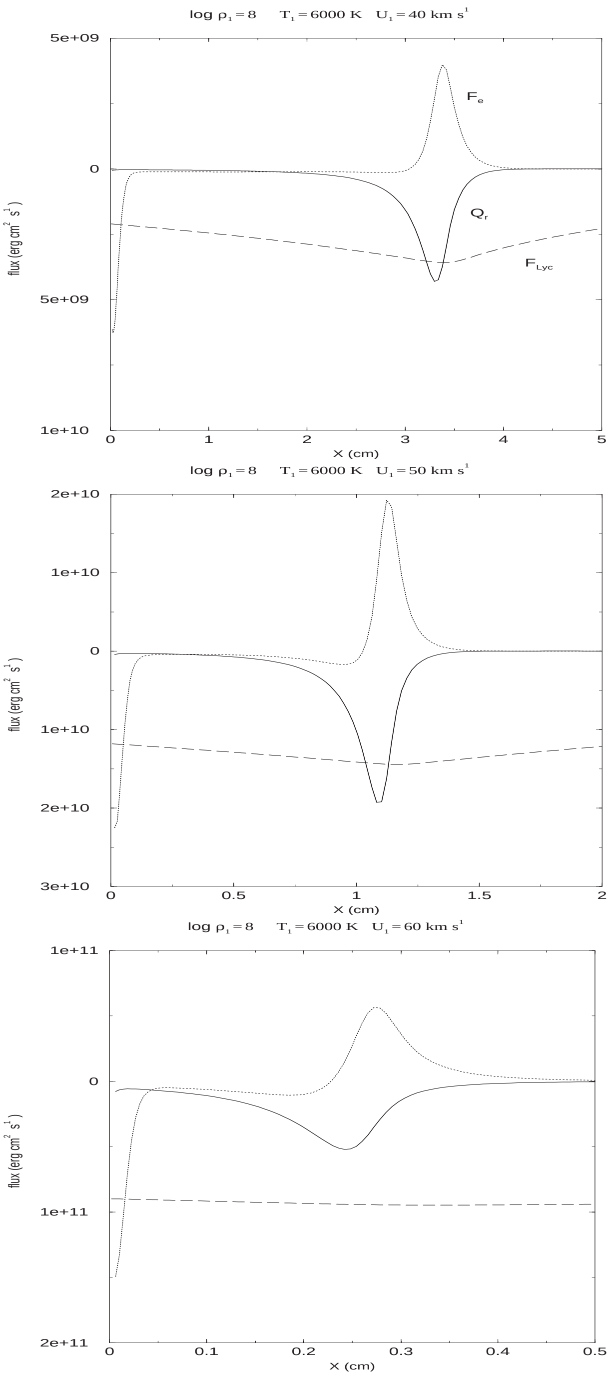

Fig. 3. Flux in the post-shock vicinity of the discontinuous jump of a shock propagating in a gas with $\rho_1 = 10^{-8}$gm cm^{-3}, $T_1 = 6000$ K and at three upstream velocities $U_1 = 40$ (upper panel), 50 (midle panel) and 60 km s^{-1} (lower panel). Dotted, solid and dashed lines are respectively for the translational electronic heat flux F_e, the reactive conductivity Q_r and the Lyman continuum flux F_Lyc.

Fadeyev et al. (2002) showed that in shock waves with $\rho_1 \simeq 10^{-10}$ gm cm^{-3} and velocities of <70 km s^{-1}, the translational electronic heat flux does not affect substantially the structure of the radiative shock wave and, in particular, does not

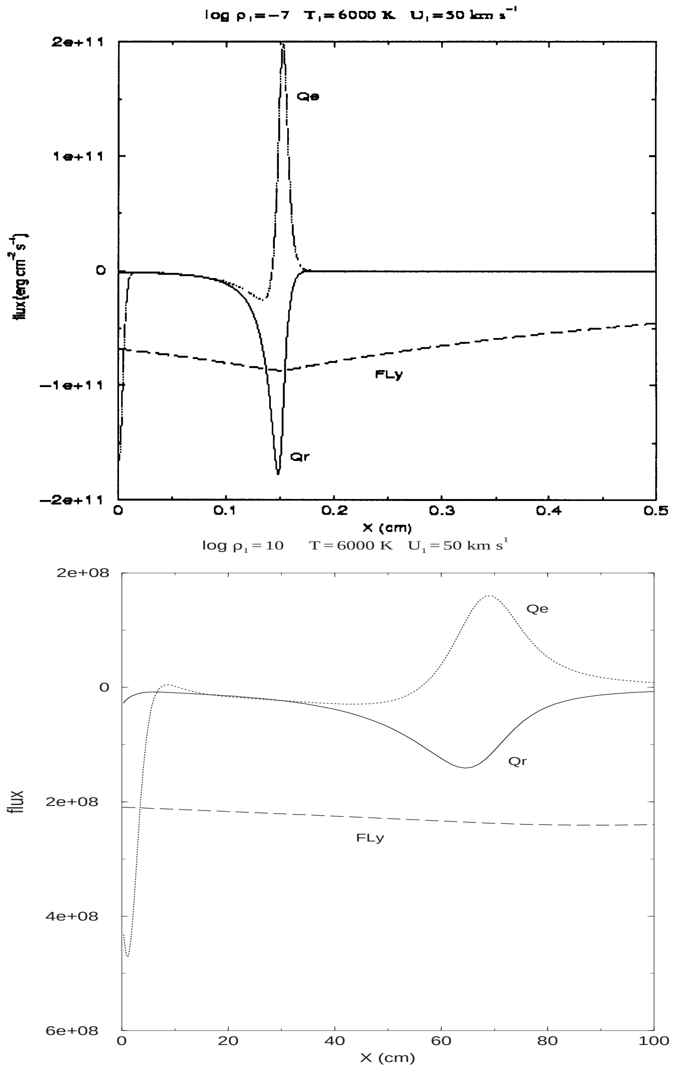

Fig. 4. The postshock flux in the vicinity of the discontinuous jump for an upstream velocities $U_1 = 50\,\mathrm{km\,s^{-1}}$, a temperature $T_1 = 6000$ K and two density $\rho_1 = 10^{-7}$ (upper panel), and 10^{-10} gm cm^{-3} (Lower panel). Dotted, solid and dashed line are respectively for the translational electronic heat flux F_e, the reactive conductivity Q_r and the Lyman continuum flux F_Lyc.

affect substantially the radiative losses. Because the reactive conductivity flux does not exceed the electronic heat flux, effects of reactive conductivity does not be seem efficient enough at the gas density of $\rho \simeq 10^{-10}$ gm cm^{-3}. However, at higher densities ($\rho \gtrsim 10^{-8}$ gm cm^{-3}), the translational electronic heat flux and the reactive conductivity may become equal or even larger than the electronic heat flux found by Fadeyev et al. (2002) in order to change the structure and the radiative losses of the shock.

4. Conclusion

In this paper, we give a system of fluid equations taking into account the diffusion velocity of ions, electrons and neutrals atoms. The electron energy equation contains a new term of reactive thermal conductivity. With ambipolar diffusion coefficients determined by Conrad & Schunk (1979) we obtained the expression for the reactive conductivity adapted to the problem of shock where the two–temperature gas (that is, the mixture of free electrons and heavy particles) and for the non–LTE ionization. For the single temperature and LTE ionization our expressions are reduced to the classical reactive thermal conductivity function of the temperature gradient given by Devoto (1967) and Nowak & Ulmschneider (1977).

The reactive thermal conductivity can be relatively strong in the post-shock ionization region but it is negligible in other regions of the shock. Nevertheless, in our shock wave model (Fadeyev & Gillet 2000), the shock front has not been correctly described in terms of fluid dynamics. The physical quantities (the temperature, velocity, density, etc.) behind the shock front are determined using the Rankine-Hugoniot equations. Thus, the temperature gradient, which can be very strong in this very narrow zone, is not well known. Also, it is impossible to evaluate the reactive thermal conductivity in our shock front model. Nevertheless, we should bear in mind that the large temperature and pressure gradients can be responsible for the ion and neutral atom diffusion velocity. Moreover, the shock front structure is complex because the viscosity phenomena have to be considered and the temperature of ions can be enough different than that of neutral atom temperature (Jaffrin 1965).

In this study we found that in the post-shock ionization zone the intensity (in absolute value) of the reactive thermal conductivity increases with both increasing density of the unperturbed gas and increasing velocity of the shock until the preshock gas is fully ionized by the Lyman flux. In order to better understand effects of the reactive thermal conductivity the self–consistent approach is needed. Thus, the next step of this work is that to compute the structure of a radiative shock wave with diffusion velocity phenomena (i.e. with reactive thermal conductivity) by using the equation system of Sect. 2.

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Appendix A: Conservation equations

Here we describe the main step in order to derive the system of equations of Sect. 2. We follow the way of Braginskii (1965) and Fontenla et al. (1990). However, in contrast to these previous works, we have in our study two energy equations: one for heavy particles (ions and neutral atoms) and another for electrons. Moreover, we present these equations in a form adapted to our shock wave model. In this appendix we give the approximations that are needed in order to find this system of equations.

The Boltzmann equation describing the evolution of the particle distribution function f_j is written as (Braginskii 1965)

$$\frac{\partial f_j}{\partial t} + \frac{\partial}{\partial x_\beta}(v_\beta f_j) + \frac{\partial}{\partial v_\beta}\left(\frac{e_j E_\beta}{m_j} f_j\right) = C_j \tag{A.1}$$

where E_β is the electric field in the β direction and e_j the charge of particles j. C_j is the change per unit time in the distribution function for particles of species j due to collisions with others particles.

A.1. The mass conservation equation

Integrating Eq. (A.1) over velocity, we find for the species j

$$\frac{\partial n_j}{\partial t} + \nabla\left(n_j \boldsymbol{U}_j\right) = \int C_j \mathrm{d}\boldsymbol{v}\,. \tag{A.2}$$

Multiplication of this equation by m_j and adding over all species j for the one–dimensional steady–state gas flow gives

$$\frac{\mathrm{d}}{\mathrm{d}x}(\rho U) = \sum_j m_j \int C_j \mathrm{d}\boldsymbol{v}\,. \tag{A.3}$$

Determining this equation we neglected the electron inertia and we replaced U_j by $u_j + U$. These velocities are defined in Sect. 2 and we also used $n_{\mathrm{H}^+}u_{\mathrm{H}^+} = -n_{\mathrm{H}}u_{\mathrm{H}}$.

$\int C_j \mathrm{d}\boldsymbol{v}$ is the number of particles j that was created or suppressed by unit time and volume with inelastic collisions. Thus, we obtain that the right side of Eq. (A.3) vanish

$$\begin{aligned}\sum_j m_j \int C_j \mathrm{d}\boldsymbol{v} \;=\; & m_{\mathrm{H}} \sum_{i=1}^{L} (P_{ki} n_{\mathrm{H}^+} - P_{ik} n_i) \\ & + m_{\mathrm{H}} \sum_{i=1}^{L} \sum_{\substack{l=1 \\ l\neq i}}^{L} (P_{li} n_l - P_{il} n_i) \\ & + m_{\mathrm{H}^+} \sum_{i=1}^{L} (P_{ik} n_i - P_{ki} n_{\mathrm{H}^+}) \\ & + m_{\mathrm{e}} \sum_{i=1}^{L} (P_{ik} n_i - P_{ki} n_{\mathrm{H}^+}) = 0\end{aligned}$$

where P_{ji} are defined in Sect. 2. Thus, including this last equation in Eq. (A.3), we have found Eq. (2).

A.2. The momentum conservation equation

The momentum conservation equation is obtained in the same manner as the mass conservation equation. We multiply the Boltzmann Eq. (A.1) by $m_j \boldsymbol{v}$ and then integrate over velocity. Assuming the one-dimensional steady-state gas flow and neglecting the stress tensor after some transformations given by Braginskii (1965) we find for j species

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(m_j n_j U_j^2\right) + \frac{\mathrm{d}}{\mathrm{d}x}(P_j) - e_j n_j E = \int m_j v C_j \,\mathrm{d}\boldsymbol{v} = R_j \tag{A.4}$$

where the pressure of species j is $P_j = n_j k T_j$.

We identify the electric field with that generated by the tendency of electrons and ions to separate. Then, adding Eq. (A.4) on all species j and with $U_j \equiv u_j + U$ we obtain

$$\dot{m}\frac{\mathrm{d}U}{\mathrm{d}X} = -\frac{\mathrm{d}P_{\mathrm{g}}}{\mathrm{d}x} + \sum_j R_j \tag{A.5}$$

where we neglect the electron inertia and assume that the diffusion velocity u_j is small in comparison with velocities of other species. u_j/U terms was neglected in front of one.

The velocity v is the some as the mean velocity U_j and the random velocity $v^{'}$ linked with thermal velocity. Thus, the collision terms $\sum_j R_j$ are

$$\sum_j R_j = \sum_j \int m_j v^{'} C_j \,\mathrm{d}\boldsymbol{v} + \sum_j U_j m_j \int C_j \mathrm{d}\boldsymbol{v}. \tag{A.6}$$

R_j is the mean change in the momentum of particles of a given species due to collisions with all other particles. The last sum at the right of the equality linked with the rate of production of particles writes

$$\sum_j U_j m_j \int C_j \mathrm{d}\boldsymbol{v} = m_{\mathrm{H}} V_{\mathrm{A}} \frac{\mathrm{d}(n_{\mathrm{H}} U_{\mathrm{H}})}{\mathrm{d}x} \tag{A.7}$$

where V_{A} is the ambipolar diffusion velocity given by Eq. (10). We have checked every where in the shock wake that this sum is very small when we compare it with $\frac{\mathrm{d}P_{\mathrm{g}}}{\mathrm{d}x}$. Thus, we can neglect this term. This shows that even at the tail of the thermalization region where ionization processes occur, inelastic collisions are not efficient enough to affect the momentum equation. Finally, if R_j is dominated by elastic processes then (Braginskii 1965)

$$\sum_j R_j = \sum_j \int m_j v^{'} C_j \,\mathrm{d}\boldsymbol{v} = 0\,. \tag{A.8}$$

Finally, if we include Eq. (A.8) into Eq. (A.5) we return to Eq. (3).

A.3. The energy conservation equations

The energy conservation equation is obtained by multiplication of the Boltzmann Eq. (A.1) by $m_j v^2/2$ and then its integrating over velocity. Assuming an one–dimensional steady–state gas flow, neglecting the stress tensor and using some transformations given by Braginskii (1965), the energy conservation equation writes

$$\nabla\left[\left(\frac{1}{2}m_j n_j U_j^2 + \frac{5}{2}P_j\right)\boldsymbol{U}_j\right] + \nabla \boldsymbol{F}_j = e_j n_j E U_j + \int \frac{m_j v^2}{2} C_j \mathrm{d}\boldsymbol{v} \tag{A.9}$$

where $\boldsymbol{F}_j$ is the translational thermal conductivity of the j species. Replacing the species j by e and U_{e} by $u_{\mathrm{e}} + U$, after some transformations we find the electron energy equation

$$\begin{aligned}U\frac{\mathrm{d}E_{\mathrm{e}}^{'}}{\mathrm{d}x} \;=\; & -P_{\mathrm{e}} U \frac{\mathrm{d}V}{\mathrm{d}x} - \frac{1}{\rho}\nabla \boldsymbol{F}_{\mathrm{e}} - \frac{1}{\rho}\nabla\left(\frac{5}{2}kT_{\mathrm{e}}\, n_{\mathrm{e}} \boldsymbol{u}_{\mathrm{e}}\right) \\ & + \frac{u_{\mathrm{e}}}{\rho}\frac{\mathrm{d}P_{\mathrm{e}}}{\mathrm{d}x} + \frac{1}{\rho}\int \frac{m_{\mathrm{e}}\, v^2}{2} C_{\mathrm{e}} \mathrm{d}\boldsymbol{v}\end{aligned} \tag{A.10}$$

where $E_{\mathrm{e}}^{'}$ is the electron thermal energy by mass unit defined in Sect. 2. To get this relation we have neglected $\frac{1}{2}m_{\mathrm{e}} n_{\mathrm{e}} U_{\mathrm{e}}^2$ in front of $\frac{5}{2}P_{\mathrm{e}}$. We can do this assumption because the small electron mass and because electrons are linked with ions due to electrostatic field, thus U_{e} is not very large. Moreover, we used the mass conservation equation (Eq. (2)), the specific volume $V \equiv \frac{1}{\rho}$ and the polarization electrostatic field $e n_{\mathrm{e}} E = -\frac{\mathrm{d}P_{\mathrm{e}}}{\mathrm{d}x}$.

Finally, the collision term can be rewritten

$$\frac{1}{\rho}\int \frac{m_\mathrm{e}\, v^2}{2} C_\mathrm{e}\mathrm{d}\boldsymbol{v} = \frac{1}{\rho}\int \frac{m_\mathrm{e}\, v'^2}{2} C_\mathrm{e}\mathrm{d}\boldsymbol{v} + \frac{U_\mathrm{e}}{\rho}\int m_\mathrm{e} v' C_\mathrm{e}\mathrm{d}\boldsymbol{v} + \frac{m_\mathrm{e}}{2}\frac{U_\mathrm{e}^2}{\rho}\int C_\mathrm{e}\mathrm{d}\boldsymbol{v}.$$

We have checked that the last term of this equation can be always neglected. If we consider only elastic collisions, the first and second terms at the right–hand–side of this equation give Q_elc the heat generated in the electrons gas as a consequence of collisions with heavy particles (Braginskii 1965).

Even if inelastic collisions are important for energy exchanges, this kind of collisions is less frequent than elastic collisions. Also, we do the assumption that we can compute Q_elc as in a gas without inelastic collisions. Finally, with inelastic collisions the collision term writes (Murty 1971; Fontenla et al. 1990)

$$\frac{1}{\rho}\int \frac{m_\mathrm{e}\, v^2}{2} C_\mathrm{e}\mathrm{d}\boldsymbol{v} = Q_\mathrm{elc} + Q_\mathrm{inc} \tag{A.11}$$

where Q_inc is given by Eq. (5). Thus, including Eq. (A.11) in Eq. (A.10) we have found the Eq. (4).

We followed the same way to find the heavy particle energy. We add the energy equations (Eq. (A.9)) for each heavy particle type (ions and neutral excited atoms), we replace U_j by $U + u_j$ and we neglected second order terms because u_j is small in comparison with velocities of other species. We used again $n_\mathrm{H} U_\mathrm{H} = -n_\mathrm{H^+} U_\mathrm{H^+}$ and the polarization electrostatic field law. For the collision term, we do the same kind of computation that in the electron energy equation. We take into account the exchange of heat linked with elastic collisions between heavy particles and electrons ($-Q_\mathrm{elc}$). We used $u_\mathrm{H^+} = u_\mathrm{e}$ and we neglected the heat created by the exchange of momentum between electrons and heavy particles. We also assume that heavy particle mass is high enough and that the inelastic collisions terms are only in the electron energy equation. With all these approximations, we get the heavy particle energy equation (Eq. (6)).

Appendix B: Computation of ambipolar diffusion coefficients

In this appendix, we give all coefficients necessary to compute the ambipolar diffusion velocity (Eq. (10)). These coefficients were given earlier by Conrad & Schunk (1979) but for the oxygen gas. Here, we have computed the ambipolar diffusion velocity for an hydrogen gas and with the assumption that the ions temperature is equal to that of neutral atoms ($T_\mathrm{H^+} = T_\mathrm{H} = T_\mathrm{a}$). The ordinary and thermal ambipolar diffusion coefficients can be computed with

$$\Delta_\mathrm{H^+H} = \frac{Z_\mathrm{H^+H}}{2n_\mathrm{H^+}kT_\mathrm{a}}\left(R_\mathrm{H^+H} + \frac{n_\mathrm{H^+}}{n_\mathrm{H}} R_\mathrm{HH^+}\right) \tag{B.1}$$

$$w = \frac{Z_\mathrm{H^+H}}{4}\frac{\nu_\mathrm{H^+H} m_\mathrm{H}}{n_\mathrm{H^+}k^2 T_\mathrm{a}}\left(K_\mathrm{H^+H} - \frac{n_\mathrm{H^+}}{n_\mathrm{H}} K'_\mathrm{H^+H}\right) \tag{B.2}$$

$$w^\star = \frac{Z_\mathrm{H^+H}}{4}\frac{\nu_\mathrm{H^+H} m_\mathrm{H}}{n_\mathrm{H^+}k^2 T_\mathrm{a}}\left(K'_\mathrm{HH^+} - \frac{n_\mathrm{H^+}}{n_\mathrm{H}} K_\mathrm{HH^+}\right) \tag{B.3}$$

$\Delta_\mathrm{H^+H}$, w and $w^\star$ have to be computed with

$$K_\mathrm{HH^+} = K_\mathrm{H^+H} = \frac{C_\mathrm{H^+H}}{H_\mathrm{H^+H}} J_\mathrm{H} \tag{B.4}$$

$$K'_\mathrm{H^+H} = -F_\mathrm{H^+H}\frac{J_\mathrm{H}}{H_\mathrm{H^+H}} \tag{B.5}$$

$$K'_\mathrm{HH^+} = -F_\mathrm{HH^+}\frac{J_\mathrm{H^+}}{H_\mathrm{HH^+}} \tag{B.6}$$

$$R_\mathrm{HH^+} = \frac{C_\mathrm{HH^+}A_\mathrm{H^+H} + F_\mathrm{H^+H}A_\mathrm{HH^+}}{H_\mathrm{HH^+}} \tag{B.7}$$

$$R_\mathrm{H^+H} = \frac{C_\mathrm{H^+H}A_\mathrm{HH^+} + F_\mathrm{HH^+}A_\mathrm{H^+H}}{H_\mathrm{H^+H}} \tag{B.8}$$

where

$$A_\mathrm{HH^+} = A_\mathrm{H^+H} = -\frac{5n_\mathrm{H}\, k\, T_\mathrm{a}\, \nu_\mathrm{HH^+}}{4} Z_\mathrm{HH^+} \tag{B.9}$$

$$F_\mathrm{HH^+} = -\frac{2}{5}Z''_\mathrm{HH}\nu_\mathrm{HH} - \nu_\mathrm{HH^+}\left[\frac{3}{4} + \frac{Z'_\mathrm{HH^+}}{4} + \frac{Z''_\mathrm{HH^+}}{5}\right] \tag{B.10}$$

$$F_\mathrm{H^+H} = -\frac{2}{5}Z''_\mathrm{H^+H^+}\nu_\mathrm{H^+H^+} - \nu_\mathrm{H^+H}\left[\frac{3}{4} + \frac{Z'_\mathrm{H^+H}}{4} + \frac{1}{5}Z''_\mathrm{H^+H}\right] \tag{B.11}$$

$$C_\mathrm{H^+H} = \frac{n_\mathrm{H^+}}{n_\mathrm{H}} C_\mathrm{HH^+} = \nu_\mathrm{H^+H}\frac{n_\mathrm{H^+}}{n_\mathrm{H}}\left[\frac{3}{4} + \frac{1}{4}Z'_\mathrm{H^+H} - \frac{Z''_\mathrm{H^+H}}{5}\right] \tag{B.12}$$

$$J_\mathrm{H^+} = \frac{n_\mathrm{H^+}}{n_\mathrm{H}} J_\mathrm{H} = \frac{5}{2}k^2\frac{n_\mathrm{H^+}T_\mathrm{a}}{m_\mathrm{H}} \tag{B.13}$$

$$H_\mathrm{HH^+} = H_\mathrm{H^+H} = F_\mathrm{H^+H}F_\mathrm{HH^+} - C_\mathrm{H^+H}C_\mathrm{HH^+} \tag{B.14}$$

where the momentum transfer collision frequency are given by

$$\nu_\mathrm{H^+H^+} = \frac{32}{3}\sqrt{\pi} n_\mathrm{H^+}\left(\frac{4kT_\mathrm{a}}{m_\mathrm{H}}\right)^{-\frac{3}{2}}\frac{e^4}{m_\mathrm{H}^2}\ln\Lambda \tag{B.15}$$

$$\nu_\mathrm{HH^+} = \frac{n_\mathrm{H^+}}{n_\mathrm{H}}\nu_\mathrm{H^+H} = \frac{8}{3}n_\mathrm{H^+}\Omega^{(1,1)}_\mathrm{HH^+} \tag{B.16}$$

$$\nu_\mathrm{HH} = \frac{8}{3}n_\mathrm{H}\sqrt{\frac{kT_\mathrm{a}}{\pi m_\mathrm{H}}}Q_\mathrm{HH}\,. \tag{B.17}$$

The average cross sections between neutral hydrogen atoms has been computed by Nowak & Ulmschneider (1977)

$$Q_\mathrm{HH} = 6.4539\times10^{-15} - 8.2913\times10^{-16}\ln T_\mathrm{a} + 2.3651\times10^{-17}\ln^2 T_\mathrm{a} \tag{B.18}$$

and where

$$Z_\mathrm{H^+H} = Z_\mathrm{HH^+} = 1 - \frac{2}{5}\frac{\Omega^{(1,2)}_\mathrm{H^+H}}{\Omega^{(1,1)}_\mathrm{H^+H}} \tag{B.19}$$

$$Z'_\mathrm{H^+H} = Z'_\mathrm{HH^+} = \frac{5}{2} + \frac{2}{5}\left[\frac{\Omega^{(1,3)}_\mathrm{H^+H} - 5\Omega^{(1,2)}_\mathrm{H^+H}}{\Omega^{(1,1)}_\mathrm{H^+H}}\right] \tag{B.20}$$

$$Z''_{\mathrm{H^+H}} = Z''_{\mathrm{HH^+}} = \frac{\Omega^{(2,2)}_{\mathrm{H^+H}}}{\Omega^{(1,1)}_{\mathrm{H^+H}}} \tag{B.21}$$

$$Z''_{\mathrm{HH}} = 2 \tag{B.22}$$

$$Z''_{\mathrm{H^+H^+}} = 2. \tag{B.23}$$

Finally, the Hydrogen collision integrals are given by

$$\begin{aligned}\Omega^{(1,1)}_{\mathrm{H^+H}} &= \sqrt{\frac{kT_{\mathrm{a}}}{\pi m_{\mathrm{H}}}}\Big(39.84B^2 - 17.85AB + 2A^2 \\ &\quad +(8.923B^2 - 2AB)\log T_{\mathrm{a}} + \frac{B^2}{2}\log^2 T_{\mathrm{a}}\Big)\end{aligned} \tag{B.24}$$

$$\begin{aligned}\Omega^{(1,2)}_{\mathrm{H^+H}} &= 3\sqrt{\frac{kT_{\mathrm{a}}}{\pi m_{\mathrm{H}}}}\Big(41.14B^2 - 18.13AB + 2A^2 \\ &\quad +(9.067B^2 - 2AB)\log T_{\mathrm{a}} + \frac{B^2}{2}\log^2 T_{\mathrm{a}}\Big)\end{aligned} \tag{B.25}$$

$$\begin{aligned}\Omega^{(1,3)}_{\mathrm{H^+H}} &= 12\sqrt{\frac{kT_{\mathrm{a}}}{\pi m_{\mathrm{H}}}}\Big(42.12B^2 - 18.35AB + 2A^2 \\ &\quad +(9.176B^2 - 2AB)\log T_{\mathrm{a}} + \frac{B^2}{2}\log^2 T_{\mathrm{a}}\Big)\end{aligned} \tag{B.26}$$

$$\Omega^{(2,2)}_{\mathrm{H^+H}} = 0.8\pi\sqrt{\left(\frac{2\eta e^2}{m_{\mathrm{H}}}\right)}. \tag{B.27}$$

For the hydrogen, $A = 2.1\times10^{-7}$ cm, $B = 2.2\times10^{-8}$ cm (Biolsi 1978) and the neutral atom polarizability that is approximately the atom's volume $\eta = 6.7\times10^{-25}$ cm^3 (Martin & Wiese 1996).

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