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Multicomponent Diffusion Coefficients of Atomic Hydrogen Plasma: Effects of Electronic Excited States and Magnetic Field

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Transport coefficients of equilibrium and non-equilibrium plasmas have been widely studied in these years due to their importance in determining the properties of high enthalpy flows. The relevant properties (thermal and electrical conductivity, viscosity, etc.) are usually determined by using higher order approximations of the Chapman-Enskog method applied to the mixture of electrons, ions and neutral species. The transport coefficients are functions of the local state of the plasma: pressure, temperature, composition and of the collision integrals that describe the interactions between the plasma constituents.

In particular, given the temperature and pressure, the composition can be obtained from the Saha equation if an equilibrium condition can be assumed or it is derived from a kinetic model of the plasma state.

Electronic excited states (EES) influence the plasma composition through the partition functions in the equilibrium case and through the collisional-radiative models under non-equilibrium conditions. On the other hand, EES do not appear in the equations for the transport coefficients of plasmas because of their low concentration. This common practice, however, underestimates the enormous increase of the transport cross sections of EES as a function of the principal quantum number. Small concentrations of EES can, in fact play an important role in affecting the transport coefficients of plasmas. This point has been recently emphasized by our group[1].

In the present work, we extend the previous calculations for atomic Hydrogen plasmas taking into account the presence of a magnetic field. Attention is devoted to the multicomponent diffusion coefficients that determine the transport of mass and of excitation and ionization energies. We show, in particular, that the H-H$^+$ diffusion

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[1] M. Capitelli, R. Celiberto, C. Gorse, A. Laricchiuta, P. Minelli, D. Pagano, *Physical Review E*, Vol. 66, 016403, 2002; M. Capitelli, R. Celiberto, C. Gorse, A. Laricchiuta, D: Pagano, P. Traversa, *Physical Review E*, Vol. 69, 026412, 2004.

coefficient, that controls the transport of ionization energy, strongly depends on the presence of EES due to resonant charge transfer processes in H(n)-H^+ collisions, the cross sections of which scale with the fourth power of the principal quantum number n. The presence of the magnetic field is shown to affect in a non-trivial way the dependence of the transport coefficients on the EES cross sections by inhibiting selectively the contribution of the electron component.

Transport coefficients for Hydrogen plasma have been obtained in the framework of the Chapman-Enskog method[2]. In order to properly account for the presence of EES, each electronic excited state of the Hydrogen atom, H(n), is considered as a separate species.

In addition, the possibility that the plasma be magnetized is considered in the calculations[2].

The composition and the populations of EES are obtained under a equilibrium assumption. Note however, that contrary to Ref. 1 in this work the two steps are consistently coupled by considering an effective maximum number of EES, determined by the Fermi cut-off criterion:

$$a_0 n_{\max}^2 < N^{-1/3} \tag{1}$$

The collision integrals for the relevant interactions among H(n), H^+ and electrons are the same used in our previous works[1]. They present a strong dependence on the principal quantum number especially for collision integrals diffusion type of H(n)-H^+ collisions. To show the role of the electronic excited states we will compare in the following the results obtained by considering the actual values of the transport coefficients ("abnormal") with those obtained by assuming the transport cross sections of EES equal to those of the ground state ("usual").

The multicomponent diffusion coefficients are defined by the following equation for the mass diffusion fluxes:

$$\mathbf{J}_{mj} = m_j \int \mathbf{C}_j f_j d\mathbf{c}_j = -\frac{\rho}{p}\frac{m_j}{m}\sum_k \mathbf{D}_j^k \cdot \mathbf{x}_k - \frac{1}{T}\rho_j \mathbf{D}_j^T \cdot \nabla T \tag{2}$$

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[2] J.H. Ferziger, H.G. Kaper, *Mathematical Theory of Transport Processes in Gases*, North Holland, Amsterdam, 1972.

where $\mathbf{x}_j = \nabla p_j - \frac{e_j}{m_j} \rho_j \cdot \left(\mathbf{E} + \mathbf{v} \times \mathbf{B} \right)$.

In the following, results are reported for the diffusion coefficient of atomic Hydrogen (including ground and electronic excited atoms) diffusing into protons. This coefficient is mainly determined by the resonant charge transfer cross sections; the latter increase roughly as n^4 with the principal quantum number. Figure 1 shows the parallel component of the diffusion coefficient $D_H^{H^+}$ (the one unaffected by the magnetic field) as a function of temperature for two pressures calculated with ("abnormal") and without ("usual") the consideration of different cross sections for the electronic excited states.

We wish to remind at this stage that, under the equilibrium assumption used in this work, the ionization degree of the plasma and the population of EES increase with the temperature; however, entropic effects prefer ionizing the system instead of exciting it. Since the first excited level of Hydrogen is 10.2 eV above the ground state, appreciable population of EES is attained only at high temperatures where, however, the ionization degree is significant. Higher pressures shift the ionization to higher temperatures where EES are more populated but the increase in pressure also means a decrease in the number of EES considered. Since the decrease in the number of EES is slower than the effect on the ionization equilibrium, increasing the pressure should enhance the effect of EES cross sections as already pointed out[1].

At relatively low temperature the "abnormal" diffusion coefficient follows the same curve as the "usual" one. After, the effect of EES becomes evident in strongly decreasing (in absolute value) the diffusion coefficient. An increase in pressure of a factor 100 corresponds to a decrease by the same order of magnitude of the diffusion coefficient in both cases. Note, however, that the differences between the two values for this coefficient, as obtained for a plasma at p=100atm, are larger up to a factor 5 than the corresponding values for the 1atm case.

Let us now analyze how the results discussed above are modified by the presence of the magnetic field. The parameter that governs the extent to which the magnetic field perturbs the results is the Hall parameter, β, that is a measure of the extent to which particle trajectories are perturbed by the Lorentz force. The components of the transport coefficients affected by the field experience the maximum effect when β (either β_e or β_{H+} or a combination of both) is of order 1 and tend to vanish when the magnetic field is high enough that the plasma becomes non-viscous. For the case under examination it is natural

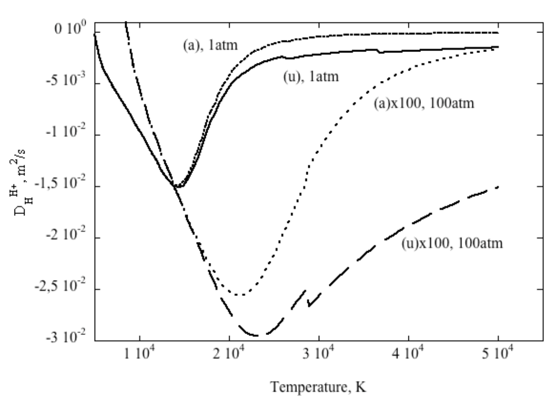

Figure 1. **Parallel component of the atom-proton diffusion coefficient as a function of temperature for the abnormal and usual cases at two pressures.**

to expect that the governing parameter should be the ion Hall parameter which is much smaller than 1 even at 1atm and with magnetic fields of several tesla. We should therefore expect the transverse component of the $D_H^{H^+}$ coefficient to be much smaller than the parallel component and to show, at fixed pressure and temperature, a monotonic increase with the magnetic field. In Fig. 2 this component of the $D_H^{H^+}$ coefficient is plotted as a function of the magnetic field strength for a plasma at 1atm and 50000K. The two curves report the results for the usual and abnormal coefficients, respectively. As expected, both curves increase as the magnetic field increases. As the electron Hall parameter becomes of order 1, however, the contribution due to electron collisions vanish and the effect is much stronger when the EES cross sections are taken into account. This is due to the fact, already mentioned, that H(n)-H$^+$ cross sections have a stronger dependence on principal quantum number than H(n)-e ones. It can also be noticed that the presence of EES cross sections slows down the effect of the magnetic field. This occurs since, for the same value of the magnetic field, the abnormal electron Hall parameter is smaller than the corresponding usual value.

Acknowledgments

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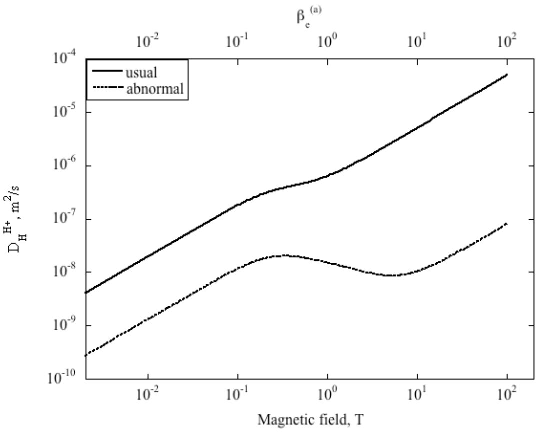

Figure 2. **Transverse component of the atom-proton diffusion coefficient as a function of the magnetic field for the abnormal and usual cases. Equilibrium Hydrogen plasma at *p*=1atm, *T*=50000K.**