

Effect of the vibrational relaxation in detached hydrogen plasma

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Introduction

The population of the vibrational states of hydrogen molecules in the edge plasma of fusion reactors is an important issue due to its influence on the volume recombination rate through the Molecular Activated Recombination (MAR) channels [1, 2]. The relation between the relaxation time of the vibrational levels and the residence time of the neutrals in the detached plasma region is essential for the determination of the excited states population. Provided that the relaxation time is much less than the residence time, collisional-radiative models (CRM) based on the quasi-steady state (QSS) approximation are standard tools to derive effective rate coefficients of collisional and radiative processes prior to the transport

simulation for the neutrals. In the opposite case the vibrational states have to be considered as distinct species in the transport code for the neutrals. In this work the relaxation times of the vibrationally excited hydrogen states are investigated under conditions expected in the linear divertor simulator Magnum-PSI [3]. As a comparison, plasma and neutral parameters representative for the detached divertor regime of fusion devices (ITER) are also considered. The linear device Magnum-PSI, that is currently being designed, is aimed at the study of plasma surface interaction in the strongly coupled regime characterized by large ion fluxes and the capture of particles released from the surface in the interaction region.

	Process
eV	$e + H_2(v) \leftrightarrow e + H_2(w)$
EV	$e + H_2(v) \rightarrow e + H_2(B^1\Sigma_u^+, C^1\Pi_u)$ $\rightarrow e + H_2(w) + h\nu$
VV	$H_2(v) + H_2(w) \leftrightarrow H_2(v-1) + H_2(w+1)$
VT	$H_2(v) + H_2 \leftrightarrow H_2(v-1) + H_2$ $H_2(v) + H \leftrightarrow H_2(v-\Delta v) + H$
eD	$e + H_2(v) \rightarrow e + H_2(b^3\Sigma_u^+, c^3\Pi_u, a^3\Sigma_g^+)$ $\rightarrow e + H + H$
eI	$e + H_2(v) \rightarrow e + H_2^+ + e$ $e + H_2(v) \rightarrow e + H^+ + H + e$
e-DA	$e + H_2(v) \rightarrow H^- + H$
e-E	$e + H_2(v) \rightarrow e + H_2(Y)$
CX	$H^+ + H_2(v) \rightarrow H_2^+(v') + H$

Table 1: Processes considered in the vibrational kinetics of the H_2 molecules

Vibrational kinetics

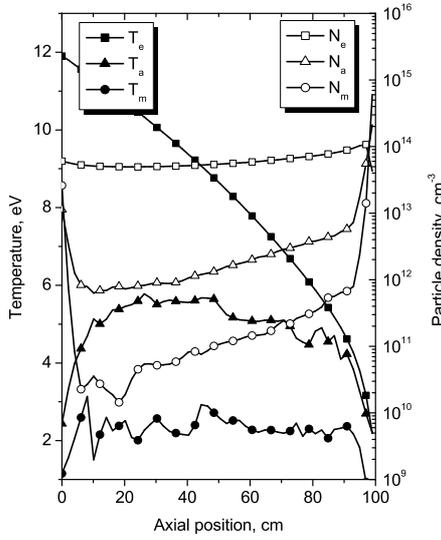


Figure 1: Axial distributions of the plasma and neutral parameters.

Processes The present study is based on the comprehensive model of molecular and atomic hydrogen [4], recently extended to consider the vibrational levels of several electronic states (X, B, E, C, a, b) as individual species. In order to obtain the temporal behavior of the population density of each state, a set of differential equations is solved. As a result, the relaxation times are evaluated and compared with the typical residence times. In what follows, a special attention is paid to the rate equations for the vibrational levels of the ground electronic state and the terms describing the vibrational kinetics are given. The temporal development of the population density of a vibrational level v in the ground state of the hydrogen molecule is described by the master equation written in the form [5]:

$$\begin{aligned} \frac{dN(v)}{dt} = & \left(\frac{dN(v)}{dt} \right)_{eV} + \left(\frac{dN(v)}{dt} \right)_{EV} + \left(\frac{dN(v)}{dt} \right)_{VV} + \left(\frac{dN(v)}{dt} \right)_{VT} \\ & + \left(\frac{dN(v)}{dt} \right)_{eD} + \left(\frac{dN(v)}{dt} \right)_{eI} + \left(\frac{dN(v)}{dt} \right)_{e-DA} + \left(\frac{dN(v)}{dt} \right)_{e-E} + \left(\frac{dN(v)}{dt} \right)_{CX} \end{aligned} \quad (1)$$

where the respective relaxation terms represent the energy exchange in the processes as summarized in Table 1. Because of the large electron density, the electron energy distribution is supposed to be Maxwellian for edge plasmas. H atoms effectively quench the $H_2(v)$ vibrationally excited states. Hence, if the lower vibrational states are populated mainly by electron impact and the population of the upper levels results from vibration-vibration (VV) exchange in competition with vibration-translation (VT) relaxation processes, the vibrational distribution of the molecular component could be of minor importance. However, in plasmas with high degree of ionization, the alternative mechanism of vibrational excitation through singlet electronic states can compete with the fast VT relaxation. As a result, the vibrational kinetics of the hydrogen molecules can persist even under conditions characterized by high atomic densities.

Vibrational population densities The temporal behavior of the vibrational population densities of the ground electronic state is calculated for various axial positions in MAGNUM-PSI using the plasma parameters (Fig. 1) obtained by B2-EIRENE simulations. The $H_2(v)$ densities after a steady-state has been established are presented in Fig. 2 for two axial positions (a) $y=0$

(plasma inlet) b) $y=99\text{cm}$ (target)). The relaxation times of the $H_2(v)$ densities are found to be $4.5\mu\text{s}$ and $100\mu\text{s}$ near the plasma inlet and the target, respectively. The corresponding residence times are significantly shorter ($\sim 0.1\mu\text{s}$ and $\sim 1\mu\text{s}$, resp.). Hence, the transport of the individual $H_2(v)$ is expected to be important. At the plasma inlet ($y = 0$), where the electron temperatures are high and the neutral densities are low, the population densities are dominated by EV-collisions. VV- and VT-collisions affect the last few vibrational levels. In front of the target ($y = 99\text{cm}$), the EV-collisions are significant for levels with $v > 5$. In this region, a weak effect of VV- and VT-collisions is also observed. In the detached plasma region in front of the target, the $H_2(v)$ densities can be well reproduced by the eV-collisions up to $v = 5$. Note that in the present version of the transport code in use (EIRENE) only this kind of vibrational excitation is accounted for.

Transport of vibrationally excited molecules

To study the effect of the vibrational relaxation in detached hydrogen plasmas, a Monte Carlo simulation of the neutrals with EIRENE is performed in two cases: 1) only the ground vibrational state is considered in the simulation. The densities of the upper levels are derived from the population coefficients as found by means of the CRM for given plasma parameters. 2) all vibrational levels are considered in the transport code as distinct species.

B2-EIRENE simulations in MAGNUM-PSI The simulation of plasma and neutrals is performed self-consistently, so that the effect of the transport of the $H_2(v)$

molecules on the plasma parameters has been considered. Fig. 3 shows the axial distribution of the total H_2 density and the population densities of the first three vibrational levels for both cases. The maximum total H_2 density decreases by a factor of ~ 2 when $H_2(v)$ are considered as distinct species in the Monte Carlo simulation. The maximum plasma density in front of the target decreases by $\sim 25\%$ and the atomic density by $\sim 40\%$. This results in lower particle sinks due to dissociation ($\times 1.2$), ionization ($\times 1.2$), molecular ($\times 5.5$) and 3-body atomic recombination ($\times 1.7$).

EIRENE simulation in ITER In this case the simulation is performed with a fixed plasma background. The results obtained show that the maximum particle sink due to molecular recom-

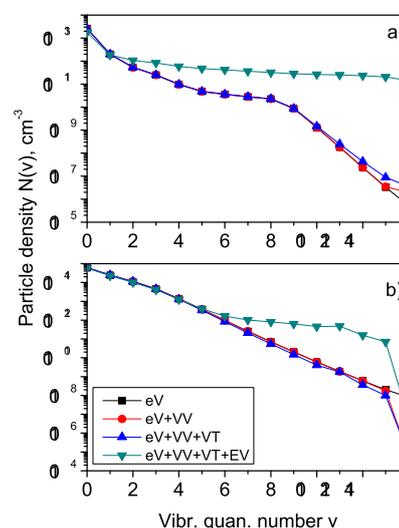


Figure 2: Stationary densities of the vibrational levels of H_2 .

bination increases by a factor of ~ 2 . The particle sink due to dissociation of H_2 molecules decreases by $\sim 20\%$ whereas the particle sink due to ionization increases by $\sim 10\%$.

Conclusion

In the detached plasma region, EV-collisions have a strong influence on the $H_2(v)$ densities for $v > 5$. In the cases under consideration, VV- and VT-collisions play a minor role. Therefore, the vibrational excitation of H_2 molecules is well reproduced even when accounting only for eV-collisions.

The relaxation times of the $H_2(v)$ densities being in the range $\sim (1 - 100)\mu s$ are longer compared to the typical residence times.

Therefore, the $H_2(v)$ have to be considered in the transport code as individual species. The results obtained show that plasma parameters and particle sinks due to recombination, dissociation, and ionization are affected due to the transport of the $H_2(v)$ molecules.

Acknowledgments

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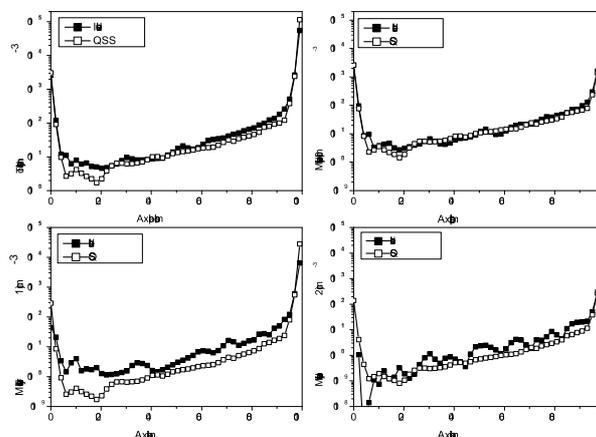


Figure 3: Axial distributions of the total molecule density and $H_2(v)$ density ($v = 0 - 2$).