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Section 5. Plasma fueling, recycling and tritium recovery

Hydrogen molecules in the divertor of ASDEX Upgrade

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Abstract

In order to reduce the power load onto the target plates detached divertor conditions are often preferred. These are characterized by volume recombination, i.e. three-body and radiative recombination. Due to low T_e (few eV) hydrogen molecules can penetrate into the plasma and may play a role in divertor dynamics. In particular, it was suggested, that molecules may assist the volume recombination process. The role of molecules in the divertor is examined here by a combination of experimental results with plasma edge simulations (B2-EIRENE) and a collisional-radiative model for hydrogen molecules. Spectroscopic diagnostics of the Fulcher transition carried out at the divertor of ASDEX Upgrade yield estimates of molecular hydrogen fluxes and the vibrational population in the ground state in detached and attached hydrogen plasmas. Good agreement with B2-EIRENE is achieved only if vibrational levels are treated as distinct (metastable) particles in the model and if the collisional-radiative model is applied to the electronically excited levels. On this basis the contribution of molecules to plasma recombination was determined to be in the order of a few 10%. The dominant molecular process is the dissociation process via H_2^+. As a consequence initially detached divertor plasmas can even re-attach if vibrationally resolved molecules are properly included in plasma edge models. A set of B2-EIRENE calculations carried out for ASDEX Upgrade is discussed. In particular the threshold upstream density for detachment was found to be up to a factor 1.5 higher than that originally expected due to these molecular effects. The transferability of the results to deuterium will be discussed.

Keywords: ASDEX-Upgrade; B2EIRENE; Collisional-radiative model; Divertor detachment; Divertor spectroscopy; Hydrogen; Volume recombination

1. Introduction

In present-day fusion experiments the power load to the target in the boundary layer and in the divertor is often reduced by radiation cooling, which leads to lower plasma temperatures. Especially in detached divertor conditions the hydrogen molecules produced at the surfaces by recombining atoms and ions can penetrate into the plasma and may affect plasma dynamics. These detached divertor plasmas are characterized by an increase in electron density and decrease in electron temperature such that the plasma flux drops with increasing upstream density ('roll-over'). This is typically accompanied by a strong increase of volume recombination. Due to the low T_e (0.5–5 eV) of these plasmas molecules survive conventionally discussed dissociation and ionization processes quite long. They can, therefore, undergo other, even resonant, reactions. The molecular assisted recombination (MAR) is one such effect in detached divertor conditions. Here vibrationally excited molecules ($H_2(v)$, $D_2(v)$) contribute to plasma volume recombination due to the following chains of reactions:

$H_2(v) + e \rightarrow H^- + H$	dissociative attachment followed by
$H^- + H^+ \rightarrow H + H^*$	mutual neutralisation

and

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$H_2(v) + H^+ \rightarrow H_2^+ + H$ ion conversion followed by

$H_2^+ + e \rightarrow H + H^*$ dissociative recombination.

In each channel an electron–ion pair is recombined into a H-atom and the molecule is dissociated. Inspecting the rate coefficients for these reactions, the ion conversion channel dominates over the negative ion channel [1,2]. Under the assumption of radiative decay of all excited atoms the amplification of volume recombination was predicted to be in the range of a factor of 30 [2,3]. However, considering both re-ionization of the electronically excited state (H^*) and decay into the ground state the recombination enhancement factor was found to be much smaller (2–3) [1]. In any case it was speculated that, e.g., for an ITER size machine, the presence of hydrogen molecules might assist detachment and lead to somewhat relaxed upstream conditions for achieving detachment. However, a detailed bookkeeping of atomic-, molecular-, surface- and transport processes has only now become possible in plasma edge codes. For this purpose a treatment of vibrationally resolved molecules is included in one of these codes. With this extension the role of molecules on divertor dynamics can now be discussed quantitatively and in more detail.

As a starting point for such assessments results from the plasma edge model (B2-EIRENE [4]) are compared with experimental results from ASDEX Upgrade, particularly with regard to hydrogen molecules. A spectroscopic method [5,6] for measuring hydrogen molecular influxes and especially the vibrational population from the radiation of the H_2 and D_2 diagonal Fulcher bands ($d^3\Pi_\mu \rightarrow a^3\Sigma_g^+$) in the divertor plasma of ASDEX Upgrade was applied. The interpretation of radiation was supported by a collisional-radiative model [7,8]. An experimental campaign of hydrogen discharges with both detached and attached divertor conditions was started. The B2-EIRENE calculations reported here were initially carried out for pure plasma conditions, with effects from impurities taken into account only implicitly via the boundary conditions. However the vibrational levels of H_2 are treated as distinct particles in the EIRENE code, a modification made necessary as compared to earlier versions by an assessment of the vibrational relaxation times vs. transport times under the relevant plasma conditions. In addition, the rates from a collisional-radiative model for the electronically excited levels were used. With these modifications of the code line-of-sight integrated and spatially resolved results have been obtained.

2. Diagnostics and calculations

In the following a more detailed discussion of the reaction chains, especially the ion conversion chain, is given. The excited atom at the end of either channel has several possibilities leading to a distinction into three processes:

MAR :	$H_2(v) + H^+ \rightarrow H_2^+ + H$	and	$H_2^+ + e \rightarrow H + H$	Molecular Assisted Recombination
MAD :	$H_2(v) + H^+ \rightarrow H_2^+ + H$	and	$H_2^+ + e \rightarrow H + H^+ + e$	Molecular Assisted Dissociaton
MAI :	$H_2(v) + H^+ \rightarrow H_2^+ + H$	and	$H_2^+ + e \rightarrow H^+ + H^+ + 2e$	Molecular Assisted Ionization

Only MAR contributes to recombination, whereas in the other two cases ions are produced, effectively leading to an increase of potential energy, quite opposite of true volume recombination. In Fig. 1 a comparison of the rate coefficients of MAR and MAD is presented with the electron density as parameter. Rate coefficients for MAI are considerably smaller and are therefore not included. MAD increases slightly with density and is always higher than MAR, which, instead, shows a steep decrease with higher densities. For detached plasma conditions, i.e. high densities and low temperature, these two rate coefficients (and also the rates themselves) differ by one or two orders of magnitude. Not only is MAR much smaller than without accounting for re-ionization of the excited fragments, more importantly the very large MAD rate coefficients lead to a rapid destruction of H_2, which, hence, is not available for MAR to happen any more. In order to obtain rates for these processes the knowledge of hydrogenic densities and vibrational populations is necessary. The latter play an important role in ion conversion due to the resonance with the $v = 4$ level of hydrogen.

For the purpose of getting a deeper insight into these various competing processes the treatment of molecules in the plasma edge model, i.e. in B2-EIRENE together

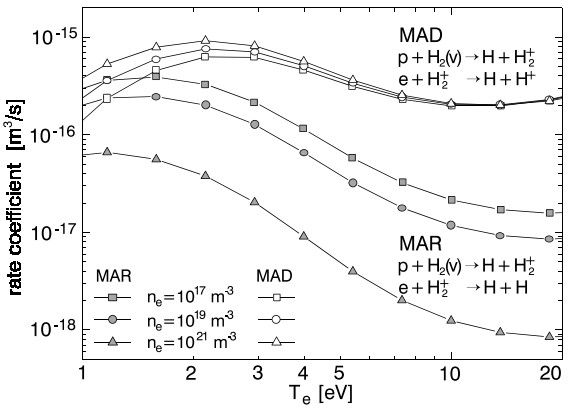

Fig. 1. Rate coefficients for molecular assisted recombination and dissociation.

with the collisional-radiative model, was checked by a comparison with the experimental data. Therefore measurement of molecular hydrogen fluxes and vibrational populations [5,6] have been performed. The emission of the Fulcher band was measured by means of a 1m spectrometer and a CCD camera providing a spectral resolution of 0.05 nm. Spatial resolution was achieved by a fibre-optical system using only the poloidal lines-of-sight (LOS). In contrast to the method described in [5,6] a vibrational temperature in the ground state was no longer assumed. The method was improved by using the vibrational populations from the collisional-radiative model matched to the experimental data. The spectroscopic method gives reliable results up to $v = 4$, for higher v it becomes insensitive due to the low population of those highly excited states. The vibrational distribution predicted by the collisional-radiative model is a function of T_e, which can thus be derived from the measured spectra. Because of the line-integrated measurements the determined T_e is the temperature in the plasma region, weighted where the molecular radiation originates. The knowledge of this value is important to determine the fluxes from the radiation of the band. The calculated numbers of ionization and dissociation processes per emitted Fulcher photon show a steep T_e dependence [5]. In addition, this ratio depends upon n_e and the vibrational population.

The investigations were carried out in hydrogen discharges at ASDEX Upgrade with a density and power ramp in L-mode. The divertor plasma moves from an attached state to a detached state and, with decreasing density and power, again to an attached state. The plasma parameters in the outer divertor region, as measured by probes, were $T_e = 5$–15 eV, $n_e \approx 4 \times 10^{19}$ m^{-3}. For the completely detached plasma phases the analysis of the Paschen and Balmer continuum radiation [9] resulted in T_e between 1 and 10 eV and n_e about 2–5×10^{20} m^{-3}. Results for the hydrogen molecular influxes as a function of time and LOS are shown in [5]. In order to achieve sufficient intensity, the measured spectra were integrated over time intervals of 0.5 s, thus representing average values for the respective time windows. The molecular flux increases with time, reaching a maximum in the detached interval with $\Gamma_{H_2} = 1.5 \times 10^{22}$ m^{-2} s^{-1}, here being in the same order as the atomic flux ($\Gamma_H = 4$–8×10^{22} m^{-2} s^{-1}). As the measurements demonstrate [5], the detached plasma is characterized by high molecular fluxes and high vibrational populations corresponding to a vibrational temperature of approximately 9000 K. The total intensity of the Fulcher system was compared directly with B2-EIRENE predictions using the electron impact emission rate coefficient. The relevant section of the computational domain of the code and the LOS used are shown in Fig. 2. On the basis of the consistent numerical solution e.g., for the molecular densities and electron temperatures, line-of-sight integrated Fulcher intensities were also calculated, directly applicable to the present experimental data. The calculated Fulcher emission was, initially, more than one order of magnitude (a factor 50) above the measured values [5]. This discrepancy can now be explained by considering the steep n_e dependence of the Fulcher emissivity rate coefficient calculated with the collisional-radiative model. Taking into account this dependence and making some improvements by considering vibrationally resolved rate coefficients for dissociation and excitations in the original collisional-radiative model [10] satisfactory agreement between measured and calculated Fulcher photon fluxes can be achieved (Fig. 3). The B2-EIRENE calculations were carried out for typical plasma discharges with a detached and an attached divertor, initially without explicit treatment of impurities. As Fig. 3 demonstrates, the calculations without accounting for vibrational states in H_2 lead to an enhancement of a factor 2–3. Including the vibrational levels as particles and testing the influence of various wall effects, the results are very robust in both plasma phases. The different wall effects distinguish between

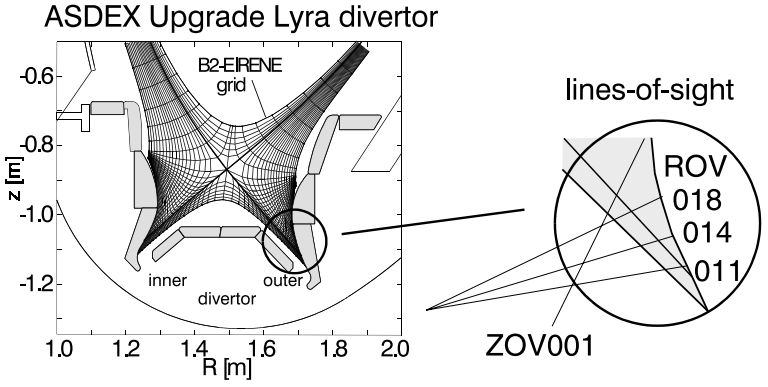

Fig. 2. Divertor geometry with the grid of the B2-EIRENE code and lines-of-sight used in measurements.

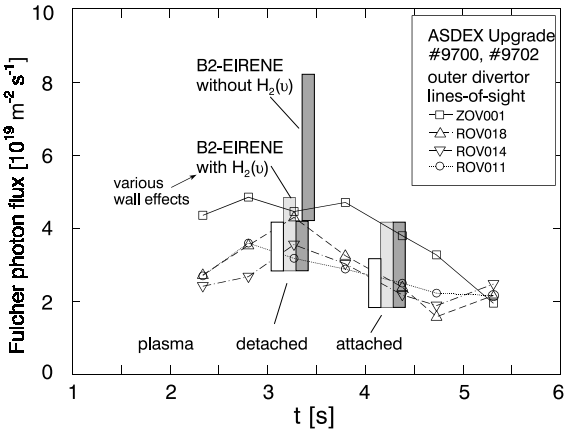

Fig. 3. Comparison of measured and calculated Fulcher photon fluxes for hydrogen discharges.

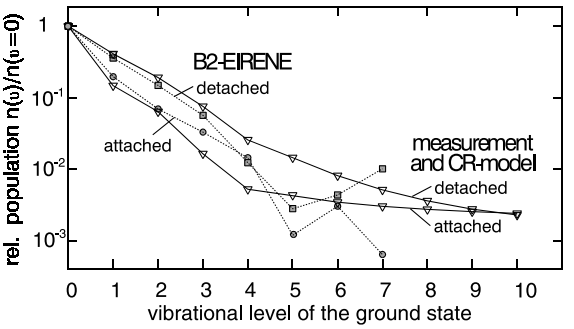

Fig. 4. Vibrational population in the ground state of hydrogen in detached and attached plasmas.

various vibrational populations of H_2 originating from recombination of particles at the wall. A detailed description is given in [10]. Fig. 4 gives a comparison of the vibrational populations in the ground state of the molecule for the detached and the attached case. Here, again, a good agreement is achieved, both methods reaching higher populations in the detached plasma than in the attached plasma phase. This indicates that vibrational populations have to be taken into account both in spectroscopic rate coefficients and in plasma edge simulations. The agreement between measurements and B2-EIRENE calculations may be taken as a first indication for a correct treatment of molecules in the code and especially for the validity of the collisional-radiative approximation for electronically excited states.

3. Results

On the basis of the overall confirmation of calculations with measurements a more detailed analysis of the

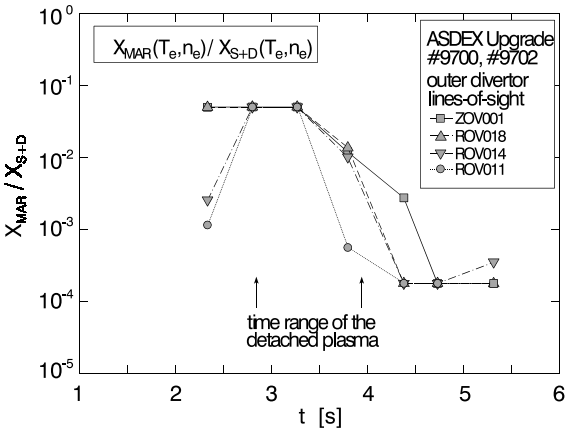

Fig. 5. Contribution of molecules to recombination.

various processes was carried out. In Fig. 5 the ratio of rate coefficients for molecules which contribute to recombination to those molecules which are destroyed by ionization and dissociation processes is given. The plasma parameters as T_e and n_e are taken from experimental data, whereas the dependence of the rate coefficients from T_e, n_e and the vibrational population originates from the collisional-radiative model. In the detached time range the contribution of molecules to recombination is in the order of a few percent and in the attached phase below 1%. This clearly confirms the picture that the molecules dissociate (MAD) and ionizate (MAI) before they have a chance to contribute to recombination (MAR). In order to get spatially resolved rates for the processes along a line-of-sight and a direct comparison with the three-body and radiative recombination R^{3+r}, B2-EIRENE data were evaluated in detail. The results are given in Fig. 6, where in the upper part of the figure the calculated densities n_e, n_{H_2} and n_H are shown together with the temperature necessary to form rates. The dependence of the molecular and atomic densities is clearly correlated with the temperature shape. In the regions of low T_e and near the surface the molecular density dominates over the atomic density until the molecules dissociate, leading to a strong decrease of n_{H_2} further inward. The atomic density is stable due to the gain from the molecules until ionization occurs. The calculated rates, i.e., processes per volume and time, for MAR, MAD and MAI are shown in the lower part of Fig. 6 and can be directly compared with the volume recombination R^{3+r}. The three-body and radiative recombination rate is nearly constant along the plasma volume whereas the MAD and MAR strongly decrease away from the divertor walls. This is due to the combination of high electron temperature and low molecular density. Again, the process of MAD dominates the molecular reaction chains. Only in a very thin layer near the walls can the molecules contribute to the plas-

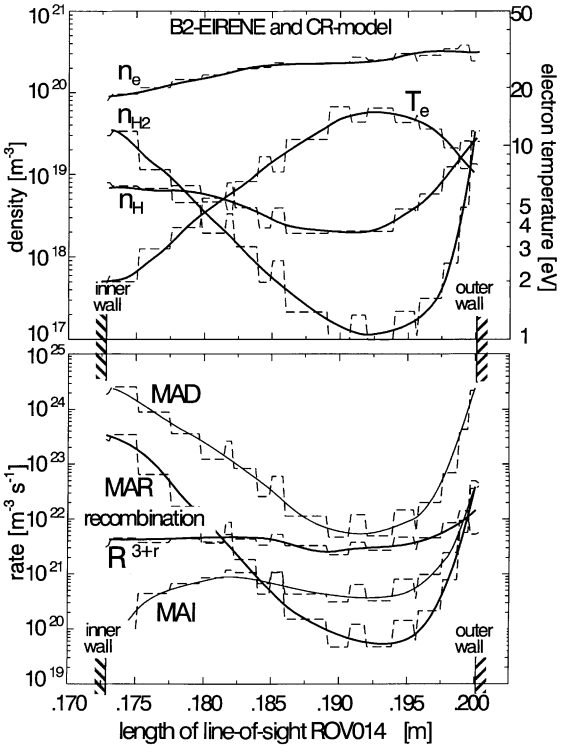

Fig. 6. Spatially resolved densities and rates for molecular enhanced recombination (MAR), dissociation (MAD) and ionization (MAI) in comparison with three-body and radiative recombination.

ma recombination. This leads to a 10% effect, corroborated by the interpretation of the measurements plotted in Fig. 5.

As mentioned above the reaction chains for the molecules lead to an increase of dissociation and ionization, in particular reducing the ionization length of the particles. As a consequence, the potential energy stored in the divertor plasma increases, the plasma reattaches.

These conclusions can also be derived from comparing the B2-EIRENE runs with and without full (vibrational) treatment of the molecules.

Starting point was a detached divertor plasma, resulting from B2-EIRENE with its conventional treatment of molecules, i.e., without accounting for vibrational excitation. Turning to the full treatment of molecules, with otherwise identical model parameters everywhere, lead to re-attachment of the divertor plasma into a moderately high recycling regime. In order to recover the initial detached state a ramp up of the midplane density was carried out. The outer target profile is plotted in Fig. 7 with the midplane density as input parameter in the calculations. First, the decrease of the divertor density is demonstrated by a comparison

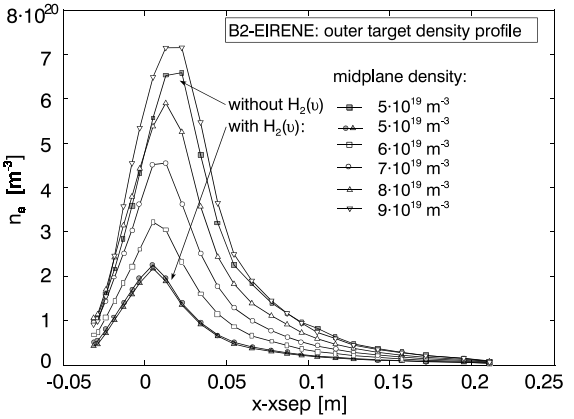

Fig. 7. Outer target density profile from B2-EIRENE calculations with and without vibrationally resolved molecules.

of the results at a density of 5×10^{19} m^{-3} with and without molecules. Increasing the density at the SOL, the starting point is recovered again only after an enhancement in the upstream density by a factor of at least 1.5.

One might speculate that the effect may be somewhat weaker, quantitatively, if impurities are explicitly taken into account as well and hence the whole burden of achieving detachment is not only on the hydrogenic species. However, the trend remains, as the first multifluid B2-EIRENE runs for the same conditions have now confirmed. This will be described next.

These other series of calculations have now been carried out, explicitly including carbon atoms and ions as impurity species. Chemical erosion is accounted for as an effective carbon-atom source in addition to the physical sputtering term. Experimental carbon radiation profiles have carefully been matched by the code. The results of calculations with the original model for hydrogen molecules have already been published [11]. They are discussed there with respect to the combination of detachment and occurrence of flow reversal. In addition, the diagnostic method for verification of flow reversal is introduced there and measurements are carried out for the same hydrogen discharges as considered above. The first analysis of this identical model case, but with proper account for the effects of vibrationally excited molecules, gives the similar results as the calculations for pure plasma conditions described above. The plasma reattaches after activating the vibrational excitation of H_2 (and resulting resonances) in the code. In addition the predicted parallel velocity shows a somewhat weaker flow reversal for CIII as compared to the case with the conventional model for H_2. In the pure plasma case mentioned above the flow reversal at the inner target has disappeared entirely after turning to the more complete treatment of molecules and re-attachment.

4. Isotope effect

Regarding the D_2 isotope the number of vibrational levels involved increases and the levels are energetically lower and closer. The potential curves and electronic states are the same as in H_2. The first point of interest is the vibrational population of D_2 in electronic ground state in comparison to H_2 at the same plasma conditions. Measurements were carried out in laboratory plasmas (ECR discharge) and give very similar populations of the levels leading to a lower vibrational temperature for D_2 [6]. The dependencies of electron temperature and pressure were found to be comparable. In order to verify these results for divertor plasmas hydrogen was puffed into deuterium discharges at ASDEX Upgrade. The LOSs viewing directly onto the divertor valve detect radiation of hydrogen, whereas another set of LOSs has the same poloidal view but in the next sector detecting deuterium. In the first step the population was assigned a vibrational temperature. During the time of the H_2 puff the derived temperatures are $T_{vib} = 4000$ K for D_2 and $T_{vib} = 5500$ K for H_2 both with an error of 500 K, representing a very similar population of the first five levels. With increasing density and power of the discharge T_{vib} of D_2 reaches 6000 K. Detailed results and a comparison of isotopes are given in [12]. As a consequence, the rate coefficients for example of ion conversion or dissociative attachment which are resonant with the vibrational level $v = 4$ for H_2 will be shifted to $v = 6$ for D_2. Due to the lower population of $v = 6$ this is likely to result in a reduced number of ion conversion processes. Ultimately for getting better information the current collisional-radiative model for H_2 has to be translated to D_2. The vibrational energies and selected rate coefficients have to be changed but the database is rather scarce. As the next step calculations and experimental results for deuterium discharges have to be compared, followed by a detailed interpretation in order to be able to make a statement about the transferability to other isotopes, in particular the fusion reactor relevant DT isotope.

5. Conclusions

In order to investigate the role of molecules in divertors and especially in detached divertor plasmas an experimental campaign at ASDEX Upgrade has been carried out. Spectroscopic diagnostic methods allow the measurements of hydrogen fluxes and of the vibrational population in the ground state for the first five levels from the radiation of the Fulcher transition. The interpretation of the radiation was supported by a collisional-radiative model for hydrogen molecules. This combination leads to a diagnostic for the electron temperature in the plasma region where the radiation originates. On the basis of this temperature the precise ratio of ionization and dissociation processes per emitted photon could be used for the determination of hydrogen fluxes. These molecular fluxes are in the detached case comparable with the atomic fluxes. The vibrational population in the detached case is significant, only 45% of the molecules are in the ground state. In attached plasmas the vibrational population is smaller which is due to higher T_e. These experimental results have been used for a comparison with the B2-EIRENE calculations. In the EIRENE code the vibrational levels have been implemented as distinct particles. The direct comparison was carried out for the Fulcher photon fluxes which could be calculated from the code using the collisional-radiative model for hydrogen as well. In addition, various wall effects (recombination of atoms and protons at the surface into various vibrationally excited levels) have been tested. The results of the code are very robust against these details. Nevertheless, a good agreement could be achieved only by including the molecules vibrationally resolved in the code and by simultaneous usage of the collisional-radiative model. After these considerations the reaction chains and especially the rates for molecular assisted processes could be determined precisely. It turned out that the molecular assisted dissociation (MAD) dominates always over the MAR. Spatially resolved results demonstrate that molecular densities are comparable to atomic densities only in a small layer near the divertor walls. A direct comparison with the volume recombination rate, i.e. three-body and radiative recombination, gives a contribution of molecules to recombination in these plasma regions. The effect in the plasma volume is more or less an effect of a few 10%. Instead of the predicted contribution of molecules to recombination the molecules dissociate and 'assist ionization'. As a consequence even initially detached plasmas can re-attach due to molecular effects. In other words, the B2-EIRENE results show that, for ASDEX Upgrade, detachment is harder to achieve with vibrationally excited molecules taken into account in the EIRENE code than without. To recover detachment an increase of the midplane density of a factor 1.5–2 was necesssary. However, most of the calculations have been carried out for pure plasma conditions. The effects of impurities must also be taken into account. This can lead to a somewhat reduced effect but the same trend is found so far. For interpretative plasma edge modelling including these molecular effects may lead to modified conclusions about the other model parameters (in particular: anomalous transport). For predictive plasma edge modelling, e.g. ITER calculations, this effect may be of importance for the threshold of upstream parameters for detachment.

Concerning the isotopes of H_2 it has to be kept in mind that quantitative predictions may be different for hydrogen and deuterium. First investigations have been

presented, which yield quite similar populations of the vibrational levels. But, as a consequence of the energetically lower lying levels such processes as ion conversion or dissociative attachment will be resonant to higher vibrational levels in deuterium as in hydrogen. Together with the lower population the rates may be estimated to be smaller. For a full treatment of these effects the collisional-radiative models have to be translated to deuterium by replacing the vibrational levels and some selected rate coefficients. However, the database is rather scarce. By performing a direct comparison of deuterium with hydrogen the isotopic relations have to be critically reviewed in order to get information about scaling laws for the other isotopes as T_2 and HD, DT molecules.

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