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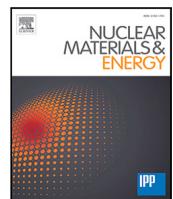
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Demonstrating the impact of ro-vibrationally excited H₂ on divertor detachment via population modelling

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ABSTRACT

EDGE2D-EIRENE profiles characteristic for low recycling, high recycling and detached plasmas are postprocessed applying a vibrationally resolved collisional radiative (CR) model based on the Yacora solver to predict excited state densities and thus the molecular Lyman-, Werner- and Fulcher band emission intensities. These emission intensities are compared to predictions from the AMJUEL database standardly used in EIRENE. Lower Fulcher band and higher Lyman- and Werner band emission is predicted by the Yacora model in comparison to AMJUEL suggesting that inconsistent results from model based evaluation of measured spectra are expected depending on which model and molecular emission band is considered. The implications on detachment rate predictions are discussed.

1. Introduction

In future fusion devices as ITER reducing the heat load onto divertor plates through detachment is essential. Detachment is achieved at high-density operation, when energy exchange of plasma particles with neutrals enables volumetric recombination leading to a reduction in the plasma temperature in front of the target plate [1]. Both experiments [2] and simulations [3] have demonstrated that not only atomic, but also (ro-)vibrational excited molecular neutrals (e.g. molecular hydrogen H₂) are important in the detachment process via their molecular reaction rates (e.g. molecular assisted recombination (MAR)), as the excitation energy required for the respective reactions is reduced for ro-vibrationally excited levels. This work focuses solely on vibrational levels. The vibrational distribution of the electronic ground state $X^1\Sigma_g^+$ is usually determined indirectly through measurements of the vibrational levels of electronically excited states.

Collisional radiative models are suited to predict both electronically and vibrationally excited state densities (n_p) balancing (de-)populating processes for each state of interest ($p = p$ (electronic state i , vibrational level v)) in the form of rate equations depending on molecular reaction probabilities as input. A general form of the rate equation for H₂ is given by Eq. (1), whereby depending on the excited level under consideration, individual terms may equal zero (e.g. the second term

for vibrational levels of the electronic ground state):

$$\frac{dn_p}{dt} = \sum_{q>p} A_{qp} n_q - \sum_{q< p} A_{pq} n_p + n_e [\sum_{q\neq p} X_{qp} n_q - \sum_{q\neq p} X_{pq} n_p + (\alpha + \beta n_e) n_{H_2^+} - S_p n_p - D_p n_p] - C_p n_{H^+} n_p \quad (1)$$

The electron density n_e , proton density n_{H^+} , H₂⁺ density $n_{H_2^+}$, ground state density of H₂ ($n_{H_2} = n(X^1\Sigma_g^+, v = 0)$), the Einstein coefficients A_{pq} and the rate coefficients for electron impact (de-)excitation X_{pq} , radiative recombination α_p , collisional three-particle recombination β_p , electron impact ionization S_p , dissociative electron attachment D_p and proton charge transfer C_p are inputs for the CR model. Eq. (1) must be extended by additional terms, if additional processes are considered. The rate coefficients are typically derived from cross sections under application of the respective energy distribution function. Several repositories of such atomic and molecular reaction probabilities are available, whereby models applying different databases show strong differences in the model predictions of excited state densities [4]. If the model predicted emission is applied to derive the plasma parameters from measured spectra, obviously incorrect model predictions result in incorrect plasma parameters. This deviation may then be directly passed on to the estimation of the detachment rates (e.g. when using n_{H_2} to calculate MAR rates). In addition, assumptions are made for

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deuterium plasmas due to the lack of reaction data for hydrogen isotopologues. While the neutral kinetic Monte Carlo code EIRENE [5] utilizes the AMJUEL database [6], for this work a vibrationally resolved CR model for H_2 based on the Yacora solver [7] has been developed applying dedicated state-of-the-art reaction data (e.g. the fully quantum-mechanical molecular convergent close-coupling (MCCC) cross sections for electron impact excitation [8]).

Excited state densities (e.g. $d^3 \Pi_u(v)$) predicted from different models are compared in the form of molecular emission (e.g. Fulcher band emission) representing the product of the excited state densities with the respective Einstein coefficients. In this work post-processing of EDGE2D-EIRENE plasma parameter profiles of the characteristic phases during the detachment process are performed to compare the predicted emission intensities from AMJUEL and the vibrationally resolved Yacora model.

2. EDGE2D-EIRENE simulations for JET L-mode plasmas

The different plasma regimes during the transition into the plasma detachment of JET ITER-like wall (tungsten in divertor, beryllium in main chamber) L-mode plasmas ($I_p = 2.5$ MA, $B_t = 2.5$ T, $P_{core} = 1.1$ MW) with hydrogen as main plasma species and impurities of beryllium have been simulated for previous studies using EDGE2D-EIRENE [9] for varying electron densities at the outer midplane separatrix $n_e^{sep,omp} = 0.6 - 2.2 \cdot 10^{19} \text{ m}^{-3}$ [10]. Fig. 1 shows the total ion current to the low field side (LFS) target plate $I_{LFS,plate}$ (solid line) in comparison to Langmuir probe measurements from JET pulse number 91 284 (open circles). As stated in [11] while $n_e^{sep,LFS,mp}$ at which the predicted $I_{LFS,plate}$ peaks agrees with the measurements within the densities' uncertainty, the absolute value of $I_{LFS,plate}$ and its relative dependence on $n_e^{sep,LFS,mp}$ differ (e.g. calculations predict a reduction of $I_{LFS,plate}$ by a factor of 2–3 from its maximum with increasing $n_e^{sep,LFS,mp}$, while measurements show a corresponding reduction by a factor of 10). Within this work three cases with distinct $n_e^{sep,omp}$ representing the characteristic stages during detachment are utilized for further analyses (see Fig. 1): the low recycling ($n_e^{sep,omp} = 0.7 \cdot 10^{19} \text{ m}^{-3}$), the high recycling ($n_e^{sep,omp} = 1.3 \cdot 10^{19} \text{ m}^{-3}$) and the detached ($n_e^{sep,omp} = 2.0 \cdot 10^{19} \text{ m}^{-3}$) regimes. As an example Fig. 2 depicts 2D profiles of the molecular hydrogen ground state density (n_{H_2}), atomic hydrogen density (n_H), electron density (n_e) and electron temperature (T_e) in the divertor region calculated with EDGE2D-EIRENE for the high recycling plasma ($n_e^{sep,omp} = 1.3 \cdot 10^{19} \text{ m}^{-3}$). In this regime vibrationally excited molecules react with the plasma through MAR before electron-ion recombination becomes more efficient [2]. While EDGE2D predicts n_e and T_e , EIRENE calculates n_H and n_{H_2} on a grid encompassing the EDGE2D grid and the halo plasma region between the outermost EDGE2D grid edge and the implemented vessel wall. The EIRENE calculations show that n_{H_2} is larger than n_H in the area close to the divertor plates. The position of the X-point is determinable from the subfigure for T_e .

3. Molecular emission predictions

Among the most intense structures in H_2 radiation in the VUV range are the Lyman- (130–170 nm) and Werner bands (<130 nm) originating from (ro-)vibrational transition between the molecular states $B^1 \Sigma_g^+$ – $X^1 \Sigma_g^+$ and $C^1 \Pi_u$ – $X^1 \Sigma_g^+$ respectively. Since the $B^1 \Sigma_g^+$ and $C^1 \Pi_u$ states belong to the same multiplet system of molecular hydrogen as the ground state $X^1 \Sigma_g^+$, the (de-)excitation between them (by electron impact) is optically allowed and therefore highly probable. Due to the close coupling, spectroscopic analyses of vibrational levels of these electronically excited states enhance the evaluation of the vibrational distribution of the electronic ground state [12]. The Fulcher- α band (500–800 nm, with the most intense structure in 600–640 nm resulting from Q-lines of diagonal vibrational transitions) is often used for molecular spectroscopy in the VIS range originating from $d^3 \Pi_u$ – $a^3 \Sigma_g^+$

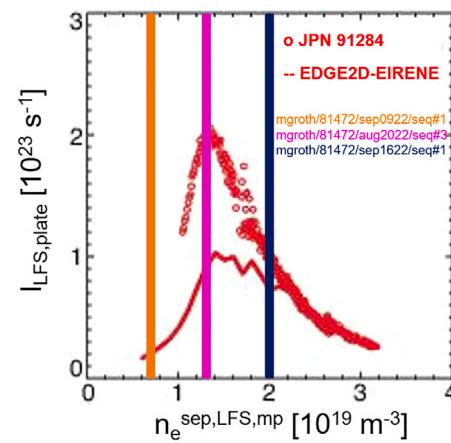


Fig. 1. Total ion current to the LFS target plate in dependence on n_e adjacent to the separatrix LFS midplane position stemming from measurements (JPN 91284) and EDGE2D-EIRENE calculations. The vertical lines indicate the plasma regimes for which the EDGE2D-EIRENE profiles are post-processed below: low recycling ($n_e^{sep,omp} = 0.7 \cdot 10^{19} \text{ m}^{-3}$), high recycling ($n_e^{sep,omp} = 1.3 \cdot 10^{19} \text{ m}^{-3}$) and the detached regime ($n_e^{sep,omp} = 2.0 \cdot 10^{19} \text{ m}^{-3}$). Figure adapted from [11].

transitions.

A more detailed description of the Lyman-, Werner- and Fulcher bands is given in e.g. [13]. Usually emission spectroscopy is not performed for both VIS and VUV at the same fusion experiment. To ensure that results derived from different devices are comparable, a model predicting consistently VIS and VUV emission is required.

In the EIRENE calculations the transport of vibrationally excited levels or electronically excited states is not modelled, but molecular effective rate coefficients from the AMJUEL database are applied, which have been derived from a pioneering CR model for H_2 (Sawada 1995) [14]. In the standard version of this model the electronic ground state is non-vibrationally resolved and for electronic states with main quantum number $n = 2$ (united atom limit) the states are resolved due to the projection of the orbital angular momentum onto the internuclear axis Λ . For some processes AMJUEL offers in addition effective rates from a modified version of the Sawada model with a vibrationally resolved electronic ground state ($H.2$ 3.2.3, $H.4$ 2.2.5 g). AMJUEL provides population coefficients \tilde{n}_p ($H.12$ 2.2.5fu, $H.12$ 2.2.5we, $H.12$ 2.2.5ly), from which the Lyman-, Werner- and Fulcher band emission (I_{pq}) is determined via $I_{pq} = A_{pq} \tilde{n}_p(n_e, T_e) n_{H_2}$. In Sawada 1995 electron impact excitation from the electronic ground state $X^1 \Sigma_g^+$ into the excited states $B^1 \Sigma_g^+$, $C^1 \Pi_u$ and $d^3 \Pi_u$ is based on semi-empirical cross sections from [15]. The model neglects the critical de-populating processes of dissociative electron attachment and proton charge transfer. Based on the Yacora solver several CR models for hydrogen aimed for different applications are available (e.g. a model for atomic hydrogen, an electronically resolved model for molecular hydrogen and a vibrationally resolved model for the electronic ground state of H_2 aimed to self-consistently calculate the vibrational ground state distribution (T_{vib}) [7,12,16]). The electronically resolved model for H_2 applies purely electronically resolved MCCC cross sections and includes several de-populating mechanisms (e.g. dissociative electron attachment and proton charge transfer). The MCCC cross sections are the most consistent data set available for electron impact excitation [8]. This electronically resolved model was compared to other input cross sections and validated for low-pressure plasmas (at electron densities up to $n_e = 3.3 \cdot 10^{16} \text{ m}^{-3}$) [12,16]. For this work a vibrationally resolved Yacora model has been developed including the same electronic states as the electronically resolved model. While the electronic states with $n \leq 3$ are resolved by the quantum number Λ in this model, the electronically excited states with $n = 4-10$ are neither vibrationally, nor Λ -resolved. Table 1 summarizes the reactions considered in the rate equations for

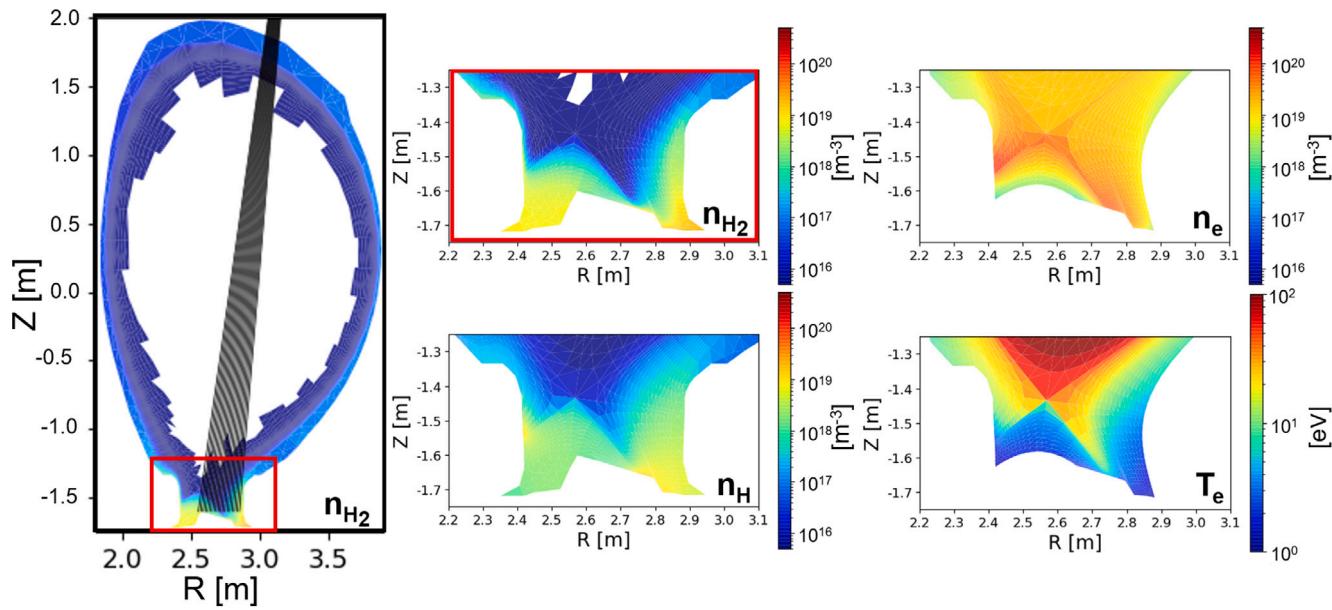


Fig. 2. Profiles for n_{H_2} , n_H , n_e and T_e simulated with EDGE2D-EIRENE for a JET ITER-like wall L-mode high recycling plasma ($n_e^{sep,omp} = 1.3 \cdot 10^{19} \text{ m}^{-3}$). The n_{H_2} overview figure also depicts synthetic lines of sight discussed later.

Table 1

Processes considered in the rate equations for the vibrational levels of the electronically excited states with initial vibrational level v of initial electronic state i and final vibrational level v' of final electronic state j .

Process	Reaction	Reference
Electron impact (de-)excitation	$H_2(i,v) + e^- \rightarrow H_2(j,v') + e^-$	[8,17]
Electron impact dissociation	$H_2(i,v) + e^- \rightarrow 2 H$	[8,17]
Spontaneous emission	$H_2(i,v) \rightarrow H_2(j,v') + h\nu$	[18]
Electron impact ionization	$H_2(i,v) + e^- \rightarrow H_2^+ + 2 e^- \text{ or } H + H^+ + 2 e^-$	[19]
Dissociative electron attachment	$H_2(i,v) + e^- \rightarrow H + H^-$	[20,21]
Proton charge transfer	$H_2(i,v) + H^+ \rightarrow H_2^+ + H$	[22]
Quenching	$H_2(d^3 \text{ or } a^1, v) + \bar{H}_2(X^1, v=0) \rightarrow 2 H_2(X^1, v=0)$	[23]

the (vibrational levels of the) electronically excited states and gives the sources for the applied input data (for processes involving the non-vibrationally resolved states $n \geq 4$ the sources are stated in section 4.2 of [16]). For the vibrational levels of the electronic ground state the following processes are considered (corresponding to the basic form of the $X^1(v)$ model from [16]): electron impact (de-)excitation, electron impact dissociation, dissociative electron attachment, proton charge transfer, electron impact ionization, radiative recombination and collisional three-particle recombination. The Yacora model of this work is applied to predict excited state densities, from which consequently the respective molecular emission is derived, through post-processing parameter profiles (n_e , n_{H_2} , n_{H^+} , $n_{H_2^+}$, T_e , T_{H^+}) obtained from the EDGE2D-EIRENE calculations.

Thereby, n_{H_2} is utilized for $n(X^1 \Sigma_g^+, v = 0)$. All excited level and state densities are determined by the Yacora model under the quasi-steady-state (QSS) approximation (e.g. setting the time derivative in the respective rate equation to zero). Consequently, the sum of all vibrational levels in the electronic ground state equals or exceeds n_{H_2} .

It should be noted that surface interaction processes (e.g. surface recombination) are not accounted for neither in the effective rates of AMJUEL nor the Yacora model, even though it was demonstrated that the vibrational ground state distribution is influenced by tungsten divertors [24].

The Yacora model generally predicts lower Fulcher band emission than AMJUEL. This is shown for 2D profiles of the Fulcher band emission calculated by both AMJUEL and Yacora for the high recycling plasma ($n_e^{sep,omp} = 1.3 \cdot 10^{19} \text{ m}^{-3}$) in Fig. 3.

To compare the spatially resolved emission predictions of the two models with measurements, synthetic lines of sight (LOS) in the form of

cones with finite etendue are introduced on the EIRENE grid pointing from the low-field side divertor towards the tokamak top half (respective orientations depicted in Fig. 2). The spatially resolved predicted emission is integrated along their respective LOS paths.

The Yacora model predicts LOS integrated about 2 times lower Fulcher band emission than AMJUEL for the low recycling plasma ($n_e^{sep,omp} = 0.7 \cdot 10^{19} \text{ m}^{-3}$) and about 5 times lower emission for the detached plasma ($n_e^{sep,omp} = 2.0 \cdot 10^{19} \text{ m}^{-3}$) (see Fig. 4). For the Lyman band the Yacora model predicts LOS integrated about 4 to 5 times higher emission than AMJUEL for all considered plasma cases. Furthermore, the Yacora model predicts LOS integrated about 1.7 times higher Werner band emission than AMJUEL for the low recycling plasma ($n_e^{sep,omp} = 0.7 \cdot 10^{19} \text{ m}^{-3}$) and up to 3.3 times higher emission for the high recycling plasma ($n_e^{sep,omp} = 1.3 \cdot 10^{19} \text{ m}^{-3}$).

The distinctly different emission intensities predicted by the two models are explained by different reaction probabilities for the same molecular processes in the two models and differing sets of processes considered in the respective models: The Yacora model applies MCCC cross sections for electron impact excitation from the ground state $X^1 \Sigma_g^+$ into the excited states $B^1 \Sigma_u^+$, $C^1 \Pi_u$ and $d^3 \Pi_u$, which are larger than the cross sections used in the Sawada 1995 model (e.g. see figure 6a in [16]). This increase in the rates would in itself result in larger Lyman-, Werner- and Fulcher band emission intensities. Dissociative electron attachment for electronically excited states is considered in the Yacora model via non-vibrationally, purely n -resolved constant rate coefficients from [20,21] ($X(n = 2) = 10^{-15} \text{ m}^3/\text{s}$, $X(n \geq 3) = 6 \cdot 10^{-11} \text{ m}^3/\text{s}$). For the $d^3 \Pi_u$ state it is among the most influential depopulating channels for high electron densities (e.g. $n_e \approx 10^{19} \text{ m}^{-3}$) causing despite the large electron impact excitation rate from the

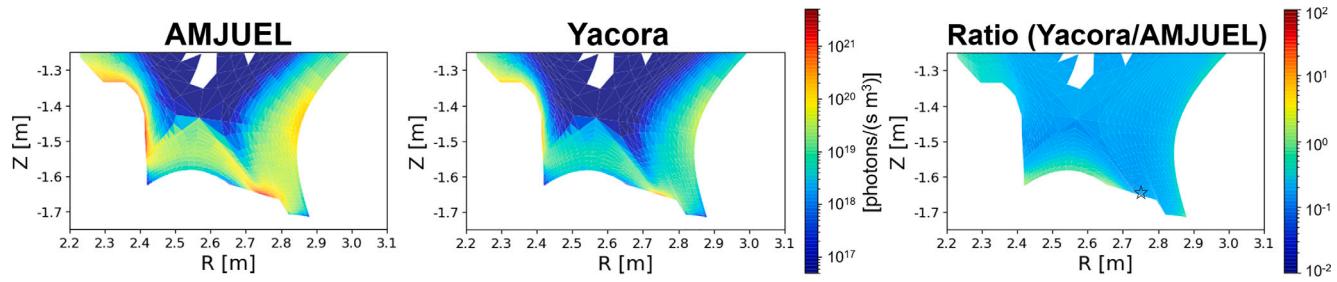


Fig. 3. Fulcher band emission predicted by AMJUEL (H.12 2.2.5fu) and the Yacora model and their ratio (Yacora/AMJUEL) for a high recycling plasma ($n_e^{sep,omp} = 1.3 \cdot 10^{19} \text{ m}^{-3}$). The star in the ratio profile marks the position for which additional Yacora model calculations are discussed below.

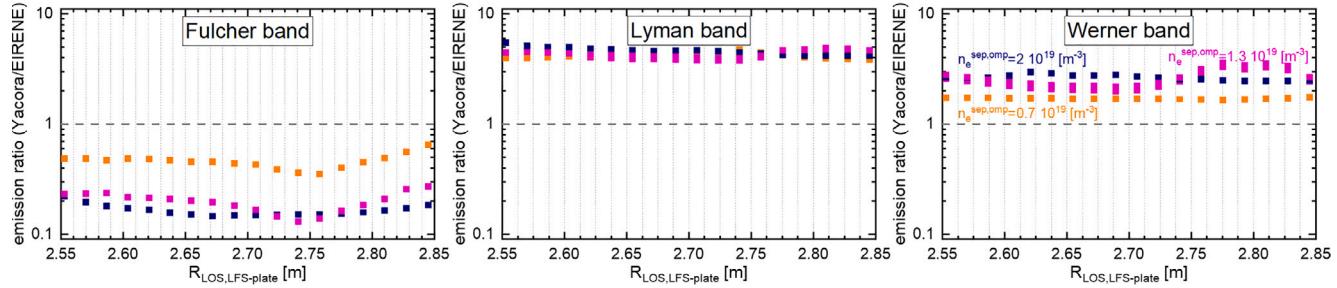


Fig. 4. Ratios of the predicted Fulcher-, Lyman- and Werner band emission between Yacora and AMJUEL (H.12 2.2.5fu, H.12 2.2.5ly, H.12 2.2.5we) integrated over the synthetic LOS directed to the LFS divertor.

ground state a lower $d^3\Pi_u$ density and thus lower Fulcher emission. Note that, since the electronically excited H_2 densities are low, not much H^- is produced. The extent to which dissociative electron attachment for electronically excited states reduces the $d^3\Pi_u$ density is demonstrated in Fig. 5 for the plasma parameters ($T_e = 4.3 \text{ eV}$, $T_H = 5 \text{ eV}$, $n_e = n_{H^+} = 5.9 \cdot 10^{19} \text{ m}^{-3}$, $n_{H_2^+} = 1.2 \cdot 10^{17} \text{ m}^{-3}$, $n_{H_2} = 9.9 \cdot 10^{18} \text{ m}^{-3}$) at the position marked in the ratio profile of Fig. 3: A model run without dissociative electron attachment for (vibrational levels of) electronically excited states results in $d^3\Pi_u$ densities increased by more than one order of magnitude. This large discrepancy underlines the importance for a benchmark with measurements, apart from the comparison of the model predictions. In addition, the $X^1\Sigma_g^+(v)$ densities are compared for a standard model run and a simulation, in which dissociative electron attachment for the ground state is deactivated, resulting in similar densities. As discussed in previous works (e.g. [22]), the dissociative electron attachment rate coefficients for excited states available in literature are controversially large. Since, to the authors knowledge, there are no other rate coefficients or cross sections available in literature, this data is included in both the electronically resolved Yacora model discussed above and the vibrationally resolved Yacora model from this work. For high electron densities the electron collision induced processes become more relevant, so that dissociative electron attachment for electronically excited states has a higher impact on the excited state population densities for divertor plasmas than for the low-density test cases discussed above. Deactivating test-wise dissociative electron attachment in the electronically resolved model leads to qualitatively similar consequences to those demonstrated here for the vibrationally resolved model. Dissociative electron attachment is not considered in the Sawada 1995 model at all (neither for the ground state, nor for electronically excited states) and consequently higher Fulcher band emission is predicted by AMJUEL compared to the Yacora model.

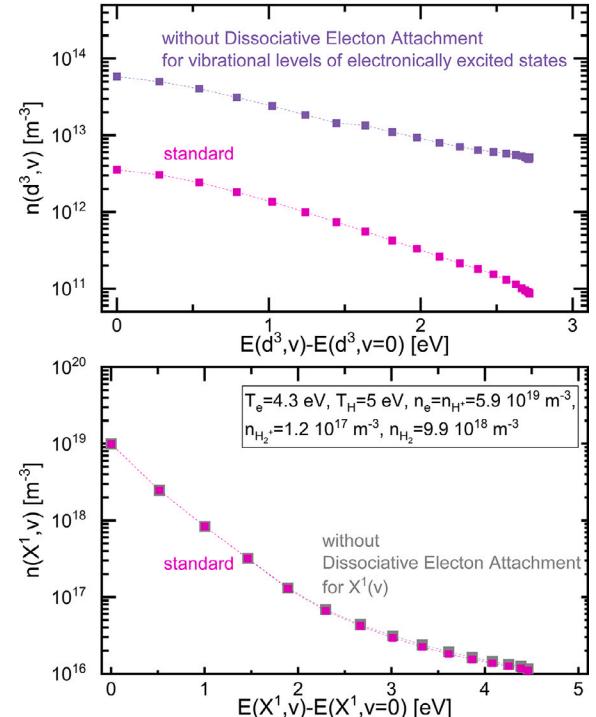


Fig. 5. $X^1\Sigma_g^+$ and $d^3\Pi_u(v)$ densities predicted from the vibrationally resolved Yacora model for the plasma parameters of a single grid cell of the high recycling plasma ($n_e^{sep,omp} = 1.3 \cdot 10^{19} \text{ m}^{-3}$) in a standard model run, a calculation without dissociative electron attachment for electronically excited states and a calculation without dissociative electron attachment for the vibrational levels of the electronic ground state.

4. Discussion

2D edge plasma transport codes coupled to neutral gas models (e.g. such as EDGE2D-EIRENE) are widely used for studying edge plasma phenomena, for the interpretation of experimental data and for the prediction of edge plasma parameters [25]. This is particularly relevant for H₂, if model predicted emission is used to derive from measured spectra the ground state density n_{H₂}. Inconsistent results are to be expected depending on which model and molecular emission band is used. Furthermore, the AMJUEL predicted Fulcher band emission is overestimated in comparison to the results from the vibrationally resolved Yacora model applying MCCC cross sections for electron impact excitation and considering additional reaction channels. This observation is in agreement with the results of [26], where it has been shown that AMJUEL overestimates the Fulcher band emission for deuterium plasmas in DIII-D. Consequently, an overestimation of the molecular emission can lead to an underprediction of the H₂ density and thus to the overprediction of MAR rates. Furthermore recent works (e.g. [2]) found that the Fulcher band emission profiles in divertor plasmas can be utilized as a proxy for the ionization region and may be employed as plasma temperature diagnostic. Based on the demonstrated strong influence of dissociative electron attachment for electronically excited states on the Fulcher band emission intensity predictions and the corresponding reaction probability under dispute, it is evident that absolute temperature predictions should be made cautiously. The large and (depending on the transition under consideration) asymmetric discrepancy between the molecular emission predicted by AMJUEL and the vibrationally resolved Yacora model demonstrate that the prediction of the total emission bands strongly depends on the implementation of all relevant reaction channels and reliable input data. Studies on vibrationally resolved dissociative electron attachment cross sections for electronically excited states are highly desirable, since their influence becomes particularly strong at high electron densities present in the divertor. In future work, an experimental benchmark is needed to clarify the difference in the model predicted emission. Furthermore, it should be kept in mind that the QSS approximation does not necessarily hold for vibrationally excited X¹Σ_g⁺ [27]. Hence, it would be more accurate to model the transport for the excited X¹Σ_g⁺(v) levels, even though this is typically not done in neutral transport codes for H₂. Instead, effective rates for fixed vibrational distributions are used (for some processes), as e.g. in the EDGE2D-EIRENE calculations, which are the basis for this work or the B2-EIRENE JET (carbon divertor) calculations from [28].

5. Conclusion

EDGE2D-EIRENE predictions representing low recycling, high recycling and detached JET ITER-like wall L-mode plasmas are post-processed with a vibrationally resolved CR model for H₂ based on the Yacora solver. The molecular emission intensities of the Lyman-, Werner- and Fulcher bands predicted by the Yacora model are compared with the emission predicted by AMJUEL in the form of synthetic LOS integrated emission (mimicking spectroscopy pointed at the LFS divertor). About 4–5 times higher Lyman band emission, about 1.7–3.3 times higher Werner band emission and 2–5 times lower Fulcher band emission is predicted by the Yacora model for the three plasma regimes compared to AMJUEL. Consequently, depending on which model and molecular emission band is used to derive the H₂ density from measurements, inconsistent particle density predictions are to be expected. The discrepancy between the model predictions is a result of different molecular reaction data (e.g. input cross sections) for the same molecular reactions and different sets of molecular reactions considered in both models. The MCCC method provides accurate and consistent sets of cross sections for electron impact excitation applied in the Yacora model. The authors would recommend their usage also for calculations directly in a CR model in EIRENE. For the Yacora model, it

was shown that the application of the dissociative electron attachment data for electronically excited states from [21] has a large impact on the Fulcher band emission prediction, while neglecting dissociative electron attachment for the vibrational levels of the electronic ground state can for certain plasma parameters hardly influence T_{vib}. As the only available data for dissociative electron attachment for electronically excited states are already under debate, vibrationally resolved cross sections for this process are highly desirable.

CRediT authorship contribution statement

Richard C. Bergmayr: Writing – original draft, Visualization, Validation, Software, Methodology, Formal analysis, Conceptualization. **Dirk Wunderlich:** Writing – review & editing, Supervision, Methodology, Conceptualization. **Mathias Groth:** Writing – review & editing, Software, Resources, Conceptualization. **Liam H. Scarlett:** Writing – review & editing, Resources. **Dmitry V. Fursa:** Writing – review & editing, Resources. **Mark C. Zammit:** Writing – review & editing, Resources. **Igor Bray:** Writing – review & editing, Resources. **Ursel Fantz:** Writing – review & editing, Supervision, Project administration, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data will be made available on request.

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