Collisional-radiative model for transport simulations of neutrals in detached conditions

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In the upcoming fusion reaction tokamaks DEMO and ITER detached operation regimes with electron temperature in the divertor even below 1eV are expected. At such low temperatures molecular processes which include physics behind detachment are shown to play a key-role. The Monte-Carlo transport solver EIRENE [1] is an established tool for edge and divertor modelling combining transport with atomic and molecular (A&M) reactions. Focusing just on A&M side one can describe the problem in terms of transitions between different species and their internal states and the resulting system of balance equations which is called collisional-radiative model (CRM). As most processes are driven by collisions with electrons as well as other species presented in the plasma, the realization of such models requires a database for reaction rates and a flexible solver of the system of equations for stationary equilibrium. An established data collection and a solver is YACORA [2] including the necessary validation. We aim to use this experience as well as EIRENE-associated data collections [3] to produce a specific CRM for detachment control modelling with EIRENE-involving packages. In this work we preset the first

Reaction	Type	Source
$H_2+e \rightarrow H_2^+ + e + e$	molecular ionization	H2vibr
$H_2+e \rightarrow H_2(b_{triplet}) \rightarrow H+H+e$	neutral dissociation	H2vibr
$H_2+e \rightarrow H+H^+ + e + e$	dissociative ionization	Amjuel
$H_2+H^+ \rightarrow H_2^+ + H$	charge exchange (CX)	H2vibr
$H+e \rightarrow H^+ + e + e$	ionization	Amjuel
$H_2^+ + e \rightarrow H+H^+ + e$	neutral dissociation (MAD)	Amjuel
$H_2^+ + e \rightarrow H^+ + H^+ + e + e$	dissociative ionization (MAI)	Amjuel
$H_2^+ + e \rightarrow H+H$	dissociative recombination (MAR)	Amjuel

Table 1: *The list of reactions: the databases for rates are Amjuel and H2vibr [3]. The CRM takes* $n_e = n_i$, $T_e = T_i$ *and molecular source* Γ_{H_2} *as parameters.*

version of the CRM applied for two representative cases (JET, $n_e = 10^{19} m^{-3}$, and EU-DEMO, $n_e = 10^{21} m^{-3}$) for a temperature range $T_e = 0.2 \div 30 eV$. These values and the list of reactions in table 1 correspond to EDGE2D-EIRENE simulations for JET [4] and SOLPS-ITER (B25-

EIRENE) simulations for EU-DEMO[5]. The databases Amjuel and H2vibr [3] are adopted for reaction rates and the flexible YACORA solver [2] is used. The relevant processes for molecules and the role of vibrational transitions are outlined, while the model contains the molecular source term as a free parameter, that can be adjusted to reproduce the molecular density obtained in the simulations. This procedure equivalent to assuming a certain molecular density is illustrated for JET case and the implications for molecular transport are discussed.

Atomic H, molecular H_2 and molecular ions H_2^+ balance equations are solved in the context of the plasma background (density and temperature). The produced H^+ is considered to be a sink in the infinite background, thus not tracked further. A reference molecular source term Γ_{H_2} is included for modelling of hydrogen gas influx to the plasma. The results of the stationary run [2] for EU-DEMO case [5] ($n_e = n_i = 10^{21} m^{-3}$) are presented in Fig.1 (similar results are obtained for JET case). Molecular density is in an equilibrium between the source term and the molecular dissociation/ionization reactions (sinks) and exhibits a rapid drop with increasing temperature at $T_e < 2eV$. The corresponding leading contribution to the loss channels is due to heavy-particles charge-exchange (CX) collisions $H_2 + H^+ \rightarrow H_2^+ + H$ (green line in (b)). This is due to the dissociation/ionization high threshold energy both above $15eV$ for electron impact reactions (blue and yellow lines in (b)). For H_2^+ the equilibrium is between dissociation reactions (dotted lines in (c)) and molecule ionization by proton and electron impact (green and orange solid lines). The former provides a peak at $T_e < 3eV$, the latter is responsible for a density increase with temperature. It is worth noting the contributions from the loss processes $H_2^+ + e \rightarrow H + H$ and $H_2^+ + e \rightarrow H + H^+ + e$ (purple and pink dotted lines in (c)) at very low temperature ($T_e < 0.5eV$) resulting in a competition between molecular activated recombination and dissociation (MAR vs MAD) reaction chains.

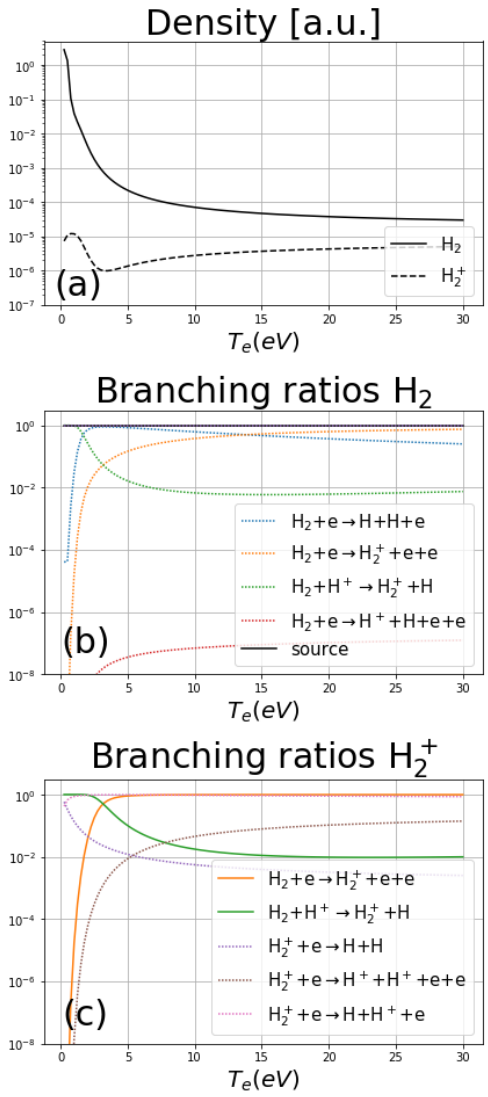

Figure 1: *The molecular and molecular ion densities (a) and the branching ratios (b,c). Dotted/solid lines are for loss/gain reactions.*

The model is extended by including vibrationally resolved molecular states $H_2(v)$, for the vibrational quantum number v ranging from 0 to 14, and electron-induced ladder-like transitions $H_2(v) + e \rightarrow H_2(v \pm 1) + e$. The resolution of vibrational meta-stable states decreases the effective molecular dissociation rate as discussed in [6]. Such a resolution is considered here with the reactions corresponding to a subset of those considered in EDGE2D-EIRENE simulations [4]. The solver runs provide the results in Fig.2 ($H_2(v = 0)$ is equivalent to H_2 in Fig.1). Plot (a) shows the density of the vibrationally resolved molecular states, each one exhibiting large values at low temperature. Plots (b) and (c) outline how the main reaction channels at low temperature ($T_e < 3eV$) are vibrational transitions (solid light-blue and dotted yellow lines). In particular, at $T_e < 1eV$, the main dissociation/ionization loss channels are three orders of magnitude lower than vibrational transitions; they become significant only at higher temperature (e.g. the dotted blue line in (b) is of the same order at $T_e > 3eV$).

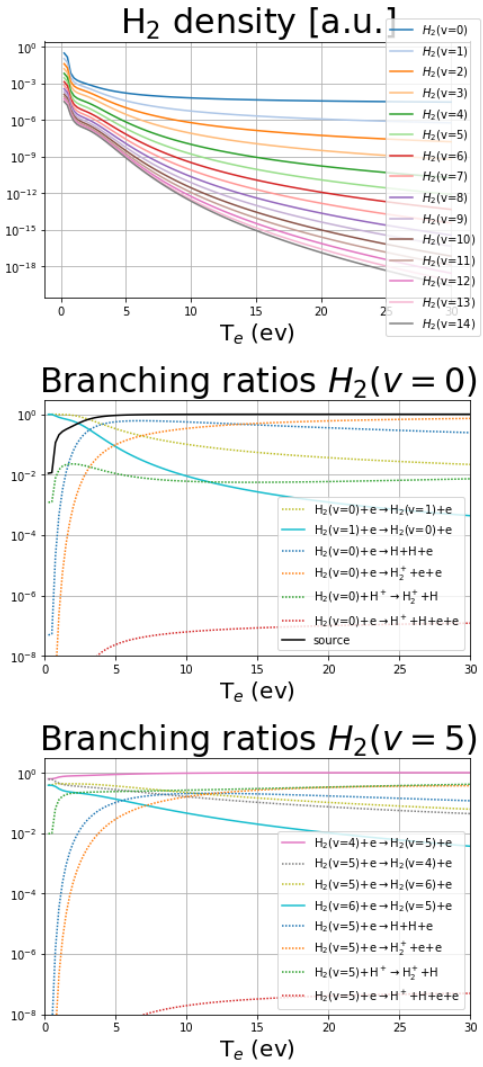

Figure 2: *The density (a), the branching ratio for the ground (b) and* $v = 5$ *excited state (c) of vibrationally resolved molecules for* $n_e = n_i = 10^{21} m^{-3}$. *Dotted/solid lines are for loss/gain reactions. The black solid line for* Γ_{H_2} *is normalized with* Γ_{H_2} *plus the contribution from the transition* $v = 1 \rightarrow v = 0$.

The source term is a free parameter and it has no impact on branching ratios. In EDGE2D-EIRENE simulations, molecules enter as Monte-Carlo test particles the main chamber in the vacuum region between the plasma and the first wall across the red surface in Fig.3. Then, they spread across the whole simulation volume (covering mainly scrape-off-layer and divertor region). The obtained equilibrium includes not just A&M reactions, but also self-consistent transport, plasma parameters and species fluxes and density distributions. An effective source term $\Gamma_{H_2}^{(eff)}$ can be determined as follows. A solver run with molecular dissociation/ionization reactions only gives the molecular density for reference source in each point of the EDGE2D-EIRENE grid. $\Gamma_{H_2}^{(eff)}$ is obtained by fitting the molecular source term in order to match the molecular density from simulations, *i.e.* by rescaling the source by the ratio of the EIRENE-simulated and

the CRM-output molecular densities. In Fig.3 $\Gamma_{H_2}^{(eff)}$ is shown in the divertor region (a) and it is compared with molecular density (b). In the characteristic region for detachment (blue box) the temperature drops below few eVs. From (b) density is nearly constant in the box. Since at low temperature CX collisions dominate and drive weaker dissociation with respect to the region above, $\Gamma_{H_2}^{(eff)}$ decreases from the upper to the lower region, as shown in (a). $\Gamma_{H_2}^{(eff)}$ is a volumetric source term that provides an estimate of the transport from the wall to the final stationary configuration. Hence, the larger the value of $\Gamma_{H_2}^{(eff)}$ in Fig.3(a) the bigger the fraction of molecules transported from the (red) injection region. The transport neglecting approach in the presented CRM still allows capturing the game-changing contributions for branching between different sets of reactions as a function of the plasma temperature (MAD vs MAR reactions chains, vibrational transitions vs dissociation/ionization). The CRM is staged for standalone use as well for becoming in the future an integral part of EIRENE in order to investigate the role of different reactions for detachment control and the impact of transport. The model must be refined to include the isotope effect for D and DT plasmas and extended for simulation of spectroscopic emission and radiation trapping (opacity).

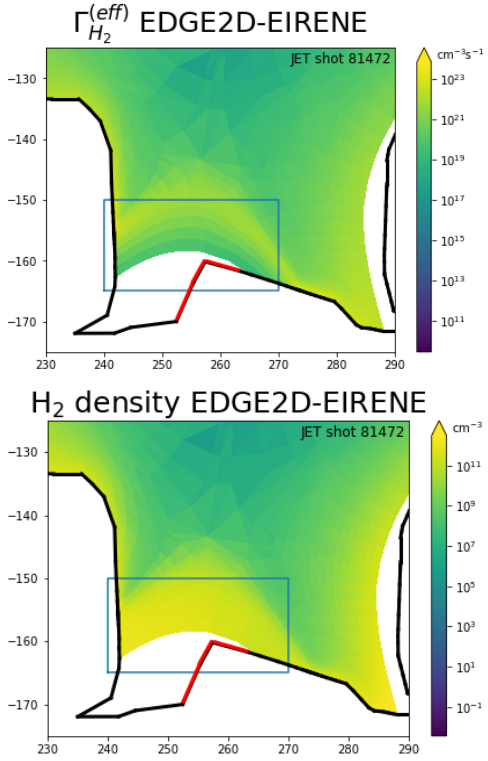

Figure 3: *The effective source (a) and the molecular density (b) in the divertor region of EDGE2D-EIRENE simulations for JET [4]. The red surface denotes the gas injection region. In the blue box the temperature ranges from* $\sim 10eV$ *(upper region) to* $\sim 1eV$ *(lower region).*

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