Molecular contribution to the Deuterium influx in Tore Supra ergodic divertor experiments

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1. Motivation and experimental set-up

The deuterium recycling processes, either back scattering or D_2 molecule extraction, determine the neutral energy distribution. As a consequence, they play an important role in the neutral penetration depth, and thus in the gas injection fuelling efficiency. Another parameter influenced by the molecular to back-scattered deuterium balance, important when interpreting spectroscopic data, is the relationship between the photon emission of a given D spectral line and the emitter density (S/XB). Up to now, few calculations and measurements [1, 2] have been reported on this subject. We have evaluated the molecular contribution in the vicinity of a neutraliser plate (NP) of the Tore Supra ergodic divertor, where the incident particle flux density is of the order of 10^{22} ions.$s^{-1}m^{-2}$. This plate is diagnosed by a Langmuir probe and by a set of 4 *in situ* optical fibres connected to a Czerny-Turner spectrometer, allowing to observe spectral lines/bands emitted by D or D_2 along 4 lines of sight roughly parallel to the NP at a distance (in the radial direction) between 1.2 and 6.4 cm. The pulses used in this study were performed in a standard resonant divertor configuration. The edge electron temperature was decreased from about 45 eV to 12 eV (and hence the density was increased from 1.5×10^{18} to 10^{19} m^{-3}) during the current plateau by means of D_2 gas injection. Since only one spectral line (or band) can be observed during a pulse, several identical pulses (in the sense that $n_e = f(T_e)$ is the same for all pulses) were performed in order to measure the Deuterium Balmer lines Dα to Dδ and a part of the D_2 Fulcher band ($3p^3\Pi_u - 2s^3\Sigma_g^+$).

2. Determination of the molecular flux by observation of the molecular spectrum

The total D_2-Fulcher band brightness is deduced from the observed spectral interval (a 60 Å interval around 6030 Å), which contains 8 rotational lines of the Q(0,0) vibrational transition. In order to sum up *all* Fulcher-band components, including those not observed due to the narrow wavelength interval of the spectrometer, the rotational temperature of the excited state (T_{rot}) was estimated from the present experiments. The rotational population was determined by a Boltzmann-fit of the diagonal Q(0,0)-branch. Six lines were included into the fitting program. In [3] a nearly linear dependence of T_{rot} on n_e (and with some restrictions also on T_e) was found. Fig. 1 shows the same trend for the present experiment , with T_{rot} ranging from 620 K at low density up to 750 K at high density. This quantity allows determinations of plasma parameters in regions which might not be accessible by other diagnostics.

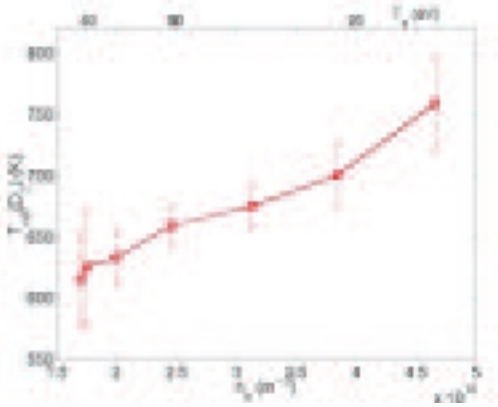

Fig. 1: Rotational temperature deduced from Fulcher band observation

From the estimate of the population of the upper vibrational state, the ground state population was recalculated by means of a collisional-radiative model calculating the population equilibrium of D

atoms originating from D_2 molecules (CRMOL-code [4]). From measurements on TEXTOR [3], where density scans in front of a test limiter were performed, a factor for the conversion from the number of photons of the (0-0)-branch to all visible branches (v′= v″ = 5) was determined. The total number of Fulcher-band photons and finally the molecular photon flux can then be calculated via the CRMOL-code, which provides the number of D_2 dissociations/ionisations per "Fulcher photon" (D/XB) as a function of n_e and T_e. The resulting molecular flux is shown on Fig. 2 (circles) as a function of the temperature, for the line of sight closest to the NP.

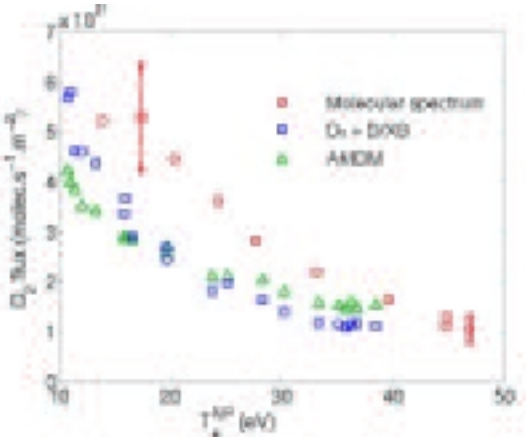

Fig. 2: Molecular flux as a function of the local electron temperature. ○: deduced from the molecular spectrum; □: deduced from the narrow Dα component; △: self-consistent method AMDM [6].

3. Determination of the molecular flux by observation of Dα

It has already been shown [5] that, in our experimental conditions, the Dα line is the sum of two contributions, of which the narrower one is consistent with the assumption of emission by the population of cold atoms originating from D_2 molecules. Adopting the formalism of [1], let us express the relation between this "cold" photon emissivity and the D_2 dissociation/ionisation rate. The former can be written as:

$$\frac{dn_{D\alpha}^{cold}}{dt} = A_{32}\, n_{D(n=3)} = A_{32}\, n_e \left(R_1(3)\, n_D^{D_2} + R_2(3)\, n_{D_2}\right)$$

The latter is the sum of the production rates of a D atom, a D^+ or a D_2^+ by electron collision with a D_2 molecule:

$$\frac{dn_{D_2}}{dt} = \left(P_D^{D_2} + P_{D^+}^{D_2} + P_{D_2^+}^{D_2}\right) n_e\, n_{D_2}$$

The resulting number of dissociations/ionisations per "cold" Dα photon is thus:

$$\frac{Dis_{D_2}}{(XB r)_{D\alpha}^{cold}} = \frac{dn_{D_2}/dt}{dn_{D\alpha}^{cold}/dt} = \frac{P_D^{D_2} + P_{D^+}^{D_2} + P_{D_2^+}^{D_2}}{A_{32}\left[R_1(3)\,\dfrac{n_D^{D_2}}{n_{D_2}} + R_2(3)\right]}$$

All the parameters in this expression are known from [1] for Hydrogen, and are assumed to be identical for Deuterium. This ratio can also be expressed in terms of flux and brightness: let us assume a constant velocity of the molecules along their trajectory and the D_2 flux (Γ_{D2}) radial dependence as a decaying exponential with an e-folding length λ. We can write:

$$\frac{dn_{D_2}}{dt} = \frac{d\Gamma_{D_2}}{dr} = -\frac{\Gamma_{D_2}}{\lambda}$$

The photon emission rate is assumed to be uniform along the line of sight, which is verified at least for the line of sight closest to the neutraliser plate. It can then be expressed as:

$$\frac{dn_{D\alpha}^{cold}}{dt} \approx \frac{4\pi B_{D\alpha}^{cold}}{l_{los.}}$$

where $l_{l.o.s.}$ is the integration length of the line of sight. These expressions allow to deduce the D_2 flux from the measured Dα brightness, taking into account the number of D_2 dissociations/ionisations per "cold" Dα photon. A more complete study of the Dα line shape, called the AMDM method [6], which takes into account both the warm and the cold components in a self-consistent way, is also used. The results of both these methods (Fig. 1, squares and triangles resp.) are in good agreement with those of the first method, taking into account a total uncertainty of 80%.

4. Comparison of calculated and measured Balmer line ratios

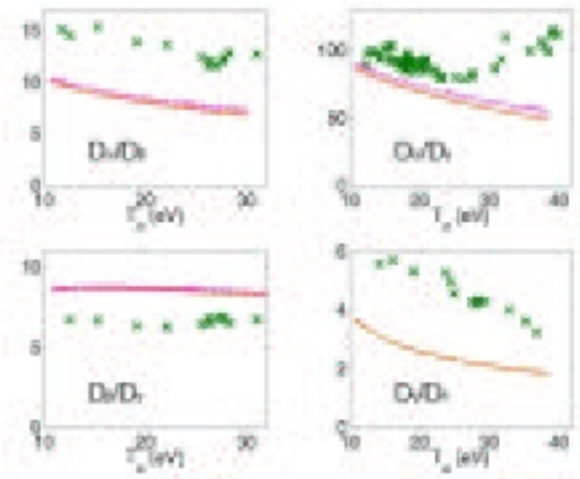

Fig. 3: Balmer line ratios. Solid and dashed line: resp. back scattered atom and molecular calculation; ×: measurements.

Due to the various processes of D_2 ionisations/dissociations, the population equilibrium, and thus the corresponding Balmer line ratios, of D atoms originating from molecules is different from the purely atomic case (as calculated in central ADAS [7] for example). Fig. 3 shows the measured line brightness ratios, for the 3rd line of sight, located 3.6 cm away from the plate. Surprisingly enough, the line ratios are approximately the same on all lines of sight. They are compared with recent collisional-radiative calculations [2] of this population equilibrium which take into account the population equilibrium of the molecule itself and the various molecule destruction processes. Fig. 3 shows the resulting Balmer line emissivity ratio predictions (no prediction is available for the Dδ line) along with the well known atomic case, taking a fairly rough estimate of the local density from the Langmuir probe measurement, assuming a density radial e-folding length of 3 cm [8]. Note that due to the high fraction of D_2 molecules producing ground state atoms (calculated from [1]), the population equilibrium is only marginally modified in our plasma conditions.

5. Modelling of Deuterium recycling and transport

The 3D Monte-Carlo code BBQ [9] contains a realistic description of the magnetic strucure in the NP vicinity computed by the code MASTOC [10]. It was modified to include the various physical processes involving Deuterium (excitation, ionisation, charge exchange; back scattering, D_2 desorption) and hydrogenic transport. BBQ is used to study the

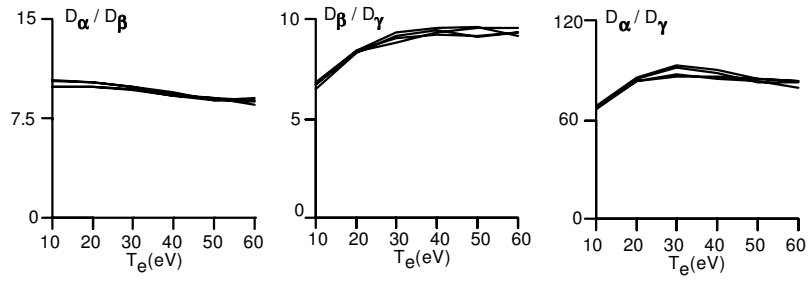

Fig. 4: Balmer line brigthness ratios modelled by BBQ for the 4 lines of sight.

effect of the density and temperature distribution non-homogeneities and of the complex structure of the NP. The back conductance of the vents in the NP is also taken into account when computing the D_2 source. Several cases have been run to cover the whole range of experimentally accessed n_e and T_e. There is little variation in the ratios between individual lines of sight, in agreement with the data and the CR predictions. Reasonable agreement is found for the D_α/D_β, D_β/D_γ and D_α/D_γ line emission ratios, taking into account that global shadowing by other neutralizers and localized flux amplification processes introduce unavoidable uncertainties. The code has also been used to calculate the expected rotational temperature for the D_2 molecules. The trend seen in the Fulcher band measurements is also found in the simulation.

6. Discussion

The measured Balmer line ratios, and particularly the T_e dependence, are in agreement with the calculations within the experimental error bars (30%, mostly due to the calibration uncertainties). It must be said here that, strictly speaking, the expected range for the line ratio values is larger since we integrate the line emissivities over a region where the atom and molecule densities probably vary. The $D\alpha/D\beta$ and $D\beta/D\gamma$ deviations from the prediction on the entire T_e range suggest that the n=4 level is less populated than expected. However, it should be kept in mind that the lack of homogeneity in the n_D, n_{D2}, n_e and T_e distributions in the NP vicinity may influence the ratios in a similar way.

From the values of the D_2 flux on the 4 lines of sight, it can be seen that its radial dependance is approximately a decreasing exponential. The corresponding molecular flux radial e-folding length is 1.2-1.6 cm. In contrast with the BBQ results, it does not depend on the edge n_e and T_e. This value is significantly larger than that given by a simple estimate of the dissociation length ($\lambda_d = v_0/(n_e<\sigma v>_{dissoc}) < 0.8$ cm), possibly because the radial density and temperature profiles in the NP region are not measured, and also because the Deuterium atomic and molecular physics is not entirely known. As T_e is decreased from 45 eV down to 13 eV (n_e from 1.5×10^{18} m^{-3} up to 7×10^{18} m^{-3}), the D_2 flux increases by a factor of 4, i.e. more than the incident particle flux (increased by a factor of 2) estimated from the Langmuir probe measurements. This indicates a change in the fraction of incident ions recycling in the form of D_2. Using the D_2 flux radial decay length estimated from the measurements of 1.2 cm, we deduce the absolute flux emitted directly on the NP. Comparing it to the Langmuir probe measurements, we estimate the fraction of incident ions being re-emitted as molecules ($2\times\Phi_{D2}/\Phi_{D+}$) to increase from about 36% at T_e = 45 eV (n_e = 1.5×10^{18} m^{-3}) up to 73% at T_e = 13 eV (n_e = 10^{19} m^{-3}), leading to a roughly constant complementary reflected atom flux of 9×10^{21} atoms.m^{-2}.s^{-1}.

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