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* See annex of J. Pamela et al, "Overview of Recent JET Results and Future Perspectives",
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ABSTRACT

At JET the properties of deuterium molecules and their contribution to the total deuteron flux in the outer divertor for the Horizontal configuration in L- and H-mode conditions have been determined. For this purpose the outer divertor was observed with several high resolution spectrometers and lines of sight directed vertically with spatial resolution from the outer vertical target plate to the centre of the MK IIB GB/SRP divertor. The rovibrational population of the Fulcher bands of the deuterium molecules could both be measured for the first five diagonal vibrational transitions. A collisional-radiative model for deuterium molecules was used to convert the measured photon fluxes into local molecular D_2-fluxes. With more than 70% of the total proton flux originating from molecular sources molecules make up a significant contribution to the fuelling in the divertor. This was found to be in agreement with the 2d-fluid/neutral particle code EDGE2D/NIMBUS.

1. INTRODUCTION

Since the detection of major fractions of hydrogen/deuterium molecules in front of limiters and in divertors with graphite surfaces via molecular spectroscopy [1, 2, 3], a growing attention has been devoted to the investigation of the interplay between atoms, molecules and their interaction with the surrounding surfaces and to the study of the resulting particle energies. On TEXTOR [2, 4, 5, 6, 7] the atom to molecule ratio and the subsequent energy distribution have been measured, on ASDEX-U [3] the contribution of deuterium molecules to recombination has been determined and on Tore-Supra [8] the potential of hydrogen/deuterium molecular spectroscopy for plasma diagnostics has been tested. The methods employed in those devices have now been used to determine the location and the strength of molecular sources in the outer divertor of JET, where a number of high resolving spectrometers are available.

2. DIAGNOSTICS AND METHODS

Figure1 shows the lines of sight of the different views into the JET outer divertor. An overview spectrometer (KS3A, resolution $\approx$3000) observes the whole outer divertor, KS3B (resolution $\approx$20000) three selected narrow angle views, whereas KT3A/B (resolution $\approx$10000) exhibit a more ore less complete, spatially well resolved coverage. The viewing locations could be absolutely calibrated by identification of a hot edge on a divertor plate during a special strike point position of the separatrix (Pulse No:61248 see below). For the observation of the molecular deuterium the Fulcher-α band emission (3p $^3\Pi_u \rightarrow$ 2s $^3\Sigma_g$) in the relatively unperturbed red spectral wavelength range around 610nm was chosen. Figure 2 displays this region for the three spectroscopic systems mentioned. One can see that for the interpretation from the KS3B spectrometer additional information is necessary in order to complete the missing bands. Although KS3A lacks detailed spectral information it may be used for qualitative impressions as it covers nearly all of the emitting volume. The deuterium atoms were conventionally detected via the emission of either the Balmer-β and -γ

lines by means of the spectrometers or the Balmer-α light via photomultipliers equipped with the appropriate interference filters.

It was shown in [5,6] that, even with the restricted information provided by a system like KS3B, a full reconstruction of the spectrum can be achieved , which is necessary for the conversion of all Fulcher-α photons into total molecular deuterium fluxes. Otherwise, the measurement the molecular deuterium lines can be very elaborate, as they are scattered over a wide spectral range, which for normal experimental condition of fusion plasma experiments cannot be measured in total within a justifiable effort.

The main steps of this extrapolation method will be only shortly outlined here and can in detail be found in the references mentioned above: From one measured vibrational branch a rotational temperature T_{rot} can be derived. If more vibrational branches can be observed – as with KT3B – a formal vibrational temperature T_{vib} of the ground state can be calculated with the help of a procedure shown in [9]. If T_{vib} can be independently determined, additional information of the temperature of the deuterium emitting surface can be obtained. In the worst case the measurement of only a single molecular line may be sufficient if T_e and ne in the emitting volume are known. With the help of these properties (T_{rot}, T_{vib}, T_e and n_e) it is then possible to include lines into the total Fulcher-α band emission, which could not be measured otherwise. With the knowledge of the latter quantities and a collisional radiative model, which provides the conversion factors D/XB, the molecular photon fluxes can then be converted into the respective particle fluxes. This extrapolation method has been already used in [8] in order to determine the molecular deuterium flux from the Tore-Supra divertor plates.

3. RESULTS
3.1 SOURCE DISTRIBUTIONS
In order to investigate the source locations of the deuterium atoms, molecules and their respective absolute and relative source strengths, the strike point of the separatrix was swept during a discharge under constant plasma conditions from the horizontal to the vertical target position. This served also for the finding of an optimum separatrix position for all diagnostics during future plasma parameter variations (L-mode, H-mode, etc.) The extreme positions are indicated in figure 1 and figure 3 which display the line emission of the atomic and molecular deuterium during such a scan. The letters refer to the different positions of the strike point on the divertor plates. Because of their different viewing capabilities there is no strict coincidence of the spatial behaviour of atomic and molecular signals in both the KS3A, KT3B spectrometers and a tangentially viewing D_α-camera. These scans show that strike point positions on the vertical divertor plates can lack information on the molecular source distribution and strength from the spectroscopic systems. Also, one can already conclude that the penetration depth of the molecules must be short and is in the order of about 1cm. Therefore, a position of the strike point on the horizontal target was chosen for further studies of atomic and molecular deuterium behaviour.

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Figure 4 shows these distributions over the horizontal target plate during the L- and H-mode of a discharge. Several features deserve special attention. First, practically all emission volumes remain fully in the view of all spectroscopic systems, second at the vertical target position, the atomic distribution displays a broader distribution than the molecular one, which is stronger localised. Obviously the molecules can move, probably as H_2^+, along the magnetic field lines before they radiate atomic emission lines. And thirdly during the H-mode a second source can be seen in the centre of the KT3-observation field, from which the molecules gradually disappear. Apparently the separatrix had been positioned too close to the outer corner of the base plate so that this edge was heated by plasma impact. From that the KT3 spectroscopic observation systems could be exactly adjusted spatially.

3.2 MOLECULAR PROPERTIES

For the determination of the magnitude of the molecular sources from a limited number of measured molecular lines the temperatures T_{rot} and T_{vib} (of the ground state) should be known. T_{rot} for every vibrational transition can be obtained via a Boltzmann plot for the individual lines of the Q-branch and the relative population of the upper vibrational states by summation. In our case the population of the first 3 diagonal transitions could be measured (see fig.2) and from that the (formal) vibrational temperature of the ground state derived from this using the procedure outlined in [9]. As the population of the first 3 branches is very sensitive to variations of T_{vib} the values are reliable, which could also be tested with identical discharges, where also the transitions v=4,5 were measured. The variation of T_{vib} during the L-mode phase with the observation line of sight is shown in fig.5. The increase to smaller radii seems to be coupled to some "heating" of the molecules the further they move away from their place of origin.

The influence of the plasma on the population of the rotational levels can also be seen in figure 6 where for one line of sight (into the strike point position) the behaviour of T_{rot} during the discharge is plotted for the 3 vibrational states. In principle T_{rot} should decrease with increasing vibrational number. This discrepancy also grows with the distance of the molecules from the location of the separatrix (fig.5).

3.3 MOLECULE TO ATOM RATIOS

The molecular properties derived in section 3.2 now permit the determination of the molecular deuterium flux and its fraction of the total (atomic and molecular) source. In fig.7 one can see the radial intensity distribution of the atomic D_γ-line together with that from the molecular Fulcher-α band which is observed via the same observation line of sight. The width of both distributions differs by a factor of 2 (6cm and 3cm respectively), which underlines the strong confinement of the molecular source. Thus, it seems more reasonable to deduce ratios for the divertor as a whole rather than for individual lines of sight, which do not cover all particles with the same origin.

What is now left is the conversion of photons into the corresponding number of particles. For this purpose we have to apply the respective conversion factors (S/XB- for atoms and D/XB-values for molecules) [10,6].

As these conversion factors conveniently vary with electron density and temperature these parameters have to be known for the outer divertor. Measurements of the D_α/D_γ ratio, which is independent of T_e in the density range of the divertor plasma yield numbers of $3 \cdot 10^{19}$ m^{-3} for the L- and $1 \cdot 10^{19}$ m^{-3} for the H-mode part. With an electron temperature of about 30eV values of S/XB for D_γ of 1500 and 690 respectively were used. The corresponding D/XB-values for the molecules, which is defined by $\Gamma_M = D/XB \cdot I^M_{Fulcher}$, can be found in [7] with 2300 and 1500. It may be noted here that in general the ratio of the S/XB and D/XB only show a variation from 1.53 to 2.17, which may be important for an assessment of the accuracy. In order to separate the contribution of the molecules and atoms to the atomic radiation ($I^A = k_1 \Gamma_A$) one has to determine the amount of atomic radiation from the (known) molecular flux $I^M_\gamma = k_2 \Gamma_A$ (for definitions see [1]). The fraction of molecules in the total proton flux $I_{tot} = \Gamma_A + 2 \cdot \Gamma_M$ is then given by:

$$R = \frac{2\Gamma_M}{\Gamma_A + 2\Gamma_M} \tag{1}$$

By expressing the fluxes in terms of Balmer line intensities one ends up using $I^M_{Fulcher} = k_3 \Gamma_M$

$$R = \frac{2}{\frac{1^{tot}_\gamma}{I^M_{Fulcher}} \frac{k_3}{k_1} - \frac{k_2}{k_1} + 2} \tag{2}$$

From [9] we know that for such plasma conditions $k_1 \approx k_2$ is valid so that (2) reduces to

$$R = \frac{2}{\frac{1^{tot}_\gamma}{I^M_{Fulcher}} \frac{S/XB_A}{D/XB} + 1} \tag{3}$$

with the replacements $k_1 = 1 / S/XB_A$ and $k_3 = 1 / D/XB$.

This function is plotted in fig.8 and shows that, for these plasma conditions, the molecular fraction is nearly always responsible for 70% to 95% of the total proton flux, which is also in accordance with modelling from EDGE2D/NIMBUS calculations [11] for a comparable discharge.

DISCUSSION AND CONCLUSION

The release of deuterium from the divertor walls of JET and its recycling takes place in the majority in the form of molecules. The penetration depth of the molecules is in the order of 1cm and their ratio to the total flux increases during the H-mode with decreasing electron density, which may indicate a change in the fraction of incident ions recycling in the form of molecules but could also be due to uncertainties in the conversion factors. For electron densities above 10^{19} m^{-3} similar ratios have been obtained at Tore-Supra [8] and TEXTOR [5,6].

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For a proper calculation of the atom fluxes a knowledge of the molecular contribution is needed, otherwise the proton influx will be underestimated by a factor of about two if only the S/XB-value for pure atomic release were adopted. As it looks as if the molecular release is the dominant process, S/XB-values near double the atomic one seems to be the more appropriate one value. The dissociation chain obviously leaves only one atom behind whereas the other one takes along the charge from intermediate molecular ion state. The latter also leads to the intensity distribution of the atomic light emission along the separatrix.

The rotational population of the different vibrational branches, however, is not strictly thermal as found e.g. in [5,6]. This might be due to the fact that a number of molecules can move freely over long distances within the divertor without being ionised and leading to non-thermal population via cascading from upper levels.

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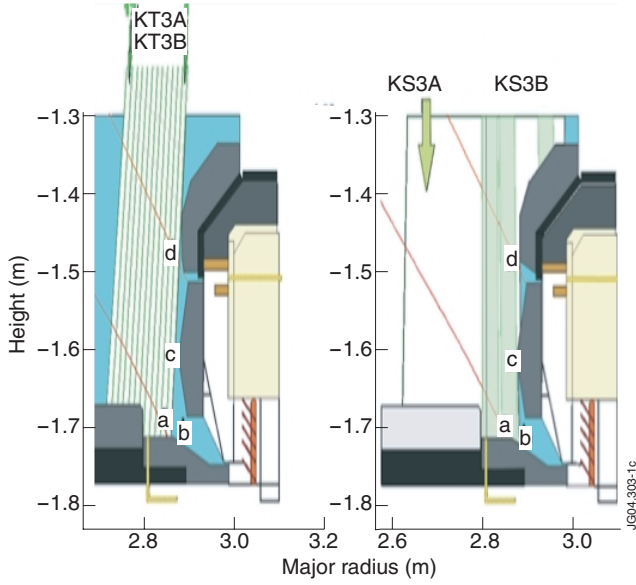
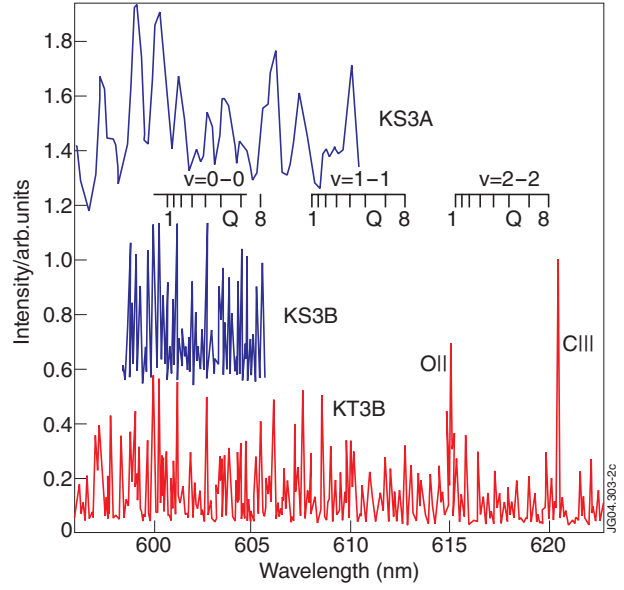Figure 1: Lines of sight for KS3A,B and KT3A,B,

Figure 2: Spectral regions for the spectroscopic systems KS3A,B and KT3B.
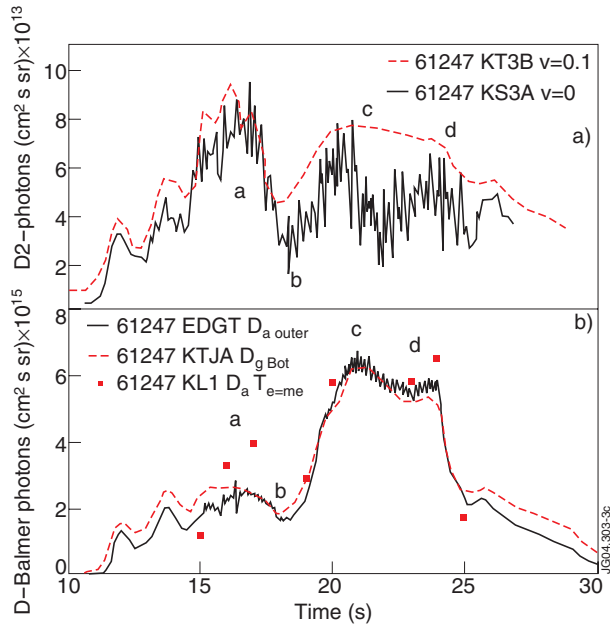

Figure 3: Behaviour of the molecular (a) and atomic (b) deuterium intensities integrated over the outer divertor region during a sweep of the separatrix from the horizontal to the outer vertical target plate in L-mode (JET Pulse No: 61247) a) full line: KS3A v=0, dashed line: KT3B v=0-1 b) full line: D_α-filter system, dashed line: D_γ from KT3A, points: D_α-camera KL1.
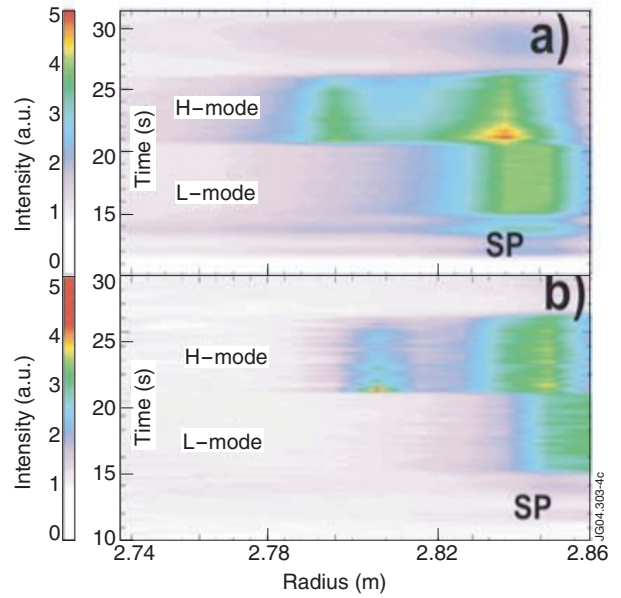
Figure 4: Atomic (a: D_γ) and molecular (b: v=0-1) intensity distributions over the horizontal target plate during the L- and H-mode for JET Pulse No: 61248 from KT3A,B.

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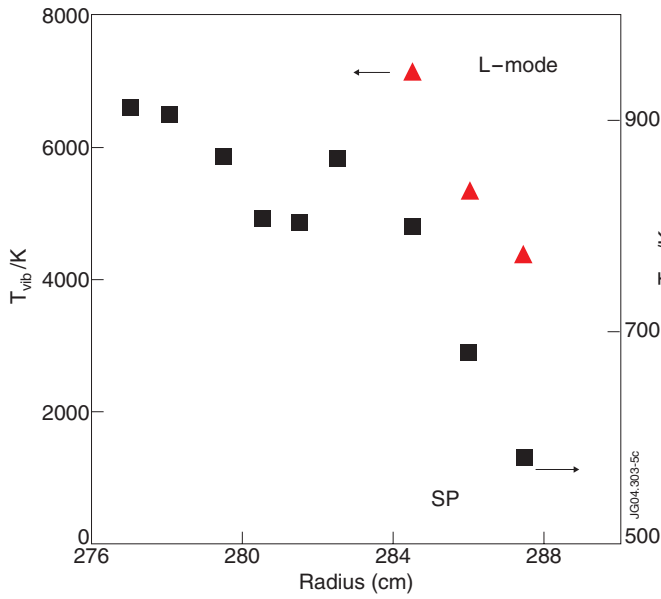*Figure 5: Spatial variation of T_{vib} (triangles) and T_{rot} (squares) during the L-mode phase of JET Pulse No: 61248*
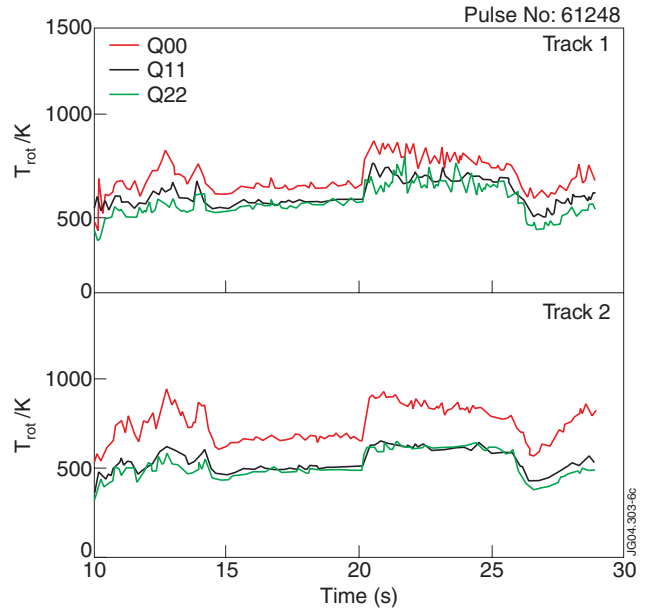

Figure 6: Behaviour of Trot during JET Pulse No: 61248 for the first 3 vibrational states for one line of sight at R=2.83m (track 2 of KT3B)
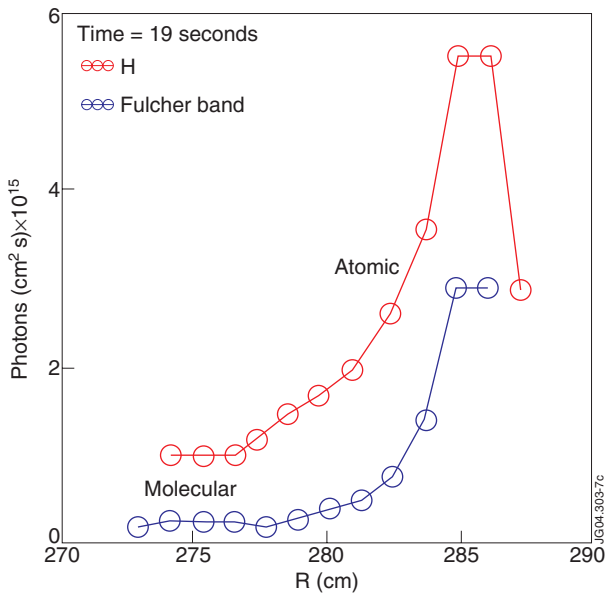

Figure 7: radial distribution of the atomic D_γ-line and the Fulcher-α emission from deuterium molecules
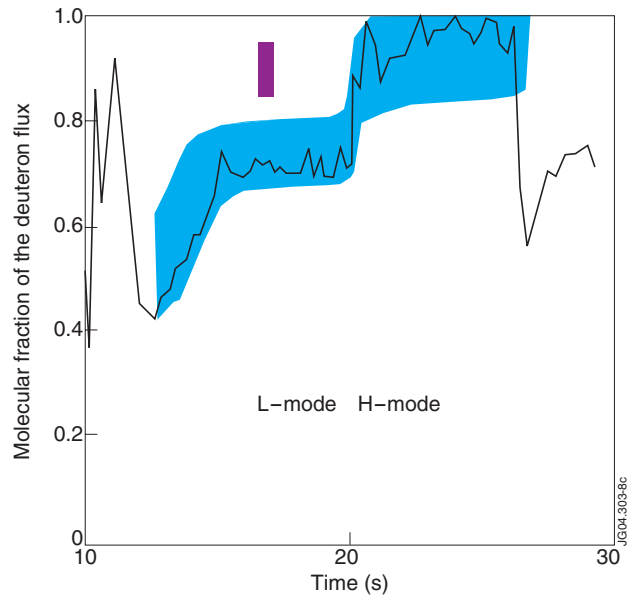

Figure 8: Ratio of protons from molecules to the total (proton) influx during JET Pulse No: 61248 in the outer divertor. The shadowed area describes the variation introduced by the inaccuracies of S/XB- and D/XB-values. The rectangle is from EDGE2D/NIMBUS calculations.

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