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Comparison of hydrogen and tritium uptake and retention in IET *

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Abstract

During previous Joint European Torus (JET) deuterium-to-tritium change-over experiments, subdivertor tritium concentrations were compared with those measured at the strike point region and found to differ significantly during the first few discharges, which was correlated with wall saturation. New deuterium-to-hydrogen fueling experiments in JET have been made and are compared to these previous experiments. Rates of hydrogenic species exchange are similar to those found in previous tritium experiments, granting differences in divertor configuration and mass ratio. In the new experiments, measurements of the CD and CH molecular band intensities near the divertor strike point monitor an intermediate stage of particle exchange between the plasma and wall. The CD/CH ratio correlates well with both the plasma and subdivertor concentration. The neutral transport code EIRENE and the wall hydrogen trapping and diffusion code WDIFFUSE have been used to evaluate the wall saturation. It appears that chemically-related processes play a role in mediating the plasma—wall exchange. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

For recent deuterium-tritium (D-T) discharges in the Joint European Torus (JET), the H-mode power and density threshold, confinement scaling, and the ability to

transfer enhanced performance scenarios from deuterium to D–T were all found to depend on the controllability of the D–T isotopic concentration [1]. In addition, if the tritium (T) retention in the wall and wall erosion products (co-deposited layers) cannot be properly controlled there can be serious consequences for the safety and environmental acceptability of future fusion reactors.

The hydrogenic inventory has previously been found to be 'dynamic,' that is, it changes substantially depending on the past history of particle fluxes to the wall and their energy dependence. This paper describes the study of the core plasma-wall exchange dynamics, between the plasma, graphite covered walls, and subdivertor region of JET, for a sequence of pulses in which 100% hydrogen (H) was injected into the JET vacuum vessel which, before the first shot, was loaded with $\sim 100\%$ deuterium (D). Using species-resolved Penning gauge measurements of H concentrations in the subdivertor,

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the dynamics of the plasma-wall exchange have been investigated by tracing the evolution of strike point and subdivertor concentrations over the first five discharges. Some of the earliest tokamak H–D changeover experiments were performed on TFR [2] and DITE [3] and demonstrated the importance of the wall contribution to the plasma composition.

Previously, similar JET experiments were performed with T, which was introduced into a D saturated wall environment [4] and this led to the development of a semi-empirical model for the rate of particle exchange due to particle-induced desorption. The systematic differences between the Penning measurements and the composition measured at the strike point by divertor spectroscopy were found to be a sensitive measure of the near-divertor wall saturation. EIRENE [5] modeling determined the relation between the plasma (strike point) and subdivertor parameters, as a function of wall status. Thus a range of values for wall recycling coefficients was determined. The code EIRENE was also used to calculate wall implantation fluxes and energies, which were used as input to the WDIFFUSE [6] wall diffusion model to calculate the wall recycling coefficients. The dynamics of the wall inventory for T were found to be related directly to the particle-induced detrapping rate, for which a semi-empirical value was inferred. The semiempirical recycling model for T can be compared with the present H measurements.

During the new H experiments, additional spectroscopic measurements were made of the relative concentrations of CH and CD molecular radicals in the divertor region, to test whether a 'chemical' path involving hydrocarbon formation was correlated with the particle exchange process. Because chemical sputtering may saturate with high particle fluence, one might expect little correlation. We tested the compatibility of particle-exchange models based on hydrocarbon formation. The modeling effort has profited from the additional information available [7] regarding the structure of a-C:H films and the variability of effective particle range and retention depending on prior history ('hard' vs 'soft' film).

2. Experimental arrangement

The JET D-H change-over experiments described here were performed with the MkII-GB (gas box divertor) while the JET D-T experiments were performed with the MkIIa divertor. A species-resolved Penning gauge was used to measure the H or T concentrations in the subdivertor region and details can be found in [8]. The H and T concentration is also measured via a divertor spectrometer (equipped with polarizing filters) which views the outer divertor strike point region (r = 2.83 m). For the H measurements reported here a

new divertor molecular spectroscopy measurement was utilized which also views the outer strike point and the molecular emission spectra of CH and CD in the wavelength region from 4240 to 4320 Å. This wavelength band covers the Q branch of the $A^2\Delta$ – $X^2\Pi$ transition. Comparisons of the CD and CH molecular spectra with model calculations from the CALCAT [9] code make it possible for H concentrations to be deduced following the techniques of [10]. Differences between the H (or T) concentration measured by the Penning gauge, divertor spectroscopy, or molecular spectroscopy are due to the species composition of the wall recycling processes as the initially D-rich walls become H (or T) rich.

3. Change-over experiments (H vs T)

Fig. 1(a) shows measured H concentrations as a function of time after pure H gas is injected between 50

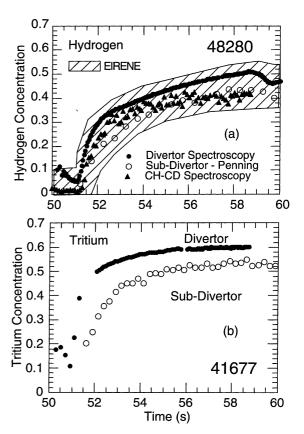


Fig. 1. (a) Comparison of the H concentration in the divertor, subdivertor, and as determined from CH–CD molecular spectroscopy vs time of the first H fueled discharge with 100% D loaded walls. (b) T concentration in the subdivertor and divertor vs time of the first T fueled discharge with 100% D loaded walls. The hatched region of (a) is the EIRENE calculation of the subdivertor H concentration utilizing the range of recycling coefficients determined in [4] for T.

and 60 s in the first, mainly ohmic, discharge (48280), as given by divertor spectroscopy of H and D, the subdivertor Penning gauge, and by the divertor molecular spectroscopy. Fig. 1(b) shows the measured T concentration for an identical discharge which was reported in [4]. Before these discharges, only D has been exposed to the tokamak walls. The difference in the H (or T) concentration between these various diagnostics is expected and was discussed in [4]. Initially, the wall is saturated with the majority species, and recycled particles of this species will dominate. As the H-input increases, H2 and HD are exchanged, as well as D2 (and possibly $C_nH_mD_1$ hydrocarbons), and the observed Penning gauge H concentration will rise. The observed behavior of the H concentration with time shown in Fig. 1 (a) is similar to that shown in Fig. 1 (b) for T.

Fig. 2 shows the variation of the H concentration for the sequence 48280–48285 in terms of accumulated time. The strong dip in the H concentration during each shot is due to 2 s of D neutral beam injection $\sim \! 10 \, \mathrm{s}$ into each discharge. Comparison of Fig. 2 with the T [4] shows that the transient behavior of H and T during these ohmic uptake experiments is quite similar.

4. Particle exchange models

As was previously described for T [4], the multispecies (D, H, D2, HD, H₂) EIRENE [5] neutral

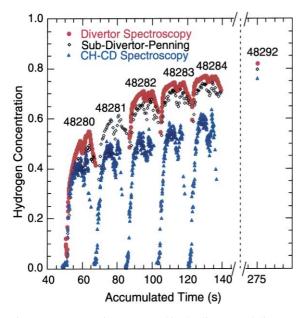


Fig. 2. H concentrations measured in the divertor, subdivertor, and via the CH–CD molecular band are shown for the first five H discharges vs accumulated time. Shot 48292 is after 12 H discharges and demonstrates that the H concentration is approaching equilibrium.

Table 1 Surface coefficients used in WDIFFUSE

Coefficient	Ehrenberg semi-empirical [4,11]
Recombination: k_0 (cm ³ s ⁻¹)	2.5×10^{-21}
Thermal detrapping: $k_{t,s}$ (s ⁻¹)	0.0
Trapping: $k_{s,t}$ (s ⁻¹)	1.0×10^{4}
Detrapping: σ_{dt} (cm ⁻²)	0.0
Particle-induced detrapping: k_d (cm ^{3/2} s ^{-1/2})	6.0×10^{-13}
Detrapping $\propto \Phi^{\alpha}$ (Φ flux); α :	0.5
Difffusivity: deuterium (m ² s ⁻¹)	1.0×10^{-7}

transport code is used to calculate the spatial distribution of charge-exchange (CX) fluxes and energies to the wall area surrounding the strike points. A model for H inventory dynamics is incorporated in the 1-D WDIF-FUSE code [6], which treats H and D and calculates the evolution of H₂, H–D, and D₂ in the surface, following the space- and time-dependent evolution of both trapped (t) and solute (s) H species under the interaction of H and D implanted fluxes. In the implantation zone (whose extent is determined by EIRENE) the model equations for the solute concentrations are described in [4] and treat trapped or solute species, whose concentration depends on the implantation rate (Σ), the recombination coefficient (k_0) , the thermal detrapping coefficient $(k_{t,s})$, the trapping coefficient $(k_{s,t})$, and the particle-induced detrapping coefficients (k_d). The Ehrenberg [11] semi-empirical particle-induced desorption rate, as discussed in [4] was found to describe the JET T

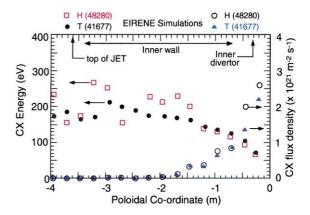


Fig. 3. EIRENE calculation of the poloidal distribution of the H (T) incident charge–exchange (CX) energy and CX flux over the vessel surface for the early phase of the H (T) change-over experiment. The species recycling coefficients used in the EIRENE modeling were $R_{\rm H}$ ($R_{\rm T}$) = 20%, $R_{\rm D}$ = 80%, with a background plasma minority concentration of $c_{\rm H}$ ($c_{\rm T}$) = 20%, $c_{\rm D}$ = 80%, for both H and T cases. The value x = 0 corresponds to the x-point location in the divertor.

change-over rate. This model (parameters in Table 1) is used in WDIFFUSE for H saturation calculations.

The long history of high-power operation in JET with inconel, graphite, and beryllium surfaces, makes precise specification of the plasma-facing materials difficult. However, recent studies [12,13] have shown that the actual surface, which is some mixture of Be, C, Ni, Cr, and Fe, has hydrogen trapping and release properties similar to graphite. Our evaluations are thus performed under this assumption.

The EIRENE calculations use experimentally measured, divertor strike-point profiles [14] of n_e and T_e . They show that the total neutral flux density is largest near the divertor strike points, $>10^{22}$ m⁻² s⁻¹, falling to $<10^{20}$ m⁻² s⁻¹ in the top half of the vessel. For comparison, peak perpendicular ion fluxes from the Langmuir probe measurements are $2.3 \times 10^{22} \text{ D m}^{-2} \text{ s}^{-1}$. Fig. 3 compares the H (T) CX flux densities and energies to the inner wall during the initial phase of the H (T) change-over in pulse 48280 (41677). The minority flux densities, shown here, are about 20% of the total. The incident neutral flux densities decay rapidly with distance from the inner divertor strike point ($x \approx -0.3$ m in Fig. 4), so that only the near-divertor area receives a significant fluence for the time period (\sim 50–60 s). Similarly, implantation energies vary strongly, from a few eV in the divertor region to ~300 eV away from the strike point, owing to the higher energy of plasma ions which produce the CX fluxes. Note that the highest energies occur in regions with the lowest flux density.

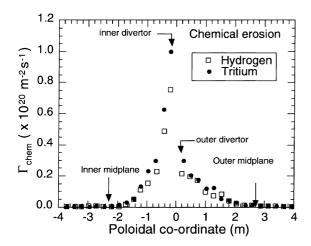


Fig. 4. Comparison (from EIRENE calculations) of an upper estimate of the poloidal distribution of the chemical sputtering flux densities over the vessel surface caused by incident D flux during an intermediate phase of the change-over. The recycling coefficients used in the modeling were $R_{\rm H}$ ($R_{\rm T}$) = 20%, $R_{\rm D}$ = 80%, with a background plasma concentration of $c_{\rm H}$ ($c_{\rm T}$) = 20%, $c_{\rm D}$ = 80%, for both H and T cases. The value x = 0 corresponds to the x-point location in the divertor.

Net implantation fluxes result after accounting for reflection of energetic atoms. The net D⁰ and H⁰ fluxes are the implantation driving terms which determine the changes in wall composition and hence in the recycling coefficient. A model for the implantation range (TRIM [15]) is used in WDIFFUSE to relate the mean energies from EIRENE to the implantation range for each surface element. The dependence of the range on the possible composition of the a-C:H film has been adopted from [7]. This range determines the size of the active wall reservoir which participates in particle exchange.

As seen in Fig. 3, the CX flux and energy to the wall as calculated by EIRENE for the D/T and D/H cases are similar. This is to be expected since plasma conditions, as reflected in the divertor Langmuir probe density $(3 \times 10^{18} \text{ m}^{-3})$ and T_e (12 eV) measurements, are also quite similar. From the discussion above it is not surprising that the semi-empirical values of particle-induced desorption coefficients inferred for the earlier T experiments are found to be valid for the H case, granting differences ~50% due to mass ratio and configuration changes. The T recycling coefficients found from this particle-exchange model in previous JET T experiments [4] are thus valid for the new experiment, allowing a prediction of the H concentration in the subdivertor. The EIRENE particle-exchange model result is displayed as the hatched area on Fig. 1(a). The agreement is quite good and the small differences in time scale are explicable by the difference in mass ratio and energy fluxes.

5. CD/CH results

Fig. 1 shows that the H concentration, as reflected in the CH/CD ratio in the outer strike point region, mirrors the divertor spectroscopy (plasma composition) and subdivertor pressure measurements during the initial discharge (48280). The concentration inferred from the CH/CD ratio initially grows at a rate intermediate between that of the plasma and the subdivertor. In subsequent discharges, however, some saturation is observed (Fig. 2). The H concentration inferred from the CH/CD ratio begins to lag and is significantly below the others after the third discharge. However the H concentration grows continually and reaches 0.76 after 12 discharges when the plasma composition is 0.84.

The previous semi-empirical model for particle-exchange, which fits these experiments, proceeds at a rate,

$$\frac{\mathrm{d}c_{\mathrm{t}}^{\mathrm{H}}}{\mathrm{d}t}_{PID} \approx -k_{\mathrm{d}}c_{\mathrm{t}}^{\mathrm{H}}(\Sigma^{\mathrm{D}} + \Sigma^{\mathrm{H}})^{1/2},\tag{1}$$

where c_t^H is the trapped concentration of H (or T) and k_d is the particle-induced detrapping coefficient as given in Table 1. This model involves particle replacement solely by hydrogenic exchange processes. As is well-known, an

alternative mechanism can produce particle-replacement: the chemical erosion of graphite plasma-facing components by the D/H CX influx. Using the EIRENEderived wall fluxes (Fig. 3) we have calculated the distribution of CD₄ emission using rates proposed in [16]. Upper levels of the rates have been adopted, by assuming a uniform (artificial) wall temperature of 750 K. The rationale is that the chemical exchange process is thought to occur at the end of the range of the energetic D or H wall penetration and so sufficient energy for the chemical rearrangement is thus available for the CX process, which is supplied by wall heating in the case of thermal particles [7]. With this estimate, particle-exchange fluxes on the order of 1-5% of the influx are possible, which can lead to a substantial contribution to the H exchange (consistent with the behavior in Fig. 1), since multiple H atoms enter in the hydrocarbons. Further, Fig. 4 shows that the calculations predict that the chemically-exchanged fluxes will be created predominantly in the inner region of JET, while the CH/CD measurements are made in the outer divertor. There are many caveats in such an estimate, but the particle-exchange rates (chemical erosion yields) are consistent with those found in [17,18].

Using the Langer–Erhardt database [19] of methane rate coefficients, and the divertor density and temperature profiles of these shots, we have calculated the rate-controlling (minimum) mean free paths for the dominant break-up channels for the hydrocarbon components in the CD₃ break-up chain leading to production of the observed CH/CD radicals. These are found to be $\sim 1-5$ mm near the peak of the divertor fluxes, with lifetimes in the microsecond range, but the mean free paths are found to be considerably longer in the region away from the peak. This is sufficient to provide time for the vibrational heating which is consistent with the spectroscopic modeling of the CH/CD band-head spectra.

6. Conclusions

D-T experiments on JET provided a unique opportunity to study the isotopic-exchange processes in a large

tokamak under the most directly relevant conditions. With the cessation of T experiments, improvements in models leading toward a predictive capability are being sought in simulation and similarity experiments, such as the one described here for H.

The D-to-H change-over was found to proceed at about the same rate as the previous JET D-to-T change-over experiment described in [4]. Wall rate coefficients from the Ehrenberg semi-empirical model are again found to give reasonable agreement with the observed H recycling transition. However, new measurement of CH/CD ratio show a continuing increase in this fraction that mirrors the D-to-H change-over. This suggests that graphite erosion processes could provide a physical mechanism for the particle-induced desorption rates, which have hitherto been based on semi-empirical fitting.

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