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Modelling of carbon deposition from CD₄ injection in the far scrape-off layer of TEXTOR

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Abstract

To analyse the impurity transport in plasma-shadowed, remote areas, methane CD₄ has been injected into the far scrape-off layer of TEXTOR through a cylinder equipped with a quartz micro balance (QMB). CD₄ transport including break-up and resulting deposition on the QMB (shot-resolved) and on the cylinder top surface (shot-integrated) has been modelled with the codes ERO and 3D-GAPS. The modelling shows good agreement with the observations if reflection coefficients based on molecular dynamics simulations are used. In contrast to plasma-wetted areas, no enhanced erosion has to be applied.

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(Some figures may appear in colour only in the online journal)

1. Introduction

The build-up of deposition layers at remote areas is of great importance for ITER and future fusion devices due to the potential of co-deposition of tritium and thus the contribution to long-term tritium retention. As effective methods of removing or cleaning layers in such regions are currently not available, it is desirable to reduce layer deposition as much as possible [1]. Thus, an understanding of the involved processes is necessary. Within this work, the modelling of a dedicated experiment performed in the far scrape-off layer (SOL) of TEXTOR is presented in detail. After a description of the experiment in section 2, the results of the modelling for impurity transport and layer deposition by means of the codes ERO and 3D-GAPS are presented in section 3.

2. Experiment

As the experiment is described in detail in [2], in this paper only the main features are summarized. A stainless steel

cylinder of diameter 10 cm, see figure 1, has been exposed to the far SOL of TEXTOR positioned at distances from the last closed flux surface (LCFS; $R = 46$ cm) between 5 and 8 cm. This corresponds to radial positions in TEXTOR between 51 and 54 cm. As the cylinder top surface was parallel to the magnetic field and far away from the plasma, ion fluxes hitting the surface can be neglected. During the discharges (Ohmic or neutral beam injection (NBI)-heated ones), a defined amount of methane CD₄ was injected through a hole within the cylinder top surface. A description of the calibration of injected CD₄ can be found in [3]. At a distance of 2.3 cm along the cylinder surface and away from the injection hole, a quartz micro balance (QMB) was mounted 7 mm below the top surface—a sketch of the QMB housing is shown in figure 1. The QMB allows shot-resolved measurement of the deposition at this location resulting from CD₄ injection. Representative radial profiles of the electron temperature and density measured with the helium beam diagnostic are presented in figure 2. The deposition on the QMB has been measured as a function of the amount of

Figure 1. Photograph of the cylinder, which has been exposed to the far SOL in TEXTOR. Also shown is a schematic view of the QMB housing.

injected CD_4 (variation between 1.23×10^{19} and 3.32×10^{20} molecules per discharge) with a fixed radial position of the cylinder at 52 cm. This measurement revealed a linear increase of deposition with the amount of injected CD_4 and thus shows that the deposition is determined by CD_4 injection, whereas background carbon deposition can be neglected. Figure 3 summarizes the measured deposition efficiencies on the QMB (i.e. deposition on the QMB relative to the amount of injected CD_4) as a function of the radial position of the cylinder for Ohmic and NBI-heated discharges. The measured efficiencies vary between 0.003 and 0.008%, with a relative measuring error of about 5%. With increasing distance from the LCFS the deposition decreases exponentially. Deposition from NBI discharges is slightly larger than from the Ohmic ones. Post-mortem analysis after exposure to the TEXTOR far SOL results in a deposition efficiency of about 1% on the top surface of the cylinder integrated over all discharges.

3. Modelling

3.1. ERO modelling

The three-dimensional (3D) Monte Carlo code ERO [4] is used to model the transport of injected CD_4 including ionization and dissociation processes within the far SOL. This modelling delivers the number of particles returning to the cylinder surface. As shown in figure 2 the measured plasma parameters are only available for radial positions R smaller than 49.5 cm, whereas the cylinder is positioned further outside. Therefore, for the modelling, constant values are assumed at locations $R > 49$ cm, corresponding to the last measured values: for Ohmic discharges $T_e = 4.3$ eV, $n_e = 1 \times 10^{11} \text{ cm}^{-3}$ and for NBI-heated discharges $T_e = 9$ eV, $n_e = 1 \times 10^{11} \text{ cm}^{-3}$. Later, the influence of variations for these parameters was studied.

Experimentally, only a very little information is available from spectroscopy. However, CD light emission has been recorded for Ohmic discharges with the cylinder surface positioned at $R = 52$ cm, i.e. 6 cm away from the LCFS. Figure 4 shows the modelled result in 2D integrated over the poloidal direction. Also shown is a radial profile of CD emission (normalized to 1), taken toroidally at the location of injection hole, in comparison with the experimental one. The agreement between modelled and observed CD profiles with respect to CD penetration and shape is very good.

Knowledge of the distribution and energy of returning species is important to draw conclusions concerning their reflection at the surface as the reflection depends on species and impact energy. Figure 5 shows the ERO-modelled

Figure 2. Measured profiles of electron temperature and density for Ohmic and NBI discharges.

Figure 3. Measured deposition efficiencies on the QMB for Ohmic and NBI discharges as a function of the radial position of the cylinder top surface. Also shown is the modelled flux of the returning species (relative to injected CD_4 flux) to the QMB aperture area.

distribution of hydrocarbons CD_x (from $x = 4$ to 0) returning to the cylinder surface for Ohmic discharge conditions and radial position of 52 cm for the cylinder surface. The simulations have been carried out using an anomalous cross-field diffusion coefficient of $D_{\perp} = 0.2 \text{ m}^2 \text{ s}^{-1}$ and zero for comparison. Due to the remote location almost no charged species can return to the cylinder surface. Only with the cross-field diffusion switched on, about 18% of returning species are ions and most of them are CD_4^+ . The energy of returning species is smaller than about 3 eV. At these low energies, reflection cannot be treated with the TRIM code but molecular dynamics (MD)-based methods have to be applied. Figure 6 presents the modelled deposition on the cylinder top surface for Ohmic discharge

Figure 4. Left: modelling of the 2D pattern of CD emission after CD_4 injection for Ohmic discharge and cylinder surface position at 52 cm. Right: modelled and observed radial profiles of CD emission normalized to 1.

Figure 5. Modelling of the distribution of species returning to the cylinder surface after CD_4 injection for Ohmic discharge with the cylinder surface positioned at 52 cm.

conditions and radial position of 52 cm of the cylinder surface. Cross-field diffusion has been neglected here. Outside the QMB aperture on the cylinder top surface, MD-based reflection coefficients [5] are used: $R_{\text{CH}_4} = R_{\text{CH}_3} = 1$, $R_{\text{CH}_2} = 0.9$, $R_{\text{CH}} = 0.6$, $R_{\text{C}} = 0.3$. Within the area of the QMB aperture a reflection coefficient of $R = 0$ is applied to assess the flux of species entering the QMB housing—this information is used as input for the 3D-GAPS code to analyse the detailed transport within the QMB housing, see section 3.2. The modelled deposition efficiency on the cylinder top surface (without QMB aperture area) of $2.2\% \pm 0.01\%$ is of the same order of magnitude as the post-mortem value of about $1\% \pm 0.2\%$, which represents an average of all discharges. The indicated error of the simulated value is of statistical nature only. Further reduction of the deposition can be caused by chemical erosion due to deuterium atoms originating from the injected CD_4 molecules (the flux of deuterium atoms in the background plasma is comparably small and can thus be neglected). The calculations show that roughly two deuterium atoms return to the top surface per returning C particle. Assuming a chemical erosion yield of 5% for a-C:D layer [6] (surface temperature around 150°C) reduces the deposition efficiency on the top cylinder surface from 2.2 to 2%. It is worth mentioning that simulations of injection experiments for plasma-wetted test limiters exposed to the SOL of TEXTOR reveal modelled deposition efficiencies typically a factor of >100 larger than the measured one if no enhanced re-erosion of re-deposits is assumed; see e.g. [7].

Figure 3 shows ERO modelling of the amount of returning carbon to the QMB aperture (relative to the amount

Figure 6. Modelled carbon deposition on the cylinder surface from CD_4 injection for Ohmic discharge with the cylinder surface positioned at 52 cm.

of injected carbon) for Ohmic and NBI discharges as a function of the radial position of the cylinder surface. Again, the cross-field diffusion is set to zero. Similar to the observed deposition on the QMB, the modelled flux of returning carbon decreases exponentially with increasing distance of the cylinder top surface to the LCFS. Also, due to a larger electron temperature within the far SOL, NBI-heated discharges lead, in the modelling, to slightly larger values of returning flux than Ohmic discharges. Compared to the observed deposition on the QMB, the modelled flux to the QMB aperture is about 15 times larger. This discrepancy will be discussed in section 3.2.

Parameter variations for radial position $R = 52$ cm of the cylinder top surface have been performed as summarized in table 1—‘standard’ refers to the parameters used so far and neglecting cross-field diffusion. Assuming in the far SOL larger electron temperature (for Ohmic) or larger density (for NBI) leads to larger deposition and flux to the QMB aperture, where the increase of electron density has the largest effect. Cross-field diffusion leads particularly to an increase of carbon flux to the QMB aperture (a factor of 1.4).

Table 1. ERO modelling of the flux to the QMB and deposition on the cylinder surface applying parameter variations, cylinder surface at $R = 52$ cm: ‘OHM standard’ refers to parameters used earlier, ‘OHM diffusion’ takes into account cross-field diffusion with $D_{\perp} = 0.2 \text{ m}^2 \text{ s}^{-1}$, ‘OHM plasma variation’ uses 9 eV in the far SOL instead of 4.3 eV and ‘NBI plasma variation’ uses $2.8 \times 10^{11} \text{ cm}^{-3}$ in the far SOL instead of $1 \times 10^{11} \text{ cm}^{-3}$.

	OHM standard (%)	OHM diffusion (%)	OHM plasma variation (%)	NBI standard (%)	NBI plasma variation (%)
Flux to QMB	6.9×10^{-2}	9.6×10^{-2}	8.7×10^{-2}	7.5×10^{-2}	14.7×10^{-2}
Deposition on cylinder	2.1	2.1	2.2	2.5	2.9

3.2. 3D-GAPS modelling

The neutral transport code 3D-GAPS [8] is applied to address detailed impurity transport within the QMB housing (as shown in figure 1) and the resulting deposition on the QMB. As input the ERO-calculated flux to the QMB aperture (exemplarily for Ohmic discharge and cylinder surface position $R = 52$ cm) is used, taking into account also the species and velocity distribution of impinging particles. The simulations show that only about 15% of incoming species is finally deposited on the QMB crystal applying MD-based reflection coefficients. This results in a deposition efficiency modelled on the QMB, which is ~ 2 times larger than the measured one. The 3D-GAPS simulations show that about 42% of incoming species is deposited on the side walls of the QMB housing and the remaining 43% leaves the housing through the aperture into the far SOL plasma. The probability that part of these lost particles return again to the QMB aperture is negligibly small.

As for the top cylinder surface, further reduction of the deposition on the QMB crystal can be expected due to chemical erosion by deuterium atoms. Assuming again an erosion yield of 5% reduces the deposition on the QMB: compared to 15% of incoming species, now about 13% is deposited on the QMB.

4. Conclusions

Modelling with ERO and 3D-GAPS of CD_4 injection experiments in the far SOL of TEXTOR results in good agreement with the observed light emission and deposition under the assumptions made. In the modelling it is important to apply MD-based reflection for hydrocarbons as they have small impact energies of less than 3 eV. This becomes evident if one uses as the extreme assumption $R = 0$ for all species (according to TRIM-like modelling, which delivers zero reflection at these low impact energies). The modelled deposition efficiency on the top cylinder surface increases with this assumption by a factor of 3 and the modelled value on the QMB increases by a factor of 2; therefore both simulated values are further away from the measured ones.

The detailed transport modelling inside the QMB housing needs to be addressed (with 3D-GAPS), whereas ERO provides the flux and species distribution of particles entering the QMB housing. The modelled deposition efficiencies reduce by roughly 10% if the erosion due to deuterium atoms is taken into account. However, the modelled values are still about a factor of 2 larger than the observed ones (for both the top cylinder surface and the QMB). This discrepancy can possibly be explained by the remaining uncertainties in the reflection coefficients used for returning species. Also, it has to be mentioned that the modelling of methane injection experiments at plasma-wetted areas [7, 9] typically leads to deposition efficiencies more than 100 times larger than those observed if no enhanced re-erosion for re-deposits is assumed. Thus, the modelling of the present work for plasma-shadowed, remote areas with no ion-impinging flux does not require any enhancement of erosion.

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