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A. Kirschner¹, J. N. Brooks², V. Philipps¹, J.P. Coad³
and contributors to the EFDA-JET workprogramme*

¹*Institut für Plasmaphysik, Forschungszentrum Jülich GmbH, EURATOM Association,
Trilateral Euregio Cluster, D-52425 Jülich*

²*Argonne National Laboratory, Argonne, Illinois 60439, USA,*

³*EURATOM/UKAEA Fusion Association, Culham Science Centre, Abingdon, Oxon OX14 3DB, UK*

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ABSTRACT

This contribution presents two dimensional Monte-Carlo simulations of the local transport of hydrocarbons that are chemically eroded in the JET MkIIa divertor. The effect of a given background carbon flux flowing from the main plasma down to the divertor is taken also into account. The influence of local plasma temperatures and densities and the influence of different assumptions for the sticking of re-deposited particles hitting the tiles is analysed. Even under the assumption that the sticking of re-deposited hydrocarbon fragments is zero, a large amount (about 75%) of the eroded particles is re-deposited in form of ionised carbon on the tiles. A reasonable agreement between the simulation and the experimental observation of the carbon deposition at the inner louvres in the MkIIa JET divertor is achieved, if high chemical erosion yields of about 20% together with a negligible effective sticking of hydrocarbons is assumed. Although there are experimental observations indicating similar high erosion yields, such high erosion yields can not be applied as a stationary value for the effective erosion since it would turn the inner divertor into a net erosion area in contrast to the experimental findings. Therefore the influence of the chemical erosion induced by low energy deuterium atoms in addition to the erosion due to ions is considered. The possibility of applying different erosion rates for (re-) deposited layers and the substrate material is discussed. First conclusions concerning the erosion and re-deposition behaviour in ITER will be drawn.

1. INTRODUCTION

In fusion research carbon-based materials are still the primary choice for plasma facing elements exposed to the high heat and particles fluxes near the strike zone areas in the lower divertor area. Thus the vertical targets in the divertor of ITER will be CFC to handle the stationary heat fluxes (up to 20 MW/m^2) but in particular the transient power pulses in ELMs or disruptions [1]. The understanding of the erosion and (re-)deposition behaviour of the carbon-based materials, especially under the low temperature plasma conditions that are typical for the divertor regions is of virtual importance. The uncertainties about the involved physical processes and the experimental database are still too large for reliable predictions of these processes for future devices. Chemical erosion is the dominant erosion process at the low electron temperatures in the divertor area - and a thorough modelling of the carbon transport and comparison with experimental results in existing devices is one of the most important issues in present PSI research. Based on a reasonable reproduction of various experimental results under different conditions in existing devices, the lifetime of the divertor targets and the tritium retention due to co-deposition of eroded hydrocarbons should be predicted for future machines like ITER.

This paper presents detailed modelling studies of the carbon transport in the divertor of JET. In the MkIIa divertor of JET a strong asymmetry of carbon deposition between inner and outer divertor leg is observed showing that the inner leg is everywhere deposition dominated - but with most of the deposition on the inner louvres - and essential no or very little deposition in the outer divertor including the louvre region. The thick carbon deposits on the inner louvres contain the majority of

the hydrogenic species retained on a long term basis. The in – out asymmetry of the particles fluxes is explained with flows in the SOL which drive particles from the SOL in the main chamber towards the inner divertor [2]. This is concluded from measurements of the Mach number [3] but also supported from the fact that beryllium, that is evaporated in the main chamber but not in the divertor region, is found only on the inner divertor tiles. Recently, moreover, ^{13}C marked methane has been injected from the top of the machine and also was found only in the inner divertor. The nature of these strong flows is not fully understood presently. Equally, the local transport of carbon inside the divertor region with the large carbon deposition at the remote, cold locations of the inner water-cooled louvres is not yet understood. Attempts to model this behaviour have been performed with an adapted version of the ERO-TEXTOR code [4] (ERO-JET). The transport of carbon towards the inner louvres is analysed applying various parameter studies such as electron temperature and density, location of the strike point and sticking assumptions for carbon ions and hydrocarbons fragments. The carbon is released from the target in form of methane and higher hydrocarbons by chemical erosion but in addition a certain amount of carbon flowing with the background plasma to the divertor surfaces is taken into account. Starting-point for the simulations are the divertor plasma parameters of a “representative” standard gas fuelled ELMy H-mode discharge (12MW heating power) of MkIIa. The density and temperature distributions are calculated from the Onion Skin model using target Langmuir data. They are shown in figure 1. The areas for which the temperature and density is plotted correspond to the calculation volume used for the simulations. The plasma represents a condition where the inner divertor plasma is partially detached whereas at the outer plate an attached plasma is formed with electron temperatures (T_e) of about 6eV at the inner strike point and 10eV at the outer strike point and densities (n_e) of about $6 \cdot 10^{13} \text{ cm}^{-3}$ and $6.5 \cdot 10^{13} \text{ cm}^{-3}$ respectively. From the T_e and n_e pattern along the plates the incoming deuterium ion flux is calculated according to $\Gamma^{\text{D}^+} = n_e \cdot c_s$ with $c_s = c_s(T_e)$ the ion flow velocity.

2. MODELLING RESULTS OF THE LOCAL CARBON TRANSPORT IN MKIIA

2.1. CHEMICALLY ERODED METHANE CD_4

To start with, the incoming deuterium ion flux is assumed to erode methane CD_4 with a fixed erosion yield of 1%. This number will be discussed later. To investigate the influence of the sticking probability of hydrocarbon fragments returning to the divertor plates the extreme cases of fully ($S = 1$) and zero sticking ($S = 0$) have been analysed. In the latter case the hydrocarbons are re-ejected as saturated methane molecules into the edge plasma. A negligible sticking of hydrocarbons cannot be explained solely with a simple energetic reflection but with a high (self)re-erosion of a soft a C:D layer built up by the hydrocarbons [5]. At first, the sticking of carbon atoms and ions has been determined using to reflection coefficients calculated with the TRIM code.

To visualise the local transport of eroded methane molecules figure 2 shows the 2D-distribution of the CD_4 and C^+ density for the assumption of sticking $S = 1$ of hydrocarbons. Due to the high electron density near to the strike points the penetration depth of CD_4 is extremely small in these

regions (~mm). At locations away from the strike points the penetration depth is in the order of a cm or slightly smaller. The C^+ ions, which are a reaction product at the end of the dissociation chain of CD_4 molecules, penetrate deeper into the plasma (~10 cm). The Coulomb interactions with the background plasma ions (friction force) tends to drive the ions back to the divertor plates or into the louvre regions via gyration around the magnetic field lines (figure 2, right hand side). The density distributions of the different species for the assumption of zero sticking $S = 0$ for hydrocarbons do not differ significantly from the case of fully sticking $S = 1$. Nevertheless, the different sticking assumptions lead to differences in the re-deposition such that the integrated amount of re-deposition relative to the amount of eroded molecules decreases in the case of zero sticking. At the inner divertor from 97% ($S = 1$) to 86% ($S = 0$). A similar behaviour is found at the outer divertor: the re-deposition decreases from 98% to 85%. The profiles of erosion and re-deposition along the plates are shown in figure 3 for the inner divertor, upper part. Only the inner divertor is shown since the simulations do not reveal significant differences between inner and outer divertor. The co-ordinate x used in figure 3 is the position along the plates with the starting point $x = 0$ corresponding to the upper corner of the vertical plate ($ZC = -148$ cm) and the end point $x = 430$ mm to the right end of the horizontal (base) plate ($RC = 255$ cm). For the case of fully sticking ($S = 1$) almost all particles eroded near to the strike point ($x \approx 400$ mm) are re-deposited locally. This is a consequence of the above mentioned short penetration of CD_4 molecules in this region. Particles eroded at the vertical plates have larger penetration depths and therefore a higher probability to be transported away from their origin. Thus at low x -values on the vertical plates the re-deposition probability is small and part of the eroded particles are transported downwards along the vertical plates and are re-deposited (at higher x -values) or enter the louvre region. Under the assumption of zero sticking the re-deposition profile near to the strike point is significantly shifted along the horizontal plates towards the louvre region (to smaller x -values). Most of the eroded molecules return to the plate near to their erosion site as hydrocarbon fragments. Due to the assumption $S = 0$ they are re-ejected into the plasma. This process is repeated until the particle is re-deposited as carbon atom or ion with a re-deposition probability according to TRIM which is significantly high under the given plasma conditions (small reflection coefficient). The repetition of these processes and the movement of the charged species along the magnetic field lines towards the plate leads to a deposition left from the erosion site deeper in the SOL (smaller x -values). In the lower part of figure 3 the resulting net-deposition and net-erosion patterns along the plates for the two sticking assumptions are shown.

Table 1 summarises the integrated amount of re-deposition at the inner and outer divertor for the different sticking assumptions. The amounts of particles entering the louvre regions show no significant difference for the inner and outer divertor. This is in strong contradiction to the observations showing large carbon deposition at the inner louvres and almost nothing at the outer. This shows evidently that additional processes determine the transport of eroded carbon. One candidate are asymmetric flows driving particles which are eroded at the main chamber and maybe also at the outer vertical tile to the inner divertor. This would result in an essentially zero carbon

background flux to the outer divertor but a large background contribution to the inner. Measurements of the Mach number at JET indicate such flows even though there is no final explanation of their origin [3]. In the outer divertor we have thus a situation with a low fraction of eroded carbon reaching the louvre as simulated with the code leading to no significant carbon deposition. But the code does not reproduce the measured amount of carbon that is deposited at the inner louvres. This amount has been estimated experimentally to be $\approx 4\%$ of the incoming deuterium ion fluence Φ_{D^+} [2]. The amounts simulated are $\approx 0.08\% \cdot \Phi_{D^+}$ for $S = 1$ and $\approx 0.5\% \cdot \Phi_{D^+}$ for $S = 0$ assuming a chemical erosion yield of $Y_{D^+ \rightarrow CD_4} = 5\%$. Thus even for $S = 0$ the simulated value is at least one order of magnitude too small keeping also in mind that only some fraction of particles entering the louvre region is finally deposited at the louvres.

Thus, for the inner divertor we will discuss the possible influence of further parameter variations while for the sticking probability of hydrocarbons only zero-sticking is considered.

a) Dynamic reflection of carbon atoms and ions

TRIM calculations of the reflection of carbon on graphite reveal zero reflection for particle energies less than ≈ 20 eV. At these low energies chemical processes become more and more important such that the binary collision model used in TRIM becomes more and more invalid. In contrast, calculations with the molecular dynamics code MolDyn [6] result in a significant reflection of carbon particles on an a:C-D layer as shown in figure 4 for an impact angle of 60 degree. Using these reflection coefficients instead those of TRIM decreases the simulated amount of re-deposition for the inner divertor from 86% to 75%. At the same time the amount of particles entering the louvre region (relative to the amount of eroded particles) increases from 9% to 12%. Although this increase tends to the right direction the absolute value of 12% is still about one order of magnitude too small (if a chemical erosion $Y_{D^+ \rightarrow CD_4} = 5\%$ is assumed) in order to explain the measurements.

b) New rate coefficients for hydrocarbons

Recently new data for the rate coefficients for electron and proton reactions of hydrocarbons were published [7, 8]. They differ significantly from the Ehrhardt-Langer data base used so far - details are discussed elsewhere [9]. Additional ERO-JET simulations have been done with the rate coefficients for electron reactions of [7] and with proton reactions of [8]. This leads to a further decrease of the re-deposition along the inner divertor plates from 75% to 69% while the simulated amount of particles towards the inner louvre region increases from 12% to about 15%.

c) Location of the strike point

In the Onion Skin Modelling of the inner divertor the strike point at the horizontal plate is located at $x \approx 400$ mm (see figure 3, maximum of erosion). Several measurements, however, indicate a shift of the strike point at the horizontal plates by ≈ 8 cm to the high field, left side [2]. Thus ERO-JET calculations were carried out for the inner divertor with an OSM plasma shifted as a whole by 8 cm to the left side along to the horizontal plate. The resulting profiles of erosion and re-deposition

(Ehrhardt-Langer data, zero sticking for hydrocarbons, dynamic reflection of carbon particles) is shown in figure 5. Compared to the “non-shifted plasma” the re-deposition increases from 75% to 82%, resulting from an increase of the average temperature and density of the shifted plasma. The amount of particles entering the louvre region increases also somewhat, from 12% to 15.3%, since more particles are eroded at locations in the vicinity to the louvre region.

d) Electron temperature and density variations

To investigate the influence of the plasma conditions on the particle transport, T_e and n_e have been varied by a factor of two keeping the plasma pressure $n_e \cdot T_e$ constant while the spatial distribution was kept unchanged. This procedure changes the incoming ion flux density ($\sim n_e \cdot T_e^{0.5}$). The results are summarised in figure 6. While the re-deposition decreases only slightly with increased incoming deuterium ion flux the amount of particles to the louvres decreases by more than a factor of two (from 16% to 6.3%). This is attributed to an increased number of particles leaving the simulation volume in positive r- and z-direction as consequence of the decreased electron temperature and is thus also partly an effect of the assumed size of the simulation volume.

2.2. CONTRIBUTION OF HIGHER HYDROCARBONS: C_2D_4

At low electron temperatures - as present in the divertor regions - the formation of higher hydrocarbons C_2D_x and C_3D_x becomes more and more important [10]. To estimate its importance simulations with chemically eroded C_2D_4 (which is one of the most important species at low temperatures, [10]) were carried out. With the “non-shifted” plasma solution, the zero-sticking assumption for hydrocarbons and dynamic reflection of carbon atoms and ions the resulting re-deposition profile is similar to the one for methane molecules (figure 3). The fraction of re-deposition is slightly smaller than the one for CD_4 erosion (69% compared to 75%). Figure 7 shows the distribution of species returning to the divertor plates from the C_2D_4 molecule (first cycle, re-ejected hydrocarbons are not included). Under those conditions, about 39% of the eroded C_2D_4 return to the plates as (charged or neutral) C_2D_x , 8% as CD and 37% as carbon atom or ion. Figure 8 presents the integrated re-deposition for the C_2D_4 molecules together with the amount of particles reaching the louvre region. The value of one for the normalized flux corresponds to the plasma conditions from the Onion Skin Model calculations. Figure 8 also includes the results for CD_4 . As for CD_4 the re-deposition of C_2D_4 shows no clear dependence on the incoming flux but the values itself are slightly smaller than those for CD_4 . The amount of particles entering the louvre decreases with increasing flux and is higher for C_2D_4 than for CD_4 .

2.3. BACKGROUND CARBON FLUX

The deposition of carbon from the background carbon flux is very important for erosion and deposition at the divertor plates. The assumption of a certain fraction of carbon flux relative to the incoming deuterium ion flux results in a deposition profile shown in figure 9. The gross-deposition is here the amount of incoming background carbon which is directly deposited. With the reflection

coefficients from the dynamic MolDyn calculations and the “non-shifted” plasma solution, 67% of the incoming carbon flux is gross-deposited and 33% is reflected. 52% of the reflected carbon is finally re-deposited so that all together around 84% of the incoming background carbon is deposited with a maximum of deposition near the strike point. Table 2 summarises the amount of gross-reflection (incoming background carbon which is directly reflected), re-deposition and particles entering the louvre region for TRIM reflection coefficients instead of MolDyn and the shifted plasma solution. Compared to MolDyn data the TRIM reflection coefficients lead to a significant decrease of the gross-reflection from 33% to less than 4%. The amount of particles which can enter the louvre region decrease by a factor of ten from 4% to 0.4%. The influence of the plasma with the shifted strike point is comparably small: With the MolDyn data the amount of gross-reflected particles does not change whereas the integrated amount of re-deposition increases slightly from 52% to 67% and the particles entering the louvre region from 4% to 6%.

3. COMPARISON WITH EXPERIMENTAL OBSERVATIONS AND DISCUSSION

The following discussion concentrates on the carbon deposition at the inner louvres whereas the in – out asymmetry of the deposition, which seems to be a global transport effect caused by asymmetric flows, is not considered. Experimentally, the amount of carbon particles contributing to the deposition at the inner louvres was estimated to $\sim 4\%$ of the incoming deuterium ion fluence Φ_{D^+} [2]. This is an integrated result of about 10.000s plasma operation in JET MkIIa. With the plasma parameter from the Onion Skin Model calculations, zero-sticking for hydrocarbons and the dynamically calculated reflection coefficients for carbon atoms and ions the ERO-JET calculations result in an amount of $0.52\% \cdot \Phi_{D^+}$ entering the louvre region with the following contributions:

- chemical erosion of CD_4 with $Y_{D^+ \rightarrow CD_4} = 1\%$ $\Rightarrow 0.12\% \cdot \Phi_{D^+}$
- chemical erosion of C_2D_4 with $Y_{D^+ \rightarrow C_2D_4} = 1\%$ $\Rightarrow 0.36\% \cdot \Phi_{D^+}$
- background carbon flux with $\Gamma_C = 1\%$ $\Rightarrow 0.04\% \cdot \Phi_{D^+}$

The value of 0.52% is a factor of 8 smaller than the measured one. However, the above values of 1% for chemical erosion caused by deuterium ions and 1% background carbon flux are rough assumptions. Indeed, measurements at JET suggest higher values that is 5% for CD_4 erosion, 7% for C_2D_4 erosion [11] and 5% for Γ_C [12]. With these values the ERO-JET simulations result in an amount of $3.3\% \cdot \Phi_{D^+}$ carbon particles entering the louvre region which is very near to the measured value of 4%. A further increase (to 4.6%) is achieved if the shifted-strike point is taken into account. Nevertheless, the involved overall chemical erosion of 19% seems to be unlikely – at least as stationary value during the whole campaign. This would automatically lead to net erosion zones near the strike point unless the background carbon flux is higher than the erosion, thus about 20%. However, the inner divertor plates are deposition dominated [2]. Therefore additional mechanisms must be considered – two are discussed in the following: First, the chemical erosion of soft (re)-deposited carbon-films can be significantly higher than of pure graphite [13]. Second, the chemical

erosion due to deuterium atoms is not included so far in the simulations but could have an important contribution in addition to deuterium ions [13]. The carbon transport in the inner divertor region could then be explained as follows. Carbon is eroded at the first wall and (partly) at the outer divertor (these are erosion dominated areas in JET) and transported – via asymmetric flows – into the inner divertor. The main part (around 80%, see chapter 2.3.) of the incoming carbon is deposited at the divertor plates in form of soft, hydrogen-rich films. These soft films are re-eroded effectively by chemical erosion – at locations with low deuterium ion fluxes away from the strike point these erosion mainly could take place via deuterium atoms. Most of the eroded carbon (around 80%, see chapter 2) is then first of all re-deposited at the divertor plates. As result of the transport of charged species along the magnetic field lines the location of re-deposition is shifted relative to the location of the erosion into the direction of the louvre region as suggested by the simulations. The repetition of these processes (erosion of re-deposited layers – transport along magnetic field lines – re-deposition) finally leads to a successive transport of the carbon particles into the inner louvre until a net-deposition of carbon takes place at the water-cooled louvres. Within this picture there is no need for chemical erosion yields of 20%. If the deuterium atom flux is in the same order as the D_+ -flux, chemical erosion yields of about 5% (which seems to be reasonable for soft layers) are sufficient. The temperature of the substrate may be an important parameter. At the divertor plates with temperatures around 200°C the soft carbon films are chemically eroded effectively whereas at the water-cooled louvres (surface temperature around 20°C) the chemical erosion yield is about a magnitude of order reduced which can lead to a significant net-deposition at these locations [13].

4. CONCLUSION

Simulations of the carbon transport in the divertor of JET MkIIa cannot reproduce the huge carbon deposition at the inner louvres if “common” assumptions (1% erosion yield due to erosion via deuterium ions) are used. However, the simulations suggest that the particle transport in the inner divertor is dominated by re-deposition and further effective erosion of soft carbon layers which finally leads to a successive transport of carbon to the louvre region. In addition to chemical erosion due to deuterium ions the erosion due to deuterium atoms seems to be important so that even at locations with low D_+ -fluxes (away from the strike point) an effective erosion of the soft carbon layers can take place. According to this picture the main part of the background carbon which enters the inner divertor is successively transported into the louvre region via (re)-deposition and erosion and leads to thick carbon layers at the inner water-cooled louvres.

In JET the main source of carbon formation seems to be the inner wall. Due to the fact that the inner divertor is net-deposition dominated the large amount of carbon which is found at the inner louvres must originate mainly from the inner wall and is transported via the above described processes. In ITER only the divertor plates are made from CFC so that the main wall cannot be a carbon source. Therefore, transferring the JET results suggest that the formation of tritium containing carbon layers via co-deposition should be less problematic in ITER.

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	Inner divertor		Outer divertor	
	Redeposition	Particles to louvre	Redeposition	Particles to louvre
S = 1	97%	1.5%	98%	1%
S = 0	86%	10%	85%	12%

Table 1: Integrated amount of re-deposition and particles entering the louvre regions for fully and zero sticking of hydrocarbons in the inner and outer divertor.

	TRIM Non-shifted plasma	Dynamic reflection Non-shifted plasma	Dynamic reflection Shifted plasma
"Gross" reflection (relative to incoming background carbon)	3.6%	33%	33%
Redeposition (relative to incoming background carbon)	74%	52%	67%
Particles to louvre (relative to incoming background carbon)	0.4%	4%	6%

Table 2: Integrated amount of re-deposition and particles entering the louvre regions for fully and zero sticking of hydrocarbons in the inner and outer divertor.

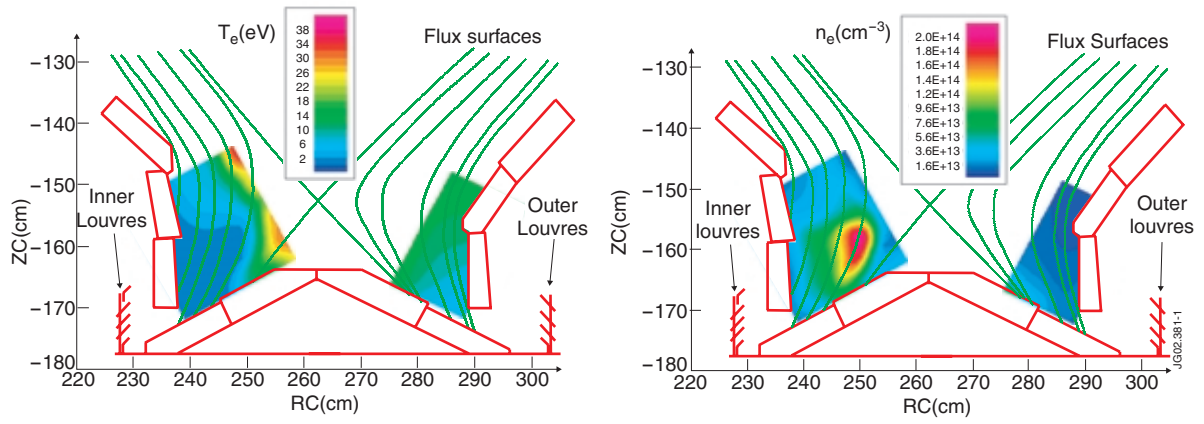


Figure 1: Electron density and temperature distribution calculated from the Onion Skin Model for a representative ELMy H discharge in JET MkIIa (Pulse No: 44029).

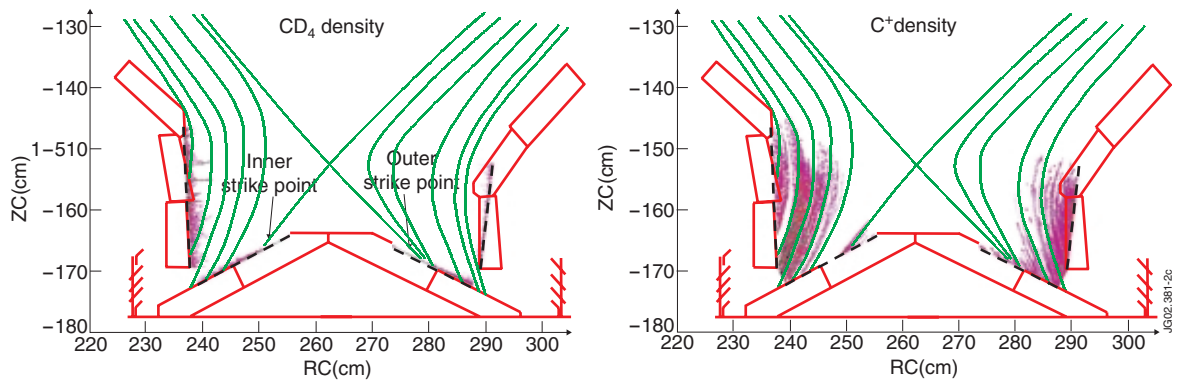


Figure 2: Simulated CD_4 (left) and C^+ (right) particle density after chemical erosion of CD_4 in the divertor of JET MkIIa under the assumption of fully sticking for hydrocarbons.

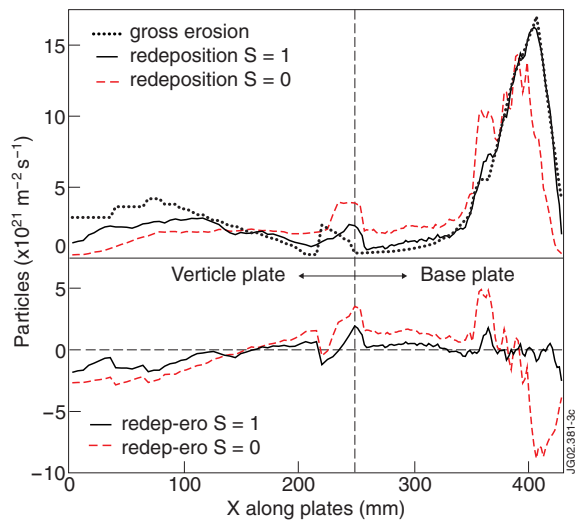


Figure 3: Profiles of erosion and re-deposition along the inner divertor plates for fully ($S = 1$) and zero ($S = 0$) sticking of hydrocarbons (upper part). Resulting profiles of re-deposition minus erosion (lower part).

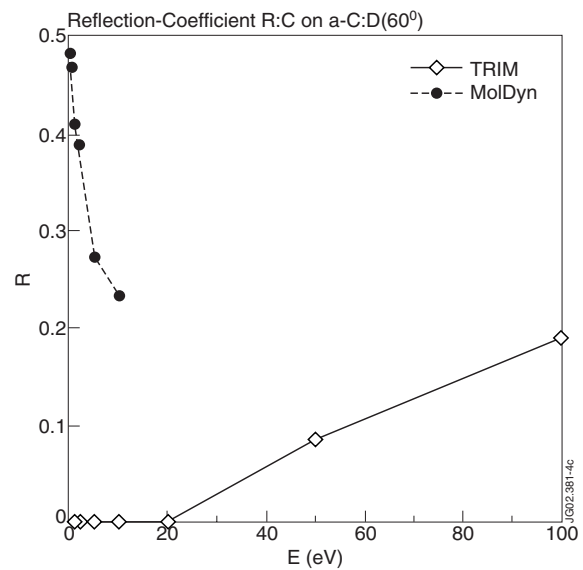


Figure 4: Reflection coefficient for “carbon on carbon” according to MolDyn [6] calculations in comparison to TRIM.

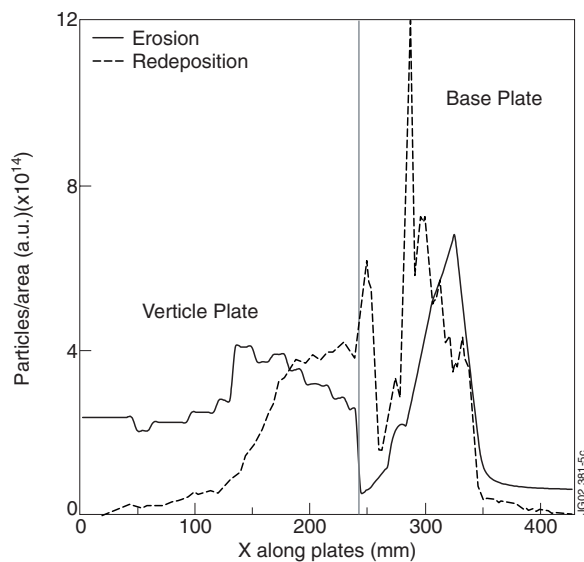


Figure 5: Profiles of erosion and re-deposition along the inner divertor plates using zero sticking for hydrocarbons, MolDyn reflection coefficients for carbon atoms/ions and the plasma with the shifted strike point.

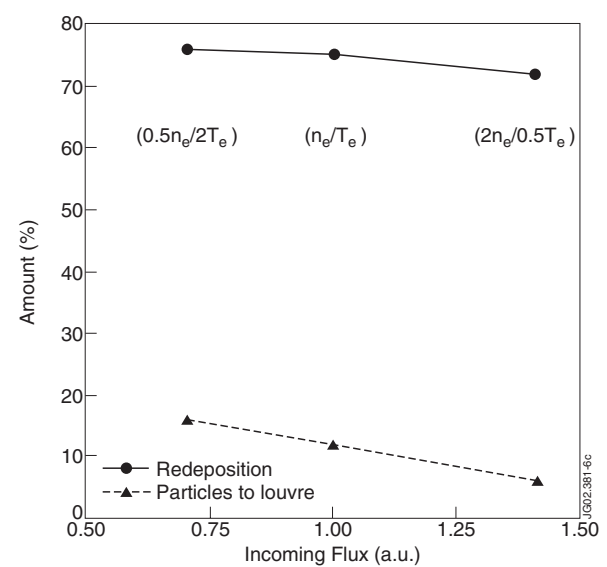


Figure 6: Influence of variations of the electron temperature and density on the integrated re-deposition and on the amount of particles entering the louvre region in the inner divertor for chemically eroded CD_4 .

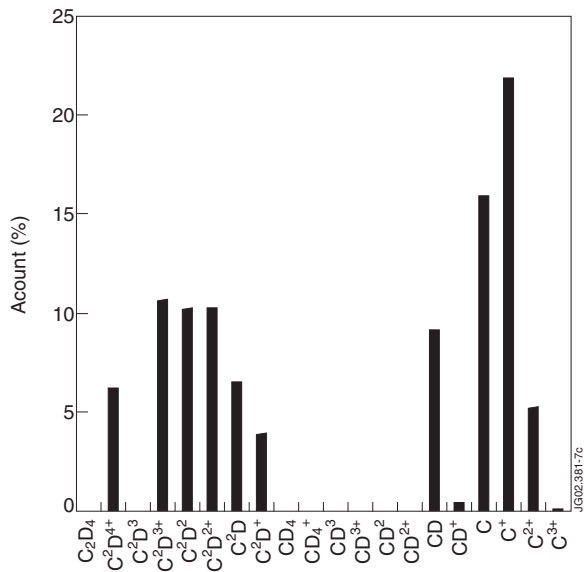


Figure 7: Simulated distribution of species returning to the inner divertor plates after chemical erosion of C_2D_4 .

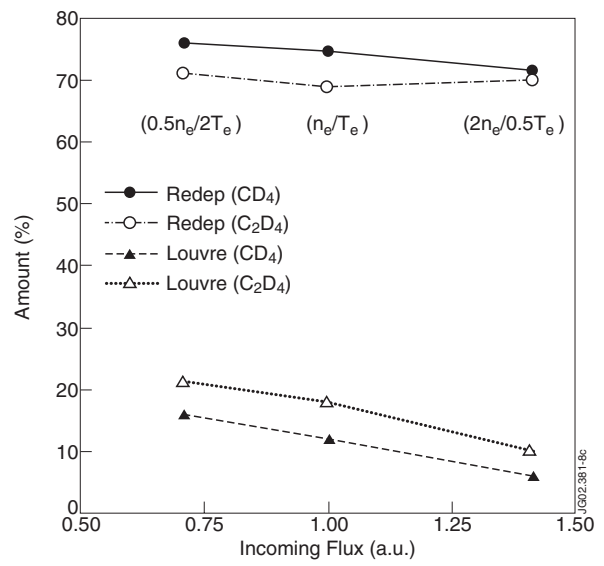


Figure 8: Influence of variations of the electron temperature and density on the integrated re-deposition and on the amount of particles entering the louvre region in the inner divertor for chemical erosion of C_2D_4 and CD_4 .

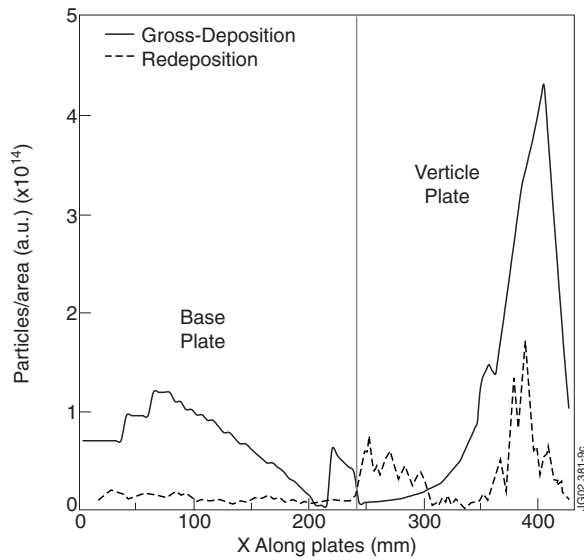


Figure 9: Simulated carbon deposition at the inner divertor plates resulting from the incoming background plasma.