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Modelling of the transport of methane and higher hydrocarbons in fusion devices

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Abstract

New Monte Carlo modelling with the ERO-TEXTOR code has been done for methane transport in the scrape off layer of TEXTOR using recently published rate coefficients of the methane family from Brooks/Janev. Compared to former used rate coefficients from Ehrhardt–Langer the new data result in significantly larger D/XB-values at plasma temperatures above ~20 eV. The computed amount of re-deposition is at high plasma temperatures up to a factor of 100 smaller with the new rate coefficients. Parameter studies of the transport of locally injected methane and C_2D_4 in the divertor MkIIa of JET with ERO-JET (adapted version of ERO-TEXTOR) show a strong influence of the location of injection on D/XB. Calculated D/XB-values can increase up to a factor of 1000 if hydrocarbons are puffed at a location inside the SOL instead at the strike point.
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1. Introduction

Chemical erosion of carbon based wall materials via formation of hydrocarbon molecules is a crucial issue in fusion devices with respect to target lifetime and tritium retention via co-deposition. There exist still large uncertainties in the dependence of the chemical erosion yield on the plasma parameters. Experimentally, the yield is determined by measuring the intensity of CD-band emission. The (inverse) photon-efficiency D/XB, which relates the amount of eroded molecules to the emitted CD-light intensity, has to be deduced from independent measurements or from simulations. Modelling of hydrocarbon transport and the resulting CD-emission is based on rate coefficients for hydrocarbon reactions with electrons and protons. Up to now the data by Ehrhardt and Langer [1] for methane and its fragments were used. Recently, new rate coefficients for methane have been published [2–4]. Thus, it is necessary to compare former modelling calculations with calculations using the new rate coefficients. For this, methane transport in the SOL of TEXTOR and resulting D/XB and the amount of re-deposition are simulated using the databases from Ehrhardt–Langer and Brooks/Janev. Calculated D/XB values are compared with measured ones.

For cold plasmas as in the divertor of fusion machines, higher hydrocarbons become more and more important [5] whereas methane comprises only ~30% of total chemical erosion yield at impact energies of 10 eV. Recently, rate coefficients also for higher hydrocarbons have been published [2–4] which will be used here for parameter studies of the transport of externally injected C_2D_4 molecules in the divertor MkIIa of JET. These calculations will be compared with simulations of CD_4 injection.

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2. Methane transport

2.1. Parameter study for a homogenous plasma

Simplifying assumptions are made for the ERO-TEXTOR [6] calculations in order to study the influence of the rate coefficients on transport of methane molecules: CD_4 molecules are thermally injected into a homogenous plasma with constant temperatures $T_{e,i}$ and density n_e. Electrical fields as well as diffusion and friction forces are not taken into account so that there is no possibility of re-deposition. Simulations carried out using rate coefficients from Ehrhardt–Langer [1] are compared to those using recent data from Brooks and coworkers [2,3] (for electron reactions) and from Janev et al. [4] (for proton reactions). Plasma temperatures of $T_{e,i} = 1$ and 30 eV have been considered. The density n_e is kept constant at 1×10^{13} cm^{-3} because the lifetime of hydrocarbon species under the simplified assumptions is proportional to $1/n_e$ (the probability of ionisation/dissociation at constant plasma temperature is proportional to the number of reaction partners and therefore to n_e).

Fig. 1(a) shows the penetration of CD_4 molecules into the plasma with $T_{e,i} = 1$ eV. Using recent rate coefficients results in a penetration depth of about a factor of 2.5 smaller compared to the Ehrhardt–Langer data. At this low temperature proton reactions dominate. Rate coefficients for reactions between protons and CD_4 molecules according to the Janev database are significantly higher than the Ehrhardt–Langer ones and result in a smaller lifetime of CD_4 molecules. As shown in Fig. 1(b) penetration of CD radicals – which are a product of the reaction chain – is now larger for rate coefficients from Janev. The rate coefficients for reactions between protons and CD_2 or CD radicals are about one order of magnitude smaller than the ones of Ehrhardt–Langer.

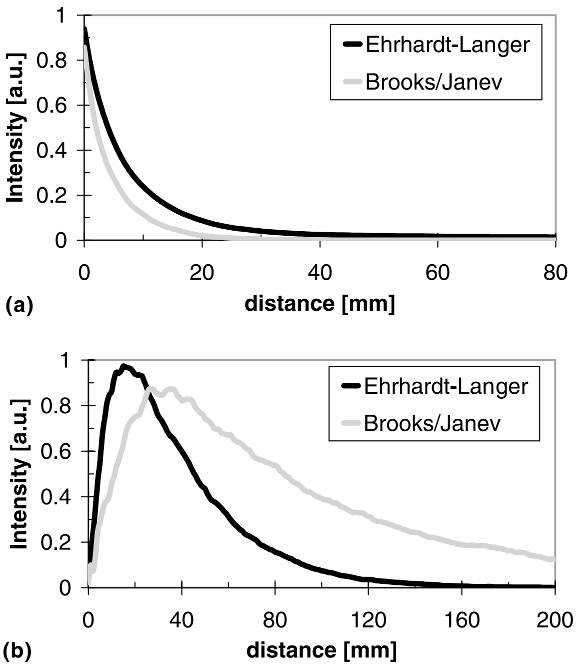

Fig. 1. Penetration of CD_4 (a) and CD (b) in a homogenous plasma using rate coefficients from the Ehrhardt–Langer database in comparison to data according to Brooks/Janev at 1 eV.

At $T_{e,i} = 30$ eV the penetration depth of CD_4 is similar in the two cases because differences in the rate coefficients are small. The main difference occurs in the rate coefficient for electronic dissociation – $CD_x + e^- \rightarrow CD_{x-1} + D + e^-$ for $x = 1$–4 – where the value in the Ehrhardt–Langer database is at $T_{e,i} = 30$ eV about a factor of 3 higher than the one in the Brooks database. In contrast to CD_4, there is a significant difference in penetration of CD radicals at 30 eV. With Ehrhardt–Langer data the penetration length is about four times smaller than with Brooks/Janev data. This can be attributed to following differences: (i) as stated out before the rate coefficients from Brooks database for electronic dissociation are at higher temperatures (>20 eV) smaller than the Ehrhardt–Langer data, (ii) several electron reactions are included merely in the Ehrhardt–Langer database ($CD_x^+ + e^- \rightarrow CD_{x-1} + D^+ + e^-$ for $x = 1$–4 and $CD_x^+ + e^- \rightarrow CD_{x-1}^+ + D + e^-$ for $x = 1$–4 and $CD + e^- \rightarrow C + D^+ + 2e^-$) and these reactions can be neglected only at temperatures smaller than several eV, (iii) as for the low temperature range rate coefficients for reactions between protons and CD_2 or CD radicals given from Janev are smaller than corresponding values according to Ehrhardt–Langer. In total, this results in smaller *total* rate coefficients for the data of Brooks/Janev and therefore in higher penetration depths.

Fig. 2 shows the influence of the different rate coefficients on photon efficiency D/XB. Only the temperature dependence is shown because the density does not affect D/XB under the simplifying assumptions. In

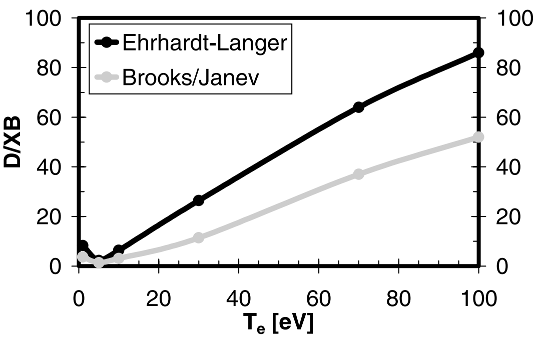

Fig. 2. D/XB for CD from CD_4 in a homogenous plasma: usage of rate coefficients from the Ehrhardt–Langer database in comparison to data according to Brooks/Janev.

general, the *total* rate coefficients according to Brooks/Janev are smaller for CD radicals. This results in longer lifetimes of these species and thus to a smaller value of D/XB compared to calculations where Ehrhardt–Langer data are used. This difference is particularly large at higher plasma temperatures but tends to decrease with decreasing temperature down to 5 eV and then increases again slightly with a further decrease of temperature. The increase of D/XB with decreasing temperature below ~5 eV is a result of a decreasing rate coefficient for excitation of the CD band [7], independent on the used rate coefficient database.

2.2. Modelling of transport of chemically eroded methane in the scrape off layer of TEXTOR

Methane transport and resulting D/XB-values may differ if instead of the simplified conditions of Section 2.1 realistic conditions are used. Hence, calculations are carried out for transport of methane molecules chemically eroded at a spherical (70 mm radius) carbon test-limiter in the scrape off layer (SOL) of TEXTOR. Input parameters are the temperatures $T_{e,i}$ and density n_e at the last closed flux surface (LCFS). The radial decay of temperature and density is described by exponential decay lengths of $\lambda_T = 25$ mm and $\lambda_n = 20$ mm. Although the minimal possible temperature near the test-limiter in TEXTOR is about 10 eV, the parameter range for modelling is extended to plasma temperatures down to 1 eV at the LCFS. Sticking of hydrocarbons hitting the surface is assumed to be zero which can be explained with a high erosion of deposited (soft) carbon layers [8].

Fig. 3 shows the spatial distribution of CD_4 and CD above the test-limiter at $T_{e,i}(\text{LCFS}) = 1$ eV and $n_e(\text{LCFS}) = 1 \times 10^{13}$ cm^{-3} for the two cases of rate coefficients, Ehrhardt–Langer and Brooks/Janev. CD_4 molecules penetrate deeper into the plasma for the Ehrhardt–Langer case. Proton reactions dominate at 1 eV and the corresponding rate coefficients for $CD_4 + p$ are smaller in the Ehrhardt–Langer than in the Janev database. The CD penetration shows an opposite behaviour: it is smaller using the Ehrhardt–Langer data. Rate coefficients for the dominant proton reactions are higher in the Ehrhardt–Langer database (especially for CD_2 and CD radicals).

At $T_{e,i}(\text{LCFS}) = 30$ eV and $n_e(\text{LCFS}) = 1 \times 10^{13}$ cm^{-3}, the spatial distributions of CD_4 molecules and CD radicals show no pronounced differences when the different databases are used. This is not surprising in case of CD_4 in view of the discussion for a homogenous plasma. From the different rate coefficients for CD, one would expect a significantly deeper penetration of CD in the Brooks/Janev case. This is not the case because dissociation and ionisation processes of hydrocarbons now mainly take place outside the LCFS. Although the hydrocarbons tend to live longer when Brooks/Janev data are used, they do not leave the SOL: friction forces drive the (ionised) species effectively back to the test-limiter. As a result the penetration of CD in radial direction is reduced.

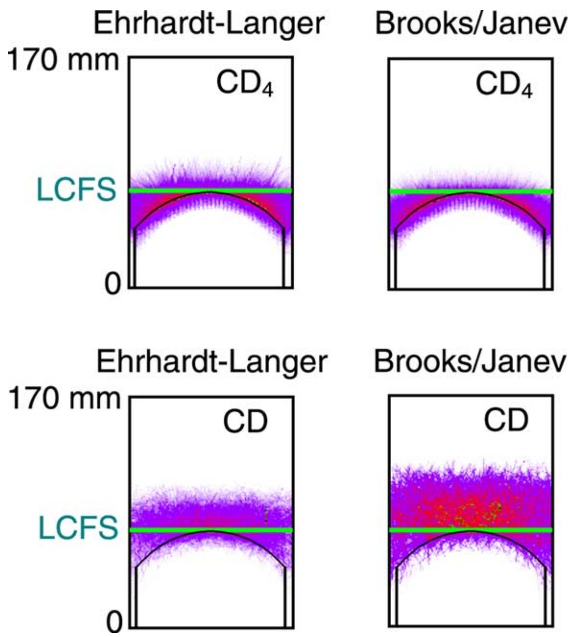

Fig. 3. Spatial distribution of CD_4 (top) and CD (bottom) as a result of chemically eroded CD_4 of a test-limiter in the SOL in TEXTOR with $T_e(\text{LCFS}) = 1$ eV and $n_e(\text{LCFS}) = 1 \times 10^{13}$ cm^{-3}: Ehrhardt–Langer data vs. Brooks/Janev data.

Fig. 4 shows the re-deposition probability at the test-limiter of chemically eroded CD_4 molecules in dependence on electron temperature for two different electron densities. For hydrocarbon radicals the assumption of zero sticking is hold. The sticking probability of carbon atoms and ions is assumed to be unity. Therefore the

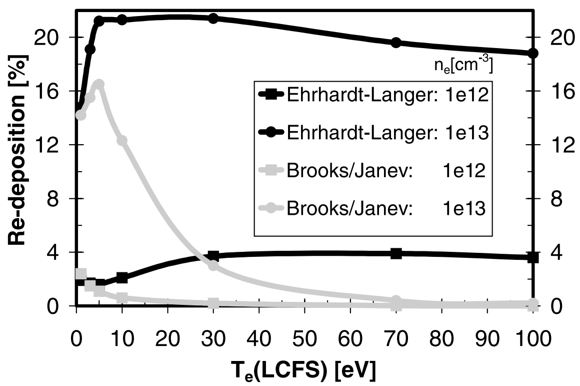

Fig. 4. Re-deposition of chemically eroded CD_4 at a TEXTOR test-limiter in dependence on T_e and n_e: Ehrhardt–Langer data vs. Brooks/Janev data.

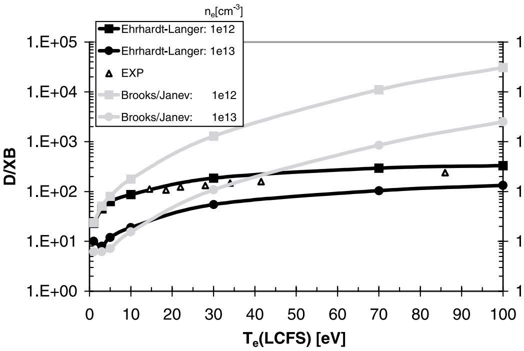

Fig. 5. D/XB for CD from CD_4 as a result of chemically eroded CD_4 at a TEXTOR test-limiter in dependence on T_e and n_e: Ehrhardt–Langer data vs. Brooks/Janev data.

re-deposition probability is here defined as the amount of carbon atoms/ions hitting the test-limiter surface relative to the amount of eroded CD_4 molecules. At high plasma temperatures the re-deposition probability of carbon approaches almost zero if Brooks/Janev data are used, whereas at temperatures smaller than about 10 eV the values do not differ much. With Brooks/Janev data eroded methane molecules return to the test-limiter still as hydrocarbon because of low rate coefficients at high temperatures. Since zero sticking is assumed, these hydrocarbons are re-ejected into the plasma as CD_4. They either return to the test-limiter or finally leave the observation volume. Also the probability of becoming a CD radical decreases with Brooks/Janev data (the majority of hydrocarbons hit the limiter even before becoming a CD) which leads to significantly higher D/XB at high temperatures (Fig. 5). Compared to experimental values [9] the modelled D/XB values are up to a factor of 100 higher for Brooks/Janev whereas the use of Ehrhardt–Langer data gives a better agreement. At smaller temperatures the difference between simulated D/XB values using Ehrhardt–Langer or Brooks/Janev data decreases and is at temperatures smaller 5 eV negligible. The extremely high D/XB values in the Brooks/Janev case at higher temperatures can mainly be attributed to the neglected reactions for charged radicals CD_x^+ in the Brooks database, see Section 2.1. From the resulting discrepancy compared to measurements (in opposite to the Ehrhardt–Langer case) one can conclude that neglecting of these reactions in the Brooks database is not justified at higher temperatures.

3. Modelling of transport of methane and C_2D_4 externally injected into the divertor MkIIa of JET

Transport of hydrocarbons in the divertor MkIIa has been investigated for standard gas fuelled ELMy H mode conditions with additional 12 MW heating. The strike points are located at the base targets. Corresponding plasma parameters (n_e,T_e) were calculated with the onion skin model (OSM) [10]. Two different locations at the base target of the inner divertor for gas injection are studied: the strike point where the maximum electron temperature and density occurs and a location about 6 cm away from the strike point into the direction of the SOL (mid point of base target). Sticking of hydrocarbons is assumed to be zero, whereas reflection of carbon atoms/ions is determined according to results of molecular dynamics calculations [11]. To investigate the sensitivity of n_e, T_e, variations of the reference case (n_e,T_e) corresponding to OSM are studied: ($0.5n_e$, $2T_e$) and ($2n_e$, $0.5T_e$). This corresponds to a flux increase of a factor of two.

Injection of thermal CD_4 molecules at the strike point using the Ehrhardt–Langer data results in deposition yields of about 88% independent on the different plasma conditions under discussion. Due to the high density and temperature the penetration of hydrocarbons into the plasma is small. This leads to narrow deposition profiles along the target plate with a width of about 5 cm. If the particles are injected at the mid point of the base target the amount of deposited carbon is reduced to values between 66% ($2n_e$, $0.5T_e$) and 76% ($0.5n_e$, $2T_e$). The decrease can be attributed to lower densities and temperatures in the region where the molecules are puffed compared to the conditions near the strike point. Moreover, the resulting deposition profiles are much broader (about 12 cm in width).

As an example, Fig. 6 compares the spatial distribution of CD radicals and C^+ ions after CD_4 injection at the strike point and the mid point of the base target for the highest flux case ($2n_e$, $0.5T_e$). When puffing at the strike point, the particle density of CD and C^+ is concentrated in a narrow region around the strike point. Injection at the mid point of the base target results in a deeper penetration into the plasma especially of C^+ ions. This finally leads to reduced deposition and broadens the profile of deposition.

Fig. 7 presents calculated D/XB values for CD band emission from externally injected CD_4 and C_2D_4 molecules for the two locations of injection in dependence on the incoming particle flux. The flux is normalised to the reference case (n_e, T_e). Increasing the particle flux, injection at the strike point causes decreasing D/XB values (from 16 to 2). There is no significant difference in D/XB between CD_4 and C_2D_4 injection. Hydrocarbon injection at the mid point of the base target results in a completely different behaviour: D/XB increases with increasing flux and therefore decreasing temperature. Extremely high values are reached at the maximum flux ($D/XB > 1000$ for CD_4). This is a consequence of lower temperatures near the puffing location and the strong decrease of the rate coefficient for CD band excitation

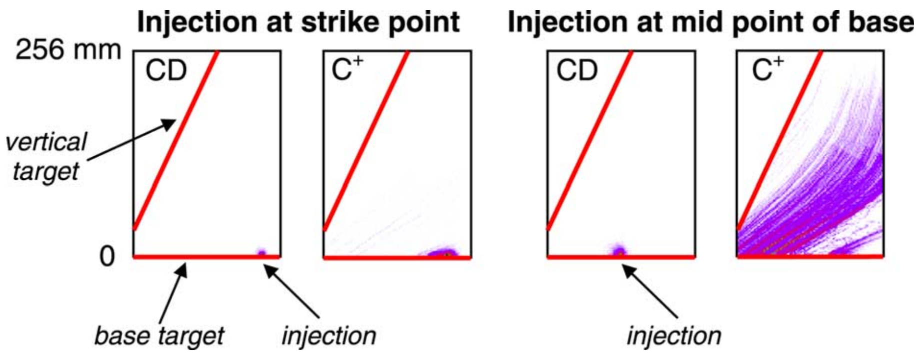

Fig. 6. Spatial distribution of CD and C^+ after external injection of CD_4 into the divertor MkIIa of JET at two different locations.

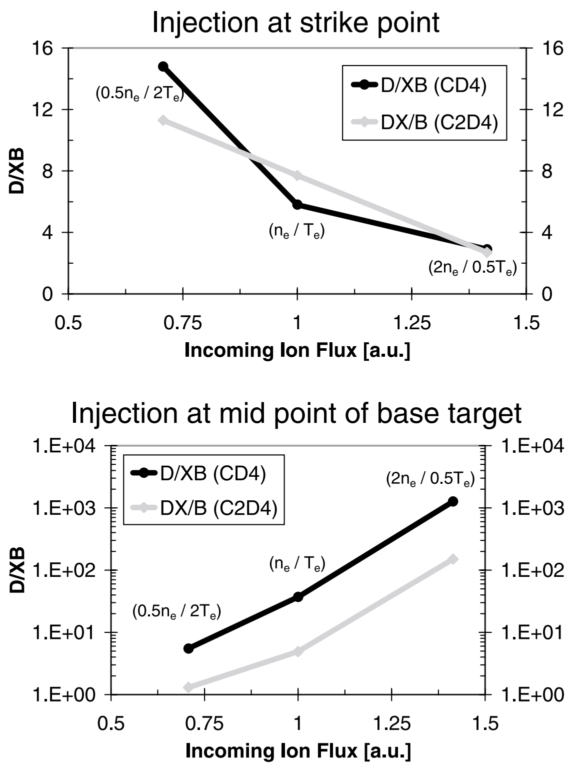

Fig. 7. D/XB for CD from externally injected CD_4 and C_2D_4 into the divertor MkIIa of JET.

with decreasing temperature for T_e smaller than 1 eV [7]. In addition, the D/XB values resulting from C_2D_4 injection are significantly smaller than for CD_4 injection.

4. Summary

Recently published rate coefficients for the methane family show significant differences compared to former used data according to Erhardt–Langer. In the modelling of hydrocarbon transport this leads to significant differences. While calculated D/XB values for TEXTOR test-limiter conditions match well experimental values if the Ehrhardt–Langer data are used, the use of Brooks/Janev data results in significantly higher values especially at temperatures greater than ~30 eV. Neglecting of certain reactions in the Brooks database (Section 2.1), which is the main reason for this discrepancy, seems therefore not to be justified for higher temperatures. However, direct comparison of the modelled penetration of various species like CD_4 and CD above the test-limiter with experimental results is necessary to get reliable information of the quality of the different databases. For this, experiments are planned at TEXTOR.

Calculated D/XB values for CD emission from externally injected hydrocarbons in JET MkIIa depend strongly on the location of injection. Injection at the strike point results in decreasing D/XB with increasing flux, whereas injection inside the SOL shows the opposite behaviour. In addition, D/XB can reach extremely high values if puffing takes place away from the strike point in plasma regions with low temperatures. Experiments at JET normally reveal increasing D/XB values with increasing flux independent on the locations of puffing analysed so far. In the future, detailed gas puffing experiments at JET are planned to study the influence of the location of puffing on D/XB. A comparison with modelling is foreseen.

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