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Modelling of the hydrocarbon transport and light emission during methane injection in TEXTOR boundary plasma using the ERO code

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Introduction. The erosion of carbon-based materials, which are foreseen as first wall elements of fusion devices including ITER, determines their life time. In addition the co-deposition of radioactive tritium has to be minimised. Thus, the general understanding of carbon erosion, transport and deposition pattern is of importance. The diagnostic for impurity fluxes is often based on the D/XB – 'decay per photon' values, which allow us to determine the fluxes of molecular species by spectroscopy.

The aim of this work is to model the hydrocarbon transport and recycling in experiments done at TEXTOR using the ERO code. In these experiments a known amount of CH_4 molecules was injected near the LCFS through cylindrically shaped gas inlets ('nozzle') with different sizes of the surrounding surface. In the experiments CH (CD) A-X band emission and also emission of several other species like C (including ions, e.g. 426.7nm CII line) and D were obtained with a spatial resolution. The CH species are a decay product of injected CH_4 or hydrocarbons recycled on the nozzle surface. In this case the D/XB values can be defined as a coefficient between the intensity of CH emission and the number of CH_4 molecules coming from the injection. These values are to be calculated and compared with the experimental ones.

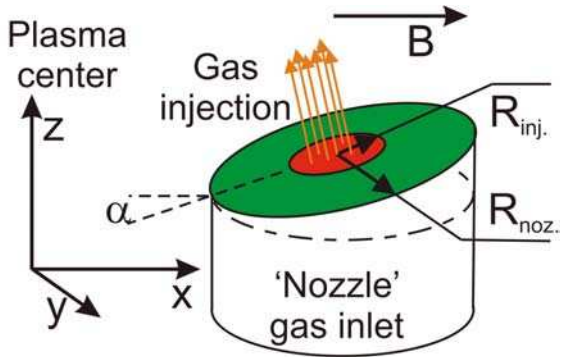

Fig. 1. Scheme of the 'nozzle' gas inlet geometry. α - inclination angle, $R_{noz.}$ – radius of the nozzle, $R_{inj.}$ – radius of the injection zone, B – toroidal magnetic field.

The model. ERO [1] is a 3D Monte-Carlo code based on the test-particle approximation. Plasma density and temperature are taken as an input and fixed. The emission is calculated using effective rate coefficients. We suppose that CH_4 is injected and CD_4 molecules are chemically sputtered by deuterium plasma from the nozzle surface if some C is deposited there. The emission of CH, CD (decay products of CH_4 and CD_4 respectively) and C^+ (which is produced after dissociation and ionization of both CD and CH) is calculated. Following CH and CD helps to distinguish and analyse the influence of different processes, though in the experiment we usually see the total emission of both. As an illustration we present (Fig. 2) the density and light emission pattern of the species in the observation volume. We see that the distribution of emission is shifted deeper into the plasma than the one of density. The distribution of C^+ is clearly influenced by the magnetic field.

The concentration of elements in the interaction layer of each surface cell is followed. If a net erosion (deposition) takes place, the content of the interaction layer is periodically

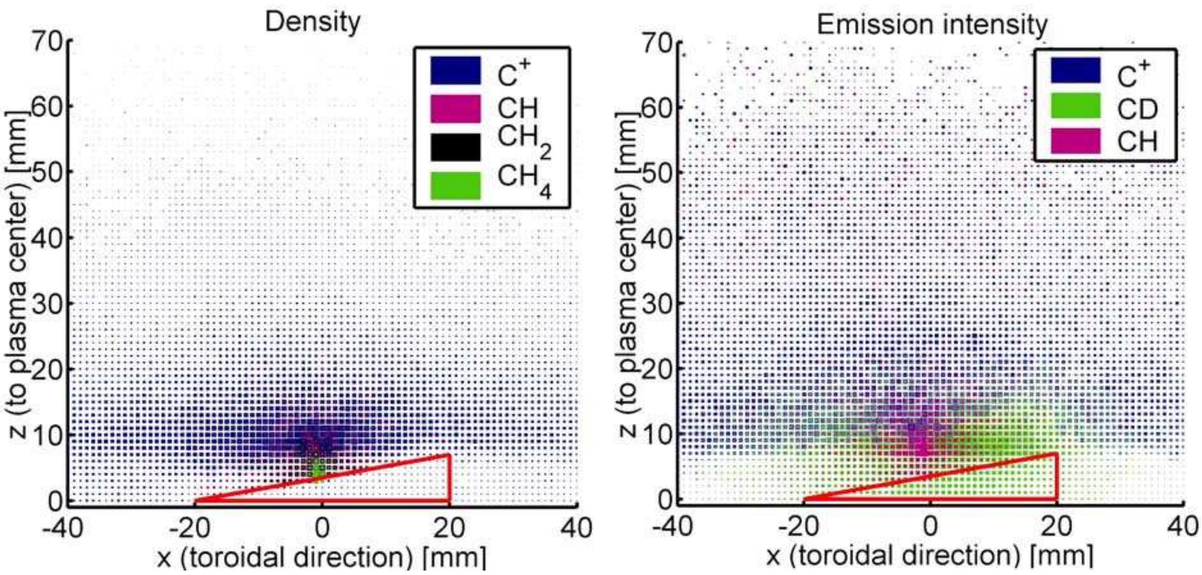

Fig. 2. Distribution of CH_4 and decay products: density (left) and light emission (right) in the observation volume (side view, 20mm nozzle radius, α=10°).

filled from (removed to) the substrate. Initially we start with a pure Fe surface (substrate material), where the C is later deposited and re-eroded. We can separate carbon deposited from the background plasma, from the injection and re-deposited. So we follow totally 4 surface species.

Nozzle geometry is similar to a cylinder (Fig. 1), however in the modelling the upper disk-like surface generally is inclined by a certain angle α. This angle is an independent parameter which can be used to analyse the influence of different effects, e.g. the zone near the nozzle, where the plasma density is smaller [2], grows if α increases. In our modelling we used α=1°, to avoid the extreme case of α=0°, where the tokomak toroidal magnetic field and, thus, the flux of plasma particles, is parallel to the surface. We have modelled the nozzle radii from 5mm to 40mm. The observation volume of 80x80x70mm is large enough to contain the most part of CD and CH particles in all cases. The disk nozzle surface was separated into cells 1x1mm. To represent a non-point source (the area, where injection took place was comparable to the total size of the nozzle surface) the test-particles of injected gas were equally split between the cells passing into the disk defined by $R_{Inj.}$ (Fig. 1). They started from the centre of each cell with a cosine distribution.

Parameter study. An important parameter of our modelling is the effective sticking of hydrocarbons to the surface. We have modelled two extreme cases: 'S1' means that every CH_x molecule coming to the surface is deposited as C. 'S0' supposes that every molecule coming to the surface triggers a new CH_4 to go into the plasma. This represents so-called self re-erosion. Atomic or ionic C is deposited or reflected according to the TRIM data. In case 'S1' the emission of CH is lower by a factor of about 2. This means that recycling can contribute a considerable part into the emission.

In the tokamak plasma boundary electron density n_e and temperature T_e decrease exponentially towards the plasma edge. They can be characterised by a decay length λ and a value at LCFS (Fig. 3). For a plasma parameter study we have taken plasma conditions obtained at TEXTOR ('Case 1') and assumed effective sticking 'S0'.

The value of n_e at LCFS was varied from $1*10^{12}$ to $8*10^{12}$ cm^{-3} (all other parameters were fixed). Due to higher dissociation and ionization rates the penetration depth of CH_4 and its decay products decreases for higher densities. This leads to a decrease of CH and C total flux in the observation volume. However that dependence is slower than the roughly linear proportionality of emission to n_e. Therefore, the emission of CH and C grows with an increase of n_e. The total flux of CD grows due to the higher chemical erosion of CD_4 on the gas inlet surface due to the higher deuterium influx. The latter is proportional to n_e and the flow velocity, which equals the sonic velocity c_s. So, the emission of CD grows even faster than the one of CH.

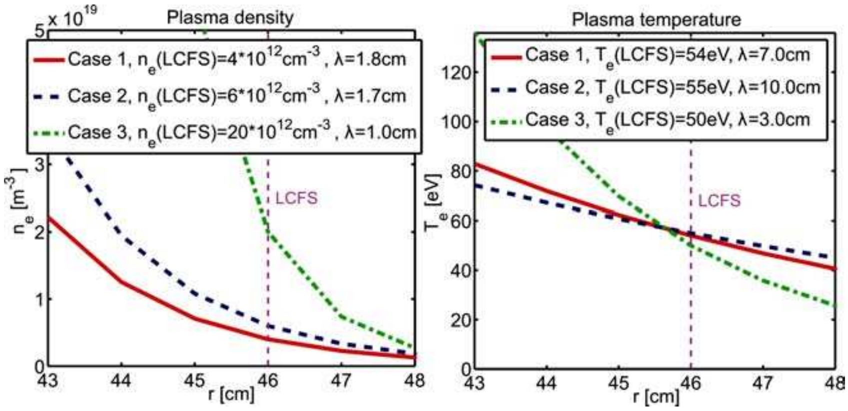

Fig. 3. 3 cases of plasma density (left) and temperature (right) in dependense of tokamak minor radius r.

The value of T_e at LCFS was varied from 10 to 100eV (all other parameters were fixed). For higher temperatures penetration depths (and so the total fluxes) of hydrocarbons decrease due to higher dissociation rates. In addition the maximum of their density moves towards the plasma edge (closer to the disk nozzle surface), where n_e is smaller. Therefore, the emission of hydrocarbons including CD decreases. At higher T_e the erosion of CD_4 increases due to the higher flow velocity $c_s \sim T_e^{1/2}$.

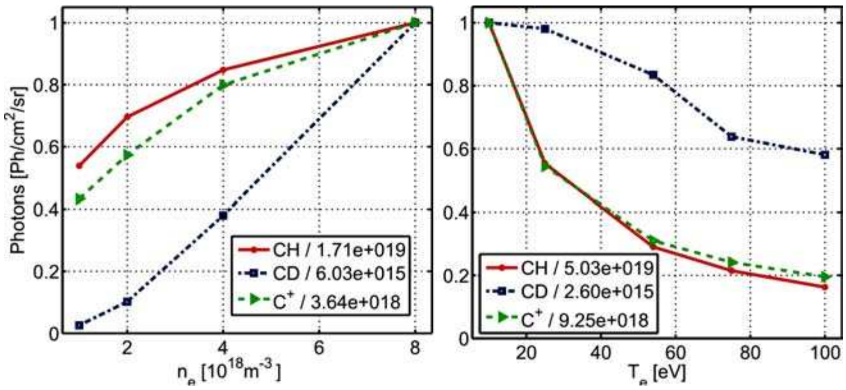

Fig. 4. Total emission of CH, CD and C^+ in dependence on the value of n_e (left) and T_e (right) at LCFS.

D/XB values are proportional to the CH_4 injection rate (in modelling it was fixed to $1.75*10^{19}$mol/s, similar in the experiment) divided over the emission intensity, thus everything that was mentioned before concerning emission is reverse to the D/XB.

One could expect that with an increase of the disk-like nozzle surface size the recycling on it should grow. Our modelling says that for a given range of plasma conditions and limiter sizes the influence of this effect on CH emission (D/XB) is negligible for any effective sticking assumptions, though the deposition rate of C in 'S1' case is much higher. The CD flux (after decay of CD_4 chemically released from surface) and its emission clearly grows, however it does not contribute much to the D/XB values. To represent the unstable deposited molecular layer the chemical re-erosion yield of CD_4 was increased by a factor of 5, which leads to an according increase of CD light. However, even by an unrealistically high chemical yield, the CD light intensity is several orders of magnitude less than the one of CH coming from the injection. By the larger surface inclination angles there is more C deposition, however even with an angle of 20° the influence of surface size on D/XB is minimal. Most part of C deposition occurs in the injection zone, or just within several mm from it. This means that even the smaller 'nozzle' is big enough to cause most part of the recycling.

It should be noted that we have not investigated the dependence on the injection rate and the influence of the higher hydrocarbons. These investigations are foreseen in the future.

Comparison with experiment. In the experiment two gas inlets were used. One had a radius of 5mm, another of 20mm. The CH_4 was injected through a number of small tubes situated inside the 4mm circle in the centre of the disk (round injection zone). The spectroscopic measurements were carried out for several series of equivalent TEXTOR discharges (with and w/o NBI). The boundary plasma n_e and T_e (Fig. 3) were measured by the He beam diagnostic [3]. In this paragraph by 'CD' we mean a combination of both CD and CH species.

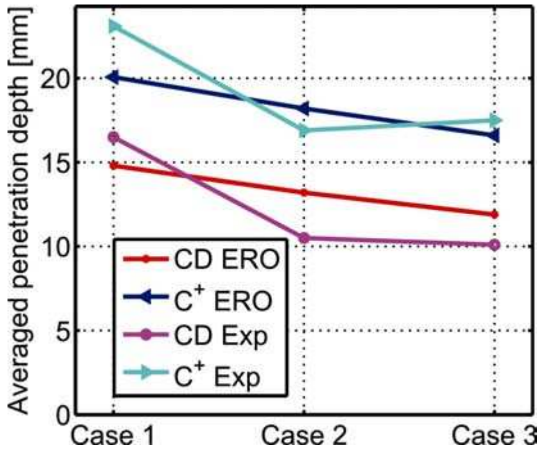

Fig. 5. Averaged penetration depth in dependence on plasma conditions.

The shape and width of the CD and C^+ profiles along the beam of injected particles are in a general agreement with the modelling. The measured profiles show the same tendencies as the modelled ones: for example the measured emission of CD injected through the larger nozzle penetrates deeper into the plasma, which is also seen in the modelling. The average penetration depths (absolute values) of species along the profile obtained for different plasma conditions are also in a good agreement with modelling (Fig. 5).

The modelling gives values of D/XB for CD of about 100, which is in general agreement with the experimental data obtained previously.

Conclusion. *The reasonability of modelled hydrocarbon transport pattern and the general agreement of modelling results with experimental data shows that ERO code can be used to calculate the D/XB values for CH and CD in boundary plasma of tokamaks. The values depend mostly on plasma parameters (decrease with increasing plasma density and increase with increasing temperature), whereas the influence of the inlet surface size is negligible (in the considered range of $R_{noz.}$ larger than 5mm and at injection rates much larger then the intrinsic hydrocarbon influx). Though the gas injection is useful for comparison between modelling and experiment, the intrinsic hydrocarbons can be modelled as well.*

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