

Modelling of $^{13}\text{CH}_4$ injection through graphite and tungsten test limiters in the scrape-off layer of TEXTOR using the coupled ERO-SDTrimSP code

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Introduction. The present choice of first wall materials in ITER [1] will lead to the formation of mixed carbon (C), tungsten (W) and beryllium (Be) layers. The influence of these layers on life time of wall components and particular on tritium retention is unclear. Therefore, predictive modelling of erosion processes, impurity transport and deposition processes is important. For this the 3D Monte-Carlo code ERO can be used [2]. ERO calculates the plasma wall interaction and follows released impurities in a given background plasma.

Until now, the surface in ERO was described as a homogeneous material mixture in a given interaction layer. To improve this simple approach, ERO has been coupled to the Monte-Carlo code SDTrimSP (a version of TRIDYN [3]). SDTrimSP uses the binary collision approximation to describe the transport of ions inside a given surface. It calculates the depth resolved material concentration caused by the implantation of particles into the solid.

Code Coupling. The SDTrimSP calculation of projectile and recoil atoms movements in the solid leads to reflected and sputtered atoms. These are in turn handed over to ERO to calculate the transport in the plasma. For a direct coupling of ERO and SDTrimSP it was necessary to increase the number of test particles followed in SDTrimSP compared to the number of test particles in ERO such that the statistical error in SDTrimSP is sufficiently small and the computation time for the coupled code remains acceptable [4]. Since SDTrimSP does not consider chemical processes, a method has been developed to implement chemical erosion of carbon by impact of hydrogen projectiles. Each time a hydrogen projectile is stopped in the surface at a certain depth there is a chance to form CH_4 . One fraction of the created CH_4 is formed at the stopping depth (reaction of thermalised ions enhanced by radiation damage [5]) and the other fraction at the upmost surface layer (ion-induced desorption of hydrocarbon radicals [5]). Additionally, the given erosion yield is proportional to the incident flux (and not to the number of stopped projectiles) and, therefore, the chemically eroded amount of carbon is scaled up to account for the reflected hydrogen projectiles.

Experiments at TEXTOR. Modelling with the coupled code ERO-SDTrimSP was compared with TEXTOR experiments which were carried out to study the formation of mixed surface layers. In these experiments methane $^{13}\text{CH}_4$ was injected through drillings in graphite and tungsten spherical limiters into the plasma. A pronounced dependence on the substrate of the deposition was observed although the experiments were carried out in identical experimental

conditions [6]. The deposition efficiency, i.e. the ratio of locally deposited carbon ^{13}C to the amount of injected one, was 4% for graphite and 0.3% for tungsten. The deposition-dominated area on the graphite limiter covers a five times larger area than on the tungsten limiter.

These experimental results could not be explained by simulations with ERO using the surface model with a homogeneous material mixture in the interaction layer which leads to ^{13}C deposition, which is only weakly dependent on the substrate material.

Comparison of experiments with ERO-SDTrimSP modelling. Measurements of electron density and temperature in the scrape-off layer of TEXTOR with a helium atomic beam diagnostic deliver the background plasma for the simulation. To benchmark ERO-SDTrimSP three independent measurements have been compared with simulations: 2D light emission of CH and CIII lines above the limiter, carbon ^{12}C deposition from the background plasma on the limiter and 2D carbon ^{13}C deposition on the limiter induced by $^{13}\text{CH}_4$ injection.

Figure 1 shows radial and toroidal profiles of the measured emission compared to simulated profiles for different positions of the last closed flux surface (LCFS) which has some uncertainty due to limited experimental accuracies (e.g. the plasma parameters are not measured

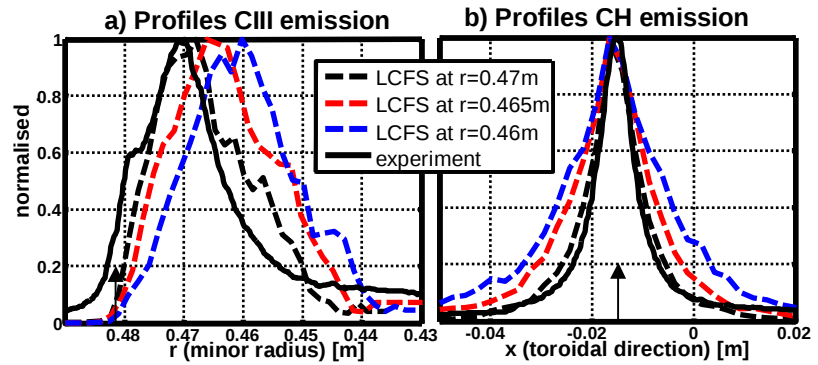


Figure 1: Comparison of light emission profiles in front of the limiter. a): radial profile of CH emission for the toroidal injection location at $x = -0.015\text{m}$, b): toroidal profiles of CIII emission at the maximum of radial profiles. The arrow indicates the location of injection.

at the poloidal position of the limiter). With the LCFS at $r = 0.46\text{m}$ and $r = 0.465$ the simulated maximum of the radial profile for CIII emission is too far away from the location of injection (Figure 1a). These assumptions for the position of the LCFS also lead to a toroidal CH emission profile, which is too broad compared to the experimental profile (Figure 1b). The best agreement is achieved with the LCFS at $r = 0.47\text{m}$: the location of the experimentally observed maximum in radial direction and also the width of the radial CIII emission is well reproduced. The toroidal profile of the CH emission for the LCFS at $r = 0.47\text{m}$ is in good agreement with experiment. Assuming that the used rate coefficients for the hydrocarbon reaction chain [7] and the excitation rate coefficients for the light emission of hydrocarbon and carbon [8] are well known, one can conclude that the transport processes through the considered plasma in the vicinity of the limiter are sufficiently well understood.

Comparison of modelling and experimental results of the ^{12}C deposition from the background plasma impurities on the limiter surface has been used to determine the ^{12}C

concentration in the background plasma. To reproduce the experimental transition from an erosion dominated zone to deposition dominated zone at a toroidal distance $x=0.02\text{m}$ to $x=0.03\text{m}$ from the middle of the limiter due to ^{12}C background impurity impact a ^{12}C concentration of about $3.5\%\pm 0.5\%$ must be assumed in the simulations.

To characterise the parameters which influence the local ^{13}C deposition from the injection a comprehensive parameter variation has been carried out. The influence of the substrate (W and C) on the deposition efficiency and pattern has been observed in the modelling for a range of the parameters: injection rate S_i , effective sticking coefficient for hydrocarbon molecules S_{eff} , chemical erosion Y_{chem} and enhanced chemical erosion of redeposited carbon Y_{RE} .

Injection rate S_i : To observe a clear influence of the substrate on the deposition it is not sufficient to simulate the flat top phase of the injection in the plasma discharge ($S_i=3.5\cdot 10^{19}\text{ s}^{-1}$ for 2s), but either a mean injection rate ($S_i=1.5\cdot 10^{19}\text{ s}^{-1}$ for the whole discharge $\sim 5\text{s}$ including periods without injection) or a time dependent injection rate (deduced from a gas test shot). A high injection rate leads to complete coverage of a larger region around the injection hole of the tungsten limiter by a thick carbon layer so that further deposition is not influenced by the substrate tungsten.

Effective sticking coefficient for hydrocarbon molecules S_{eff} : If one assumes non-negligible effective sticking of hydrocarbon molecules returning to the surface the modelled deposition efficiency shows as well no substrate dependence and is too high compared with the measurements (e.g. for $S_{eff}=0.5$ the deposition efficiency becomes $\sim 40\%$ on both limiters). $S_{eff}=0$ must be used instead which can be explained by the assumption that every hydrocarbon molecule hitting the surface first enters a weakly bond precursor state which will suffer from immediate ion-induced re-erosion preventing deposition.

Enhanced chemical erosion of redeposited carbon Y_{RE} : While the chemical erosion Y_{chem} of graphite in the order of 1-3% does not have a big influence on the deposition efficiency, the enhanced chemical erosion of redeposited carbon Y_{RE} directly influences the deposition efficiency (figure [2]). For $Y_{RE}=Y_{chem}=0.015$ the deposition pattern and efficiency on the carbon and tungsten test limiter is very similar at around 10%. At about $Y_{RE}=0.15$ the difference of the deposition on the two limiters reaches a maximum. At very high values for Y_{RE} the tungsten and also the carbon test limiter are erosion dominated apart from a very small area close to the injection location. Therefore, at these high values of Y_{RE} the substrate dependence of the deposition decreases again. Laboratory

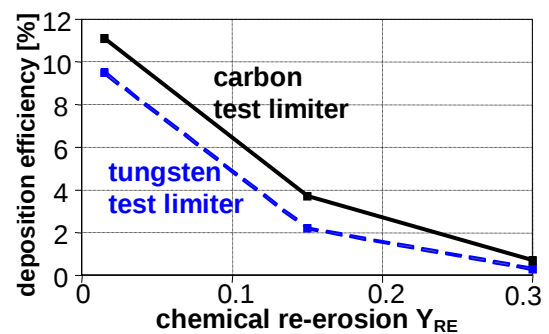


Figure 2: Deposition efficiency in dependence on the chemical erosion of deposited carbon on the carbon and tungsten test limiter.

experiments and earlier modelling of Tokamak experiments showed that especially soft amorphous hydrocarbon layers can have chemical erosion yields of the order of 0.15 similar as the modelling suggests [9,10].

The best match of the deposition pattern of the ^{13}C deposition on the limiter of the experiment compared to the simulation can be seen in figure [3]. The shape and the spread of the deposition are in fair

agreement. Analysis of profiles through the patterns reveal that the

maximum of the carbon deposition in the simulation is generally 3-5mm too far away from the injection location at $s=0\text{mm}$ and especially the overall deposition on the graphite limiter is not high enough (deposition efficiency on graphite 1.8%, on tungsten 0.3%).

Conclusions. Modelling with the coupled code shows clear substrate dependence and a well reproduced deposition efficiency of about 2% on the graphite and about 0.3% on the tungsten limiter. One reason for the substrate dependence is due to the higher physical sputtering yield of a thin carbon film on top of tungsten substrate compared to the yield of pure C. The remaining discrepancy of the C deposition on graphite to the experiment can be accounted to the higher surface roughness of the graphite limiter, which is not yet included into the model. To reproduce the deposition with ERO-SDTrimSP it is necessary to assume negligible effective sticking of hydrocarbon radicals on plasma facing surfaces and also a largely enhanced erosion of re-deposited C (yield about 0.15) compared with the erosion of substrate C. This can be explained by the enhanced erosion of formed amorphous C-layers with high hydrogen content as a result of C redeposition with low energy.

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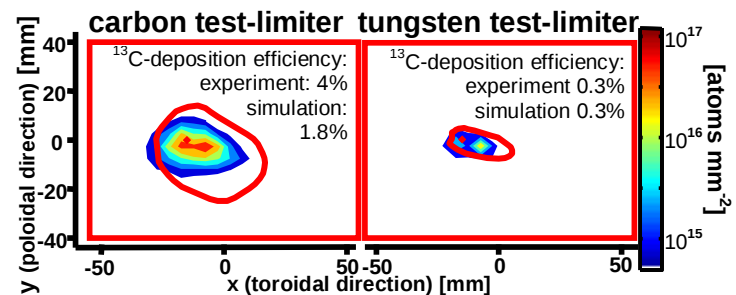


Figure 3: Comparison of measured and simulated 2D ^{13}C -deposition on the carbon and tungsten test limiters – view from above. False colour contour is the simulated deposition (lower than the detection limit of colour fringe analysis is not shown: $5 \cdot 10^{14}$ atoms mm^{-2} ~10nm layer thickness), the red curve shows the boundary of the deposition pattern from experimental colour fringe analysis.