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**Review on global migration, fuel retention and modelling after TEXTOR decommission**

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Review on global migration, fuel retention and modelling after TEXTOR decommission


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ABSTRACT

Before decommissioning of the TEXTOR tokamak in 2013, the machine was conditioned with a comprehensive migration experiment where MoF6 and 15N2 were injected on the very last operation day. Thereafter, all plasma-facing components (PFCs) were available for extensive studies of both local and global migration of impurities – Mo, W, Inconel alloy constituents, 15 N, F – and fuel retention studies. Measurements were performed on 140 limiter tiles out of 864 throughout the whole machine to map global transport. One fifth of the introduced molybdenum could be found. Wherever possible, the findings are compared to results obtained previously in other machines. This review incorporates both published and unpublished results from this TEXTOR study and combines findings with analytical methods as well as modelling results from two codes, ERO and ASCOT. The main findings are:

• Both local and global molybdenum transport can be explained by toroidal plasma flow and E × B drift. The suggested transport scheme for molybdenum holds also for other analysed species, namely tungsten from previous experiments and medium-Z metals (Cr-Cu) introduced on various occasions.
• Analytical interpretation of several deposition profile features is possible with basic geometrical and plasma physics considerations. These are deposition profiles on the collector probe, the lower part of the inner bumper limiter, the poloidal cross-section of the inner bumper limiter, and the poloidal limiter.
• Any deposition pattern found in this TEXTOR study, including fuel retention, has neither poloidal nor toroidal symmetry, which is often assumed when determining deposition profiles on global scale.
• Fuel retention is highly inhomogeneous due to local variation of plasma parameters – by auxiliary heating systems and impurity injection – and PFC temperature.
• Local modelling with ERO yields good qualitative agreement but too high local deposition efficiency.
• Global modelling with ASCOT shows that the radial electric field and source form have a high impact on global deposition patterns, while toroidal flow has little influence. Some of the experimental findings could be reproduced. Still, qualitative differences between simulated and experimental global deposition patterns remain.

The review closes with lessons learnt during this extensive TEXTOR study which might be helpful for future scientific exploitation of other tokamaks to be decommissioned.

1. Introduction

For future energy production, fusion is considered a viable option due to abundant supply of raw materials needed for fusion power production, namely lithium and deuterium, and due to the absence of both greenhouse gases and long-lived radioactive waste [1,2]. But for fusion to be successful it must also be economically viable. Power production increases with the volume of the fusion plasma [3]. On the
other hand, the fusion reactor itself should be as small as practically achievable for economic reasons; especially the reactor wall should be a close fit to the plasma boundary to reduce material costs, e.g. for magnetic systems. This in turn would increase the interaction between the hot fusion plasma and the reactor wall, accelerating wall erosion and requiring maintenance during lengthy and expensive shut-downs. Plasma-wall interaction (PWI) is thus a key area of research within fusion plasma physics to make energy production by fusion not only possible, but also cost-efficient.

PWI is a combination of many different physical and chemical effects, varying greatly with the plasma facing material (PFM) of interest. Comprehensive literature on PWI can be found for instance in [4]. PFMs are selected mainly due to high melting point, good thermal conductivity, low erosion under plasma particle impact and chemical inertness in a hydrogen-rich environment. Behaviour under high neutron irradiation is another very important topic when considering PFMs, due to transmutation and material damage effects, but is ignored in this paper because TEXTOR did not produce significant amounts of neutrons during its lifetime. A comprehensive list of which qualities make a good PFM can be found for instance in [5]. No known material can fulfill the full set of requirements to become an optimal PFM. It is thus crucial to select a material whose drawbacks can be handled in a future fusion reactor. At the time of writing, the first choice for a reactor PFM is tungsten [6].

Tungsten is characterised by its high atomic number, melting point and thermal conductivity, as well as low sputter yield, low fuel retention and low activation by neutrons. On the other hand, it causes high radiative power loss [7], plasma dilution by introducing large numbers of electrons [8] and under certain condition accumulates in the plasma centre where it is most harmful [9]. Benefits and drawbacks of tungsten as PFM are extensively covered in the literature, e.g. in [10–17]. It is clear that erosion of any PFM cannot be avoided in a tokamak, and that tungsten is superior to many other elements in this regard. However, it must not be transported into the confined plasma region if the largest impurities is removed from PWI. What governs this transport? And is there a qualitative difference between high-Z elements and others?

To answer these questions numerous experiments were conducted in several tokamaks over the last decades – a selection can be found in [14,18–23]. The most comprehensive one however was the mapping of several elements throughout a complete tokamak, i.e. the plasma-facing components (PFCs) study after the decommissioning of TEXTOR. Directly before the decommissioning, TEXTOR was conditioned with a tracer experiment comprising MoF₆ and ¹⁵N injection. We will describe the findings of this study concerning all analysed species – the volatiles deuterium, nitrogen, fluoride (volatile by forming fluorocarbons [24]) as well as the non-recycling metals tungsten, molybdenum and the metals ranging from chromium to copper – and compare them to results from other studies. In this paper, the species are classified as low-Z (≤ 10), medium-Z (11 ≤ Z ≤ 36) or high-Z (Z > 36). We will compare the findings to modelling of high-Z transport of eroded impurities in the plasma edge and the scrape-off layer (SOL) in TEXTOR. Lessons learnt from the decommissioning of a machine and the subsequent scientific exploitation will finalise the paper.

2. Experimental

In this section the machine TEXTOR is introduced where the research was carried out, followed by a description of the very last high-Z tracer experiment prior to decommissioning. We will then introduce the methods used for analysis with their advantages and shortcomings, and how the raw data was treated to retrieve the sought information. The section closes with a discussion about uncertainties.

2.1. The TEXTOR tokamak

The TEXTOR tokamak had been chosen for several reasons for this study. First, the planned decommissioning offered the opportunity of access to all PFCs. Second, it was a machine dedicated to PWI research and offered flexible tools for material transport investigation: test limiter with a gas inlet [25] and monitoring spectroscopy [26], a collector probe [27,28], movable main limiters [29] and movable poloidal limiters with gas inlet. In this study, the two first tools were the most important ones. A comprehensive review of PWI studies at TEXTOR can be found in [30]. The third reason to choose TEXTOR was its PFM: the tokamak was a carbon machine. From the analysis point of view, carbon as a PFM makes it easy to trace heavier impurities with conventional ion beam analysis (IBA) methods which were also employed in this study. As will be discussed in Section 4.4, results from the TEXTOR limiter plasma gives implications for divertor machines as well, with some limitations.

Fig. 1a shows a view in the direction of the magnetic field with the different components explained in Fig. 1b. TEXTOR had a pumped belt limiter as main PFC, an inner bumper limiter, a set of poloidal limiters and a set of divertor limiters with gas inlet. In this study, the two first tools were the most useful access to all PFCs. Second, it was a machine dedicated to PWI research and presented flexible tools for material transport investigation: test limiter with a gas inlet [25] and monitoring spectroscopy [26], a collector probe [27,28], movable main limiters [29] and movable poloidal limiters with gas inlet. In this study, the two first tools were the most important ones. A comprehensive review of PWI studies at TEXTOR can be found in [30]. The third reason to choose TEXTOR was its PFM: the tokamak was a carbon machine. From the analysis point of view, carbon as a PFM makes it easy to trace heavier impurities with conventional ion beam analysis (IBA) methods which were also employed in this study. As will be discussed in Section 4.4, results from the TEXTOR limiter plasma gives implications for divertor machines as well, with some limitations.

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The largest PFC was the inner bumper limiter (IBL), covering the inner circumference by 120° poloidally. There were 64 tile rows in the toroidal direction with 10 tiles each in the poloidal direction, covering a total area of 8,7 m². The radius of curvature in the poloidal direction was 0.49 m [36], i.e. different from the plasma radius of curvature of 0.46 m. This detail will become important in later discussions of deposition profiles.

The poloidal limiters were situated at one toroidal position, with two arrays at the top and bottom of the vessel and 2 cm behind the LCFS at the time of the experiment. Each array consisted of five “stones”, semi-circular carbon bricks of 6,5 cm radius and 4,5 cm width. Its area was roughly 0,1 m² and hence insignificant in comparison to other limiters.

Finally, there was the possibility to insert different test limiters through a limiter lock at the vessel bottom, connected to a gas reservoir for gas injection [25] and monitored from the side by four spectroscopic systems [26]. The test limiter used in this study was a single-roof shaped graphite block, with a polished graphite collector plate on top [42]. All limiters are depicted schematically in Fig. 2 while Fig. 3 shows photographs of PFCs.

2.2. The MoF₆ tracer experiment

As final experiment before the decommissioning of TEXTOR a tracer experiment was conducted with MoF₆ and ¹⁵N₂ (shots no. 120 964 – 121 007, also including preparation and calibration shots). The aim was to create molybdenum and ¹⁵N deposition patterns on the PFCs for subsequent studies when all PFCs have become available due to the decommissioning, with the emphasis on molybdenum. The reason to use molybdenum instead of the actual element of interest, tungsten, was that an undetermined background of tungsten deposition from previous WF₆ injection – from a WF₆ experiment described in [23] and from spectroscopy calibration – was expected. Molybdenum background due to previous experiments with molybdenum test PFCs and due to the molybdenum concentration in the liner Inconel were assumed to be smaller and also more homogeneous. The reason not to use a neighbouring element of tungsten was both the small mass resolution for high-Z elements with IBA methods, as described below, and the fact that no neighbouring element can be contained in gaseous molecules at room temperature. An overview of issues related to tracer experiments and their evaluation is summarised in [43]. The discharges used were standard NBI discharges with 350 kA plasma current, a toroidal field of 2,25 T and 1,7 MW co-injected NBI power. The minor plasma radius was 0.46 m. Neither ICRH nor DED was in operation during the experiment. A discharge time line is displayed in Fig. 4a.

MoF₆ was injected for 1 s through the gas channel in the single-roof test limiter described above (see also Fig. 3) during the 5 s flat-top phase of 31 discharges of 6–7 s duration. The gas injection was monitored from the side by cameras and imaging spectrometers (Acton Research Corporation, SpectraPro 500) with a filter for 395 nm to monitor FII and MoI lines at 402 nm and 390 nm, respectively. Line intensities for molybdenum and fluorine can be seen in Fig. 4b. The overall amount that left the calibrated volume during these integrated 201,5 s was ca. 1.4 · 10²¹ molecules, whereof only 40% or 5.7 · 10²⁰ molecules reached the vessel through the gas inlet in the test limiter. Hence only these 40% were introduced into the tokamak while the rest was lost in the piping. This number was obtained by analysing the MoI line radiation at 390 nm and calculating the amount of injected molybdenum atoms via the so-called S/XB values which relate line intensity with the inward flux of atoms [44]. Signal analysis of the in-vessel pressure gauge yielded a comparable value of one third of the 1.4 · 10²¹ molecules. We want to stress that such problem was not experienced with WF₆ and hence is due to the difference between MoF₆ and WF₆, most probably the higher boiling point of MoF₆. The issue is further discussed in [42] and Section 3. In the following, relative molybdenum amounts always refer to the injected amount, i.e. with respect to the 5.7 · 10²⁰ molecules which evidently reached the inside of TEXTOR.
Apart from MoF₆, also $^{15}$N₂ was injected 90° toroidally away from the test limiter. Impurity seeding is a method for improved edge radiation (cooling) especially in operation with high-Z plasma-facing components (PFC) [45–47]. The injection of neon (Ne), argon (Ar), or nitrogen (N₂) is performed for that purpose. Nitrogen-assisted glow discharge cleaning was also considered for fuel removal [48]. It has been noticed that a fraction of the injected species is retained in the wall [49,50]. In the case of ex-situ analyses of nitrogen in PFC there was a question whether the measured amount was reflecting the amount of gas retained during the tokamak operation nitrogen or adsorbed from air when samples were exposed to air. To resolve this problem tracer experiments with a rare isotope of nitrogen ($^{15}$N, natural abundance 0.37% versus 99.63% of $^{14}$N) were proposed and performed first at TEXTOR [23,51] [52] and then in several other machines, like ASDEX Upgrade [53] and JET with the ITER-Like Wall [54].

The total amount of injected nitrogen atoms was $5.3 \cdot 10^{21}$. Memory effects caused accumulation of nitrogen in the plasma and led to two disruptions, see Fig. 4c. Such memory effects were experienced before at TEXTOR [50] and also at JET [55,56], hence it is a common problem with nitrogen. $^{15}$N₂ was hence only puffed during 22 discharges. Helium GD cleaning was performed between every 3–5 discharges for five minutes with a 300 V wall potential. The test limiter was retracted during GD cleaning. The last disruption occurred 11 shots before the end of the experiment. No memory effect could be seen for fluorine, see also Fig. 4c.

After the experiment, venting and machine clearance, the first action was dust sampling with carbon stickers (details on sampling and analysis are given in [57]), thereafter all PFCs were dismounted and packed in plastic bags. The Inconel ALT blades were then removed for deposit scraping from backsides and neutraliser plates for later analysis. Finally, pieces from the liner were cut with a circular saw for studying this structural component (details on sampling and analysis are given in [58]). The PFC, liner and dust samples were then shipped to the Ångström Laboratory at Uppsala University, Sweden, for IBA studies, cataloguing and re-distribution to other laboratories.

2.3. Analysis

Most analysis was conducted with IBA at the Tandem Laboratory at Uppsala University. IBA methods were: Rutherford backscattering...
yielding 571 measurement points. We employed a 4He\(^2\) beam at 2140 tiles from ALT-II and IBL, plus further PFCs from other locations, and the SIMNRA program [61]. An exemplary RBS spectrum from a TEXTOR main PFC is shown in Fig. 5a. Under the assumption that all elements have homogeneous depth distributions except for a surface peak or depletion in the first 50 - 150 µm, and representing all medium- to heavy elements, one of the heavier main constituents, nickel, for calculation purposes, identification of all elements with their substrate concentration plus their surface enrichment or depletion is straightforward. In some cases, highly inhomogeneous elemental depth distributions make RBS spectra rather challenging for interpretation, as can be seen in Fig. 5b.

Another important IBA method, complementary to RBS, is ERDA. The system used for the measurements in this study was built in the investigation period. Most measurements were conducted with the system described in [62], whereas an improved system described in [63] became only available in the experiment described above. Since it should document local deposition profiles, a dense mapping was required, which is easier to archive with electron beam methods. Here, EPMA was employed to measure concentrations of B, N, O, F, Ti and Mo with one point of measurement every 2 mm. Titanium was used on catcher plates at the sides of the test limiter. EPMA measurements were conducted with a 15 keV electron beam using wavelength dispersive spectroscopy. Close to the gas inlet (ca. 1 cm) the re-deposited film was too thick to be penetrated by the electron beam even at 30 keV. The film thickness was thus probed with SIMS at two different positions, yielding a deposited layer of up to 6 µm thickness which built up during the 31 tracer injections. SIMS is not quantitative for films with a priori unknown properties and cannot be employed to assess the overall amount of deposited elements, which was crucial for molybdenum. Therefore EPMA at Ångström laboratory was used to quantify at least the molybdenum amount. In our case, protons at 2 MeV were used which increases the depth range to ca. 15 µm instead of about 2 µm with 4He RBS. The disadvantage is a greatly reduced energy resolution, which makes it only possible to separate light from heavy elements. EPMA was thus solely used to quantify molybdenum as sole heavy element on the catcher plate.

2.4. Uncertainties and data treatment

Uncertainties for RBS and NRA are a combination of three effects: uncertainties in the beam current integrator (10% relative), uncertainties in beam-target cross-sections (around 10% relative), and
statistical uncertainties (around 6%). For RBS the signal overlaps from different elements create some ambiguity in analysis. For ERDA ambiguity arises due to multiple scattering, roughness, and stopping power uncertainties, the latter being maximum 10% for iodine in most materials [64]. Quantification errors by multiple scattering and surface roughness are hard to account for—extensive literature exists for treating this topic, e.g. [65,66,67] and references therein. Due to the fact that the investigated samples are mostly of graphite, a rough light material, roughness dominates the uncertainty. Estimations of roughness impact on quantification with SIMNRA [68] together with roughness studies of TEXTOR samples in [69] yield an uncertainty in quantification of 30%, i.e. the total uncertainty for ERDA is 35%. Quantification can thus be trusted within ± 20% for molybdenum and tungsten, for the IBA methods applied.

SIMS is not quantifiable in this study. Uncertainties in depth profiling could be assessed by studying the SIMS crater with stylus profilometry, showing inhomogeneous sputtering with height variations at the crater bottom of approximately ± 5 µm [42].

EPMA can quantify elements with about 5% uncertainty, plus another maximum 15% due to surface roughness. In total this yields ± 16% uncertainty for the quantification with EPMA on the graphite collector plate from the test limiter. Adequate data visualisation was crucial in this study to understand impurity transport patterns. Interpolation was used to cast the data points into a deposition map. For interpolation radial basis functions (RBFs) were used. RBFs can be used to interpolate any set measurement values $y(x)$ as functions of measurement position through sums of a certain type of function $f(r)$ where

$$y(x) = \sum_{i=1}^{n} w_i f(r) = ||x - x_i||$$

(1)

with $w_i$ being a weight factor, $n$ the amount of measured data points, and $||·||$ is a norm, usually Euclidean [70]. In this case $f(r) = r$ was used, i.e. a linear RBF, as simplest adequate function.

The deviation of the interpolation $y(x)$ from measured data varies strongly with position, see Fig. 8a. The scatter is not an artefact of the employed IBA method or the spectra evaluation but resembles how strongly tracer amounts can vary on centimetre scale. While the cause is discussed further in Section 3, for now it is important to note that these small scale (order of centimetres) variations near the source are not accounted for in the interpolation for due to smoothing. Such smoothing can be introduced by subtracting a fraction of the diagonal terms in the linear system of equations for calculation of $y(x)$. A certain level of smoothing is necessary to avoid negative concentration in some areas which is unphysical. However, smoothing at a too high level would erase valuable information about deposition patterns, see Fig. 8b. We chose the smallest smoothing yielding non-negative concentrations at all interpolated positions. The maps obtained from interpolation are used for qualitative discussion only while all quantitative analysis is based on the actual measured concentrations.

Discussion of results and physical interpretation in the subsequent sections is often done with the aid of fitted functions to the measured data. Fitting was performed with least square calculation for finding the
optimal fit. Those functions are used to describe and relate measured data, not for statistical purposes. The accuracy of fits is thus not discussed further but can be judged from the respective figures.

2.5. Expected species

TEXTOR was mainly operated with deuterium and hence fuel retention is measured by the amount of deuterium in the samples. The main PFCs were made out of carbon. The machine itself was wall-conditioned with deuterium and helium GD cleaning, and boronisation as well as siliconisation. Furthermore the liner and the ALT-II blade structure was made of Inconel 625 with composition given in Table 2.

The ICRH antennas were covered with stainless steel Faraday shields. The NBI systems had beam scrapers made of water cooled copper plates.

On top of that, despite GD cleaning usual impurities in vacuum systems are oxygen and hydrogen from water and residual air. These are the so-called “intrinsic” elements since they are introduced into the vessel by normal operation and maintenance. During experiments, many more elements and isotopes were introduced into TEXTOR over the course of years and decades. Table 3 lists all species together with their origin and further reading while Fig. 9 displays their positions. The table also shows which elements or isotopes released in the final TEXTOR experiment have in fact been found with IBA. Apparently, most of the listed elements and isotopes are traceable, in many cases with hints or even clear links to their point of origin. This is both a good and a bad message concerning impurity transport experiments: we are able to link the place of deposition to the origin for heavier elements (around iron and heavier) years after their introduction which encourages scientific exploitation of other tokamaks’ decommissioning; on the other hand, even lighter elements stay long in the vessel and make tracer experiments increasingly difficult as the “background” of leftover species gradually increases. In Section 4 it will become clearer how one can treat such background in the case of molybdenum, and how long residence times of elements in tokamaks can be turned to an advantage to develop and verify transport models.

2.6. Part I – experimental results and discussion

In the following sections, positions are described using minor radius (in centimetres, measured from the geometrical centre of the torus cross-section), toroidal distance (in degrees, zero at the molybdenum source, increasing in the direction of plasma current) and poloidal distance (in degrees, zero at the outer mid-plane, increasing in the counter-clockwise direction when looking in positive toroidal direction).

3. Tracer injection and local deposition

The injection of MoF$_6$ took place in the line-of-sight for the horizontal observation system described in [26], yielding two valuable pieces of information: (i) the amount of overall injected MoF$_6$, (ii) the radial distribution of molybdenum from the MoI line radiation. Fig. 10a shows the MoI line radiation during MoF$_6$ injection through the test limiter, Fig. 10b the cumulated intensity during one shot (no. 120,975) over radius at one lateral position. It can be described adequately by a Cauchy distribution [71]

\[
C(r) = A \frac{s^2}{s^2 + (r - r_0)^2}
\]

(2)

with 2 s as full-width-half-maximum (FWHM) and $r_0$ as centre. This can be understood when the gas is assumed to not form a directed jet normal to the inlet, but rather to expand isotropically. In such a case the amount of gas molecules per angle is constant and it follows for a projection on a radial line according to Fig. 10c:

\[
\frac{dn}{dp} = \text{const.} \Rightarrow \frac{dn}{dr} = \frac{dn}{dp} \frac{dp}{dr} = A \frac{s^2}{s^2 + (r - r_0)^2} \text{with } p = \arctan \left( \frac{r - r_0}{s} \right)
\]

Fitting parameters for the curve in Fig. 10b are: $s = 6, 3$ mm, $r_0 = 48, 3$ cm. The fit has been obtained directly at the lateral position of the gas inlet in Fig. 10a (red line) which shows that $s$ in reality does not only depend on the distance of projection as implied by Fig. 10c, because at the gas inlet $s$ would be zero. The maximum of measured MoI radiation is a bit closer to the gas inlet, at $r_0 = 48, 5$ cm.

When looking in the toroidal direction (horizontally in Fig. 10a) 6 mm above the inlet (i.e. $r = 48, 7$ cm), which is roughly at the position of highest intensity, the MoI radiation distribution is best described by a Cauchy distribution ($s = 5, 2$ mm, $x_0 = -10$ mm w.r.t. the inlet) multiplied by an exponential function with 7 cm e-folding length. The exponential component may be due to re-erosion taking place at the test limiter tip.

Local deposition of different elements is shown in Fig. 11, together with the obtained layer thickness. The plots are based on EPMA data,

<table>
<thead>
<tr>
<th>Element</th>
<th>Wt%</th>
<th>At%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ni</td>
<td>58</td>
<td>58</td>
</tr>
<tr>
<td>Cr</td>
<td>20-23</td>
<td>20,5</td>
</tr>
<tr>
<td>Fe</td>
<td>Max. 5</td>
<td>Max. 4,5</td>
</tr>
<tr>
<td>Mo</td>
<td>8-10</td>
<td>Ca. 4,7</td>
</tr>
<tr>
<td>Nb (+ Ta)</td>
<td>3,15-5,15</td>
<td>Ca. 2</td>
</tr>
<tr>
<td>Co</td>
<td>Max. 1</td>
<td>0,8</td>
</tr>
<tr>
<td>Mn</td>
<td>Max. 0,5</td>
<td>0,5</td>
</tr>
<tr>
<td>Al</td>
<td>Max. 0,4</td>
<td>0,7</td>
</tr>
<tr>
<td>Ti</td>
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<tr>
<td>Si</td>
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<td>0,9</td>
</tr>
<tr>
<td>C</td>
<td>Max. 0,1</td>
<td>0,4</td>
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</table>
Table 3
List of elements and isotopes in TEXTOR, their origin, literature (if available), and whether they were found during PFC analysis in this study. Found status: “Yes” – element/isotope was found after TEXTOR shutdown, “No” – no indication of this element found, “Unclear” – indication found but not enough for conclusiveness.

<table>
<thead>
<tr>
<th>Species</th>
<th>Origin</th>
<th>Literature</th>
<th>Found?</th>
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<td>D</td>
<td>Plasma (homogeneous)</td>
<td>[128]</td>
<td>Yes</td>
</tr>
<tr>
<td></td>
<td>GD cleaning</td>
<td></td>
<td>Yes&lt;sup&gt;1&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>Ion cyclotron wall conditioning</td>
<td>[129]</td>
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<tr>
<td></td>
<td>Boronisation/siliconisation</td>
<td>[128]</td>
<td>Yes&lt;sup&gt;1&lt;/sup&gt;</td>
</tr>
<tr>
<td>He</td>
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<td>[128]</td>
<td>Yes&lt;sup&gt;2&lt;/sup&gt;</td>
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<td></td>
<td>Ion cyclotron wall conditioning (Rutherford Scattering beam)</td>
<td>[74]</td>
<td></td>
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<tr>
<td>Li</td>
<td>Li beam</td>
<td>[58,131]</td>
<td>Yes</td>
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<tr>
<td>B</td>
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<td>[69,128]</td>
<td>Yes</td>
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<tr>
<td>C</td>
<td>Limiters</td>
<td></td>
<td>Yes</td>
</tr>
<tr>
<td>N</td>
<td>Air, plasma edge cooling experiments</td>
<td>[50, 69], [129], this paper</td>
<td>Yes</td>
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<tr>
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<td>[23, 69, 132], this paper</td>
<td>Yes</td>
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<tr>
<td>O</td>
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<td></td>
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<td>[129]</td>
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<td>Cover during test limiter experiments</td>
<td>[107]</td>
<td>Unclear</td>
</tr>
<tr>
<td>Si</td>
<td>Siliconisation</td>
<td>[128]</td>
<td>Yes</td>
</tr>
<tr>
<td>Cl</td>
<td>Shutdown work?</td>
<td></td>
<td>Yes</td>
</tr>
<tr>
<td>Ar</td>
<td>Plasma edge cooling experiments</td>
<td>[135–137]</td>
<td>Yes</td>
</tr>
<tr>
<td>Inconel, stainless steel</td>
<td>Liner, struct. components of ALT-II, ICRH Faraday shields,</td>
<td>[34], [73]</td>
<td>Yes</td>
</tr>
<tr>
<td></td>
<td>Test limiter experiments (LL1)&lt;sup&gt;3&lt;/sup&gt;</td>
<td>[118]</td>
<td>Unclear</td>
</tr>
<tr>
<td></td>
<td>Test limiter experiments (LL3)&lt;sup&gt;4&lt;/sup&gt;</td>
<td></td>
<td>Unclear</td>
</tr>
<tr>
<td>Cu</td>
<td>NBI scraper</td>
<td>[32]</td>
<td>Unclear</td>
</tr>
<tr>
<td></td>
<td>Poloidal limiter experiments for W7X</td>
<td>[88]</td>
<td>Yes</td>
</tr>
<tr>
<td></td>
<td>Test limiter experiments</td>
<td>[73]</td>
<td>Unclear</td>
</tr>
<tr>
<td>Mo</td>
<td>Mo test limiter experiments</td>
<td>[72, 84, 139]</td>
<td>Yes</td>
</tr>
<tr>
<td></td>
<td>Inconel components</td>
<td></td>
<td>Yes</td>
</tr>
<tr>
<td></td>
<td>MoF&lt;sub&gt;6&lt;/sub&gt; injection through test limiter</td>
<td>This paper</td>
<td>Yes</td>
</tr>
<tr>
<td>Ta</td>
<td>Collector probe cap (see Fig. 1a)</td>
<td>[28]</td>
<td>No</td>
</tr>
<tr>
<td>W</td>
<td>W poloidal limiter experiments</td>
<td>[85, 86]</td>
<td>Yes</td>
</tr>
<tr>
<td></td>
<td>W test limiter experiments</td>
<td>[72, 84, 86, 87, 101, 133]</td>
<td>Yes</td>
</tr>
<tr>
<td></td>
<td>WF&lt;sub&gt;6&lt;/sub&gt; injection through test limiter</td>
<td>[23]</td>
<td>Unclear</td>
</tr>
<tr>
<td></td>
<td>WF&lt;sub&gt;6&lt;/sub&gt; for calibration</td>
<td>[133]</td>
<td>Unclear</td>
</tr>
<tr>
<td>Re</td>
<td>Layer erosion at test limiters</td>
<td>[107]</td>
<td>No</td>
</tr>
<tr>
<td></td>
<td>Interlayer on poloidal limiters</td>
<td>[85]</td>
<td>Unclear</td>
</tr>
</tbody>
</table>

<sup>1</sup> D from the respective sources cannot be distinguished from other sources, but both GD and ICRH antennas have an impact on the deuterium deposition profile.

<sup>2</sup> He was found all around the vessel, but no link to the actual source can be drawn, neither to the impact of sub-systems.

<sup>3</sup> Limiter Lock 1, injection position of MoF<sub>6</sub> at 0° toroidally and 90° poloidally (bottom).

<sup>4</sup> Limiter Lock 3, at −112,5° toroidally and +90° poloidally (top).

Fig. 9. Schematic drawing of element sources in TEXTOR which will be relevant for later discussion – top view. The same orientation will be used in later interpolation maps.
combined with EPS data in the case of molybdenum. Most deposition takes place around the gas inlet, with molybdenum as main impurity (note that the colour bar is in $10^{18}$ cm$^{-2}$ instead of $10^{16}$ cm$^{-2}$ for all other elements). Although only MoF$_6$ was injected at the indicated position in Fig. 11 (arrow), also nitrogen and oxygen could be found. Nitrogen deposition exhibits a similar pattern to molybdenum and the deposition thickness. It was most probably deposited during the discharge along with molybdenum. ERDA analysis close to the gas inlet yields $^{15}$N/($^{15}$N + $^{14}$N) < 10%, i.e. most nitrogen is not from the simultaneous $^{15}$N tracer injection but in fact $^{14}$N, probably from earlier experiments and residual air in TEXTOR. Oxygen levels are very high only at the gas inlet itself. Titanium catcher plates were mounted on the side of the test limiter but hardly any titanium was deposited on the collector plate, without any correlation to the other elements. 6% of the injected

![Fig. 10.](image_url)

Fig. 10. a) Spectroscopic image of the MoI line radiation summed over all frames in shot no. 120 975, with fitting position (red vertical line) and test limiter (white dashed line); b) measured MoI line intensity (black, taken from Fig. 10a at the red vertical line) and fitted by a Cauchy distribution (red); c) isotropic point source, yielding a Cauchy distribution whenever the particle amount is projected on a vertical line at some distance s. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

![Fig. 11.](image_url)

Fig. 11. Deposition patterns on the collector plate on top of the test limiter, showing deposition thickness and the areal concentrations of molybdenum, nitrogen, fluorine, oxygen and titanium. The arrow indicates the position of the gas inlet. The plasma current goes from left to right, i.e. the limiter tip is to the right (see also Fig. 2a), and the HFS is to the top.
The deposited amount of molybdenum exhibits a Cauchy distribution both in toroidal and poloidal direction. Fits to the EPS data are displayed in Fig. 12. As with the MoI line, the fit in the toroidal direction is better for \( C(x) \cdot \exp(-x/\lambda) \) while in poloidal direction an unmodified Cauchy distribution suffices. Fit parameters are: \( s = 4, 6 \text{ mm} \), \( x_0 = -0, 2 \text{ mm} \), \( \lambda = 15 \text{ mm} \) (toroidally) and \( s = 3, 9 \text{ mm} \), \( x_0 = -0, 2 \text{ mm} \) (poloidally). Any constant offset is negligible.

Both the radial MoI line distribution and the lateral molybdenum deposition exhibit a Cauchy distribution, and therefore one might expect that the molybdenum simply moved down to the collector plate along the field lines. However, the lateral deposition on the collector plate cannot be obtained by projecting the radial MoI line distribution onto the collector plate along the magnetic field lines. The spreads of the deposition are smaller than for MoI (they should be about the same in poloidal direction, and a bit larger in toroidal direction due to projection at around 20°), and the toroidal distance from the gas inlet \( x_0 \)'s too small (it should be more than a factor 10 bigger).

As can be seen from Fig. 11, the molybdenum deposition is elongated towards the upper right corner, i.e. towards the high-field side (HFS, upwards in Fig. 11) and in the direction of the plasma current (to the right in Fig. 11). Such a pattern has been recorded also for methane [72] and silane injection experiments [73] as well as for tungsten [23] (for tungsten more details below). The elongation deviates almost exactly 45° from the toroidal direction in Fig. 11. Taking the test limiter inclination of 20° into account the real value is 48°. Hence the movement of the molybdenum atoms is equally fast in toroidal and poloidal directions. This movement cannot be explained by the magnetic field direction alone. In [72] and [73] the elongation is explained by combined SOL flow in toroidal direction and \( \vec{E} \times \vec{B} \) drift in poloidal direction due to a radial electric field. For various plasma scenarios the toroidal velocity of the plasma at the LCFS is in the order of a few km/s [74–76] (without DED). The poloidal velocity of the plasma in the SOL is also around a few km/s for different scenarios, with a flow reversal at or slightly inside the LCFS [75–77] for using nBI. More detailed information cannot be provided, considering error bars given in [75] and the fact that only one of the aforementioned sources (the oldest one: [74]) has data from the same plasma scenario. In any case all sources agree that the toroidal and poloidal velocities of measured impurities are within the same order of magnitude, which is in line with the deposition profile seen in Fig. 11 for molybdenum. Velocities of molybdenum ions moving along field lines, i.e. in the direction of \( \vec{E} \times \vec{B} \) (to the right in Fig. 11), would be in the order of 1 km/s for a few eV of kinetic energy from dissociation and collisions, just as the \( \vec{E} \times \vec{B} \) drift for a few kV/m electric field and 2.25 T magnetic field.

There is a coincidence between injected and deposited molybdenum, as can be seen from a SIMS depth profile measured 2 mm away from the gas inlet, Fig. 13. The maxima in the molybdenum depth profile correspond to enhanced injection quantities, as measured by the pressure gauge at the calibrated volume of the injection system. Similar depth profiles were only found on a few other PFCs with high molybdenum concentration and less clear coincidence. In all other cases the deposited layers were too thin in order to be resolved and one may assume a more or less homogeneous deposition profile further away from the impurity source, except for an eventual surface peak.

Evaluating data from a previous experiment with WF6 [23] shows a Cauchy distribution of the deposited tungsten as well, see Fig. 14. A Gaussian fit is displayed for comparison, proving that a Cauchy distribution fits the data better. The spread \( s \) is larger than for molybdenum, with \( s = 7, 7 \text{ mm} \). The typical elongation in the direction of plasma current and HFS was also observed, see Fig. 2 in [23], though with higher elongation in the poloidal direction than for molybdenum. The local deposition efficiency for tungsten was 1–3% [23] and hence smaller than for molybdenum (6%).

It was previously mentioned that only about 40% of MoF6 released from the calibrated volume eventually reached the vessel. We assume a substantial part of the remaining 60% could have decomposed in the inlet system. Therefore the test limiter was cut into pieces and RBS measurements were conducted along the injection channels. Both molybdenum and tungsten from MoF6 and WF6 injections could be detected, but only in negligible amounts. Details of the test limiter analysis are given in [42]. The rest of the inlet system was not available for analysis and hence it can only be speculated what exactly happened in the piping between calibrated volume and test limiter. The piping itself, starting at the calibrated volume and proceeding towards the vessel, consisted of a 0.3 m pipe with 6 mm outer diameter, a flexible metallic vacuum hose of 0, 4 m length and ca. 8, 5 mm outer diameter, connected via CF16 flange to a 2,35m pipe of 10 mm inner diameter which is finally connected to the test limiter. Overall, the piping surface area was minimum ca. 0.2 m². Assuming the lost \( 8.4 \times 10^{20} \) molecules were deposited evenly, one obtains \( 10^{22} \text{ cm}^{-3} \) when counting one molybdenum atom and six fluorine atoms per molecule. Taking the crystal density of MoF6, as 3.5 g/cm³ and a molar mass of 210 g/mol [78], one obtains ca. \( 10^{22} \text{ cm}^{-3} \) or a layer thickness of 3 μm.

4. Global transport of heavy impurities

4.1. Molybdenum

The 571 points of RBS measurement are displayed in Fig. 15a, with
at least 3 points of measurement on each tile. The deposited molybdenum was quantified as described in [79]. 32 points were cross-checked with ERDA for quantification, yielding agreement within the error bars. The results are:

1) The ALT-II limiter harbours 1–2% of the injected molybdenum on the plasma-facing sides according to RBS, and 2% according to ERDA. Deposition on the ALT-II tile backsides yields additional 0,4% of molybdenum, whereof more than half was deposited on the four corner tile backsides next to the injection point. Deposition on ALT-II backsides will be addressed again in Section 9 about global modelling.

2) On the IBL 7–10% of injected molybdenum was deposited according to RBS, and 11% according to ERDA.

3) Measurements on the poloidal limiter yields maximum 1% of the injected molybdenum (assuming 3 nm/s deposition rate). Measurements have only been performed with RBS due to very rough, flaky deposits and unfavourable sample geometry, see Fig. 3a.

4) Contributions from the collector probe, the liner [58] and PFC sides are negligible.

Together with the locally found 6% [42], only 20% ± 5% of the injected molybdenum could be found. An attempt was made to measure molybdenum in the dust from the neutraliser plates in the ALT-II pump ducts through which the vessel is pumped under operation. Particle-induced X-ray emission (PIXE) analysis did not yield a significant amount of molybdenum in the pump ducts: 1:20 ratio of molybdenum to other Inconel components, i.e. the same ratio as molybdenum in the Inconel alloy. It is questionable that the MoF₆ injection could cause a detectable increase of molybdenum with respect to the continuous background level from the liner erosion at all, due to the long duty time of the neutraliser plates.

Local deposition patterns were explained by knowledge about the injection, the SOL flow in toroidal direction and the $\vec{E} \times \vec{B}$ drift in poloidal direction. The same can be done for global deposition patterns. Depending on the radial position, different parts of the molybdenum “cloud” are moved in different directions with different proportions of covered distances (in metres) $\Delta d_{tor}$ and $\Delta d_{pol}$ in toroidal and poloidal direction, respectively. As seen from local deposition, radially close to the injection point toroidal flow and poloidal drift are about equal and towards the HFS, leading to deposition on the lower part of the IBL with $\Delta d_{tor} \approx \Delta d_{pol} \approx 1$. At around the LCFS at $r = 46 \, \text{cm}$ the flow reversal takes place and the molybdenum is now transported towards ALT-II, but with $\Delta d_{tor} / \Delta d_{pol} \approx 8$. In other words, for the transport of molybdenum towards...
ALT-II the poloidal velocity is significantly higher than the toroidal one, which is supported by modelling in [80]. For the deposition peak on the IBL top, \( d_{\text{pol}} \approx 0.5 \), i.e. it probably originates from molybdenum revolving around the plasma several centimetres outside the LCFS, either from re-erosion or from molybdenum not sticking to the IBL bottom. Such a transport scheme can also explain the deposition of most molybdenum on the IBL since the injection “cloud” contains most molybdenum at \( r > 46 \) cm. The cumulative MoI light intensity below the LCFS is 6.5 times the cumulative MoI light intensity above the LCFS for the measured values (9.3 for the Cauchy fit). In comparison, between \( \frac{75}{37} \approx 3 \) to \( \frac{115}{37} \approx 11 \) times more molybdenum was deposited on IBL than on ALT-II, i.e. deposition efficiencies agree with the transport scheme sketched above. Fig. 16 depicts all information merged into one transport scheme.

- After injection at the test limiter, point (0) in Fig. 16, the MoF\(_6\) decomposes and the excited molybdenum first radiates MoI line radiation, giving us a coarse hint on the radial molybdenum distribution above the inlet.
- The molybdenum below the LCFS poloidally follows the \( \vec{E} \times \vec{B} \) drift direction at that radial position, namely clockwise when seen in the direction of the plasma current. The motion creates a local deposition profile tilted towards the HFS in Fig. 11. It also causes the
• The deposition profiles decay in the toroidal direction roughly exponentially, with e-folding lengths summarised in Table 4 [79]. A significant broadening with e-folding lengths up to a metre has been reached after only 31 shots for molybdenum. This effect may be due to re-erosion – re-deposition steps as suggested in [81], due to radial diffusion across magnetic field lines, or both. The latter process is examined and discussed further with the ERO code in Section 8.

It will be seen later that the transport scheme sketched above can be also applied to other impurities, namely tungsten and medium-Z metals. But first we will examine four positions in more detail in the attempt to understand the molybdenum deposition patterns analytically. These four positions are: the collector probe, the IBL bottom, the IBL poloidal cross-section at the gas inlet, and the poloidal limiters.

4.1.1. Collector probe

The radial deposition profile on the collector probe head is the easiest one to understand. Its position is schematically depicted in Fig. 2a. Deposition took place on a range of \( r = 49, 5 \text{ cm} \) to \( r = 54 \text{ cm} \). Exposures were either during a 1 s time window of a discharge, usually between 0.5 and 1.5 s on the timeline in Fig. 4a, or for a substantial part of the flat-top phase, up to 3.5 s. Deposition on the collector probe tiles

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**Table 4**
e-folding lengths of exponential concentration decay in the toroidal direction for molybdenum and tungsten (first published in [79]). The e-folding lengths in the co- and counter-directions have different values (errors in parentheses).

<table>
<thead>
<tr>
<th>PFC</th>
<th>Mo (co) [cm]</th>
<th>Mo (counter) [cm]</th>
<th>W (co) [cm]</th>
<th>W (counter) [cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALT-II limiter</td>
<td>12(5)</td>
<td>26(7)</td>
<td>52(12)</td>
<td>35(9)</td>
</tr>
<tr>
<td>IBL (top)</td>
<td>103(21)</td>
<td>66(14)</td>
<td>179(40)</td>
<td>155(34)</td>
</tr>
<tr>
<td>IBL (bottom)</td>
<td>105(21)</td>
<td>84(18)</td>
<td>124(28)</td>
<td>166(37)</td>
</tr>
</tbody>
</table>

---

**Fig. 17.** a) detailed geometry of a poloidal TEXTOR cross-section, showing the relation between distance from the plasma centre and distance from the IBL curvature centre; b) the impact angle \( \alpha \) for impurities and positive \( \Delta \) (plasma centre shifted towards HFS) and c) negative \( \Delta \) (plasma centre shifted towards LFS).
were used to determine the radial molybdenum distribution in the SOL. At least several seconds of exposure were necessary to yield amounts traceable for RBS with a sensitivity of a few tens of ppm for molybdenum on carbon. Hence, only two sets of samples, one in co- and one in counter-direction, captured enough molybdenum for subsequent analysis. Both sides showed an exponential decay of molybdenum concentration as one would expect for a SOL particle source with \( r < 49, 5 \text{ cm} \). The decay on the side facing the plasma current (and hence the SOL flow) had an e-folding length of \( \lambda = 11 \text{ mm} \) and higher concentration of molybdenum, while the side facing away from the plasma current had an e-folding length of \( \lambda = 29 \text{ mm} \) and about five times less molybdenum. As we have seen on the collector plate the molybdenum moved with the SOL flow and consequently \( \lambda = 11 \text{ mm} \) will be assumed throughout the rest of the paper.

4.1.2. IBL bottom

Secondly, we will focus on the IBL bottom next to the test limiter, as can be seen in Fig. 2d. The idea that the \( E \times B \) drift carried the centre part of the Cauchy distribution from the inlet towards the HFS sparked a question: is it possible to find a Cauchy distribution on the bottom of the IBL? We indeed found a – slightly distorted – Cauchy distribution also in radial direction at the very bottom of the IBL. First, let us look at the geometry of the plasma with respect to the IBL, see Fig. 17a. Impurities move in the poloidal direction with respect to the plasma centre \( \varphi \), while the geometry we use for plotting follows the machine layout, and its centre \( \varphi \) is likely to be off-set with respect to the plasma centre. The result is the following: as an impurity moves in the poloidal direction at a constant distance towards the LCFS, the IBL comes closer and closer, has maximum proximity with the LCFS at the inner mid-plane and then recedes again. One can express the radial position \( r(\varphi) \) of the IBL surface with respect to the plasma centre as:

\[
r(\varphi) = \sqrt{\Delta^2 + b^2 + 2b\Delta \cos(\varphi)}
\]

(3)

with \( b \) being the IBL curvature radius and \( \Delta \) the distance between the IBL curvature centre and the plasma centre, \( \varphi \), respectively. \( \varphi \) starts at the outer mid-plane and continues in counter-clockwise direction as seen in the plasma current direction. Eq. (3) also applies for plasma shifts away from the IBL, i.e. negative \( \Delta \). The offset of the plasma centre during this experiment varied during a discharge according to EFIT: \( \Delta \approx \pm 4 \text{ cm} \). Although it is difficult to guess from the data at hand which value \( \Delta \) predominantly took, one can say with certainty that it is not zero, see next sub-section. Fits in the next subsection suggest \( |\Delta| \) being mainly between 2 and 3 cm.

We examined the lower side of the bottom tile along radial direction, yellow stars in Fig. 18, which had much higher molybdenum concentration than the plasma-facing sides. The poloidal positions from the other examined tile fronts above (green stars in Fig. 18) were translated into radii with the help of Eq. (3) in order to combine them with the measurements from the lower side of the bottom tile. The best fit to the measured data could be obtained by a distorted Cauchy distribution, i.e. multiplied by an exponential decay with \( \lambda = 10 \text{ mm} \), see Fig. 18 red curve. Without this modification the best fit does not match the tails of the function, see Fig. 18 blue curve.

4.1.3. IBL poloidal cross-section

If the centres of the plasma column and the IBL curvature do not coincide, i.e. \( \Delta = 0 \), the areal molybdenum concentration must vary with the poloidal angle. We begin with the areal concentration as a function of the intersection angle \( \alpha \) between a circular trajectory of an impurity at \( r(\varphi) \) and the IBL surface. The intersection angle can be expressed by the cosine rule regardless of the sign of \( \Delta \), as shown in Fig. 17b and c. Knowing that the flux to an area depends on \( \sin(\alpha) \) and using \( \sin(\arccos(x)) = \sqrt{1 - x^2} \), one obtains:

\[
\sin(\alpha) = \sqrt{1 - \left(\frac{b^2 + r(\varphi)^2 - \Delta^2}{2br(\varphi)}\right)^2}.
\]

(4)

With a function \( f(r) \) describing the radial molybdenum concentration in the SOL, the areal molybdenum concentration on the IBL in the poloidal direction is:

\[
M_\text{o}(\varphi) = M_\text{o}_0 \sin(\alpha)f(r(\varphi))
\]

(5)

with \( M_\text{o}_0 \) being a constant, \( f(r) \) a radial distribution function describing radial molybdenum distribution in the plasma edge, and \( r \) as function of \( \varphi \). With \( f(r) \) being a Cauchy distribution, e.g. as seen at the injection position, or an exponential function, e.g. as seen with the collector probe, one obtains comparable patterns. The molybdenum concentration should either resemble a “double-hump” or a “funnel”, depending on whether \( \Delta \) is positive or negative. A similar case is discussed in [82], Section 25.2. Both shapes are observed in the five evaluated poloidal cross-sections: the “funnel” appears in four positions to varying degrees, the “double-hump” is observed once – toroidally on the far side of TEXTOR with respect to the gas inlet.

A comparison of \( M_\text{o}(\varphi) \) with actual values at the toroidal position of the test limiter can be seen in Fig. 19 for \( \Delta = 2 \text{ cm} \) and \( f(r) = C(r) \) (blue curve). Due to the sheath potential an impact angle \( \alpha \) smaller than ca. 1° is unrealistic, and setting the minimum angle to 1° yields the red curve in Fig. 19. \( f(r) = \exp(-\frac{r^2}{2\kappa^2}) \) performs equally well (green curve). The large scatter of data comes from measurements at different positions on one tile. Obviously, the molybdenum concentration exhibits local variation not only on ALT-II.

4.1.4. Poloidal limiters

Finally, let us look at the poloidal limiters which are displayed in Fig. 2b and positioned 45° toroidally away from the test limiter. Due to their semi-circular shape, the impact angle is again a function of radius. Fig. 20a displays the geometry which in combination with a radial distribution function \( f(r) \) yields the molybdenum concentration as a function of radius:

\[
M_\text{o}(r) = M_\text{o}_0 \sqrt{\frac{\varphi + \kappa - r}{\kappa}} f(r)
\]

(6)

Here, \( \kappa = 6, 5 \text{ cm} \) is the radius of poloidal limiter curvature, \( \varphi = 48 \text{ cm} \) is the radial position of the limiter tip, and \( M_\text{o}_0 \) is the concentration for \( \varphi = 90^\circ \). Six poloidal limiter stones were measured on both sides facing co- and counter-direction with respect to the plasma current. Each stone showed a different radial pattern with co-counter asymmetry. However, the asymmetries of all stones combined did not have a clear preference towards co- or counter-direction, i.e. there is no clear co- or counter-deposition pattern. Fig. 20b shows data from all stones, depicting the surface concentration of molybdenum (negative values indicate lower surface concentration than background concentration) and fits of Eq. (6) with exponential (blue) and Cauchy distribution (red) as \( f(r) \). The latter has better agreement with the data. Because of the large scatter due to very rough surface and local concentration fluctuation, the agreement is only qualitative.

4.2. Tungsten

Tungsten concentration was measured at the positions indicated in Fig. 15a. No attempt was made to absolutely quantify the amounts of tungsten and hence the unit to express concentration is given in parts per million, ppm, relative to other surface constituents. The deposition pattern interpolated from the measured values is displayed in Fig. 21. Strongest peaks appear on the IBL top and bottom close to the poloidal limiter. Table 3 and Fig. 9 suggest that most of the tungsten may have been introduced during tungsten limiter experiments described in [83]. The radial position had varied between a rest position 3 cm behind the LCFS
and immersion in the plasma for 1.7 s. A subset of limiter stones had been replaced after showing exfoliation. The tungsten peaks on the IBL top and bottom are toroidally close to its main source, the poloidal limiter. In [83] it is mentioned that for the upper poloidal limiter (source A in Fig. 22) all stones had been replaced with freshly tungsten coated stones at some point during the experiment while only one stone was replaced on the lower limiter (source B). This indicates that the upper limiter experienced higher damage and must have been a stronger source of tungsten, yielding a higher amount of tungsten on the IBL top than on the IBL bottom when assuming transport within the LCFS. Another tungsten deposition peak appears close to the test limiter on the ALT-II limiter. There is no clearly enhanced tungsten deposition on the IBL on that place, contrary to the situation with molybdenum. Hence there must have been a tungsten exposure qualitatively different to that of the MoF₆ injection. Such an exposure has taken place multiple times with a solid tungsten or tungsten covered test limiter either at or inside the LCFS [84–87], (source C in Fig. 22). As a result the eroded tungsten moved in the direction of the $\vec{E} \times \vec{B}$ drift within the LCFS, namely counter-clockwise towards the ALT-II limiter (plasma current in normal direction). In the toroidal direction all tungsten deposition peaks are wider than the ones of molybdenum, most probably due to the longer residence time of tungsten impurities in TEXTOR from previous experiments. Also here a roughly exponential behaviour is observed, with e-folding lengths summarised in Table 4. In general, high-Z metals are deposited close to their point of origin.

4.3. Medium-Z metals

We define as “medium-Z metals” all the elements between chromium and copper. The applied RBS and ERDA analysis methods cannot separate them clearly,¹ and since the sources of most of the elements (except copper) are roughly the same – Inconel liner and stainless steel structures – no effort was taken to measure them separately with other methods. Points of measurements are the same as for molybdenum and

(¹ For ERDA one must make a distinction between measurements with the old [62] and the new [63] ERDA detector. The new detector is capable of separating lighter medium-Z elements like chromium from heavier ones like nickel. However, the new detector became only available during the last part of the measurements.)
tungsten, see Fig. 15a. The global deposition pattern is depicted in Fig. 23a. The first important observation is: the medium-Z deposition is not at all uniform. Consequently the liner, being a more or less symmetric (at least toroidally), cannot be the main medium-Z source. All of the features must be explained through local sources.

The strongest peak appears close to the poloidal limiters and can be associated with a poloidal limiter experiment where B$_4$C covered copper pieces had been tested [88]. These limiters had been exposed to SOL plasma 1 cm outside the LCFS and experienced strong unipolar arcing with penetration of the B$_4$C layers down to the copper substrate [89]. Subsequent investigation had shown that copper from the substrate had been lifted out of the arc craters. With unipolar arcs lifting copper from the poloidal limiter substrate through holes in the B$_4$C coating the copper should mainly end up around the LCFS and hence follow the $E \times B$ drift towards the upper IBL, just as for tungsten. Splashing of molten copper should yield comparable copper amounts on the IBL top and bottom at the same toroidal position as the poloidal limiters, which is not the case: the majority of medium-Z metals is found on the upper IBL with a toroidal shift, indicating that movement with the plasma had been involved. Some of the copper seems to be also deposited on the ALT-II (Fig. 23a, close to co-NBI). Hence the same transport scheme as for tungsten applies, see Fig. 22, with the sources A and B, and the deposition areas 1 and 2.

Apart from the strong deposition peaking close to the poloidal limiters, there are several other areas of increased medium-Z concentration on the IBL, namely close to one ICRH antenna and to the counter-NBI injection position. Investigation of the previous IBL (1994–2003) with beta backscattering [90] had already shown areas with increased metal deposition, see Fig. 23b (extracted from [90], modified and oriented as Fig. 23a). It is mentioned in [90] that the two areas (in Fig. 23b) with increased metal deposition coincide with the toroidal positions of one NBI port (at coil 7) and one GD antenna (at coil 16) and that liner damage had been observed at those positions. The areas of increased metal deposition in Fig. 23a and 23b do coincide,
disregarding the influence of the poloidal limiter in Fig. 23a. It can thus be speculated that the sources must have been the same, in 1990 and again 23 years later, which indeed is the case for at least two out of three: NBI (1986 [32]), ICRH antennas (1987 [34]), and GD antennas (no information available). This and the toroidal proximity indicate that the named subsystems are indeed the sources for medium-Z impurities found in either case. In an ICRH experiment [91] the effect of ICRH heating on SOL parameters, impurity release and hydrogen recycling had been studied, amongst others. It had been found that ICRH heating influences the SOL parameters and increases iron fluxes to the wall. It had been further noticed that at least the influence on the SOL can be observed only in the neighbourhood of the antenna, within a distance of about 1 m. These findings are in line with studies of deposited layers at the ICRH antennas of TEXTOR where metal deposition is much higher on the antennas than on the ALT-II limiter, and the metal deposition increases during ICRH operation [92]. This can explain local medium-Z impurity deposition on the IBL near to one ICRH antenna, as seen in Fig. 23a, but it does still not explain the absence near the other ICRH antenna.

4.4. Metals: comparison to other machines

After establishing a transport scheme for molybdenum and testing it on other species, namely tungsten and medium-Z elements, it will now be checked against findings in other machines. Findings from JT-60 U, TFTR, ASDEX Upgrade (AUG) and Alcator C-Mod will be compared to our results. The reversed field pinch (RFP) device EXTRAP T2R is equipped with molybdenum limiters but molybdenum measurements were only related to radial transport [93].

The first example is from JT-60 U where a toroidal tile section of the outer divertor was changed from the usual carbon to tungsten for two campaigns, followed by divertor tile analysis [22]. A toroidal spread of tungsten was observed on the so called outer wing, located in the private divertor region (see Fig. 2, 8 and 9 in [22]). The tungsten was spread toroidally, with the maximum toroidally close to the tungsten source, just as for TEXTOR. The e-folding lengths are shorter though, possibly due to only two years of exposure to plasma and the different nature of the source: in JT-60 U it had the form of bulk tungsten tiles which were present throughout these two years, while the source in TEXTOR was non-permanent. Obtained poloidal patterns at the toroidal position of the tungsten tiles can be interpreted as a result of \( \vec{E} \times \vec{B} \) drift through the private plasma from the outer to the inner divertor (see Fig. 2 and 6 in [22]) due to radial electric field [94]. This is in accordance with findings in TEXTOR.

The next example is from the IBL of TFTR analysed by beta backscattering for metallic depositions [95] which were later modelled [96]. The deposition profile of metals could be explained by a model that relied on the same formula as Eq. 5 (Eq. 1 in [96]). However, the deposition on the IBL was symmetric in toroidal direction with respect to the PFC periodicity (Fig. 3 in [95]) which is not the case in this study.

![Fig. 22. Tungsten transport along poloidal flows (black solid arrows) from the poloidal limiter top (A), with minor contributions (dashed arrows) from the bottom (B), and from the test limiter (C). Sub-systems except the test limiter (red) and the poloidal limiter (blue) are omitted for clarity. The point of view is illustrated in Fig. 21. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)](image)

![Fig. 23. a) Global medium-Z deposition pattern. The IBL is the inner closed ring with the top towards the centre and the bottom towards the ALT-II; b) metal deposition on the previous IBL (1994–2003) from [90] (rearranged and oriented), as obtained with beta backscattering. The white dashed lines indicate the directions of the neutral beams.](image)
Another example is from AUG, with a study conducted during the stepwise transformation from an all-carbon to an all-tungsten machine [20]. One part of the study was focused on the tungsten re-deposition in the divertor which could be explained due to transport along magnetic field lines: source and sink had a direct magnetic connection. This is a disagreement with results obtained in this study which shows no clear impurity transport along magnetic field lines. However, another study combining experiment [97] and modelling [98] could only reproduce experimental erosion-deposition profiles of tungsten in the AUG divertor by including the $E \times B$ drift, indicating its importance for high-Z migration.

The last example is from Alcator C-Mod which had a full molybdenum wall. Molybdenum erosion-deposition studies for a set of 21 tiles from divertor and IBL was conducted after 1090 discharges or 1200 plasma-seconds [99]. The obtained results show highest erosion at the outer strikepoint and deposition above the inner strikepoint as well as on the IBL. Disregarding the difference in the nature of the molybdenum source (gas injection in TEXTOR versus tile erosion in Alcator C-Mod), it is noteworthy that most deposition, also of boron and deuterium, takes place on the IBL. We will see later that the IBL in TEXTOR is the main repository not only for heavy species but also for lighter ones, including deuterium.

The main ingredients for the transport scheme sketched for metals in this paper are the radial electric field profile and re-erosion/reflection, both of which also occur in divertor machines. However, strong temperature gradients along divertor SOLs and detached plasma conditions would lead to somewhat altered transport schemes for divertor machines due to the temperature gradient force and neutralisation. The former would increase transport along field lines, the latter would enhance transport perpendicular to the field lines. In short, in addition to the radial electric field profile, also the parallel temperature profile and the divertor plasma parameters have a strong influence not only on amount of transported impurities, but also on deposition patterns. As a consequence, transport in divertor machines can be more complex and requires more knowledge about SOL plasma parameters. Especially the comparisons with JT-60 U and AUG highlight both the similarities and differences to the transport scheme sketched above.

5. Global transport of light impurities

5.1. Nitrogen

$^{15}$N was seeded simultaneously with MoF$_6$, but 90° toroidally away from the test limiter, see Fig. 9 (light blue). During the experiment it created a memory effect with consecutive build-up of higher and higher nitrogen amounts in the plasma, see Fig. 4c. Such behaviour is known from previous injections [50].

Overall 5, $3 \cdot 10^{21}$ $^{15}$N atoms were introduced during 22 pulses, whereas a maximum of 26% deposited on the walls can be deduced from measured concentrations. The local deposition profile of nitrogen is shown in Fig. 11, which is very similar to the molybdenum deposition profile although the nitrogen source was at a completely different position, indicating deposition alongside molybdenum. The same effect was also found on ALT tiles near the injection [69]. Averaging over all measured points, the N/Mo ratio is about 0,16. The absolute amount of nitrogen deposited on the test limiter was negligible, $4 \cdot 10^{19}$ atoms, which was mostly $^{14}$N. Only about 10% of the nitrogen was $^{15}$N, corresponding to maximum 1‰ of the injected amount of $^{15}$N. This value and all the following ones are an upper estimate because $^{15}$N had been introduced into TEXTOR before and, unlike the case for molybdenum, no background estimate was available.

On global scale nitrogen deposition on the ALT-II and the IBL were studied. The deposition in toroidal direction is shown in Fig. 24 for both limiters. On ALT-II the deposition peaks at two positions: close to the test limiter due to deposition with molybdenum, and on a misaligned blade due to a few millimetres increased distance from the plasma and hence lower heat flux onto the limiter surfaces. The total amount deposited on the ALT-II limiter is $3 \cdot 10^{20}$ atoms or maximum 5,7% of the injected amount. On the IBL the $^{15}$N deposition does not correlate with any other deposited species investigated in this study, neither toroidally nor poloidally. The total amount of $^{15}$N deposited on the IBL is ca. $1,1 \cdot 10^{21}$ atoms or maximum 20,6% of the injected amount. The ratio between the total amounts found on IBL and ALT-II is $3,6 \pm 1$ whereas the ratio between the PPC area of IBL and ALT-II is 2,6. Hence a preferred deposition of nitrogen on more remote PPCs (as the IBL) is likely, yet not significant when considering the measurement uncertainty of 35%. The deposition of $^{15}$N cannot be explained by the transport scheme developed for metals in the previous section. Instead, co-deposition and plasma wetting seem to play the significant roles in nitrogen deposition.

5.2. Fluorine

Fluorine was introduced into TEXTOR in several experiments in the form of hexafluorides through the test limiter. Hence as for $^{15}$N, the numbers given here with respect to the fluorine released during this study are upper estimates since information about background fluorine is missing. The overall amount of released fluorine during this study was six times the amount of released molybdenum, i.e. $3,4 \cdot 10^{23}$ atoms. No memory effect was observed, i.e. fluorine levels did not build up during the discharges, see Fig. 4c and [23]. This may be due to the high chemical reactivity of fluorine which may have caused quick and effective removal of fluorine in a carbon wall machine, e.g. by hydrofluorocarbons. Locally, fluorine was deposited only directly at the gas inlet, see Fig. 11. There was no deposition alongside molybdenum despite their simultaneous release at the same position. The total amount...
of locally deposited fluorine was 1 \cdot 10^{19} \text{ atoms} or 0.3\% of the injected amount. The deposition on ALT-II and IBL in toroidal direction is illustrated in Fig. 24. As for nitrogen, fluorine deposition on the ALT-II limiter peaks close to the test limiter and on the misaligned blade. The total amount of fluorine deposited on ALT-II is 2.3 \cdot 10^{20} \text{ atoms or maximum 6.8\% of the injected amount}. On the IBL fluorine deposition does not coincide with any other species analysed in this study, just as for nitrogen. The total amount of fluorine deposited on the IBL is 4.2 \cdot 10^{20} \text{ atoms or maximum 12.4\% of the injected amount}. The ratio between fluorine amounts on IBL and ALT-II is 1.8 \pm 0.5, and is hence significantly smaller than the limiter area ratio, i.e. the deposition of fluorine took place preferentially on ALT-II.

Deposition of nitrogen and fluorine is similar on the main PFCs, see Fig. 24a, while exhibiting differing behaviour on the more remote IBL, see Fig. 24b, and locally on the test limiter, see Fig. 11. Qualitatively, deposition alongside other elements seems to play a larger role for both elements than deposition on lower temperature PFCs, as can be seen from the peak heights at 0° and 110° toroidally in Fig. 24a. The behaviour regarding recycling is different, with nitrogen showing a clear memory effect while fluorine does not, see Fig. 4c. For TEXTOR, the amount of recovered light elements is of the same order of magnitude as deposition on ALT-II. Deposition on ALT-II shows toroidal and poloidal asymmetry in fuel retention. This is both due to overall higher deuterium concentration in some areas, but also due to varying layer thickness, as shown in Section 6.2. On average the areal deuterium concentration is 3.2 \cdot 10^{18} \text{ cm}^{-2}, i.e. eight times higher than on the ALT-II.

The combined inventory on these two PFCs is thus ca. 3 \cdot 10^{23} deuterium atoms or 1 g.

6.1. Fuel retention on ALT-II

On ALT-II the fuel was deposited in the first 1–2 \mu, including the misaligned blade, see Fig. 26a. The deuterium fraction in these layers was usually between 2 and 6\%, and 14\% on the misaligned blade. One investigated tile exhibited thick debris with a metallic appearance on parts of its surface which had a large influence on the fuel retention and deuterium depth profiles: retention is measured even beyond the range of 10 \mu with a remarkably homogeneous deuterium fraction of 4–7\% in the debris, see Fig. 26a. The debris itself is mainly carbon despite its metallic appearance. Fig. 26b shows the detected deuterium concentration at different points of measurement on the tile with debris. Deuterium concentration along the poloidal direction was also analysed on ALT-II, see Fig. 26c. With respect to the error bars the poloidal fuel distribution is flat, in contrast to findings in a previous fuel retention study of ALT-II [100]. However, this can be explained by the selection of tiles: the tiles analysed in this study were from regions with small differences in incident flux, see Fig. 26d (adapted from Fig. 4 in [39]) while the tiles studied in [100] possibly came from a region with stronger flux gradients. It is not possible to resolve the fuel retention pattern imposed by magnetic field ripple with the amount of data points available in this study because the spatial resolution of measured points in this study is below the flux variations expected from [39]; hence the interpolation pattern in Fig. 25b only shows variations on metre scale. Bearing this in mind, the amount of retained fuel on ALT-II may be larger than anticipated above, yet the overall figure hardly changes because of the much higher fuel retention contribution from the IBL, see next section.

6.2. Fuel retention on the IBL

Fuel retention on the IBL is more complex than on ALT for the following reason. Contrary to the ALT-II tiles the IBL tiles were never cleaned and have hence accumulated a decade of fuel retention history which cannot be linked to specific events.

The thicknesses of deuterium containing layers on the IBL are up to 8–9 \mu with most of the deuterium in the upper half of the layers, but in some cases also with non-negligible contributions from deeper layers, see Fig. 27a. There can be also great variations between neighbouring tiles. Note the difference between two tiles spaced only ca. 15 cm apart, i.e. 444 and 446 (for positions see Fig. 27c). Deuterium is depleted in the topmost 1–2 \mu on all IBL tiles. Deuterium-to-carbon (D/C) ratios of the order of 0.01 – 0.1 indicate that the IBL surface was heated up to at least 700 K under plasma impact [109]. At positions with high fuel retention the deuterium levels are usually elevated over the whole depth range, proving that fuel retention has been built up continuously. Hence, the cause of the inhomogeneous fuel retention pattern had to be
either permanently present over the IBL lifetime or regularly occurring. Such possible causes are: (i) plasma heating by NBI and ICRH, influencing the SOL and thus the fuel retention behaviour; (ii) local release of impurities, e.g. at the poloidal or test limiter position, and thus increase of co-deposition; (iii) inhomogeneity of wall conditioning methods such as GD cleaning, or boronisation and siliconisation with deuterated molecules. We will now investigate each of these possible causes (i) – (iii).

**Cause (i): auxiliary heating**

Auxiliary heating systems can influence fuel retention in two ways: first, they represent local impurity sources for limiter materials (carbon limiters at the ICRH antennas of TEXTOR) and metallic impurities (NBI scrapers, ICRH Faraday shields) for co-deposition of deuterium; second, local heating of the SOL by just a fraction of the wave power can increase PFC temperature and trigger release of deuterium. Both effects have been found in [91] where ICRH leads to an increase of iron flux and temperature in the SOL. This temperature increase was found to be highest at \( r = 49 \text{ cm} \) (Fig. 6 in [91]), i.e. the radial position of the IBL, and locally restricted (ca. 1 m) which explains local deuterium depletion on the IBL near the ICRH antennas in Fig. 25b. Lessons learnt from ALT-II analysis shows that temperature seems to influence fuel retention more than co-deposition, leading to an overall negative effect of ICRH on local fuel retention and thus explaining the drop of deuterium concentration on IBL next to the antennas. This is in line with previous examinations of both deposits [92] and dust in the vicinity of ICRH antennas [57]. Also, impurity influx is not considerably increased due to ICRH [91]. Depth profiles from two tiles are plotted in Fig. 27a (tiles 71 and 76, see Fig. 27c for positions), again showing great differences.

**Fig. 25.** Fuel retention – a) position of measured points, b) fuel retention pattern. The IBL is the inner closed ring with the top towards the centre and the bottom towards the ALT-II.

**Fig. 26.** Fuel retention on the ALT-II main limiter – a) depth profiles from each blade, treating the misaligned Blade 3 and Blade 6 with metallic debris separately; b) fuel retention along Tile 21 of Blade 6 with debris; c) usual poloidal distribution of fuel retention of Tile 21 from different blades (Blade 3 and 6 are omitted as special cases); d) modified Fig. 4e from [39] with the line of analysis in this study (insert, yellow dashed). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
in fuel retention possibly due to different radial distances to the plasma (see Fig. 17).

NBI heating increases the density and particle flux in the SOL, but not so much the temperature [110]. Additionally, the carbon deposition is increased with power, leading to increased co-deposition [111]. Hence, contrary to ICRH the NBI should increase fuel retention in the wall. Assuming a priori that this effect is also local, the observed higher fuel retention along the co-NBI injection path can be explained, see Fig. 25b. The counter-NBI was not used as regularly which explains asymmetry between the two NBI positions.

**Cause (ii): co-deposition by impurity release**

Deposition both at the poloidal limiter position and the test limiter position is enhanced for high- and medium-Z elements, see Section 4. It is thus likely that eroded carbon from these limiters behaved similarly and was deposited on the IBL toroidally close to both limiter positions as well. This should manifest itself on enhanced amount of particle deposition. Indeed, when analysing the widths of surface peaks as indicators for impurity particle flux one can observe the following trend: higher fuel retention coincides with wider surface peaks, see Fig. 27. This trend only holds on the IBL, proving yet again that the outgassing due to higher PFC temperature on ALT-II dominates over co-deposition. On the IBL where temperatures are lower, co-deposition can enhance fuel retention considerably. A depth profile of the tile closest to the test limiter is shown in Fig 28a (tile 400, see Fig. 27c for position).

**Cause (iii): inhomogeneity of wall conditioning methods**

Homogeneity of wall conditioning by carbonisation in TEXTOR has been investigated in [112] and was shown to be inhomogeneous. On average, carbon films are thicker close to the GD antennas than further away (Fig. 38 in [112]). Toroidal inhomogeneity exists also for boronisation [113]. Since there is no symmetry of fuel retention either with respect to the GD antennas or the gas source of diboride, asymmetry in wall conditioning did not seem to play a major role in fuel retention pattern development.

6.3. Fuel retention: comparison to other machines

Fuel retention has been examined in great detail also in other machines. We will focus on three machines where larger areas were examined, namely TFTR, JT-60 U, Tore Supra (now WEST) and Alcator C-Mod.

The first example is from investigation of the carbon IBL in TFTR [19]. The thickness of deposits was similar with up to ca. 10 µm. Deuterium concentration varied both poloidally and toroidally, ranging from 3 to 60 \( \cdot 10^{17} \) cm\(^{-2} \) which is comparable to what was found in this study. Comparing Fig. 1 and 2 in [19] shows that areas with large amounts of deposition (in this case metals) also had high amounts of fuel retention. The biggest disagreement is found in the deuterium depth profiles which do not exhibit surface depletion in [19]. Furthermore the maximum D/C ratio in TFTR exceeded 0.2 while it was maximum 0.12 in this study.

The second example is from JT-60 U where retention from different hydrogen isotopes was studied in the divertor [114]. A linear relationship between fuel retention and deposited layer thickness was found. This is in accordance with our findings on the TEXTOR IBL. (H + D)/C ranges from 0.02 up to 0.13, hence the ratios found in JT-60 U in [114] and in TEXTOR in this study are of the same order. Depth profiles exhibit deuterium surface depletion for the first 0.1 µm instead of 1 µm as found in this study. The discrepancy can be explained only partly by surface roughness which was about 1 µm for JT-60 U and 3 µm for TEXTOR.

The next example is from Tore Supra where the fuel retention of the main PFC in a time interval of 2002–2007 was studied [115]. In contrary to the main PFC in this study, the D/(D + C) ratio in Tore Supra was an order of magnitude higher, probably because it operated with actively cooled main PFC. The depth profiles found in Tore Supra were qualitatively similar to those found in this study (see Fig. 3a in [115]), with deuterium depletion in the first 1–3 µm followed by a...
concentration peak, running out in a tail of decreasing deuterium concentration. Depth profiling in [115] yielded a good agreement between operation history and depth profiles.

The last example is from Alcator C-Mod and points to PFC analysis already introduced in Section 4.4 [99]. As already mentioned above, deuterium retention was highest on the IBL of Alcator C-Mod which is in qualitative agreement of what we found in TEXTOR.

6.4. Part II – Comparison with modelling and summary

7. Local modelling with ERO

Modelling of tracer injection and local deposition was undertaken with the Monte Carlo code ERO described in [116]. MoF$_6$ from this study and WF$_6$ from the study in [23] were modelled in [117]. No data on molecular dissociation of the two hexafluorides was available. Instead the ionisation of impurity atoms was adapted so the simulated line emission matched the observed one, see Fig. 2 and 3 in [117]. From helium beam measurements during the WF$_6$ injection experiment the radial SOL profiles of $T_e$ and $n_e$ were available, showing exponential decay 

$$T_e(LCFS) = 30eV; \ \ T_i(LCFS) = 60eV; \ \ \lambda_F = 40mm; \ \ n_e(LCFS) = 5 \times 10^{12}cm^{-3}; \ \ \lambda_{eff} = 30mm$$

These profiles were used for modelling of both species since the plasma parameters were similar. Plasma parameter studies were also conducted on $T_e$ and $n_e$ where the values named above yielded best qualitative agreement with respect to the obtained deposition patterns. As impurities, 5.2% carbon and 1% oxygen were assumed. Enhanced re-erosion of deposited impurities was necessary to obtain quantitative agreement, as is frequently observed in such kind of combined experiment-modelling efforts [118]. On top of that, it was assumed that for each heavy impurity (Mo or W) six fluorine ions return to the test limiter surface.

The modelled deposition pattern of molybdenum yields an elongated shape along the SOL flow in the toroidal direction and the $\vec{E} \times \vec{B}$ drift roughly in the poloidal direction, just as in the experiment. A comparison between best modelled and experimental molybdenum deposition profiles on the test limiter is given in Fig. 28a and b, using a tenfold increased re-erosion factor of molybdenum in order to obtain a net deposition efficiency close to 6%. Without increased re-erosion the re-deposited molybdenum in the simulation is 56%, i.e. ten times higher than in reality, and the tail is too pronounced, see Fig. 28c. A possible reason for such enhanced re-erosion of molybdenum is the fact that it was partly embedded into a matrix of lighter atoms, which increases re-erosion yields [119].

For tungsten, the same problem concerning quantification was observed in ERO. Without further assumptions the tungsten deposition efficiency was 26% instead of the experimentally observed 1%. With sputtering by fluorine and an enhanced re-erosion factor of 20 the modelled deposition efficiency dropped to 3%. The toroidal deposition profiles of both ERO modelled and experimentally measured tungsten on the test limiter are shown in Fig. 28d. The ERO profile is divided by 3 to match the experimental concentration.

Modelling of both molybdenum and tungsten locally with ERO, and from previous efforts in modelling $^{13}$C and Si deposition [118,120] suggests that the local transport is reasonably well understood. Even the missing dissociation data for exotic molecules like MoF$_6$ or WF$_6$ can be compensated by careful adjustment of dissociation coefficients in the modelling when spectroscopic information of the injection is available. What remains an area of active research in recent years is the correct quantification. Results published in [118] suggest that the substrate might considerably influence re-erosion yields, which is in line with the ERO modelling results presented here, and with findings in [119].

8. Modelling of diffusion effects on global patterns with ERO

In Section 4.1 an approximately exponential decay of molybdenum...
concentration away from the inlet was observed on ALT-II, see Fig. 8a. Two explanations were offered above for the exponential decay: re-erosion – re-deposition steps and diffusion across field lines. The latter has been investigated with ERO modelling [79] and will be presented in this section.

Plasma parameters as in the local modelling were used, adding also toroidal flow of $1 \times 10^{4} \text{ m/s}$, a perpendicular diffusion coefficient of $D = 0.2 \text{ m}^{2}/\text{s}$ in accordance with [5,121] and a grazing incidence angle of the magnetic field onto the PFC of 0.01°. The sound velocity for the chosen plasma parameters was $5 \times 10^{3} \text{ m/s}$. For parameter studies, a ten times lower diffusion coefficient was modelled as well. The simulation environment is shown in Fig. 29a. The PFC in the simulation resembles an exaggerated ALT blade with 6 m length. No re-erosion was considered in order to monitor the impact of diffusion on molybdenum deposition only. One million particles were simulated. More details are given in [79].

The resulting toroidal deposition patterns are displayed in Fig. 29b, both showing exponential decay. For $D = 0.2 \text{ m}^{2}/\text{s}$ the e-folding length is 15 cm which is close to the experimentally observed value of 12 cm on the ALT-II in toroidal co-direction, see Table 4. The deposited amount of molybdenum was 84% of the injected amount without re-erosion. For $D = 0.02 \text{ m}^{2}/\text{s}$ the e-folding length is 130 cm with 60% deposition efficiency. Hence, the diffusion coefficient value of 0.2 m²/s in TEXTOR gives good agreement with what is seen in the experimental deposition patterns on ALT-II in the toroidal direction, but not on the IBL. Furthermore the deposition efficiency in the simulation is more than an order of magnitude higher than the observed one.

A possible explanation would be the following. On ALT-II, re-erosion – re-deposition steps hardly occur because the high sputtering causes re-erosion of most molybdenum without significant (permanent) re-deposition. However, at the IBL the temperature and hence sputtering efficiency is lower and permanent re-deposition can take place, broadening the diffusion-smeared deposition profile further by around a factor of 5, see Table 4.

9. Global modelling with ASCOT

The Monte Carlo code ASCOT [122] can be used to model an entire tokamak with full 3D features for both the magnetic field and first wall geometry [123,124]. ASCOT follows either the guiding centres or full gyro orbits of the test particles, later referred to as markers. Each marker can represent a different number of real particles. This number is given by a weight factor assigned to each marker.

In this work the full gyro orbits of the markers were followed. For the orbit integration ASCOT has two different options: a fourth-order Runge-Kutta method with fifth-order error estimation, and leap-frog Boris. The latter was used here to guarantee energy conservation. Magnetic drifts and radial electric field are accounted for in the simulations. Coulomb interaction of the markers with the background plasma (slowing down, pitch angle scattering) is accomplished using binomially distributed Monte Carlo operators derived from the Fokker–Planck equation. The effect of flows is accounted for by carrying out the collision operations in the frame of reference moving with the flow. ASCOT uses the ADAS database to account for ionization and recombination processes. A neutralized marker will follow a ballistic trajectory until possible re-ionization. ASCOT simulations assume static background plasma and magnetic field. These background profiles are given on a discrete mesh and are interpolated during run time. The background needed for the simulations (equilibrium, plasma profiles) was obtained from previous discharges conducted with the same or similar engineering parameters: radial profiles of electron and ion temperature and density [74,117,125,126], toroidal plasma rotation profiles [74,75], and magnetic field profiles as EFIT output from the MoF experiment discharges. The plasma itself was assumed to be pure deuterium. Together with quasi-neutrality this yields $n_e = n_i$. Experimental temperature and density profiles were assumed to have parabolic shapes within the LCFS. In the SOL, electron density was assumed to fall off exponentially while the temperature was modelled by an inverted parabola, according to experimental values in [101]. As markers, Mo$^+$ ions were introduced into the simulation environment at the start of the simulation. The full gyro orbits were followed for 2 ms in the case of preparatory runs, and 10 ms in the case of full simulations. Longer simulation times were not necessary as deposition of more than 90% of the markers happened within 10 ms. In the following, preparatory cases are denoted with lowercase Latin numbers while full simulation cases are denoted with uppercase Latin numbers.

The preparatory 2 ms simulations were to determine the relative significance of various physical processes to the migration of Mo ions. To simplify the interpretation of the results, a point source was used for the markers at $r = 48 \text{ cm}$, i.e., $1.3 \text{ cm}$ above the real inlet position, with Mo$^+$ at an energy of 1 eV. The following cases were analysed and compared: (i) no interactions, i.e. deterministic Newtonian motion dictated by the magnetic geometry, (ii) atomic processes only, i.e. ionisation and recombination by background plasma, (iii) Coulomb collisions only, i.e. momentum and energy transfer by collisions with background plasma species, (iv) both atomic processes and Coulomb collisions. The obtained deposition profiles are displayed in Fig. 30. In Case (i), deposition is only local on the collector plate where it intersects the magnetic field line at the point source, Fig. 30a. The length scale of the deposition pattern is thus of the order of the gyro radius.
which is around 0.6 mm. In Case (ii), changing ionisation status alters the gyro radius, plus neutralisation makes it possible for the markers to detach from the field lines. The result is a broadened deposition profile in the order of the ionisation length, a few millimetres, but still completely local on the collector plate, see Fig. 30b. Coulomb collisions enable a more effective movement across field lines, both due to pitch scattering and increase in the kinetic energy, leading to larger gyro radii. Case (iii) thus displays a broader deposition profile than Case (ii),
and for the first time deposition takes place on global scale, i.e. on the IBL bottom, see Fig. 30c. In the last Case (iv), atomic processes and Coulomb collisions are combined, leading to deposition on the collector plate, IBL, ALT-II limiter and the liner, see Fig. 30d. The local deposition pattern is not influenced greatly, whereas the global deposition changes dramatically under the combined effect of atomic processes and Coulomb collisions. However, the deposition in Case (iv) takes place close to the field line going through the point source, as can be seen in Fig. 31. Within the simulated 2 ms, about half of the markers are deposited in all four cases, most of them locally on the collector plate, IBL, ALT-II limiter and the liner, see Fig. 30d. The local modelling outcome was checked experimentally by RBS measurements on ALT tiles and could be reproduced, see Fig. 30c. In the last Case (iv), atomic processes and Coulomb collisions are combined, leading to deposition on the collector plate, IBL, ALT-II limiter and the liner, see Fig. 30d. The local deposition pattern is not influenced greatly, whereas the global deposition changes dramatically under the combined effect of atomic processes and Coulomb collisions. However, the deposition in Case (iv) takes place close to the field line going through the point source, as can be seen in Fig. 31. Within the simulated 2 ms, about half of the markers are deposited in all four cases, most of them locally on the collector plate, IBL, ALT-II limiter and the liner, see Fig. 30d. The local modelling outcome was checked experimentally by RBS measurements on ALT tiles and could be confirmed, see Section 4.1, finding no. 1).

Four full simulations were conducted with point source, and toggling radial electric field (and hence the $E \times B$ drift) as well as toroidal plasma rotation on or off. The different cases are listed in Table 5. The following trends were discovered.

- Without electric field (Cases I and II), 64% of all markers end up locally on the collector plate while the rest is deposited on liner (20%) and IBL (5–6%) along the magnetic field lines. ALT-II receives only negligible deposition: ca. 1%. The toroidal rotation has some effect on deposition patterns but not on deposition efficiency of the different structures and PFCs. Case I is illustrated in Fig. 32a.

- With electric field (Cases III and IV), considerably less markers get deposited locally, only around 20%. More than half of all markers are transported to the HFS and are deposited right below the IBL. The two large limiters, IBL and ALT-II, in total receive only 1% of all markers on their plasma-facing sides. The deposition efficiency is unaffected by the electric field and is still at 21%. The deposition patterns are almost identical, hence the toroidal flow has no influence whatsoever. Case IV is illustrated in Fig. 32b.

The agreement between simulation and experiment is better for Cases III and IV, both with respect to the deposition efficiencies and obtained deposition patterns – but it is not satisfactory: deposition efficiencies on IBL and ALT-II are far too low while it is too high for the collector plate (local deposition); the simulated deposition pattern lacks two out of three deposition maxima present in the experimental results, compare Fig. 15b and 32b.

One key aspect in explaining the experimentally observed patterns was the radial molybdenum distribution displayed in Fig. 10b. Therefore, the simulations were repeated with radially extended source at different marker starting energies, 1 and 10 eV (Case V and VI, see Table 5). The starting energy did not have any major effect on the deposition pattern which is displayed in Fig. 32c for the 1 eV case. The extended source results in deposition mainly taking place at the bottom of the IBL, just as for Cases III and IV, but more outspread in the toroidal direction. Deposition efficiencies for the extended source are close to the experimentally determined deposition efficiencies: 0.9% on the ALT (1–2% in the experiment), 8.2% on the IBL (7–11%) and 7.8% locally (6%). These numbers should however be treated with caution since especially for the global deposition on ALT and IBL the deposition patterns do not resemble reality.

In summary, the following findings were made with the ASCOT simulations.

- Qualitatively, Case III and IV (with electric field and point source, with and without toroidal flow) match the experimental findings best. However, their quantitative agreement is poor: globally, the deposition efficiencies are a factor 10–12 too small.
- Quantitatively, Case V and VI (with radial electric field, toroidal flow and extended source) perform best, with deposition efficiencies agreeing with experimental values when taking the measurement uncertainties into account. Here the qualitative agreement is poor: the deposition pattern does not at all resemble reality.
- The following experimentally observed deposition features could be reproduced: deposition of molybdenum on the ALT backside, very high deposition on the IBL bottom (also around the tile corner), local deposition profile stretching to the HFS due to $E \times B$ drift. Additionally, the shape of the deposition pattern on the IBL bottom could be reproduced, see Fig. 33.
- The following features could not be reproduced: high deposition peak on ALT close to the source, deposition peak at the IBL top.
- Most of the markers ended up right below the IBL, i.e. not on the PFCs. This could explain at least part of the unexplained balance that was found experimentally: maximum 20% of the injected molybdenum was found on PFCs. It is possible that a substantial part of injected molybdenum has been deposited on the metallic structure just below the IBL and was therefore neither assessable by IBL tile analysis nor liner sample analysis.

Some of the discrepancies above could be resolved by introducing a missing piece of physics. In these simulations the re-erosion of molybdenum has not been taken into account because of the difficulty to implement it in ASCOT. By introducing a sticking coefficient with value less than one this effect could be coarsely mimicked, and may lead to changes in the deposition profile. However, the value of this coefficient ought not to be constant but, rather, it should depend on the position relative to the plasma.

Table 5
full ASCOT simulation cases, with the included physics listed.

<table>
<thead>
<tr>
<th>Source type</th>
<th>Electric field?</th>
<th>Tor. rotation?</th>
<th>Starting energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case I</td>
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<td>No</td>
<td>No</td>
</tr>
<tr>
<td>Case II</td>
<td>Point</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>Case III</td>
<td>Point</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>Case IV</td>
<td>Point</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Case V</td>
<td>Radial Cauchy  (Fig. 10b)</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Case VI</td>
<td>Radial Cauchy  (Fig. 10b)</td>
<td>Yes</td>
<td>Yes</td>
</tr>
</tbody>
</table>

Fig. 31. 3D plot of Case (iv) with atomic and Coulomb collisions, angled top view. The markers (blue dots) follow the field line (red) from their starting point (arrow) very closely until being deposited on the different limiters (black grid) and liner. Outside numbers are ALT blade numbers while inside numbers denote IBL column numbers. Grid size: 1 m × 1 m × 1 m. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
10. Summary

10.1. Lessons learnt from TEXTOR mapping

Due to the uniqueness of the study presented here, no best practice on how to conduct a global material migration study on all tokamak PFCs exists. We would therefore like to stress some of the lessons learnt for the benefit of similar activities in the future.

For selection of tracers, one must know which elements (or even isotopes) have been used where in the machine, together with their

Fig. 32. Full simulation cases with marker positions in blue as seen diagonally from the top (left) and with resulting deposition profile in arbitrary units (right) – a) without toroidal flow or radial electric field (Case I in Table 5), b) with both toroidal flow and radial electric field (Case IV), c) with all previously named physics plus extended source (Case V). Case I and II are qualitatively similar, Case III and IV as well as V and VI are almost identical. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
concentration. As could be seen above, non-recycling tracers stay in the machine for many years close to the point of origin. Modelling activities should be set up as early as possible since the time to set up a simulation environment can be equally long as the time needed for experimental evaluation. The kind of source and its volume expansion must be taken into consideration when interpreting deposition patterns – the more local the pattern, the more important the source form. Concerning PFC measurements, PFC selection should be based on knowledge about magnetic field topology (including field ripple when volatile species or fuel retention is of interest), drifts (especially $\vec{E} \times \vec{B}$ drift) and plasma flows together with their radial variations, and sub-system positions. No toroidal or poloidal symmetry can be assumed a priori for any species, not even the most volatile ones. Concentration of deposited tracers can vary on centimetre scale, even for heavy species, i.e. several measurements per tile are necessary to allow estimations for the surface concentration of a whole tile, especially when the PFC-plasma distance varies along the tile surface.

Detailed modelling – and interpretation of results – may require information which has not been anticipated and may not even be available in published form. It then has to be retrieved from unpublished sources most possibly on site (laboratory notes, CAD drawings, staff members experience and remembrance). This must be done as soon as possible, especially for a decommissioned machine where invaluable (undocumented) information based on personal experience may become unavailable due to staff retirement.

10.2. Suggestions for improvement

From the overall TEXTOR study, a range of open questions remains: (i) the role of magnetic field ripple and hence variations in local particle fluxes, which may have caused an underestimation of fuel retention on ALT-II, and which might explain local variation of areal molybdenum concentration on ALT-II near the gas inlet; (ii) heating systems as (local) sources of metallic impurities and their influence on local fuel retention which has been discussed only qualitatively here; (iii) deposition profile broadening due to diffusion and re-erosion – re-deposition, whose importance is seen both in experiment and modelling but which are hard to distinguish from each other with certainty.

For the ASCOT simulations themselves, parameter studies remain where physical quantities are varied to estimate their importance on (simulated) transport. The following physics aspects should be included for improvements: re-erosion together with sheath potential in front of PFCs, anomalous diffusion, temperature gradient force. At least part of these points will be addressed with further studies in the near future.

10.3. Summary of results

The complete studies on TEXTOR wall components and on local and global high-Z transport have been reviewed in recent publications and complemented by hitherto unpublished data. Extensive modelling, both on local and global scale, has been carried out to deepen the understanding of the obtained deposition patterns. In some cases, analytical treatment of the determined deposition profiles was possible by considering the PFC geometry, the particle distribution at the source and the flow patterns. In the field of PWI research, the following milestones and major conclusions could be reached:

- For the first time, results from PFC tiles and liner pieces were combined to obtain a complete material migration pattern including deposition profiles and efficiencies.
- About 20% of all molybdenum tracer species released during the very last TEXTOR experiment could be found by analysing molybdenum concentration in 571 points on 140 wall tiles (17% of the total number) throughout the whole machine.
- Several features of the determined deposition patterns could be explained analytically by basic consideration of PFC geometry, SOL physics and radial particle distribution at the source. The radial marker distribution at the source together with the $\vec{E} \times \vec{B}$ drift and toroidal plasma flow define the relative marker deposition efficiencies on PFCs.
- A transport scheme was derived from molybdenum deposition and knowledge about drift and flow directions, which is also applicable to other non-recycling species, namely tungsten and medium-Z metals (Cr – Cu) introduced into the plasma in previous experiments and through continuous machine operation.
- For the first time, a full machine fuel retention map was obtained including all major PFCs, based on 94 measurement points throughout the whole machine. It exhibits a poloidally and toroidally asymmetric retention pattern, due to auxiliary heating systems, PFC distance to the plasma and local deposition rate variation e.g. through impurity injection. Due to large distances between analysed points, only features with decimetre length scale or higher could be resolved.
- Local simulations show qualitative agreement with experimental results. Quantitative differences would be overcome by enhanced re-erosion yields.
- Global simulations show the importance of diffusion coefficients, $\vec{E} \times \vec{B}$ drift and the source form (point source versus radially extended source). However, achieving qualitative and quantitative agreement remains a challenge.

Nitrogen injection for edge cooling has resulted in a noticeable memory effect during the last TEXTOR experiment. This is in accordance with lessons learnt from other machines. A maximum of 26% of the injected $^{15}$N was retained on all PFCs. Fluorine from the injected MoF$_6$ did not produce a memory effect, also in accordance with observations from other experiments. A maximum of 19% of the injected fluorine was retained on all PFCs.

In summary, the study took the effort of several years, many weeks of beam time and another year in total for several modelling approaches. It proves that scientific exploitation of a decommissioned tokamak is a major research project in its own right. However, the knowledge gained is very valuable and difficult to obtain otherwise. We thus encourage similar projects in conjunction with the decommissioning of other medium-size tokamaks in the future.

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This study mainly rests on results from weeks of beam time and equipment provided by the Ion Technology Centre of Uppsala University. Furthermore, all the PFCs and other objects of this study have been retrieved from TEXTOR by technicians who also contributed with their hands-on experience and documentation of PFCs to this undertaking. We are very thankful to Jonas Åström (Ion Technology Centre) for constant efforts in maintaining the accelerator at best performance, as well as Matthias Schumacher and Thomas Krings (Forschungszentrum Jülich) for retrieving the large amount of samples from TEXTOR. We would like to thank Harry Reimer (Forschungszentrum Jülich) for his skills in photography which yielded following photos in Figs. 1, 3 and 4.

Reference


