
Physics affecting heavy impurity migration in tokamaks

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Physics affecting heavy impurity migration in tokamaks: Benchmarking test-ion code ASCOT against TEXTOR tracer experiment


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ABSTRACT

Erosion, transport and deposition of wall impurities are major concerns in future magnetic fusion devices, both from the perspective of the fusion plasma and the machine wall. An extensive study on molybdenum transport and deposition performed in the TEXTOR tokamak yielded a detailed deposition map that is ideal for benchmark deposition studies. A qualitative benchmark is attempted in this article with the ASCOT code.

We set up a full 3D model of the TEXTOR tokamak and studied the influence of different physical mechanisms and their strengths on molybdenum deposition patterns on the simulated plasma-facing components: atomic processes, Coulomb collisions, scrape-off layer (SOL) profiles, source distribution, marker starting energy, radial electric field strength, SOL flow and toroidal plasma rotation. The outcome comprises 13 simulations, each with 100,000 markers.

The findings are:

• Toroidal plasma movement, either within the LCFS or as SOL flow, is negligible.
• SOL profile and marker starting energy have modest impact on deposition.
• Source distribution has a large impact in combination with radial electric field profiles.
• The $E \times B$ drift has the highest impact on the deposition profiles.

1. Introduction

In fusion machines – nowadays in research devices and even more so in future reactors – interactions between fusion plasma and wall components will cause erosion, transport of eroded material into the plasma, and deposition of the material on other wall components. This plasma-wall interaction (PWI) and the resulting transport of impurity particles in the plasma leads to undesirable effects both for plasma-facing components (PFCs) and the plasma itself. Understanding PWI and transport has thus become a major goal within fusion research which is addressed both experimentally and by modelling. Increased experimental and computational capabilities have led to a combination of both approaches where usually a transport experiment is conducted and later modelled in computer simulations to benchmark the applied code or to better understand experimental results.

This work is based on combined effort where a molybdenum tracer experiment was conducted in the tokamak TEXTOR which was dismantled directly thereafter and had its PFCs analysed in order to map the tracer deposition patterns [1–3]. The experimental results were thus a perfect opportunity for modelling because deposition data from the whole machine was available. Furthermore, the tracer experiment itself had been conducted in TEXTOR under well-established standard neutral beam injection (NBI) conditions.

Subsequent modelling on both local and global scale was undertaken with ERO [4] and ASCOT for code benchmarking and understanding the experimentally obtained deposition patterns. In this article we will focus on the exploitation of the ASCOT model.

ASCOT is a Monte Carlo code capable of modelling an entire tokamak with full 3D wall structures and magnetic fields, tracing either the guiding centres or full gyro orbits of impurity particles in a predefined background plasma [5]. Plasma flows, drifts, Coulomb collisions and atomic processes can be simulated in order to cover most relevant processes for impurity transport.

We attempted to reproduce the global molybdenum deposition patterns found on the PFCs of TEXTOR by using first principle physics only, i.e. no tuning of free parameters to reproduce the measured deposition patterns. Full gyro orbits were simulated, i.e. curvature and grad(B) drifts were inherent due to the simulated 3D magnetic field.

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The attempt to reproduce experimental results yielded very interesting insights into the physics of impurity transport.

In this article we will explore the ASCOT model of the very last TEXTOR molybdenum tracer experiment, show the impact of different physical mechanisms that can be toggled on and off at will in a computer simulation, and evaluate the impact of different physical mechanisms: atomic processes, Coulomb collisions, scrape-off-layer (SOL) profiles, marker source distributions, marker starting energies, radial electric field strength, SOL flow and toroidal plasma rotation. The aim is to investigate the importance – or unimportance – of different plasma physical mechanisms on modelled deposition patterns and to illustrate where transport models must be detailed, and where using simpler parametrisation is sufficient without compromising the simulation outcome.

PWI including sputtering, re-erosion or reflection is important for formation of deposition profiles. However, those effects are not supported by ASCOT and will not be treated here. Furthermore, the focus is on qualitative deposition pattern simulation – no quantitative analysis was possible with the present version of ASCOT (ASCOT4 [5]).

2. Methods

The tracer experiment in TEXTOR and its evaluation have been described in depth elsewhere [1–3,6]. For convenience, a short outline is given here. The investigated tokamak was a carbon limiter machine with major radius of 1.75 m and minor radius of 0.46 m. Experimental conditions are given in Table 1. Only NBI of 1.7 MW in co-direction was used for auxiliary heating. Injected amounts of tracers were 5.7·10^20 of MoF6 and 5.3·10^21 of \( \text{N}_2 \). Directly after the experiment, TEXTOR was decommissioned, the PFCs dismantled and shipped to the Tandem Laboratory at Uppsala University, Sweden, for subsequent ion beam analysis (IBA) to obtain the amount of deposited tracers on the different PFC tiles. Overall, 140 tiles from the ALT-II main limiter and the inner bumper limiter (IBL) throughout the whole machine were analysed. The focus of the ASCOT study was on the molybdenum transport and deposition.

ASCOT stands for Accelerated Simulation of Charged particle Orbits in TEXTOR and has been developed for more than 20 years [7]. It is a Monte Carlo code, solving for the Fokker-Planck equation by calculating the movement of minority species through phase space, including drifts, collisions and background plasma flow [5]. These markers can be followed either along their guiding centres or with their full gyro motion, with the latter one using either a fourth-order Runge–Kutta method or a modified leap-frog method to solve the equations of motion [8]. Rates for atomic interactions – neutralisation and ionisation – are included from the ADAS database [9].

The geometry is a 3D model of TEXTOR, including all PFCs and the injection limiter (test limiter). The simulation environment is illustrated in Fig. 1. Both magnetic field and background plasma are fixed and given as input. The magnetic topology was extracted from EFIT output for the experimental discharges. The background plasma was obtained from values of previous measurements with comparable engineering parameters, fitting parabolic profiles to experimental flow velocity, temperature and density values. It was furthermore assumed that the plasma is made of pure deuterium, quasi-neutral and hence obeys \( n_e = n_i \). The kinetic profiles are given in Fig. 2.

The influence of the following physical mechanisms was studied:

- Atomic processes, i.e. ionisation and recombination (on/off),
- Coulomb collisions (on/off),
- Radial electric field in whole simulation volume (on/off),
- Bulk plasma rotation (on/off),

Table 1

| Experimental conditions for the molybdenum tracer experiment on the last operation day of TEXTOR (shots #120964 – 121007, including preparation and calibration shots). |
|----------------------------------|------------------|
| Plasma current                   | 350 kA           |
| Toroidal field strength          | 2.25 T           |
| Discharge duration               | 6–7 s (5 s flat-top) |
| Auxiliary heating                | 1.7 MW (co-NBI), no ICRH |
| MoF6 injection:                  |                   |
| - Position                       | Limitter Lock 1 (Fig. 1) |
| - Amount                         | 5.7·10^{20} molecules |
| - No. of discharges              | 31 discharges with injection |

- Source distribution (point source at \( r = 48 \text{ cm} \), radially extended source, see Fig. 2f)
- Marker starting energy (1 eV, 10 eV)
- Strength of SOL radial electric potential (0, \( T_e, 3T_e \))
- Strength of SOL toroidal velocity (0, sound speed)
- SOL profile (exponential, linear)

For atomic processes, the cross-sections are obtained from the ADAS database [9]. Coulomb collision cross-sections are derived from the Fokker-Planck equation, using binomially distributed Monte Carlo operators. The radial electric field is a fourth order polynomial fit to experimental data obtained in [10]. Parabolic fits were used for bulk plasma rotation to data in [10,11], for ion and electron temperatures to data in [10–13], respectively, and for electron and ion density to data in [12,14,15]. Used formulas are listed in Table 2. The source was either a point source at \( r = 48 \text{ cm} \) (i.e. 2 cm outside the LCFS and 1.3 cm above the gas inlet), or a radially extended source consisting of 100,000 markers, fitted with weight factors according to a spectroscopically obtained Mo profile during MoF6 injection [6]. The marker starting energy is either 1 or 10 eV since the dissociation energy of MoF6 is ca. 5 eV for each F atom, of which only a fraction is transferred to the Mo atom (or the Mo atom containing molecule fragment) [16]. The markers start as singly charged ions in all simulations. The electric potential in the SOL was set equal to the electron temperature with and without sheath potential drop, i.e. 3\( T_e \) and \( T_e \), respectively. The former case leads to an exaggeration since the sheath potential drop hardly influences the particle trajectory on the last few Debye lengths away from the target; it was therefore used as a “worst case” scenario. As toroidal velocity in the SOL the sound speed \( c_s \) was used to estimate the maximum possible influence of plasma flow along field lines towards the targets. Finally, two kinds of SOL profile shapes for \( T_e \) and \( n_e \) were used to estimate the impact of SOL profile shape on the marker transport: a realistic one based on experimental values in [4,17], with \( T_e\text{(LCFS)} = 30 \text{ eV} \) (e-folding length: 40 mm) and \( n_e\text{(LCFS)} = 5 \cdot 10^{18} \text{ m}^{-3} \) (e-folding length: 30 mm), and a linear one with \( T_e\text{(LCFS)} \) and \( n_e\text{(LCFS)} \) decreasing from their LCFS values down to almost zero at \( r = 56 \text{ cm} \).

For a direct comparison of experimental [6] and simulated deposition profiles, the final marker positions in the ASCOT output were mapped in the same way as the experimental values. The approach is described in detail in [6].

3. Results and discussions

For easy identification, the different cases are labelled with Latin numbers (I)–(XIII). An overview of the simulations and the parameters used is given in Table 3.

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1 In this paper, “tracer” denotes molybdenum atoms/ions injected in the real experiment whereas “marker” denotes simulated molybdenum in ASCOT.

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3.1. Gyration, atomic processes and Coulomb collision

The first Simulation (I) was done with markers released from a point source, starting at an injection energy of 1 eV and only following the field lines. No other physics was included but the gyro motion. The markers get deposited quickly on the test limiter, with a circular deposition profile of 0.5 mm in width. This profile is due to the gyro motion. In the other direction, the field line ends below the IBL and no deposition is seen globally, i.e. beyond the test limiter.

Including atomic processes only in Simulation (II), the local deposition profile is broadened on the test limiter to a few millimetres due to cross-field movement of neutralised markers, but again no global deposition is seen globally, i.e. beyond the test limiter.

When both atomic processes and Coulomb collisions are combined in Simulation (IV), we see global deposition for the first time. This deposition takes place on the IBL bottom tiles since markers, which otherwise would have ended up below the IBL tiles, now can traverse the magnetic field lines quickly enough by diffusion and neutralisation in order to enter field lines ending on the IBL tiles.

3.2. Central plasma rotation and electric field

After atomic processes and Coulomb collisions, we investigated the impact of radial electric field \( E(r) \), as found experimentally in [10], and plasma rotation, as found experimentally in [10,11] (both inside and outside LCFS). The profiles are given in Fig. 2. The following cases were treated: toroidal rotation only (V), radial electric field only (VI), both rotation and field (VII).

The rotation of the centre plasma had virtually no effect on the deposition profile, see Fig. 3. This is because the most markers stay well outside the region of strong toroidal rotation. The amount of markers which go beyond the LCFS is small compared to the amount staying in the SOL.

Introducing the electric field (VI) makes a huge difference and immediately brings the global deposition maximum closer to the injection. The \( \mathbf{E} \times \mathbf{B} \) drift causes a fast poloidal movement towards the high field side, and the markers intercept the IBL earlier than before where movement along the magnetic field clearly dominated, see Fig. 4. However, the central plasma rotation still has very low influence on the deposition (VII).

3.3. Source distribution and marker starting energy

The molybdenum in the real experiment was injected in the form of MoF\(_6\). The molybdenum source is not a point source but rather a three-dimensional cloud of particles. The molybdenum-containing particle distribution can be approximated to first order by MoI line radiation, and has been successfully reproduced already with ERO modelling [4]. In this work, we approximate the extended source by a radial distribution with weighted markers, see Fig. 2f.

The molybdenum-containing deposits can be formed both by molybdenum from completely dissociated molecules, or from molecule fragments containing molybdenum. The dissociation energy for each step is ca. 5 eV [16], where the kinetic energy from dissociation alone can range from 0.5 eV (MoF\(_6\) → MoF\(_5\) + F) to 3.7 eV (MoF\(_6\) → ... → 6F + Mo). Different processes (Coulomb collisions, radiation absorption, ionisation) can lead to higher kinetic energy.

We therefore explored the impact of a radially extended source and the marker starting energy on the deposition pattern. Introducing the extended source led to a slightly stronger spreading on the bottom IBL in clockwise direction, compare Fig. 4 (VII) and Fig. 5 (VIII). With a radially extended source, more than one magnetic field line is populated with markers, leading to broadened deposition profiles due to slightly different intersection points between different populated field lines and PFCs in the SOL. However, this is only the case for a strong electric field, resulting from a potential of 3T over the entire SOL. For a more realistic case given by 1T, the situation changes, as will be seen later. Concerning starting energy, we find only modest influence between 1 eV (VIII) and 10 eV (IX), see Fig. 5. The deposition maximum is shifted a few degrees in toroidal direction since the ratio between the...
 drift velocity (radial electric field was always active) and thermal velocity along field lines is different for different starting energies. The SOL potentials have been exaggerated for clear visibility of effect, leading to an electric field which is three times higher than the electron temperature in eV. 

When changing to a more realistic electric field (X) the deposition on the IBL moves toroidally further away, see Fig. 6(X): about 60° as compared to 20° with three times too strong field (Fig. 5). Still no deposition on the ALT-II limiter is visible. When extending the radial source to 44 cm (X-b; otherwise it terminates at 46.5 cm, see Fig. 2f) we see deposition on the ALT-II limiter for the first time, see Fig. 6(X-b). The markers now start also from positions inside the LCFS and are therefore more likely to be deposited on the ALT-II limiter top. As will be seen in the next section, this is not the only

Table 2
Plasma profiles used in the ASCOT simulation, with \( \rho = r/a \) and \( a = 46 \) cm.

<table>
<thead>
<tr>
<th>Profile</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radial electric field ([\text{V/m}]) (whole simulation volume)</td>
<td>(633 - 3962 \rho + 9236 \rho^2 - 9343 \rho^3 + 3436 \rho^4)</td>
</tr>
<tr>
<td>Bulk plasma rotation inside LCFS ([\text{km/s}])</td>
<td>(120 (1 - \rho^2)^2)</td>
</tr>
<tr>
<td>Electron temperature ([\text{eV}])</td>
<td>(1700 (1 - \rho)^{3.5} + 10)</td>
</tr>
<tr>
<td>Ion temperature ([\text{eV}])</td>
<td>(2890 (1 - \rho)^{3.5} + 50)</td>
</tr>
<tr>
<td>Electron and ion densities ([\text{m}^{-3}])</td>
<td>(2.7 \times 10^{15} (1 - \rho)^{3.5} + 5 \times 10^{16})</td>
</tr>
<tr>
<td>Radial source ([\text{cm}^{-1}])</td>
<td>(2.97 \times 10^{-4} (1.876 \times 10^{-1} + (\rho - 1.05)^2)^{-1})</td>
</tr>
<tr>
<td>Electron density in the SOL ([\text{m}^{-3}])</td>
<td>(5 \times 10^{13} \exp(-152 (\rho - 1)))</td>
</tr>
<tr>
<td>Electron temperature in the SOL ([\text{eV}])</td>
<td>(30(1 - 121 \times 4331^2(1 - \rho)^2))</td>
</tr>
</tbody>
</table>
possibility to get deposition on the ALT-II.

3.4. SOL flow and profiles: potential, temperature, density

Especially for tracer experiments with source in the SOL, the properties of the SOL are very important for particle transport. However, implementing the details of the SOL – e.g. flows, potential, temperature and density profiles – can be challenging, either due to the lack of experimental data or limited possibilities of implementing detailed profiles in the simulation. This is also the case for ASCOT: there is no plasma sheath in front of the PFCs, and SOL flow as function of distance from the PFC is difficult to implement.

In the recent two simulations (X, X-b) we set the SOL potential to 1 Te, which is more realistic than the formerly used 3 Te. This reduces the $E \times B$ drift by a factor of 3.

Next we implemented a toroidal velocity in the SOL with sound speed $c_s$, in order to investigate the impact of flow velocity on the marker deposition for a “worst case” scenario (XI). For direct comparison with previous cases, and for emphasising the SOL transport, we again set the radial source as in Fig. 2f, i.e. terminating at $r = 46.5$ cm.

The electric field was deactivated for case (XI) in order to have a direct comparison to simulations (IV) and (V) with point source and SOL flow equal zero for both cases. As in the case for central plasma velocity, no major impact can be detected. The deposition on the IBL is hardly affected by the SOL flow, see Fig. 7(XI). On the other hand, switching from a point source to a radial source, in combination with deactivating the electric field, leads to deposition on the ALT-II limiter because traceable amounts of markers now can cross the LCFS before being deposited on the IBL. The deposition takes place where it would be expected with a safety factor of about 4: the lower edge of the ALT-II blades is 30° away in poloidal direction (against $-B_{pol}$), leading to a distance of 120° in toroidal direction (against $-B_{tor}$) for deposition, which is observed in the simulation. Notably, this is the same position as in case (X-b) with electric field and extended source.

When activating the electric field again, this time with a potential of $1T_e$, in combination with the SOL flow (XII), the deposition on the IBL is the same as in case (X) (similar to XII, just without SOL flow) while the deposition on the ALT-II limiter decreases drastically, yet it stays at the same place as before, see Fig. 7(XII). The main difference between (XII) and (X-b) is the source extension: 46.5 cm versus 44 cm, respectively. This indicates that the radial electric field and the radial source are the main drivers behind position and quantity of deposited markers, not so much the toroidal plasma movement.

When changing the exponential profile of the SOL to a linear one (XIII) while keeping everything else the same as in Simulation (XII), a slight change appears in deposited quantities: the deposition on ALT-II increases while the deposition on the IBL decreases, see Fig. 8(XIII). The qualitative picture remains unchanged as compared to Simulation (XII). Hence, a linear SOL increases chances for markers to cross the LCFS, probably due to higher Coulomb collision probability than in the exponential case ($\nu_{ei} \propto n^{-3/2}$, hence a flatter increase in $T$ yields higher $\nu_{ei}$, see e.g. [18]).

<table>
<thead>
<tr>
<th>Simulation index</th>
<th>I</th>
<th>II</th>
<th>III</th>
<th>IV</th>
<th>V</th>
<th>VI</th>
<th>VII</th>
<th>VIII</th>
<th>IX</th>
<th>X</th>
<th>X-b</th>
<th>XI</th>
<th>XII</th>
<th>XIII</th>
</tr>
</thead>
<tbody>
<tr>
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<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
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<td>X</td>
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<td>Coulomb collisions</td>
<td>–</td>
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<td>X</td>
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<tr>
<td>$E(r)$</td>
<td>–</td>
<td>–</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
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<td>–</td>
<td>–</td>
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<td>X</td>
<td>X</td>
<td>X</td>
<td>3</td>
<td>–</td>
<td>1</td>
<td>1</td>
<td>1</td>
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<tr>
<td>Source ($P/R$)</td>
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<td>P</td>
<td>P</td>
<td>P</td>
<td>P</td>
<td>P</td>
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<tr>
<td>$E_{start}$ [eV]</td>
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</tr>
<tr>
<td>$SOL\ (E/L)$</td>
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<td>E</td>
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<td>E</td>
<td>E</td>
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<td>E</td>
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<td>E</td>
<td>E</td>
<td>L</td>
</tr>
</tbody>
</table>

* $P = $ point source, $R = $ radially extended source.
* $E = $ exponential, $L = $ linear.
* Radial source extends to $r = 44$ cm instead of 46.5 cm.

Fig. 3. Simulations (IV) and (V). Influence of the toroidal plasma rotation within the LCFS is non-existent. The “stripe”-like deposition along the $x = 0$ position is an interpolation artefact. The concentration is in arbitrary units. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
4. Comparison with experimental results

The Mo deposition patterns in the MoF₆ experiment exhibit three main features (see also Fig. 8) which can be directly compared to the simulation outcomes described above.

1. The deposition on the ALT-II limiter takes place at the same toroidal position as the injection and decreases exponentially in both toroidal directions, with the longer e-folding length being in the direction of the plasma flow.
2. The deposition on the IBL takes place also at the same toroidal position as the injection, with depositions at top and bottom of the IBL but not on the midplane, with exponential decrease in both toroidal directions.
3. Most Mo tracers were found on the IBL (7–11%), then locally on the test limiter (6%) and only a minor fraction on the main PFC, the ALT-II limiter (1–2%).

Fig. 4. Simulations (VI) and (VII). Influence of the radial electric field is large because of the resulting $E \times B$ drift. The impact of toroidal plasma rotation stays low. The concentration is in arbitrary units. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 5. Simulations (VIII) and (IX). Influence of the marker starting energy on the deposition pattern is modest, causing a few degrees shift along the toroidal direction for 10 eV due to lower $E \times B$ drift velocity relative to overall marker velocity. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
No single simulated scenario could reproduce these three points simultaneously. One needs atomic processes in combination with Coulomb collision to create global deposition (Simulation IV) on the IBL, and a three times too strong electric field to create it in the approximately right position. However, the deposition on the IBL only appears at the bottom, never on the top. In [1], a transport scheme is proposed that involves reflection and re-erosion in order to explain deposition on the IBL top. Both mechanisms were not investigated which could be a reason for the absence of this feature.

Deposition on the ALT limiter proves to be even more difficult to realise and only appears when either the marker source is extended beyond the LCFS to $r = 44$ cm, or when the electric field is deactivated in combination with a source up to $r = 46.5$ cm. In either case, the deposition on the ALT-II limiter is determined by the safety factor and thus takes place ca. 120° toroidally away from the source. In [1], the proposed transport scheme proposes tracers inside the LCFS in combination with $\vec{E} \times \vec{B}$ drift reversal as the main reason for the observed pattern. One would thus expect a deposition close to the source for Case

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Fig. 6. Simulations (X) and (X-b). Setting the electric potential in the SOL to $1T_e$ instead of $3T_e$ decreases the poloidal movement. Extending the source from $r = 46.5$ cm (see Fig. 2) to $r = 44$ cm gives deposition on ALT-II. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 7. Simulations (XI) and (XII). No electric field also gives same deposition on the ALT-II limiter as in case (X-b) but different deposition on IBL. Realistic electric field plus “worst case” flow is rather similar to case (X) where there is no flow at all. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
X-b where the markers started inside the LCFS and the electric field with a field reversal at the LCFS (see Fig. 2e) was present. However, the deposition took place too far away toroidally. It is possible that a three times too strong electric field together with markers up to \( r = 44 \text{ cm} \) could have reproduced the experimental pattern since also on the IBL a too strong field led to a more realistic positioning of the marker deposition.

In either case, IBL and ALT-II limiter both show too large e-folding lengths as compared to the experiment, except for the IBL in Cases VI to IX with three times too strong electric field. Qualitatively, the simulation cases VI to VIII come closest to the experimentally obtained deposition patterns.

Quantification was not possible in the ASCOT code, however a relative comparison is possible between the amount of marker hits on IBL, ALT-II limiter and test limiter (local deposition). The relative amounts in Simulation VIII are closest to the experimental values with ca. 1\% on the ALT-II limiter (1–2\% in the experiment), 8\% on IBL (7–11\%) and 8\% locally on the test limiter (6\%). Simulations prior to VIII produce too much local deposition, 20–60\%, and too little global deposition on the IBL and ALT-II limiter, altogether 1–6\%. Simulations posterior to VIII also have too much local deposition, around 40–60\%, and less Mo on the IBL than on the ALT-II limiter, about a factor 2–5, contrary to the experimental results.

One feature where ASCOT results were verified with measurements after the simulation concerns deposition on the ALT-II backside. The simulations yielding deposition on the ALT-II limiter also had a considerable contribution on the limiter backsides. This was confirmed by measurements where about 15–30\% of the tracers on the ALT-II limiter were deposited on its back.

5. Conclusion

We used the TEXTOR MoF\(_6\) marker experiment as a setting for extensive ASCOT simulations, studying the importance of various physical mechanisms. The following conclusions are drawn.

- Toroidal plasma movement, either in central plasma due to NBI or in the SOL due to flow towards the PFCs, has very small influence on high-Z marker deposition.
- The \( E \times B \) drift is one of the most important parameters for global marker transport, and hence exact knowledge of radial electric field profiles is needed for proper impurity transport code benchmarking.
- The source distribution is another important parameter, yet its impact on simulation results depends on the strength of the radial electric field.
- Marker starting energy has a modest influence on deposition. For detailed studies one therefore needs to simulate also the dissociation of molecules. For rather coarse assessments, approximations might be feasible.
- While changing the SOL profile does not change the qualitative picture, the deposition efficiencies are notably altered.

Finally, when comparing the qualitative results with experimentally obtained results, see Fig. 8, the closest match is obtained by Simulations (VI)–(VIII), albeit with three times too strong electric field. This illustrates that the closest match between experiment and simulation is not necessarily obtained by the most realistic set of simulation parameters. The most realistic set of parameters investigated in ASCOT was in Simulation case (X-b). Still, substantial features of the experimental deposition patterns could not be obtained: deposition on the ALT-II limiter next to the gas inlet, and deposition on top of the IBL. This indicates the importance of PWI effects neglected in the present ASCOT simulations, namely reflection and re-erosion. We therefore encourage benchmarking and parameter studies with other 3D codes including PWI processes, e.g. ERO 2.0.

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