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# Modelling of deposition and erosion of injected $WF_6$ and $MoF_6$ in TEXTOR

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## Abstract

Tracer injection experiments in TEXTOR with $MoF_6$ and $WF_6$ lead to local deposition of about 6% for Mo and about 1% for W relative to the injected amount of Mo and W atoms. Modelling of these experiments has been done with ERO applying updated data for physical sputtering. The dissociation of the injected molecules has been treated in a simplified manner due to the lack of dissociation rate coefficients. However, with this it was possible to reproduce the observed radial penetration of Mo and W atoms into the plasma. The modelled local deposition efficiencies are about 50% for Mo and 60% for W assuming typical plasma parameters for the experimental conditions used. To reproduce the measured deposition efficiencies an enhancement factor for the erosion of deposited Mo and W has to be assumed (~10 for Mo and ~25 for W). Due to the rather low electron temperature $T_e$ of these plasma conditions ($T_e$~15 eV at the location of injection), Mo and W are mostly sputtered by impurities whereas sputtering due to deuterium is negligible. A parameter study applying larger electron temperature leads to increased sputtering and thus to reduced local deposition efficiencies of about 30% for Mo and 5% for W. Though, even under these conditions enhanced erosion, albeit with reduced enhancement factors, is needed in the modelling to obtain the small measured deposition efficiencies.

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## 1. Introduction

The erosion and deposition of plasma-facing components in fusion devices are critical issues due to reduced wall life time and long-term tritium retention by means of co-deposition. At the locations of highest heat and particle loads, like the divertor of ITER, tungsten is the preferred material given that it has the highest melting point and low physical sputtering. Moreover, high-Z materials benefit from prompt deposition, which lowers the net erosion.
Local injection experiments at TEXTOR together with modelling indicated that carbon deposited at plasma-wetted areas can suffer from significantly larger in-situ erosion than comparable bulk material, i.e. enhanced erosion during the deposition process [1, 2]. The level of enhancement depends on the flux and energy of depositing particles, the surface roughness and on the surface temperature [3]. Maximum enhancement factors for the erosion of up to 30 have been reported. Additional tracer injection experiments at other fusion devices like JET or ASDEX Upgrade also indicated the effect of enhanced erosion of deposited carbon [4, 5].
However, most of these experiments have been performed with carbon-based tracer species. To study the possibly enhanced in-situ erosion of deposited tungsten particles, tungsten hexafluoride ($WF_6$) has been injected through a graphite test limiter exposed to the edge plasma of TEXTOR. For comparison with another high-Z material, an additional injection experiment has been carried out with molybdenum hexafluoride ($MoF_6$). The present contribution gives a brief overview of these experiments and describes in detail the according modelling. The focus here will be on the local transport and resulting deposition near the injection inlet on the test limiter surfaces. Global migration aspects of molybdenum (Mo) and tungsten (W) are discussed in detail in [6].

## 2. $MoF_6$ and $WF_6$ injection experiments in TEXTOR

An extensive description of the $WF_6$ and $MoF_6$ injection experiments can be found in [7, 8], therefore here only some basic information is summarised. $WF_6$ has been injected through test limiters in two different experiments; the contribution at hand focuses on the first one, which is denoted as Exp. 1 in [7]. The $MoF_6$ experiment has been performed during the very last operation day of TEXTOR. Both $WF_6$ and $MoF_6$ have been injected through roof-like test limiters (20° inclination angle) exposed to the scrape-off layer (SOL) of TEXTOR. The tips of the test limiters were located at minor plasma radius of 47.5 cm, which is 1.5 cm inside the SOL. The test limiters were covered with polished graphite plates to ease the post-mortem analysis of the deposition. The experiments have been executed with Neutral Beam Injection heating of about 1.5 MW during the flat top phases of the discharges. The $WF_6$ and $MoF_6$ injection rates were about 3E19 molecules/s with opening the injection valve at the beginning of the flat top phase of the discharges and keeping the valve open for 1 s. In case of $WF_6$ 7 injections have been done, in case of $MoF_6$ 31. Part of the injected molecules entered the vessel after the plasma discharges due to the significant length of the injection system; however, this has been considered for the estimation of the deposition efficiencies. Spectroscopic observations of different species have been done during the discharges. In particular the radiation of the neutral species W and Mo has been used to benchmark with the modelling. Various post-mortem analysis techniques like SIMS, EPMA, RBS, ERDA, EPS, have been applied to measure the resulting deposition on the graphite plates after removal of the test limiters out of TEXTOR. From these the local deposition efficiencies, i.e. the total number of atoms deposited on the graphite plates relative to the total number of atoms injected, have been estimated to ~1% for W and ~6% for Mo. For the sake of completeness it is noted that the second $WF_6$ experiment had been performed under similar plasma conditions

but with the test limiter located slightly deeper inside the SOL at plasma radius of 48 cm. The local W deposition efficiency on the test limiter surface was 1-2%.

## 3. Modelling of $MoF_6$ and $WF_6$ injection experiments in TEXTOR

The three dimensional Monte-Carlo impurity transport and plasma-wall interaction code ERO [9] is used to model these experiments. Preliminary modelling results have been presented earlier in [2] for $WF_6$ and in [8] for $MoF_6$. For these former modelling the physical sputtering yields for traced test particles hitting the limiter surface have been calculated with the revised Bohdansky formula for the impact energy dependence and the Yamamura formula for the impact angle dependence [10]. However, it is known that the Yamamura formula is not valid in particular for self-sputtering and for heavy projectiles near the threshold as described e.g. in [10]. Thus, for the new simulations the sputter yield is calculated according to the so-called Eckstein fit as described in [11, 12]. The necessary fit parameters are provided for a number of projectile and substrate combinations in [12]. In case of missing combinations, like carbon on tungsten or carbon on molybdenum and vice versa, or too narrow energy ranges provided in [12], SDTrimSP [13] simulations have been carried out and from these the required fit parameters have been determined. As example figure 1 shows the resulting angular dependence of the sputter yield for carbon on molybdenum for an impact energy of 300 eV. Plasma background ions (deuterium D, carbon C and oxygen O) are typically not traced in ERO for which the impact angles and energies are not exactly known. However, test runs injecting these species away from the test limiter have been performed showing that an average impact angle of 60° is a good assumption for typical TEXTOR edge plasma conditions. SDTrimSP simulations have been done to produce a data base of sputtering yields for the background species hitting W, Mo and C substrates under 60° impact assuming Maxwellian energy distributed projectiles with mean charge states of Z=1 for D ions, Z=4 for C ions and Z=5 for O ions. The acceleration in the sheath potential has been considered in these SDTrimSP simulations.

In the previous simulations of these injection experiments no dissociation of the injected molecules has been considered as no complete sets of dissociation data for $WF_6$ and $MoF_6$ are available. Instead, the atoms W and Mo have been injected and the ionisation rate coefficients of these injected atoms have been adapted to match the measured radial penetration from the emission of the atoms (WI line and MoI line) [2, 8]. However, this approach resulted in a clear mismatch of the toroidal distribution between observed and simulated WI and MoI emission. The simulated emission was much more localised in toroidal direction compared to the observed ones. Within the present work isotropic velocity change of the W and Mo atoms after the dissociation of the molecules (which occurs already thermally around 300°C) is taken into account by considering one effective dissociation process. To mimic the observed 2D radiation patterns of WI and MoI, the effective dissociation rate coefficient and the released dissociation energy are chosen by input parameters to match the observed WI and MoI emission. Formally still W and Mo atoms are injected within the simulation but the line radiation of the atoms is only calculated for species after the effective dissociation process.

Both experiments have been performed under similar plasma conditions. Helium beam measurements of the radial profiles of the electron temperature $T_e$ and density $n_e$ are available for the $WF_6$ injection experiment. These data have been fitted with exponential functions with decay length $\lambda$ resulting in the following parameters: $T_e$(LCFS) = 30 eV and $\lambda_{Te}$ = 40 mm, $n_e$(LCFS) = 5E12 $cm^{-3}$ and $\lambda_{ne}$ = 30 mm, where the Last Closed Flux Surface (LCFS) is located at the minor plasma radius of 46 cm. These parameters result in rather low electron temperature of about 15 eV at locations near to the injection inlet of the test limiter. Therefore, sputtering of W and Mo will be dominated by impurities whereas erosion due to deuterium plasma ions is negligible. It has to be kept in mind that the He beam measurements

In TEXTOR were made at a position different from the test limiter and measurements of the plasma conditions directly located at the test limiter are not available. Also, local plasma disturbances due to the injection cannot be excluded. The latter effect has been studied for $^{13}CH_4$ injection and it has been concluded that possible local plasma disturbances are likely but do not significantly influence the modelling results of the local deposition for typical injection rates applied in TEXTOR [14]. Thus, local plasma disturbances will not be discussed here; however, plasma parameter variations have been addressed as parameter study. Of particular interest is the influence of increased electron temperature such that W and Mo erosion due to deuterium ions can occur. For this, data of NBI heated plasmas in TEXTOR from literature [15] have been assessed and following parameters have been used to compare with the above-mentioned ones: $T_e$(LCFS) = 80 eV, $n_e$(LCFS) = 7E12 $cm^{-3}$ with the same exponential decay lengths as before.
For both sets of plasma parameters the ion temperature $T_i$ is assumed to be twice as large as the electron temperature [16]. The main impurities in TEXTOR are carbon and oxygen. Their concentrations within the plasma are needed for the modelling to consider the erosion due to these species. For the $MoF_6$ and $WF_6$ experiments no concentration measurements of these impurities are available wherefore here the following assumptions are made according to earlier publications [14, 17, 18]: concentrations at the LCFS of 5.2% for carbon and 1% for oxygen with negative exponential decay lengths (leading to increasing concentrations farther in the SOL) of -139 mm for carbon and -70 mm for oxygen. The mean charge states are assumed to be 4 for carbon and 5 for oxygen. The assumptions reflect upper values of the impurity concentrations and thus lead maximum erosion of deposited Mo and W atoms.

### 3.1. Modelling results for the $MoF_6$ injection experiment

At first, simulations have been done using the first plasma parameter set (30 eV, 5E12 $cm^{-3}$). Adapting the effective dissociation of injected molecules results in a 2D emission pattern of MoI line presented in figure 2. The dissociation leads to a certain distribution of MoI in toroidal direction which is similar to the one observed in the experiment. Besides the main MoI pattern near to the injection inlet an additional emission is visible – both in the simulation and the experiment – at the top of the test limiter at plasma radius 47.5 cm (dashed-dotted line). This comes from the erosion of before-hand deposited Mo. The more detailed comparison of the simulated and observed radial penetration of MoI into the plasma is shown in figure 3 and indicates a good agreement. The profiles are taken at the toroidal location of the injection inlet and their intensities are normalised to one as here the comparison of their shapes is of main interest.
The simulations reveal that about 56% of the injected Mo atoms return to the test limiter surface. As the reflection of Mo on carbon is rather small, almost all of these returning atoms are first of all deposited. To simulate the ultimate deposition of injected Mo atoms on the test limiter, erosion due to the background species deuterium, carbon and oxygen is taken into account. In addition, eroded particles returning to the test limiter can re-erode new particles and finally the erosion due to fluorine atoms coming from the dissociation of $MoF_6$ is considered. As fluorine is not tracked in the simulations it is assumed that 6 fluorine atoms return to the test limiter surface together with each returning Mo atom. This is an extreme assumption to consider a maximum erosion effect due to fluorine. According to the Eckstein fit formula $Y_{F\_Mo}$ is in the percent range for an impact energy of 45 eV ($3ZT_e$ with Z=1 and $T_e$=15 eV around the injection inlet). Thus, for the sputtering of Mo due to F a yield of $Y_{F\_Mo}$ = 1% is assumed. However, considering all these erosion processes results in a deposition efficiency of injected Mo of about 47% and thus about 8 times larger than the observed one. It is seen that Mo sputtering by deuterium is negligible as the electron temperature is rather small. Main Mo sputtering is due to oxygen and fluorine and to a smaller portion due to the

background carbon ions and re-erosion due to returning of formerly eroded particles. The simulated 2D pattern of Mo deposition on the test limiter, presented in figure 4, reveals a rather extended distribution in toroidal direction. Also visible is a certain distortion in poloidal direction which is the result of E×B transport. To obtain the smaller observed deposition efficiency an enhanced (related to substrate Mo) erosion of deposited Mo atoms has to be assumed. With an enhancement factor $f_{enh}$ = 10 for physical sputtering the deposition efficiency is reduced to about 9% which is near to the measured one. The 2D Mo deposition pattern is now much more localised compared to the case without enhanced sputtering, see figure 4. The resulting Mo deposition profiles for the simulation with enhanced erosion are shown in figure 5 in toroidal and poloidal direction in comparison to the EPMA measurements. The profiles are taken along lines near to the injection inlet and show rather good agreement between simulation and experiment with a tendency of the modelled profiles being a bit broader than the measured ones.
Additional variations of the parameter $f_{enh}$ have been done showing that a value of 15 further decreases the Mo deposition efficiency to about 4%. The modelled deposition profiles with $f_{enh}$=15 fairly agree with the measured ones, however, maximum deposition is about 2 times smaller than the measured one. Altogether it can be concluded that enhanced erosion of deposited Mo is necessary to be assumed and the enhancement is between 10 and 15.

To study the influence of an increased electron temperature simulations have been done with the second plasma set (80 eV, 7E12 $cm^{-3}$). As before, the effective dissociation of $MoF_6$ has been adapted to match the radial profile of the MoI emission observed. Due to the increased electron temperature Mo sputtering due to deuterium becomes significant; however, the overall sputtering is dominated by eroded particles returning to the limiter surface and by background ions and fluorine. The increased electron temperature and density leads to a slightly increased amount of returning Mo to the surface: now about 70% compared to 56% with the previously used plasma parameters. The simulation without enhanced erosion of Mo now gives a deposition efficiency of about 29%, which is still 5 times larger than the measured one. Therefore, again enhanced erosion of deposited has to be applied to lower the deposition efficiency to the observed one. Though, compared to the previous simulations with lower electron temperature the enhancement factor is smaller: a value of $f_{enh}$ = 3 gives a Mo deposition efficiency of about 5%, i.e. almost the measured value of 6%. But the resulting Mo deposition profile is clearly more peaked than the measured one with the modelled maximum deposition nearly 4 times larger than the measured one. It thus can be speculated that the first parameter set used represents the plasma conditions of the Mo injection experiment better than the second one with increased electron temperature. In any case, enhanced erosion of at least a factor of 3 is a necessary assumption to reproduce the small measured deposition efficiency.

### 3.2. Modelling results for the $WF_6$ injection experiment

The modelling of the $WF_6$ experiment followed the same strategy as the one for the $MoF_6$ injection, which has been described in detail in the previous section. Therefore, here only the main results will be summarised. For the sputtering of tungsten due to fluorine the same assumptions as for $MoF_6$ are made (6 F atoms returning per deposited W and a sputtering yield for F on W of 1% is used). As before, the radially observed WI profile has been matched by the modelling by means of adapting the effective dissociation of the injected W. Applying the first plasma parameter set (30 eV, 5E12 $cm^{-3}$) results in a W deposition of about 26%, which is about 26 times larger than the measured one. Assuming enhanced erosion of W with $f_{enh}$ = 20 leads to about 3% deposition efficiency which is near to the measured value of 1%.

The modelled deposition profile for this case in toroidal direction is shown in figure 6 together with the measured one demonstrating the good agreement of their shapes.
Using the second plasma parameter set (80 eV, 7E12 $cm^{-3}$) with increased sputtering leads to W deposition efficiency of about 5% and thus about 5 times larger than the measured one. With these plasma parameters the modelled deposition efficiency is reduced to about 1% if an enhanced erosion of deposited tungsten $f_{enh} = 3$ is assumed. As for the Mo modelling with these plasma parameters, also the modelled W deposition profile is much more peaked with maximum deposition about 10 times larger than the measured one.

## 4. Summary and conclusions

New modelling of Mo and W deposition from $MoF_6$ and $WF_6$ injection experiments in TEXTOR has been presented. Main focus was on the local deposition on the test limiter surfaces near to the injection hole. For the modelling, updated data for physical sputtering yields were used and an effective dissociation of the injected molecules was implemented. It was seen that the modelled amounts of deposited Mo and W atoms were significantly larger than the measured ones (8 times for Mo and 26 times for W). It has to be noted that for these simulations already upper values for the impurity concentrations (carbon and oxygen) in the edge plasma have been assumed and an extreme assumption for the sputtering due to fluorine from the injected molecules. Sputtering of deposited Mo and W is dominated by these impurities and partly by self-sputtering due to returning Mo and W ions whereas sputtering due to deuterium ions is negligible. To match the measured deposition efficiency of injected atoms an enhanced erosion of deposits had to be assumed with enhancement factors of about 10 for Mo and 20 for W. For testing, a higher electron temperature was assumed for the modelling such that the overall sputtering increases and also sputtering due to deuterium ions becomes important. However, even under these extreme plasma parameters still the assumption of enhanced erosion is necessary to match the observed deposition efficiencies albeit the enhancement factors are significantly smaller than before (3 for both Mo and W re-erosion).
Such enhanced erosion was introduced already earlier for the simulation of $^{13}CH_4$ injection experiments and interpreted as an in-situ increased erosion during the deposition process itself. The deposition flux has been identified as one determining factor of the enhanced erosion showing larger enhanced erosion at increasing deposition fluxes. From the modelling it is seen that the local Mo and W deposition fluxes near the injection inlet are about 5E21 atoms/$m^2$s. The depositing flux of sputtered tungsten in fusion devices is typically much smaller, which would decrease the enhanced erosion effect or even eliminate it. Further studies under well-defined conditions e.g. in laboratory experiments would be necessary to clarify the process of enhanced erosion.

## Acknowledgements

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## References

[1] A. Kirschner et al., J. Nucl. Mat. 328 (2004) 62
[2] A. Kirschner et al., J. Nucl. Mat. 415 (2011) S239
[3] A. Kirschner et al., J. Nucl. Mat. 438 (2013) S723

[4] M. Airila et al., Phys. Scripta T138 (2009) 014021
[5] L. Aho-Mantila et al., J. Nucl. Mat. 415 (2011) S231
[6] A. Weckmann et al., this conference
[7] M. Rubel et al., J. Nucl. Mat. 438 (2013) S170
[8] A. Weckmann et al., Phys. Scripta T167 (2016) 014058
[9] A. Kirschner et al., Nucl. Fus. 50 (2000) 989
[10] C. García-Rosales et al., J. Nucl. Mat. 218 (1994) 8
[11] W. Eckstein, Vacuum 82 (2008) 930
[12] R. Behrisch, W. Eckstein W, editors: Sputtering by particle bombardment, Top. Appl. Phys. 110 (2007)
[13] W. Eckstein et al., *SDTrimSP: A Monte-Carlo Code for Calculating Collision Phenomena in Randomized Targets*, IPP Report 12/3 (2007)
[14] R. Ding et al., Plasma Phys. Contr. Fus. 52 (2010) 045005
[15] O. Schmitz et al., Plasma Phys. Contr. Fus. 50 (2008) 115004
[16] A. Huber et al., Plasma Phys. Contr. Fus. 42 (2000) 569
[17] S. Droste et al., Plasma Phys. Contr. Fus, 50 (2008) 015006
[18] S. Brezinsek et al., Phys. Scripta 145 (2011) 014016

## Figure captions:

**Figure 1** Sputter yield in dependence on the impact angle: carbon ions impinging molybdenum and tungsten at 300 eV.

**Figure 2** Simulated (left) and observed (right) distribution of MoI emission. The dotted line indicates the location of the LCFS at plasma radius of 46 cm.

**Figure 3** Normalised radial profiles of observed (Exp) and modelled (ERO) MoI emission. The red line in the right picture of figure 2 indicates the location at which the radial profiles have been taken.

**Figure 4** Modelled 2D distribution of Mo deposition on the test limiter without enhanced erosion (left) and with 10 times enhanced erosion (right). The simulations represent the distributions after having reached steady state conditions.

**Figure 5** Modelled (ERO) and measured (Exp) Mo deposition profiles in toroidal and poloidal direction. For the modelling 10 times enhanced erosion of deposited atoms is assumed.

**Figure 6** Modelled (ERO) and measured (Exp) W deposition profiles in toroidal direction. For the modelling 20 times enhanced erosion of deposited atoms is assumed. Note that the modelled profile has been divided by 3 to normalise its maximum to the measured one.

## Figures:

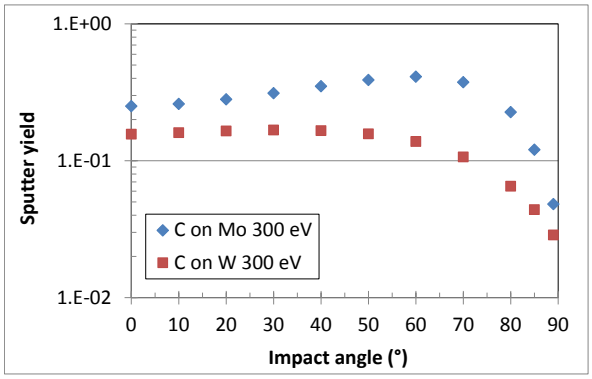


**Figure 1**

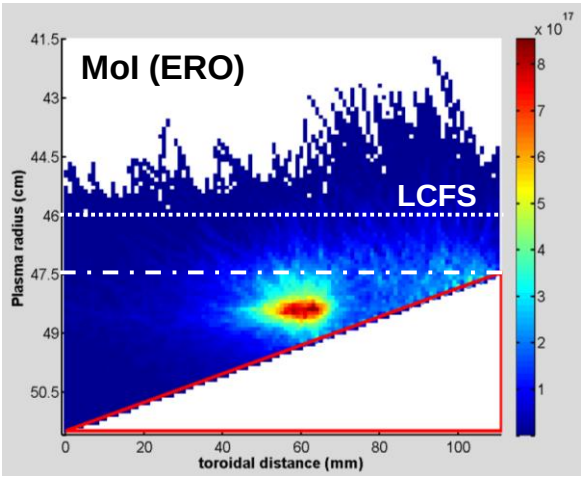


**Figure 2**

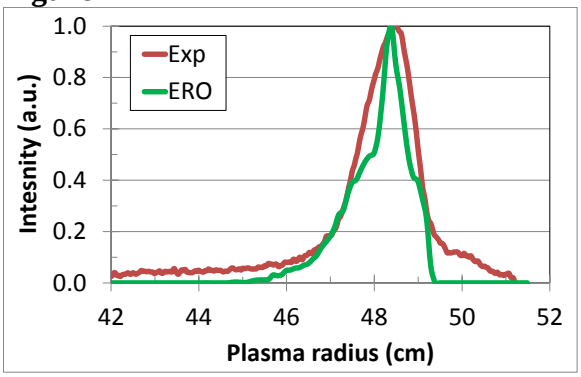


**Figure 3**

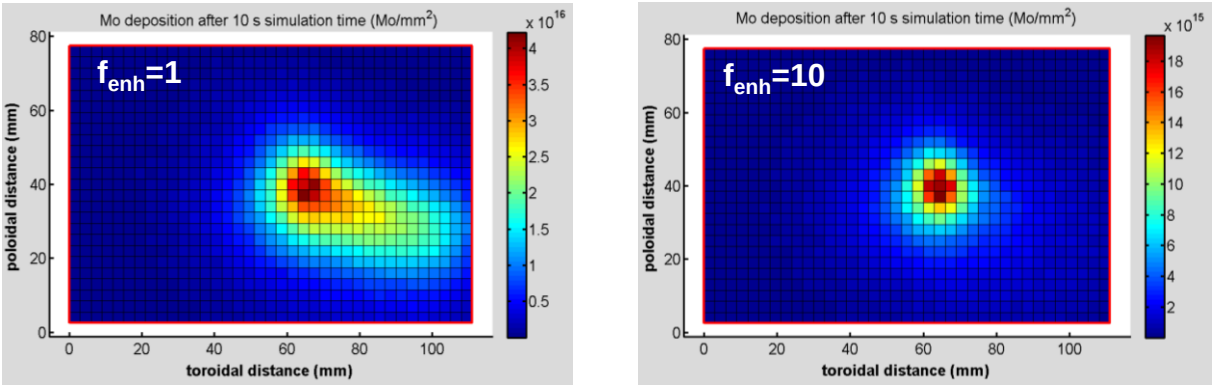


**Figure 4**

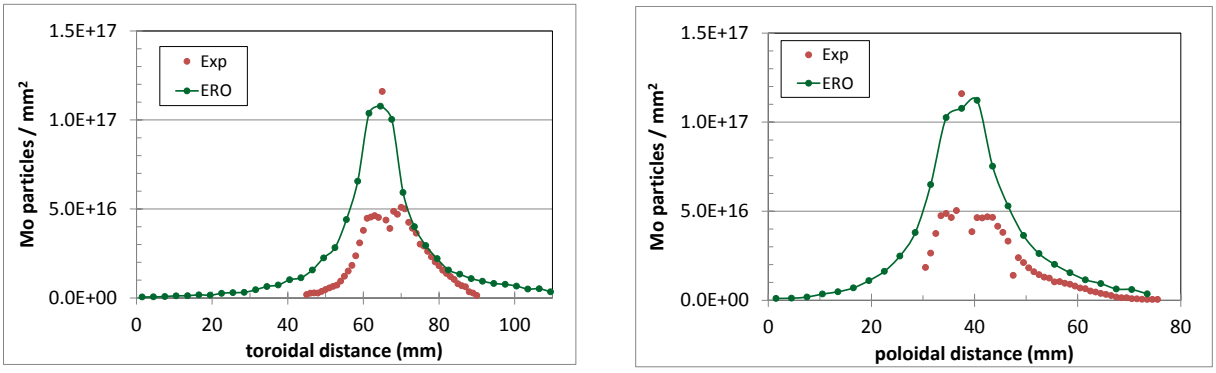

**Figure 5**

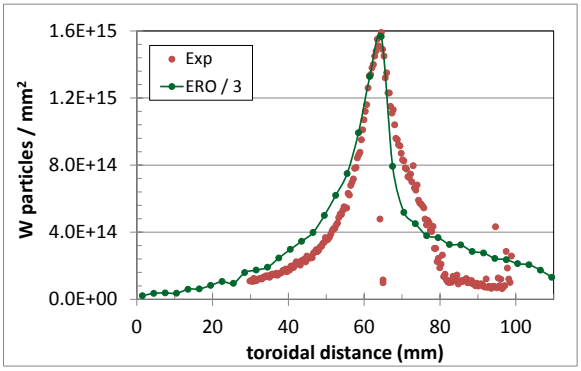


**Figure 6**