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## Retention and Release of Hydrogen Isotopes in Tungsten Plasma Facing Components: Understanding and Controlling with an Integrated Approach

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**Abstract.** Fusion fuel retention (trapping) and release (desorption) from plasma facing components is one of the critical issues for ITER and for any future industrial demonstration reactor such as DEMO. Therefore, understanding fundamental mechanisms behind hydrogen isotopes retention in first wall and divertor materials is necessary. We developed an approach that couples dedicated experimental studies with modelling at all relevant scales, from microscopic elementary steps to macroscopic observables, in order to: 1. gain insight in the fundamental interactions between fusion fuel and wall materials; 2. build a reliable and predictive fusion reactor walls model. This integrated approach is applied to ITER divertor material (tungsten) and advances in the development of the wall model are presented. An experimental dataset, including Temperature Programmed Desorption and isothermal desorption, is exploited to initialize a Macroscopic Rate Equations (MRE) model resolved by the MHIMS code, which includes all elementary steps: implantation of fusion fuel, fuel diffusion in the bulk or towards the surface, fuel trapping on defects and release of trapped fuel during a thermal excursion of PFC. We were able to unambiguously show that a single trap type – single detrapping energy model is not able to reproduce an extended parameter space study of a well characterized sample exhibiting a single desorption peak. It is therefore justified to use Density Functional Theory to guide the initialization of a single trap type – multi-detrapping energy model to simulate the hydrogen isotopes retention behaviour of tungsten.

### 1. Introduction

For ITER, tritium poses both nuclear regulation and economic issues due to, respectively, its radioactivity and the scarcity of its resources. These reasons impose to control the tritium inventory in the tokamak, especially in Plasma Facing Components (PFC) of the machine where most of particles flux are expected and which are composed of beryllium and tungsten. In order to preserve a high duty cycle in ITER, a direct detailed control of the tritium inventory in PFC cannot be routine. It is therefore important to develop a reliable first wall and divertor model to estimate the tritium content of PFC at any time.

In this paper, we report on the development of a Macroscopic Rate Equations (MRE) model for tungsten-based PFC. Our integrated approach consists in devising model experiments where a large parameter space can be explored on a single tungsten sample. This way sample-to-sample variability is avoided and MRE model development is more accurate. In section 2, we first describe the experimental methods we used and give an overview of the experimentally explored parameter space. Then we present the MRE code MHIMS [1] which is used to construct a tungsten wall model. In section 3, we elaborate on the parametrization of the MHIMS code based mostly on experimental inputs. Then, we estimate how far the model is able to reproduce experimental observations and draw conclusions on its partial failure. Finally, we discuss how MHIMS-reservoir [2], a code evolution which allows to model multi-hydrogen isotopes trapping on a single defect trap, can be parametrized based on Density Functional Theory (DFT) inputs, i.e. only from a theoretical microscopic description of fundamental processes. This paper ends on a summary and a perspective about our MRE wall model development.

## 2. Methods

To reach the goal of an accurate description of PFC behavior regarding hydrogen isotopes retention, an integrated approach is preferred. This is the reason why a large set of complementary techniques must be used in order to grasp as much information on bulk and on surface PFC processes as possible. A selection of some of these experimental techniques will be described in section 2.1 and we will focus particularly on the *in situ* implantation/thermo-desorption setup used at Aix-Marseille Université [3]. These experimental inputs should then be confronted to a multi-scale modeling, from the microscopic scale (DFT) to the macroscopic scale (MRE). In section 2.2, we will specifically describe the calculation setup of the latter which is at the core of the first wall and divertor model development.

### 2.1.Experiments

Tungsten PFC in ITER will be located in the divertor region of the tokamak and will contain polycrystalline tungsten with specific grain elongation in order to optimize heat transfer to the cooling structures [4]. However, in our experimental approach we need a model sample which can withstand multiple implantations and thermo-desorption cycles (typically around 100) without structure evolution affecting neither its retention nor its thermal release of hydrogen isotopes. Therefore, we used recrystallized polycrystalline tungsten (99.99 wt.% purity, A.L.M.T. corp, Japan) with typical grain size of about  $\sim 30 \mu\text{m}$ . The sample ( $10 \times 10 \times 0.4 \text{ mm}^3$ ) was subjected to several polishing and cleaning procedures before to be introduced in the Ultra High Vacuum (UHV) implantation/thermo-desorption setup at Aix-Marseille Université (base pressure  $< 4 \cdot 10^{-8} \text{ Pa}$ ). The sample was thoroughly degassed at 1300 K in UHV before any experimental campaign. A typical experiment consisted, first, in implanting the tungsten sample at 320 K with 500 eV  $\text{D}_2^+$  ions with a flux of  $2 \cdot 10^{16} \text{ D}^+ \cdot \text{m}^{-2} \cdot \text{s}^{-1}$ . This low flux insured that there was no thermal gradient on the sample during implantation. Then, a minimum storage time of 2 hours at room temperature and at a base pressure of  $< 10^{-7} \text{ Pa}$  was used before the sample was transferred back in the thermo-desorption setup. Finally, the sample temperature was increased at a rate of  $1 \text{ K} \cdot \text{s}^{-1}$  while a differentially-pumped quadrupole mass spectrometer was measuring in line-of-sight HD and  $\text{D}_2$  molecules emitted by the sample. This last step is a Temperature Programmed Desorption (TPD), also known as Thermal Desorption Spectroscopy (TDS), and provides information regarding hydrogen isotopes retention and detrapping energies. Further details can be found in the recent article by Bisson *et al.* [3].

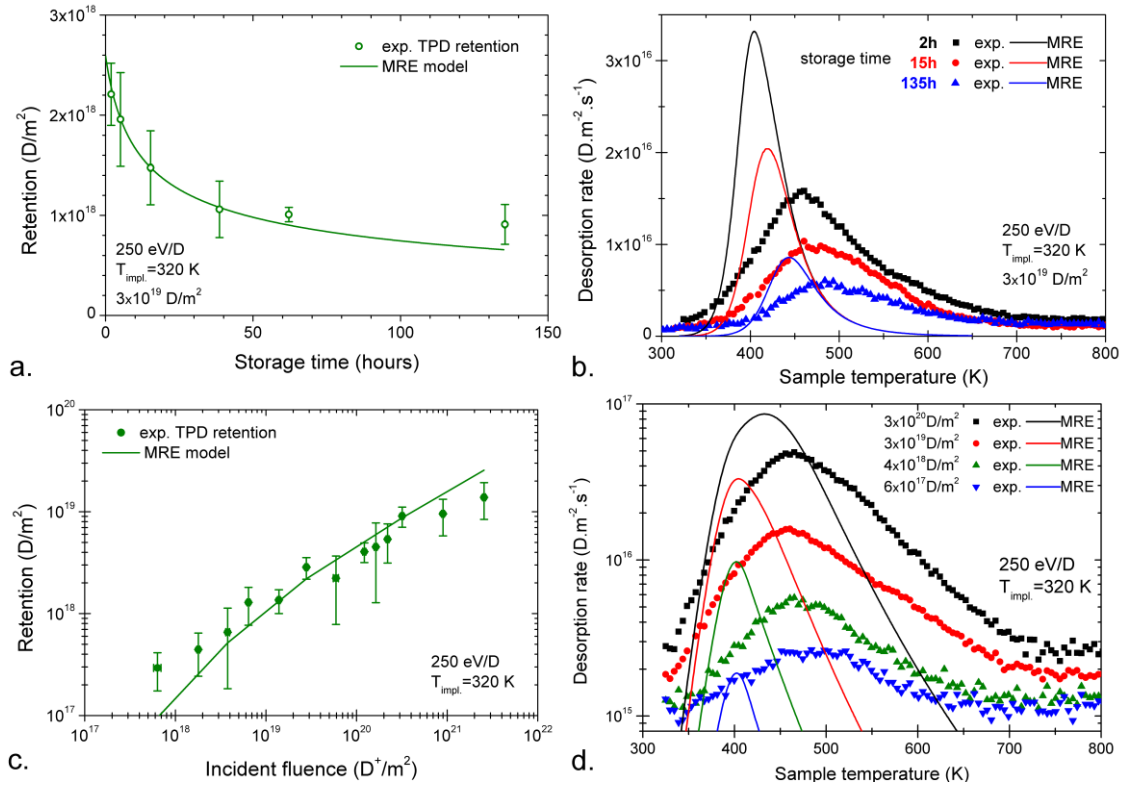


FIG. 1. Comparison between experimental data (symbols) and MRE results (lines) for a single trap type – single detrapping energy model. Experimental data in a., c. and d. adapted from [3].

With this setup, an extended parameter space study has been performed (see FIG. 1.). TPD measurements have been realized after various implantation duration, allowing to explore how fluence affects hydrogen isotopes retention (through integration of the TPD curve, see FIG. 1.c.) and detrapping energy (through the shape and width of the TPD curve, see FIG. 1.d.). Desorption and bulk diffusion might play a role since fluence is spanned at a constant flux and implantation durations vary from a few minutes to tens of hours. To explore the importance of desorption and diffusion at 320 K, measurements have been realized at a constant fluence for various storage times (see FIG. 1.a. and 1.b.) which constitutes an isothermal desorption experiment. Nuclear Reaction Analysis (NRA) has also been performed to access the bulk distribution of implanted deuterium as well as Auger Electron Spectroscopy (AES) to check any surface chemistry change. Because of the limited space available in the proceedings these other results will be presented in a future article.

While the details of the experimental results will be described in Section 3, it is important to note that the originality of this data set, obtained from room temperature implantation of low energy deuterium ions, is to exhibit a single desorption peak. This feature allows to test the usual assumption that the number of trap types present in a material is (at least) equal to the number of desorption peaks.

## 2.2. Macroscopic Rate Equations models: MHIMS

One dimensional (1D) MRE codes are commonly used to extracting energetic information about PFC materials interaction with ions beams and plasmas [5–7]. We have recently developed such a code, MHIMS for Migration of Hydrogen Isotopes in Materials [1], which describes numerous elementary steps encountered in real experiments. With MHIMS, one can simulate the implantation of hydrogen isotopes below the surface with their subsequent diffusion into the bulk or toward the surface and their trapping on bulk defects. Detrapping of

hydrogen isotopes and diffusion are thermally activated processes, thus they are active during the whole simulation i.e. from the beginning of the implantation to the end of a Temperature Programmed Desorption experiment, including all the practical steps in between such as the storage time described in Section 2.1.

Even though an arbitrary number of types of defects can be implemented in the MHIMS code, in the present paper we will setup only one type of defect. Indeed, one is generally able to fit any observable with a model that includes a large number of free parameters. However, we aim at testing if the simplest model can reproduce our extensive experimental data set and learn from its eventual failure in order to guide the construction of a more complex model.

We will now describe briefly the MHIMS code [1]. A simple diagram such as the one shown in FIG. 2. represents the potential energy experienced by a trapped hydrogen isotope on its path to desorption. In order to escape a trap, the hydrogen isotope needs to overcome a detrapping barrier  $E_{\text{detrapp}}$ . Then, it has to surmount diffusion barriers  $E_{\text{diff}}$  to reach the surface, go deeper in the bulk or become trapped in another defect site. Finally, if two hydrogen isotopes reach the surface, they can recombine and form a desorbing molecule. The latter process has been shown not to be rate limiting in experiments [3] simulated in this paper and thus the desorption process is considered to be instantaneous in the present simulations. However, we inform the reader that the description of surface processes has been included in a recent upgrade of the MHIMS code [8]. Every barrier is surmounted with thermal energy, so we use the following Arrhenius formulation of kinetic rates:  $v_{\text{process}} = v_{\text{process}}^0 \cdot \exp(-E_{\text{barrier}}/k_{\text{B}}T)$ , where  $E_{\text{barrier}}$  can be one of the process barriers listed above,  $v_{\text{process}}^0$  is the rate constant of the process,  $k_{\text{B}}$  is the Boltzmann constant and  $T$  is the sample temperature.

These rates are used to make evolve the concentrations (in  $\text{m}^{-3}$ ) of hydrogen isotopes trapped in defects,  $c_t$ , as well as the concentration of hydrogen isotopes diffusing as interstitial atoms in the bulk,  $c_m$ , with the following set of equations:

$$\partial c_m / \partial t = \varphi \cdot (1 - r) \cdot f(x) + v_{\text{diff}} \cdot \partial^2 c_m / \partial x^2 - \partial c_t / \partial t \quad (1)$$

$$\partial c_t / \partial t = v_{\text{trap}} \cdot (c_m / n_m) \cdot (n_t - c_t) - v_{\text{detrapp}} \cdot c_t \quad (2)$$

where  $t$  and  $x$  are the temporal and spatial variables. Desorption of hydrogen isotopes occurs when particles arrive at  $c_m(x=0)$  and the boundary condition is set to  $c_m(x=0) = 0$  (instantaneous desorption).

On the right-hand side of EQ. 1, the first term describes the implantation of impinging hydrogen isotope ions at a flux  $\varphi$  (in  $\text{m}^{-2} \cdot \text{s}^{-1}$ ) having a reflection probability  $r$  and being deposited in the bulk as diffusing particles with an implantation profile  $f(x)$  (in  $\text{m}^{-1}$ ). The second term is Fick's law of diffusion with  $v_{\text{diff}}$  the temperature dependent diffusion coefficient. The third term expresses loss/gain of diffusing hydrogen isotopes into/from defect traps at a rate defined by EQ.2.

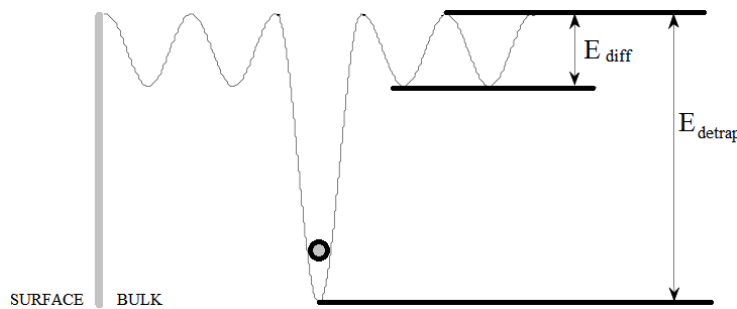


FIG. 2. Potential energy diagram of a hydrogen isotope (represented by a filled circle) in tungsten trapped at a defect.  $E_{\text{detrapp}}$  and  $E_{\text{diff}}$  are explained in the text.

In the right-hand side of EQ. 2, the first term defines the increase in concentration of trapped hydrogen isotopes to be proportional to the fraction of bulk interstitial sites containing a diffusing hydrogen isotope ( $c_m/n_m$ ) and to the concentration of empty trapping site ( $n_t - c_t$ ).  $n_m$  is the constant concentration of bulk interstitial sites where hydrogen isotopes can reside between two diffusion processes, the tetrahedral interstitial sites in tungsten [9] with 6 sites per unit cell of this body centered cubic crystal.  $n_t$  is the constant concentration of defect trapping site which depends on the sample under study, which is assumed to be uniformly distributed throughout the bulk. The second term describes the decrease in concentration of trapped hydrogen isotopes following a simple thermal detrapping process.

Rate constants are defined in the following way:

$v_{diff}^0 = D_H/\sqrt{m_{HI}}$ , where  $D_H$  is the temperature independent hydrogen diffusion coefficient (in  $m^2 \cdot s^{-1}$ ) and  $m_{HI}$  is the ratio of mass of the hydrogen isotope to hydrogen.  $m_{HI} = 2$  here,

$v_{trap}^0 = v_{diff}^0 / (\lambda^2)$ , where defect trapping of the diffusing hydrogen isotope occurs from a tetrahedral interstitial site with  $\lambda$  the distance between two of these sites,

$v_{detrapp}^0$  is the usual first-order pre-exponential factor of a thermally activated process.

### 3. Results and Discussion

#### 3.1. Single trap type – single detrapping energy: MHIMS code parametrization

The purpose of the work presented here is to test if the single trap type – single detrapping energy MRE model, the simplest model one can devise, can reproduce the experimental data set described previously when its parameters are initialized with experimental observations typical for our sample. Therefore, we set MRE parameters according to the following decreasing order of preference: 1. experimentally derived parameters ( $\phi$ ,  $D_H$ ,  $E_{diff}$ ,  $E_{detrapp}$ ), 2. parameters from a binary collisions code (SRIM [10]) bench-marked on experimental observations ( $r$ ,  $f(x)$ ), 3. DFT values ( $\lambda$ ,  $v_{detrapp}^0$ ,  $n_m$ ); see Table I. The only free parameter left is the density of trapping sites in our sample,  $n_t$ .

TABLE I: Initialization of parameters for the 1 trap – 1 energy MRE model.  $\rho_w = 6.3 \cdot 10^{28} m^{-3}$ .

MRE parameters	Values	References
$\phi$	$2 \cdot 10^{16} m^{-2} \cdot s^{-1}$	Exp [3]
$r$	0.55	SRIM [10]
$f(x)$	approximated by a gaussian profile with a mean depth of 4.5 nm and a standard deviation of 2.5 nm	SRIM [10]
$D_H$	$4.1 \cdot 10^{-7} m^2 \cdot s^{-1}$	Exp [11]
$E_{diff} = E_{trap}$	0.39 eV	Exp [11]
$E_{detrapp}$	1.1 eV	Exp [3]
$\lambda$	$1.1 \cdot 10^{-10} m$	DFT [9]
$v_{detrapp}^0$	$10^{13} s^{-1}$	DFT [9]
$n_m$	$6 \cdot \rho_w$	DFT [9]
$n_t$	$10^{-3} \cdot \rho_w$	Free parameter



### 3.2.MHIMS results and comparison with experiments

In order to converge the MHIMS simulation, we minimized the difference between the simulation results and the experimental data describing the retention as a function of the storage time (*see FIG. 1.a.*) and as a function of incident ion fluence (*see FIG. 1.c.*). By doing so we determined the only free parameter,  $n_t$ , i.e. the concentration of uniformly distributed defect trapping sites. The agreement is quantitative for both set of measurements. However, if the prediction of the hydrogen isotopes retention, i.e. the integral of the TPD measurements, is quantitatively correct, the TPD simulations do not agree quantitatively with measurements.

*FIG. 1.b.* shows that TPD simulation results reproduce only qualitatively the experimental observation. Both in experiments and simulations, the maximum rate of desorption shifts by about 30 K to higher temperature as the storage time is increased from 2 h to 135 h. This behavior can be explained by hydrogen isotopes diffusing deeper in the bulk (not shown) as the storage time increases. However, the obvious difference between simulations and experiments is the difference in the width of desorption peaks. The width of the simulated TPD peaks (FWHM  $\sim 75$  K) is systematically smaller than the width of the experimental TPD peaks (FWHM  $\sim 150$  K). Such difference cannot be ascribed to a difference in  $E_{diff}$ , since decreasing  $E_{diff}$  to the DFT value of 0.2 eV [9] does not change significantly the hydrogen isotopes bulk distribution neither the width of simulated TPD peaks (not shown). The simulated TPD peaks width can approach the experimental ones if the  $E_{detrap}$  value is lowered, which increases the depth range that deuterium reaches. However, lowering  $E_{detrap}$  results in a disagreement on absolute deuterium retention and its storage time dependency. Thus another physical process should be found to fix the difference of TPD peak width.

The usual way to deal with a TPD peak width discrepancy and/or some shallow bumps in the TPD is to invoke additional types of trapping sites with slightly different (0.2 – 0.3 eV) detrapping energy [1, 6, 7]. However, careful analysis of *FIG. 1.d.* can lead to a different physical explanation that keeps the number of traps in the MRE model to only one, i.e. to the same number of TPD peaks observed experimentally.

A striking experimental results from *FIG. 1.d.* is the observation that the maximum rate of desorption shifts to lower temperature and then stays put as the hydrogen fluence is increased. As shown by Bisson *et al.* [3], this behavior cannot be explained by a second order surface rate limiting step but instead a bulk property may be invoked. Indeed, recent DFT studies have demonstrated that a single defect site can trap multiple hydrogen isotopes and that the detrapping energy from the defect site is dependent on the number of trapped hydrogen isotopes. Several types of defects exhibit this behavior, such as tungsten vacancies [9, 12, 13], poly-crystal grain boundaries [14] and tungsten vacancy-impurity complexes [15].

Given the polycrystalline nature of the sample used in the present study, it is natural to focus on defects that are related to grain boundaries. Xiao and Geng calculations have shown that a  $\Sigma 3(111)$  grain boundary defect site can accommodate up to 7 hydrogen isotopes [14] with detrapping energies  $E_{detrap}$  ranging from 1.5 eV to 0.9 eV ( $E_{diff}$  from [9] has been added to the binding energy from [14]). In particular, it is shown that  $E_{detrap}$  is decreasing when the number of trapped hydrogen isotopes increases from 1 to 3. This trend is consistent with the experimental observation of *FIG 1.d.* where the TPD peak position is decreasing to lower temperature when the deuterium fluence increases. Therefore, it seems a good lead to follow in order to develop a MRE model that keeps the one TPD peak – one type of defect trap correspondence.



### 3.3.DFT insight and single trap type – multi-detrapping energy MRE model

Various DFT calculations of tungsten defects have shown that the detrapping energy from a defect site can vary with the number of hydrogen isotopes bound to the defect. This behavior has been recently included in MRE model codes [2, 16]. The implementation of Hodille *et al.* used in the present work, called MHIMS-reservoir [2], will be presented in a future article. Here we will simply expose the principle of the code implementation as shown in FIG. 3. Each trap in the bulk is able to bind to several deuterium atoms and hence each trap is described with a filling level  $l$  representative of the number of bound deuterium atoms. To each filling level corresponds a different detrapping energy. Because the implementation of this single trap type – multi-detrapping energy MRE model has been inspired from theoretical calculations, we parametrized the MHIMS-reservoir code according to a different order of preference than in Section 3.2, which was mostly experimentally-set. Here, we want to test if a purely theoretical approach for the development of a MRE model is able to improve the simulation results i.e. if selecting the right physics is able to render the trends of experimental observations. Therefore, the MRE parameters are set according to the following decreasing order of preference: 1. DFT values ( $D_H$ ,  $E_{diff}$ ,  $E_{detrapp}$ ,  $\lambda$ ,  $v_{detrapp}^0$ ,  $n_m$ ), 2. parameters from the SRIM code ( $r$ ,  $f(x)$ ), 3. Experimentally derived parameters ( $\phi$ ). The only free parameter left is the density of trapping site in our sample,  $n_t$ . The results obtained will be described in a future article.

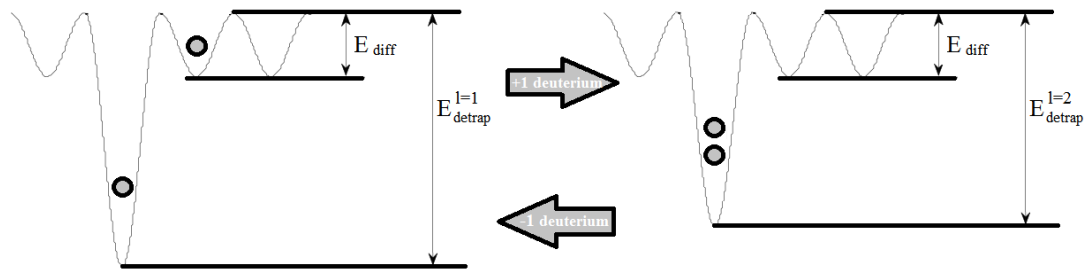


FIG. 3. Principle of the single trap type – multi-detrapping energy MRE model: each trap has a hydrogen isotope filling level  $l$  which value determines the detrapping energy. Filled circles represent deuterium atoms.

## 4. Summary and perspectives

We presented joint experiment-simulation study of deuterium retention in recrystallized polycrystalline tungsten aimed at guiding the development of a Macroscopic Rate Equations model for PFC used in all metal tokamaks. These model experiments probed a large parameter space on a single sample and always exhibited a single desorption peak. The latter observation allows the development of a MRE model in a systematic manner. Starting with the simplest model possible, a single trap type with a single detrapping energy, we found that it is possible to reproduce quantitatively or qualitatively only 3 of the 4 experimental results. The failure of the simplest model to reproduce the TPD peak shift to lower temperature with increasing fluence was analyzed and we argued that it is possible to keep the simplicity of a single trap type model to rationalize all experimental observations. Indeed, a physical interpretation was found from the *ab initio* DFT literature: defects in tungsten can accommodate more than one hydrogen isotope per defect site, and the detrapping energy is dependent of the number of hydrogen isotopes bound to the defect site. Because the experimental dataset has been obtained from polycrystalline tungsten, we described the setup of a single trap type MRE model based on a grain boundary defect. The results of this DFT-based simple MRE model will be presented in a future publication. These results will allow to justify further development of the Macroscopic Rate Equations tungsten divertor model as

well as to propose new model experiments. This interplay between well-controlled model experiments and the systematic test and development of a MRE model supported by multi-scale modeling is the foundation of our integrated approach and gives solid results.

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