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Modelling of Be transport in PSI experiments at PISCES-B

D. Borodin^{a,*}, A. Kirschner^a, A. Kreter^a, V. Philipps^a, A. Pospieszczyk^a, R. Ding^a, R. Doerner^b, D. Nishijima^b, J. Yu^b

^a Institut für Energieforschung – Plasmaphysik, Forschungszentrum Jülich GmbH, Association EURATOM-FZJ, Trilateral Euregio Cluster, D-52425 Jülich, Germany ^b University of California, San Diego, CA 92093-0417, La Jolla, USA

ARTICLE INFO	ABSTRACT
PACS: 52.40.Hf 52.20.Hv	Light emission patterns of BeI and BeII in the PISCES-B divertor simulator were simulated using the 3D Monte-Carlo code ERO. Many additional physical effects, e.g. Be collisions with neutral particles, were implemented into the code and tested alongside with the underlying data (e.g. ionization rates) by detailed comparison with experimental observations. This analysis is important to fully understand the Be impurity transport, deposition and re-erosion in PISCES-B, which will form the basis to model the Be behaviour in the LET LIW project and LTEP.

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1. Introduction

Erosion and deposition processes of plasma-facing components (PFC) in ITER, which will be made of beryllium (Be), tungsten (W) and carbon (C), determine the long term tritium retention rate and their lifetime. A detailed understanding of these processes and validated modelling is needed to make reliable predictions for ITER, understand experimental observations and develop control mechanism. Of particular importance is to understand the interplay of erosion, material transport, and material mixing in PFCs including chemical processes [1].

Modelling of PISCES-B (linear divertor simulator) experiments plays a particular role, because this is the only device, which allows relevant plasma experiments with toxic Be. In addition, it has a simple geometry and continuous plasma operation. PISCES-B has an exchangeable and cooled target with variable biasing, which defines the impinging energy of plasma ions. Beryllium is introduced into the plasma column using either a Be-effusion cell or by erosion from the Be target.

ERO is a 3D Monte-Carlo code, which simulates erosion, deposition, local impurity transport and their light emission. Recently, a special version was developed for PISCES-B and first modelling results were presented in [2]. Several additional effects were added to the code and proved to be of importance, e.g. elastic collisions (EC) of Be with the neutral background gas of the plasma constitute (D₂) and physical sputtering by molecular ions (D₂⁺, D₃⁺). To reproduce the mitigation of chemical erosion of the carbon target by Be deposition, which is of large importance for ITER operation [3], a model has been used in which Be–C carbide formation appears instantaneously. This assumption could reproduce qualitatively

* Corresponding author. E-mail address: d.borodin@fz-juelich.de (D. Borodin). some experimental observations. The main disagreement is the much larger experimental time scale of the mitigation, which we account to slow changes of surface morphology and chemical reactions in the surface affected by diffusion. The complete mitigation, which is observed experimentally, can be reproduced by modelling only at larger Be plasma concentrations than in the experiment (several percent in modelling versus less than 1% in experiment).

This work presents improved modelling of experimentally measured Bel and Bell line intensity profiles in PISCES-B. Spectroscopy is used to characterise the Be transport through the plasma, which is a key part in understanding the beryllium flux to and from the target and thus plasma surface interaction (PSI) processes. Spectroscopic measurements allow also tracking the temporal evolution, whereas surface analysis characterises usually only the final state of the system.

2. Simulations, comparison with experiment, discussion

2.1. PISCES-B experiments

PISCES-B has a cylindrical vessel with a radius of about 20 cm. The plasma column confined by axial B-field impinges on an exchangeable target (Fig. 1). The electron density n_e slightly drops approaching the target and has a Gaussian profile in radial direction with a characteristic width of 50 mm. The electron temperature is constant along the axis and has a 72 mm wide plateau in radial direction. The data used are an approximation from multiple experimental data [4] resulting in fitting formulas that are anchored to the value at the axis at z = 150 mm, which is measured routinely. Typically $n_e \sim 1 \div 3 \times 10^{12}$ cm⁻³, $T_e \sim 4 \div 12$ eV.

Be is injected from side using a special oven (effusion cell). The spectroscopic patterns of Bel, Bell and other species are measured





Fig. 1. Plasma parameters in the cross-section of PISCES-B taken through the axis [4]. The target and the Be injection from the oven (situated at 195 mm from the axis) are marked. The remaining part of the vessel is filled with neutral gas.

with a 2D camera with narrow band filters and also with a spectrometer. The latter allows taking linear profiles both along and perpendicular to the magnetic field (PISCES-B axis).

2.2. Elastic collisions with neutrals

Elastic collisions (EC) with neutral D_2 gas play an important role for the transport of neutral Be. They lead to a broad distribution of Be along the whole PISCES-B volume. As a result of EC, the influence of initial angle and energy distribution of the injected Be becomes mostly negligible. As only the Be impurities are tracked by ERO the velocity vector of D_2 is randomly generated with a Maxwell distribution at room temperature. The oppositely directed velocity directions after the collision are assumed to be isotropically random in the centre of mass system.

The ERO EC model and the underlying data were tested by the modelling of dedicated experiments in which Be was seeded into the volume but without plasma. The Be oven aperture has a cone-like shape with a very sharp angle of about 12° such that the Be stream entering the PSICES-B device is strongly collimated. Thus, the Be flux that can impinge on the target itself is only due to EC (Fig. 2). The ERO simulations were used to correlate the seeding rates with the Be-deposition on the target, assuming full sticking of Be. The Be rate estimation based on this correlation and the exper-



Fig. 2. Density of neutral Be inside PISCES-B vessel (right) illustrating the transport of injected Be to the target. The calibration of deposition to the injected rate based on ERO simulations determines the injection rate corresponding to the experimental weight gain.



Fig. 3. Comparison of normalized to maximum Bel line intensity profiles. The electron density used as input for ERO is also shown to illustrate plasma column position and width. The target and Be seeding direction are marked.

imentally measured weight gain $(1.5 \times 10^{-4} \text{ g in } 2400 \text{ s})$ of the target due to Be-deposition are in a good agreement with the amount of Be filled into the oven for Be-seeding (2 g of Be is spent in more than 10 h). The first estimation (Fig. 2) gives a rate of 4.03×10^{18} Be/s, the second – 3.7×10^{18} Be/s.

2.3. Radial profiles

Recently, dedicated experiments for the characterisation of Be transport were carried out by tracking the Bel, Bell and D_{γ} light intensity profiles perpendicular to the PISCES-B axis using a spectrometer at 150, 100, 50 and 20 mm distance from the target at different plasma conditions: 'low density' case ($n_e = 1.2 \times 10^{12} \text{ cm}^{-3}$, $T_e = 10.5 \text{ eV}$) and 'high density' case ($n_e = 2.9 \times 10^{12} \text{ cm}^{-3}$, $T_e = 8 \text{ eV}$).

Fig. 3 illustrates the comparison of simulated and experimental profiles for the 'low density' case. The $n_{\rm e}$ profiles mark the plasma column position and width. The injection rate in the modelling is fitted to reproduce the measured Bel intensity at maximum. The resulting axial profiles taken from the intensity at the axis from the radial profiles are also shown in Fig. 3 as a projection to the rear plane. The simulated profiles have similar asymmetric shape and width, however, they are more shifted to the direction of the injection. The penetration depth of the neutral Be especially near the oven is strongly influenced by the ionization, determined by the effective rate depending on $n_{\rm e}$, $T_{\rm e}$.

The simulated ratio between BeII (467 nm) and BeI (457 nm) line intensity profile (Fig. 4) has a maximum of similar width as the respective experimental one. It is asymmetric due to shift of neutral Be density distribution towards the oven, whereas Be⁺ density and light emission is practically axial symmetric in both experiment and ERO modelling. However, the simulated ratio is smaller than in the experiment (though it has the same order of magnitude), showing that the BeII density calculated by ERO is obviously too large. This is another indication in the direction that the used ionization rates might be too large.

In our previous calculations [2] Be ionization rates according to the '93' ADAS [5] dataset have been used while the present modelling makes use of the '96' dataset based on data from [6]. In the plasma parameter range relevant for PISCES-B the new rates are smaller by a factor of about 2 (Fig 5). This leads to a better agreement with experiment, though the Bell intensity is still overestimated.



Fig. 5. Effective ionization rates used by the ERO code; 2 sets of data from ADAS: '93' (used previously) and '96' are compared. In addition the rates estimated by the Lotz formula are plotted.

It should be noted that the pattern of Bell can be affected also by other factors, e.g. the radial electric field (determined by the Gaussian radial plasma potential of $-2T_e$; directed to the PISCES-B axis) and the cross-filed diffusion (Bohm diffusion was assumed, as confirmed by experiments). The Bel emission can also be affected by the initial population of the $1s^22s2p$ ³P metastable state and its evolution on the way from the oven through the neutral gas and the plasma. Another uncertainty comes from the presence of Be-D molecules in plasma. Their light emission is registered experimentally showing a more or less complete filling of the vacuum volume. However, they are not followed in the ERO calculations and consequently the influence of Be-D molecules on the Be transport is not reflected in the modelling.

However, the most important reason for deviations is probably uncertainties in plasma parameters. As the temperature has a wide radial plateau the D_{γ} emission should theoretically characterise the



Fig. 4. Radial profiles of neutral and ionized Be line intensity ratios perpendicular to the PISCES-B axis at z = 150 mm (near the Be oven); comparison of experimental and simulated results.

plasma density. However, its radial profile has a quite different shape compared to the Gaussian density, which ERO uses as input: it is narrower and also hollow close to the plasma axis (we suppose that the dim at x = 0 is artificial, resulting from uncertainties in the intensity calibration there).

The comparison of the simulated and experimental results for the 'high density' case leads to similar conclusions as for the low density case, shown in Figs. 3 and 4. The comparison of Bel light pattern registered independently by the 2D camera with the respective ERO simulation is in line with the results obtained using the spectrometer.

3. Summary and outlook

The ERO modelling for PISCES-B was significantly improved (the model for elastic collisions, new atomic data from ADAS, etc.) and benchmarked again by experiments, leading to better agreement. Some discrepancies remain which can be accounted most probably to uncertainties in the underlying data, e.g. the plasma parameters, though they can also be determined by physical effects not yet implemented into the model, such as the influence of metastable Be states.

Understanding and modelling of the beryllium transport is a necessary step before proceeding with further simulations of PSI experiments, in which the slow time evolution of the surface chemical erosion of graphite targets plays a key role. It is essential to correctly interpret the transport of seeded Be and eroded particles from the target.

The next important improvement for ERO would be the introduction of metastable states for Be. The respective atomic data indicates that this effect can influence strongly the emission of BeI. The implementation of Be–D molecules transport is also of importance, however, it is complicated due to the lack of the respective atomic data.

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