Validation of EDGE2D-EIRENE and DIVIMP for W SOL transport in JET

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Abstract. Tungsten sputtering and density profiles predicted using the edge plasma codes EDGE2D-EIRENE and DIVIMP are found to agree within a factor of 2 with measurements of singly-ionized W spectral line emission in the JET low-field side (LFS) divertor, and with SXR, VUV, and bolometric calculations of the W density in the main plasma. The studied plasmas include attached L-mode and type-I ELMy H-mode conditions typical for JET. To reproduce the spectroscopically inferred W sputtering rates in EDGE2D-EIRENE, imposing the experimentally observed Be concentration of order 0.5% in the divertor is necessary. However, the predicted W density in the main plasma is found to be insensitive to whether or not W is sputtered by Be at the divertor targets. Instead, the majority of the predicted core W originated in L-mode from sputtering due to fast D charge-exchange atoms at the W-coated tiles above the LFS divertor, and in H-mode due to D ions at the targets during ELMs.

Keywords: Impurity transport, tungsten, scrape-off layer, code validation, Joint European Torus, spectroscopy, fluid simulation

1. Introduction

Tungsten (W) is the material of divertor plasma-facing components in ITER and the JET ITER-like wall [1], and a strong candidate for use in future fusion reactors. The erosion and transport of tungsten from the divertor plates into the core plasma is detrimental to the fusion performance due to the high radiation factor of W ions in the keV-MeV range [2]. Therefore, the design of viable fusion reactors greatly benefits from the ability to predict the W erosion rate, the W screening by the scrape-off layer (SOL) and the main plasma W density as a function of time.

This study uses recent calculations [3] based on JET W diagnostics to quantitatively assess the ability of the 2D edge plasma codes EDGE2D-EIRENE [4, 5] and DIVIMP [6, 7] to predict the spatially resolved W sputtering rates and the main plasma W density in JET. The electron density and temperature profiles as well as the beryllium densities are matched against data from existing JET L-mode and H-mode experiments. The transport of W across closed flux surfaces is modelled by coupling the JETTO and SANCO core transport codes with EDGE2D-EIRENE. All information from the W diagnostics is reserved solely for validation and not used as input in the W transport simulations.

2. Methods

Discharge	B_t	I_p	P_{NBI}	P_{Ohmic}	$n_{\mathrm{e,core}}$
#81472	2.5 T	2.5 MA	1.0 MW	1.5 MW	$2.8 \cdot 10^{19}$ m^{-3}
#82486	2.0 T	2.0 MA	10.0 MW	1.0 MW	$7 \cdot 10^{19}$ m^{-3}

Table 1. The main parameters of the studied JET discharges JPN 81472 at 9 s in L-mode and JPN 82486 at 14 s in H-mode.

One L-mode and one H-mode discharge (Table 1) with steady magnetic field, plasma current, heating power and electron density were selected for this study. Discharges with a horizontal low-field side strike point configuration were chosen due to the availability of high fidelity Langmuir probe and spectroscopic data for validation. While this configuration is not typical of the highest-performance JET discharges, the selected scenarios are similar to several other JET experiments. The focus of this study is on attached divertor conditions, due to the prevalence of W erosion in this regime and due to the limited reliability of the Langmuir probe data in detached plasmas.

In addition to the divertor conditions, also the upstream electron density and temperature were fitted to measurements by high resolution Thomson scattering [8], lithium beam [9] and reciprocating Langmuir probe [10] diagnostics when available (Fig. 1, 2).

2.1. EDGE2D-EIRENE simulation setup

The multi-fluid edge plasma/kinetic neutral code EDGE2D-EIRENE is used in this work to model the SOL plasma conditions, including intrinsic beryllium and tungsten impurities. The source of W is the predicted sputtering of divertor W surfaces due to D, Be and W. The Be concentration is based on the predicted sputtering of beryllium surfaces in the JET main chamber. The 74 W ion charge states were bundled [11] to 6 fluid species for computational stability.

The applied heating power and fuelling rate were based on the experiments, taking into account the power losses due to radiation in the core plasma. For calculating the pumping rate, an effective albedo of 0.8 was specified for neutral particles at the LFS pumping plenum leading to the subdivertor. The HFS pumping plenum was assumed

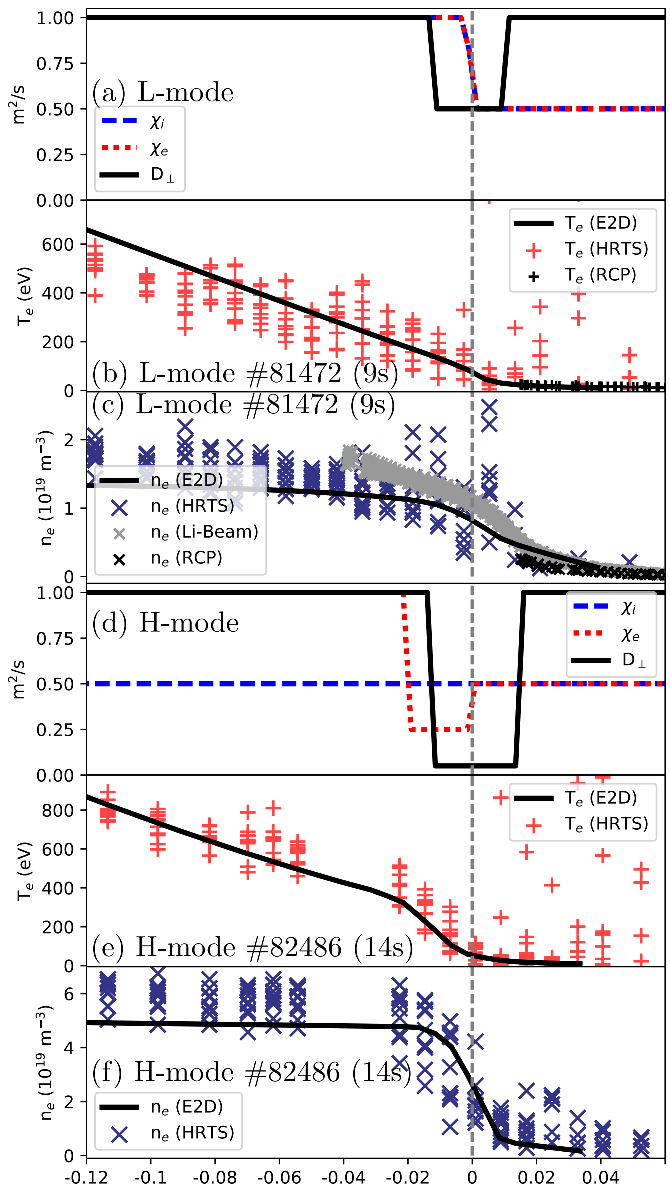

Figure 1. Ion and electron cross-field heat and particle diffusion coefficients (a,d) used in EDGE2D to reproduce the electron density and temperature profiles measured by high-resolution Thomson scattering, Li-beam, and reciprocating probe along the LFS mid-plane (b,c,e,f) in the L-mode (a-c) and inter-ELM H-mode (d-f) scenarios.

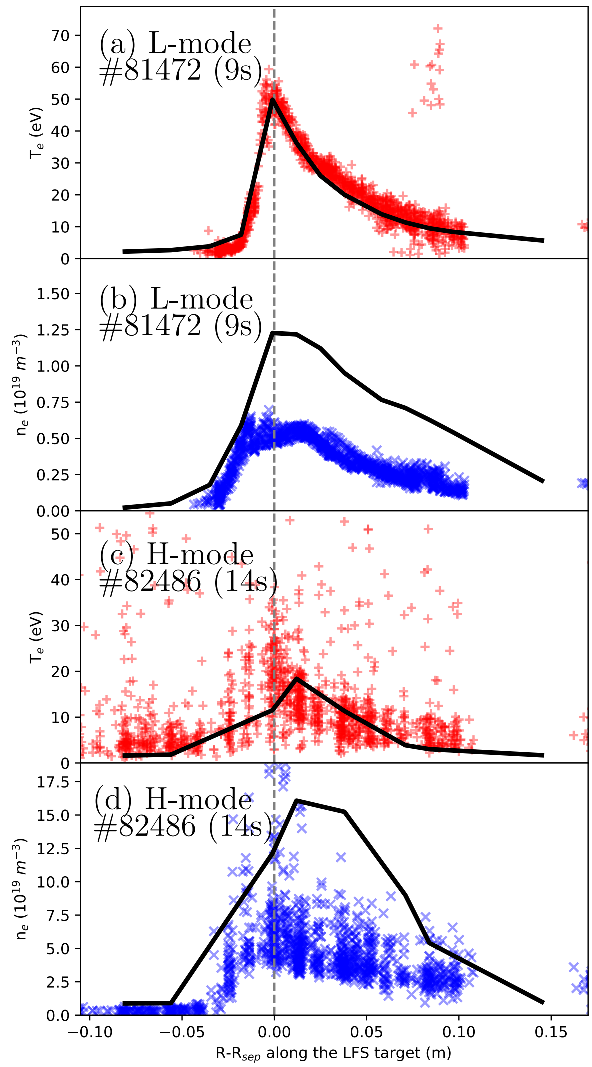

Figure 2. Electron temperature (a,c) and density (b,d) profiles predicted by EDGE2D-EIRENE (solid lines) compared to Langmuir probe measurements (markers) along the LFS target in the L-mode (a,b) and H-mode (c,d) scenarios. The predicted target electron temperatures closely match the measurements, whereas the target electron densities are overestimated by a factor of 2.

ineffective. These assumed albedo values are justified by earlier analysis of EDGE2D-EIRENE simulations with the subdivertor module included [12].

The anomalous cross-field transport coefficients for electrons and deuterium ions in the main SOL were selected to reproduce the experimental electron density and temperature profiles measured by high-resolution Thomson scattering (HRTS) along the LFS mid-plane (Fig. 1). In the divertor SOL, the transport coefficients were set to 1 m^2/s. For impurities, a constant $D_\perp$ of 1 m^2/s was used in both the divertor and the main chamber. The pinch velocity was assumed 0 for all species.

In the H-mode scenario, ELMs are simulated with a frequency of 28 Hz and parameters based on earlier work [13]. The particle and thermal diffusivities are multiplied by a factor of 10 and 30 respectively within an ELM-affected region on the LFS, extending radially from 0 to 7 cm inside the separatrix. Time-dependent kinetic correction factors [14] for the heat flux limiters were included, however corrections for the sheath heat transmission coefficients are neglected due to their adverse impact on the simulation time step when W is included. The duration of each ELM is specified as 1 ms. The recycling coefficient was assumed constant, neglecting any dynamic changes in the outgassing of the PFCs. Although this description of ELMs is very simplified and only applicable when the parameters are fitted to experiment, the goal here is to simply obtain background plasmas for W transport rather than attempting to predict the detailed ELM characteristics. The ELM parameters used in this study have been validated against statistical analysis of 53 similar JET type-I ELMy H-mode discharges with 12 MW of NBI heating power [13]. Comparison of simulations with and without ELMs revealed that the increase in W erosion due to ELMs constitutes 80% of the predicted W in the main plasma, highlighting the importance of constraining the ELM parameters with accurate measurement data. This is consistent with earlier studies [15].

Test simulations were executed for L-mode and ELM-free H-mode with cross-field drifts included. However, the drifts were not observed to improve the agreement between the predicted and measured plasma conditions, and were thus excluded from the simulations in this work in favor of numerical stability. Generally, in other scenarios beyond this work, the drifts may be instrumental to reproducing the observed divertor conditions. Dynamic ELM simulations with drifts and tungsten are not considered feasible using the current version of EDGE2D-EIRENE (v191219).

2.2. DIVIMP simulation setup

One significant advantage of the Monte Carlo code DIVIMP compared to the multi-fluid code EDGE2D-EIRENE is that all of the ionized states of tungsten can be individually tracked without adversely affecting the execution time and the stability of the simulation. DIVIMP has been observed to predict consistently 50% higher W density than EDGE2D-EIRENE in JET L-mode and H-mode scenarios, primarily due to the bundling of W charge states in EDGE2D-EIRENE [16]. Furthermore, EDGE2D-EIRENE simulations with both tungsten and cross-field drifts included tend to be unstable whereas in DIVIMP the inclusion of drifts has a negligible computational cost. These factors and the short execution time of DIVIMP make it an attractive option to use EDGE2D-EIRENE solely for the background plasma while replacing the computationally more demanding multi-fluid treatment of W with DIVIMP predictions, especially when drifts and/or ELMs are involved.

In this work, the background plasma conditions and the 2D neutral W ionization profiles are imported to DIVIMP from the EDGE2D-EIRENE simulations. Singly-ionized W test particles are launched at initial positions sampled from the W ionization profile. The code version, boundary conditions and other options used are the same as in earlier comparisons between the two codes [16].

2.3. Integrated core-edge modelling setup

The experiment-based calculations [3] of the main plasma W density in JET are valid in the plasma region with normalized minor radius < 0.6. The SOL transport codes used in this work are not well suited to predict W transport in the core, hence the gap between the edge and core W densities is bridged by coupling EDGE2D-EIRENE to the 1.5D core transport codes JETTO and SANCO, the full system of codes collectively referred to as JINTRAC [17]. The neutral particles in the JETTO domain are described by a model called FRANTIC [18] and neutral beam heating is modelled using the PENCIL code [19].

The coupling interface between the EDGE2D-EIRENE and JETTO domains in the L-mode simulation is placed at a flux surface located 6 cm inside the separatrix at the LFS mid-plane. Coupling at the separatrix, while better justified by the transport models, excludes W erosion by D atoms from the confined plasma, because the kinetic distribution of neutral particles is not transferred across the interface. Including the 6 cm wide confined plasma region in EDGE2D-EIRENE is sufficient to reproduce the majority of the W sputtering by atoms observed in the standalone EDGE2D-EIRENE case. In the H-mode simulation, the interface is placed at the separatrix, because W erosion by D atoms has a low impact on the main plasma W density compared to the impact of the ELMs.

The neoclassical and anomalous cross-field transport is predicted using the standard NCLASS [20] and Bohm/gyro-Bohm transport models [21] respectively. The transport coefficients predicted by the core transport codes are also used as a core boundary condition in EDGE2D-EIRENE. In the H-mode simulation, a 2 cm wide edge transport barrier is set up in JETTO with local anomalous transport multipliers of 0.1, 0.03 and 0.025 for the electron thermal, ion thermal, and particle diffusivites respectively. ELMs are modelled by JETTO, using the same transport multipliers as in the standalone EDGE2D-EIRENE case but with a Gaussian-shaped 5 cm wide ELM region centered at normalized radius 0.97. This approach was tested to produce similar heat and particle loads at the targets as the EDGE2D-EIRENE approach. No JETTO transport barrier or ELMs are applied to the integrated L-mode scenario.

3. Results

If EDGE2D-EIRENE is used to predict the Be flux to the LFS target by only considering erosion and transport from Be components in the main chamber, the resulting Be II line emission is lower than measured by a factor of 200 (Fig. 3a), black line). The primary reason for this result is that the re-erosion of Be from W surfaces is neglected and all of the deposited Be vanishes from the simulation. Earlier studies [23] have established that Be ions are the dominant cause of W erosion in typical attached JET L-mode scenarios and that a 0.5% concentration of Be^{2+} at the LFS target is consistent with the observed W sputtering rate. As expected, simulations with an unrealistically low Be concentration

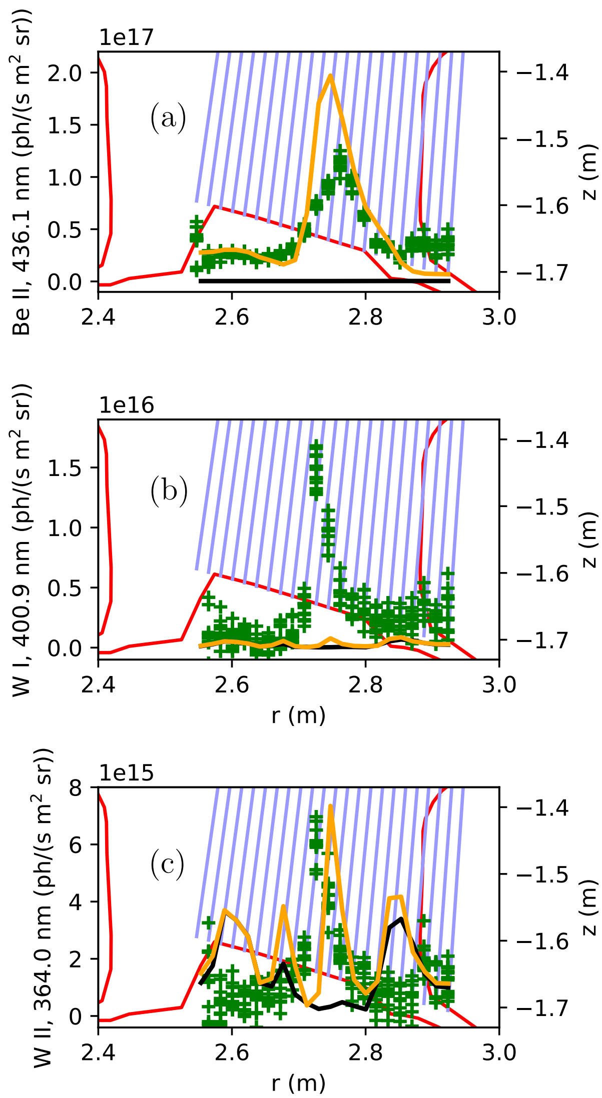

Figure 3. Comparison of a) Be II, b) W I, and c) W II spectral line emission from JPN 81472 at 9.5-10.0 s measured by the high-resolution Czerney-Turner spectrometer *KT3* (green markers) and EDGE2D-EIRENE predictions with only intrinsic Be directly from the main chamber (black lines) and with 10^{20} Be atoms/second injected at the targets to emulate Be re-erosion (orange lines). The JET divertor geometry is shown in red and the spectrometer lines-of-sight in blue. The predicted line emission was calculated using the pyproc post-processor [22].

predict negligible W erosion at the strike point, contrary to experiment (Fig. 3b) and c), black line).

The lack of a Be re-erosion model in EDGE2D-EIRENE can be compensated by injecting additional neutral Be at the targets to achieve the expected 0.5% concentration. In this case, both the predicted and observed Be II line emission profiles show a peak of similar shape, with the predicted Be II intensity 60% higher than the measurement (Fig. 3a), orange line). The predicted W I emission is then one order of magnitude lower than observed (Fig. 3b), orange line), but the predicted peak W II emission agrees with the measurement within a few percent (Fig. 3c), orange line).

Accurately reproducing both the W I and W II lines would require accounting for the prompt redeposition of W, for example by tracking the first few gyro-orbits of W ionized near surfaces. Instead, EDGE2D-EIRENE calculates an effective sputtering yield in which the neutral W influx from the surface represents the sputtered but not promptly-redeposited W. Noting that prompt redeposition is expected for >90% of the W eroded under the studied plasma conditions [23], the result is consistent with the discrepancy in Fig. 3b). For the purposes of W transport simulations using this model, matching the experimental W II emission is therefore far more relevant than the W I emission.

The four rightmost spectrometer lines-of-sight intersecting with the outer vertical divertor indicate a second peak in the W I and W II emission, approximately one order of magnitude weaker than the peak emission at the strike point, despite the several orders of magnitude lower thermal load and incident ion flux in the far SOL. The EDGE2D-EIRENE simulations suggest that the W erosion in this region is dominated by charge-exchange D atoms from the confined plasma and that this region is the largest contributor to the W influx across the separatrix in L-mode and inter-ELM scenarios. In contrast, the W erosion rate at the strike points is predicted to have a negligible impact on the main plasma W density due to efficient W screening by the SOL (Fig. 4), except during ELMs when the W screening is weaker (Fig. 6).

The flux-surface averaged main plasma W density predicted by integrated modelling agrees with the experiment-based calculation within 25% throughout its regime of validity (Fig. 4). Such a close agreement can be attributed to coincidence, because even a 10-15% uncertainty in the upstream SOL electron density would be enough to cause a 50% deviation in the predicted W density. Despite the sensitivity to the input parameters, the EDGE2D-EIRENE and DIVIMP predictions lie approximately within a factor of 2 from the extrapolated experimental result, demonstrating that they provide a viable boundary condition for predicting the main plasma W density. The 60% difference between DIVIMP and EDGE2D-EIRENE predictions is mostly due to the bundling of W charge states to 6 fluid species in EDGE2D-EIRENE [16].

The toroidal rotation of the plasma causes a centrifugal effect which creates an asymmetry of up to one order of magnitude between the HFS and LFS main plasma W densities (Fig. 5). When a rotation velocity of 50 km/s is applied as a boundary condition at the core boundary in EDGE2D-EIRENE, the asymmetry is reproduced to

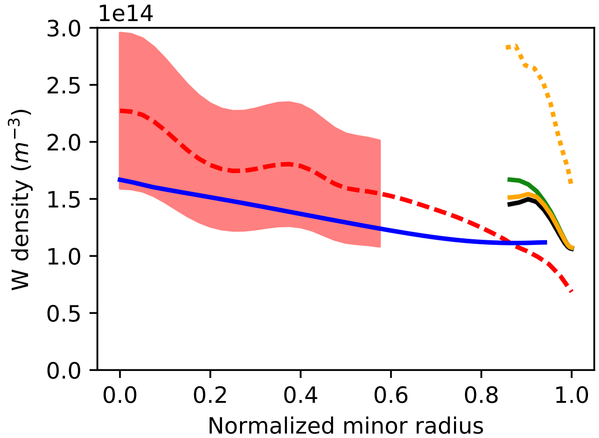

Figure 4. Flux-surface averaged W density in L-mode JPN 81472 at 9 s, calculated from diagnostics (red dashed line with shaded 30% confidence intervals), compared to code predictions. Orange solid and dotted lines: EDGE2D-EIRENE and DIVIMP respectively with 0.5% Be concentration at targets. Blue solid line: SANCO output from integrated modelling. Black solid line: EDGE2D-EIRENE without Be injection at targets. Green solid line: EDGE2D-EIRENE assuming zero toroidal plasma rotation.

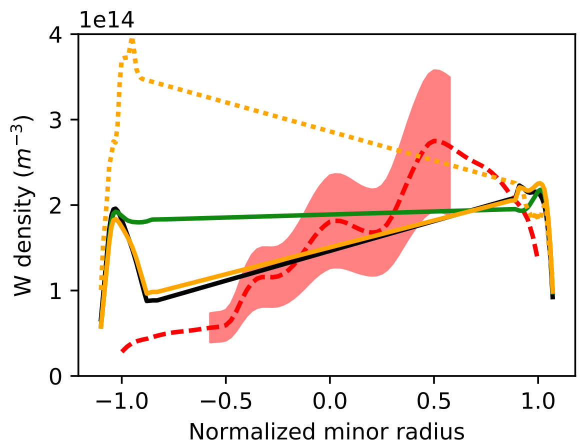

Figure 5. W density along the mid-plane in L-mode JPN 81472 at 9 s. Negative radii correspond to the HFS and positive to the LFS. Linear interpolation is used to connect the EDGE2D-EIRENE predictions across the core region. See Fig. 4 for legend.

within a factor of 2 on the closed flux surfaces (-1 < normalized radius < 1). DIVIMP does not include the centrifugal effect, which is why it predicts an opposite asymmetry driven by parallel-B SOL transport. The impact of rotation on the W density is only significant on the closed flux surfaces, due to parallel-B temperature gradients and inter-species friction playing a more dominant role in the SOL. The extrapolated experimental calculation outwards of normalized radius 0.6 is ambiguous and cannot be used to draw conclusions about the W density in the SOL. The W density profile predicted by the core

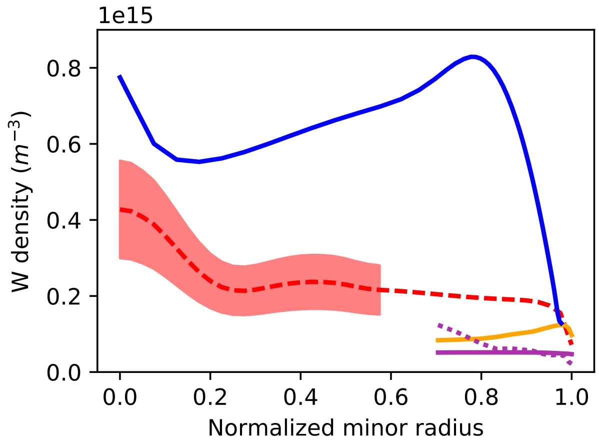

Figure 6. Flux-surface averaged W density in L-mode JPN 81472 at 9 s, calculated from diagnostics (red dashed line with shaded 30% confidence intervals), compared to code predictions. Orange solid line: EDGE2D-EIRENE with ELMs. Blue solid line: SANCO output from integrated modelling with ELMs. Purple solid and dotted line: EDGE2D-EIRENE and DIVIMP respectively without ELMs.

transport codes is one-dimensional, hence poloidal W asymmetries are not reproduced by the integrated modelling scenarios studied in this work.

The ELMy H-mode integrated modelling scenario overestimates the experimental W density by a factor of 2 near the magnetic axis and by a factor of 3 to 4 at normalized radii from 0.2 to 0.6 (Fig. 6). Since it predicts a much larger W density gradient across the pedestal region than the edge codes and the measurements, the overestimation appears to be a feature of the core transport models in conjunction with the imposed ELMs and the edge transport barrier, rather than overestimated W influx by EDGE2D-EIRENE. The standalone EDGE2D-EIRENE and DIVIMP W density predictions are intended to be valid for the SOL, but of limited use far inside the separatrix due to the purely diffusive radial transport model.

4. Conclusions

When the background plasma conditions are fitted to JET L-mode and type-I ELMy H-mode attached plasmas, the edge plasma codes EDGE2D-EIRENE and DIVIMP demonstrated the ability to predict the singly-ionized W emission in the LFS divertor and the upstream W density to within a factor of 2 of the experimental values. The validity of the main plasma W predictions is supported by integrated core-edge modelling, using JETTO and SANCO for core transport. Keeping in mind that the codes used in this work involve simplifications which are not necessarily accurate under all circumstances, further validation is recommended when extrapolating these results to vastly different plasma conditions.

The uncertainties resulting from the simulation parameters in predicting the W density are greater than the observed discrepancy between the predictions and the experiments. The predicted main plasma W density is particularly sensitive to the upstream electron density, the ELM transport multipliers and the width of the ELM-affected region. For predicting the W density in future discharges, it is thus very beneficial to constrain these parameters as accurately as possible using the available data from existing discharges. W predictions for future devices, involving considerable uncertainty in the ELM parameters, should be taken as order-of-magnitude estimates at best. On the other hand, improvements in the ability to predict the background plasma conditions can also be expected to increase the confidence in W predictions by EDGE2D-EIRENE and DIVIMP.

Acknowledgments

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 and 2019-2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

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Appendix A: Catalogue of simulations

Catalogue ID	Comments
hkumpul/81472/apr0120/seq#2	L-mode reference
hkumpul/81472/apr0120/seq#1	L-mode, no plasma rotation
hkumpul/81472/mar3120/seq#1	L-mode, no added Be
hkumpul/81472/may2120/seq#1	L-mode, integrated core+edge
hkumpul/82486/apr1120/seq#1	H-mode reference
hkumpul/82486/sep3019/seq#1	H-mode, no ELMs, no added Be
hkumpul/82486/apr1920/seq#1	H-mode, integrated core+edge

Table 2. Catalogue identifiers of the EDGE2D-EIRENE and integrated core+edge JINTRAC simulations stored on the JET Heimdall cluster (July 2020). The DIVIMP simulations with corresponding identifiers are stored on the IPP Garching TOK cluster and on the Aalto University Triton cluster.