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Comparison of DIVIMP and EDGE2D-EIRENE tungsten transport predictions in JET edge plasmas



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ABSTRACT

The average tungsten concentrations in the pedestal region (c_w) predicted by the Monte Carlo code DIVIMP and the coupled multi-fluid plasma/kinetic neutral code EDGE2D-EIRENE are found to agree within a factor of 2 for a range of JET-ILW L-mode and H-mode plasma conditions. Under attached divertor conditions with c_w exceeding 10^{-6} , the c_w predicted by DIVIMP is consistently ~50% higher than by EDGE2D-EIRENE. In colder plasma scenarios with c_w < 10^{-6} , stochastic variations exceed the systematic disagreement between the two codes. The average tungsten charge predicted by EDGE2D-EIRENE in the upstream scrape-off layer is lower by 40–50% due to the bundling of the 74 tungsten ion charge states into 6 fluid species, which explains the reduced tungsten accumulation in the main plasma compared to the DIVIMP predictions.

1. Introduction

Tungsten (W) has been chosen as the divertor plasma-facing material for ITER, and for the JET ITER-like wall [1], primarily due to its low tritium retention, high melting point, and low erosion [2]. For fusionrelevant plasma operation with W divertors, it is essential to maintain the W concentration in the core plasma below the upper limit of a few 10^{-5} to mitigate the cooling effect of W radiation [3].

The core W concentration is determined by the net erosion rate at W surfaces as well as transport in the scrape-off layer (SOL) and across the closed flux surfaces into and out of the core plasma. In this work, predictions of tungsten transport in the SOL of JET plasmas are compared using multi-fluid EDGE2D-EIRENE and Monte Carlo DIVIMP treatment of tungsten ions.

Both EDGE2D-EIRENE and DIVIMP have been used in previous W transport studies in JET edge plasmas [4–9]. A particularly surprising result is that the core plasma W density has been predicted to vary by only 20% when the 74 charge states of W ions are modelled using 2 to 13 fluid species in EDGE2D-EIRENE [4]. This paper discusses the implications of bundling the W charge states in further detail.

The comparison between DIVIMP and EDGE2D-EIRENE is motivated by the desire to understand the impact of the differing approximations made by each code, and to find the level of agreement between the code predictions under a wide range of plasma conditions. While diagnostics of W exist, and can be used to further validate the codes, they are not used in this work due to imperfect agreement between the measured and simulated background plasma conditions. By applying as-similar-as-possible parameters and boundary conditions to both codes, the majority of potential uncertainty sources is eliminated and the attainable level of accuracy is consequently higher than for a code-experiment comparison.

Understanding the reason behind any diverging predictions allows the identification of potential ways to improve the prediction accuracy of the core W influx using edge fluid simulations. Additionally, this study serves as a W transport benchmark of both codes in typical JET Lmode and inter-ELM H-mode plasmas, enabling further comparisons against diagnostics or other codes with different transport models. Although ELMs generally dominate the dynamics of W transport in JET H-mode [10], the ability to predict W transport in ELM-free regimes is potentially more relevant than in type-I ELMy H-mode for larger future machines such as DEMO.

2. Methods

2.1. Description of plasma conditions in the L-mode and H-mode discharges

The studied scenarios are based on two JET discharge series: lowconfinement mode (L-mode) JET pulse number (JPN) 81472 at plasma current and toroidal magnetic field of 2.5 MA and 2.5 T, respectively, and the inter-ELM high-confinement mode (H-mode) phase of the Be

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Table 1

The main parameters of the studied JET discharges #81472 at 9 s in L-mode and #83393 at 21 s in H-mode.

Discharge	B_t	I_p	P _{NBI}	P _{Ohmic}
#81472	2.5 T	2.5 MA	1.0 MW	1.5 MW
#83393	2.0 T	2.0 MA	6.0 MW	1.0 MW



Fig. 1. Poloidal reconstruction of the magnetic configuration of the JET discharges #81472 and #83393. The diagnostic positions and lines of sight are: high resolution Thomson scattering (HRTS, green), lithium atom beam (Libeam, black), reciprocating Langmuir probe (RCP, black), and divertor Langmuir probes (LPs, orange). The HFS strike point is on divertor tile 3 and the LFS strike point on tile 5/C.

monitoring discharge [11] JPN 83393 at plasma current and toroidal magnetic field of 2.0 MA and 2.0 T, respectively (Table 1). Both scenarios are well diagnosed and they have been repeated multiple times during several JET campaigns. Discharges with different heating power, magnetic field and current were included to investigate whether the level of agreement between EDGE2D-EIRENE and DIVIMP predictions is sensitive to these parameters.

The strike point locations in both discharges were on the vertical divertor tile 3 on the high-field side (HFS) and on horizontal tile 5/C on the low-field side (LFS) (Fig. 1). Electron density and temperature measurements by high resolution Thomson scattering [12], lithium beam [13], reciprocating Langmuir probe [14], and divertor Langmuir probes were used for the simulation setup and validation of the simulated plasma conditions.

2.2. EDGE2D-EIRENE simulation setup

The coupled 2D multi-fluid plasma/kinetic neutral code EDGE2D-EIRENE [15,16] solves the particle, momentum and energy conservation equations by Braginskii [17] in the parallel magnetic field direction simultaneously for the electrons, main ions and each impurity species. The computational domain consists of a simulation grid representing a 2D poloidal cross-section of the SOL, pedestal and private plasma regions with toroidal symmetry assumed. The temperatures of all main and impurity ion species are assumed equal.

The EDGE2D-EIRENE simulations of the studied JET discharges are based on earlier work [18,19]. The electron density was assigned a constant value at the LFS mid-plane separatrix and maintained in the simulations by adjusting the deuterium fuelling into the private flux region (L-mode) or from the top of the main chamber (H-mode). The applied boundary conditions are explained in Appendix A.1. For both the L-mode and the H-mode cases, a range of low-recycling, high-recycling and partially detached divertor conditions was studied by altering the prescribed electron density while maintaining constant heating power, transport coefficients and boundary conditions. The EDGE2D-EIRENE version used was v280818 for all L-mode simulations and v121218 for all H-mode simulations.

Cross-field drifts were not included in this study, instead particle and energy transport across flux surfaces was treated as purely diffusive with no convective pinch velocity. 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. 2). In the divertor SOL (region below the X-point), the transport coefficients were set to 1 m²/s. For impurities, a constant D_{perp} of 1 m²/s was used in all plasma regions. The 74 W ion charge states were bundled [4] to 6 fluid species representing charges 1, 2–6, 7–12, 13–22, 23–73 and 74. Impurity recombination to neutral state was disabled. In the H-mode simulations, the edge-localized modes (ELMs) were excluded and the inter-ELM periods of the discharge were simulated based on conditionally averaged electron density and temperature profiles.

The EDGE2D-EIRENE predictions of the L-mode electron temperature and H-mode electron density profiles at the LFS target are consistent with Langmuir probe measurements (Fig. 3a, d). However, EDGE2D-EIRENE overestimates the H-mode electron temperature at the strike point by a factor of 4 and the L-mode electron density by a factor of 2 (Fig. 3b, c). Predictions more consistent with the measured divertor conditions could be obtained by including cross-field drifts in the simulations, at the expense of code execution time and stability. For the purpose of W transport code-code comparison, these discrepancies between measured and predicted target conditions were not deemed critical, because the same background plasmas were used for both codes.

The source of W in the EDGE2D-EIRENE simulations is sputtering from divertor surfaces due to D, Be and W. The Be concentration is based on the predicted erosion of beryllium surfaces in the JET main chamber. Each of the 4 ionized states of Be was treated as a fluid species in EDGE2D-EIRENE.

2.3. DIVIMP simulation setup

In the DIVIMP [20,21] 2D Monte Carlo simulations, tungsten test particles were injected in a singly ionized state with a 2D probability distribution based on the neutral W ionization profile calculated by EDGE2D-EIRENE. The background plasma conditions for each DIVIMP simulation were imported from the EDGE2D-EIRENE solution. Previously [5,6,8], the DIVIMP W source distribution was taken from DI-VIMP W sputtering predictions, preventing a direct comparison of W



Fig. 2. 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 H-mode (d–f) scenarios.

transport between DIVIMP and EDGE2D-EIRENE due to different W sources. In this work, after normalizing the DIVIMP results with the total W ionization rate, the only difference between the W ion sources in DIVIMP and EDGE2D-EIRENE is Monte Carlo noise. The initial velocities of the injected W ions were sampled based on the Maxwellian



Fig. 3. 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 H-mode peak electron temperature (c) is overestimated due to not including cross-field drifts in the simulations.

ion temperature profile from EDGE2D-EIRENE. The boundary conditions used for DIVIMP are given in Appendix A.2. The IPP version of DIVIMP, installed on the TOK cluster at IPP Garching as of March 2020, was used in this work. The W ionization and recombination rates were obtained using the same ADAS [22] data (year 42) as in the EDGE2D-EIRENE simulations. W recombination to neutral state was disabled, as in the EDGE2D-EIRENE cases. Likewise, the value used for D_{perp} was the same constant 1 m²/s for both codes.

DIVIMP employs the trace-impurity approximation, that is, the predicted impurity density has no effect on the background plasma. However, beryllium and tungsten are included in the simulations of the EDGE2D fluid background used as input for DIVIMP, and sputtering by D, Be and W is taken into account in the EIRENE calculations of the DIVIMP W source. Including W in the EDGE2D-EIRENE background plasma simulations has a negligible impact on the scrape-off layer electron temperature and density profiles in the studied scenarios.

Impurity transport along magnetic field lines is modelled in DIVIMP

based on a force balance model [23] which is nearly equivalent to the momentum conservation equation solved by EDGE2D. A potentially significant difference between the transport models in DIVIMP and EDGE2D is that the DIVIMP impurity pressure gradient force FPG = -dp/ds is replaced by velocity diffusion [21]

$$\Delta v = \sqrt{\frac{-2ln(x_1)\Delta t}{\tau_{\parallel}} \frac{2kT_Z}{m_Z}} \cos(2\pi x_2)$$
(1)

where x_1 and x_2 are uniform random variables in the range [0,1], Δt is the time step and

$$\tau_{\parallel} = m_Z \sqrt{\frac{T_i}{m_i}} \frac{T_Z}{6.8 \cdot 10^4 n_i Z^2 \Lambda} \left(1 + \frac{m_i}{m_Z} \right)$$
(2)

The EDGE2D pressure gradient term is directly proportional to the ion temperature T_i and independent of the ion density n_i and the impurity charge *Z*. In contrast, its diffusive DIVIMP counterpart (Eq. 1) is proportional to $T_i^{-1/4}$, $n_i^{1/2}$ and *Z*. This means that the change in impurity momentum predicted by these two models can only be equal under a specific set of plasma conditions. The impurity temperature T_Z also appears in the DIVIMP Eqs. (1) and (2), but the two instances cancel out. Λ is the Coulomb logarithm.

It is important to point out that even if the equations for all the force terms were identical in both codes, differences in the predicted density



Fig. 4. Spatial average of the tungsten concentration in the pedestal region (the closed flux surfaces at r/a > 0.8) predicted by DIVIMP and EDGE2D-EIRENE in the L-mode (a) and the H-mode (b) scenarios as function of electron temperature at the LFS strike point ($T_{e,OSP}$, bottom axis) and electron density at the LFS mid-plane separatrix ($n_{e,sep,OMP}$, top axis).

and velocity profiles would still arise due to the fact that the velocity and charge distributions of the test particles in DIVIMP are not necessarily equal to the flow velocity and charge of the impurity fluid species in EDGE2D-EIRENE. This is in part due to DIVIMP not requiring the impurities to be instantly thermalized with the main ions, and in part due to the charge state bundling by EDGE2D-EIRENE.

3. Comparison of the DIVIMP and EDGE2D-EIRENE predictions

The W concentration predicted by DIVIMP in the pedestal region is consistently ~50% higher than by EDGE2D-EIRENE under low- and high-recycling divertor conditions in both the L-mode and the H-mode scenarios (Fig. 4). In cases with average pedestal W concentration below 10⁻⁶ ($T_{e,OSP}$ < 5 eV in L-mode, $T_{e,OSP}$ < 35 eV in H-mode), the systematic disagreement is lower compared to the statistical variations, predominantly due to Monte Carlo noise in the EIRENE-calculated W source.

In cases with low tungsten concentration (<10⁻⁷, high-density and low-temperature cases), the numerical error terms in the EDGE2D-EIRENE particle and momentum conservation equations tend to be large compared to the physical terms, indicating the limit of the expected validity regime of the code. The error terms are residuals indicating imperfect conservation of W ions or momentum. It means that the code does not reliably describe tungsten transport in regimes with virtually no tungsten. The most relevant cases in terms of core W contamination are the low-density, high-temperature cases ($n_{e.sep,OMP} < 10^{19}$ m⁻³ in L-mode, $n_{e.sep,OMP} < 3.5 \cdot 10^{19}$ m⁻³ in H-mode, $T_{e.OSP} > 40$ eV) in which the numerical errors and the Monte Carlo noise are negligible.

The W densities predicted by DIVIMP and EDGE2D-EIRENE are nearly identical on the LFS, whereas on the HFS DIVIMP predicts up to more than twice the W density of EDGE2D-EIRENE in the pedestal, the upstream SOL and the divertor far SOL regions (Fig. 5). The DIVIMPpredicted W densities are also slightly higher and more localized near the LFS vertical divertor. The differences in the pedestal and upstream SOL are attributed to the W force balance, as the thermal and frictional forces on W depend significantly on the W charge and velocity profiles in each code. In the divertor, the main factors explaining the differences are considered to be the impurity pressure gradient models and the velocity boundary conditions. DIVIMP predicts less W than EDGE2D-EIRENE near the X-point, where the W density in both simulations is negligible compared to other regions due to strong temperature gradient forces towards the upstream.

The bundling of the 74 W ion charge states into 6 fluid species in EDGE2D-EIRENE decreases the average W charge in the upstream SOL region by 40–50% in both L-mode and H-mode compared to the DIVIMP predictions (the 6-fluid scheme, Fig. 6a,c). The predicted W charge profiles matched in the divertor (1 eV $T_e < 60$ eV, 1 $< Z_W < 6$) and in the pedestal region ($T_e > 100$ eV, $Z_W > 13$). The upstream SOL displays a hysteresis effect, more pronounced in the DIVIMP than the EDGE2D-EIRENE results, in which W ions are transported at a lower average charge (7–12) inwards and at a higher charge (13–17) outwards across the separatrix at similar electron temperatures. This is explained by the W ions not reaching ionization equilibrium when transported across the SOL, thus their charge state at a given temperature in the near SOL depends on whether they are coming from the far SOL or from the main plasma.

Including all individual W charge states from 1 + up to 20 + as separate fluid species in EDGE2D-EIRENE (the 22-fluid scheme, Fig. 6b, d) results in a W charge profile far more similar to the DIVIMP predictions than using the 6-fluid scheme. However, the momentum balance with the 22-fluid scheme has large error terms due to numerical



Fig. 5. a) 2D W density profile predicted by EDGE2D-EIRENE and b) 2D-resolved DIVIMP-to-EDGE2D-EIRENE ratio of the predicted W density profiles in the L-mode scenario ($n_{e,sep,OMP} = 0.8 \cdot 10^{19} \text{ m}^{-3}$) with 6 EDGE2D fluid species for W ions.

issues as the EDGE2D-EIRENE runs become unstable, requiring several attempts to obtain a converged solution. With the default 6-fluid W scheme, these same issues are encountered only when the plasma density is increased to the partially detached regime, in which the W densities are negligible. Due to not conserving W momentum as a result of the numerical errors, the 22-fluid scheme does not reproduce the DIVIMP W velocity and density profiles despite matching the W charge profiles.

EDGE2D with 6 W fluids predicts weaker forces on W than DIVIMP and EDGE2D with 22 W fluids (Fig. 7) due to the lower W charge in the main chamber SOL. The differences in the forces predicted by EDGE2D with 22 W fluids and DIVIMP are primarily due to the W velocity profiles (Fig. 8), which affect the friction between W and the background plasma. Considering that both codes use the same W sources and background plasma, and the predicted W charge states are similar, then also the forces, velocities, and densities of W predicted by DIVIMP and EDGE2D-EIRENE with the 22-fluid scheme should be approximately equal if not for the error terms in the 22-fluid scheme momentum balance.

Despite the net forces being significantly stronger for 22 W fluids than for 6, the W flow velocities predicted by the 6-fluid and 22-fluid schemes are almost identical on the HFS (Fig. 8). This is only possible because the W momentum balance was violated in the 22-fluid scheme. The region between the HFS mid-plane and the X-point (at parallel-B distance 60–70 m) is particularly interesting for W accumulation, because DIVIMP predicts a W velocity directed towards the upstream, whereas both 6-fluid and 22-fluid EDGE2D-EIRENE W velocities are towards the HFS target. It results in W being confined in the parallel-B direction and therefore able to escape from this SOL flux surface only by cross-field transport in DIVIMP, whereas in EDGE2D-EIRENE W also flows directly along the field lines into the HFS divertor. This explains why the pedestal W density is higher in DIVIMP than in EDGE2D-EIRENE, particularly on the HFS (Fig. 5).

4. Conclusions

The DIVIMP and EDGE2D-EIRENE predictions of the W density in

the confined plasma region for typical JET L-mode and H-mode plasmas were found to agree within a factor of 2, provided that identical plasma conditions and near-equivalent parameters and options were used for both codes. The average W densities predicted by DIVIMP are consistently 50% higher than by EDGE2D-EIRENE for both L-mode and Hmode plasmas under low- and high-recycling divertor conditions. This level of agreement can be considered very reasonable when taking into account the different underlying code assumptions, namely the bundled-Maxwellian-fluid treatment of W and the Bohm condition by EDGE2D-EIRENE, and the trace-impurity approximation and the parallel-B velocity diffusion model by DIVIMP.

When the upstream electron density was increased to reach lower temperatures and W sputtering rates in the divertor, no significant systematic disagreement between DIVIMP and EDGE2D-EIRENE was observed, although the low W densities made the EDGE2D-EIRENE simulations unstable and the numerical errors were considerably larger than under attached conditions.

A consistent decrease of 40–50% in the average charge of W in the main chamber SOL was observed due to the bundling of charge states into fluid species in EDGE2D-EIRENE compared to DIVIMP. Using a more highly resolved bundling scheme with 22 W fluids instead of 6, EDGE2D-EIRENE reproduced the W charge profile predicted by DIVIMP within a few percent. However, the increased amount of fluid species led to larger numerical errors in the particle and momentum balance and turned the EDGE2D-EIRENE simulations unstable. Because the 22-fluid scheme output is unphysical due to the numerical error terms, the 6-fluid scheme for W can be considered more appropriate than the 22-fluid scheme, despite the less realistic W charge profile.

The presented results suggest that, apart from the problems induced by charge bundling, there is no significant difference in the accuracy of EDGE2D-EIRENE multi-fluid and DIVIMP Monte Carlo W transport predictions. The impact of charge bundling was found to be systematic, and as such it could in principle even be accounted for by empirically adjusting the code output. The consistent level of agreement suggests that a comparison between experimental measurements and W predictions by either code is sufficient to verify or disprove the accuracy of both codes, assuming that the applied parameters and boundary



Fig. 6. The average charge state of W ions in each grid cell plotted against the local electron temperature for DIVIMP and EDGE2D-EIRENE in the L-mode (a, b) and H-mode (c, d) scenarios ($n_{e,sep,OMP} = 0.9 \cdot 10^{19} \text{ m}^{-3}$ and $3.5 \cdot 10^{19} \text{ m}^{-3}$ respectively). The 74 W charge states in EDGE2D-EIRENE are bundled into 6 (a, c) and 22 (b, d) fluid species.

conditions are similar to those specified in this paper. To increase the confidence that the codes produce valid predictions also for future reactors, a similar benchmark and validation could be carried out for a number of existing tokamaks.

CRediT authorship contribution statement

H.A. Kumpulainen: Formal analysis, Investigation, Visualization,
Writing - original draft, Data curation. M. Groth: Supervision,
Conceptualization, Writing - review & editing, Project administration.
M. Fontell: Software, Investigation. A.E. Jaervinen: Software,
Conceptualization, Writing - review & editing. G. Corrigan:
Methodology, Software. D. Harting: Methodology, Software.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.



Fig. 7. The average net force acting on W ions predicted by DIVIMP and EDGE2D-EIRENE with 6 and 22 W fluids in the L-mode (a) and H-mode (b) scenarios as a function of distance along a SOL magnetic field line, located 8 mm outside the separatrix at the LFS mid-plane. The positive direction is towards the HFS target and negative towards the LFS target. (O = outer, I = inner, T = target, MP = mid-plane).



Fig. 8. The average velocity of W ions predicted by DIVIMP and EDGE2D-EIRENE with 6 and 22 W fluids in the L-mode (a) and H-mode (b) scenarios along the same magnetic field line as in Fig. 7.

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Appendix A. Supplementary data

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