A study of the atomic and molecular power loss terms in EDGE2D-EIRENE simulations of JET ITER-like wall L-mode discharges

K.D. Lawson\(^a\), M. Groth\(^b\), D. Harting\(^c\), S. Menmuir\(^a\), D. Reiter\(^c\), S. Brezinsek\(^c\), G. Corrigan\(^a\), P. Drewelow\(^d\), C.F. Maggi\(^a\), A.G. Meigs\(^a\), J. Simpson\(^a\), M.F. Stamp\(^a\), S. Wiesen\(^c\)

\(^a\) Culham Science Centre, Abingdon OX14 3DB, UK
\(^b\) Aalto University, Otakaari 1, Espoo 02150, Finland
\(^c\) Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung - Plasmafysik 52425 Jülich, Germany
\(^d\) MPI für Plasmaphysik, 17491 Greifswald, Germany

Contributors\(^{\text{a,b}}\)

ABSTRACT

A discrepancy in the divertor radiated powers between EDGE2D-EIRENE simulations and JET-ILW experiments employing a set of NBI-heated L-mode discharges with step-wise density variation is investigated. The analysis shows the importance of the contributions from the deuterium fuel to the divertor radiated power, making these discharges ideal for this study. Molecular radiation losses from D\(_2\) molecules have been included for the first time and the present simulations allow the atomic and molecular electron power loss terms in EIRENE to be independently scaled in order to understand their importance in determining the simulated electron temperatures and distribution of radiated power.

1. Introduction

An understanding of the behaviour of the plasma edge and divertor physics is essential for the design of next-step machines such as ITER, for which JET with its ITER-Like Wall (ILW) of Be in the main chamber and W in the divertor is ideally suited. Both fuel and edge impurities affect the power balance, thus determining the power reaching the divertor-target plates, which is limited by the mechanical and thermal properties of the plates. A study\(^1\) of L-mode discharges during the present JET-ILW campaign and previous JET-C campaigns, in which the plasma-facing surfaces were C based materials (Carbon-Fibre Composite), has consistently shown a shortfall in the radiated power in the Scrape-Off Layer (SOL) and divertor calculated from EDGE2D-EIRENE simulations\(^2\) below that measured by bolometry. A similar result is found for unseeded ELMy H-mode discharges by Järvinen et al.\(^3\). In order to gain understanding of this discrepancy, the contributions to the divertor radiated power (\(P_{\text{rad}}\)) as predicted by the simulations have been quantified and the results compared with measurements from bolometry for a density scan series of L-mode discharges run in JET-ILW. The simulations include for the first time molecular radiation losses from the D\(_2\) molecules and allow the atomic and molecular power loss to the electrons to be independently scaled.

2. Simulations

The simulations of the JET-ILW, L-mode, NBI-heated discharges of Groth et al.\(^1\) have been used to determine \(P_{\text{rad}}\) contributions (Table 1). They apply to a density scan series of 2.5 MA / 2.5 T discharges (\(81,472\)–\(81,492\)) heated with 1, 1.2 or 1.6 MW of NBI. The simulation geometry is taken from discharge 81,472, the fuel being D with Be and W impurities. A range of outer midplane separatrix densities, \(n_e\text{sep} = (7 \times 10^{19})\ m^{-3}\) up to the maximum at which the simulations converge of 2–2.2 \(\times 10^{20}\ m^{-3}\) and of powers transported across the separatrix into the SOL (2.2–2.8 MW) was considered. Since little sensitivity to the power transported across the separatrix was found, only the 2.2 MW case is illustrated in this paper. The version of the EDGE2D-EIRENE code adapted to include D\(_2\) and D\(_2^+\) molecules was used and, for the first time here, molecular radiation losses from the D\(_2\) molecules are included in the
Table 1
Contributions to the divertor radiated power ($P_{rad}$).

<table>
<thead>
<tr>
<th>Contributions</th>
<th>Estimated $P_{rad}$ contributions</th>
<th>$\text{Ly}<em>\alpha \sim 85$–90%, $\text{Ly}</em>\beta \sim 10$% and other lines $\sim 3%$.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Line radiation from D.</td>
<td>C and O impurity radiation.</td>
<td>$\sim 10^{-3}$ of D line radiation.</td>
</tr>
<tr>
<td>D line radiation due to recombination directly populating excited D atomic levels.</td>
<td>High Z impurity (Ni, Cu and W) line radiation.</td>
<td>$\sim 10$% of D line radiation.</td>
</tr>
<tr>
<td>Line radiation from $D_2^+$ molecules.</td>
<td>Ly$\alpha$ and line impurity radiation.</td>
<td>$\sim 3$% of D line radiation.</td>
</tr>
<tr>
<td>Radiative recombination to D followed by cascading within D atoms + Bremsstrahlung.</td>
<td>Radiative recombination to D followed by cascading within D atoms + Bremsstrahlung.</td>
<td>$\sim 10^{-2}$ at low $n_{\text{sep}}$, rising to $\sim 30%$ at high $n_{\text{sep}}$.</td>
</tr>
<tr>
<td>Be impurity radiation.</td>
<td>Variable - few % in cases considered.</td>
<td>Generally smaller than low Z elements at the low $T_e$ of the divertor.</td>
</tr>
</tbody>
</table>

Fig. 1. Lines-of-sight of the bolometer.

Fig. 2. D line power, radiative recombination and total rate coefficients, AMJUEL.

The full ITER reference atomic and molecular datasets were used as detailed by Kotov et al. [4]. The simulations use a diffusive transport model in which the radially varying particle and thermal diffusivities are illustrated in Fig. 9 of [1]. These were determined for the lowest density case considered in the study ($n_{\text{sep}} = 7 \times 10^{18}$ m$^{-3}$), the same model being applied to the higher density simulations. Ballooning transport and cross-field drifts are not included in the present simulations, although the latter have been discussed by [5] and [6]. For the present cases, drifts increase the radiated power of a feature in the inner divertor (at $R = 2.42$ m) by at most $\sim 30%$, this percentage decreasing with increasing density. Since no broadening of this feature was observed, the omission of drifts did not explain the discrepancy between measured and simulated radiated powers. Ballooning transport is also expected to influence the inner - outer divertor asymmetry and will be assessed in a later publication. To allow comparisons with the bolometric measurements, contributions to the radiated power are integrated along the diagnostic lines-of-sight (Fig. 1).
3. Contributions to the divertor radiated power ($P_{\text{rad}}$)

Table 1 details the contributions to the divertor $P_{\text{rad}}$ and the importance of deuterium is evident, the impurities each accounting for no more than a few per cent [7]. These pulses therefore provide a stringent test of the simulations for the D fuel. Among the atomic D contributions, the largest component is due to D (Lyman) line radiation, in particular from the Ly$\alpha$ line. $P_{\text{rad}}$ due to free electron recombination, which for D is radiative recombination, can also be significant at temperatures less than $\sim 1$ eV (Fig. 2). In these first simulations the number of $D_2$ and $D_2^+$ molecules was small, typically being $\sim 10$% and 3% of the number of D atoms, although significant variations from these values are seen in different regions of the divertor and as $n_{\text{e,sep}}$ increases. Lawson et al. [8] concluded that the simulated $T_e$ tended to be too high in these simulations. Lowering $T_e$ would result in higher atomic and molecular densities, which in turn would lead to higher radiation, although this in part may be offset by falling excitation rates at the lower $T_e$. However, increasing the volume of plasma with temperatures of less than $\sim 1$ eV would both increase the radiation and broaden the divertor emission features through the radiative recombination channel.

4. Variation of the atomic and molecular electron power loss terms

The sensitivity of the simulations to the electron power loss terms was investigated by scaling the terms for the D atoms and $D_2$ molecules independently. Temperature dependent scalings were used, which were defined by quadratic polynomials in $T_e$ biased towards lower temperatures and applied to the radiated power in the EIRENE code. The electron power loss due to the D atoms is

$$P_{\text{atom}, \text{e,loss}} = 13.6 \times n_0 + P_{\text{D, line}\text{eVm}^3\text{s}^{-1}}.$$  

while that for the $D_2$ molecules is

$$P_{\text{molecule}, \text{e,loss}} = 15.4 \times n_0 + 9.9 \times d_0 + P_{\text{D}, \text{electronic eVm}^3\text{s}^{-1}}.$$  

where $s$ and $d$ are the ionization and dissociation rate coefficients and $P$ the power loss due to radiation, which for atoms is dominated by Ly$\alpha$ and for molecules the Werner and Lyman band emission [8]. It is noted that the molecular radiation losses are due to radiative processes within the molecular state, a 'direct' molecular contribution. An 'indirect' molecular contribution due to dissociation into excited (rather than ground) states and subsequent radiation will be investigated and reported on in a later publication. Figs. 2 and 3 compare atomic data from the AMJUEL [9] and ADAS [10] databases at two densities, $n_0 = 10^{19}$ and $10^{20}$ m$^{-3}$. Fig. 2 illustrating the line power and radiative recombination rate coefficients and Fig. 3 giving ratios of data from the two databases. Included in the latter are the D line power, $P_{\text{D, line}}$, the total power loss, $P_{\text{atoms, e,loss}}$, ionization rates and radiative recombination rates. Although ionization rates for the two databases show significant differences (Fig. 3), this occurs at temperatures where the contributions due to ionization are small, resulting in only small differences in the total power loss term. Fig. 4 illustrates the total and radiative losses for the $D_2$ molecules at $n_0 = 10^{19}$ and $10^{20}$ m$^{-3}$.

Four scalings of the atomic power loss term were tested: 1) AMJUEL rates, 2) AMJUEL rates + 3%, 3) AMJUEL rates + 5% and 4) AMJUEL rates + 10%, the percentages corresponding to approximate averages of the increase in the power loss term. The last corresponds to the expected accuracy of the electron collisional excitation rates, which largely determine the dominant line power term, and it is noted that case 2 is most like the ADAS rates. The
molecular behaviour is more complicated and a wider variation is explored: 1) AMJUEL rates, 2) AMJUEL rates +20% and 3) AMJUEL rates −50%, all of which include molecular radiation losses.

A strong sensitivity to the atomic power loss term is found in these new simulations, a small change in this term resulting in significantly lower electron temperatures and higher D2 molecular densities. It should be emphasized that the four atomic cases considered are within the expected accuracy of the atomic data used. The sensitivity is illustrated in Figs. 5 and 6, which show, respectively, the peak electron temperature at a height of z = −1.5 m in the outer divertor and the D2 molecular density at the same radius for three n_{e,sep} 1.4 × 10^{19}, 1.5 × 10^{19} and 1.8 × 10^{19} m\(^{-3}\). At z = −1.5 m the private flux region - SOL boundary is at R = 2.63 m, while the major radius of the peak electron temperature varies between R = 2.65 and 2.69 m. The change is so marked between atomic cases 1 and 2 that additional simulations for the molecular case 1 at an n_{e,sep} of 1.5 × 10^{19} m\(^{-3}\) have been made in order to increase the resolution at the lowest percentage change in the atomic power loss term. Fig. 7 illustrates the peak T_e at z = −1.5 m in the outer divertor and the peak T_e along the outer target plate. The latter is usually displaced outwards from the strike point (R = 2.735 m) falling at major radii of up to ∼2.765 m. Looking for the peak T_e in the inner divertor usually led to flux surfaces that ended at the top of the inner divertor targets in the divertor throat. Consequently, it was thought more representative to compare the data at the same position in the inner divertor. T_e on the inner divertor target plate at R = 2.42 m, z = −1.54 m and in the inner divertor volume at R = 2.46 m, z = −1.5 m are illustrated. A significant step fall or transition in the electron temperature with a small increase in the atomic power loss term is observed, together with some recovery in T_e as the loss term is increased further. The changes in electron temperature affect the radiated power distribution within the divertor and this is illustrated in Figs. 8 and 9 which contrast the distribution of T_e and the power radiated by D atoms, respectively, in atomic cases 1 and 4 (molecular case 1) at n_{e,sep} = 1.8 × 10^{19} m\(^{-3}\). It can be seen that the lower temperatures of case 4 result in the emission from close to the divertor legs seen in case 1 moving up towards the X-point, with a consequent broadening of the radiation features. In these simulations the temperatures do not fall below 1 eV over large enough volumes in which the densities are high to boost significantly the radiation through radiative recombination.

Reconstruction of the bolometric profiles allow direct comparisons with measurements to be made (Figs. 10–12) and the effect on the initial simulations of including the molecular radiation can be seen for the three n_{e,sep} already illustrated. The effect of the molecular radiation is small at the lowest n_{e,sep}, but more significant at higher n_{e,sep}. This is explained by the comparatively small number of D2 molecules in the initial simulations at low n_{e,sep}. In contrast, increasing the atomic power loss term results in a marked change at all densities, affecting the inner/outer divertor balance of the P_{rad} profile and as seen in Figs. 8 and 9 tending to broaden the radiation features, the new simulations better reflecting the overall profile of the bolometric measurements. Since there can be a significant variation in the measured profiles, four profiles are il-
illustrated in these figures. It was necessary to subtract a contribution of $1.3 \times 10^4 \text{W/m}^2$ from the measured bolometric signals to account for core radiation, although as can be seen in these figures the emission comes predominately from the divertor region. Varying the molecular power loss term has the greatest effect in atomic case 1 at high $n_{e,sep}$. It is noted that modifying the molecular power loss term alone would not allow the lowest temperatures found in these simulations to be reached. Despite the improvement in the profile shape a $P_{\text{rad}}$ deficit still remains.

5. Conclusions

Comparisons between EDGE2D-EIRENE simulations and measurements of $P_{\text{rad}}$ in a density scan series of L-mode, NBI-heated discharges emphasize the importance of atomic and molecular D in determining the radiated power. Independent scalings of the atomic and molecular electron power loss terms have been used to gain understanding of a shortfall in the simulated radiated power compared with bolometric measurements. A strong sensitivity to the atomic power loss term, in particular, is found which allows a lower temperature parameter space to be accessed, with broadened radiation profiles closer to those measured, although still with a deficit in the divertor radiated power. Inclusion of molecular radiation losses from the $D_2$ molecules had a small effect on the initial low density simulations, becoming more important with increasing $n_{e,sep}$ with their lower temperatures and higher molecular densities. The new parameter space will be exploited in the first instance by extending the analysis of the L-mode regime with comparisons of line radiation profiles and molecular densities and in the longer term will be tested in other regimes.

Fig. 8. (a) Simulated 2D distribution of electron temperature for $n_{e,sep} = 1.8 \times 10^{19} \text{m}^{-3}$, atomic and molecular cases 1, with $D_2$ molecular radiation. Simulation has 2.2 MW power to SOL. (b) Simulated 2D distribution of electron temperature for $n_{e,sep} = 1.8 \times 10^{19} \text{m}^{-3}$, scaled atomic case 4 and molecular case 1, with $D_2$ molecular radiation. Simulation has 2.2 MW power to SOL.
Fig. 9. (a) Simulated 2D distribution of radiated power due to atomic D for $n_{sep} = 1.8 \times 10^{19} \text{ m}^{-3}$, atomic and molecular cases 1, with $D_2$ molecular radiation. Simulation has 2.2 MW power to SOL. (b) Simulated 2D distribution of radiated power due to atomic D for $n_{sep} = 1.8 \times 10^{19} \text{ m}^{-3}$, scaled atomic case 4 and molecular case 1, with $D_2$ molecular radiation. Simulation has 2.2 MW power to SOL.
Fig. 10. Bolometric profiles for pulse 81,480 at ~ 17 s, \( n_{\text{sep}} = 1.4 \times 10^{20} \text{ m}^{-3} \). Measured data, 4 curves without symbols (in black). \( 1.3 \times 10^9 \text{ W/m}^2 \) core emission subtracted (---), initial simulation, with D\(_2\) molecular radiation. All simulations have 2.2 MW power to SOL.

Fig. 11. Bolometric profiles for pulse 81,472 at ~ 13 s, \( n_{\text{sep}} = 1.5 \times 10^{19} \text{ m}^{-3} \). Measured data, 4 curves without symbols (in black). \( 1.3 \times 10^9 \text{ W/m}^2 \) core emission subtracted (---), initial simulation, with D\(_2\) molecular radiation. All simulations have 2.2 MW power to SOL.

Fig. 12. Bolometric profiles for pulse 81,472 at ~ 16 s, \( n_{\text{sep}} = 1.8 \times 10^{19} \text{ m}^{-3} \). Measured data, 4 curves without symbols (in black). \( 1.3 \times 10^9 \text{ W/m}^2 \) core emission subtracted (---), initial simulation, with D\(_2\) molecular radiation. All simulations have 2.2 MW power to SOL.

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References