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Use of the Culham He model He II atomic data in JET EDGE2D-EIRENE simulations

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1. Introduction

Present-day large plasma machines use a divertor containing a cold, dense plasma to act as a buffer between the hot core and the plasma-facing material surfaces, providing protection for the latter. The behaviour of the divertor plasma, including the power radiated by fuel and impurity species, is therefore crucial in determining the performance of the next-step machines such as ITER, requiring transport modelling of the plasma edge and divertor. Transport codes that simulate the edge and divertor plasmas rely on the availability of accurate atomic and molecular data both for the fuel and impurity species. It is important to understand the sensitivity of the simulations to these data, since this determines the quality of the atomic and molecular data required. Recent work has led to the generation of the CHEM (Culham He Model) atomic dataset for hydrogenic He II (He^{+}) [1,2]. The sensitivity of the simulation codes to the atomic data is being tested by comparing their use in EDGE2D-EIRENE simulations with the presently used data from the ADAS database [3]. Helium is widely used in laboratory fusion experiments both as a fuel as in the first, non-nuclear phase of ITER, as a minority gas for RF heating and will occur as ash from the thermonuclear reactions. The atomic physics of He II is in many ways similar to that of D I, so this study will inform work on D fuelled simulations. He rather than D is considered first, since the former presents a more tractable atomic physics problem in that the heavy particle collisions [1] involve ions rather than neutrals. The use of He simulations also avoids the complications that can result from molecular emissions, allowing easier comparisons with experiment. However, it should be noted that the present simulation results are not compared with measurements in this paper.

The study is pertinent in that simulations by Groth et al. [4] of L-mode discharges run in JET have consistently shown a shortfall in the radiated power at low temperatures below that measured by bolometry. This applies both to the earlier JET-C campaigns in which the plasma-facing surfaces were predominately C, as well as more recent ones undertaken after the installation in JET of an ITER-like wall (ILW). In JET-ILW, the plasma-facing surfaces in the divertor are W, with a Be wall in the main chamber. Similar results are found for unseeded ELMy H-mode discharges by Järvinen et al. [5]. The shortfall brings into question predictions for the radiated power and cooling of a radiative divertor in a next-step machine.

An analysis of DIII-D He discharges by Canik et al. [6] showed a smaller 25–35% shortfall in radiation, with the simulated divertor density being consistently 40% lower than measurement by the Divertor Thompson Scattering (DTS) system. By matching the divertor densities agreement between the simulated and measured divertor radiated powers was found. This matching was achieved by increasing the upstream density, but in doing so losing the connection between the divertor and main Scrape-off Layer (SOL), which Canik *et al.* regarded as the outstanding issue in simulations in which there was a shortfall. However, temperatures must also be considered, since it is rare for the simulated temperature to reach the low values (~2 eV in He) necessary to bring about the large radiated powers expected from recombination-driven populations in the atoms. In the absence of MARFES, this is the most likely explanation of the intense, spatially localized features observed close to the inner divertor targets in JET [4,7]. Although there is general agreement between the DIII-D simulated and DTS measurements of temperature [6], it is noted that the simulated temperature (~4–6 eV) nevertheless lies above the measurements (~2–4 eV) close to

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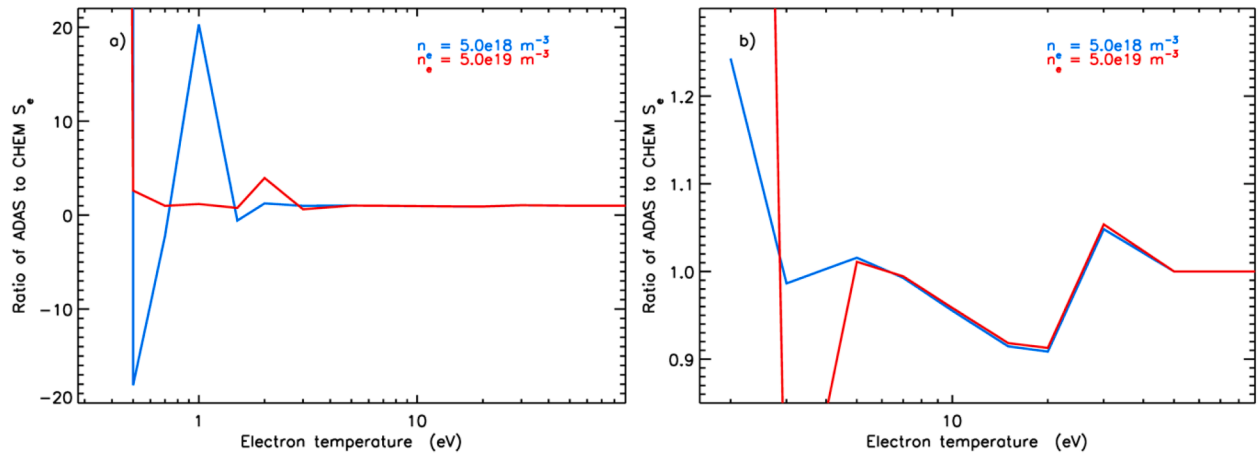

Fig. 1. Ratios of S_e calculated from ADAS 96 and CHEM data in Eq. (1). a) Shows the full temperature range for which data is available, the higher temperature section being redrawn on a larger scale in b).

the target in the highest density simulation, only reaching ~ 2 eV at the target. It is the atomic physics that is important in determining the simulated temperatures and this study looks into the extent to which these data might limit the temperatures reached in the simulations by using the most recent atomic data with particular attention to that at low temperatures.

2. Atomic physics

The CHEM atomic physics model is described by Lawson et al. [1,2]. This collisional-radiative model considers the dominant populating channels for energy levels in a hydrogenic species, in this case He II, including electron and heavy particle collisional excitation and deexcitation, radiative decay, direct electron collisional ionization, radiative and three-body recombination. At present it is available for all densities of interest and an electron temperature range of 0.2 to 30 eV, this including the temperatures of most importance for high density simulations. It can be run as a stand-alone program, with different populating channels readily switched on and off so as to show the importance of their contributions. The model makes use of the most recent atomic data, including recently generated electron and heavy particle collisional excitation and direct collisional ionization rate coefficients, the latter also determining the three body recombination rate coefficients. The heavy particle collisional excitation rate coefficients are only available in the CHEM database.

EDGE2D uses atomic data to define the ionization balance and for the calculation of the energy loss terms, these usually being calculated from the ADAS database [3]. The ionization balance is given by the ionization and recombination rate coefficients, SCD and ACD, respectively, which give the effective rates at which these processes take place [8]. For hydrogenic species the electron power loss term is given by

$$S_e(z, T_e, n_e) = n_e n_z I_H SCD(z) - n_e n_{z+1} I_H ACD(z+1) + n_e n_z PLT(z) + n_e n_{z+1} PRB(z+1) \quad (1)$$

where z corresponds to the hydrogenic charge state and $z+1$ that of the fully stripped ion. In addition to the SCD and ACD functions, this involves the low-level line power coefficient, PLT, and the recombination-bremsstrahlung power coefficient, PRB [8]. SCD, ACD, PLT and PRB are all tabulated as functions of density and temperature. The power loss term, S_e, should include only kinetic energy components, since it is these that affect transport. However, it is noted that the ACD function contains a component relating to the potential energy of the system.

The simplest way of including the CHEM data in the EDGE2D simulations is to generate look-alike SCD, ACD, PLT and PRB functions from the CHEM database. This was done for the temperature range 0.2 to 30 eV and for densities of 5×10^{13} to 2×10^{21} m^{-3}, which is the range of densities included in the ADAS 96 functions. For temperatures higher than 30 eV ADAS 96 data is used to supplement the CHEM data. The SCD and ACD functions are calculated as described by Summers et al. [8] so as to preserve the ionization balance. Eq. (1) is then used to determine S_e, but with the PLT and PRB functions adjusted so as to give a precise calculation of the power loss due only to kinetic terms. This is achieved by summing the contributions to the power loss or gain channels, which include electron collisional excitation (loss) and deexcitation (gain), direct collisional ionization (loss), three-body recombination (gain), bremsstrahlung (loss) and radiative recombination (loss). For the latter, the power loss does not correspond to the radiated power, which includes a component ($I_H - E_i$) removed from the potential energy reservoir of the simulations. In this expression I_H is the ionization potential and E_i the energy of level i. It is also noted that the energy loss is smaller than would be expected from using the mean of the Maxwellian electron energy distribution, $1.5kT_e$, the multiplier varying with temperature (~0.9 to 0.7 over a temperature range 0.3 to 20 eV). Fig. 1 shows ratios of S_e calculated from ADAS 96 and CHEM data, evaluated for electron densities of 5×10^{18} and 5×10^{19} m^{-3}. The ground state He II and fully ionized He densities are 1×10^{18} and 2×10^{18} m^{-3}, respectively, for the 5×10^{18} m^{-3} case and 1×10^{19} and 2×10^{19} m^{-3}, respectively for the 5×10^{19} m^{-3} case, these being typical values taken from the simulations described in the next section. It is noted that a fitting error in the ACD function for the data at 0.2 and 0.3 eV results in the sharp rise in the ratio at low temperatures in Fig. 1a. It has been confirmed that this error has no effect on the final ADAS result. The ADAS 96 data called by EDGE2D is somewhat different to the ADAS 96 data in the central ADAS repository and OPEN-ADAS, with this error being corrected in the latter.

3. Simulations

D-fuelled EDGE2D-EIRENE simulations [9] in which the impurity was He were run at a number of densities, those at the highest being most relevant to ITER and used in the present study. In these the D density in the divertor was typically ~ 4% of that of the He impurity. Both D and He were puffed into the scrape-off layer at the top of the machine. A comparison is made between simulations in which the ADAS 96 and CHEM databases are used to provide atomic data for He II (the latter in the electron temperature range 0.2 to 30 eV, this range including the temperatures of most importance for high density simulations). The setup of the simulations was otherwise the same. D and neutral He (He I) are simulated with the EIRENE code which employs AMJUEL atomic data [10]. Since the motivation of the study is to assess whether significant changes in the simulations are observed when different atomic datasets are used, changing only the He II data is

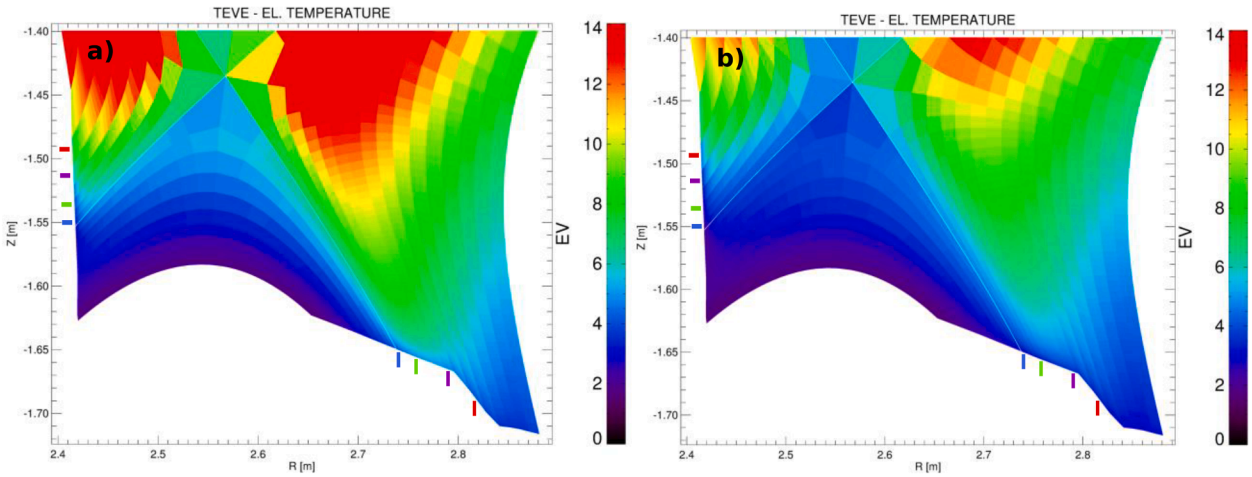

Fig. 2. Electron temperatures from simulations that use a) ADAS, b) CHEM He II atomic data. Coloured marker lines indicate the beginning of field lines used in Figs. 4 and 5.

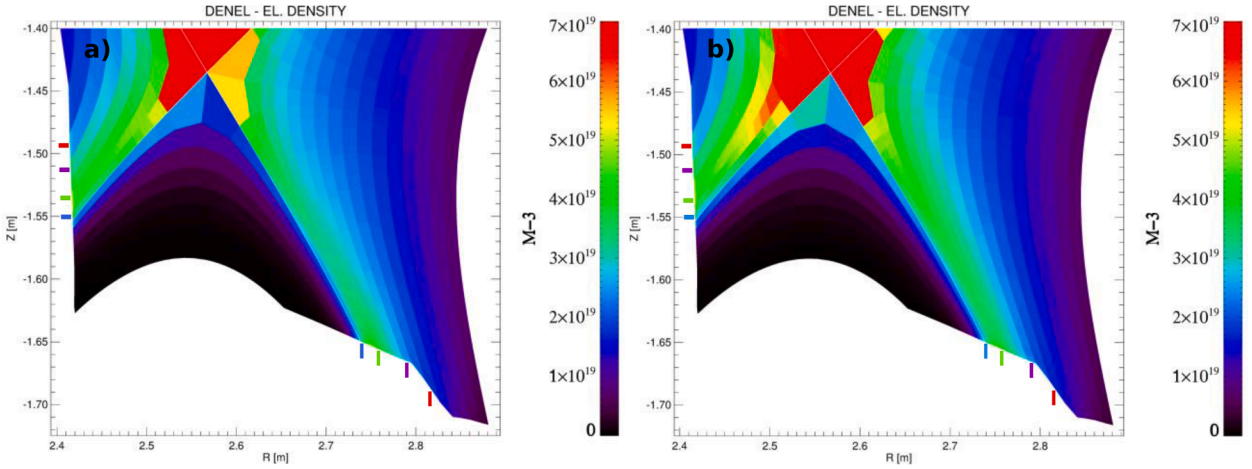

Fig. 3. Electron densities from simulations that use a) ADAS, b) CHEM He II atomic data. Coloured marker lines indicate the beginning of field lines used in Figs. 4 and 5.

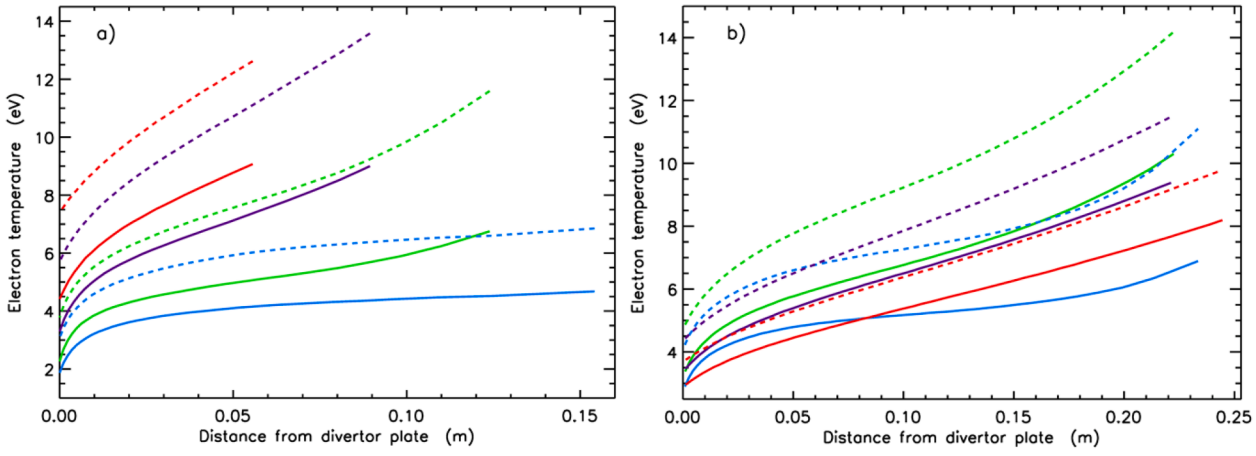

Fig. 4. Simulated electron temperatures along field lines for a) the inner divertor and b) the outer divertor: full lines CHEM database, dotted lines ADAS database. The coloured marker lines in Figs. 2 and 3 show the starting point of the field lines at the divertor plates.

regarded as a useful first step. It is noted that in JET pulses the He II emission dominates the VUV spectrum. This shows its importance in its contribution to the radiated power of the He impurity. This observation is consistent with the present simulations in which the He I to He II ratio of radiated powers in many cells is significantly below unity.

4. Results

The simulations used in the comparison are catalogued under JET pulse 81472, that using ADAS 96 data as '/jan2721/seq#3' and the CHEM data as '/jan2921/seq#1'. 2D electron temperature and density profiles are shown in Figs. 2 and 3, respectively. It is evident that the use

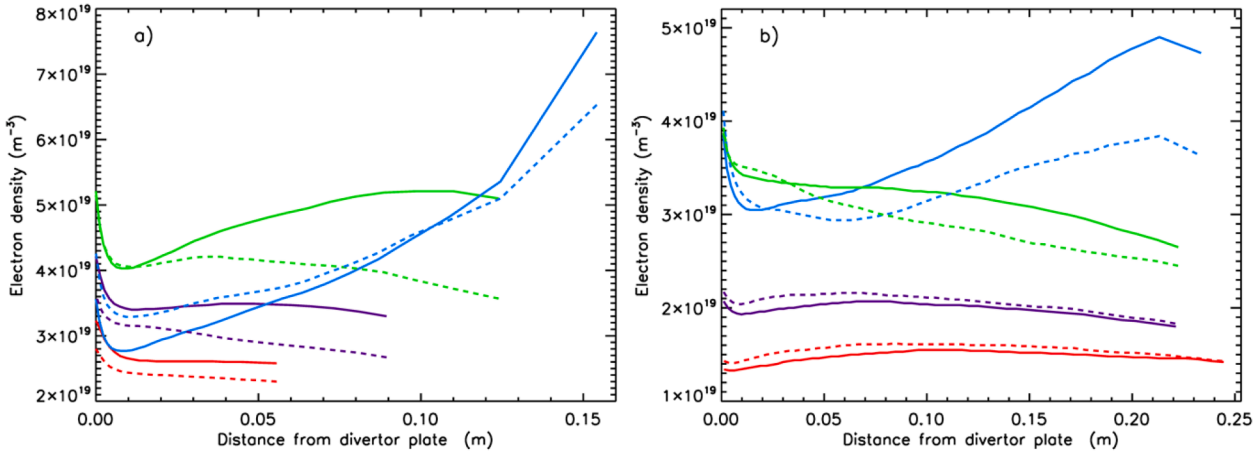

Fig. 5. Simulated electron densities along field lines for a) the inner divertor and b) the outer divertor: full lines CHEM database, dotted lines ADAS database. The coloured marker lines in Figs. 2 and 3 show the starting point of the field lines at the divertor plates.

of the CHEM data results in lower temperatures throughout the divertor volume. The temperatures along field lines in the inner and outer divertor are illustrated in Fig. 4 and it can be seen that this reduction is particularly marked for the inner divertor, being typically 30 to 40%, and reaching temperatures as low as ~ 2 eV. In this diagram the field lines are followed from points on the divertor plates to cells at roughly the height of the X-point. The reductions are smaller in the outer divertor, typically 15 to 30%, but in some cells up to 35% lower and reaching temperatures ~ 3 eV at the target plates. In Fig. 5 it can be seen that the outer divertor electron densities increase by up to ~ 30% close to the separatrix, although with smaller reductions with increasing major radius and becoming a ~ 10% reduction in the outer cells of the simulation. The changes in the inner divertor are larger, varying from a 15% reduction to a 50% increase. The processes driving these changes vary with temperature. At temperatures above ~ 8 eV excitation from the ground state is the dominant channel whereas below temperatures of ~ 3 eV recombination is dominant. At intermediate temperatures there is a balance between these two processes. The significant reduction in temperatures leads to an overall reduction in the radiated power by between 50 and 80%. However, at the lowest temperatures of ~ 2 eV radiation due to recombination becomes of particular importance and increases in radiation is seen in both He ionization stages, up to 70% in He I and 40% in He II.

5. Conclusions

A comparison of EDGE2D-EIRENE He simulations which differ only in the atomic data used demonstrates the importance of these data in determining the temperatures achieved in the simulations. It is made using newly compiled He II CHEM datasets and the ADAS 96 data which would normally be used in these simulations. The temperatures using the CHEM datasets were reduced throughout the divertor volume by 30 to 40% in the inner divertor region and 15 to 30% in the outer divertor, reaching ~ 2 eV close to the target plates in the inner divertor. This is the temperature at which recombination-driven populations lead to significant increases in the radiated power, which is thought to be the most likely explanation of intense, spatially localized features observed close to the inner divertor target plates in JET. In these comparisons changes have only been made to the He II atomic data, although the results would suggest that checks on the He I data are desirable to see if this leads to further reductions in the simulated temperatures. Extending the regions in which the temperatures are close to ~ 2 eV in He simulations (in D ~ 1 eV) would significantly increase the radiated power from the divertor and reduce the simulated radiation shortfall. Indeed, in D-fuelled discharges, it is necessary to reach these low temperatures before radiation due to the D molecules will become significant. This analysis clearly demonstrates the need for the highest quality atomic data to be used in order to give reliable edge transport simulations.

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CRediT authorship contribution statement

K.D. Lawson: Conceptualization, Investigation, Methodology, Writing. **M. Groth:** Conceptualization, Methodology. **D. Harting:** Software, Formal analysis. **S. Menmuir:** Validation, Investigation. **D. Reiter:** Conceptualization, Investigation, Methodology. **K.M. Aggarwal:** Formal analysis. **S. Brezinsek:** Conceptualization, Methodology. **I. H. Coffey:** Validation, Investigation. **G. Corrigan:** Software. **F.P. Keenan:** Conceptualization. **C.F. Maggi:** Conceptualization. **A.G. Meigs:** Validation, Investigation. **M.G. O'Mullane:** Software, Formal analysis, Data curation. **J. Simpson:** Software. **S. Wiesen:** Conceptualization, Methodology.

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.

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