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Comparisons of new He II atomic data with JET line ratio measurements and their application to EDGE2D-EIRENE simulations

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Application of new He II atomic data to EDGE2D simulations

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1. Introduction

An understanding of the plasma edge and divertor is essential for predicting the performance of next-step machines such as ITER. Transport codes used to study the divertor behaviour [1] employ atomic physics data in two applications. The first is to predict the power radiated by the fuel and impurity atoms, which is carried out as a post-processing option, while the second use is in calculating the atomic power loss term. This forms part of the transport calculations and in D fuelled simulations it has been shown that the simulated temperatures are sensitive to this term [2]. A new He II (He^+) atomic database [3,4] is used to check the application of the atomic data in the EDGE2D code.

2. Atomic physics model

A stand-alone atomic physics model has been developed for He II that includes the dominant populating channels of the energy levels in this hydrogenic species. These are electron and heavy particle collisional excitation and deexcitation, radiative decay, direct electron collisional ionization, radiative and three-body recombination. A schematic diagram is shown in figure 1. A *J*-resolved description (*J* the total angular momentum) is used for the spectroscopic levels and *n*-resolution for higher shells up to the maximum considered of n=16. This is above the collision limit for these species at all densities of interest, where the probability of the atom being ionized exceeds 50%. The model allows populations, line intensities and radiated powers to be calculated with different processes easily switched on or off.

3. Use of atomic data in EDGE2D

Radiated powers are calculated as a post-processing option of EDGE2D using the ADAS [5] *PLT* and *PRB* functions, the low-level line power and recombination-bremsstrahlung power coefficient. These are calculated by summing the radiated powers driven by excitation and recombination, respectively. For the *PLT* function the agreement between ADAS and the new He II database is within 20% throughout most of the temperature range, rising to ~25% at the highest

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temperatures and density considered of ~20-30 eV and 10^{21} m^{-3}. At temperatures below 0.6 eV larger discrepancies are found, although these are unimportant due to the very small value of the function. A similar agreement of ±20% is found for the *PRB* function at temperatures >2-3 eV, although this rises to ~×2 at lower temperatures and to ×3.5 at the lowest temperature and density considered of 0.2 eV and 10^{18} m^{-3}, with ADAS tending to be higher at low n_e and vice versa.
Atomic data are also used to calculate the ADAS electron power loss term, S_e,

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

where n_e, n_z and n_{z+1} are the electron, ion and continuum densities and I_H is the ionization potential. *SCD* and *ACD* are the effective ionization and recombination rates. There are much larger discrepancies for these functions, which are shown in figures 2 and 3. Burgess and Summers [6] give the rate equations for the population of the *i*th level in the form

$$\sum_j C_{ij} n_j = n_e n_{z+1} r_i - \frac{dn_i}{dt}.$$

C_{ij} represents all processes connecting levels i and j, including radiative decay, collisional excitation and deexcitation and C_{ii} all loss channels from level i, which in addition includes direct collisional ionization. The terms n_j and r_i represent the density of level j and recombination to level i, respectively, the latter both radiative and three body. Assuming that the populations of the excited levels reach equilibrium on a much faster timescale than changes in the ground state

$$\sum_j C_{ij} n_j = n_e n_{z+1} r_i \quad \text{for} \quad i \neq 1 \quad \text{and} \quad \sum_j C_{1j} n_j = n_e n_{z+1} r_1 - \frac{dn_1}{dt}.$$

SCD and *ACD* are then defined by

$$n_e \, SCD \, n_1 = n_e n_{z+1} \, ACD - \frac{dn_1}{dt}$$

It can be shown that

$$SCD = n_e^{-1} \left(C_{11} - \sum_i \frac{C_{1i} C_{i1}}{C_{ii}} \right) \quad \text{and} \quad ACD = r_1 - \sum_i \frac{C_{1i} r_i}{C_{ii}}. \qquad (2)$$

This treatment omits populating channels from excited levels, a complete description being given by matrix inversion, which in steady state leads to

$$\begin{pmatrix} n_1 \\ n_2 \\ \dots \\ n_j \\ \dots \end{pmatrix} = n_e n_{z+1} \begin{pmatrix} C_{11} C_{12} \dots C_{1j} \dots \\ C_{21} C_{22} \dots C_{2j} \dots \\ \dots \\ C_{i1} C_{i2} \dots C_{ij} \dots \\ \dots \end{pmatrix}^{-1} \begin{pmatrix} r_1 \\ r_2 \\ \dots \\ r_j \\ \dots \end{pmatrix},$$

from which

$$SCD = 1 / (n_e (C_{11})^{-1}) \quad \text{and} \quad ACD = r_1 + \sum_j \frac{(C_{1j})^{-1} r_j}{(C_{11})^{-1}}. \qquad (3)$$

$(C_{ij})^{-1}$ is the *ij*th element of the inverse of the matrix. As a check on the calculation of the *SCD* and *ACD* functions using the new He II data they have been determined from both equations 2 and 3 and found to be within ~50% of each other.

4. Contributions to the kinetic energy

Only terms that affect the kinetic energy should be included in the power loss term. There is also a potential energy reservoir for which no precise calculation is made, since changes to the potential energy have no direct effect on the transport. For example, the emission of radiation does not affect the kinetic energy. The electron fluid will, however, lose kinetic energy through collisional excitation and gain energy through collisional deexcitation, the power loss being

$$P_{exc} = \sum_i n_i \sum_{j>i} q_{ij} E_{ij} - \sum_j n_j \sum_{i<j} q_{ji} E_{ij}$$

where q_{ij} is the collisional excitation rate coefficient between levels i and j and $E_{ij} = E_j - E_i$ the transition energy. Direct collisional ionization will also lead to a kinetic energy loss

$$E_{initial} - (E_{final1} + E_{final2}) = (I_H - E_i)$$

with the power loss and the power gain for the reverse reaction, three-body recombination, being

$$P_{ci} = \sum_i n_i s_i (I_H - E_i) \quad \text{and} \quad P_{3b} = \sum_i \alpha_i^{3b} (I_H - E_i),$$

where s_i and α_i^{3b} are the ionization and three-body recombination rate coefficients for level i and, in these reactions, the energy (I_H - E_i) is either added or removed from the potential energy reservoir. Although the emitted photon energy in radiative recombination is $h\nu = E_{init} + (I_H - E_i)$, the kinetic energy change is only E_{init}, the power loss being

$$P_{rr} = \sum_i E_i^{Max} = a(T_e)\, T_e \sum_i \alpha_i^{rr} .$$

E_i^{Max} is the energy lost from a Maxwellian distribution of temperature T_e and α_i^{rr} the radiative recombination rate coefficient, with the constant a varying from ~1-0.7 for T_e 0.3-20 eV. If P_{br} is the power lost through Bremsstrahlung, which is usually small, the total power loss is

$$S_e = n_e n_z P_{exc} + n_e n_z P_{ci} + n_e n_{z+1} P_{rr} - n_e^2 n_{z+1} P_{3b} + n_e n_{z+1} P_{br} \qquad (4)$$

The value of S_e can be calculated from equations (1) and (4) and figure 4 gives the ratio for a range of parameters. In an exact, algebraic comparison made for the special case of a single excited state, using equation (2) to give *SCD* and *ACD*, it is seen that equation (1) contains terms such as $n_e n_{z+1} (\alpha_z^{rr} + \alpha_1^{rr}) I_H$, which relate to changes in the potential rather than kinetic energy.

5. Conclusions

Comparisons between the ADAS *PLT*, *PRB*, *SCD* and *ACD* functions and those derived using a new He II database show agreement for the first two, but significant differences for the *SCD* and *ACD* functions. As a check the latter have been calculated by two different methods with

reasonable agreement between the results. Further the formula being used to calculate the power loss term in the EDGE2D simulations is not found to agree with a direct calculation from the new database, differing by more than an order of magnitude in some cases. In it are terms relating to changes in potential energy, which have no effect on transport. He simulations are being carried out at present to see the effect of using the new He II database on the simulated parameters.

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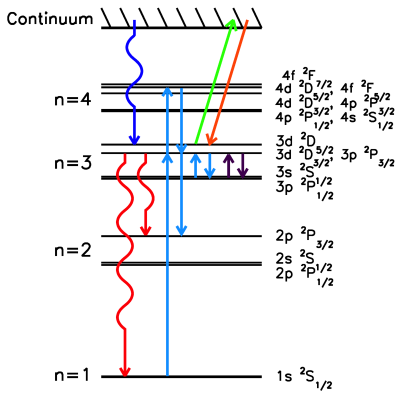

Figure 1. Schematic diagram of the hydrogenic energy levels showing populating and depopulating channels. These include radiative decay, electron and heavy particle collisions, direct collisional ionization, radiative recombination and three-body recombination.

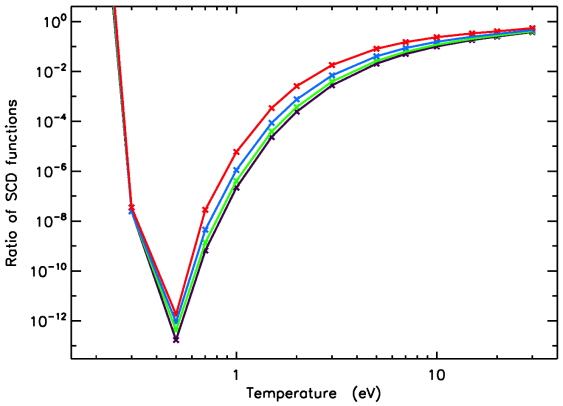

Figure 2. Ratio of the ADAS SCD function to that calculated from the new He II atomic database. n_e = 10^{18}, 10^{19}, 10^{20} and 10^{21} m^{-3}.

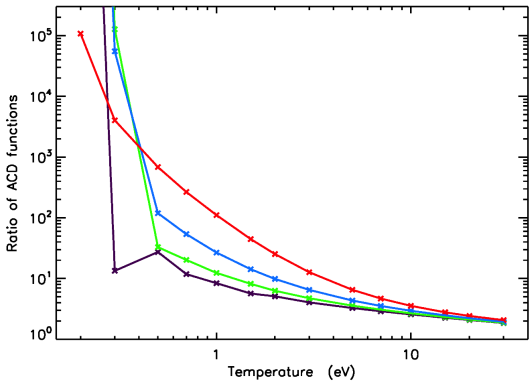

Figure 3. Ratio of the ADAS ACD function to that calculated from the new He II atomic database. n_e = 10^{18}, 10^{19}, 10^{20} and 10^{21} m^{-3}.

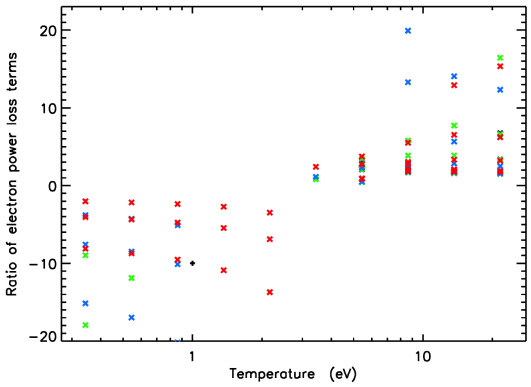

Figure 4. Ratio of the electron power loss term calculated by equations (1) and (4). n_e = 10^{18}, 10^{19}, 10^{20} and 10^{21} m^{-3}.