Applications of Atomic Data to JET Spectroscopic Measurements

Kerry Lawson

Introduction

The presentation will concentrate on 3 distinct topics, illustrating various atomic data that are required:

- C IV emission from the JET divertor is used to check the consistency of a collisional-radiative model. For this it is necessary to use measurements from the earlier JET campaigns when the plasma-facing components were carbon. Nevertheless, the results are highly topical to JET with its ITER-like wall and nitrogen and carbon machines.

- Assumptions about electron collisional ionization are examined, in particular whether ionization can affect excited state populations.

- A-particle collisional excitation — fast a-particles are found to have unexpectedly high excitation rates — could this affect the power balance of burning plasma machines?

The emphasis will be on the diagnostic or so-called 'spectroscopic' energy levels — i.e. for which the principal quantum number n ≤ 5, rather than on high n levels.

Energy level populations

Energy levels: Index

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- In a more accurate treatment, the steady state rate equations form a set of simultaneous linear equations.

- At low densities and over a wide temperature range, collisions between excited states can be still be neglected.

- However, it is essential to include radiative cascading from higher energy levels (e.g. in C IV, populations increased ~ 10%).

- In steady state, the rate equation is

\[
\frac{dn_i}{dt} = \sum n_j A_{ji} - n_i A_{ij} - \sum n_k A_{ki} + \sum n_l A_{li} + \chi
\]

Electron collisional excitation, \( q_e \)

Electron collisional excitation from ground state

Radiative cascading from higher levels

Application to JET divertor plasmas - measurements

- Spectra recorded on a CFPED spectrometer during JET C campaigns.

- Spectral range 140 Å to 245 Å

- Spectral resolution ~ 1 Å

Application to JET divertor plasmas — VUV calibrations

- Analysis involves VUV measurements, since only 1 useful visible C IV line.

- VUV range of XUV / VUV × 40-100 compared with 2 for visible — more information in XUV/VUV.

- VUV absolutely less difficult to use and often sensitivity calibration more difficult to determine.

- In-situ calibration used on JET — relative calibration given by line ratios.

- Relative calibration from Na- and Li-like ratios and from C IV ratios.

- Absolute sensitivity calibration problematic, mainly because of difficulty in obtaining reliable visible calibrations — e.g. unable to fit a calibration source in space available, etc.

- Useful confirmation of XUV / VUV absolute calibrations provided by elemental cooling rates.

- On JET, one measurement of the W concentration is calibrated using the W cooling rates.

Acknowledgements

Co-authors

K. D. Lawson1, K. M. Aggarwal2, J. H. Coutts2, A. Czarnacka2, F. P. Kaeber2, I. Kasprzak2, B. M. McLaughlin2, R. H. G. Reid2 and JET contributors

EUROfusion Consortium, JET, Culham Science Centre, Abingdon, OX14 3DB, UK
1 CCFE, Culham Science Centre, Abingdon, OX14 3DB, UK
2 Astrophysics Research Centre, School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, UK.
3 Institute of Plasma Physics and Laser Microfusion, Henry 23 St, 01-497 Warsaw, Poland
4 Institute of Physics, Opole University, ul.Čwieków 48, 45-052 Opole, Poland.
5 Centre for Theoretical Atomic, Molecular and Optical Physics, School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, UK.


J. H. Coutts2, A. Czarnacka2, F. P. Kaeber2, I. Kasprzak2, B. M. McLaughlin2, R. H. G. Reid2 and JET contributors

EUROfusion Consortium, JET, Culham Science Centre, Abingdon, OX14 3DB, UK
1 CCFE, Culham Science Centre, Abingdon, OX14 3DB, UK
2 Astrophysics Research Centre, School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, UK.
3 Institute of Plasma Physics and Laser Microfusion, Henry 23 St, 01-497 Warsaw, Poland
4 Institute of Physics, Opole University, ul.Čwieków 48, 45-052 Opole, Poland.
5 Centre for Theoretical Atomic, Molecular and Optical Physics, School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, UK.

**Application to JET divertor plasmas - analysis**

- Necessary to include collisional recombination in the analysis. Most conveniently done using the ADAS Photon Emissivity Coefficient (PEC) formalism.
- The PECs for excitation (already described), free electron recombination and charge exchange (CX) recombination, $\nu_{rec}$, is the ground state population of the next higher ionization stage and $\nu_e$ the D density. The PECs are functions of $\nu_e$ and $T_e$.
- Line ratios provide the most stringent test. No absolute calibration required.
- A much larger database of A-values is required (C IV Li-like with single outer electron).
- Free electron recombination rates not used for spectroscopic measurements.
- A-values reliable (C IV Li-like with single outer electron).

**Application to JET divertor plasmas - results**

- Database of 86-Chrom, 70 Low confinement (L) mode, 56 ELMy High confinement (H) mode and 38 ELMy H-mode pulses, all with D fuel.
- For this database the minimization is not sensitive to $n_e$ or $n_\text{rec}$, the parameter relating to free electron recombination.
- Only CX recombination is important for the spectroscopic levels in (i): $T_e$ (eV) ranges from 17 to 65 eV.
- Highest CX contribution (11-21%) to 1s2p^3P level. Also small contribution (4-6%) to 1s2p^1S level.
- Free electron recombination, which includes dielectronic, radiative and 3-body recombinations, only becomes significant at low $T_e$ (~1-2 eV).

**Application to JET divertor plasmas - atomic data**

- Analysis used spectroscopic measurements.
- Line intensity ratios and atomic data.
- Ionization probabilities.
- Electron collisional excitation rates, from ground state to D CX rates.
- Free electron recombination rates not used for 'spectroscopic' levels.
- A-values reliable (C IV Li-like with single outer electron).
- Can electron collisional excitation rates make a difference?
- 3-R-matrix calculations for C IV:
- Burke calculations are for limited T_e range (~21 eV).
- Griffin uses R-matrix with pseudo-states method.

**C IV Analysis - Summary**

- The most important atomic data used in the analysis are A-values and electron collisional excitation rates.
- The highest quality R-matrix calculations of electron collisional rates are essential – it makes a difference!
- Charge exchange recombination is the only significant recombination channel. Limited availability of D CX rates other than for C IV?
- Is there a way of exploiting the importance of electron collision from the ground state as opposed to those between excited states in further R-matrix calculations?
- Heavy particle excitation/de-excitation rates required when metastable levels present.
- Spectrometer sensitivity/calibrations make use of elemental cooling rates.

**Electron collisional ionization – from excited level**

- Generally assumed that the main ionization channel is from ground state to ground state, the effect on excited states being small.
- Can electron collisional ionization affect excited state populations of the spectroscopic levels?
- Very little data exists for ionization from or to excited levels, even for elements such as C.
- Flexible Atomic Code (FAC) calculations generated distorted wave ionization rates for C II, C IV and C V.
- Comparison of A-values and ionization rates showed that ionization from an excited level does not significantly affect the populations (≤ 2×10^{-4} of radiative decay).

**Electron collisional ionization – to excited level**

- However, ionization in the spectroscopic levels produced larger contributions to the populations than expected from the ‘ground state to ground state’ scenario.
- E.g., for the C IV 1s2p^3P levels, the ionization to excitation PEC ratio reaches >7% even in steady state, when $n_e$ / $n_g$ ~ 1, due to the C II 1s2p^1S bound state.
- During impurity influxes when $n_e$ / $n_g$ ~ 1, ionization would be expected to make larger contributions to the populations.
- Brendan McLoughlin (QUB) has carried out R-matrix calculations for C IV and a C V ionization rates as a check on the accuracy of the FAC calculations and to see the importance of indirect recombination processes.
- In the long term, experiments with injected impurities could be used to study perpendicular transport in the plasma edge.

**Summary**

- A much larger database of ionization rate coefficients both from (for the ionization balance) and to excited states than is available now is required.
• Preliminary work on a possible α-particle diagnostic using Kr line intensity ratios to give n_e produced unexpected results.
• Thermal heavy particles (D, T or He) excite levels, which are close, usually forbidden transitions.
• However, the fast α-particle excitation rates for allowed transitions in Kr XXVIII are ×10−20 larger than for the forbidden transition.
• Further, the fast α rates are ×6 larger than the electron rates.
• The fast β-particles act as an 'extra' population of electrons, but with largely unknown excitation rates – none for W.

Summary
• Development of IFXN code desirable, with calculation of α-particle cross-sections for Kr and W.

Conclusions
• An extensive and highly accurate analysis of C IV JET divertor emission illustrates the importance of various atomic processes.
• The most important atomic data used in the analysis are A-values and electron collisional excitation rates, particularly those from the ground state. Significant differences were found between the 3 R-matrix calculations of electron collisional rates available for C IV.
• Free electron recombination was not found to be significant for C IV. Charge exchange recombination rates allowed the contribution towards the populations to be determined and are essential when the density product n_D n_g+1/n_e n_g is not known.
• Free electron recombination is important for D and low ionization stages of impurities (T_e ~ 1-2 eV).
• Accurate heavy particle collisional rates are required when metastable levels are present.
• Elemental cooling rates have been used on JET for spectrometer sensitivity calibrations.
• Electron collisional ionization to the 'spectroscopic' levels (n=5) should be considered, particularly during influxes.
• R-matrix calculations of collisional ionization have just become available and will be used to confirm the accuracy of previous FAC calculations.
• Development of the IFXN heavy particle collisional excitation code is required to assess the importance of fast α-particles to the power balance in a burning plasma with W.
• This code would also provide data for sensitivity studies of a possible α-particle diagnostic.