EUROfusion

Applications of Atomic Data to JET Spectroscopic Measurements

Kerry Lawson

CCFE

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement number 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

Acknowledgements

Co-authors

K. D. Lawson[1], K. M. Aggarwal[2], I. H. Coffey[2], A. Czarnecka[3], F. P. Keenan[2], I. Książek[4], B. M. McLaughlin[5], R. H. G. Reid[5] and JET contributors*

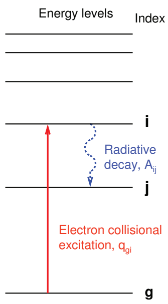
EUROfusion Consortium, JET, Culham Science Centre, Abingdon, OX14 3DB, UK
[1] CCFE, Culham Science Centre, Abingdon, OX14 3DB, UK
[2] Astrophysics Research Centre, School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, UK
[3] Institute of Plasma Physics and Laser Microfusion, Hery 23 St, 01-497 Warsaw, Poland
[4] Institute of Physics, Opole University, ul.Oleska 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
* See the Appendix of F. Romanelli et al., Proceedings of the 25th IAEA Fusion Energy Conference 2014, Saint Petersburg, Russia

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 neon radiative divertor experiments.
- Assumptions about electron collisional ionization are examined, in particular whether ionization can affect excited state populations.
- α-particle collisional excitation – fast α-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 level populations, n_i, derived from the rate equation

$$\frac{dn_i}{dt} = n_e \sum_{j\neq i} n_j q_{ji} + \sum_{j>i} n_j A_{ji} - n_i \sum_{j<i} A_{ij} + \alpha - s$$

where α and s represent contributions from recombination and ionization.

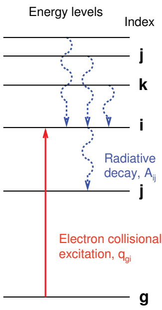
- In steady state $\frac{dn_i}{dt} = 0$
- In low density plasmas excited state populations are small (e.g. for C IV $1s^2 2p$ level $n_i < 2\times10^{-3} n_g$ and for higher levels $n_i \le 10^{-6} n_g$). Hence collisions between excited states can usually be neglected.
- Neglecting recombination and ionization

$$n_i \approx \frac{n_e n_g q_{gi}}{\sum_{j<i} A_{ij}}$$

- If there is a single dominant radiative decay *i* -> *j*, the line intensity

$$I_{ij} \approx n_e n_g q_{gi}$$

Energy level populations



- 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 still be neglected (Accuracy of n_i, a few % – e.g. in C IV ~ 1%),
- However, it is essential to include radiative cascading from higher energy levels (e.g. in C IV, populations increased ~ 10%).

$$n_i \sum_{j<i} A_{ij} = n_e n_g q_{gi} + \sum_{j>i} n_j A_{ji}$$

$$= n_e n_g q_{gi} + \sum_{j>i} \frac{n_e n_g q_{gj} A_{ji}}{\sum_{k<j} A_{jk}}$$

Electron collisional excitation from ground state — Radiative cascading from higher levels

Line intensities

- Spectral line intensity of transition *i* -> *j* :-

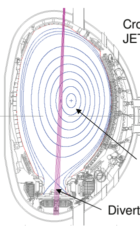
$$I_{ij} = n_i A_{ij} = \frac{n_e n_g A_{ij}}{\sum_{j<i} A_{ij}} \left[q_{gi} + \sum_{j>i} \frac{q_{gj} A_{ji}}{\sum_{k<j} A_{jk}} \right]$$

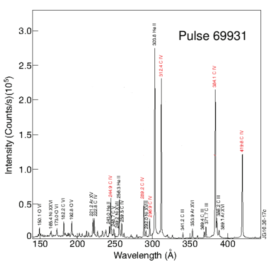
Electron collisional excitation from ground state — Radiative cascading from higher levels

- A metastable level acts as a 'second ground state'.
- Its population may be difficult to determine.
- Usually require heavy particle collisional rates for the transitions between the close low-lying energy levels.

Application to JET divertor plasmas - measurements

- Spectra recorded with a SPRED spectrometer during JET-C campaigns.
- Vertical line-of-sight.
- Spectral range 140 Å to 443 Å.
- Spectral resolution ~ 1Å.

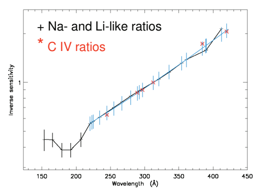




- Spectrum of JET pulse 69931 averaged between times 12.3 and 12.6 s showing the 6 VUV C IV spectral lines used, at wavelengths of 245 Å, 289 Å, 297Å, 312 Å, 384 Å and 420 Å.

Application to JET divertor plasmas – VUV calibrations

- Analysis involves VUV measurements, since only 1 useful visible C IV line observed.
- Energy range of XUV / VUV ×40-100 compared with ×2 for visible – more information in XUV/VUV.
- VUV experimentally more difficult than visible and often sensitivity calibration more difficult to determine.
- *In-situ* calibration used on JET
  - relative calibration given by line ratios.
  - absolute calibration from branching ratios with calibrated visible spectrum.
- Relative calibration from Na- and Li-like line intensity ratios and from C IV ratios.
- Error bars ± 10% – high accuracy!



Spectrometer sensitivity calibration
Lawson *et al.*, 2009, JET Report JET-RE(09)5

- 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.

Application to JET divertor plasmas - analysis

- Necessary to include recombination in the analysis. Most conveniently done using the ADAS Photon Emissivity Coefficient (PEC) formulation.

$$I = n_e n_g \varepsilon^{exc} + n_e n_{g+1} \varepsilon^{rec} + n_D n_{g+1} \varepsilon^{cx}$$

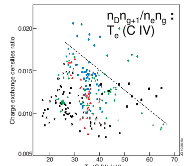
- ε^{exc}, ε^{rec} and ε^{cx} are the PECs for excitation (already described), free electron recombination and charge exchange (CX) recombination. n_{g+1} is the ground state population of the next higher ionization stage and n_D the D density. The PECs are functions of n_e and T_e.
- Line ratios provide the most stringent test. No absolute calibration required. $n_e n_g$ cancels from the dominant terms.

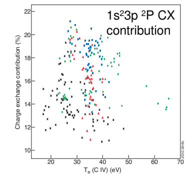
$$\frac{I_1}{I_2} = \frac{\varepsilon_1^{exc} + \frac{n_{g+1}}{n_g}\varepsilon_1^{rec} + \frac{n_D n_{g+1}}{n_e n_g}\varepsilon_1^{cx}}{\varepsilon_2^{exc} + \frac{n_{g+1}}{n_g}\varepsilon_2^{rec} + \frac{n_D n_{g+1}}{n_e n_g}\varepsilon_2^{cx}}$$

- The RMS of the differences between the 5 measured and theoretical line intensity ratios was minimized by varying T_e, $\log_{10} n_e$, n_{g+1}/n_g and $n_D n_{g+1}/n_e n_g$.
- Allows the T_e of the plasma emitting the C IV radiation, T_e (C IV), to be determined.

Application to JET divertor plasmas - results

- Database of 86 Ohmic, 70 Low-confinement (L) mode, 59 ELMy High-confinement (H) mode and 36 ELM-free H-mode pulses, all with D fuel.
- For this database the minimization is not sensitive to n_e or n_{g+1}/n_g, the parameter relating to free electron recombination.
- Only CX recombination is important for the spectroscopic levels (n ≤5).
- T_e (CIV) ranges from 17 to 65 eV.
- Highest CX contribution (11-21%) to 1s²3p ²P level. Also small contribution (1-4%) to 1s²3d ²D level.
- Free electron recombination, which includes dielectronic, radiative and 3-body recombination contributions, only becomes significant at low T_e (~1-2 eV).

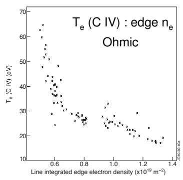


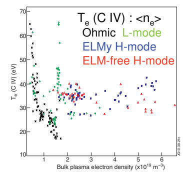


Application to JET divertor plasmas - results

- Clear dependencies of T_e (C IV) on bulk plasma parameters are found.
- C IV occurs in the Scrape-Off Layer (SOL) of JET plasmas, outside the L- and H-mode transport barriers.
- Hence, no clear separation of the data for the different regimes.
- Parallel transport will be the most important transport mechanism.
- Nevertheless, 2 clear trends are observed. For $n_e < 1.5\times10^{19}$ m^{-3} :- $\text{Log}(T_e\text{(C IV)}) = 1.47 - 0.56{*}\text{Log}(n_e)$ and for $n_e > 1.7\times10^{19}$ m^{-3} :- $T_e\text{(C IV)} = 33.2 + 0.24{*}n_e$

K D Lawson *et al.*, 2011, PPCF, **53**, 015002

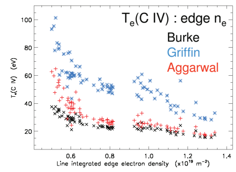




Application to JET divertor plasmas – atomic data

- Analysis used spectroscopic measurements
  - line intensity ratios

  and atomic data
  - transitions probabilities
  - electron collisional excitation rates, from ground state
  - 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, 1992, J.Phys. B, **25**, 4917
  - Griffin *et al.*, 2000, J. Phys. B, **33**, 1013
  - Aggarwal & Keenan, 2004, Phys. Scripta, **69**, 385
- Burke calculations are for limited T_e range (≤ 31 eV).
- Griffin uses R-matrix with pseudo-states method.



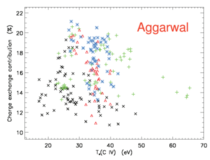
- RMS difference from minimization
  - Burke 4 - 5%
  - Griffin 9 - 10%
  - Aggarwal 4 - 5%
- Griffin results in ~ × 2 higher T_e and larger scatter in data.

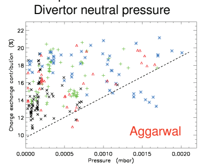
Application to JET divertor plasmas – atomic data

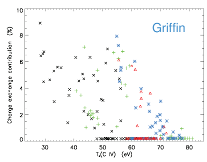
- Higher T_e(C IV) of Griffin case lead to unexpectedly small CX contributions (≤ 9% for 1s²3p ²P level).
- Diagrams compare Griffin and Aggarwal CX contributions to 1s²3p ²P level as function of T_e (C IV) and the divertor neutral pressure.
- Clear difference found for the R-matrix calculations. Aggarwal preferred.

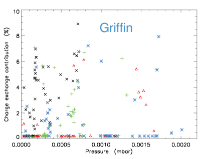
1s²3p ²P CX contribution : T_e(C IV)

1s²3p ²P CX contribution : Divertor neutral pressure









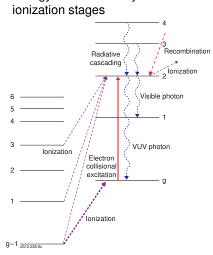
C IV Analysis - Summary

- 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?
- Is there a way of exploiting the importance of electron collisions 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 III, 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).

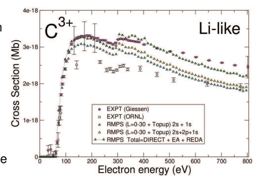
Energy levels for 2 adjacent ionization stages



Lawson *et al.*, 2013, J. Phys. B, **46**, 035701

Electron collisional ionization – *to* excited level

- However, ionization *to* 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 1s²2p ²P levels, the ionization to excitation PEC ratio reaches ~7% even in steady state, when $n_{g-1} / n_g \sim 1$, due to the C III 1s²2s2p ³P metastable levels.
- During impurity influxes when $n_{g-1} / n_g > 1$, ionization would be expected to make larger contributions to the populations.



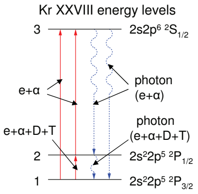
- Brendan McLaughlin (QUB) has carried out R-matrix calculations for C IV and N V ionization rates as a check on the accuracy of the FAC calculations and to see the importance of indirect resonant processes.
- In the long term, experiments with injected impurities could be used to study perpendicular transport in the plasma edge.

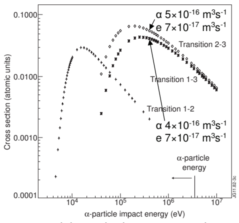
Summary

- A much larger database of ionization rate coefficients both *from* (for the ionization balance) and *to* excited states than is available now is required.

α-particle collisional excitation

- Preliminary work on a possible α-particle diagnostic using Kr line intensity ratios to give n_α 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.





α-particle excitation cross sections

- Further, the fast α rates are ~×6 larger than the electron rates.
- The fast α-particles act as an 'extra' population of electrons, but with largely unknown excitation rates – none for W.
- In a burning plasma, the 'extra' radiation is also unknown.

α-particle collisional excitation

- For W, it is desirable to determine this 'extra' radiation to see if there is a significant effect on the power balance of the burning plasma.
- The Kr rates were produced by an early version of the heavy particle IFXN code, which is being developed at QUB.
- The IFXN code has a close-coupled, symmetrised, semi-classical collision formulation, with short-range behaviour taken into account.
- It is the only code that we know of that accurately treats heavy particle excitation of both forbidden and allowed transitions.
- It is hoped to continue code development with the subsequent calculation of rates for W (for burning plasma power balance) and Kr (for sensitivity of the α-particle diagnostic).
- This diagnostic covers the α-particle energy range 0.1-1 MeV, where a reliable diagnostic is still required.

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.