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Scientific progress report 2

30 June 2010

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Scientific progress report 2

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Abstract: *The report reviews scientific task completion for project months 7-12*

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Preface

This scientific report is the second of a series of six such reports, deliverable under the ADAS-EU project, which summarise the scientific achievements of the project over the preceding six months.

H P Summers
30 June 2010

Chapter 1

Overview and milestones SCI22, SCI23

The milestone SCI22 concerns ‘merging of high bundle-n model with low l-mixing model accomplished and functioning for arbitrarily highly charged CXS receiver ions’. The bundle-n model has been fully implemented and works effectively for very highly charged heavy receiver ions. The merging with the basic low l-mixing model has not been implemented. A different scientific method, more suited to l-subshell cross-section examination is being developed. In consequence the milestone SCI22 for this last part should be reset to month 24 (see the discussion of section 2.4 below).

Milestone SCI23 concerning ‘universal scaled state selective CX data fully linked to bundle-n/l-mixing models, delivering complete synthetic CXS feature emissivities for heavy element ions’ has been met. But the linking is to the bundle-n model and l-mixing models separately and it is the bundle-n model which has been carried to complete synthetic feature emissivity generation. This has proved very effective and predictions have been carried through to tungsten in ITER. The procedures and data have been placed in ADAS and OPEN-ADAS for general use.

The timings of placement PDRA staff engagement, the timings of sub-contract placement and management staff loss are slowing the progress of certain work packages. Compensatory increase of other management staff time allocations to ADAS-EU and temporary compensating PDRA staff employment are speeding up other work packages. This will become evident in the next report SCIENCE3. Staffing adjustments will be detailed in the 18 month report REVIEW1. From the perspective of the primary ADAS-EU themes, theme 1 (heavy species) is significantly in advance, theme 2 (charge exchange) is in some respects behind, theme 3 (beam stopping and emission) is in part behind and in part in advance, theme 4 is substantially in advance and theme 5 is a little behind.

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Chapter 2

Work package reports

2.1 Work package 1-2

The work package concerns including configuration average structure computation as part of the automatic scripted complex atom handling. The configuration average solutions are to be used to size the full intermediate coupling structure calculations to computer resources and top up total radiated power. This has been accomplished and enabled in ADAS. The implementation is sophisticated in that the promotion rules are used to optimise the precision of the power estimates, by seeking to include the dominant power contributions within the intermediate coupling part of the solution. The extended description and instructions for use are given in PUBL3. For completeness, the front pages and contents page of PUBL3 are attached as Appendix A [1] to this report. Chapter 2, sections 2.4 is apposite to work package 1-2. PUBL3 must have restricted access at this stage.

2.2 Work package 2-1

The work package task concerns managing spectral complexity, that is allowing the handling of massive line sets from heavy specie ion emitters. This introduces the concept of accumulating all the lines in a spectral interval and then treating the spectral interval as a whole. The relevant theoretical quantity is a 'feature emissivity coefficient' which is a function of electron density, electron temperature and pixel number in wavelength space (new ADAS data format adf40). Strong lines continue to be described by photon emissivity coefficients (adf15) as before. This has been fully enabled and is part of the outputs from scripted automatic operation of the complex atom codes. PUBL3 (see Appendix A, chapter 1, section 1.3 and chapter 2, section 2.2 are apposite to work package 2-1. ADAS releases now include adf40 data for heavy species. ADAS release v3.1 is to be principally a data release, including substantial heavy element data. It is scheduled for month 20 (August 2010)

2.3 Work package 2-3

Although complex atom and ion feature emissivity data are now available for a number of elements and new elements can be added in a matter of days, the experimental exploitation is only proceeding at a modest pace. The recommencement of the JET Facility after completion of the new ITER-like wall will enable comprehensive tungsten observational spectroscopy. AUG at this time is the main test bed for tungsten and the ADAS tungsten data release has been made available there.

2.4 Work package 6-4

For the CXSFIT part of work package 6-4, see early completion report in document SCIENCE1, section 2.2.

2.5 Work package 7-2 and 7-3

In work package task 7-2, it was planned to project bundle-n CX modelling onto the l-redistributive cascade model (used for light element receivers) below the collision limit. In a later work package task, 8-1, the more complete bundle-nl model was to be activated. It has been decided to modify these intentions, in light of the likely continuing relatively high uncertainties of l-substate charge transfer cross-sections for heavy element highly ionised receivers and the ongoing calculations relating to this at sub-contractors. The older l-redistributive cascade incorporated a sophisticated inversion algorithm which allowed comment on the precision of n-shell selective charge transfer cross-sections if a number of CXS lines were simultaneously observed. Modern computer resources suggest that a similar procedure can be enabled for the l-shell capture, albeit with heavier and more memory demanding computations. We shall take this path expecting delivery of the revised 7-2 and 8-1 around the original 8-1 delivery date. Analytic work is underway and can be followed in PUBL1 (see Appendix B chapter 2 sections 2.2 and 2.3).

At this point of time, the mass production using the bundle-n model is adequate for forward prediction studies for ITER. Thus the objective of task 7-3 has been fully enabled by generation of necessary adf12 and adf40 data sets - in particular for tungsten. Some results are shown in Appendix C for illustration.

2.6 Work package 17-1

Work package 17.1 requires more ADAS-EU staff time than originally expected. Also, the three month delay in the start of Dr. Francisco Guzman at FZ Juelich and the one year delay in the first appointment period of Prof. Ratko Janev has necessitated slowing of this development. At this stage, definition of the ADAS formats was expected and transcription into these formats. These definitions have been constructed and the transcription of the electron collisional part is virtually complete. These use new ADAS molecular data formats, mdf02 and mdf04. The ion impact part remain to be done. Procedures and sub-routines in ADAS to read these new data formats have been written. The presentation of Dr. Guzman, reproduced in SETUP2 appendix B [3], summarises the status at Mar 2010. For physics-based verification tests, it has been decided that a basic molecular collisional radiative model for hydrogen must be prepared for ADAS. This development is the work package 18, but it has just started. So completion of the molecular extension is not expected before month 24.

2.7 Work package 26-1-2

The work package task comprises the completion of this report.

Appendix A

ADAS-EU Theme 3 supplementary material for the report

[1] ADAS-EU/REPORTS_PUBL/PUBL.3/ pages 1-6

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ADAS-EU R(09)01

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Hugh Summers, Adam Foster, Stuart Loch, Martin O'Mullane
and Allan Whiteford

**Heavy species in fusion plasma modelling
and spectral analysis**

25 May 2010

Workpackages :
Category :

Heavy species in fusion plasma modelling and spectral analysis

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Abstract: *The derived data for usual application in fusion, from the perspective of light elements, are hugely unwieldy for heavy elements, preventing the immediacy and handleability to which ADAS aspires for the experimental diagnostic analyst. So additional work must be done within ADAS in the direction of spectral synthesis for the spectroscopist and in the direction of enhanced condensation for the plasma computational modeller. The purpose of this article is to put all these steps in the hands of the ADAS user who wishes to become expert and, for the more application oriented user of ADAS, to explain what is available now for heavy species in ADAS, how to access it and use it correctly.*

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Appendix B

ADAS-EU Theme 1 supplementary material for the report

[1] ADAS-EU/REPORTS_PUBL/PUBL.1/ pages 1-6

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Adam Foster, Martin O'Mullane and Hugh Summers

Charge exchange spectroscopy for fusion plasmas

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Charge exchange spectroscopy for fusion plasmas

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Abstract: *Charge exchange spectroscopy (CXS) using fast neutral beams has a history of nearly thirty years. CXS is now a principle diagnostic on most fusion machines of proven effectiveness. Most of this application has been to the bare nuclei of light elements of nuclear charge $z_0 \leq 10$ as the charge exchange receiver and with neutral deuterium, D^0 , as the donor. Present and future application, with a view to ITER, is focussed on heavier elements - argon and above - and also on partially stripped receivers occurring towards the periphery of the plasma. The present work is concerned with re-examining and elaborating the older CXS models and with extension and critical reassessment of the fundamental atomic reaction database for heavier elements. The work comprises part of the the redesign/re-orientation of ADAS for heavy species and ITER. Therefore it also lays out the comprehensive atomic modelling and fundamental/derived data environment for medium/heavy species for fusion application which ADAS will support and on which further more refined developments will be made.*

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Appendix C

Emission from tungsten

C.1 Emission Estimates

An example of the emission calculated for a single stage, W^{+40} , is shown in figure C.1. The reference temperature, 2376eV, is chosen as this is the core temperature obtained from the MAST-Upgrade simulations. In the final plot in this figure the fraction of the beam in the ground and excited states is used to modify the relative emissivity from the two processes, and the $n = 1$ contribution is found to dominate. The fraction of the beam deuterium in each state is determined by collisions between beam ions (initially all in the ground state) and plasma ions, and it is found that approximately 0.2% of the beam neutrals are in the $n=2$ state in the plasma core.

It is clear that in a real plasma there will be more than one ionisation state of tungsten present at any given time. Applying a steady state ionisation balance to the tungsten for the same plasma conditions (figure C.2) already produces a mass of spectral lines covering the entire visible spectrum. .

The line of sight integrated results across the plasma are shown in figure C.3. It is found that the CX and the Bremsstrahlung emission are of the same order of magnitude, and therefore there is likely to be significant interference in measurements of such background quantities.

C.2 Application to ITER and conclusions

The same model was applied to ITER plasmas, using a vertical line of sight crossing one of the neutral beams. It is found (figure C.4) for a vertical line of sight that the ratio of the CX to the Bremsstrahlung emission is similar, with peaks arising to about 15-20% of the Bremsstrahlung levels.

Given the typically narrow spectral regions which are used for measurements of Z_{eff} (the MAST system uses a 1nm bandpass filter) care must be taken to select an appropriate region of the plasma with no such emission. This in turn may prove difficult given the sheer number of lines present, and the change in wavelengths depending on the area of the plasma viewed (and therefore the underlying impurity ionisation balance).

While the results of this section are of modest accuracy due to the extrapolations which these data are based upon, it is likely that these will mostly affect the intensities of the lines present, not their wavelengths. Therefore the potential problems that these lines pose are likely to be real effects, and they should be taken into account in future diagnostic design.

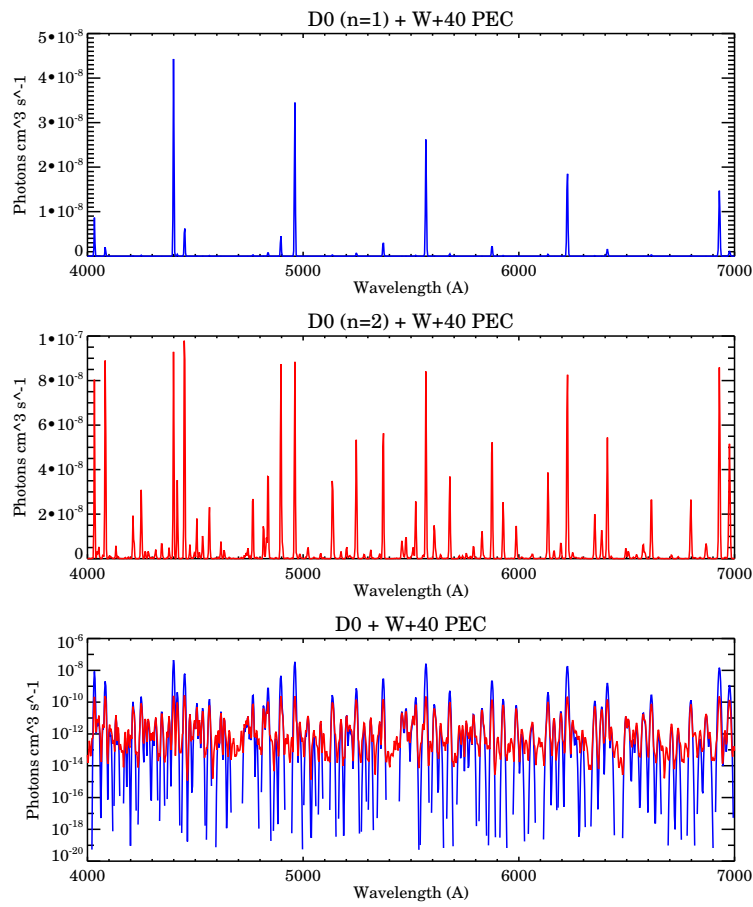


Figure C.1: The predicted emission from one ionisation stage of tungsten at $T_e \approx 2.4\text{keV}$. In the final graph the spectra have been multiplied by the fraction of the beam deuterium in the ground and excited states.

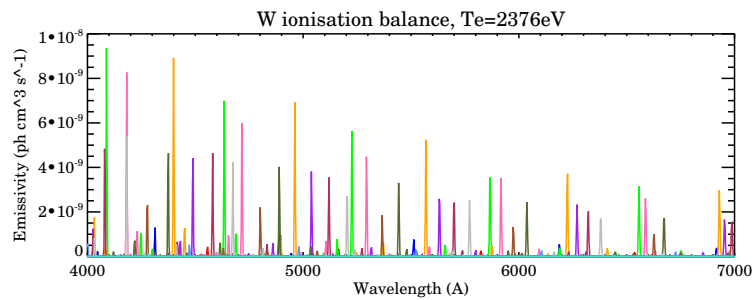


Figure C.2: The predicted emission from a steady state ionisation balance of tungsten at $T_e \approx 2.4\text{keV}$. The different colours indicate different stages of tungsten.

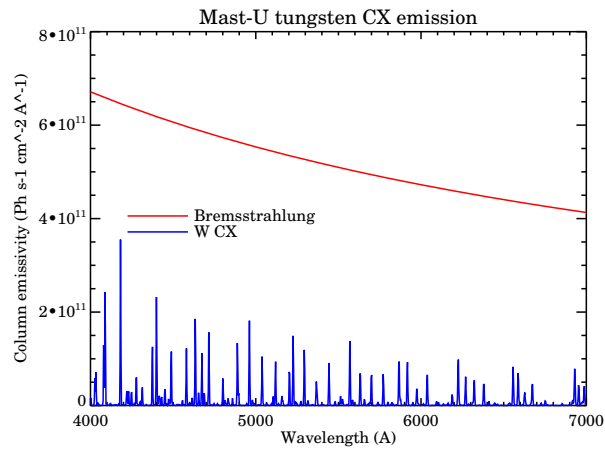


Figure C.3: The predicted line integrated tungsten charge exchange and Bremsstrahlung emission for a chord on MAST-U. While the Bremsstrahlung level is greater than the charge exchange estimates, the CX emission is of the same order of magnitude, and therefore it is likely that it will interfere with background measurements of Z_{eff}

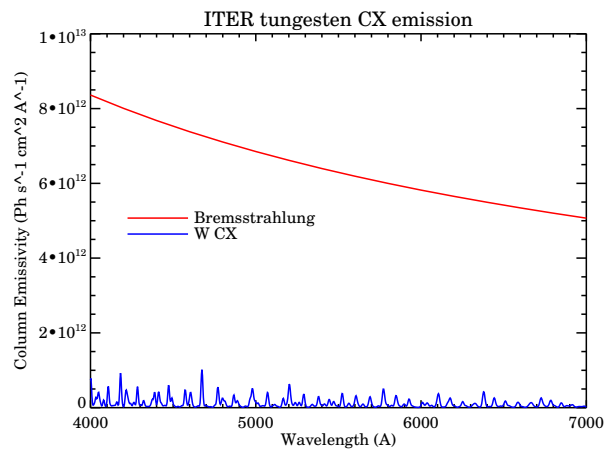


Figure C.4: The predicted line integrated tungsten charge exchange and Bremsstrahlung emission for a vertical chord on ITER viewing the diagnostic neutral beam through the core of the plasma. Again, as for MAST Upgrade the CX emission is found to be a significant fraction of the background.