

Hugh Summers, Nigel Badnell, Martin O'Mullane, Francisco Guzmán, Luis Menchero and
Alessandra Giunta

Review 2

8 Feb 2012

Workpackages : 26-5-2, 27-1*, 27-2*, 28-1*, 28-2*
Category : DRAFT

This document has been prepared as part of the ADAS-EU Project. It is subject to change without notice. Please contact the authors before referencing it in peer-reviewed literature.
© Copyright, The ADAS Project.

Review 2

Hugh Summers, Nigel Badnell, Martin O'Mullane, Francisco Guzmán, Luis Menchero and
Alessandra Giunta

Department of Physics, University of Strathclyde, Glasgow, UK

Abstract: *Review of reporting period: months 19-36*

Contents

1	Overview	3
1.1	Staffing	5
1.2	Computation	5
1.3	Forward planning	6
1.4	Finances	7
1.5	Publications	7
1.6	Reports	7
A	Reports	11
A.1	Reports: SCIENCE4, SCIENCE5, SCIENCE6	13
A.2	Report: OPEN2	21
A.3	Report: SETUP3	23
A.4	Report: DISSEM2	25
A.5	Report: ECWP1, SUBC1, ITER1	29
A.6	Reports in development: PUBL1, PUBL2, PUBL3, PUBL4, PUBL5, PUBL6	37
B	ADAS/ADAS-EU computing equipment review and status	61

-

Chapter 1

Overview

In this middle period of the ADAS-EU project, the broad objectives for the period have largely been met. The international fusion programme, nonetheless, evolves and the specific needs from atomic physics modelling change and evolve with this. In particular, the momentum build-up with ITER is of note and its need for early support in the conceptual design phase for spectroscopic diagnostics. ADAS-EU was specifically mandated to support ITER and the European contribution to it, and has responded strongly to these needs. Dr. O'Mullane has carried almost the entire burden of this support, with frequent visits to the ITER site in France and direct participation in conceptual design reviews (see report DISSEM2 and the summaries therein, also the individual person entries in the six-monthly science reports SCIENCE4, SCIENCE5 and SCIENCE6). Another feature of the evolving European scene, has been the forming up into group projects, such as the Integrated Tokamak Modelling activity (ITM) under FP7, with participation of many European universities and laboratories from both the West and East of Europe. Then ADAS-EU support and point of contact has optimally been to ITM rather than to each university/laboratory separately. ADAS-EU has again responded in this middle period.

Another main part of dissemination is the ADAS-EU Courses. These were planned as annual events, linked in time and location to the ADAS Workshop. In 2010, the ADAS Workshop was held at Armagh Observatory in Northern Ireland, recognising ADAS connection with both fusion and astrophysics. It was then convenient to hold the 2nd ADAS-EU Course, scheduled for November 2010 within this reporting period, at EFDA-JET. A complexity has been the popularity of the ADAS training courses, but coupled to a wish to have them not only in Europe and also to have versions of them tuned to specific local interest. This is in spite of the fact that the ADAS-EU course, as originally mandated, did allow for participation by any ADAS sponsored participant - not just European. A version of the ADAS-EU course, called ADAS-US and unfunded by ADAS-EU, was held at Auburn University, Alabama in July 2010. Then in 2011, the ADAS Workshop was held at Auburn University, Alabama, recognising the increasingly international nature of ADAS. The spin-off course ADAS-US was therefore held again at Auburn in October 2011. In the light of the paragraph below on academic underpinning of ADAS-EU, ADAS/ADAS-EU staff were very willing to contribute in this way. ITER Organisation was also enthusiastic to have a local, tailored version of the course. The ADAS-EU-ITER course was held at Cadarache in December 2010. The main ADAS-EU course for 2011, also within this reporting period, was planned to be held at RFX Padua in December 2011, but machine operations and consequent availability of RFX staff and resources induced a change of date to March 2012, falling outside this reporting period. The fourth and last of the ADAS-EU courses will be held also in 2012, in September along with the 17th ADAS Workshop at Cadarache. Details of these dissemination activities are in report DISSEM2.

The academic atomic physics underpinning of ADAS-EU, that is the production and making available of responsive fundamental atomic reaction cross-section data to feed into current plasma atomic models and spectroscopic diagnostic analysis, relies on the university academic activities of Professors Summers and Badnell, outwith their time commitment to ADAS-EU. Badnell guides an international group of co-working scientists calculating key atomic reactions, which is probably the most productive in the world at this time. Loch, Ballance, Pindzola and Griffin at Auburn University, USA and Liang of Strathclyde University and the National Astronomical Observatories Beijing China deserve special mention. These data flow into the ADAS databases and thence into the ADAS-EU support action. The last eighteen months has been an outstanding period, with penetration into the most difficult atomic cases, such as tungsten for ITER, JET and AUG, as well as large scale production for simpler general systems. Summers, in

the more applied atomic physics territory covered by ADAS, has guided the PhD work of Giunta and Nicholas, which completed in this period. Nicholas built and completed the advanced special feature spectroscopic analysis capability which has been provided for ADAS/ADAS-EU and is one of the main themes of ADAS-EU. Report PUBL2 is in essence the thesis of Nicholas. Giunta worked in the solar astrophysical area, analysing spectral measurements from the chromosphere/corona. A core part of Giunta work was the extended construction of the generalised-collisional-radiative (GCR) model for medium weight elements. Report PUBL5 is in essence the thesis of Giunta. Dr. Giunta has now joined the ADAS-EU/ADAS team (see section 1.1). This work, also supported by Badnell, is key to current fusion needs for highest quality modelling for species, such as argon and the iron group, and feeds directly into ADAS/ADAS-EU. The medium-weight element GCR work is on-going and a substantial and important extension to ADAS-EU theme 1. For this the new work packages 27-1 (level 1 and 2 AUTOSTRUCTURE/distorted wave, called AS/DW, collisional rate inclusion in ADAS), 27-2 (level 1 and 2 AS/DW mass data production), 28-1 (level 1 and 2 GCR ionisation) and 28-2 (level 1 and 2 GCR recombination) have been added to the ADAS-EU Project.

The OPEN-ADAS web site, which is the pathway for public domain release of data from ADAS-EU has proved very popular. There has been a very large number of users and downloads (The website is <http://open.adas.ac.uk>). A considerable problem occurred in mid-2011, when the OPEN-ADAS website was attacked and damaged by the frivolous actions of the so-called LutzSec group. This pointless exercise, since OPEN-ADAS is open, compromised user sign-in information and usage statistics. OPEN-ADAS had to be taken off-line for about two months for protective re-coding. This unexpected and arduous task was handled by Dr. O'Mullane in the absence of Dr. Whiteford - the original programmer. OPEN-ADAS is back in action, but without the sign-in and statistics aspects which were there before. Nonetheless, indications are that OPEN-ADAS remains very popular and is now seen as an essential resource world-wide. See report OPEN2 for further details.

As discussed in the previous review, a problem was created for implementation of some of the ADAS-EU plans by the unexpected, early departure of Dr. Alan Whiteford from the project. Dr. Whiteford was the intended person to direct the Electron Collision Working Party (ECWP). This activity was designed to assist and enable paths of communication between theoretical/computational atomic physicists calculating electron impact collisional cross-section data and the utilisation framework of ADAS-EU and ADAS. In October 2010, Professor Badnell of Strathclyde University, one of the leading such theorists in world, was freed up enough to assign 20% of his time to ADAS-EU and bring into play the ECWP. An extra report ECWP1 summarises its activity over the present reporting period. It is noted here, that Badnell was able to coordinate substantial efforts on some of the most difficult cases in fusion, such as the ion W^{+20} , and to engage deeply with sub-contractors of ADAS-EU in the electron collision area. This has optimised benefit from sub-contractors. But particularly, Badnell and the ECWP have succeeded in breaking down some of these difficult problems such that we feel confident that the quality of content of the ADAS electron impact databases at the end of ADAS-EU will be unparalleled. The product and scientific detail of this work will enter particularly reports PUBL3 and PUBL5.

Six out of the eight planned ADAS-EU sub-contracts were placed in the first reporting period. Five of these delivered in the second half of 2011. The sixth had an agreed termination in a partly completed state. At this point in time, two sub-contracts remain unplaced and three-quarters of a sub-contract value was retained from sub-contract six. The delay in placing the last two stems from the late starting of ECWP and because further exploitation of the special feature infrastructure at this time could not be supported. The revised residual sub-contract intentions are detailed in section 1.3 below. The quality of delivery on the sub-contracts, although later than expected, and the effectiveness and relevance of their integration into the ADAS modelling has exceeded all expectations. The extra report SUBC1 gives more detail and includes copies of the completion reports. The sub-contracts were split between the electron collision side (for ionisation, recombination and excitation) and the ion collision side (for charge exchange recombination and beam excitation). For the latter, we now have sufficient information and consistency of data to forward model as far as tungsten as an impurity species in the core of ITER, in ionisation stages as high as W^{+60} . On the electron collision side, we now can model emission of tungsten as an inflowing neutral W^0 , as a divertor species, such as W^{+20} and as a core species, such as W^{+44} .

The detailed reports due at this time have been assembled and are available as separate documents (see section 1.6). The titles and front pages are included in appendices for information. Attention is drawn to the PUBL series of reports. These contain the full scientific and computational application details of the main themes of ADAS-EU and are due for completion and publication towards the end of the ADAS-EU project. They are works 'in progress'. As a scientific work package item and its background theory are completed, the appropriate chapters and sections are written up in the relevant PUBL. They are available to the scrutinisers and the Governance Committee of ADAS-EU but should not be released further at this stage. Reference is made in the SCIENCE reports to sections of the PUBL documents which

may be helpful or clarifying. It is noted that the work of ADAS-EU theme 5, which has proved more substantial than originally expected, now has its own summative science and computational document PUBL6.

1.1 Staffing

As noted in REVIEW1, an emergency increase of assigned time to 40% FTE by Professor Summers was made from 1 Nov 2009, following the resignation of Dr. Whiteford. Also Dr. O'Mullane increased his time to 30% FTE. On 1 Oct 2010, Professor Summers reduced his assigned time to 20% and simultaneously Professor Badnell joined the ADAS-EU team at 20% FTE. Professor Badnell is based at the Department of Physics, University of Strathclyde and took over the direction of the ECWP.

On 1 Jan 2011, Professor Summers reduced his assigned time to 10% FTE and Dr O'Mullane increased his assigned time to 40%. This restored Professor Summers to the originally planned assignment of time in the late stages of ADAS-EU. Dr. O'Mullane has in effect now taken over the role of Dr. Whiteford.

A further year having elapsed, it was decided to seek to appoint another postdoctoral scientist on a two-year contract from 1 July 2011, the post to be funded 30% FTE from ADAS-EU and 70% by the ADAS project. The 30% from ADAS-EU comprises the 7 months of lost postdoctoral scientific input identified in REVIEW1 and will be used in the period up to 31 Dec. 2012. The position specification had both fusion and astrophysical components matching the funding ratio between ADAS-EU and ADAS and the ADAS obligations to both fusion and astrophysics.

The position was advertised. Details of the appointment processes and procedures are given in the report SETUP3. The quality of candidature for the position was outstanding. Two candidates were deemed appointable. The highest placed candidate, Dr. Alessandra Giunta, was offered and accepted the position. Her appointment dates from 1 Jul. 2011 as planned. Dr Giunta brings ideal talents to the project, already having connections with the MAST SuperX divertor planning team at CCFE Culham Laboratory. Dr Giunta will spend two days per week at Culham Laboratory and three days at Rutherford Appleton Laboratory.

With the postdoctoral positions now all filled, ADAS-EU has post-doctoral staff in place at IPP Garching, CEA Cadarache/ITER and CCFE Culham Laboratory/EFDA-JET.

1.2 Computation

The ADAS-EU project plan budgetted for a number of items of computer support equipment.

Laptops for the ADAS-EU postdoctoral staff, of sufficient power to carry the complete ADAS system, were required. These have allowed the ADAS-EU staff to function most effectively in their support and demonstration roles when visiting remote sites. Four machines were purchased in the last reporting period, but a fifth, along with necessary software, was purchased in the present period for Dr. Giunta. These machines individually came in below expected cost, so that the five machines (rather than the four originally expected) were within the budgetted limits.

Fixed servers, located and maintained at the Department of Physics, Strathclyde University, supply the web services, OPEN-ADAS and ADAS, provide the primary SVN and CVS archives of ADAS-EU and ADAS, and backup. The replacement and upgrading of these machines was anticipated as part of ADAS-EU and expected to be necessary at some point in the four year duration of ADAS-EU. Machine failure commenced in 2011, with lack of sufficient protective backup occurring in late 2011. The replacement plan was then put in motion. Also in late 2011, results on the more complex of the atomic physics background research tasks (this is funded independently of ADAS-EU) put into play as part of the ADAS-EU themes came to fruition. Especially, the influx studies for W^0 , the dielectronic studies for medium-charge heavy ions such as W^{+20} , and the needs of advanced collisional-radiative modelling for heavy ion charge exchange with beams and for diatomic molecules (H_2 and H_2^+) identified a problem. This is the need for a moderate power machine, but of very large memory assigned to each processor to pilot advanced models, in advance of their finalising and organising for massively parallel computer systems (but typically of modest attached memory per processor). It was decided in late 2011 that the requirements could be met by three moderate power, large backing store, machines as servers and one high capacity machine for pilot calculations. The details of the new

ADAS-EU/ADAS provision is detailed appendix A. The cost of the high capacity machine and the set of three servers were about equal and divided between ADAS-EU and ADAS consistent with the equipment plan and assigned budget of ADAS-EU.

It was noted in the overview that hacking caused problems for OPEN-ADAS and waste of staff time in 2011. It is also noted that the electrical services to the Department of Physics have been subject to unplanned interruptions and to voltage swings which trigger resets. These appear to be a feature of Scottish Power services at this time. Such unforwarned events can and do damage disk systems and were contributory to the failures discussed above. The new systems will be held in a rack system in a more protected environment, with central University backup (see appendix B).

1.3 Forward planning

From a scientific point of view, the main objective of the final period of ADAS-EU through to the end of 2012, is the summative developments of the main themes. This will be the scientific legacy of ADAS-EU which will be the completed documents PUBL1 - PUBL6 and the incorporation of their methods and results as codes and data within ADAS. On charge exchange with beams (PUBL1), we are confident that the fundamental database will be complete and at the precision levels needed for all current fusion devices and ITER through to its end. The completion of the derived, effective data for arbitrarily heavy species of receiver charge $> \sim 18$ requires the incorporation of the bundle-nl population model, driven by *adf42*. This task, to be completed by Summers, will follow the pattern of inclusion of the bundle-n model and difficulties are not anticipated. In essence, we believe that the theoretical inputs for all beam charge exchange spectroscopy will be available and complete by the end of ADAS-EU.

Theme 2, on special features and spectral analysis is complete from the point-of-view of the infra-structure. The creation of theoretical special feature constructs in ADAS for its exploitation is open-ended. The finishing point for ADAS-EU will be the complete driver data sets for the He-like/Li-like dielectronic satellite line special feature. We are in a position to produce these routinely now, but the raw theoretical model and data needs to be refined with precision wavelengths for experimental spectroscopy. In the the final period, this modest completion and update should be done.

Theme 3 on heavy species went forward quickly and well, largely due to the efforts and PhD. work of Adam Foster. The last part of this theme was again, the open-ended lifting of the database from baseline, where possible, to so-called precision levels 1 and 2. In this respect, we have greatly exceeded expectations in finding convincing paths into the most difficult systems. In parallel with this and to somewhat less heavy systems, Alessandra Giunta has moved generalised-collisional-radiative (GCR) modelling forward strongly. Thus we can now envisage carrying this high precision modelling up to an beyond the iron period elements. Because of this, GCR has become a theme in its own right and PUBL5 added to the list of summative documents. These areas are tied closely to the activities of the Electron Collision Working Party (ECWP) and it is the ECWP which we really envisage growing and taking over from ADAS-EU after the end of 2012. ADAS-EU will leave the infrastructure for fusion and ECWP will refine it and connect it also with the infrastructure for astrophysical atomic analysis. Atomic physics for fusion and astrophysics should not be two separate things, but united following the philosophy of ADAS and its origins.

Development of theme 4 was initially led by Summers and Henderson, but was then taken over by Menchero when he moved into post for ADAS-EU. The theme was broadened by Summers and Henderson to cover the situation of mixed magnetic and electric fields rather than only a motional-Stark electric field. There is justification for this in the abiguities of experiment with respect to residual circular polarisation and meaningful observables. Menchero continued in this direction, but has exposed the limitations of perturbation theory (taken to 2nd order in the Stark field), especially if field ionisation rates are to be obtained at typical fusion neutral beam speeds. Menchero is following the complex variable approach to obtaining an eigenstate basis for beam modelling. We shall continue forward in this direction with the theme, but it is a substantial task which we do not expect to be completed until the end of ADAS-EU.

The molecular theme, PUBL6, has been a much larger task than anticipated and is still further delayed from the estimate of REVIEW1. Completion of the reaction sets, filling the many gaps, was a slow process. Guzmán, leading this part, was also engaged with experiment plans at CEA Cadarache - a good and appropriate activity in ADAS-EU support terms. This has meant that the molecular collisional-radiative model is not yet in place, with the working

version now expected around June 2012. This meant that the planned month's support by Prof. Janev of the molecular modelling could not be justified for 2011. This is now re-scheduled for the second half of 2012.

The completion of themes 4 and 6 and the associated PUBL4 and PUBL6 is now a priority. If residual staff funds remain in the last half-year of ADAS-EU, it may be appropriate for Summers to increase his ADAS-EU time from the current 10% to assist in these completions.

It is planned to reassign the remaining 2.75 of sub-contract monies, responding to the success of the completed sub-contracts and the opportunities created by some of them for extensions. These extension will exploit the methods previously developed and give very high return in database growth to ADAS. Thus it is planned to give extension contracts to ITPA, University of Vilnius and to Department of Physics, University of Mons-Hainaut. The plan, but delayed, sub-contract with Queen's University, Belfast will be put in place and target high power supercomputer R-matrix calculations of the tungsten ions identified earlier in this report. Provided these sub-contacts are in place by the end of February 2012, completion in time for incorporation in the ADAS-EU PUBL series and the ADAS databases will be possible.

1.4 Finances

1.5 Publications

Publications in this period connected to ADAS-EU include works by Badnell ([1],[2], [3]), Giunta ([4], [5],[3]), Guzman ([6], [7], [8], [3]), Menchero ([3]), O'Mullane([9], [10], [11], [1], [12], [13], [14], [15], [16], [17], [18],[19], [3]) and Summers ([1], [5], [17], [10], [19], [3]). The references are to the bibliography of this review on pages 9 and 10. There are nineteen independent titles. Several of these publications have shared authorship

1.6 Reports

Reports available for release at this time comprise:

- SCIENCE4, SCIENCE5, SCIENCE6 (see Appendix A.1)
- OPEN2 (see Appendix A.2)
- SETUP3 (see Appendix A.3)
- DISSEM2 (see Appendix A.4)
- ECWP1, SUBC1, ITER1 (see Appendix A.5)

Reports in preparation, not for release at this time, comprise:

- PUBL1, PUBL2, PUBL3, PUBL4, PUBL5, PUBL6 (see Appendix A.6)

The frontispiece and contents pages only of the reports are given in the appendices. The full reports will placed on the ADAS-EU web site (www.adas-fusion.eu).

-

Bibliography

- [1] N. R. Badnell, A. Foster, D. C. Griffin, D. Kilbane, M. O'Mullane and H. P. Summers. 'Dielectronic recombination of heavy species: the tin $4p^64d^q - 4p^64d^{(q-1)}4f + 4p^54d^{(q+1)}$ transition arrays for $q = 1 - 10$ '. *J. Phys. B*, **44** (2011) 135201. doi:[10.1088/0953-4075/44/13/135201](https://doi.org/10.1088/0953-4075/44/13/135201)
- [2] N. R. Badnell. 'A Breit-Pauli distorted wave implementation for AUTOSTRUCTURE'. *Comput. Phys. Commun.*, **182**(7) (2011) 1528–1535. doi:[10.1016/j.cpc.2011.03.023](https://doi.org/10.1016/j.cpc.2011.03.023)
- [3] H. Summers, N. R. Badnell, A. R. Foster, F. Guzmán, L. Menchero, C. H. Nicholas, M. G. O'Mullane, A. D. Whiteford, A. Meigs and JET-EFDA Contributors. 'Modelling spectral emission from fusion plasma'. *AIP Conf. Proc. ATOMIC PROCESSES IN PLASMAS: Proceedings of the 17th International Conference on Atomic Processes in Plasmas*, **1438** (2012) –in press
- [4] M. M. Bisi, A. R. Breen, B. V. Jackson, R. A. Fallows, A. P. Walsh, Z. Miki, P. Riley, C. J. Owen, A. Gonzalez-Esparza, E. Aguilar-Rodriguez, H. Morgan, E. A. Jensen, A. G. Wood, M. J. Owens, M. Tokumaru, P. K. Manoharan, I. V. Chashei, A. S. Giunta, J. A. Linker, V. I. Shishov, S. A. Tyulbashev, G. Agalya, S. K. Glubokova, M. S. Hamilton, K. Fujiki, P. P. Hick, J. M. Clover and B. Pintér. 'From the Sun to the Earth: The 13 May 2005 Coronal Mass Ejection, 2010'. *Solar Physics*, **265**(1) (2010) 49–127. doi:[10.1007/s11207-010-9602-8](https://doi.org/10.1007/s11207-010-9602-8)
- [5] A. S. Giunta, A. Fludra, M. G. O'Mullane and H. P. Summers. 'Comparison between observed and theoretical O iv line ratios in the UV/EUV solar spectrum as derived by SUMER, CDS and EIS'. *Astron. Astrophys.*, **538** (2012) A88. doi:[10.1051/0004-6361/201118178](https://doi.org/10.1051/0004-6361/201118178)
- [6] F. L. Tabarés, D. Tafalla, J. A. Ferreira and F. Guzmán. 'Frequency-fluctuation model for line-shape calculations in plasma spectroscopy'. *Rev. Sci. Instrum.*, **81** (2010) 10D708. doi:[10.1063/1.3464462](https://doi.org/10.1063/1.3464462)
- [7] P. Barragán, L. F. Errea, F. Guzmán, L. Méndez, I. Rabadán and I. Ben-Itzhak. 'Resonances in electron-capture total cross sections for C4+ and B5+ collisions with H(1s)'. *Phys. Rev. A*, **81** (2010) 062712. doi:[10.1103/PhysRevA.81.062712](https://doi.org/10.1103/PhysRevA.81.062712)
- [8] F. Guzmán, L. F. Errea, C. Illescas, L. Méndez and B. Pons. 'Calculation of total cross sections and effective emission coefficients for B 5 + collisions with ground-state and excited hydrogen'. *J. Phys. B*, **43**(14) (2010) 144007. doi:[10.1088/0953-4075/43/14/144007](https://doi.org/10.1088/0953-4075/43/14/144007)
- [9] C. Guillemaut, R. Pitts, A. Kukushkin and M. O'Mullane. 'Radiative power loading in the ITER divertor'. *Fusion Engineering and Design*, **86**(12) (2011) 2954 – 2964. doi:[10.1016/j.fusengdes.2011.07.008](https://doi.org/10.1016/j.fusengdes.2011.07.008)
- [10] J. D. Strachan, G. Corrigan, D. Harting, L. Lauro-Taroni, C. F. Maggi, G. F. Matthews, M. O'Mullane, D. Reiter, J. Seebacher, J. Spence, H. Summers, S. Wiesen and J.-E. Contributors. 'EDGE2D comparisons of JET tungsten and carbon screening'. *J. Nucl. Mater.*, **415**(1) (2011) S501–S504. doi:[10.1016/j.jnucmat.2010.08.028](https://doi.org/10.1016/j.jnucmat.2010.08.028)
- [11] S. Brezinsek, S. Jachmich, J. Rapp, A. G. Meigs, C. Nicholas, M. O'Mullane, A. Pospieszczyk, G. van Rooij and J.-E. contributors. 'Impact of Nitrogen Seeding on Carbon Erosion in the JET Divertor'. *J. Nucl. Mater.*, **417** (2011) 624–628. doi:[10.1016/j.jnucmat.2010.12.097](https://doi.org/10.1016/j.jnucmat.2010.12.097)
- [12] G. Telesca, R. Zagorski, S. Brezinsek, W. Fundamenski, C. Giroud, G. Maddison, M. O'Mullane, J. Rapp, M. Stamp, G. V. Oost and JET EFDA contributors. 'Simulation with the COREDIV code of nitrogen-seeded H-mode discharges at JET'. *Plasma Phys. Control. Fusion*, **53** (2011) 115002. doi:[10.1088/0741-3335/53/11/115002](https://doi.org/10.1088/0741-3335/53/11/115002)

- [13] T. W. Versloot, P. C. de Vries, C. Giroud, M. Brix, M. G. von Hellermann, P. J. Lomas, D. Moulton, M. O'Mullane, I. M. Nunes, A. Salmi, T. Tala, I. Voitsekhovitch, K.-D. Zastrow and JET-EFDA Contributors. 'Momentum losses by charge exchange with neutral particles in H-mode discharges at JET'. *Plasma Physics and Controlled Fusion*, **53** (2011) 065017. doi:10.1088/0741-3335/53/6/065017
- [14] K. D. Lawson, K. M. Aggarwal, I. H. Coffey, F. P. Keenan, M. G. O'Mullane, L. Ryc, J. Zacks and JET-EFDA Contributors. 'An analysis of VUV C IV emission from the JET divertor giving measurements of electron temperatures'. *Plasma Phys. Control. Fusion*, **53** (2011) 015002. doi:10.1088/0741-3335/53/1/015002
- [15] A. Czarnecka, K.-D. Zastrow, J. Rzakiewicz, I. H. Coffey, K. D. Lawson, M. G. O'Mullane and JET-EFDA Contributors. 'Determination of metal impurity density, ΔZ_{eff} and dilution on JET by VUV emission spectroscopy'. *Plasma Phys. Control. Fusion*, **53**(3) (2011) 035009. doi:10.1088/0741-3335/53/3/035009
- [16] E. Delabie, M. Brix, C. Giroud, R. J. E. Jaspers, O. Marchuk, M. G. O'Mullane, Y. Ralchenko, E. Surrey, M. G. von Hellermann, K.-D. Zastrow and JET-EFDA Contributors. 'Consistency of atomic data for the interpretation of beam emission spectra'. *Plasma Phys. Control. Fusion*, **52**(3) (2010) 125008. doi:10.1088/0741-3335/52/12/125008
- [17] T. Pütterich, R. Neu, R. Dux, A. Whiteford, M. O'Mullane, H. Summers and the ASDEX Upgrade Team. 'Calculation and experimental test of the cooling factor of tungsten'. *Nucl. Fusion*, **50**(2) (2010) 025012. doi:10.1088/0029-5515/50/2/025012
- [18] K. W. Hill, M. Bitter, L. Delgado-Aparicio, D. Johnson, R. Feder, P. Beiersdorfer, J. Dunn, K. Morris, E. Wang, M. Reinke, Y. Podpaly, J. E. Rice, R. Barnsley, M. O'Mullane and S. G. Lee. 'Development of a spatially resolving x-ray crystal spectrometer for measurement of ion-temperature (Ti) and rotation-velocity (v) profiles in ITER'. *rsi*, **81** (2010) 10E322. doi:10.1063/1.3492414
- [19] H. P. Summers and M. G. O'Mullane. 'Atomic data and modelling for fusion: The ADAS Project'. *AIP Conf. Proc. ATOMIC AND MOLECULAR DATA AND THEIR APPLICATIONS: 7th International Conference on Atomic and Molecular Data and Their Applications (ICAMDATA-2010)*, **1344** (2011) 179–187. doi:10.1063/1.3585817

Appendix A

Reports

-

A.1 Reports: SCIENCE4, SCIENCE5, SCIENCE6

ADAS-EU R(10)SC04

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Hugh Summers, Martin O'Mullane, Francisco Guzman and Luis Menchero

Scientific progress report 4

April 13, 2012

Workpackages : 3-3, 4-1, 8-4, 9-1, 9-2, 9-3, 11-1, 26-1-4,S1, S4
Category : DRAFT

Contents

1 Overview	3
2 Individual contributions	4
2.1 Hugh Summers: Dielectronic recombination for special features and BBGP	4
2.1.1 Doubly excited states and adf04 datasets	4
2.1.2 Preparing BBGP drivers	5
2.2 Martin O'Mullane: Code developments and ITER engagements	5
2.3 Francisco Guzmán: Molecular CR modelling	5
2.3.1 Ion impact excitation data	6
2.3.2 Ar MGI time dependent model	6
2.3.3 Completion of report science_4	6
2.4 Luis Menchero: Atomic structure of beam atoms in fields	6
2.4.1 Data of ion-impact excitation adf02	6
2.4.2 Preparation of a programming code to calculate differential cross-sections	7
2.5 Nigel Badnell: Electron impact collision cross sections	7
A ADAS Theme 5 supplementary material for the report	8
B Excitation cross sections from classical and semiclassical methods in a wide energy range for the reactions	
$(\text{Li}^{3+}, \text{Ne}^{10+}, \text{Ar}^{18+}) + \text{H}(1s) \rightarrow (\text{Li}^{3+}, \text{Ne}^{10+}, \text{Ar}^{18+}) + \text{H}(n)$	14

ADAS-EU R(10)SC05

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Hugh Summers, Martin O'Mullane, Francisco Guzman and Luis Fernández-Menchero

Scientific progress report 5

February 3, 2012

Workpackages :
Category : DRAFT

Contents

1	Overview	3
2	Individual contributions	4
2.1	Luis Fernández-Mencheró: Atomic structure of beam atoms in fields	4
2.1.1	Study of Stark effect in terms of perturbation theory	4
2.1.2	Improvement of the FORTRAN routine fldizn	4
2.1.3	Programming of the ADAS305a package in FORTRAN	5
2.1.4	Conclusions	5
2.1.5	Future work	5
2.2	Hugh Summers: Continued BBGP development and Culham SuperX studies	5
2.2.1	BBGP development	5
2.2.2	Culham SuperX studies	6
2.3	Martin O'Mullane: Code developments and ITER engagements	6
2.4	Francisco Guzmán: Molecular CR modelling	6
2.4.1	Advances in Molecular CR modelling	6
2.4.2	Ion impact atomic data	7
2.4.3	TORE SUPRA Ar experiment	7
2.4.4	ITER collaborations	7
2.4.5	Recall to JET	8
2.5	Alessandra Giunta: GCR studies	8
2.6	Nigel Badnell: Electron impact collision cross sections	8
3	Work package reports	9
3.1	Work package 8-1	9
3.2	Work package 10-1	9
3.3	Work package 10-2	9

ADAS-EU R(10)SC06

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Hugh Summers, Martin O'Mullane, Francisco Guzman, Luis Menchero and Alessandra Giunta

Scientific progress report 6

/today

Workpackages : 8-2, 8-3, 15-1, 15-2, 16-1, 16-2, 16-3, 26-1-6
Category : DRAFT

Contents

1 Overview	2
2 Individual contributions	3
2.1 Alessandra Giunta: GCR studies	3
2.1.1 Spectral analysis of the solar atmosphere	3
2.1.2 Oxygen analysis	4
2.1.3 GCR developments	4
2.1.4 Transient ionisation in the solar atmosphere	4
2.1.5 MAST Super-X divertor modelling	5
2.2 Hugh Summers: Raising the ADAS GCR baseline to level 1 for medium weight elements	5
2.2.1 Feature emissivities for SANCO and EDGE2D transport codes	5
2.2.2 ADAS database raising to level 1	6
2.2.3 adf04 type conversion	7
2.3 Martin O'Mullane: Code developments and ITER engagements	7
2.4 Francisco Guzmán: Molecular CR modelling	7
2.4.1 ADAS molecular CR modelling time scales generation tool	7
2.4.2 ADAS molecular CR modelling stage 3: adding new data	8
2.4.3 ADAS molecular CR modelling stage 4: population model and CR coefficients	8
2.4.4 Ion impact atomic data	9
2.4.5 ITM collaboration	9
2.5 Luis Menchero: Atomic structure of beam atoms in fields	9
2.6 Nigel Badnell: Electron impact collision cross sections	9
A ADAS data formats	10
B PSI 2012 conference submitted abstract	17

C Seminar on MATLAB version of CHEAP code given on November 2011	20
D Experimental quality assessment of Ar CX density profiles	56
E ADAS-EU travel report: ITM workshop Cyprus 3-13 October	64

-

A.2 Report: OPEN2

ADAS-EU R(12)OP02

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Hugh Summers, Martin O'Mullane, Francisco Guzman and Luis Menchero

OPEN-ADAS report 2

February 2012

Workpackages : 26-2-2
Category : PU

Contents

1 Overview	3
2 Work package reports	5
2.1 Work package 26-2-1	5

A.3 Report: SETUP3

ADAS-EU R(12)SE03

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Hugh Summers, Nigel Badnell, Martin O'Mullane, Francisco Guzmán, Luis Menchero and
Alessandra Giunta

ADAS-EU setup report 3

8 February 2012

Workpackages : 22-1-3, 22-2-3, 23-1-3, 23-2-3, 24-1, 25-1-3, 25-2-3, 26-3-3, S1, S5, S7
Category : DRAFT

Contents

A.4 Report: DISSEM2

ADAS-EU R(11)DI02

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Hugh Summers, Martin O'Mullane, Francisco Guzman and Luis Menchero

Dissemination report 2

January 27, 2012

Workpackages : 20-1-2, 20-2-2, 21-1-2, 21-2-2, 26-4-2
Category : DRAFT

Contents

- 1 Overview and milestones DSM2** **3**

- 2 Work package reports** **5**
 - 2.1 Work packages 20-1-2 and 20-2-2 5
 - 2.2 Work package 21-1-2 and 21-2-2 5
 - 2.3 Work package 26-4-2 6

- A ADAS data formats** **7**

Preface

The report is the second of a series of three such reports, deliverable under the ADAS-EU project, which summarise dissemination of ADAS capabilities during the period.

H P Summers
January 27, 2012

-

A.5 Report: ECWP1, SUBC1, ITER1

ADAS-EU R(12)SU01

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Hugh Summers, Nigel Badnell, Martin O'Mullane, Francisco Guzman,
Luis Menchero and Alessandra Giunta

ECWP1: Electron Collision Working Party Report 1

20 Jan 2012

Workpackages : ??-??-??
Category : DRAFT – CONFIDENTIAL

Contents

1	Introduction	2
2	Review of progress 2011	3
A	Electron impact data initiative	4
A.1	Electron impact data generation and exploitation for fusion and ITER: Proposal: 8 Sept 2010	4
A.2	Planning Meeting: Queen's Belfast: 10.00am Wed 6 Oct. 2010	6
A.3	Draft Working Document for 2nd ECWP meeting: EFDA-JET Facility: 12 April 2011	7

ADAS-EU R(12)SU01

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Hugh Summers, Nigel Badnell, Martin O'Mullane, Francisco Guzman,
Luis Menchero and Alessandra Giunta

**SUBC1: Sub-contract specifications, deliverables,
integration and analysis**

18 Jan 2012

Workpackages : ??-??-??
Category : DRAFT – CONFIDENTIAL

Contents

1	Introduction	3
2	Influx of low ionisation stages of tungsten	6
2.1	Background	6
2.2	Atomic structure calculations in W, W ⁺ and W ⁺² ions	6
2.3	Integration of W I-III data into ADAS	7
2.4	Perspectives and recommendations	7
2.5	References	7
3	Electron-ion recombination and electron-ion impact ionisation of many-electron atomic ions	9
3.1	Background	9
3.2	Electron impact ionization of many-electron ions up to high charge states	9
3.3	Recombination of many-electron ions with electrons	11
3.4	References	14
4	Atomic structure and electron data for heavy element ions	16
4.1	Introduction	16
4.2	Electron-impact excitation of tungsten ions	17
4.2.1	Energy spectra calculation in quasirelativistic approach	17
4.2.2	Electron-impact excitation of ions	18
4.3	Peculiarities of spectroscopic properties of W ⁺⁸	24
4.3.1	Theory	24
4.3.2	Large scale calculations	24
4.4	Multiple ionization of tungsten ions	28
4.4.1	Multiple electron ionisation rate coefficients, with special emphasis on 4d, 4f and 5d, 5f open-shell systems	28

ADAS-EU R(12)SU03

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Martin O'Mullane

**ITER1: ITER visits and support activities
Report 1**

10 Feb 2012

Workpackages : 2-3 and 3-4
Category : DRAFT – CONFIDENTIAL

Contents

1	Overview	3
2	ITER plasma scenarios	4
2.1	Magnetic geometry and background plasma profiles	4
2.2	Impurity transport model	5
2.3	Transport coefficients adopted for the simulations	6
2.4	Sensitivity of emission model to transport	7
2.5	Plasma models of SOL and divertor	8
3	Edge VUV Imaging	10
3.1	Instrument and wavelength range	10
3.2	Emission predictions	10
4	VUV core survey spectrometer	15
4.1	Instrument	15
4.2	Possible emission lines	16
5	VUV divertor survey spectrometer	17
5.1	Instrument	17
5.2	Synthetic spectra	18
6	Upper port X-ray spectrometer	20
6.1	Instrument and lines of sight	20
6.2	Tungsten emission line in X-ray region	21
7	H-α (and visible spectroscopy) viewing system	24
7.1	Instrument	24
7.2	Fuel and impurity emission	25

-

A.6 Reports in development: PUBL1, PUBL2, PUBL3, PUBL4, PUBL5, PUBL6

ADAS-EU R(10)PU01

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Adam Foster, Martin O'Mullane and Hugh Summers

Charge exchange spectroscopy for fusion plasmas

17 June 2010

Workpackages : 2.34
Category : DRAFT

Contents

1	Introduction	4
2	Collision-radiative modelling environments	6
2.1	The n-shell redistributive/cascade model	9
2.1.1	Effective emission coefficients	10
2.1.2	Average emission measure and spectral analysis	10
2.2	Extending the model scope	10
2.2.1	The bundle-n model	10
2.2.2	The bundle-nl model	11
2.3	Condensation, projection and inversion for advanced charge exchange modelling	11
3	Extending the fundamental charge exchange cross-section calculations	12
3.1	Comparison of methods	12
3.2	State selective ion impact cross-sections	12
3.3	Lifting the ADAS fundamental charge exchange cross-section database	12
4	A universal baseline of fundamental charge exchange data	13
4.1	The scaled total cross-section, $\bar{\sigma}_{tot}(\epsilon)$	14
4.2	The scaled n-shell resolved cross-section, $\bar{\sigma}_v(\epsilon)$	17
4.3	The scaled nl-shell resolved cross-section, $\bar{\sigma}_{v,l}(\epsilon)$	18
4.4	The code adas315 and formats adf49, adf01	18
4.5	The code adas316 and formats adf12, adf25 and adf26	19
5	ADAS codes and data formats for level 1 and level 2 modelling	29
A	ADAS data formats	30
A.1	<i>adf00</i> : configurations and ionisation potentials	30
A.2	<i>adf01</i> : bundle-n and bundle-nl charge exchange cross-sections	33

B IDL procedures	38
C FORTRAN subroutines	39
D Shell scripts	40

-

ADAS-EU R(10)PU02

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Christopher Nicholas, Hugh Summers and Martin O'Mullane

PUBL2: Special features and spectral analysis for fusion plasmas

22 Jun 2010

Workpackages : 26-6-1
Category : DRAFT

Contents

1 Introduction	3
1.1 Existing Analysis Systems	6
1.1.1 Package for Interactive Analysis of Line Emission (PINTofALE)	6
1.1.2 Charge Exchange Spectroscopy Fitting (CXSFIT)	6
1.1.3 CHIANTI Atomic Database	6
1.1.4 Atomic Data Analysis Structure (ADAS)	6
1.1.5 Object-oriented modelling for numerical fitting	7
1.2 Improving on Existing Software	7
1.3 Temperature and Density Measurement in the Divertor	8
1.3.1 Langmuir Probes	8
1.3.2 Balmer Series	8
2 Special Feature Modelling for Nuclear Fusion	9
2.1 Introduction	9
2.2 Population Modelling	9
2.2.1 The Orientation Problem	10
2.2.2 Thermal Emission and Resolution	13
2.3 Helium-like soft x-ray resonance and satellite lines	14
2.3.1 The population calculations	16
2.3.2 Electron-impact rate coefficients	18
2.3.3 Computational details	21
2.4 The background continuum	21
2.5 Primary special features for consideration	22
2.5.1 Heavy Species Envelope Emission	22
2.5.2 Motional Stark Multiplet Features of H and D Beams	22
2.5.3 Stark Broadening and Series Limits: Balmer and Paschen series	24
2.5.4 Helium-like Soft X-ray Resonance and Satellite Line Regions	25
2.6 Charge Exchange Spectra (Carbon, Helium/Beryllium ?)	26
3 ADAS Special Feature Application Programming Interface	27
3.1 ADAS Feature Generator (AFG)	27

3.2	ADAS605 — GUI to AFG	33
4	Combinations of functions for Spectral Fitting	39
4.1	Introduction	40
4.2	Functions considered	40
4.2.1	Un-broadened line	40
4.2.2	Gaussian	40
4.2.3	Doppler	41
4.2.4	Lorentzian	42
4.2.5	Voigt	43
4.2.6	Linear Background	46
4.2.7	Addition operator	46
4.2.8	Scaling (multiplication) operator	47
4.2.9	Shift operator	47
4.2.10	AFG	47
4.3	Practical Examples	48
4.3.1	Convolution of two normalized, un-shifted Gaussian functions	48
4.3.2	Convolution of N-Gaussian profile with Gaussian	49
4.4	Framework for Feature Synthesis	50
4.5	Model Definition Language	51
4.6	Parameter Coupling	53
4.7	Optimisation of the Model	57
4.8	Typical Examples for Fitting	62
4.9	Non-linear Least Squares Fitting	62
4.10	Validation of Results	64
4.11	Analytic / Numerical fitting Speed Comparison	64
5	Experimental Analysis	66
5.1	Initial Validation	66
5.2	An Illustration from SOHO-CDS	68
5.3	Divertor Detachment Experiment at JET	72
5.4	Zeeman Split Feature in JET Divertor	77
5.5	Diatomic Molecular Spectra in the JET Divertor	79
6	Conclusions	80
A	Mathematical Notes	82
A.1	Convolution; definition and basic properties	82
A.2	Area of convolved functions	82
A.3	Raw moments of convolved functions	82

A.3.1	1 st raw moment	83
A.3.2	2 nd raw moment	83
A.4	Gaussian Line Widths	84
A.5	Delta function	84
A.6	Error function	85
A.6.1	Definition	85
A.7	Complementary Error function	85
A.7.1	Definition	85
A.7.2	Derivative	86
A.8	Complex Error Function	87
A.8.1	Definition	87
A.8.2	Derivative	88

Draft

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 :

Contents

1	Introduction	4
1.1	Atomic nomenclatures	4
1.2	Population structure	6
1.2.1	Some algebra	6
1.3	Emissivities	9
1.3.1	Some more algebra	10
1.4	Primary ADAS data for heavy species	12
2	Complex atom calculations	14
2.1	Promotional rules	14
2.2	Structure, populations and emissivities	18
2.3	Automatic running and naming conventions	22
2.4	Optimised sizing for computer systems	30
3	Ionisation state of heavy elements	37
3.1	Ionisation	38
3.1.1	Parametric forms	38
3.1.2	Configuration average distorted wave ionisation	42
3.2	Recombination	46
3.2.1	Radiative recombination	47
3.2.2	Dielectronic recombination	49
3.3	Finite density heavy species collisional-radiative coefficients	53
4	Superstages and flexible partitioning	55
4.1	The natural partition and spectroscopy	59
4.2	Superstage condensation and plasma transport models	62
4.3	Generating the superstage	63

5	Lifting the baseline	66
A	ADAS data formats	71
A.1	<i>adf00</i> : configurations and ionisation potentials	71
A.2	<i>adf03</i> : recombination, ionisation and power parameters	74
A.3	<i>adf04</i> : resolved specific ion data collections	81
A.4	<i>adf07</i> : direct resolved electron impact ionis. data collections	85
A.5	<i>adf08</i> : direct resolved radiative recombination coefficients	89
A.6	<i>adf09</i> : state selective dielectronic recombination coefficients	93
A.7	<i>adf11</i> : iso-nuclear master files	104
A.8	<i>adf15</i> : photon emissivity coefficients	105
A.9	<i>adf23</i> : state selective electron impact ionisation coefficients	106
A.10	<i>adf32</i> : drivers for ADAS802 ionisation calculations	112
A.11	<i>adf34</i> : drivers for ADAS801 structure calculations	113
A.12	<i>adf40</i> : envelope feature photon emissivity coefficients	116
A.13	<i>adf42</i> : driver data sets for ADAS810 emissivity calculations	120
A.14	<i>adf46</i> : driver data sets for BBGP for dielectronic recombination	121
A.15	<i>adf48</i> : state selective radiative recombination coefficients	127
A.16	<i>adf54</i> : general promotional rule sets	128
A.17	<i>adf55</i> : general dielectronic recombination promotional rules	132
A.18	<i>adf56</i> : general ionisation promotional rules	136
B	IDL procedures	140
C	FORTRAN subroutines	183
D	Shell scripts	231

-

ADAS-EU R(10)PU04

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Luis Fernández-Menchero, Stuart Henderson and Hugh Summers

PUBL4: Neutral Beam Emission: The Motional Stark Effect

01 Feb 2012

Workpackages : 26-6-4
Category : DRAFT – CONFIDENTIAL

Contents

1	Introduction	5
1.1	Neutral Beam Characteristics	6
1.1.1	JET Positive Ion Neutral Injection	7
1.1.2	ITER Negative Ion Neutral Injection	8
1.2	Beam Emission and Spectroscopy	8
1.3	Motional Stark Effect	11
1.4	Diagnostics	12
2	Field Perturbation	14
2.1	Paschen-Back Effect	16
2.2	Fine structure	17
2.3	Zeeman Effect	17
2.4	Linear Stark Effect	18
2.5	Matrix elements of Stark perturbations	21
2.6	Polarization	22
2.7	Motional Stark Effect	22
3	Field Ionization	33
3.1	Classical Ionization Limit	33
3.2	Potential Barrier Penetration	34
3.3	Below Potential Barrier	36
3.4	Near Potential Barrier	37
3.5	Implementing Code	38
4	Exact Stark effect, the complex coordinate method	45
4.1	Inconsistencies of perturbation theory for Stark effect	45
4.2	The complex coordinate rotation	45

4.3	Method to solve the eigenvalue equations	47
4.4	The choose of a basis set	47
5	Population Modeling	50
5.1	Radiative Decay Rates	50
5.2	Cascade Effects	51
5.3	N-Shell Expansion	52
5.4	Results	52
5.5	Implementing Code	52
6	Asymmetric Cross Sections	59
6.1	Isotropic Atom	59
6.1.1	Transition Probability	60
6.1.2	Neutral Atoms	60
6.1.3	Charged Atoms	62
6.2	Asymmetric Atoms	63
6.2.1	Transition Probability	63
6.2.2	Coordinate Transformation	64
6.2.3	Cross Sections	65
6.3	Implementation	66
6.3.1	Transition Probability	66
6.3.2	Differential Cross Sections	67
6.3.3	Strong Coupling	68
6.3.4	Total Cross Sections	69
7	Summary	84
7.1	Improvements	84
7.2	Future Work	85
7.3	Conclusions	85
A	Coding	89
A.1	Adas305 Expansion	89
A.2	fldizn	90
A.3	getpn	91
A.4	gamaf1	91

-

ADAS-EU R(10)PU05

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Alessandra Giunta

**Spectral analysis of the solar atmosphere at the chromosphere-corona
boundary**

August 24, 2010

Workpackages :
Category : DRAFT

Contents

1	Introduction	1
2	Background	4
2.1	The solar upper atmosphere	4
2.2	Spectrometric and related instrumentations for the solar atmosphere	6
2.3	The behaviour of EUV helium line intensities	9
2.4	Spectral diagnostics and atomic physics	14
3	New observations	15
3.1	Missions and instrumentation	15
3.1.1	Outline of capabilities of SUMER and CDS on SoHO	15
3.1.2	Outline of capabilities of EIS on Hinode	19
3.2	Observations	21
3.2.1	Solar Joint Programme	21
3.2.2	Spatial co-alignment and cross-calibration	22
3.2.3	Profile fitting procedure	22
4	Atomic physics and data developments	23
4.1	The collisional-radiative modelling environment	25
4.1.1	Solving the collisional-radiative equations	25
4.2	Data status and the solar requirements	31
4.3	New atomic calculations	31
4.3.1	Step 1 - state selective ionisation rate coefficients	31
4.3.2	Step 2 - specific ion files for low levels	39
4.3.3	Step 3 - specific ion file supplementation with s- and r-lines	39
4.4	Comparison of data sources, methods and data precision	39

5 Revised integrated analysis	43
5.1 Differential emission measure	43
5.2 Comparative line ratios	43
5.3 On enhancement factors	43
6 Conclusions	44

-

ADAS-EU R(12)PU06

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

F. Guzmán

PUBL6: The ADAS molecular population model for fusion plasmas

1 Feb 2012

Workpackages : 26-6-6
Category : DRAFT – CONFIDENTIAL

Contents

1	Introduction	4
1.1	Molecules in plasmas	4
1.2	H ₂ System	4
1.3	Isotopic Scaling	4
2	H₂ data	5
2.1	Type of data and quality	5
2.2	Fitting formulas	5
2.3	Scaling and classical models	5
2.3.1	Scaling	5
2.3.2	Classical Models	5
2.4	Maxwell rates	5
2.4.1	Single maxwellian integrations for electron-impact collisions	5
2.4.2	Double maxwellian integrations for ion-impact collisions	5
3	Collisional-Radiative model for molecules	6
3.1	Molecular Generalized Collisional-Radiative Model	6
3.1.1	Time Scales	6
3.1.2	Collisional Radiative model	11
3.1.3	Vibrational resolution in molecular GCR	12
3.2	Source terms	12
3.3	Other Molecular Collisional-Radiative Models	12
4	ADAS9xx: The molecular ADAS	13
4.1	Structure and Diagrams	13
4.1.1	MDF: The Molecular ADAS format	13
4.1.2	Index of parameters in <i>mdf</i> files	17

4.2	The Molecular ADAS routines	17
4.2.1	Scaling, widening and resolving	17
4.2.2	The collisional-radiative routines	17
5	Results	18
5.1	Checking in the experimental plasma	18
5.2	The molecular challenge. ADAS9xx: a general molecular software	18
A	MDF data formats	20
A.1	<i>mdf00</i> : general parameter information files and potentials curves	20
A.1.1	potentials	20
A.1.2	vibrational energies	20
A.1.3	Franck-Condon Factors	24
B	IDL procedures	26
C	FORTRAN subroutines	27
C.1	ADAS902	27
C.1.1	adas902.for	28
C.1.2	thermrat.for	46
C.1.3	intrap.for	53
C.1.4	extrap.for	57
C.1.5	dstform.for	61
C.1.6	wrt_mdf04.for	63
C.1.7	fcf.for	67
C.1.8	rd_enu.for	69
D	Shell scripts	71
E	Fitting Formulas	72

-

Appendix B

ADAS/ADAS-EU computing equipment review and status

ADAS/ADAS-EU/OPEN-ADAS Computer Resources

1. The provision of computer resources for ADAS-EU staff, central ADAS services, OPEN-ADAS web services, computational services for students and high performance computational facilities is financed from a mixture of ADAS funds, student support grants, ADAS-EU and department funds.
2. The present computer servers located at the University of Strathclyde:

Machine	Services	Status
ferro.phys.strath.ac.uk	/home/ file system CVS, svn server	operational 92% capacity
x-wing.phys.strath.ac.uk	access machine general computation	failed hard disk
ripley.phys.strath.ac.uk	general computation	failed hard disk
open.adas.ac.uk	OPEN-ADAS server	operational

3. The University of Strathclyde provides infrastructure support and covers all internet bandwidth costs.
4. The ADAS-EU researchers have multi-place work locations and mobility is expected. The ability to to work effectively is enabled by providing software and sufficiently powerful laptop computers capable of running ADAS and complementary codes. This is backed up by ADAS specific servers housed at the University of Strathclyde.
5. In 2011 laptop computers were provided to ADAS-EU researcher Dr. A. Giunta and student Stuart Henderson. The specification:

Role	Model	CPU	Cache	Memory	Disk	Cost
Laptop	E640	Intel Core i5-560M 2.66Ghz	3Mb	8Gb	320Gb	£780.00 × 2

Price is ex-VAT.

6. The gui of ADAS and much of the user programability of ADAS is provisioned via IDL, the Interactive Data Language from Exelis. This scientific programming language has an annual license fee. The ADAS group purchases 7 licenses per year split between 4 floating seats on the ADAS servers and node-locked licenses on laptops. The renewal cost in 2011 was £1267.83 (inc VAT) of which £423.00 was apportioned to the ADAS-EU budget.
7. The www.adas-fusion.eu domain name attracts an annual renewal fee of £17.99 (inc VAT).
8. Large scale calculations in support of ADAS-EU programmes and ADAS are carried out on various facilities:
 - JET Analysis Cluster at EFDA-JET.
 - HPC parallel systems at the University of Strathclyde.

- HPC-FF, the High Performance Computing for Fusion which is part of the JuRoPA supercomputer (Jülich Research on Petaflop Architectures) a European supported programme with access for ADAS staff provided via CCFE, the UK Euratom Association.
9. In the past year a number of computer related issues have become matters of increasing concern:
- The present ADAS computer infrastructure is nearing its end of life and two servers have suffered hard disk failure.
 - The hardware is not adequate to support the R-matrix repository plans.
 - The current backup provision is too ad-hoc a process for the increased scale of the ADAS activities.
 - The physical security of the computers can be compromised by estate re-allocation within the physics department.
 - ADAS-EU collaborations identified the need for a facility with large amounts of addressable memory. For the first few ionisation stages of the heavy species large memory serial calculations are required. This is against the trend of supercomputer centres where large number of CPUs with modest attached memory is the norm.
10. Following discussions the Physics Department will supply a server rack and housing in a secure location. Backup facilities to separate departmental and university NAS services can be purchased for a modest one-off fee of the order of £200/500Gb.
11. The following rack mounted servers have been ordered from Dell, one of the preferred suppliers to the university, satisfies the mid-term future needs of ADAS, ADAS-EU and OPEN-ADAS:

Role	Model	CPU	Cache	Memory	Disk	Cost
Computational node	R510	Intel Xenon X5650 6 core, 2.66Ghz	12Mb	96Gb	5 × 2Tb	£6221.52
Internet server	R310	Intel Xenon X3430 4 core, 2.4Ghz	8Mb	8Gb	4 × 2Tb	£2116.80 × 3

Prices are ex-VAT. The R501 was delivered 11th January and the others are expected to arrive in February.

12. It was felt prudent to keep an off-site backup of the ADAS CVS repository, the ADAS-EU shared document repository and web-site and the OPEN-ADAS database. A 1Tb disk (£89.99. inc VAT ADAS budget) is kept at EFDA-JET for this purpose. We note that if it is required there may be greater problems than missing disks.

MO'M
Jan. 2011