

ADAS-EU

ADAS for fusion in Europe

Grant: 224607

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

Review 3

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Workpackages : 26-5-3, 27-1*, 27-2*, 28-1*, 28-2*

Category : DRAFT

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Review 3

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Abstract: *Review of reporting period: months 37-48*

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Chapter 1

Overview

The final and summative period of the ADAS-EU project sees the broad sweep of themes, deliverables and milestones of ADAS-EU met. However, as discussed in REVIEW2, some adjustments of the details of the themes was appropriate in a project of such duration to meet evolving needs/interests and maintain relevance to current fusion in Europe. Also, special studies, which were part of ADAS-EU or ADAS-EU sub-contracts in some cases gave surprising results which had to be followed up. Some of these issues were noted in the forward planning section of REVIEW2, including special features and spectral analysis, generalised-collisional-radiative modelling for medium-weight species, advanced Stark modelling of beam atoms and extensions of the molecular theme to rovibrational spectral prediction. Also it has been important to continue to increase the engagement and application of the expanding ADAS-EU capabilities with laboratory studies. This period was markedly successful in this respect at EFDA-JET, ITER, IPP-Garching and CEA Cadarache with work flowing into new, interesting analyses or predictions and exploiting some of the less familiar aspects of ADAS, such as differential emission measure and transient situations. It is clear that ADAS-EU, with delivery into ADAS and its public domain outlets worldwide has brought a large body of very sophisticated atomic modelling, data and descriptions into play for fusion. Considerable attention was given to the dissemination pathways from ADAS-EU and these have been very successful. Some aspects are summarised in the following paragraphs. More details can be found in the reports from this period, namely, SCIENCE7, SCIENCE8, DISSEM3, OPEN3, SUBC2, ITER2 and ECWP2.

It has been clear from the earlier periods of ADAS-EU that the dissemination programme was working well, especially the ADAS-EU workshop/training courses. The scheduled third course, because of timing issues with RFX operation at Padua, came into this last period (in March 2012) along with the final course at CEA Cadarache in late September-early October 2012. These courses have been very international, with participants from all over the world. and have been motivating for participants, lecturers and tutors alike. See DISSEM3 for details. It has been good to see the ongoing contacts and collaborations, which were initiated at the ADAS-EU courses, between and among participants and tutors. It became evident in 2012 that there would be some underspend in ADAS-EU because of currency fluctuations and artificially low salary inflation during the economic recession in Europe and the USA. It was agreed to put in place Amendment no. 2 to the ADAS-EU specification to allow extension of ADAS-EU from 1 January 2013 to 30 September 2013 for further ADAS-EU Workshop/advanced training courses world-wide. A separate report, DISSEM4, has been delivered on the extended dissemination programme. It was fulfilled by Prof. Summers, Dr. O'Mullane and Dr. Giunta, who continued in part ADAS-EU funded employment at the University of Strathclyde for a further nine months in 2013.

As indicated in REVIEW2, it has been possible to bring into play some additional atomic physics resources for ADAS-EU beyond what was originally planned, as reflected in the extra theme 6 on medium-weight element generalised-collisional-radiative modelling and its associated workpackages 27 and 28. The objectives have been to raise the baseline quality of atomic collision cross-section entering collisional-radiative modelling, to ensure completeness for primary GCR couplings and to span the range of medium-weight elements of interest to fusion. These objectives have been realised and have entailed an enormous increase in the ADAS databases (~10 Gbytes). Furthermore these developments are not exclusive to medium-weight elements, but, by utilising relativistically corrected orbitals (κ -averaged) and intermediate coupling (*ic*) extends also to heavy elements. It has been noted on a number of occasions that the neutral and near neutral ionisation stages of elements are troublesome and so this has been given special

attention. A key aspect has been the orbital optimisation strategy and the alignment of energy levels with experimental values. The ADAS-EU reference for the latter is the National Institute for Standards in Technology energy tables, which are automatically downloaded and prepared in ADAS data formats and then used in corrections to the ADAS Autotstructure distorted wave Hamiltonian. Additional benchmarking has been done, especially for tungsten ions, as described in sub-contract reports (SUBC2) and the report of the electron collision working party (ECWP2). Attention is also drawn in ECWP2 to the hybrid approach to complex system dielectronic recombination, complementary to *bbgp* techniques. The addition of the *cadw* distorted wave ionisation cross-section inclusion into GCR modelling (see Giunta's summary in SCIENCE8 and the details in PUBL6) means that we now have an internally consistent basis for all the GCR collisional-processes at the distorted wave level. Work of our university team and colleagues in the USA and China with the R-matrix approach puts the final refinement on key ions and iso-electronic sequences [1],[2], [3], [4], [5], [6],[7], [8], [9], [10].

1.1 Staffing

There were no special staffing issues in the third period. Following the re-organisations of period 2, ADAS-EU had the full post-doctoral staff in place at IPP Garching, CEA Cadarache/ITER and CCFE Culham Laboratory/EFDA-JET for the third period. Also Dr. O'Mullane continued his strong support for ITER. As summarised in reports SCIENCE7, SCIENCE8 and ITER2 engagement in the fusion research programmes at these laboratories proceeded very well and interfacing of requisite atomic physics was achieved.

The completion of period 3 marked the end of the ADAS-EU post-doctoral appointments of Dr. Guzman and Dr. Menchero. Dr Guzman continues as a postdoctoral researcher in the field in a position with the Laboratoire de Physique des Interactions Ioniques et Moleculaires (PIIM) jointly operated by University of Aix - Marseille and CNRS. He continues with his molecular modelling for fusion and maintains links to the Integrated Tokamak Modelling task force. He has also commenced new work in the topical field of transient ionisation behaviour in turbulent cells in the vicinity of transport barriers. Dr Menchero has taken up a post-doctoral position at the Department of Physics, University of Strathclyde with Professor Badnell - who chaired the Electron Collision Working Party of ADAS-EU. Dr Menchero continues his work on advanced beam emission models, but his primary role is now R-matrix calculations of electron collision data for astrophysics and fusion interest. His work continues to flow into the ADAS databases. Dr Giunta, Dr. O'Mullane and Professor Summers continued with part-time work for ADAS-EU agreement under amendment 2, until 30 Sep 2013. Dr. Giunta then took up full-time employment for the Space Science department of Rutherford Appleton Laboratory in the UK as a Solar Physicist with responsibilities for the SPICE spectrometer on the up-coming Solar Orbiter spacecraft. She continues to promote her interest in the shared atomic physics between fusion and solar astrophysics and maintains her links with CCFE Culham Laboratory and the JET Facility.

1.2 Computation

The ADAS-EU computer support equipment purchased towards the end of period 2, that is the primary servers supporting ADAS-EU science and the connected OPEN-ADAS and ADAS provisions, have operated without problem over period 3. It is the expectation that these systems will continue to host the OPEN-ADAS and associated ADAS-EU infrastructure through to at least 2017. The update of the OPEN-ADAS web site in this last period 3 was timely. The new interface (see report SUBC2) is both attractive and powerful. The University of Strathclyde will also continue to hold the 'www.adas-fusion.eu' domain name until at least 2017 and maintain the OPEN-ADAS provision.

1.3 The future

The ADAS-EU Support Action has enabled the enhanced on-site atomic physics support at European fusion laboratories intended. It has also allowed effective evolution and direction of atomic physics input to the ITER project and the European contribution to it. Also, because of the linkage of ADAS-EU to ADAS and to the latter's international stance, it has been straightforward to connect with all the partner countries in ITER outside Europe. Amendment 2 to the ADAS-EU agreement gave strong extra momentum to this. The special knowledge exchange and advanced ADAS

training courses were very well received. This willing European contribution to atomic physics for fusion internationally was recognised. Thirdly, ADAS-EU did, in addition, permit the ADAS-EU staff to oversee very large extensions to the ADAS atomic physics capabilities for fusion and growth of its databases, while simultaneously acting as a unifying and coordinating force amongst the European university specialists. The ADAS community is now probably the largest producer of atomic physics data for fusion application in the world.

It is hoped that this momentum will continue to ITER. However changes are occurring. Professor Summers will move into full retirement in June 2014. Funding for fusion in Europe is changing with the new EuroFusion organisation. Also ITER is in a transitional phase as it moves from conceptual diagnostic design to actual system manufacturer by the domestic agencies, testing, integration and finally operation. It is the declared intention of the ADAS community that ADAS should continue. The ADAS Steering Committee and directorate are pursuing appropriate funding, collaborations and actions to secure this.

1.4 Finances

1.5 Publications

Publications in this period connected to ADAS-EU include works by Badnell ([1],[2], [3], [4], [5], [6],[7], [8], [9], [10]), Guzman ([11], [12]), O'Mullane ([13], [14], [15], [16], [17], [11], [18], [19]), Menchero ([20], [21], [22]), Giunta ([16], [17]) and Summers ([20], [21], [17], [16], [11],[18], [19]). The references are to the bibliography of this review on pages 9 and 10. There are twenty-two independent titles. Two articles from late 2011, not included in REVIEW2, are included here for completeness. Also some articles due to appear in 2013 and 2014 for which the work was done in the ADAS-EU timeframe are included. Several of these publications have shared authorship

1.6 Reports

Reports available for release at this time comprise:

- SCIENCE7, SCIENCE8 (see Appendix [A.1](#))
- OPEN3 (see Appendix [A.2](#))
- DISSEM3 (see Appendix [A.3](#))
- ECWP2, SUBC2, ITER2 (see Appendix [A.4](#))

Reports for EFDA-JET laboratory publication, comprise:

- PUBL1, PUBL2, PUBL3, PUBL4, PUBL5, PUBL6 (see Appendix [A.5](#))

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

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Bibliography

- [1] G. Y. Liang, N. R. Badnell, G. Zhao, J. Y. Zhong and F. L. Wang. ‘R-matrix electron-impact excitation data for astrophysically abundant sulphur ions’. *Astron. Astrophys.*, **533** (2011) A87(13)
- [2] G. Y. Liang and N. R. Badnell. ‘R-matrix electron-impact excitation data for the Li-like iso-electronic sequence with Auger- plus radiation-damping’. *Astron. Astrophys.*, **528** (2011) A69(15)
- [3] S. A. Abdel-Naby, D. Nikolic, T. W. Gorczyca, K. T. Korista and N. R. Badnell. ‘Dielectronic recombination data for dynamic finite-density plasmas XIV. The aluminium isoelectronic sequence’. *Astron. Astrophys.*, **537** (2012) A40(12)
- [4] N. R. Badnell, C. P. Ballance, D. C. Griffin and M. O’Mullane. ‘Dielectronic recombination of W^{20+} ($4d^{10}4f^8$): Addressing the half-open f shell’. *Phys. Rev. A*, **85** (2012) 052716. doi:10.1103/PhysRevA.85.052716
- [5] C. P. Ballance, D. C. Griffin, S. D. Loch and N. R. Badnell. ‘Dielectronic recombination of Au^{20+} : a theoretical description of the resonances at low electron energies’. *J. Phys. B*, **45**(4) (2012) 045001. doi:10.1088/0953-4075/45/4/045001
- [6] M. Lestinsky, N. R. Badnell, D. Bernhardt, D. Bing, M. Grieser, M. Hahn, J. Hoffmann, B.Jordon-Thaden, C. Krantz, O. Novotny, D. A.Orlov, R. Repnow, A. Shornikov, A. Mueller, S. Schippers, A. Wolf and D. W. Savin. ‘Electron-ion recombination of Mg^{6+} forming Mg^{5+} and of Mg^{7+} forming Mg^{6+} : Laboratory measurements and theoretical calculations’. *Astrophys. J.*, **758** (2012) 40(13)
- [7] G. Y. Liang, N. R. Badnell and G. Zhao. ‘R-matrix electron-impact excitation data for the B-like iso-electronic sequence’. *Astron. Astrophys.*, **547** (2012) A87(12)
- [8] O. Novotny, N. R. Badnell, D. Bernhardt, M. Grieser, M. Hahn, C. Krantz, M. L. and A. Mueller, R. Repnow, S. Schippers, A. Wolf and D. W. Savin. ‘Electron-ion recombination of Fe XII forming Fe XI: laboratory measurements and theoretical calculations’. *Astrophys. J.*, **753** (2012) 57(11)
- [9] G. Y. Liang, N. R. Badnell and G. Zhao. ‘Evaluation of electron-impact excitation data along isoelectronic sequences’. *Fusion Sci. Technol.*, **63** (2013) 372–376
- [10] D. Nikolic, T. W. Gorczyca, K. T. Korista, G. Ferland and N. R. Badnell. ‘Suppression of dielectronic recombination due to finite density effects’. *Astrophys. J.*, **768** (2013) 82(9)
- [11] F. Guzmán, M. O’Mullane and H. Summers. ‘ADAS tools for collisional-radiative modelling of molecules’. *J. Nucl. Mater.*, **438** (2013) S585–S588. Proceedings of the 20th International Conference on Plasma-Surface Interactions in Controlled Fusion Devices. doi:10.1016/j.jnucmat.2013.01.073
- [12] J. Suarez, F. Guzman, B. Pons and L. F. Errea. ‘Excitation cross-sections for Li^{3+} , Ne^{10+} and $Ar^{18+} + H(1s)$ collisions of interest in fusion plasma diagnostics’. *J. Phys. B: At. Mol. Opt. Phys.*, **46** (2013) 095701
- [13] S. T. A. Kumar, D. J. D. Hartog, B. E. Chapman, M. O’Mullane, M. Nornberg, D. Craig, S. Eilerman, G. Fiksel, E. Parke and J. Reusch. ‘High resolution charge-exchange spectroscopic measurements of aluminium impurity ions in a high temperature plasma’. *Plasma Phys. Control. Fusion*, **54** (2012) 012002. doi:10.1088/0953-4075/21/6/014
- [14] S. Henderson, M. O’Mullane, H. Summers, L. Garzotti, H. Meyer, A. Patel and M. Valovic. ‘Low-Z impurity transport analysis by transient gas puff experiments’. In ‘54th Annual Meeting of the APS Division of Plasma Physics’, (2012). Available from: <http://meetings.aps.org/link/BAPS.2012.DPP.G06.5>

- [15] S. K. Varshney, R. Barnsley, M. G. O'Mullane and S. Jakhar. 'Bragg x-ray survey spectrometer for ITER'. *Rev. Sci. Instrum.*, **83**(10) (2012) 10E126. doi:10.1063/1.4738747
- [16] J. G. Doyle, A. Giunta, A. Singh, M. S. Madjarska, H. Summers, B. J. Kellett and M. O'Mullane. 'The Diagnostic Potential of Transition Region Lines Undergoing Transient Ionization in Dynamic Events'. *Solar Phys.*, **280** (2012) 111–124. doi:10.1007/s11207-012-0025-6
- [17] 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
- [18] S. Henderson, L. Garzotti, F. J. Casson, D. Dickinson, M. O'Mullane, A. Patel, C. Roach, H. P. Summers, M. Valovic and the MAST team. 'Low-Z perturbative impurity transport and microstability analysis on MAST'. In 'Europhysics Conference Abstracts (CD-ROM, Proc. of the 40th EPS Conference on Plasma Physics, Espoo, Finland, 2013)', volume 37D, 4.146 (2013)
- [19] S. S. Henderson, L. Garzotti, F. J. Casson, D. Dickinson, M. Fox, M. O'Mullane, A. Patel, C. M. Roach, H. P. Summers, M. Valovic and the MAST team. 'Neoclassical and anomalous analysis of perturbative helium transport experiments on MAST'. *Nucl. Fusion*, ??(??) (2014) ??
- [20] L. F. Menchero and H. P. Summers. 'Ab initio study of the Stark effect in neutral hydrogen'. IPP-10/49, Max Planck Institute for Plasma Physics, EURATOM Association (2013). Available from: <http://edoc.mpg.de/display.epl?mode=doc&id=656145>
- [21] L. Fernández-Menchero and H. P. Summers. 'Stark effect in neutral hydrogen by direct integration of the Hamiltonian in parabolic coordinates'. *Phys. Rev. A*, **88** (2013) 022509. doi:10.1103/PhysRevA.88.022509
- [22] F. J. Casson, R. M. McDermott, C. Angioni, Y. Camenen, R. Dux, B. Geiger, E. Fable, R. Fischer, B. Geiger, P. Manas, L. Menchero, G. Tardini and ASDEX Upgrade team. 'Validation of gyrokinetic modelling of light impurity transport including rotation in ASDEX Upgrade'. *Nucl. Fusion*, **53** (2013) 063026. doi:10.1088/0029-5515/53/6/063026

Appendix A

Reports

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A.1 Reports: SCIENCE7, SCIENCE8

ADAS-EU R(13)SC07

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

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

Scientific progress report 7

22 February 2013

Workpackages : 1-2, 2-3, 6-4, 7-2, 8-1, 8-2, 9-1, 11-1, 16-3, 20, 21, 26-1-7, 28-1
Category : DRAFT

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ADAS-EU R(14)SC08

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

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

Scientific progress report 8

21 February 2013

Workpackages : 2-3, 8-4, 8-4, 9-1, 9-3, 11-1, 11-2, 16-3, 17-1, 18-3, 18-4,
19, 20, 21, 22-2, 26-1-8, 27, 28-2

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A.2 Report: OPEN3

ADAS-EU R(13)OP03

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Hugh Summers

OPEN-ADAS report 3

December 2013

Workpackages : 26-2-3
Category : PU

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A.3 Report: DISSEM3

ADAS-EU R(13)DI03

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

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

Dissemination report 3

6 June 2013

Workpackages : 20-1-3, 20-2-3, 21-1-3, 21-2-3, 26-4-3
Category : DRAFT

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A.4 Report: ECWP2, SUBC2, ITER2

ADAS-EU R(13)SU01

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

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

ECWP2: Electron Collision Working Party Report 2

20 Dec 2013

Workpackages : 4-2, 5-1, 5-2, 5-3, 27-1*, 27-2*, 28-1* and 28-2*

Category : DRAFT – CONFIDENTIAL

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ADAS-EU R(13)SU02

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

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

**SUBC2: Sub-contract specifications, deliverables,
integration and analysis**

21 Feb 2013

Workpackages : 5-1, 5-3, 9-1, 9-3, 10-1 and 10-2; see also S1, S6, S7,
S9

Category : DRAFT – CONFIDENTIAL

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ADAS-EU R(XX)SUXX

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Martin O'Mullane

**ITER2: ITER visits and support activities
Report 2**

10 Feb 2014

Workpackages : 2-3 and 3-4

Category : DRAFT – CONFIDENTIAL

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A.5 Report: PUBL1, PUBL2, PUBL3, PUBL4, PUBL5, PUBL6

ADAS-EU R(10)PU01

ADAS-EU
ADAS for fusion in Europe

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Adam Foster, F. Guzmán, Martin O'Mullane and Hugh Summers

PUBL1: Charge exchange spectroscopy for fusion plasmas

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Christopher Nicholas, Andrew Meigs, Martin O'Mullane, Hugh Summers and Allan Whiteford.

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

**PUBL3: Heavy species in fusion plasma modelling
and spectral analysis**

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Luis Fernández-Menchero, Stuart Henderson and Hugh Summers

PUBL4: Neutral Beam Emission: The Motional Stark Effect

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Alessandra Giunta, Hugh Summers, Paul Bryans and Martin O'Mullane

**Generalised-collisional-modelling for light- and medium-weight
elements**

December 7, 2012

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Category : DRAFT

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F. Guzmán, M. G. O'Mullane, K. H. Behringer and H. P. Summers

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