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

Scientific progress report 5

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

Department of Physics, University of Strathclyde, Glasgow, UK

Abstract: *The report reviews scientific task completion for project months 25-30*

Contents

Chapter 1

Overview

Chapter 2

Individual contributions

2.1 Luis Fernández-Menchero: Atomic structure of beam atoms in fields

The study of Dr. Luis Fernández Menchero during the year 2011 was centred in obtaining the energies, widths and wave functions of neutral hydrogen under a constant electric field. Such electric field is usually a virtual one, produced by the motion of the atoms coming from the Neutral Beam Injectors (NBI) in the intense magnetic field present in tokamaks and stellarators, then the derived Lorentz field $\boldsymbol{F} = \boldsymbol{v} \times \boldsymbol{B}$ is the largest perturbation which receives the atomic system.

2.1.1 Study of Stark effect in terms of perturbation theory

The first option to treat the problem of a hydrogen atom under a constant electric field is to include it as a perturbation of the coulomb potential.

We solve the unperturbed Schrödinger equation for the hydrogen atom in parabolic coordinates, so we obtain the unperturbed energies and wave functions in terms of the parabolic quantum numbers $|nkm\rangle$. Then we apply the perturbation theory to obtain in different orders the energy of the levels and the wave function. This is shown in detail in the PUBL4 of the present project.

As perturbation theory is not able to obtain the state widths of the Stark states, then a semiempirical method should be used for that goal.

In PUBL4 it is shown that perturbation theory has several theoretical inconsistencies and does not lead to acceptable results, so an alternative more rigorous method should be used. We are nowadays making this work in terms of the complex coordinate integration.

2.1.2 Improvement of the FORTRAN routine fldizn

The routine fldizn calculates energies and wave functions of the hydrogen atom under a constant electric field in terms of perturbation theory, and state widths by a semiempirical method. This routine was written by Stuart Henderson, and Luis Fernández Menchero included some improvements to optimize its working.

The results obtained with fldizn can be used as input functions for the other routines of ADAS305, which are able to calculate the other weaker perturbation terms: magnetic and fine structure.

2.1.3 Programming of the ADAS305a package in FORTRAN

ADAS305 is a package to be included in the ADAS series 3, for charge exchange processes, the goal of ADAS305 is to build a general collision radiative model for the hydrogen atoms coming from the NBI, taking in account they are moving in an intense magnetic field and they are interacting with the radiation, electrons, ions and impurities of the plasma. This GCR matrix is very important to build models of beam emission and beam stopping.

The package ADAS305 is divided in two subpackages:

ADAS305a static part, which calculates just the atomic structure of the hydrogen atom under the simultaneous electric and magnetic fields.

ADAS305b dynamical part, which calculates the collision radiative matrix.

The package ADAS305a is divided in several routines, and it is programmed to calculate energies, widths and wave functions for hydrogen atoms under simultaneous constant electric and magnetic fields. It takes as input a collection of zero-order wave functions, which are the hydrogen Stark functions, which should be previously calculated for any method, and it applies the perturbation theory to calculate the additional terms: magnetic and fine structure. As output it gives the new perturbed energies, widths and wave functions.

2.1.4 Conclusions

In publication 4 it is shown the inconsistencies of perturbation theory for the Stark effect problem, mainly the present fields in tokamaks are competitive with the Coulomb potential for lowly excited states $n \gtrsim 3$, and the perturbation potential dominates in the asymptotic region at high distances of the nucleus, no matter how small the field is. In conclusion Stark functions calculated in terms of perturbation theory can not be used as input for ADAS305a.

In the other hand, conditions to use perturbation theory are fulfilled for the magnetic and fine structure terms, in this case we can use it.

2.1.5 Future work

The work for the second semester of 2011 and 2012 centers in obtaining reasonable Stark functions to be used as zero-order for ADAS305a. These functions will be stored in a data file, which will be explored for ADAS305a, in the file they will be stored energies, widths and wave functions as a linear expansion in a basis set of parabolic wave functions for the field-free hydrogen atom $|nkm\rangle$.

We use the method of the complex coordinate integration, with it we can obtain *ab initio* the searched wave functions as a linear combination of a determined basis set. Method and results will be exposed in publication 4.

2.2 Hugh Summers: Continued BBGP development and Culham SuperX studies

2.2.1 BBGP development

A strategic decision has been made that BBGP dielectronic recombination production should give as output standard ADAS *adf09* datasets. It is recognised that bundling will be necessary to limit the size of the *adf09* output, but this will be implemented in the BBGP *adf46* driver. It is also noted that the *adf09* dataset from BBGP is at a specific selected finite density, unlike the usual *adf09* datasets from AUTOSTRUCTURE. They will be normally treated as transient (for a calculation) and will not be archived in central ADAS database libraries. Firstly, in Jan., some further provision

to *process_adf04_adf46.for* was made for different configuration formats and the quantum defect and dipole polarisability extractions were filled in. Further work in Jun. made some verifications on the polarisabilities, which are used to infer energy levels of high angular momentum spectator electrons built on excited cores in BBGP. The attention was moved to BBGP processing itself. This activity is assigned to ADAS708. *g8bbgp.for* is the primary subroutine and is of some complexity. It can follow Auger/cascade down through a sequence of parents, but also evaluates the redistribution in *l* of the spectator electron. This redistribion, induced primarily by ion collisions rather than electrons, uses internally calculated cross-sections by subroutines (*cxripv.for* and *gxpeng.for*) reworked to the latest ADAS standards. The code *g8bbgp.for* now operates in test mode with suppression of some its the extended capabilities , such as non-dipole and spin-changing parent transitions. Available *adf04* datasets for the complex systems under test are prepared from PBW baseline *adf04* datasets which exclude spin-changing cross-sections. A further major upgrade in the sophistication has become possible. This is the in-house distorted wave cross-section of Badnell's AUTOSTRUCTURE code. *g8bbgp.for* has up until now used a default of Bethe approximation correction factors stemming from the work of Burgess and Summers [**?**] and Summers [**?**]. Ion specific correction factors can now be prepared in *g8bbgp.for* from AUTOSTRUCTURE partial collision strengths archived in a new *adf04 type 5* format. The mechanism to use these has been put in place in this period. The production mechanisms of the *adf04 type 5* will be addressed in the next period.

2.2.2 Culham SuperX studies

Together with Giunta, Summers has engaged with the SuperX divertor for MAST planners at Culham Laboratory, UK, to assist in prediction of the spectral emission in the divertor and to assess opportunities for improved spectral coverage depending upon the results. Following on a first meeting in Dec. 2010, further meetings took place in Mar. and May 2011. The SuperX concept has considerable interest and opportunity for atomic physics, due to the extended volume at low density, the substantial neutral hydrogen presence and the transient character of the plasma during formation of the X-point and sweep of the plasma into the divertor, and during ELMs. Reconstructions of the electron temperature and electron temperature on a 2-d grid were made available, sufficient for the ionisation stage distributions in the ADAS equilibrium collisional-radiative model to be prepared on the grid by Giunta. This was done for helium, carbon and oxygen impurities. Further work took place on forming line-of-sight integrals of emissivities, but the gridding was too coarse for strong conclusions on low ionisation stages. This area will be pursued in further time periods with finer grids which are in preparation.

2.3 Martin O'Mullane: Code developments and ITER engagements

2.4 Francisco Guzmán: Molecular CR modelling

This period was devoted mainly to advances in Molecular CR modelling (section 2.4.1. Concerning to the ion impact collisions there were new charge exchange data from subcontract which were analysed and put into ADAS (section 2.4.2). An experimental injection of Ar was performed in Tore Supra in order to analyse the impurity density profile and compare with the Soft-X ray to discriminate between the discrepant Ar cross section sets in ADAS (section 2.4.3). Lastly a recall travel to JET to analyse the progress with ADAS team was performed in June 2011.

2.4.1 Advances in Molecular CR modelling

This period is marked by the finalization of ADAS902 set of subroutines. These interrogate the *mdf02* format files and integrate the cross section in them to provide a collection of rates from external sources in the correct resolution in the formats *mdf33* (electron impact) and *mdf34* (ion impact).

These routines should "expand" the total electronic cross section into the vibrational levels in the vibrational resolved case and "compress" the vibronic cross section into the electronic ones in the non-resolved case. That is done using the Franck-Condon factors which apply in the energy range under study here. Thus, the Franck-Condon factors

should be stored in some format to be used but the different routines. The chosen directories are *mdf00/FCF/* and the reading routines have been created which were called *read_fcf* but have been changed to *xxdatm_00*.

Dipole integral for spontaneous transition have also been stored in *mdf00* together with the vibrational energy values. They are in the directories *mdf00/aval* and *mdf00/enu* respectively. The routine *xdatm_00* reads A-values files as well as their format is very similar to the Franck-Condon factors. However, it is needed a new routine *rd_enu* for obtain the vibrational energies.

ADAS 902 creates the vibrational resolved or non-resolved ADAS format *mdf33/34* files and also can do the Maxwell integration of the *mdf02* files without care for any resolution at all. That can be good in case only maxwellian rates are required from a specially prepared *mdf02* file.

That constitute the second stage (after creation of data base) for the construction of a CR model in ADAS. The document that will contain all the developments and structure is created as a public review document PUBL6 and its outline is in Appendix **??**. **These actions correspond to the partial completion of milestone SCI52 which concerns the completion of molecule/ hydrogen atom population and spectral modelling successfully available in ADAS**.

2.4.2 Ion impact atomic data

Data form subcontracts **S5** and **S6 (?)** have been released. These correspond to Kr^{36+} + H(1s) CX cross sections and N^{7+} + H(1s,n = 2) CX cross sections respectively. The former have been calculated by the improved CTMC method using an hydrogenic distribution and the latter with the AOCC using pseudostates to describe the continuum. These data have been given to F. Guzman who has check the quality and put them in *adf01* format.

Krypton data were in a good energy grid and had electron capture up to $n = 60$ of Kr^{35+} using 100000 classic trajectories. Some correction were done to keep the cross section were capture cross section were corresponding to above 100 trajectories to guarantee statistical significance. I this order $n = 60 - 70$ were removed from the original calculations. **This works concerns to task 9-1**.

Nitrogen data were given for $n = 2 - 11$ capture with H(1s) and H($n = 2$) donors. These data had a good quality but in a very rough energy grid. Data in a finer grid were provided later to other ADAS staff.

2.4.3 TORE SUPRA Ar experiment

Charge exchange recombination spectroscopy is the most direct technique to determine the argon density in a fusion plasma. This technique requires knowledge of the Ar charge-exchange (CX) cross-sections. New calculations of Ar cross-sections using an improved hydrogenic description of the initial distribution [**?**] (the previous sets come from calculation that used a microcanonical distribution [**?**]) have been released in ADAS. A big discrepancy has been found between the different calculations reaching up to two orders of magnitude depending on the beam energy.

A experiment has been carried in the fusion device Tore Supra where Ar was injected in the vessel during operation. This experiment is the starting point of a collaboration were ADAS researcher, Dr Francisco Guzmán will analyse the CXRS Ar data to obtain the impurity profiles of Ar and CEA researcher, Dr. Remy Guirlet in collaboration with G. Mondet from Laboratoire Aimé Cotton, Université Paris XI will analyse the Soft X-rays profiles together with the application of the transport code ITM (Internal Transport Model) to be able to compare the Ar profile and discriminate between the two discrepant CX sets.

Calculations of electron impact Ar data will be compared with the ones performed by G. Mondet and analysed inside the ITM model. **The actions 2.4.3 are included in the partial completion of revision of fiducial CXS data (work package task 9-4**.

2.4.4 ITER collaborations

Some scientific collaboration have been performed with ITER scientific staff. These concern to atomic data in simulation analysis and a model for radiated power in gas injections to avoid disruption.

Study of the differences in atomic data between STRAHL and ADAS

Dr. A. Kukushkin provided some ionization, recombination and PLT data used by simulation code STRAHL for C and He elements. He was not very sure where these data come. He thought they were ADAS data though very old.

A comparison of the rates coefficients used in STRAHL with those present in ADAS was performed by Dr. F. Guzmán. No significative differences were found in ionization. Recombination coeffcients were different due that STRAHL does not presumably account for dielectronic recombination or at least understimates ADAS calculations of that. Radiated Power Line coeffcients were in good agreement for C but under the ADAS calculation for He case. A report was done and given to Dr. Kukushkin. This report is in Appendix C.

Gas injection Model for FPSS

Fusion Power Shutdown System (FPSS) is a Safety Important Component (SIC) which must be extremely simple and reliable. It is imposed upon ITER by the French Nuclear Regulator. It is a high Z gas injector which will dump some highly radiating gas (e.g. Ne) into the plasma at a relatively slow rate (hundreds of ms) from a reservoir. It will be limited to about a 10 bar pressure (or lower) and use the same gas lines as we will use for the ordinary gas injection. Dr. Pitts contacted with Dr. F. Guzmán for a model which would do an estimation of the radiating power of the injected gas (once the gas is totally injected in the plasma) in order to know what kind of gas is necessary to be absolutely sure of terminating a full energy plasma at full current in the case that we lost control of it or there was a LOCA event (loss of confinement accident).

F. Guzmán prepared an IDL code which makes use of ADAS subroutines ADAS405 and get the total radiated power and fractional abundances of an homogeneously distributed gas in a plasma for a profile of temperature and density pairs. This program was handed to Dr. Pitts who used it.

2.4.5 Recall to JET

A recall to JET was made to F. Guzmán to make a series of progress discussions. The recall report is given in Appendix D.

2.5 Alessandra Giunta: GCR studies

2.6 Nigel Badnell: Electron impact collision cross sections

Chapter 3

Work package reports

3.1 Work package 8-1

Work package 8: transport and multiple charge states CXS.

Task 1: Enable adjustment of l-mixing cascade models for CXS emission by medium weight partially stripped species through improved level energy separation from static polarizabilities.

3.2 Work package 10-1

Work package 10: lithium beam diagnostic.

Task 1: procure and embed TUW lithium beam iterative electron density determination model as an ADAS code under ADAS maintenance. Provide ADAS-EU support of the application.

3.3 Work package 10-2

Work package 10: lithium beam diagnostic.

Task 2: Procure and embed the lithium beam collision cross-section database as a new adf41 format in the ADAS database.

3.4 Work package 10-3

Work package 10: lithium beam diagnostic.

Task 3: Experimental exploitation and validation. Timing is subject to experimental campaigns and indeterminate at this stage.

3.5 Work package 11-2

Work package 11: Stark manifold and projection merging.

Task 2: Map projection matrices to Stark manifold GCR population and emissivity model.

3.6 Work package 13-1

Work package 13: Zeeman feature enabling.

Task 1: Write and realise routines for acquisition of Zeeman. Paschen features emissivities in IDL, MATLAB and FORTRAN language from C language precursor. Write and release IDL display primitive for the special feature.

3.7 Work package 14-1

Work package 14: Soft X-ray He-/Li-like feature enabling.

Task 1: The creation step will release for general use and perform selective runs of a code package executing the two step chain of ADF04 file creation followed by ADF31 feature file creation. The first step assembles the extended form of ADF04 file which includes auto-ionising levels and autoionisation rates from AUTOSTRUCTURE calculation combined with electron impact excitation and ionisation rate coefficients. The second step in the chain is the extended collisional-radiative population code enabled for doubly-excited states.

3.8 Work package 14-2

Work package 14: Soft X-ray He-/Li-like feature enabling.

Task 2: Write and release routines for acquisition and interpolation of ADF31 feature files in IDL, MATLAB and FORTRAN language. Write and release and IDL display primitive for the special feature.

3.9 Work package 22-2-3

Work package 22: ADAS-EU central supervised work.

Task 2: Attendance at annual update training by each PDRA at UKAEA/JET.

Milestone STS2.

3.10 Work package 23-2-3

Work package 23: ADAS-EU on-site orientation.

Task 2: Obtain local feedback on quality and effectiveness of ADAS-EU on-site support. Review with local staff current fusion targets and appropriate atomic model and data inputs. Adjust and/or extend work packages and allocate contingency time as appropriate.

Milestone STS2.

3.11 Work package 22-2-4

3.12 Work package 23-2-4

3.13 Work package 26-1-5

Work package 26: ADAS-EU primary report assembly.

Task 1: Collation of concluding documents for each support work package task completed in each six month reporting period. For each report prepare a commentary on the use of the and benefits from the task applications in fusion and critical assessment of the achievement of scientific milestones falling in the reporting period.

Report SCIENCE5.

3.14 Work package S6

Work package S6: Lithium beam support data base update.

3.15 Work package S7

Work package S7: Multiple perturber PPP broadening data.

Appendix A

Diagrams

Appendix B

ADAS Theme 5 supplementary material for the report

[1] ADAS-EU/REPORTS_PUBL/PUBL_6/ pages 1-6

-

ADAS-EU R(10)PU06

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

F. Guzmán

The Molecular ADAS: Molecular population model for fusion plasmas

26 July 2010

Workpackages : –
Category : DRAFT

The Molecular ADAS: Molecular population model for fusion plasmas

F. Guzmán

Department of Physics, University of Strathclyde, Glasgow, UK

Abstract: *Public report for ADAS_EU*

Contents

-

Appendix C

F. Guzmán report about STRAHL data

Study of the differences between ionization, recombination and radiated power rates coefficients in STRAHL and ADAS for C and He ions

F. Guzmán
ADAS-EU, Department of Physics, Strathclyde University

May 6, 2011

Abstract

A comparison of the rates coefficients used in STRAHL with those present in ADAS is performed. No significative differences are found in ionization. Recombination coefficients are different due that STRAHL does not presumably account for dielectronic recombination or at least understimates ADAS calculations of that. Radiated Power Line coefficients are in good agreement for C but under the ADAS calculation for He case.

1 ADAS types of data

The effective ionization, recombination and line power rates are stored in *adf11* format files in ADAS. These are called SCD, ACD and PLT respectively and can have a collisional radiative treatment and so depend on density.

For He and C sets of data ADAS have the following type of data named by the year of the main contribution of these:

Data class 74. These correspond to collisional radiative data (i.e. density dependent) from the zero density calculation of Summers (1974)[1].

Data class 85. Collisonal radiative data coming from the calculations of [2].

Data class 89. JET base line data. These correspond to calcullations performed using the Lotz formula [3] for ionization and Burgess zero density general formula [4] with the dielectronic recombination part added [4].

Data class 93. Prepared by W.J. Dickson using JETXTLE code.

Data class 96. General collisional radiative model data [5]. These data can be resolved or unresolved in energy shells.

The data have also a quality assertion in which the calculations using semiclassical methods (74 and 85) have a medium quality, the semiempirical (class 89) formula has a low quality and the quantal and GCR method have a high quality.

2 Comparison of data 21

2.1 Ionization

2.1.1 Carbon

Ionization data are plotted together with ADAS data in figure 1. Here, is possible to see how the STRAHL data correspond exactly to the Lotz formula from ADAS for all the

ionization stages. It is straigthforward to infer from here that STRAHL is using Lotz formula to get ionization data.

2.1.2 Helium

Data also coincide here with ADAS 89 class as is seen in figure 2.The small difference, without more information from STRAHL, can response on the difference of precissions between programs and computers.

2.2 Recombination

2.2.1 Carbon

Recombination data are plotted together with ADAS data in figures 3,4,5,6 and 7.

In the figures 3,4 and 7. STRAHL data coincide with recombination data class ADAS-89. In figures 5 and 6 the ADAS-89 data class departs from STRAHL data as that is including dielectronic recombination that become important having a maximum around 200 eV as can be seen in figure 9 where dielectronic and radiative recombination for C^{4+} are plotted. In this figure the recombination coefficients only depend on electronic temperature but is representative for have an idea of which process dominates. It is normal to expect that dielectronic recombination becomes more important when density is higher.

In C^{3+} and C+2 dielectronic recombination is one order of magnitud smaller than radiative recombination which dominates and the maximum is displaced to 10 eV.

Furthermore, it can be seen in figure 7 how in the case of C^{6+} where there is no dielectronic recombination possible STRAHL and the rest of data sets fully coincide.

In figure 4 top left it is possible to see some kinks at high energies in the non formula (different form ADAS-89) calculations which could be due to problems of extrapolation at low densities. This is under study.

2.2.2 Helium

Data have a good agreement with ADAS-74, ADAS-85 and ADAS-96 classes as is seen in figure 8. It also have the same shape than in ADAS-89 while having a systematic difference that could be due to a difference on the parameters of the formulas used here. Only radiative recombination is possible here.

2.3 Line Radiated power coefficients (PLT)

2.3.1 Carbon

Radiated power coefficients are ploted together with available ADAS data in figure 10. Here, STRAHL data corresponds exactly to the formula from ADAS-89 for all the ionization stages. This formula have been calculated using dipole approximation specified by an oscilator stregth and a gaunt factor [4].

2.3.2 Helium

PLTs are plotted in figure 11. Data is not coincident here with ADAS data sets which are twice the values given by STRAHL. Not being available the way how STRAHL obtain these data is not possible to know what are the causes of this systematic differences.

3 Conclusions

No big differences are found in ionization data between ADAS and STRAHL calculations. The exact correspondence between ADAS-89 and STRAHL calculations let to the inference that STRAHL is using Lotz formula for this calculations. Other calculations present in ADAS agree well with the formula.

Recombination data agree whenever radiative recombination is dominant. In the case in which dielectronic recombination become dominant big differences are found. A problem of a difference with formula calculated recombination ADAS-89 arises in He in a difference of factor of two, but STRAHL data agrees well with the other collisional radiative calculations. Nothing about the causes of this disagreement can be said with no more information about the origin of the data form STRAHL.

PLTs correspond to ADAS-89 data in case of C but a factor of two systematic difference is obtained in He case.

More information from STRAHL origin of fundamental data is needed to determine what are the causes of the disagreement presented above.

References

[1] H. P. Summers. The ionization equilibrium of hydrogen-like to argon-like ions of elements. *Mon. Not. R. astr. Soc.*, 169:663–680, 1974.

[2] M. Arnaud and R. Rothenflug. *Astronomy and Astrophysics Supplement Series*, 60:425–457, 1985.

[3] W. Lichten. *Phys. Rev.*, 164:131, 1967.

[4] H. P. Summers, 2007. Atomic Data and Analysis Structure User Manual.

[5] H. P. Summers, W. J. Dickson, M. G. O'Mullane, N. R. Badnell, A. D. Whiteford, D. H. Brooks, J. Lang, S. D. Loch, and D. C. Griffin. *Plasma Phys. Control. Fusion*, 48(2):263–293, 2006.

Figures

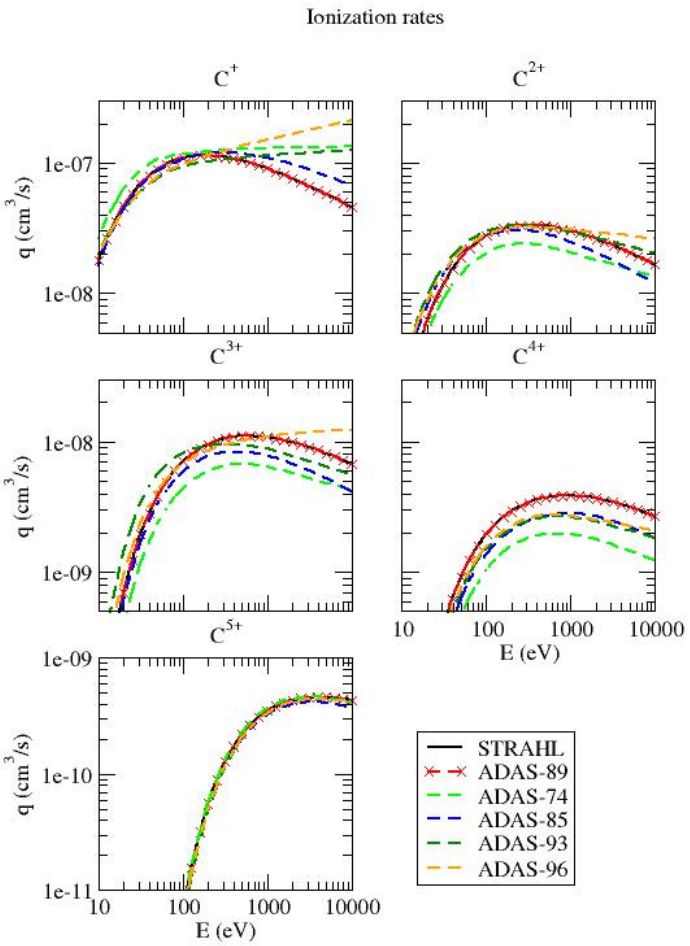

Figure 1: Effective ionization rates from *adf11* format files in ADAS for the various ionization stages of C and data form STRAHL. ADAS89 and STRAHL sets coincide.

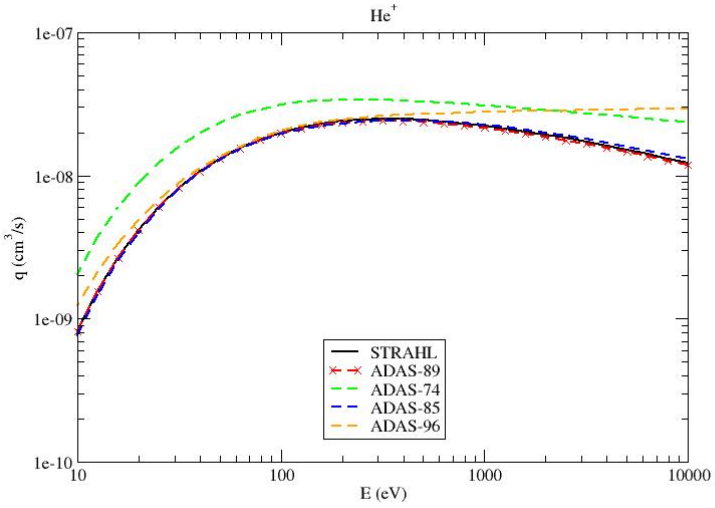

Figure 2: Effective ionization rates from *adf11* format files in ADAS for He^+ and data form STRAHL. ADAS89 and STRAHL sets coincide.

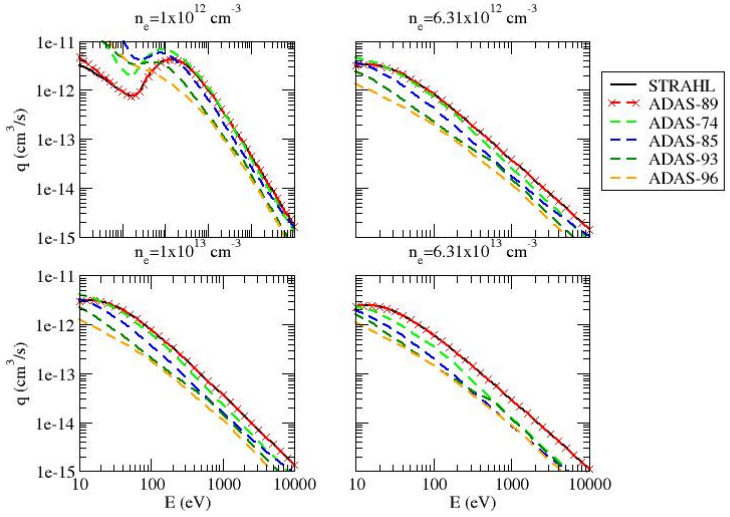

Figure 3: Effective recombination rates from *adf11* format files in ADAS for C^{2+} and data form STRAHL. ADAS89 and STRAHL sets coincide.

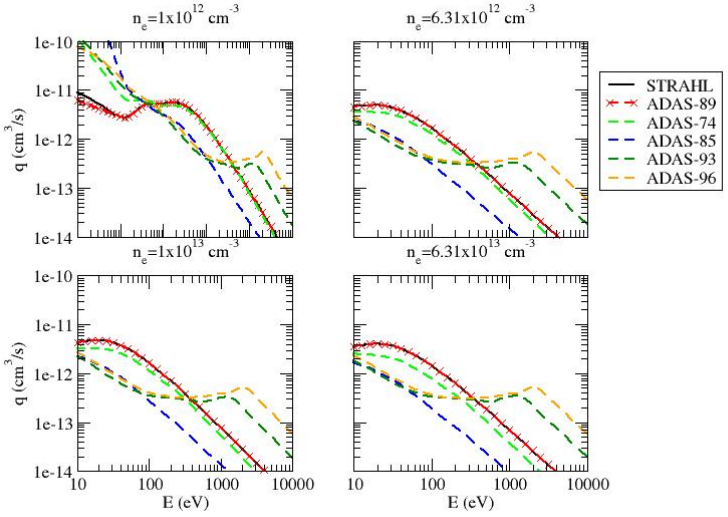

Figure 4: Effective recombination rates from *adf11* format files in ADAS for C^{3+} and data form STRAHL. ADAS89 and STRAHL sets coincide.

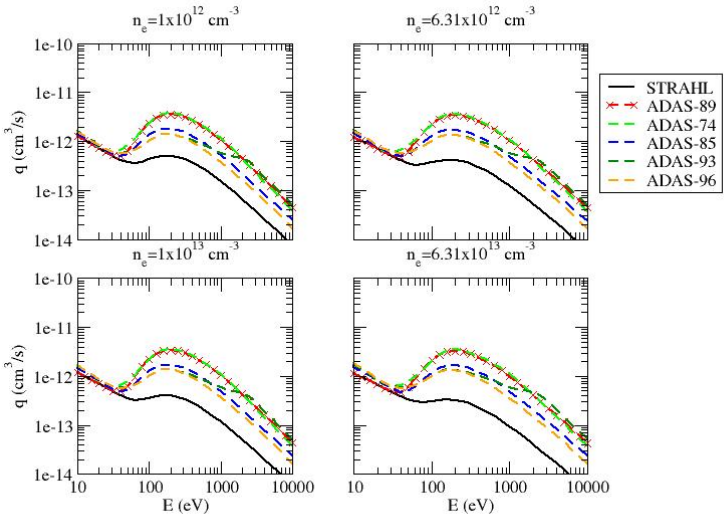

Figure 5: Effective recombination rates from *adf11* format files in ADAS for C^{4+} and data form STRAHL. Dielectronic recombination is here dominant (see text).

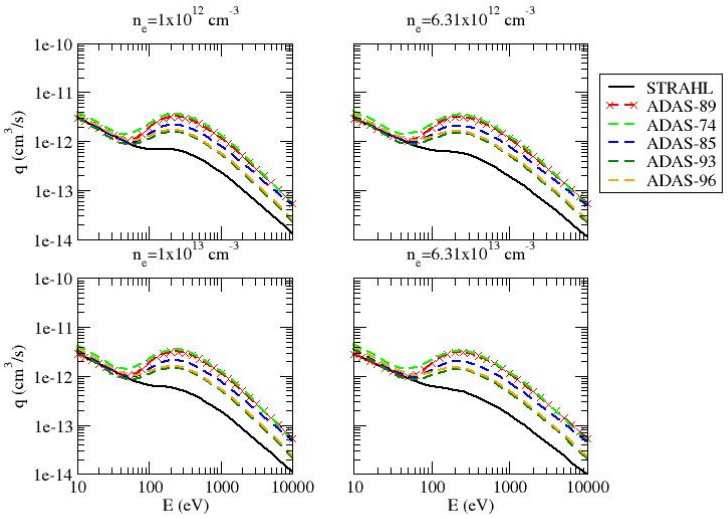

Figure 6: Effective recombination rates from *adf11* format files in ADAS for C^{5+} and data form STRAHL. Dielectronic recombination is here dominant (see text).

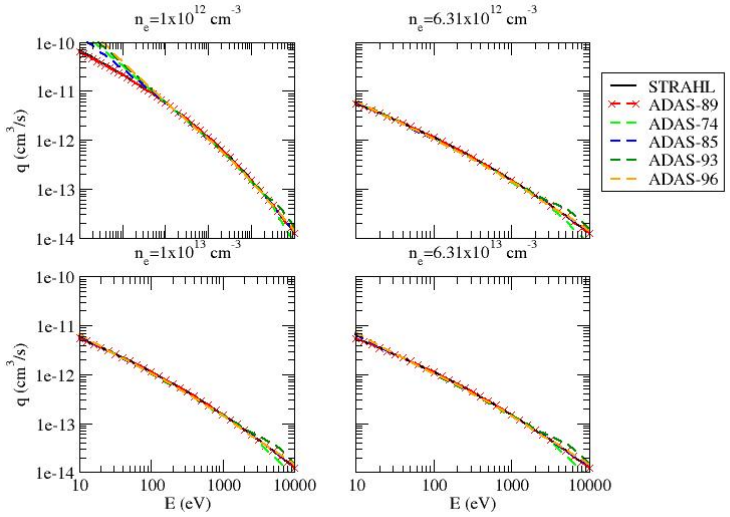

Figure 7: Effective recombination rates from *adf11* format files in ADAS for C^{6+} and data form STRAHL. Only radiative recombination is possible here.

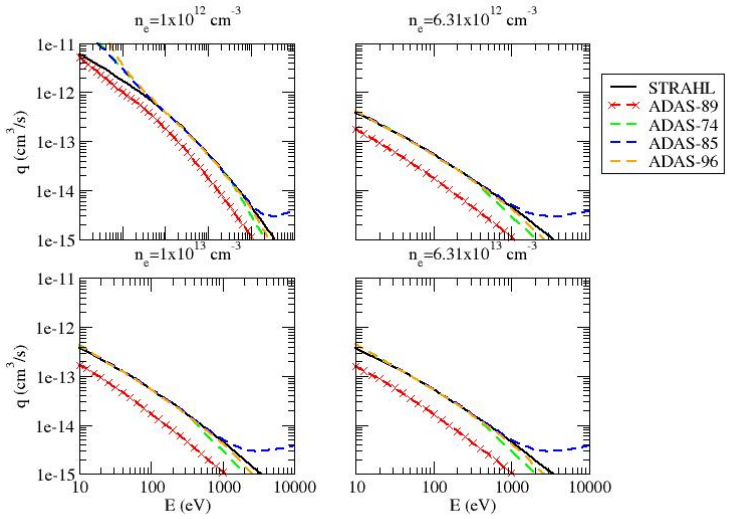

Figure 8: Effective recombination rates from *adf11* format files in ADAS for He^{2+} and data form STRAHL. Only radiative recombination is possible here. ADAS-89 data are a factor of two under the rest of sets.

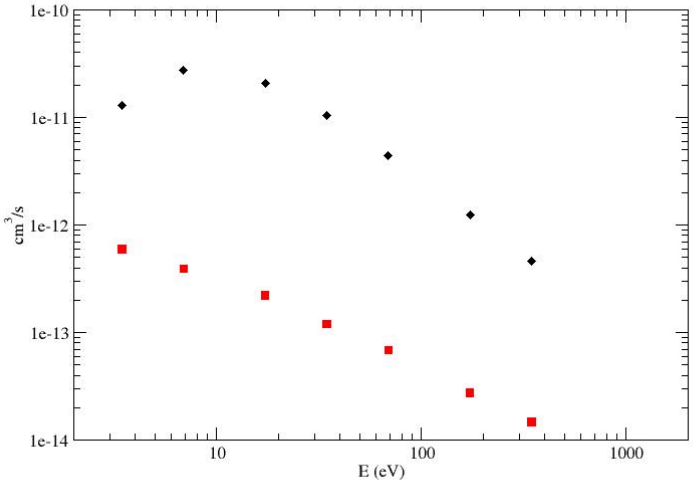

Figure 9: Black diamonts: Total dielectronic recombination $\alpha(T)$ from *adf09* format files in ADAS obtained with ADAS410 for C^{4+} before collisional radiative treatment; red squares: $(2s^2 \rightarrow 2s^2 2p)$ radiative recombination from *adf09* format files in ADAS obtained with ADAS410 for C^{4+} before collisional radiative treatment. Dielectronic recombination dominates.

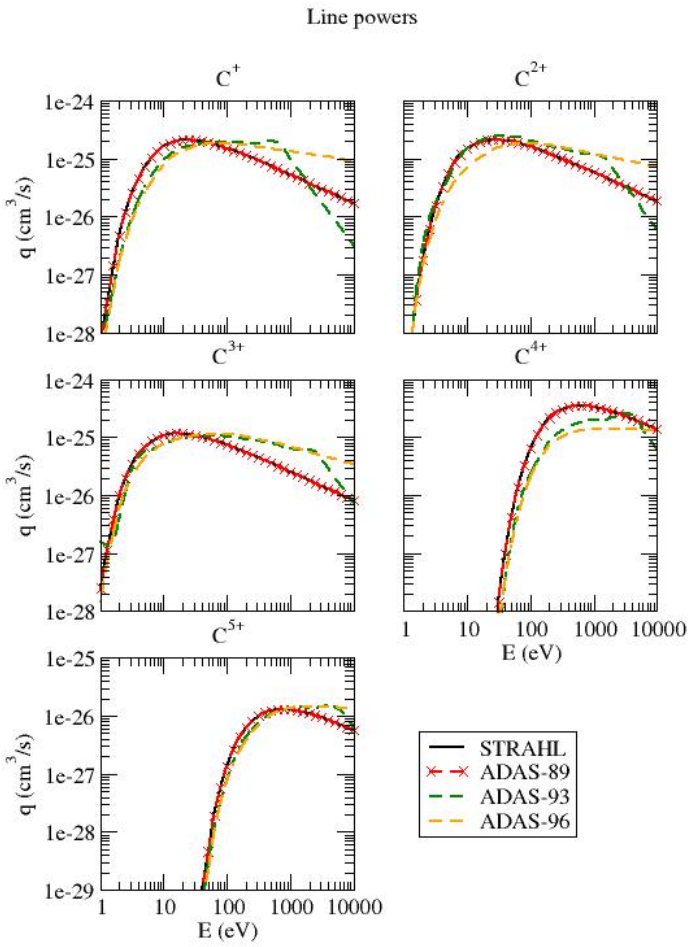

Figure 10: PLTs from *adf11* format files in ADAS for the various ionization stages of C and data form STRAHL. ADAS89 and STRAHL sets coincide.

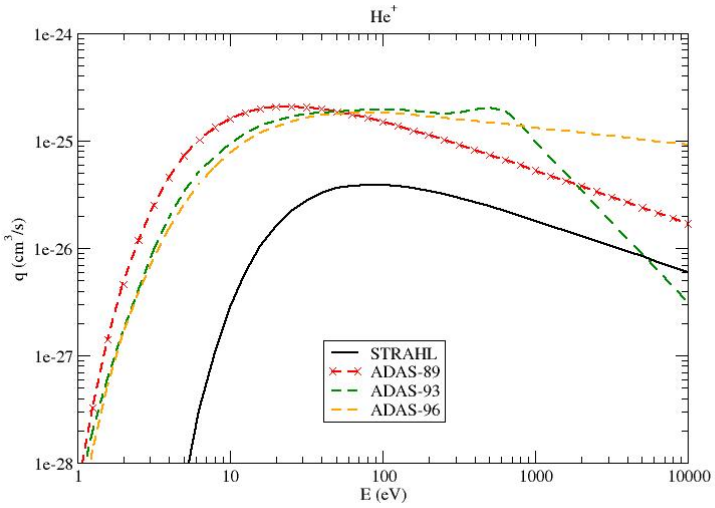

Figure 11: PLTs from *adf11* format files in ADAS for He^+ and data form STRAHL. ADAS89 and STRAHL sets disagree in a factor of two.

Appendix D

ADAS-EU recall report

ADAS-EU Recall Travel Report

Location: EFDA-JET Facility,CCFE Culham Laboratory, Abingdon, UK.
Date: 13-14 June 2011.
ADAS-EU staff: Martin O'Mullane, Hugh Summers, Francisco Guzman (A. Giunta - part)
Purpose: F. Guzman periodic recall, work review and forward planning

Items:

(1) Discussion of progress in the ADAS-EU molecular data and collisional-radiative modelling theme.
(2) Discussion of critical physics issues impacting model and data advance (2nd session).
(3) Planning and scheduling of periodic video-conference and recall meetings for improved coordination and guidance (4th session).
(4) Update on state selective charge exchange data extension for medium/heavy species (3rd session).

ADAS-EU molecular data (1st session):

(5) Fran opening the meeting sessions with a viewgraph presentation updating the principal aspects of his development of the theme. The presentation is appended to this report.
(6) A molecular ADAS development environment, called MADAS, organised in a manner paralleling ADAS itself has been set up by Fran. This is available for exploration of the development by team members. Codes in development at this stage are in Fortran language and are numbered as ADAS901, ADAS902 etc. The development will eventually be incorporated in ADAS as series 9.
(7) Data formats for molecular data have been allocated 'mdf' numbers, again in analogy with 'adf' numbers. It is planned that the 'mdf' formats will exist as such in the ADAS databases.
(8) Molecular data formats in use are:
   a. mdf00: reference data in sub-directories spanning A-values, isotopic vibrational energy level structure and Franck-Condon factors arranged by diatomic system
   b. mdf02: electron and ion impact collisional cross-section data between electronic states.
   c. mdf33 and mdf34 : Maxwell averaged rate coefficients between electronic states, derived from mdf02 for electron collisions and ion collisions respectively.
   d. mdf04: accumulated energy level, A-values and collisional rate coefficients in vibronic resolution.
(9) ADAS902 is the collision cross-section to Maxwell averaged rate coefficient convertor which handles both electron (single Maxwellian) and ion (double Maxwellian) collisions. At the moment, input driver data are assembled in the madas/pass directory for testing. ADAS902 is designed to process a set set of electron collision data from mdf02 to (1-d temperature vector set - T_e) mdf33 and a set of ion collision data from mdf02 to (2-d temperature array set - T_i/T_{mol}) mdf34.
(10) An initial look at the Fortran coding of ADAS902 was made by Martin and Hugh to assess compliance with ADAS layout, particularly of header comments etc. Broadly this is good, but needs to be done in a more complete way for all of series 9 and also for all the new 'mdf' formats for final matching into ADAS. It is proposed to start these detailed adjustments now and record matters in a running document to accompany the planning and meeting evolution of the molecular theme following item (3) - see later comments.
(11) ADAS90,1, the mdf04 display and exploration code, is in progress but was not presented at the meeting.
(12) Fran outlined his proposed timeline for development, which progressed through data expansion and handling using ADAS901 and ADAS902 over the next few months, onto the molecular collisional-radiative model for H_2 towards the end of the year. Hugh expressed anxiety with this schedule, since he felt that the collisional-radiative model was of central importance for the theme delivery and that in his experience, an early model

(13) Fran felt that more guidance from Hugh and Martin would be helpful in the theme development. Hugh, explained about the gap in supervisory capability because of Allan's departure, Martin's engagement with ITER and his own obligation to the completing PhD students. With the very successful delivery of Chris Nicholas and Alessandra Giunta's theses, Hugh expressed the view that the light/medium weight element GCR theme and the special feature themes of ADAS-EU were now in a stable and secure state for final write-up and he felt confident that better systematic supervisory attention could now be given to the molecular and charge exchange themes.

(14) Hugh was strongly of the opinion that the work-up of the molecular collisional-radiative model should not be delayed. He outlined a first set of steps towards bringing the model into realisation. These included evaluation of H_2 , H_2^+ , H and H^+ ground state on-diagonal relaxation time constants resolved by type of process, Extension to excited electronic states and then to ground vibrational states of H_2 and H_2^+. He felt that plots of these values as contours in temperature/density plane would clarify the primary partitioning of the whole collisional-radiative matrix. The next step would be evaluation of the coupling matrix partitions linking the H_2 and H_2^+ systems to the excited states of H. It was agreed that Fran would try to follow these indicative directions in the next weeks. The details and progress will be recorded in the running document as mentioned in (10) above.

(15) Fran indicated a need to fill in a range of data between excited vibronic states for which primary sources were not available. Gryzinski's approximations along with IPRATE from ADAS had been used for such transitions by Fantz and Wunderlich. Fran considered whether ECIP and or EIQIP from ADAS might be suitable. Hugh outlined the basis of both ECIP and EIQIP. In particular he pointed out the dipole only character of EIQIP and some of its special features for handling the strong coupling regime, its use of hyperbolic orbits for collisions with targets of positive charge and its application to positive ion colliders as well as electrons. Hugh also elaborated on ECIP including its connecting of a classical binary encounter exchange model for close collisions with a semi-classical impact parameter treatment for distant collisions. He also explained the use of threshold and equivalent electron manipulation of ECIP to handle auto-ionisation. Hugh felt this had relevance to pre-dissociation. Martin has been working on tiding EIQIP and it seems therefore appropriate to include EIQIP and ECIP exploration in the molecular theme.

Improved Coordination and support

(16) It was agreed by all that the molecular theme now needs to be pushed fairly quickly to completion, since it has implications for the next visit by Ratko Janev and for a possible ADAS-EU sub-contract for specific high grade electron impact molecular cross-section data. A number of procedures were discussed and it was agreed to implement the following:

a. An approximately monthly tele-conference between Martin, Hugh, Fran and Luis to examine progress and completions over the month.
b. A recall of Fran to JET for detailed work and analysis at three month intervals through to the completion of ADAS-EU.
c. The activation of a running working document recording decisions, intentions and completions of agreed items for execution. This document will include selected results, figures, charts etc. as necessary to allow all to keep up to speed and measure progress.
d. The primary ADAS-EU molecular theme publication/manual PUBL-6 should be started immediately so that completed items such as molecular data format specifications, code descriptors, exploratory figures and theoretical developments can be assembled in a timely manner.

(17) It was agreed that Fran would circulate dates for the first tele-conference and that Hugh would write-up the meeting minutes and prepare the running document and PUBL-6 structures and first entries.

State selective charge exchange data:

(18) Fran drew attention to the improved CTMC for krpton, Kr^{+36} for which Clara has now produced an ADAS adf01 dataset. Fran commented that the density of energy points

was a little low in the key 40-80keV/amu region, but that he had asked Clara to expand in that regime. It was noted that the data extended to very high n-shell.

(19) Martin was keen to complete this to the derived adf12 data and to make comparisons with the universal CX parametric form and data developed by Adam and Hugh. Also the universal form parameters should be re-assessed and updated.

(20) Martin and Fran drew attention to the additional light element state selective CX data in adf01 format from Katherina Igenbergs for N^{+7} and Fran's work on B^{+5} and his update on Be^{+4} Some of these are already validated and included in ADAS. This work needs to be completed, combined with the universal parametric form adjustment and passed through to adf12. The Universal form parameter optimisation code, which updates adf49 needs to be brought into the ADAS series 3 code framework.

(21) Hugh again stressed the importance of the write-up and publications from this work. He suggested that there was the material for an publication, probably in PPCF with Clara, Katherina, Adam, Martin and Fran as authors. He wished to see the material also incorporated coherently in the PUBL_1 as soon as possible. There was general recognition of these necessities.

(22) It seemed appropriate to incorporate these items, their scheduling and progress in the working/running document referred to earlier in (17).

Actions and other issues

(23) Hugh, while recognising the range of interesting queries coming from the different ITER divisions and also our wish to get involved, was concerned that ADAS/ADAS-EU should present a single consistent accurate interface to ITER. It appeared that somewhat similar questions could come to Martin and Fran, without cross-awareness, possibly leading to different replies and even inconsistency with best ADAS practice. . Also, some suggested routes for engagement of Fran with ITER transport were felt by Hugh not to play to ADAS-EU group strengths, and would probably remain very peripheral. These issues can be resolved by working the ADAS-EU line management correctly. All ITER queries and suggestions must be discussed between Fran and Martin, with Hugh also brought in if necessary, so that a properly based management decision to proceed or not can be made.

(24) Fran will check up and notify about the date for the first video-link meeting.

(25) Hugh will set up the working document and prepare an initial list of actions and timescales for their execution, to be agreed or modified in discussion with participants.

HPS
17 June 2011

-