ADAS-EU R(13)DI03

ADAS-EU

ADAS for fusion in Europe

Grant: 224607

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Dissemination report 3

6 June 2013

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

Dissemination report 3

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Abstract: *The report reviews dissemination task completion for project months 36-48. It includes the third ADAS-EU course, which was held in Padua, and the fourth ADAS-EU course, which was held at CEA Cadarache.*

Contents

Chapter 1

Overview and milestone DSM3

As discussed in report DISSEM2, the third ADAS-EU course, originally scheduled for 2011 was held at RFX Padua on 26-30 March 2012, to fit in with RFX operations. The fourth and final course was presented at CEA Cadarache on 26 September to 4 October 2012 following the 2012 ADAS Workshop.

1.1 ADAS-EU Courses: Work packages 20-1-3 and 20-2-3

The Padua course was one of the most enjoyable of the whole set of courses. It brought together very motivated participants from all over the world who engaged very strongly with the spectral diagnostic impact of the material of course. They came with local applications, interpretations and questions. Many contacts and interactions were made, which have continued. Also, at the Padua couse, Dr Antidormi, the overseeing scientific officer of ADAS-EU at the EU Commission, was able to attend and give a presentation indicating in person the Commission's interest and support of the ADAS-EU international collaborative perspectives. The practice, adopted at ADAS-EU courses, of taking sufficient time for each participant to describe his/her research activities in some detail to the whole group and then engage in consequential group discussion of it, has proved very fruitful and unifying. Amongst many, the contributions of Mark Holmberg (Madison, Wisconsin USA) and Bharathi Punyapu (IPR, Gandhinagar, India) are noted. The agenda, participant and presentation details are in appendices A and B. The provision of facilties at RFX Padua is gratefully acknowledged.

The CEA Cadarache course participation was a little smaller. Of special note was the participation for three days of Prof. Gary Ferland, a noted astrophyicist who had also participated in the ADAS Workshop. This laid some special emphasis on atomic modelling of dielectronic recombination in low temperature plasma and allowed fuller discussion with participants and Prof. Badnell for ADAS-EU, a specialist course presenter in this area. In the group discussions, the wide-ranging contribution of Juan Huang (ASIPP, Hefei, China) is noted.The agenda, participant and presentation details are in appendices C and D. The provision of facilties at CEA Cadarache is gratefully acknowledged.

The requirements of the work packages have been met.

1.2 ADAS-EU external visits/contacts: Work packages 21-1-3 and 21-2-3

A special meeting, focussed on tungsten ions, was held at the EFDA-JET Facility, Culaham Laboratory, UK on 26-27 April 2012. This had a dual purpose of disseminating the information obtained in ADAS-EU and its associated sub-contracts on tungsten to the diagnostic and modelling task forces at EFDA-JET in a joint session on 27 April. As such, it brought together task forces leaders, spectroscopists and spectral analysts from EFDA-JET and CCFE, Culham and the specialist university teams from Strathclyde, Vilnius and Mons-Hainaut. Secondly, it brought the specialist teams together for a two-day period to consider and plan on-going research on tungsten ions, in the light of the interests and needs of the JET fusion programme and the implications of the sub-contract delivery which had already been made

in this area. The presentation made to the joint meeting by Dr. O'Mullane on the state of tungsten modelling is in appendix E. The overall meeting short report is also in appendix E.

Dr Guzman made two visits in May 2012, firstly to present the status of the ADAS-EU molecular collisional- radiative modelling at the 2012 Plasma Surface Interaction Conference, Aachen 21-25 May 2012, followed by a visit to FZ Juelich on 29 May 2012 to discuss the integration of the upgraded molecular database and the collisional-radaiive modelling derived data at Juelich. The conference presentation and travel report are given appendix F.

Dr. O'Mullane, as part of the dissemination from ADAS-EU participated in the IAEA Technical Meeting on Atomic and Molecular Data Validation at Daejeon, Korea 4-7 September 2012. The whole meeting summary and conclusion are available as'Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion ', a Joint IAEA-NFRI Technical Meeting (report: https://www-amdis.iaea.org/publications/INDC/INDC_NDS-627.pdf). He also participated in the Integrated Tokamak modelling meeting in Innsbruck 3-7 December. The travel for both of these meetings was not funded from ADAS-EU. See appendix G for details of these presentations.

Dr O'Mullane has continued with his frequent visits to ITER. During the period of this report, the conceptual design phase for ITER spectroscopic diagnostics has been continuing, with atomic model predictions very much required. Such studies link ADAS strongly with the ITER Domestic Agency teams of the countries responsible for the design and construction of the various diagnostics. It is therefore a key part of the dissemination programme. The contact with Korea and India is of special note. In particular the contact with Korea has deepend and has included a special working visit in support of transport modelling, by Stuart Henderson (a PhD student of Prof. Summers and Dr. O'Mullane) to NFRI, Daejeon (independently funded). The ITER engagement of ADAS-EU, through Dr O'Mullane, is described separately for this period in report ITER2.

It is concluded that the dissemination plans of ADAS-EU and the associated spread of European atomic physics influence in the fusion plasma world are continuing to progress well. The requirements of the work packages have been met.

1.3 Work package 26-4-3

The work package task comprises the preparation of this report.

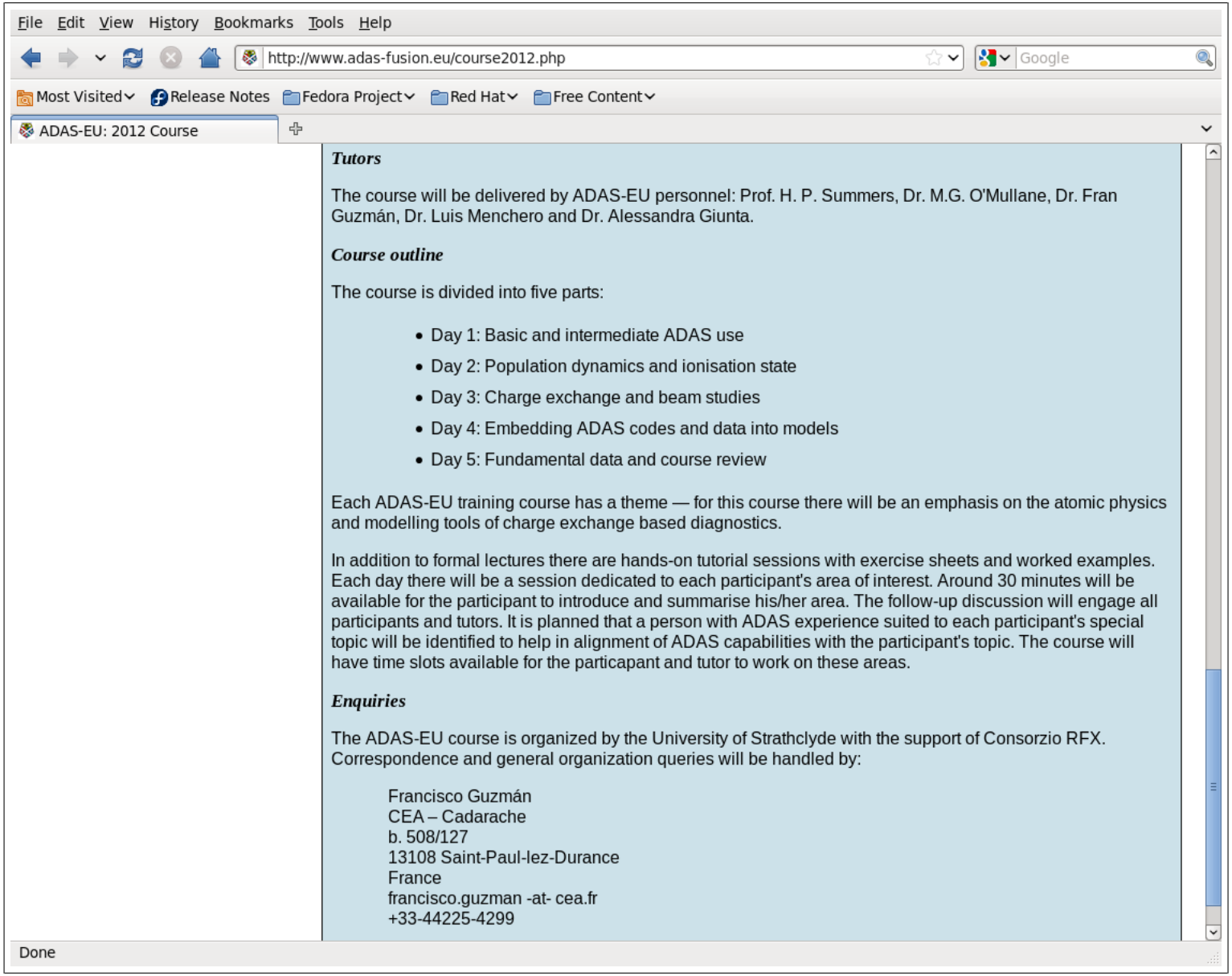
Appendix A

ADAS-EU course 2012a announcements, agenda and participants

[1] ADAS-EU_course_2012a
[2] ADAS-EU_course_agenda_2012a
[3] adas-eu_course_participants_2012a

A.1 Announcement

File Edit View History Bookmarks Tools Help
http://www.adas-fusion.eu/course2012.php
Google
Most Visited
Release Notes
Fedora Project
Red Hat
Free Content
ADAS-EU: 2012 Course
Eligibility and numbers
The course is open to researchers in the area of magnetic confinement fusion at associated laboratories of the European Fusion Programme (EURATOM) or at European Universities. Participants may also be nominated by any institution, world-wide, which is a member of the ADAS Project. The maximum number of participants is ten, with three places reserved for the hosting institution (Consorzio RFX). Preference will be given to persons who can attend the full course. There is no other participant selection process. Applications received after the lists are filled will be reserved in order of receipt, in case places are freed in either of the first two categories.
Time and place for the course
The course will take place at Consorzio RFX located in Padua, Italy. It will commence at 9.00 on Monday 26 March and finish at 15.00 on Friday 30 March. It is expected that participants will attend for the full duration of the course. Each day will have a number of lectures and hands-on tutorial sessions. Round table discussions on participants interests are a key feature of ADAS-EU training courses.
Accommodation and travel
Details on how to travel to RFX are here.
The closest airport is Marco Polo, Venice (VCE). There are two ways to travel from the airport to Padua:
The AirService pooled taxi service. The one-way cost is €30/person for transfer direct to your hotel in 30 minutes. However it must be booked in advance via their website.
There is a regular SITA coach which costs €8 and takes 40 minute and terminates at the city train station which is a 15–20 minute walk to the hotels. Tickets can be purchased from the ATVO desk at the airport. Buses run once per hour and the last bus on Sunday is at 21:40.
There is hotel accommodation either close by the laboratory or in nearby Padua. The latter is more pleasant and we recommend that you stay here so that we can meet up in the evenings. Two hotels are recommended:
Hotel Giotto
Hotel Igea
which are mid-price downtown hotels. Most of the ADAS tutors will be staying at the Hotel Giotto but Hotel Igea is just 200m away.
Unfortunately Consorzio RFX is located in a fairly anonymous industrial area but it is well served by the number 7 bus which has a stop very close to the hotels. The cost of a single journey is €1.20.
Done



Tutors

The course will be delivered by ADAS-EU personnel: Prof. H. P. Summers, Dr. M.G. O'Mullane, Dr. Fran Guzmán, Dr. Luis Menchero and Dr. Alessandra Giunta.

Course outline

The course is divided into five parts:

- Day 1: Basic and intermediate ADAS use
- Day 2: Population dynamics and ionisation state
- Day 3: Charge exchange and beam studies
- Day 4: Embedding ADAS codes and data into models
- Day 5: Fundamental data and course review

Each ADAS-EU training course has a theme — for this course there will be an emphasis on the atomic physics and modelling tools of charge exchange based diagnostics.

In addition to formal lectures there are hands-on tutorial sessions with exercise sheets and worked examples. Each day there will be a session dedicated to each participant's area of interest. Around 30 minutes will be available for the participant to introduce and summarise his/her area. The follow-up discussion will engage all participants and tutors. It is planned that a person with ADAS experience suited to each participant's special topic will be identified to help in alignment of ADAS capabilities with the participant's topic. The course will have time slots available for the particapant and tutor to work on these areas.

Enquiries

The ADAS-EU course is organized by the University of Strathclyde with the support of Consorzio RFX. Correspondence and general organization queries will be handled by:

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13108 Saint-Paul-lez-Durance
France
francisco.guzman -at- cea.fr
+33-44225-4299

A.2 Agenda

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Monday:    Welcome from Lorella Carraro (RFX)
           Introduction to ADAS (MOM)
           Interactive ADAS (LFM)
           Coffee and computer setup
           First Tutorial
           Lunch
           Round-table (1-1.5 hrs)
           Population modelling (AG)
           Coffee
           Tutorial and one-to-one instruction

Tuesday:   Embedding ADAS in other codes (MOM)
           Ionization state (AG)
           Coffee
           Tutorial
           Lunch
           Round-table (1-1.5 hrs)
           Impurity transport (MOM)
           Coffee
           Tutorial and one-to-one instruction

Wednesday: Charge exchange (HPS)
           Developments in CX data (FG)
           Coffee
           Tutorial
           Lunch
           Round-table (1-1.5 hrs)
           Beam models in ADAS (MOM)
           Coffee
           Developments in beam models (LFM)
           Tutorial and one-to-one instruction

Thursday:  Argon experiments and approach to analysis (FG)
           State of CX analysis tools (MOM)
           Coffee
           Tutorial
           Lunch
           Round-table (1-1.5 hrs)
           Coffee
           Advanced population models (HPS)
           Tutorial and one-to-one instruction

Friday:    Non-interactive ADAS and fundamental data (MOM)
           Preview of molecular population models (FG)
           Tutorial
           Coffee
           Round-table round-up
           Lunch
           ADAS-EU achievements (HPS)
           EU fostering of collaborative research (RA)
           Coffee
           End of course
           ADAS-EU meeting

MOM : Martin O'Mullane
HPS : Hugh Summers
FG  : Francisco Guzman
AG  : Alessandra Giunta
LFM : Luis Menchera
RA  : Rosa Antidormi (EU Commission)
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A.3 Participants

ADAS-EU course

Consorzio RFX Padua

26-30 March 2012

Participants

Tullio Barbui	RFX, Padua	tullio.barbui@igi.cnr.it
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Robert Toth	Uinv. of Tech. & Econ., Budapest	trobertino@gmail.com
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Francisco Guzman	Univ. of Strathclyde, Glasgow	francisco.guzman@cea.fr
Luis Menchero	Univ. of Strathclyde, Glasgow	luis.menchero@ipp.mpg.de
Alessandra Giunta	Univ. of Strathclyde, Glasgow	alessandra.giunta@phys.strath.ac.uk
Rosa Antidormi	European Commission	rosa.antidormi@ec.europa.eu

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Appendix B

ADAS-EU course 2012a lectures and tutorial exercises

[1] adas-eu_lec_introduction_2012a (first page)
[2] adas-eu_lec_interactive_adas_2012a (first page)
[3] adas-eu_lec_excited_population_structure_2012a (first page)
[4] adas-eu_lec_callable_adas_2012a (first page)
[5] adas-eu_lec_ionstate_1_2012a (first page)
[6] adas-eu_lec_impurity_transport_2012a (first page)
[7] adas-eu_lec_charge_exchange-spectroscopy_2012a(first page)
[8] adas-eu_lec_charge_exchange_data_2012a (first page)
[9] adas-eu_lec_adas_beam_codes_2012a (first page)
[10] adas-eu_lec_stark_state_advanced_modelling_2012a (first page)
[11] adas-eu_lec_argon_experiments_and_analysis_2012a (first page)
[12] adas-eu_lec_cx_analysis_tools_2012a (first page)
[13] adas-eu_lec_advanced_population_models_2012a (first pages)
[14] adas-eu_lec_fundamental_data_production_2012a.pdf (first page)
[15] adas-eu_lec_hydrogen_molecular_modelling_2012a (first pages)
[16] adas-eu_lec_achievements_2012a.pdf (first page)
[17] adas-eu_lec_eu_research_2012a.pdf (first page)

[18] ADAS-EU_tut1-ex_overview_2012a
[19] ADAS-EU_tut2-ex_excited_population_models_2012a
[20] ADAS-EU_tut3-ex_ionization_state_2012a
[21] ADAS-EU_tut4-ex_charge_exchange_spectroscopy_2012a
[22] ADAS-EU_tut5-ex_beam_stopping_and_emission_2012a
[23] ADAS-EU_tut6-ex_exercises_2012a

B.1 Lectures

University of
Strathclyde
Glasgow
Background to ADAS
Martin O'Mullane
Department of Physics
University of Strathclyde
ADAS-EU course, Consorzio RFX, Italy 26-March-2012

Interactive ADAS

L. Fernández-Menchero

ADAS, University of Strathclyde. United Kingdom.
Institut Max Plank für Plasmaphysik. Garching, Germany.

ADAS Course 2012, Consorzio, Padova, Italy.
March 26th, 2012

2b. The interactive system – working with excited population structure

- Datasets of class ADF04 contain all the information necessary to evaluate excited populations of an ion. It is called a ‘specific ion file’.
- Code ADAS205 computes the populations at temperatures and densities of your choice.
- The input, data set selection, screen is very similar to that for ADAS201

Callable ADAS

Martin O'Mullane
Department of Physics
University of Strathclyde

The ionisation state of ions in a plasma part 1

- Effective ionisation and recombination coefficients
  - » Data sets of class ADF11
  - » Interrogating ADF11 using ADAS402.
- Equilibrium ionisation balance
  - » Using adas405 to examine the temperature and density dependent equilibrium ionisation balance

Impurity data analysis using UTC

K-D Zastrow and M O'Mullane

Charge exchange spectroscopy

- Preliminaries
- ADAS series 5/series2 - thermal charge transfer
- ADAS series 3 - charge transfer with neutral beams

Developments in CX data.

Francisco Guzmán

ADAS-EU
University of Strathclyde

ADAS-EU course – 26 – 30 Mars 2012

Beam stopping and Beam emission spectroscopy

- Extracting effective beam stopping coefficients or beam emission coefficients using ADAS304.
- Calculating the beam population structure using ADAS310
- Details of beam emission with adas305_get_stark.pro

Developments in beam models

L. Fernández-Menchero

ADAS, University of Strathclyde. United Kingdom.
Institut Max Plank für Plasmaphysik. Garching, Germany.

ADAS Course 2012, Consorzio, Padova, Italy.
March 28th, 2012

Ar experiments and analysis

Francisco Guzmán

ADAS-EU
University of Strathclyde

ADAS-EU course – 26 – 30 Mars 2012

State of CX analysis tools

Martin O'Mullane
Department of Physics
University of Strathclyde

Advanced population modelling

Hugh Summers

University of Strathclyde

29 Mar. 2012
ADAS-EU Course, Padua

Non-interactive ADAS and fundamental data

Martin O'Mullane
Department of Physics
University of Strathclyde

Preview of molecular population models

Francisco Guzmán

ADAS-EU
University of Strathclyde

ADAS-EU course – 26 – 30 Mars 2012

ADAS-EU and ADAS fusion support

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

University of Strathclyde
CCFE Culham/JET

30 Mar. 2012
RFX Padua

The European fusion energy research programme: status & outlook

Rosa Antidormi
European Commission

ADAS EU course 2012
Padova, RFX, 30 March 2012

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B.2 Tutorial exercises

Tutorial session 1 examples

1. Initial set up

1. The tutorial assumes ADAS is set up for operation from your terminal and that your personal */home/<uid>/adas/* directory and sub-directories *pass/* and *defaults/* have been initialised
2. The *pass/* directory is used for data sets created by ADAS, which you choose finally how to dispose of. The *defaults/* directory remembers all the settings you selected on your last run of every ADAS code. Since ADAS codes may have changed, if you have already used ADAS, your *defaults*/ directory files may be out of date. This will cause codes to crash, so it may be best to delete all the files in the *defaults*/ directory and start afresh.
3. Move to the central adas file space [*cd /home/adas*]. Look at the directories at this level [*ls*]. You will see the directory *doc*/. Move into it and look again [*cd docs; ls*]. You should see the various sub-directories including *bulletin*/ and *manual*/. Move into the bulletins and look again [*cd bulletin; ls*]. You will see all the bulletins including the one *sep25_09.pdf*.
4. Bring up a acrobat viewer for *.pdf* files [*acroread &*] to look at the *sep25_09.pdf* bulletin. 'Bug fix' releases and the associated bulletin comes out annually or occasionally more frequently. New code releases are separate and occur when ready.
5. Return to the Terminal window, move into the *docs*/ subdirectory *manual*/ and list the files. *appxa* files describe the ADAS data and the others describe the ADAS codes. Use the acrobat reader to look at *chap5-03.pdf* and at *appxa-15.pdf*.
6. Move to the directory */work/projects/adas/*. Notice the *fortran*/ and *idl*/ subdirectories. Move into *fortran*/ and list and then down into *adas5xx*/ look again. Finally move down into *adas501*/ for a final look. You are now at the FORTRAN codes themselves. Note that on your own site the source fortran may not be accessible to the ordinary user.
7. Now move to the directory */work/projects/adas/adas/* and list. This is the database itself. Look down into ADAS data format *adf04*. Actual datasets rather than directories have the terminator *.dat*.
8. Move back to your own *pass/* directory [*cd ~/adas/pass/*]. Start up ADAS [*adas*]. The main ADAS menu pops up.
9. Note that it is best to start ADAS from your sub-directory */.../<uid>/adas/pass*. Graph and text hardcopy files created by ADAS will appear in the directory from which you launch ADAS.

2. Starting interactive ADAS and using its general GUI widgets

1. Move to your sub-directory */.../<uid>/adas/pass*. Graph and text hardcopy will consequently appear here. Start ADAS [type *adas*]and go to the ADAS5 series sub-menu. Click with the mouse on the first button in adas5 series for ADAS501. The Input window for ADAS501 pops up.
2. Click on *Central Data*, the data root to data class ADF13 should appear dimmed in the window above. Click on the directory name *sxb93#cr* in the datafile list window. *sxb93#cr* appears above in the selection window. Click on *sxb93#cr_llu#cr0.dat*. It appears in the selection window.
3. Click the *Browse comments* button. Information of what is in the file *sxb93#cr_llu#cr0.dat* is displayed. Click *Done* to restore the Input window. Click *Done* and the ADAS501 Processing window appears.
4. Click on the *Fit polynomial* button, then type [*5 {return}*] in the adjacent active editable box. Click on the first transition at 4270.7Å in the transition list window. It appears in the selection window above.
5. Click on the *Default Temperatures Values* button. If a warning pop-up appears, click *Confirm* on it. A set of density values appears in a pop-up window. Click on 1.000E+13. The temperature and density output values appear in the table.
6. Click on the *Done* button to proceed to the Output options window.
7. Click on the button for *Graphical Output*.
8. Select *Post-Script* out put by clicking on it in the Select Device list window. Click on the button for *Enable Hard Copy*. Enter a File Name such as graph.ps. Remember to press {*return*}. A warning widget appears if *graph.ps* already exits. If so click on *Replace*.
9. Click on the button for *Text Output*. Type in *paper.txt* - this is the standard text output File Name. [On many Output windows, there is a *Default File Name* button. You can click on it to enter *paper.txt* as the standard text output File Name.] Then click *Done*.

ADAS-EU Course at RFX 26-30 March 2012

10. The graph appears in the next window. Click on *Print* to send a copy of the graph to the *graph.ps* file. Click *Done* to return to the Output Options window. Click on *the Exit to Menu* icon at the bottom left corner to restore the ADAS5 series menu. Finally click on the *Exit* button on the sub-menu and main menu windows to exit ADAS.
11. [*ls*] to see the files. You may wish to list *paper.txt* to see its format.

3. Using the Table Editor widget

1. Repeat steps 1-3 above. Click on *Edit Table* on the processing screen. Table Editor pops up.
2. The values in italic font are your input data. Click in any of these boxes to edit the number within it. The workstation cut, paste and copy keys operate. Press the *return* key on the keyboard to record any change. This is the normal editing mode.
3. The set of round and square buttons below the table are designed to help in some editing tasks. You must be careful to remember the sequence of operations since it is different from that on personal computers. **Activate** the appropriate button, **position** the mouse text cursor or drag over required digits, **press** the *return* key on the keyboard to complete the sequence.
4. The *Default* round button is the reset to normal editing mode. The *Delete* button allows deletion of the value in a box, leaving an empty box; the *Remove* button allows deletion of a value with the column then being pushed up; the *Insert* button creates a new empty box, pushing the column down. These buttons stay active until you click *Default*.
5. The *Copy* and *Paste* round buttons operate for the next immediate action only.
6. Square buttons have a continuing effect until an alternative is pressed. The *Row_skip* button causes a jump to the next editable box in a row when the *return* key on the keyboard is pressed; *Column_skip* causes jumping to next box in a column. *Scroll up* moves the whole window down. Note that the window only shows ten values in a column, but the whole table may be longer that this.
7. Preferred Temperature units for working with may be chosen. Changing units causes the Inputs from the file to change to the new units. It **does not** change any Output values already typed in. It merely interprets Output values in the selected units.
8. Press the *Done* button to record the changes and return to the screen from which Table Editor was initiated. The *Cancel* button prevents the new values being substituted on return.

9. You may be interested to try some of the more advanced widgets used by ADAS501. On the processing screen click Value selection by Display. A description of how to use this is in the user manual *introduction.pdf*.
10. On the graphical display, you may like to try the *Retain* and *Adjust* buttons. Again details of use are in the user manual *introduction.pdf*.

Tutorial session 2 examples

1. **ADF04**
   1.1. Explore the /…/adas/adas/adf04 database. Note that a summary of the data base is given in the ADAS User manual *appxa-04.pdf*.

2. **ADAS201 Test Case**
   2.1. Move to your sub-directory */.../<uid>/adas/pass*. Graph and text hardcopy will consequently appear here. Start ADAS [type *adas*] and go to the ADAS2 series sub-menu. Start ADAS201.
   2.2. Click on *Central Data*, the data root to data class ADF04 should appear dimmed in the window above. Click on the directory name *adas#7* in the datafile list window. Note the designations. The 'ic' denotes J-resolved intermediate coupling system. 'ls' denotes a term resolution system. The 'n' case is a special bundled –n system for the hydrogen-like ion. The degeneracy ensures very strong mixing by ion collisions which can be assumed complete.
   2.3. Select *cop98#7_ic#n3.dat* . Click the *Browse comments* button. Information on the content and quality of the data set can be reviewed.. Click *Done* to restore the Input window. Click *Done* and the ADA201 Processing window appears.
   2.4. You may select to have a polynomial fit by clicking *Fit polynomial* button, and selecting a accuarcy (%) in the adjacent active editable box..
   2.5. Activate the *Select Temperaturesfor output file* button to obtain a numerical tabulation of results. Either edit in the temperatures you wish or click the *Default Temperatures Values* button.
   2.6. Click on the *Done* button to proceed to the Output options window and *Graphical Output*.
   2.7. Select *Post-Script* and *Enable Hard Copy* and assign an output graph file.
   2.8. Click on the button for *Text Output*. And route output to *paper.txt*, the standard text output File Name. Then click *Done*.
   2.9. The graph appears in the next window. Click on *Print* to send a copy of the graph file. Click *Done* to return to the Output Options window. Click on *the Exit to Menu* icon at the bottom left corner to restore the ADAS5 series menu. *paper.txt* is not viewable with an editor until you exit.
   2.10. You may wish to examine the *paper.txt* file to see its format.

3. **Additional exercise**
   3.1. Restart ADAS201 and again select the adas#7 sub-directory. Select the *cop98#7_ls#n3.dat* file. Browse the comments. Note that this file is obtained by bundling the level resolved 'ic' file you fist chose into terms. This procedure you will observe in the comments was done by ADAS209. You may wish to try ADAS209. The operation is described in the ADAS User manual Chap3-09.

4. **ADAS811 Test case**
   4.1. ADAS811 is a new and more sophisticated interrogation code on ADF04 files. It allows not only display of single collision rates but comparison of such data from different ADF04 files. [Note this code uses the configuration information and quantum numbers to match transitions between different files. If you use a non-standard (that is not *ADAS Standard* or *Eissner*) form, the code will fail to match – it is quite sensitive.
   4.2. For this test we shall compare a high grade assessed boron-like ion of oxygen (*adas#8/cop98#8_ls#o3.dat* with a much older impact parameter cross-section based data set (*copss#b/copss#b_ss#o3l.dat*) built on a SUPERSTRUCTURE calculation.
   4.3. Select the first data set in the in the upper part of the Input window. The second data set is selected in the lower part and uses a more standard Unix file selection so that files can be tested during construction when not located in your ADAS space. You can choose a third file if you wish (e.g. the Born baseline *copmm#8/ls#o3.dat*).
   4.4. There is only a further display screen which incorporates selection and controls. At this stage we are only concerned with electron impact excitation data. This is the default *e-exc* in the Type of Plot. The Type of e-exc plot is selectable. Note the usual Upsilon (gamma) and excitation rate coefficient, but also the Burgess C-plot.

4.5. At the top of the window, select the file whose transitions youn wish to step through. The code will attempt to match transitions from the other file to it – which may nit be successful indeed the transition may not exist in the other files.
4.6. Note the tape recorder controls at the bottom. The upper and lower indices of a particular transition may be entered in the editable boxes. Then click *Show*.
4.7. We find it convenient to have the files open in an editor as we do the examination.
4.8. Note the cursor is active for reading of values.
4.9. *Print* will send the displayed transition to a file (via a pop-up dialogue). Be cautious of using the *Print All* button – there may be a lot of electron impact excitation transitions.

5. ADAS205 Test Case

5.1. Move to your sub-directory */.../<uid>/adas/pass*. ADAS205.
5.2. Click on *Central Data*. Select the Be-like oxygen case *adas#8/cop98#8_ls#o4.dat*.
5.3. Click on the *Default Temperatures button* and *Default Densities* button.
5.4. Click on the *Selections* button for metastable states. A pop-up list of all the levels appears. Click on the button beside the first level. Note that it darkens. It is a click on/click off button. Then click on its *Done* button to restore the full Processing options window.
5.5. Click on the *Done* button to proceed to the Output options window.
5.6. Click on the button for *Graphics* to display the graphics choices then click on the button for *Graphical Output*. Select *Graph Temperature* by clicking on the one you wish in the list. Choose the fifth one [1e5]. Click on the *Text* button to display the output data set choices. Click on the *Contour File* button and enter *contour.pass* in the File Name editable window. Then click *Done*. The graph pops up. There are several graphs to look at. Finally click *Done* to restore the Output options window. Click the *Exit to Menu* icon to finish up. Finally click on the *Exit* button on the sub-menu and main menu windows to exit ADAS.
5.7. Note the files created includes the collection file *contour.pass.* You may wish look at its format.

6. ADAS207 Test Case

6.1. Move to your sub-directory */.../<uid>/adas/pass*. Make sure you have a *contour.pass* file there. Start ADAS and go to the ADAS2 series sub-menu. Click with the mouse on the seventh button in adas2 series for ADAS207. The Input window for ADAS207 pops up.
6.2. Click on *User Data*, the data root to you /pass sub-directory should appear in the window alongside. Click on *contour.pass* in the file list window. It appears in the selection window.
6.3. Click *Done* and the ADAS207 Processing window appears.
6.4. Click on the *Selections* button for the 1st composite line assembly. The window with the full list of lines pops up. Click on the buttons alongside the lines you wish for the numerator of the line ratio. These are on/off buttons. Note a button is darkened when activated and the program remembers the choice you made if you have had a previous run. Select transition 2 for the test. Click the *Done* button.
6.5. Click on the *Selections* button for the 2nd composite line assembly. The window with the full list of lines pops up. Click on the buttons alongside the lines you wish for the numerator of the line ratio. Select transition 26 for the test. Click the *Done* button.
6.6. Click on the *Done* button to proceed to the Output options window.
6.7. Click on the button for *Graphical Output*. Click on the *Diagnostic Contour Plot* button. This brings up contour plot choices. Click on the *Default Contour Scaling* button if not already selected. Then click *Done*. The graph pops up.
6.8. An object of such a plot is to detect diagnostic line ratios, that is ratios senitive to density or temperature. Note that the contour plot gives an overview but is coarse.

Example 7

6.9. Experiment with the same data set in ADAS205 but edit in a relevant range of electron temperatures and densities for the density sensitive region. Proceed to form the *contour.pass* file. Now run ADAS207 with this *contour.pass* file. Try adding more lines to the two composites or changing the lines.

Example 8

6.10. Repeat the above but at the metastable selection in the ADAS205 Processing options window, select the first and second levels. Follow through the consequences to ADAS207. Remember to obtain a contour output file from ADAS205.

6.11. Note that with two metastables, we have the opportunity to shift their relative number densities from that in equilibrium. Generally a dynamic ionisation balance provides this, but note that disequilibrium can confuse an apparent density sensitivity.

Tutorial session 3 examples

1. ADAS402 Test Case

1. Move to your directory */.../<uid>/adas/pass/* . Start ADAS402.
2. The Input window is different from the usual you have encountered so far.
3. In the top part of the screen you can choose a data set to interrogate directly. Try */.../adas/adf11/acd89/acd89_n.dat* for nitrogen.
4. Then try to lower screen search method. Select iso-nuclear master c-r class ACD. Then enter *96* as the year, *89* as the default year and *n* as the element. Select *Standard* for the type for master file. Click the *Search* button.
5. On the pop-up choose one of the files offered and click Select to return to the input screen.
6. On the processing screen you can make the usual choices of temperature and density pairs by default or using the editor.
7. Move on to the output screen and finally obtain the graph.
8. You may like to go into the data base and explore ADF11 a bit further. Also look at the ADAS User manual entry *appxa-11*.

1. ADAS405 Test Case

9. Move to your directory */.../<uid>/adas/scripts405/*. Check if you have files *NULL* and *rfx_test_c*. If not, copy them both from */.../adas/adas/scripts405/*.
10. Move back to your */.../<uid>/adas/pass/* directory. Start ADAS and move to the ADAS4 series menu. Select ADAS405.
11. The Input window is complex. Note the Isonuclear Classes - click the *SELECT* button. On the drop down choice click on the buttons for *ACD, SCD, PRB, QCD, XCD, PLT*. then click *Done*.
12. Note the Select directory branch - click on the button and select *Central*.
13. Enter Year of data [96{return}]. Enter Default year *96*.
14. Enter Isonuclear element symbol *c*.
15. Note Type of master files - click on the button and select *Partial*. Note the Specify partial type code - click on the button and select *Resolved*.
16. Look at the lower section on the Line and Analysis Selection File. Click on the button for *User data*. Select the file NULL. Click *Done* to move to the processing window.
17. Click the *Default temperature/density* values button. You will need to choose an electron density, 1.00E9 say, and a hydrogen density, 1.00 say. Then click *Done* to move to the Output options window.
18. Click the button for *Graphical output*. Then click the button for *Fractional abundance plot*. Finally click *Done* to see the graph.
19. Click *Done* to return to the Output options screen. You can *Exit to menu* using the icon in this program.

2. ADAS 407 Test Case

1. Move back to your *pass* directory */.../<uid>/adas/pass*. Start ADAS407
2. The code can operate in interactive or automatic mode. On the Analysis Choice window select Interactive
3. The code works on the adf04 files for adjacent ionisation stages. These adf04 files must have recognizable Eissner configuration format. In practice this restricts you to */copmm#<nucchg>* libraries.
4. On the upper part of the Input screen select *copmm#54/ls#xe10.dat*. If a *copmm#<nucchg>* file is selcted then the adjacent ionised ion file is automatically selected in the lower part of the screen. Otherwise you must make an explicit choice.
5. On the upper left side of the Processing window, click Selections. You must choose the lowest level, that is the ground state. (ADAS407 has another mode for which additional metastable choices are required).
6. On the upper right side of the Processing window the same for the ionised ion.
7. On the Parameter Form section, select A for all items.
8. On the Matching Temperature part, select 2.420e+06.

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9. Click on the select ionising ion ground state, just above the Selection button on the upper left side. This sets transitions in the lower right sub-window.
10. You assign a bundle index to each transition in turn in the lower right editable box. {Return} to record the value on the list. You can re-edit your choices.
11. Choose a Specific Line Index also and then click *Done*.
12. On the Output window, select the ATOMPARS Passing File and the usual paper.txt file.
13. Click *View graph*
14. Click *Done* and then on the Output window click *Output files and back to input*.
15. Exit and look at the ATOMPARS passing file.
16. Note the top line of the ATOMPARS passing file. There are two sets of ?? marks. Edit 10 into both these locations, that is the initial and final ion charge state – you have only done one stage so both are 10.

4. ADAS 408 Test Case

17. Move back to your *pass* directory */.../<uid>/adas/pass*. Start ADAS and move to the ADAS4 series menu. Select ADAS408.
18. Click on *Central Data*. Click on *atompars* in the selection window and then on *atompars_mm#c.dat*. This is and atomic parameter data set for carbon. Choose a filter if you wish.
19. Click *Done* to advance to the Processing options window.
20. Enter a *Title for Run* at the top of the window.
21. In the top left box, enter 12.0 for the *Impurity element isotopic mass* and 2.0 for the *Neutral hydrogen isotopic mass*.
22. In the lower left box for electron temperature, enter *Lower limit* 1.0, *Upper limit* 100.0, *No. of temps* 10.
23. In the lower right box for electron density, enter *Lower limit* 1.00e+10, *Upper limit* 1.00e+15, *No. of dens.* 11.
24. Click *Done* to advance to the Output window.
25. Enter 30 for the two-digit year number. Make sure there are no blanks. The Passing file template changes accordingly. It is editable.
26. Select *Text Output* and *Default File Name* and click *Done*.
27. Note the list of passing files which will be created is shown in an information widget. Click *OK* to accept the list.
28. Click on the *Escape to Menu* button to finish
29. Look at acd30#c.pass. Note that it is fully formed ADF11 unresolved type file.

3. Example 1

Repeat ADAS405, but this time select the file *iter_test_c*. Everything else is the same. You will see a line selection choice now on the processing options window. Select one of these. On the Output options window you should look at the other graphs.

5. Example 2

ADAS405 has a very wide scope. Feel free to try it. You will probably need to look at the manual to appreciate its full capabilities and the range of data which it can access.

Tutorial session 4 examples

1. ADF01 and ADF12

1. Explore the ADAS database for these formats. Note that the specification is in the ADAS User manual (*appxa-01* and *appxa-12*).

2. ADAS301 Test Case

2. Move to your sub-directory */.../<uid>/adas/pass*. Start ADAS301.
3. Click on *Central Data*, and select *qcx#h0/qcx#h0_old#n7.dat*.
4. Click the *Browse comments* button to see the list of transitions present in the file *qcx#h0/qcx#h0_old#n7.dat.* Move onto ADAS301 Processing window.
5. Select *Fit polynomial* at the 5% level. Click on the n=8 - n'=7 transition in the transition list window. You will need to use the scroll-bar on the right.
6. Click on *Select Velocities/Energies for Output File* button.
7. Now put in default values in the Table. Note the units in use. It is preferred to units of eV/amu. You need to edit the table to change the units.
8. Click on the *Select Quantum Numbers for Processing* button. Select the 7f shell. Note that you can select total and partial cross-sections – see the key to the right.
9. Click on the *Done* button to proceed to the Output options window.
10. Click on the button for *Graphical Output*. Then click *Done* to see the graph.
11. Have a look at the output text file after completion

3. ADAS303 Test Case

12. Move to your sub-directory */.../<uid>/adas/pass*. Start ADAS303.
13. Click on *Central Data*, and select *qef93#h/qef93#h_c6.dat*.
14. Click the *Browse comments* button to see what is in the file *qef93#h_c6.dat.* Move onto ADAS303 Processing window.
15. Select *Fit polynomial* at the 5% level. Click on the n=8 - n'=7 transition in the transition list window. You will need to use the scroll-bar on the right.
16. Click on the *Default Energy/Velocity Values* button. A set of energies appears in the Output energies column. Note the units in use. You need to edit the table to change the units.
17. Click on the *Select supplementary plasma parameters* button. Now type in Output Values for Ion Density, Ion Temperature, Z effective and B Magnetic. Note the reference value and valid ranges for each of these parameters are given. The reference values are good values to start with.
18. Click on the *Done* button to proceed to the Output options window.
19. Click on the button for *Graphical Output*. Then click *Done* to see the graph.
20. Have a look at the output text file after completion

4 ADAS 308 Test Case

1. Move to your directory */.../<uid>/adas/pass*. Start ADAS and move to the ADAS3 series menu. Select ADAS308.
2. Click on *Central Data*, the data root to data class ADF01 should appear in the window alongside. Click on the directory name *qcx#h0* in the file list window. *qcx#h0* appears above in the selection window. Click on *qcx#h0_old#n7.dat*. It appears in the selection window [you may need to scroll down].
3. Click the *Browse comments* button. Information of what is in the file *qcx#h0_old#n7.dat* is displayed. Click *Done* to restore the Input window. Click *Done* and the ADAS308 Processing window appears.
4. The Processing window is complex. Note the information on donor and receiver near the top. To the right enter the Atomic mass of the receiver (14.0). Remember to press {*return*}.
5. Next Input the plasma parameters, for example, T_i=5.0e3, T_e=5.0e3, N_i=2.5e13, N_e=5.0e13, Z_{eff}=2.0, B=3.0.

6. Now Select charge exchange theory. This is a drop down menu. Click *Use input data set*. [Note programs have built in default activation on some buttons. If the button is darkened it is activated]. Now Select emission measure model. This is also a drop down menu. Click *Charge exchange*.
7. Now turn to the Input of beam and spectrum line information and click first on the button for *Beam parameter information*. The appropriate table appears below for editing. Click Edit to bring up Table Editor and enter appropriate values, for example

   0.85 8.0E4
   0.12 4.0E4
   0.03 2.7E4

   and then *Done*.
8. Similarly, click the button for Observed spectrum lines and edit it's table. Try

   9 8 1.00E12

   and click *Done*.
9. Finally click the button for Required emissivity prediction and edit it's table. Try

   9 8 1
   8 7 2
   7 6 2
   6 5

   and click *Done*.
10. All is now ready. Click *Done* to move to the Output options window.
11. Click the button for *Graphical output.* You may also *Enable Hard Copy* and *Text Output*. Finally click *Done* to see the graph.
12. Click *Done* to return to the Output options screen. Click on the *Exit to Menu* icon to finish up. Finally click on the *Exit* button on the sub-menu and main menu windows to exit ADAS.

5. ADAS 304 Test Case

21. Move to your directory /.../*<uid>/adas/pass*. Start ADAS and move to the ADAS3 series menu. Select ADAS304.
22. The Input window is different from the usual. Click *on Central Data*, the data root to the data class ADF21 should appear in the window above. Now enter the Group name for input files. This is the directory of the look-up tables of stopping data for a particular beam species. Type *bms93#h*. Remember the {*return*}.
23. Now you must decide on the mixture of impurity nuclei (and hydrogen nuclei) which cause the total stopping. Click the button *Select Ion List*. The button incidentally becomes *Reselect Ion List* on later passes through. A button table pops up. Click on the buttons for the nuclei you wish to include, for example, Be4, C6, H1 and click *Done*. Note the Stopping Ion List. Click *Done* to advance to the Processing Options window.
24. Click on the *Fit polynomial* button, then type 5 in the adjacent active editable box
25. Now move to the Stopping ion fractions. Click on the *Edit Table* button to activate Table Editor. Enter 0.1,0.1,0.8 for Be, C, H respectively and click *Done*.
26. Now Select the co-ordinate type for the output graph. Click the *Energy* button for the first try.
27. Click on the *Default Output Values* button. You may find a warning widget pops up. If so, click the *Confirm* button.
28. Click the button for *Graphical output.* Finally click *Done* to see the graph.
29. Click *Done* to return to the Output options screen. You may *Exit to menu* using the icon in this program.

6. ADAS 310 Test Case

13. Move to your directory /.../*<uid>/adas/pass*. Start ADAS and move to the ADAS3 series menu. Select ADAS310.
14. The Input window is considerably different from the usual. Enter beam species details (H for hydrogen and its isotopes) and the atomic charge of the beam species.
15. There are two files to be selected, the expansion file and the charge exchange file. To select the expansion file, click on the *Central Data* button, the *Data root* to the data class ADF18 should appear in the window above. Now select the data file *bndlen_exp#h0.dat*.

To select the charge exchange file, click on *Central Data*, the *Data root* to data class ADF01 should appear in the window. Select *qcx#h0*. Now select the data file *qcx#h0_e2p#h1.dat*. Click on the *Done* button to advance to the Proessing options window.

16. The control parameters of the collisional-radiative calculation are organised into three groups, selected in turn by the buttons *genera*l, *switches (I)* and *switches (II)*.
    General button: Click on the *general* button to view the general parameter settings. The default values are reasonable.
    Switches (I) button: Click on the *switches (I)* button to view the settings associated with electron collisions. Working down the list set the parameters to the following: 2, 3, NO, YES.
    Switches (II) button: Click on the *switches (II)* button to view the settings associated with the ion collisions. Working down the list set the parameters to the following: YES, 0, YES, YES.
17. Now you must decide what range of principal quantum numbers that you want to include in the calculation. Click on the *Representative N-shells* button . Enter 1 and 110 as the minimum and maximum n-shells. Now click on the *Edit Table* button and enter the following values into the editor: 1,2,3,4,5,6,7,8,9,10,12,15,20,30,40,50,60,70,80,90,100. Click on *Done* to return to the processing widget.
18. Now you need to decide the impurity content of the target plasma. Click on the *Impurity information* button. Now click on the *Selection mode* button and choose *Multiple impurities*. Click on the *Edit Table* button and enter the following information into the editor

H	1.0	0.9
C	12.0	0.05
Be	11.0	0.05

    Click on the *Done* button to return to the processing window.
19. Click on the e*lectron/proton density scan* button to choose the range of plasma densities. In the usual manner enter the following values into the table editor.

1.0e13	1.0
2.0e13	2.0
3.0e13	3.0
4.0e13	4.0
5.0e13	5.0

    Click Done to return to the processing window. Enter the value 3 as the *Index for the reference density*.
20. Now click on the e*lectron/proton temperature* button and enter the following values ino the text editor

    1.0e3
    2.0e3
    3.0e3
    4.0e3
    5.0e3

    Click on the *Done* button to return to the processing widget. Enter the value 3 as the *Index for the reference temperature*.
21. Click on the *beam energy scan* button and eneter the following values into the table editor

    2.0e4
    3.0e4
    4.0e4
    5.0e4
    6.0e4

    Click on the *Done* button to return to the processing widget. Ernter the value 3 for the *Index for the reference beam energy* and 1.0e8 as the *Beam density.*
    Now click on *Done* to advance to the Output window.
22. There are several possible outputs but our interest is in the contents of the first passing file. The first passing file is of type ADF26 and contains the tabulated population structure and effective stopping coefficients as a function of plasma parameters. It should be noted that the fourth passing file contains the stopping coefficients assembled

according to format ADF21. The preferred route to obtaining the stopping coefficients is via ADAS312.

23. Click on the *First passing file* button and enter a filename. Now click on *Run now*. An Information widget appears. After the calculation, click on the *Exit to Menu* button to return to the ADAS3 series menu.

Tutorial session 5 examples

1. ADAS 304 Test Case

1. Move to your directory /.../*<uid>/adas/pass*. Start ADAS and move to the ADAS3 series menu. Select ADAS304.
2. The Input window is different from the usual. Click *on Central Data*, the data root to the data class ADF21 should appear in the window above. Now enter the Group name for input files. This is the directory of the look-up tables of stopping data for a particular beam species. Type *bms93#h*. Remember the {*return*}.
3. Now you must decide on the mixture of impurity nuclei (and hydrogen nuclei) which cause the total stopping. Click the button *Select Ion List*. The button incidentally becomes *Reselect Ion List* on later passes through. A button table pops up. Click on the buttons for the nuclei you wish to include, for example, Be4, C6, H1 and click *Done*. Note the Stopping Ion List. Click *Done* to advance to the Processing Options window.
4. Click on the *Fit polynomial* button, then type 5 in the adjacent active editable box
5. Now move to the Stopping ion fractions. Click on the *Edit Table* button to activate Table Editor. Enter 0.1,0.1,0.8 for Be, C, H respectively and click *Done*.
6. Now Select the co-ordinate type for the output graph. Click the *Energy* button for the first try.
7. Click on the *Default Output Values* button. You may find a warning widget pops up. If so, click the *Confirm* button.
8. Click the button for *Graphical output.* Finally click *Done* to see the graph.
9. Click *Done* to return to the Output options screen. You may *Exit to menu* using the icon in this program.

2. ADAS 310 Test Case

1. Move to your directory /.../*<uid>/adas/pass*. Start ADAS and move to the ADAS3 series menu. Select ADAS310.
2. The Input window is considerably different from the usual. Enter beam species details (H for hydrogen and its isotopes) and the atomic charge of the beam species.
3. There are two files to be selected, the expansion file and the charge exchange file. To select the expansion file, click on the *Central Data* button, the *Data root* to the data class ADF18 should appear in the window above. Now select the data file *bndlen_exp#h0.dat*. To select the charge exchange file, click on *Central Data*, the *Data root* to data class ADF01 should appear in the window. Select *qcx#h0*. Now select the data file *qcx#h0_e2p#h1.dat*. Click on the *Done* button to advance to the Proessing options window.
4. The control parameters of the collisional-radiative calculation are organised into three groups, selected in turn by the buttons *genera*l, *switches (I)* and *switches (II)*.
   General button: Click on the *general* button to view the general parameter settings. The default values are reasonable.
   Switches (I) button: Click on the *switches (I)* button to view the settings associated with electron collisions. Working down the list set the parameters to the following: 2, 3, NO, YES.
   Switches (II) button: Click on the *switches (II)* button to view the settings associated with the ion collisions. Working down the list set the parameters to the following: YES, 0, YES, YES.
5. Now you must decide what range of principal quantum numbers that you want to include in the calculation. Click on the *Representative N-shells* button . Enter 1 and 110 as the minimum and maximum n-shells. Now click on the *Edit Table* button and enter the following values into the editor: 1,2,3,4,5,6,7,8,9,10,12,15,20,30,40,50,60,70,80,90,100. Click on *Done* to return to the processing widget.
6. Now you need to decide the impurity content of the target plasma. Click on the *Impurity information* button. Now click on the *Selection mode* button and choose *Multiple impurities*. Click on the *Edit Table* button and enter the following information into the editor

H	1.0	0.9
C	12.0	0.05
Be	11.0	0.05

Click on the *Done* button to return to the processing window.

7. Click on the e*lectron/proton density scan* button to choose the range of plasma densities. In the usual manner enter the following values into the table editor.

1.0e13	1.0
2.0e13	2.0
3.0e13	3.0
4.0e13	4.0
5.0e13	5.0

Click Done to return to the processing window. Enter the value 3 as the *Index for the reference density*.

8. Now click on the e*lectron/proton temperature* button and enter the following values ino the text editor

1.0e3
2.0e3
3.0e3
4.0e3
5.0e3

Click on the *Done* button to return to the processing widget. Enter the value 3 as the *Index for the reference temperature*.

9. Click on the *beam energy scan* button and eneter the following values into the table editor

2.0e4
3.0e4
4.0e4
5.0e4
6.0e4

Click on the *Done* button to return to the processing widget. Ernter the value 3 for the *Index for the reference beam energy* and 1.0e8 as the *Beam density.*
Now click on *Done* to advance to the Output window.

10. There are several possible outputs but our interest is in the contents of the first passing file. The first passing file is of type ADF26 and contains the tabulated population structure and effective stopping coefficients as a function of plasma parameters. It should be noted that the fourth passing file contains the stopping coefficients assembled according to format ADF21. The preferred route to obtaining the stopping coefficients is via ADAS312.
11. Click on the *First passing file* button and enter a filename. Now click on *Run now*. An Information widget appears. After the calculation, click on the *Exit to Menu* button to return to the ADAS3 series menu.

Callable ADAS — Exercises

March, 2012

1 Aim

The aim is to familiarise you with callable ADAS, mainly in an IDL environment but also using Fortran. Please feel free to expand any of the tasks or change them slightly to deal with your favourite ion! The sub tasks should be considered optional and are often more difficult (marked with 🌶s) so don't spend too much time on them unless they are of particular interest — getting the main tasks done is more important.

2 Tasks

1. Use `run_adas208` to explore the population structure of boron-like neon.
   - Find the approximate density where the systems switches from coronal to CR and from CR to LTE.
   - Produce a PEC file for the system🌶.
2. Use `read_adf11` to read ionisation and recombination coefficients for carbon.
   - Plot the temperature where the ionisation and recombination rates are equal as a function of ion charge 🌶🌶.
3. Use `run_adas405` to generate an equilibrium ionisation balance for carbon.
   - Compare the temperature of peak abundance (as a function of ion charge) with the points where the rates are equal (see above) 🌶🌶🌶.
   - Contrast `run_adas405` (time independent) with `run_adas406` (time dependent)🌶🌶🌶🌶.
   - See if you can feed the results into `write_adf19` to produce a PZD file🌶🌶🌶.
4. Use `read_adf15` to read data for the $1s^2\ ^1S - 1s2p\ ^1P$ and $1s^2\ ^1S - 1s2p\ ^3S$ in He-like argon.
   - Produce a contour plot over a sensible temperature and density range🌶.
   - Hence show that the ratio is a useful density diagnostic🌶.

5. Use `read_adf15` to read the PEC for the 977Å line of C^{+2}
   - Compare the power radiated in this line with the total line power for C3+ in coronal equilibrium conditions 🌶🌶🌶.
6. Using the fortran routine `r8ah`, write a small Fortran program which prints out the A-value of the 8p - 3s transition in hydrogen.
   - Extend the program to print out the A-value of the whole $n = 8$ to $n = 3$ transition🌶.
   - Do the same in IDL.
7. Combine `run_adas405` and `read_adf15` to produce an emission profile over the device (fusion machine, star, blob of tin) of your choosing.
   - Integrate over the data to simulate a spectrometer🌶.
   - Automatically produce an adaptive grid of points where the emission is highest🌶🌶🌶.
8. Use `run_adas416` to produce partitioned data using the file `/home/ITER/omullam/ADAS_course/partition_example.dat`.
   - Modify the partition and explore how the various ions move in and out of being bundled🌶.
9. Use `read_adf12` to read effective charge exchange emission coefficients for the $n = 8 \rightarrow n = 7$ transition of CVI.
   - Write a program which can turn a fitted line area into a carbon concentration given a known beam energy, beam density and plasma parameters🌶🌶🌶.
10. Use `read_adf22` to read beam populations (`BMP`) for a hydrogen beam, look at the relative populations of $n = 2$ to $n = 1$ as a function of energy.
    - Combine these populations with two ADF12 files (via `read_adf12`) and explore the variation with energy, compare it with just assuming $n = 1$ population🌶🌶.
11. Read beam stopping coefficients for a neutral beam passing through a hydrogen plasma with a 3% neon content.
    - Find the dependence on the stopping as a function of neon content.
    - Integrate a real beam over a sensible profile, find the penetration depth as a function of neon concentration🌶🌶🌶🌶🌶.
12. Use `run_adas306` to compare active CX emission and excitation driven emission for CVI 8-7.
    - Plot the Doppler broadened feature (see `c5dplr.pro`) along with the components which make it up🌶.
    - Write a program which finds where the two emission processes become comparable🌶🌶🌶.

3 Hints

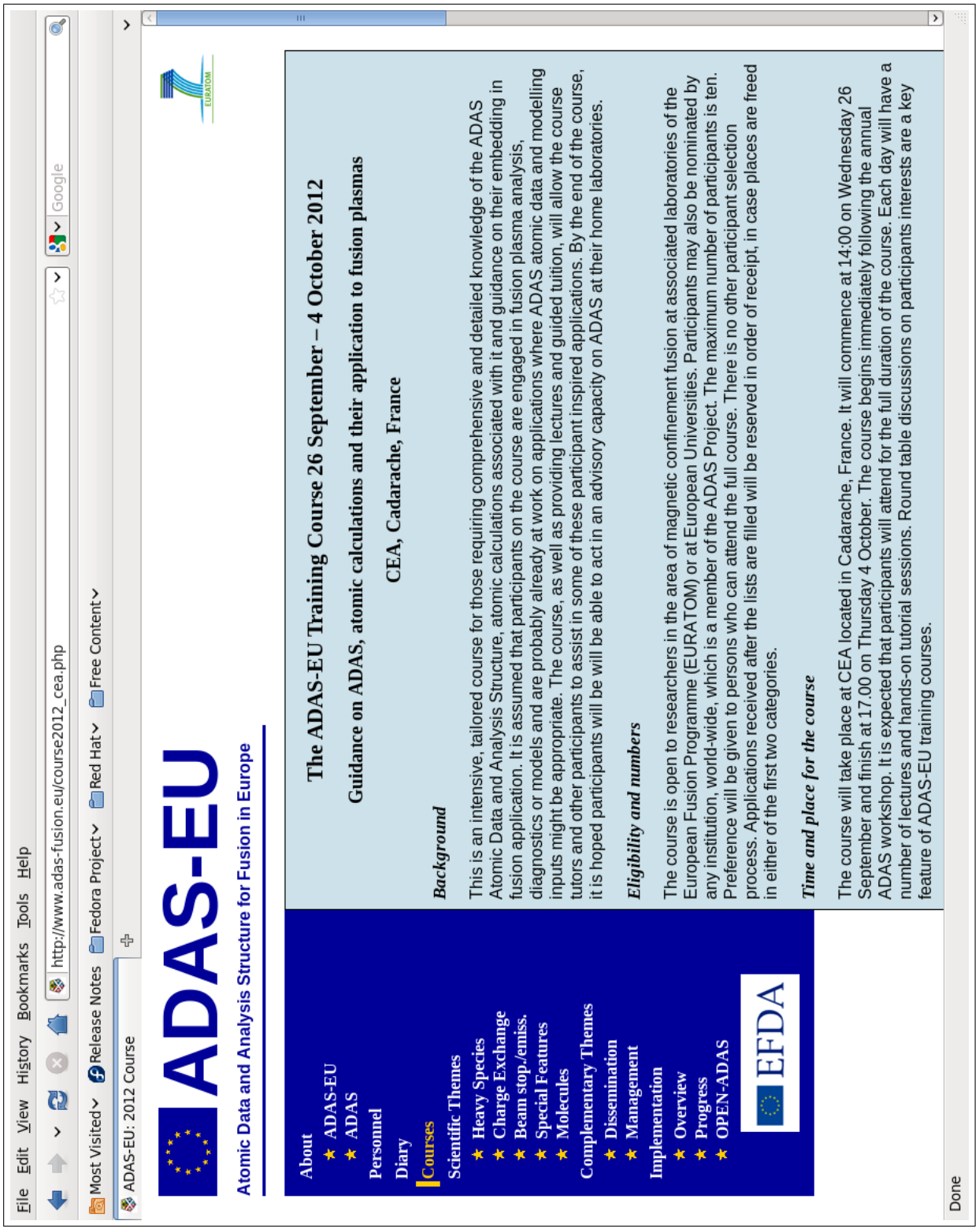
- Many IDL routines will give you help if you type their name followed by `,/help` (e.g. `run_adas405,/help`). Source is also available.
- You can search for r8ah online.
- IDL has built-in integration routines, type 'idlhelp' to see it.
- The `adas_vector` function can provide help in producing lists of numbers, see: `/home/adas/idl/adaslib/util/adas_vector.pro`.

Appendix C

ADAS-EU course 2012b announcements, agenda and participants

[1] ADAS-EU_course_2012b
[2] ADAS-EU_course_agenda_2012b
[3] adas-eu_course_participants_2012b

C.1 Announcement



File Edit View History Bookmarks Tools Help
http://www.adas-fusion.eu/course2012_cea.php
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ADAS-EU: 2012 Course
Access to CEA site
Security is important at Cadarache and advanced notice is required for visitors. We need confirmation before 6th September to complete administrative issues. Return this form if you will attend the course.
Accommodation and travel
Details on the travelling to CEA at Cadarache are here.
The closest airport is Marseille (MRS) and there is a TGV station in nearby Aix-en-Provence. There are buses from the airport to Aix and from there to Cadarache during the week. Travel by public transport during the weekend is more difficult.
Please contact the organizers if you require accommodation. We will stay either in Aix or in one of the villages closer to the laboratory.
Costs
There is no charge for the ADAS-EU course. Participants in the course will be able to use the cafeteria and restaurant facilities of the laboratory.
Tutors
The course will be delivered by ADAS-EU personnel: Prof. H. P. Summers, Dr. M.G. O'Mullane, Dr. Fran Guzmán and Dr. Alessandra Giunta.
Course outline
The course is divided into five parts:
Day 1: Introduction and setup
Day 2: Basic and intermediate ADAS use
Day 3: Fundamental data production with ADAS
Day 4: Population dynamics and ionisation state
Day 5: Introduction to molecular models and data in ADAS
Day 6: Embedding ADAS codes and data into models
Day 7: Charge exchange and beam models. Course review
Done

File Edit View History Bookmarks Tools Help
http://www.adas-fusion.eu/course2012_cea.php
Google
Most Visited Release Notes Fedora Project Red Hat Free Content
ADAS-EU: 2012 Course
Each ADAS-EU training course has a theme — for this course we will introduce a new element of ADAS, the population modelling of molecular species.
In addition to formal lectures there are hands-on tutorial sessions with exercise sheets and worked examples. Each day there will be a session dedicated to each participant's area of interest. Around 30 minutes will be available for the participant to introduce and summarise his/her area. The follow-up discussion will engage all participants and tutors. It is planned that a person with ADAS experience suited to each participant's special topic will be identified to help in alignment of ADAS capabilities with the participant's topic. The course will have time slots available for the participant and tutor to work on these areas.
Enquiries
The ADAS-EU course is organized by the University of Strathclyde with the support of le Commissariat à l'Energie Atomique (CEA). Correspondence and general organization queries will be handled by:
Francisco Guzmán
CEA – Cadarache
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+33-44225-4299
For comments and questions see: Contact Details
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Done

C.2 Agenda

ADAS-EU course 2012 – CEA Cadarache

Agenda

Wednesday 26 September		
14:00 – 14:30	Computer set up	
14:30 – 15:00	Introduction	MOM
15:00 – 15:30	Interactive system	LFM
Thursday 27 September		
9:30 – 9:45	Computing instructions for CEA	MOM
9:45 – 10:30	Excited population structure	ASG
10:30 – 10:45	*Coffee*	
10:45 – 12:30	Tutorial (ADAS introduction, series 2)	
12:30 – 13:30	*Lunch*	
13:30 – 14:00	Advanced population models	HPS
14:00 – 15:00	Tutorial	
15:00 – 15:30	*Coffee*	
15:30 – 16:00	Charge exchange for population models	HPS
Friday 28 September		
9:30 – 10:15	Overview of Atomic Structure and Collision Theory	NRB
10:10 – 10:30	*Coffee*	
10:30 – 11:00	ADAS and fundamental data generation	MOM
11:00 – 12:20	Tutorial (ADAS series 8)	
12:20 – 14:00	*Lunch*	
14:00 – 16:00	Round table	
Monday 1 October		
9:30 – 10:15	Embedding ADAS in other codes	MOM
10:15 – 10:30	*Coffee*	
10:30 – 11:00	Ionisation state	ASG
11:00 – 12:20	Tutorial (ADAS series 4, Exercise)	
12:20 – 14:00	*Lunch*	
14:00 – 14:30	Making data for ionisation state studies	MOM

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14:30 – 16:00	Round table	
Tuesday 2 October		
9:30 – 10:15	Introduction of molecular models and data in ADAS	FG
10:15 – 10:30	*Coffee*	
10:30 – 12:20	ADAS series 9 and tutorial	FG
12:20 – 14:00	*Lunch*	
14:00 – 15:00	Round table	
15:00 – 16:00	Tutorial	
Wednesday 3 October		
9:30 – 10:15	ADAS special features	MOM
10:15 – 10:30	*Coffee*	
10:30 – 11:15	Differential Emission Measure	ASG
12:20 – 14:00	*Lunch*	
14:00 – 15:00	Round table	
15:00 – 16:00	Tutorial	
Thursday 4 October		
9:30 – 10:15	Charge exchange spectroscopy	MOM
10:15 – 10:30	*Coffee*	
10:30 – 12:20	Beam stopping and beam emission spectroscopy	LFM
12:20 – 14:00	*Lunch*	
14:00 – 15:00	Tutorial	
15:00 – 16:00	Course review	

MOM : Martin O'Mullane

HPS : Hugh Summers

NRB : Nigel Badnell

FG : Francisco Guzmán

ASG : Alessandra Giunta

LFM : Luis Menchero

C.3 Participants

ADAS-EU course 2012 – CEA Cadarache

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Appendix D

ADAS-EU course 2012b lectures and tutorial exercises

[1] adas-eu_lec_introduction_2012b (first page)
[2] adas-eu_lec_interactive_adas_2012b (first page)
[3] adas-eu_lec_excited_population_structure_2012b (first page)
[4] adas-eu_lec_advanced_population_models_2012b (first pages)
[5] adas-eu_lec_charge_exchange_for_population_models_2012b (first page)
[6] adas-eu_lec_overview_of_atomic_structure_and_collisional_theory _2012b (first page)
[8] adas-eu_lec_callable_adas_2012b (first page)
[9] adas-eu_lec_ionisation_state_2012b (first page)
[10] adas-eu_lec_ionis_state_2_2012b (first page)
[11] adas-eu_lec_introduction_of_molecular_model_2012b (first page)
[12] adas-eu_lec_ADAS_special_features_2012b (first page)
[13] adas-eu_lec_differential_emission_measure_analysis_2012b (first pages)
[14] adas-eu_lec_charge_exchange_spectroscopy_2012b (first page)
[15] adas-eu_lec_adas_beam_codes_2012b (first pages)

[18] ADAS-EU_tut1-ex_overview_2012b
[19] ADAS-EU_tut2-ex_excited_population_models_2012b
[20] ADAS-EU_tut3-ex_ionization_state_2012b
[21] ADAS-EU_tut4-ex_charge_exchange_spectroscopy_2012b
[22] ADAS-EU_tut5-ex_beam_stopping_and_emission_2012b
[23] ADAS-EU_tutorial_series_9_2012b

D.1 Lectures

University of
Strathclyde
Glasgow
Background to ADAS
Martin O'Mullane
Department of Physics
University of Strathclyde
ADAS-EU course, CEA, France 26-September-2012

Interactive ADAS

L. Fernández-Menchero

ADAS, University of Strathclyde. United Kingdom.
Institut Max Plank für Plasmaphysik. Garching, Germany.

ADAS Course 2012,CEA Cadarache, France.

Working with excited population structure

- Datasets of class ADF04 contain all the information necessary to evaluate excited populations of an ion. It is called a ‘specific ion file’.
- Code ADAS205 computes the populations at temperatures and densities of your choice.
- The input, data set selection, screen is very similar to that for ADAS201

Advanced population modelling

Hugh Summers

University of Strathclyde

27 Sept. 2012
CEA Cadarache

Charge exchange for population modelling

Hugh Summers

University of Strathclyde

27 Sept. 2012
CEA Cadarache

Overview of Atomic Structure and Collision Theory

Nigel Badnell

Department of Physics
University of Strathclyde
Glasgow, UK

– ADAS 2012 –

University of Strathclyde Glasgow

Callable ADAS

Martin O'Mullane
Department of Physics
University of Strathclyde

The ionisation state of ions in a plasma

- Effective ionisation and recombination
  - » Data sets of class ADF11
  - » Interrogating ADF11 using ADAS402.
- Equilibrium ionisation balance
  - » Using adas405 to examine the temperature and density dependent equilibrium ionisation balance

3b. The ionisation state of ions in a plasma – part 2

- Superstage compression
  - » Extension of the ADF11 data classes
  - » The root partitions and specification of a new partition
  - » ADAS416

- Setting up baseline ‘89’ ADF11 data for an element
  - » Using ADAS407 to obtain atomic parameter sets of format ADF03
  - » Using ADAS408 to produce ADF11 baseline data

ADAS-EU
ADAS for fusion in Europe

An overview of the molecular extension of ADAS: ADAS900 series

Francisco Guzmán

ADAS-EU
University of Strathclyde

ADAS-EU course Cadarache, 26 Sept. – 4 Oct. 2012

Spectral features in ADAS

Martin O'Mullane

Differential Emission Measure (DEM) analysis

- One of the most widely used methods available for the interpretation of astronomical spectral lines is the Differential Emission Measure (DEM) technique.

- Although this method is less familiar in spectroscopic studies of fusion plasma, it can be applied to determine impurity concentration, impurity variation in time and impurity influx in fusion.

Charge exchange spectroscopy

- Preliminaries
- ADAS series 5/series2 - thermal charge transfer
- ADAS series 3 - charge transfer with neutral beams

Beam stopping and Beam emission spectroscopy

- Extracting effective beam stopping coefficients or beam emission coefficients using ADAS304.
- Calculating the beam population structure using ADAS310
- Details of beam emission with adas305_get_stark.pro

D.2 Tutorial exercises

Tutorial session 1 examples

1. Initial set up

1. The tutorial assumes ADAS is set up for operation from your terminal and that your personal */home/<uid>/adas/* directory and sub-directories *pass/* and *defaults/* have been initialised
2. The *pass/* directory is used for data sets created by ADAS, which you choose finally how to dispose of. The *defaults/* directory remembers all the settings you selected on your last run of every ADAS code. Since ADAS codes may have changed, if you have already used ADAS, your *defaults*/ directory files may be out of date. This will cause codes to crash, so it may be best to delete all the files in the *defaults*/ directory and start afresh.
3. Move to the central adas file space [*cd /home/adas*]. Look at the directories at this level [*ls*]. You will see the directory *doc*/. Move into it and look again [*cd docs; ls*]. You should see the various sub-directories including *bulletin*/ and *manual*/. Move into the bulletins and look again [*cd bulletin; ls*]. You will see all the bulletins including the one *sep25_09.pdf*.
4. Bring up a acrobat viewer for *.pdf* files [*acroread &*] to look at the *sep25_09.pdf* bulletin. 'Bug fix' releases and the associated bulletin comes out annually or occasionally more frequently. New code releases are separate and occur when ready.
5. Return to the Terminal window, move into the *docs*/ subdirectory *manual*/ and list the files. *appxa* files describe the ADAS data and the others describe the ADAS codes. Use the acrobat reader to look at *chap5-03.pdf* and at *appxa-15.pdf*.
6. Move to the directory */work/projects/adas/*. Notice the *fortran*/ and *idl*/ subdirectories. Move into *fortran*/ and list and then down into *adas5xx*/ look again. Finally move down into *adas501*/ for a final look. You are now at the FORTRAN codes themselves. Note that on your own site the source fortran may not be accessible to the ordinary user.
7. Now move to the directory */work/projects/adas/adas/* and list. This is the database itself. Look down into ADAS data format *adf04*. Actual datasets rather than directories have the terminator *.dat*.
8. Move back to your own *pass/* directory [*cd ~/adas/pass/*]. Start up ADAS [*adas*]. The main ADAS menu pops up.
9. Note that it is best to start ADAS from your sub-directory */.../<uid>/adas/pass*. Graph and text hardcopy files created by ADAS will appear in the directory from which you launch ADAS.

2. Starting interactive ADAS and using its general GUI widgets

1. Move to your sub-directory */.../<uid>/adas/pass*. Graph and text hardcopy will consequently appear here. Start ADAS [type *adas*]and go to the ADAS5 series sub-menu. Click with the mouse on the first button in adas5 series for ADAS501. The Input window for ADAS501 pops up.
2. Click on *Central Data*, the data root to data class ADF13 should appear dimmed in the window above. Click on the directory name *sxb93#cr* in the datafile list window. *sxb93#cr* appears above in the selection window. Click on *sxb93#cr_llu#cr0.dat*. It appears in the selection window.
3. Click the *Browse comments* button. Information of what is in the file *sxb93#cr_llu#cr0.dat* is displayed. Click *Done* to restore the Input window. Click *Done* and the ADAS501 Processing window appears.
4. Click on the *Fit polynomial* button, then type [*5 {return}*] in the adjacent active editable box. Click on the first transition at 4270.7Å in the transition list window. It appears in the selection window above.
5. Click on the *Default Temperatures Values* button. If a warning pop-up appears, click *Confirm* on it. A set of density values appears in a pop-up window. Click on 1.000E+13. The temperature and density output values appear in the table.
6. Click on the *Done* button to proceed to the Output options window.
7. Click on the button for *Graphical Output*.
8. Select *Post-Script* out put by clicking on it in the Select Device list window. Click on the button for *Enable Hard Copy*. Enter a File Name such as graph.ps. Remember to press {*return*}. A warning widget appears if *graph.ps* already exits. If so click on *Replace*.
9. Click on the button for *Text Output*. Type in *paper.txt* - this is the standard text output File Name. [On many Output windows, there is a *Default File Name* button. You can click on it to enter *paper.txt* as the standard text output File Name.] Then click *Done*.

10. The graph appears in the next window. Click on *Print* to send a copy of the graph to the *graph.ps* file. Click *Done* to return to the Output Options window. Click on *the Exit to Menu* icon at the bottom left corner to restore the ADAS5 series menu. Finally click on the *Exit* button on the sub-menu and main menu windows to exit ADAS.
11. [*ls*] to see the files. You may wish to list *paper.txt* to see its format.

3. Using the Table Editor widget

1. Repeat steps 1-3 above. Click on *Edit Table* on the processing screen. Table Editor pops up.
2. The values in italic font are your input data. Click in any of these boxes to edit the number within it. The workstation cut, paste and copy keys operate. Press the *return* key on the keyboard to record any change. This is the normal editing mode.
3. The set of round and square buttons below the table are designed to help in some editing tasks. You must be careful to remember the sequence of operations since it is different from that on personal computers. **Activate** the appropriate button, **position** the mouse text cursor or drag over required digits, **press** the *return* key on the keyboard to complete the sequence.
4. The *Default* round button is the reset to normal editing mode. The *Delete* button allows deletion of the value in a box, leaving an empty box; the *Remove* button allows deletion of a value with the column then being pushed up; the *Insert* button creates a new empty box, pushing the column down. These buttons stay active until you click *Default*.
5. The *Copy* and *Paste* round buttons operate for the next immediate action only.
6. Square buttons have a continuing effect until an alternative is pressed. The *Row_skip* button causes a jump to the next editable box in a row when the *return* key on the keyboard is pressed; *Column_skip* causes jumping to next box in a column. *Scroll up* moves the whole window down. Note that the window only shows ten values in a column, but the whole table may be longer that this.
7. Preferred Temperature units for working with may be chosen. Changing units causes the Inputs from the file to change to the new units. It **does not** change any Output values already typed in. It merely interprets Output values in the selected units.
8. Press the *Done* button to record the changes and return to the screen from which Table Editor was initiated. The *Cancel* button prevents the new values being substituted on return.

9. You may be interested to try some of the more advanced widgets used by ADAS501. On the processing screen click Value selection by Display. A description of how to use this is in the user manual *introduction.pdf*.
10. On the graphical display, you may like to try the *Retain* and *Adjust* buttons. Again details of use are in the user manual *introduction.pdf*.

Tutorial session 2 examples

1. **ADF04**
   1.1. Explore the /…/adas/adas/adf04 database. Note that a summary of the data base is given in the ADAS User manual *appxa-04.pdf*.

2. **ADAS201 Test Case**
   2.1. Move to your sub-directory */.../<uid>/adas/pass*. Graph and text hardcopy will consequently appear here. Start ADAS [type *adas*] and go to the ADAS2 series sub-menu. Start ADAS201.
   2.2. Click on *Central Data*, the data root to data class ADF04 should appear dimmed in the window above. Click on the directory name *adas#7* in the datafile list window. Note the designations. The 'ic' denotes J-resolved intermediate coupling system. 'ls' denotes a term resolution system. The 'n' case is a special bundled –n system for the hydrogen-like ion. The degeneracy ensures very strong mixing by ion collisions which can be assumed complete.
   2.3. Select *cop98#7_ic#n3.dat* . Click the *Browse comments* button. Information on the content and quality of the data set can be reviewed.. Click *Done* to restore the Input window. Click *Done* and the ADA201 Processing window appears.
   2.4. You may select to have a polynomial fit by clicking *Fit polynomial* button, and selecting a accuarcy (%) in the adjacent active editable box..
   2.5. Activate the *Select Temperaturesfor output file* button to obtain a numerical tabulation of results. Either edit in the temperatures you wish or click the *Default Temperatures Values* button.
   2.6. Click on the *Done* button to proceed to the Output options window and *Graphical Output*.
   2.7. Select *Post-Script* and *Enable Hard Copy* and assign an output graph file.
   2.8. Click on the button for *Text Output*. And route output to *paper.txt*, the standard text output File Name. Then click *Done*.
   2.9. The graph appears in the next window. Click on *Print* to send a copy of the graph file. Click *Done* to return to the Output Options window. Click on *the Exit to Menu* icon at the bottom left corner to restore the ADAS5 series menu. *paper.txt* is not viewable with an editor until you exit.
   2.10. You may wish to examine the *paper.txt* file to see its format.

3. **Additional exercise**
   3.1. Restart ADAS201 and again select the adas#7 sub-directory. Select the *cop98#7_ls#n3.dat* file. Browse the comments. Note that this file is obtained by bundling the level resolved 'ic' file you fist chose into terms. This procedure you will observe in the comments was done by ADAS209. You may wish to try ADAS209. The operation is described in the ADAS User manual Chap3-09.

4. **ADAS811 Test case**
   4.1. ADAS811 is a new and more sophisticated interrogation code on ADF04 files. It allows not only display of single collision rates but comparison of such data from different ADF04 files. [Note this code uses the configuration information and quantum numbers to match transitions between different files. If you use a non-standard (that is not *ADAS Standard* or *Eissner*) form, the code will fail to match – it is quite sensitive.
   4.2. For this test we shall compare a high grade assessed boron-like ion of oxygen (*adas#8/cop98#8_ls#o3.dat* with a much older impact parameter cross-section based data set (*copss#b/copss#b_ss#o3l.dat*) built on a SUPERSTRUCTURE calculation.
   4.3. Select the first data set in the in the upper part of the Input window. The second data set is selected in the lower part and uses a more standard Unix file selection so that files can be tested during construction when not located in your ADAS space. You can choose a third file if you wish (e.g. the Born baseline *copmm#8/ls#o3.dat*).
   4.4. There is only a further display screen which incorporates selection and controls. At this stage we are only concerned with electron impact excitation data. This is the default *e-exc* in the Type of Plot. The Type of e-exc plot is selectable. Note the usual Upsilon (gamma) and excitation rate coefficient, but also the Burgess C-plot.

4.5. At the top of the window, select the file whose transitions youn wish to step through. The code will attempt to match transitions from the other file to it – which may nit be successful indeed the transition may not exist in the other files.
4.6. Note the tape recorder controls at the bottom. The upper and lower indices of a particular transition may be entered in the editable boxes. Then click *Show*.
4.7. We find it convenient to have the files open in an editor as we do the examination.
4.8. Note the cursor is active for reading of values.
4.9. *Print* will send the displayed transition to a file (via a pop-up dialogue). Be cautious of using the *Print All* button – there may be a lot of electron impact excitation transitions.

5. ADAS205 Test Case

5.1. Move to your sub-directory */.../<uid>/adas/pass*. ADAS205.
5.2. Click on *Central Data*. Select the Be-like oxygen case *adas#8/cop98#8_ls#o4.dat*.
5.3. Click on the *Default Temperatures button* and *Default Densities* button.
5.4. Click on the *Selections* button for metastable states. A pop-up list of all the levels appears. Click on the button beside the first level. Note that it darkens. It is a click on/click off button. Then click on its *Done* button to restore the full Processing options window.
5.5. Click on the *Done* button to proceed to the Output options window.
5.6. Click on the button for *Graphics* to display the graphics choices then click on the button for *Graphical Output*. Select *Graph Temperature* by clicking on the one you wish in the list. Choose the fifth one [1e5]. Click on the *Text* button to display the output data set choices. Click on the *Contour File* button and enter *contour.pass* in the File Name editable window. Then click *Done*. The graph pops up. There are several graphs to look at. Finally click *Done* to restore the Output options window. Click the *Exit to Menu* icon to finish up. Finally click on the *Exit* button on the sub-menu and main menu windows to exit ADAS.
5.7. Note the files created includes the collection file *contour.pass.* You may wish look at its format.

6. ADAS207 Test Case

6.1. Move to your sub-directory */.../<uid>/adas/pass*. Make sure you have a *contour.pass* file there. Start ADAS and go to the ADAS2 series sub-menu. Click with the mouse on the seventh button in adas2 series for ADAS207. The Input window for ADAS207 pops up.
6.2. Click on *User Data*, the data root to you /pass sub-directory should appear in the window alongside. Click on *contour.pass* in the file list window. It appears in the selection window.
6.3. Click *Done* and the ADAS207 Processing window appears.
6.4. Click on the *Selections* button for the 1st composite line assembly. The window with the full list of lines pops up. Click on the buttons alongside the lines you wish for the numerator of the line ratio. These are on/off buttons. Note a button is darkened when activated and the program remembers the choice you made if you have had a previous run. Select transition 2 for the test. Click the *Done* button.
6.5. Click on the *Selections* button for the 2nd composite line assembly. The window with the full list of lines pops up. Click on the buttons alongside the lines you wish for the numerator of the line ratio. Select transition 26 for the test. Click the *Done* button.
6.6. Click on the *Done* button to proceed to the Output options window.
6.7. Click on the button for *Graphical Output*. Click on the *Diagnostic Contour Plot* button. This brings up contour plot choices. Click on the *Default Contour Scaling* button if not already selected. Then click *Done*. The graph pops up.
6.8. An object of such a plot is to detect diagnostic line ratios, that is ratios senitive to density or temperature. Note that the contour plot gives an overview but is coarse.

Example 7

6.9. Experiment with the same data set in ADAS205 but edit in a relevant range of electron temperatures and densities for the density sensitive region. Proceed to form the *contour.pass* file. Now run ADAS207 with this *contour.pass* file. Try adding more lines to the two composites or changing the lines.

Example 8

6.10. Repeat the above but at the metastable selection in the ADAS205 Processing options window, select the first and second levels. Follow through the consequences to ADAS207. Remember to obtain a contour output file from ADAS205.

6.11. Note that with two metastables, we have the opportunity to shift their relative number densities from that in equilibrium. Generally a dynamic ionisation balance provides this, but note that disequilibrium can confuse an apparent density sensitivity.

Tutorial session 3 examples

1. ADAS402 Test Case

1. Move to your directory */.../<uid>/adas/pass/* . Start ADAS402.
2. The Input window is different from the usual you have encountered so far.
3. In the top part of the screen you can choose a data set to interrogate directly. Try */.../adas/adf11/acd89/acd89_n.dat* for nitrogen.
4. Then try to lower screen search method. Select iso-nuclear master c-r class ACD. Then enter *96* as the year, *89* as the default year and *n* as the element. Select *Standard* for the type for master file. Click the *Search* button.
5. On the pop-up choose one of the files offered and click Select to return to the input screen.
6. On the processing screen you can make the usual choices of temperature and density pairs by default or using the editor.
7. Move on to the output screen and finally obtain the graph.
8. You may like to go into the data base and explore ADF11 a bit further. Also look at the ADAS User manual entry *appxa-11*.

1. ADAS405 Test Case

9. Move to your directory */.../<uid>/adas/scripts405/*. Check if you have files *NULL* and *rfx_test_c*. If not, copy them both from */.../adas/adas/scripts405/*.
10. Move back to your */.../<uid>/adas/pass/* directory. Start ADAS and move to the ADAS4 series menu. Select ADAS405.
11. The Input window is complex. Note the Isonuclear Classes - click the *SELECT* button. On the drop down choice click on the buttons for *ACD, SCD, PRB, QCD, XCD, PLT*. then click *Done*.
12. Note the Select directory branch - click on the button and select *Central*.
13. Enter Year of data [96{return}]. Enter Default year *96*.
14. Enter Isonuclear element symbol *c*.
15. Note Type of master files - click on the button and select *Partial*. Note the Specify partial type code - click on the button and select *Resolved*.
16. Look at the lower section on the Line and Analysis Selection File. Click on the button for *User data*. Select the file NULL. Click *Done* to move to the processing window.
17. Click the *Default temperature/density* values button. You will need to choose an electron density, 1.00E9 say, and a hydrogen density, 1.00 say. Then click *Done* to move to the Output options window.
18. Click the button for *Graphical output*. Then click the button for *Fractional abundance plot*. Finally click *Done* to see the graph.
19. Click *Done* to return to the Output options screen. You can *Exit to menu* using the icon in this program.

2. ADAS 407 Test Case

1. Move back to your *pass* directory */.../<uid>/adas/pass*. Start ADAS407
2. The code can operate in interactive or automatic mode. On the Analysis Choice window select Interactive
3. The code works on the adf04 files for adjacent ionisation stages. These adf04 files must have recognizable Eissner configuration format. In practice this restricts you to */copmm#<nucchg>* libraries.
4. On the upper part of the Input screen select *copmm#54/ls#xe10.dat*. If a *copmm#<nucchg>* file is selcted then the adjacent ionised ion file is automatically selected in the lower part of the screen. Otherwise you must make an explicit choice.
5. On the upper left side of the Processing window, click Selections. You must choose the lowest level, that is the ground state. (ADAS407 has another mode for which additional metastable choices are required).
6. On the upper right side of the Processing window the same for the ionised ion.
7. On the Parameter Form section, select A for all items.
8. On the Matching Temperature part, select 2.420e+06.

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9. Click on the select ionising ion ground state, just above the Selection button on the upper left side. This sets transitions in the lower right sub-window.
10. You assign a bundle index to each transition in turn in the lower right editable box. {Return} to record the value on the list. You can re-edit your choices.
11. Choose a Specific Line Index also and then click *Done*.
12. On the Output window, select the ATOMPARS Passing File and the usual paper.txt file.
13. Click *View graph*
14. Click *Done* and then on the Output window click *Output files and back to input*.
15. Exit and look at the ATOMPARS passing file.
16. Note the top line of the ATOMPARS passing file. There are two sets of ?? marks. Edit 10 into both these locations, that is the initial and final ion charge state – you have only done one stage so both are 10.

4. ADAS 408 Test Case

17. Move back to your *pass* directory */.../<uid>/adas/pass*. Start ADAS and move to the ADAS4 series menu. Select ADAS408.
18. Click on *Central Data*. Click on *atompars* in the selection window and then on *atompars_mm#c.dat*. This is and atomic parameter data set for carbon. Choose a filter if you wish.
19. Click *Done* to advance to the Processing options window.
20. Enter a *Title for Run* at the top of the window.
21. In the top left box, enter 12.0 for the *Impurity element isotopic mass* and 2.0 for the *Neutral hydrogen isotopic mass*.
22. In the lower left box for electron temperature, enter *Lower limit* 1.0, *Upper limit* 100.0, *No. of temps* 10.
23. In the lower right box for electron density, enter *Lower limit* 1.00e+10, *Upper limit* 1.00e+15, *No. of dens.* 11.
24. Click *Done* to advance to the Output window.
25. Enter 30 for the two-digit year number. Make sure there are no blanks. The Passing file template changes accordingly. It is editable.
26. Select *Text Output* and *Default File Name* and click *Done*.
27. Note the list of passing files which will be created is shown in an information widget. Click *OK* to accept the list.
28. Click on the *Escape to Menu* button to finish
29. Look at acd30#c.pass. Note that it is fully formed ADF11 unresolved type file.

3. Example 1

Repeat ADAS405, but this time select the file *iter_test_c*. Everything else is the same. You will see a line selection choice now on the processing options window. Select one of these. On the Output options window you should look at the other graphs.

5. Example 2

ADAS405 has a very wide scope. Feel free to try it. You will probably need to look at the manual to appreciate its full capabilities and the range of data which it can access.

Tutorial session 4 examples

1. ADF01 and ADF12

1. Explore the ADAS database for these formats. Note that the specification is in the ADAS User manual (*appxa-01* and *appxa-12*).

2. ADAS301 Test Case

2. Move to your sub-directory */.../<uid>/adas/pass*. Start ADAS301.
3. Click on *Central Data*, and select *qcx#h0/qcx#h0_old#n7.dat*.
4. Click the *Browse comments* button to see the list of transitions present in the file *qcx#h0/qcx#h0_old#n7.dat.* Move onto ADAS301 Processing window.
5. Select *Fit polynomial* at the 5% level. Click on the n=8 - n'=7 transition in the transition list window. You will need to use the scroll-bar on the right.
6. Click on *Select Velocities/Energies for Output File* button.
7. Now put in default values in the Table. Note the units in use. It is preferred to units of eV/amu. You need to edit the table to change the units.
8. Click on the *Select Quantum Numbers for Processing* button. Select the 7f shell. Note that you can select total and partial cross-sections – see the key to the right.
9. Click on the *Done* button to proceed to the Output options window.
10. Click on the button for *Graphical Output*. Then click *Done* to see the graph.
11. Have a look at the output text file after completion

3. ADAS303 Test Case

12. Move to your sub-directory */.../<uid>/adas/pass*. Start ADAS303.
13. Click on *Central Data*, and select *qef93#h/qef93#h_c6.dat*.
14. Click the *Browse comments* button to see what is in the file *qef93#h_c6.dat.* Move onto ADAS303 Processing window.
15. Select *Fit polynomial* at the 5% level. Click on the n=8 - n'=7 transition in the transition list window. You will need to use the scroll-bar on the right.
16. Click on the *Default Energy/Velocity Values* button. A set of energies appears in the Output energies column. Note the units in use. You need to edit the table to change the units.
17. Click on the *Select supplementary plasma parameters* button. Now type in Output Values for Ion Density, Ion Temperature, Z effective and B Magnetic. Note the reference value and valid ranges for each of these parameters are given. The reference values are good values to start with.
18. Click on the *Done* button to proceed to the Output options window.
19. Click on the button for *Graphical Output*. Then click *Done* to see the graph.
20. Have a look at the output text file after completion

4 ADAS 308 Test Case

1. Move to your directory */.../<uid>/adas/pass*. Start ADAS and move to the ADAS3 series menu. Select ADAS308.
2. Click on *Central Data*, the data root to data class ADF01 should appear in the window alongside. Click on the directory name *qcx#h0* in the file list window. *qcx#h0* appears above in the selection window. Click on *qcx#h0_old#n7.dat*. It appears in the selection window [you may need to scroll down].
3. Click the *Browse comments* button. Information of what is in the file *qcx#h0_old#n7.dat* is displayed. Click *Done* to restore the Input window. Click *Done* and the ADAS308 Processing window appears.
4. The Processing window is complex. Note the information on donor and receiver near the top. To the right enter the Atomic mass of the receiver (14.0). Remember to press {*return*}.
5. Next Input the plasma parameters, for example, T_i=5.0e3, T_e=5.0e3, N_i=2.5e13, N_e=5.0e13, Z_{eff}=2.0, B=3.0.

6. Now Select charge exchange theory. This is a drop down menu. Click *Use input data set*. [Note programs have built in default activation on some buttons. If the button is darkened it is activated]. Now Select emission measure model. This is also a drop down menu. Click *Charge exchange*.
7. Now turn to the Input of beam and spectrum line information and click first on the button for *Beam parameter information*. The appropriate table appears below for editing. Click Edit to bring up Table Editor and enter appropriate values, for example

   0.85 8.0E4
   0.12 4.0E4
   0.03 2.7E4

   and then *Done*.
8. Similarly, click the button for Observed spectrum lines and edit it's table. Try

   9 8 1.00E12

   and click *Done*.
9. Finally click the button for Required emissivity prediction and edit it's table. Try

   9 8 1
   8 7 2
   7 6 2
   6 5

   and click *Done*.
10. All is now ready. Click *Done* to move to the Output options window.
11. Click the button for *Graphical output.* You may also *Enable Hard Copy* and *Text Output*. Finally click *Done* to see the graph.
12. Click *Done* to return to the Output options screen. Click on the *Exit to Menu* icon to finish up. Finally click on the *Exit* button on the sub-menu and main menu windows to exit ADAS.

5. ADAS 304 Test Case

21. Move to your directory /.../*<uid>/adas/pass*. Start ADAS and move to the ADAS3 series menu. Select ADAS304.
22. The Input window is different from the usual. Click *on Central Data*, the data root to the data class ADF21 should appear in the window above. Now enter the Group name for input files. This is the directory of the look-up tables of stopping data for a particular beam species. Type *bms93#h*. Remember the {*return*}.
23. Now you must decide on the mixture of impurity nuclei (and hydrogen nuclei) which cause the total stopping. Click the button *Select Ion List*. The button incidentally becomes *Reselect Ion List* on later passes through. A button table pops up. Click on the buttons for the nuclei you wish to include, for example, Be4, C6, H1 and click *Done*. Note the Stopping Ion List. Click *Done* to advance to the Processing Options window.
24. Click on the *Fit polynomial* button, then type 5 in the adjacent active editable box
25. Now move to the Stopping ion fractions. Click on the *Edit Table* button to activate Table Editor. Enter 0.1,0.1,0.8 for Be, C, H respectively and click *Done*.
26. Now Select the co-ordinate type for the output graph. Click the *Energy* button for the first try.
27. Click on the *Default Output Values* button. You may find a warning widget pops up. If so, click the *Confirm* button.
28. Click the button for *Graphical output.* Finally click *Done* to see the graph.
29. Click *Done* to return to the Output options screen. You may *Exit to menu* using the icon in this program.

6. ADAS 310 Test Case

13. Move to your directory /.../*<uid>/adas/pass*. Start ADAS and move to the ADAS3 series menu. Select ADAS310.
14. The Input window is considerably different from the usual. Enter beam species details (H for hydrogen and its isotopes) and the atomic charge of the beam species.
15. There are two files to be selected, the expansion file and the charge exchange file. To select the expansion file, click on the *Central Data* button, the *Data root* to the data class ADF18 should appear in the window above. Now select the data file *bndlen_exp#h0.dat*.

To select the charge exchange file, click on *Central Data*, the *Data root* to data class ADF01 should appear in the window. Select *qcx#h0*. Now select the data file *qcx#h0_e2p#h1.dat*. Click on the *Done* button to advance to the Proessing options window.

16. The control parameters of the collisional-radiative calculation are organised into three groups, selected in turn by the buttons *genera*l, *switches (I)* and *switches (II)*.
    General button: Click on the *general* button to view the general parameter settings. The default values are reasonable.
    Switches (I) button: Click on the *switches (I)* button to view the settings associated with electron collisions. Working down the list set the parameters to the following: 2, 3, NO, YES.
    Switches (II) button: Click on the *switches (II)* button to view the settings associated with the ion collisions. Working down the list set the parameters to the following: YES, 0, YES, YES.
17. Now you must decide what range of principal quantum numbers that you want to include in the calculation. Click on the *Representative N-shells* button . Enter 1 and 110 as the minimum and maximum n-shells. Now click on the *Edit Table* button and enter the following values into the editor: 1,2,3,4,5,6,7,8,9,10,12,15,20,30,40,50,60,70,80,90,100. Click on *Done* to return to the processing widget.
18. Now you need to decide the impurity content of the target plasma. Click on the *Impurity information* button. Now click on the *Selection mode* button and choose *Multiple impurities*. Click on the *Edit Table* button and enter the following information into the editor

H	1.0	0.9
C	12.0	0.05
Be	11.0	0.05

    Click on the *Done* button to return to the processing window.
19. Click on the e*lectron/proton density scan* button to choose the range of plasma densities. In the usual manner enter the following values into the table editor.

1.0e13	1.0
2.0e13	2.0
3.0e13	3.0
4.0e13	4.0
5.0e13	5.0

    Click Done to return to the processing window. Enter the value 3 as the *Index for the reference density*.
20. Now click on the e*lectron/proton temperature* button and enter the following values ino the text editor

    1.0e3
    2.0e3
    3.0e3
    4.0e3
    5.0e3

    Click on the *Done* button to return to the processing widget. Enter the value 3 as the *Index for the reference temperature*.
21. Click on the *beam energy scan* button and eneter the following values into the table editor

    2.0e4
    3.0e4
    4.0e4
    5.0e4
    6.0e4

    Click on the *Done* button to return to the processing widget. Ernter the value 3 for the *Index for the reference beam energy* and 1.0e8 as the *Beam density.*
    Now click on *Done* to advance to the Output window.
22. There are several possible outputs but our interest is in the contents of the first passing file. The first passing file is of type ADF26 and contains the tabulated population structure and effective stopping coefficients as a function of plasma parameters. It should be noted that the fourth passing file contains the stopping coefficients assembled

according to format ADF21. The preferred route to obtaining the stopping coefficients is via ADAS312.

23. Click on the *First passing file* button and enter a filename. Now click on *Run now*. An Information widget appears. After the calculation, click on the *Exit to Menu* button to return to the ADAS3 series menu.

Tutorial session 5 examples

1. ADAS 304 Test Case

1. Move to your directory /.../*<uid>/adas/pass*. Start ADAS and move to the ADAS3 series menu. Select ADAS304.
2. The Input window is different from the usual. Click *on Central Data*, the data root to the data class ADF21 should appear in the window above. Now enter the Group name for input files. This is the directory of the look-up tables of stopping data for a particular beam species. Type *bms93#h*. Remember the {*return*}.
3. Now you must decide on the mixture of impurity nuclei (and hydrogen nuclei) which cause the total stopping. Click the button *Select Ion List*. The button incidentally becomes *Reselect Ion List* on later passes through. A button table pops up. Click on the buttons for the nuclei you wish to include, for example, Be4, C6, H1 and click *Done*. Note the Stopping Ion List. Click *Done* to advance to the Processing Options window.
4. Click on the *Fit polynomial* button, then type 5 in the adjacent active editable box
5. Now move to the Stopping ion fractions. Click on the *Edit Table* button to activate Table Editor. Enter 0.1,0.1,0.8 for Be, C, H respectively and click *Done*.
6. Now Select the co-ordinate type for the output graph. Click the *Energy* button for the first try.
7. Click on the *Default Output Values* button. You may find a warning widget pops up. If so, click the *Confirm* button.
8. Click the button for *Graphical output.* Finally click *Done* to see the graph.
9. Click *Done* to return to the Output options screen. You may *Exit to menu* using the icon in this program.

2. ADAS 310 Test Case

1. Move to your directory /.../*<uid>/adas/pass*. Start ADAS and move to the ADAS3 series menu. Select ADAS310.
2. The Input window is considerably different from the usual. Enter beam species details (H for hydrogen and its isotopes) and the atomic charge of the beam species.
3. There are two files to be selected, the expansion file and the charge exchange file. To select the expansion file, click on the *Central Data* button, the *Data root* to the data class ADF18 should appear in the window above. Now select the data file *bndlen_exp#h0.dat*. To select the charge exchange file, click on *Central Data*, the *Data root* to data class ADF01 should appear in the window. Select *qcx#h0*. Now select the data file *qcx#h0_e2p#h1.dat*. Click on the *Done* button to advance to the Proessing options window.
4. The control parameters of the collisional-radiative calculation are organised into three groups, selected in turn by the buttons *genera*l, *switches (I)* and *switches (II)*.
   General button: Click on the *general* button to view the general parameter settings. The default values are reasonable.
   Switches (I) button: Click on the *switches (I)* button to view the settings associated with electron collisions. Working down the list set the parameters to the following: 2, 3, NO, YES.
   Switches (II) button: Click on the *switches (II)* button to view the settings associated with the ion collisions. Working down the list set the parameters to the following: YES, 0, YES, YES.
5. Now you must decide what range of principal quantum numbers that you want to include in the calculation. Click on the *Representative N-shells* button . Enter 1 and 110 as the minimum and maximum n-shells. Now click on the *Edit Table* button and enter the following values into the editor: 1,2,3,4,5,6,7,8,9,10,12,15,20,30,40,50,60,70,80,90,100. Click on *Done* to return to the processing widget.
6. Now you need to decide the impurity content of the target plasma. Click on the *Impurity information* button. Now click on the *Selection mode* button and choose *Multiple impurities*. Click on the *Edit Table* button and enter the following information into the editor

H	1.0	0.9
C	12.0	0.05
Be	11.0	0.05

Click on the *Done* button to return to the processing window.

7. Click on the e*lectron/proton density scan* button to choose the range of plasma densities. In the usual manner enter the following values into the table editor.

1.0e13	1.0
2.0e13	2.0
3.0e13	3.0
4.0e13	4.0
5.0e13	5.0

Click Done to return to the processing window. Enter the value 3 as the *Index for the reference density*.

8. Now click on the e*lectron/proton temperature* button and enter the following values ino the text editor

1.0e3
2.0e3
3.0e3
4.0e3
5.0e3

Click on the *Done* button to return to the processing widget. Enter the value 3 as the *Index for the reference temperature*.

9. Click on the *beam energy scan* button and eneter the following values into the table editor

2.0e4
3.0e4
4.0e4
5.0e4
6.0e4

Click on the *Done* button to return to the processing widget. Ernter the value 3 for the *Index for the reference beam energy* and 1.0e8 as the *Beam density.*
Now click on *Done* to advance to the Output window.

10. There are several possible outputs but our interest is in the contents of the first passing file. The first passing file is of type ADF26 and contains the tabulated population structure and effective stopping coefficients as a function of plasma parameters. It should be noted that the fourth passing file contains the stopping coefficients assembled according to format ADF21. The preferred route to obtaining the stopping coefficients is via ADAS312.
11. Click on the *First passing file* button and enter a filename. Now click on *Run now*. An Information widget appears. After the calculation, click on the *Exit to Menu* button to return to the ADAS3 series menu.

Callable ADAS — Exercises

March, 2012

1 Aim

The aim is to familiarise you with callable ADAS, mainly in an IDL environment but also using Fortran. Please feel free to expand any of the tasks or change them slightly to deal with your favourite ion! The sub tasks should be considered optional and are often more difficult (marked with 🌶s) so don't spend too much time on them unless they are of particular interest — getting the main tasks done is more important.

2 Tasks

1. Use `run_adas208` to explore the population structure of boron-like neon.
   - Find the approximate density where the systems switches from coronal to CR and from CR to LTE.
   - Produce a PEC file for the system🌶.
2. Use `read_adf11` to read ionisation and recombination coefficients for carbon.
   - Plot the temperature where the ionisation and recombination rates are equal as a function of ion charge 🌶🌶.
3. Use `run_adas405` to generate an equilibrium ionisation balance for carbon.
   - Compare the temperature of peak abundance (as a function of ion charge) with the points where the rates are equal (see above) 🌶🌶🌶.
   - Contrast `run_adas405` (time independent) with `run_adas406` (time dependent)🌶🌶🌶🌶.
   - See if you can feed the results into `write_adf19` to produce a PZD file🌶🌶🌶.
4. Use `read_adf15` to read data for the $1s^2\ ^1S - 1s2p\ ^1P$ and $1s^2\ ^1S - 1s2p\ ^3S$ in He-like argon.
   - Produce a contour plot over a sensible temperature and density range🌶.
   - Hence show that the ratio is a useful density diagnostic🌶.

5. Use `read_adf15` to read the PEC for the 977Å line of C^{+2}
   - Compare the power radiated in this line with the total line power for C3+ in coronal equilibrium conditions 🌶🌶🌶.
6. Using the fortran routine `r8ah`, write a small Fortran program which prints out the A-value of the 8p - 3s transition in hydrogen.
   - Extend the program to print out the A-value of the whole $n = 8$ to $n = 3$ transition🌶.
   - Do the same in IDL.
7. Combine `run_adas405` and `read_adf15` to produce an emission profile over the device (fusion machine, star, blob of tin) of your choosing.
   - Integrate over the data to simulate a spectrometer🌶.
   - Automatically produce an adaptive grid of points where the emission is highest🌶🌶🌶.
8. Use `run_adas416` to produce partitioned data using the file `/home/ITER/omullam/ADAS_course/partition_example.dat`.
   - Modify the partition and explore how the various ions move in and out of being bundled🌶.
9. Use `read_adf12` to read effective charge exchange emission coefficients for the $n = 8 \rightarrow n = 7$ transition of CVI.
   - Write a program which can turn a fitted line area into a carbon concentration given a known beam energy, beam density and plasma parameters🌶🌶🌶.
10. Use `read_adf22` to read beam populations (`BMP`) for a hydrogen beam, look at the relative populations of $n = 2$ to $n = 1$ as a function of energy.
    - Combine these populations with two ADF12 files (via `read_adf12`) and explore the variation with energy, compare it with just assuming $n = 1$ population🌶🌶.
11. Read beam stopping coefficients for a neutral beam passing through a hydrogen plasma with a 3% neon content.
    - Find the dependence on the stopping as a function of neon content.
    - Integrate a real beam over a sensible profile, find the penetration depth as a function of neon concentration🌶🌶🌶🌶🌶.
12. Use `run_adas306` to compare active CX emission and excitation driven emission for CVI 8-7.
    - Plot the Doppler broadened feature (see `c5dplr.pro`) along with the components which make it up🌶.
    - Write a program which finds where the two emission processes become comparable🌶🌶🌶.

3 Hints

- Many IDL routines will give you help if you type their name followed by `,/help` (e.g. `run_adas405,/help`). Source is also available.
- You can search for r8ah online.
- IDL has built-in integration routines, type 'idlhelp' to see it.
- The `adas_vector` function can provide help in producing lists of numbers, see: `/home/adas/idl/adaslib/util/adas_vector.pro`.

ADAS900 SERIES TUTORIAL

- Explore central ADAS900 directories on /home/sccp/gttm/FG300612/dev_adas/madas/
- The data file is inside .../madas/
- The executables are on .../bin/, To run them be sure that you are on your own directory and then type '/home/sccp/gttm/FG300612/dev_adas/madas/bin/<adas9xx.out>. The input file must be in your working directory.
- copy directory /home/sccp/gttm/FG300612/DEMO to your own directory.
- Input files are inside .../DEMO/inputs/
- Explanation of input files are inside .../DEMO/tutorial/

Exercises:

1. Create input902.dat and run adas902.out with the specific settings that you'd like. Think what are the mdf02 files you would like to include in the calculations. Remember that the states you keep in the mdf02 file are the ones which will be conserved through the whole sequence.
2. Explore the output file. Identify the metastables selected on the input 902.
3. Create the itaus.dat to obtain the maxwellian time constants from mdf33. Use IDL to produce graphical plot from the output files (you will find an example of IDL program in the tutorial/ directory)
4. Create input903.dat and run adas903.out. Explore mdf04.pass.
5. Create input904.dat and run adas904.out. Look at the mdf11 files. Why are the DXCD values null? Look at the table 1 to know what type of terms are writen on the mdf11 files
6. Create the new type of itaus.dat to output your desired effective coefficients. Plot them using IDL.
7. Create ipop.dat to read the populations. Plot them using IDL.

Quantity	Description
MQCD	Molecular excitation CR coefficient
MSCD	Molecular ionization CR coefficient.
MACD	Molecular recombination CR coefficient.
MXCD	Molecular cross coupling (through ionization) CR coefficient.
PDCD	Partial (from a molecular specie) dissociation CR coefficient.
PXDCD	Partial (from a molecular specie) cross-coupling (through recombination) dissociation CR coefficient.
PXSDCD	Partial (from a molecular specie) double cross-coupling (through molecular recombination and atomic ionization) dissociation CR coefficient.
DXCD	Partial cross-coupling (through atomic ionisation) dissociation CR coefficient.
SCD	Atomic ionization CR coefficient.
ACD	Atomic recombination CR coefficient.
QCD	Atomic excitation CR coefficient.
XCD	Atomic cross-coupling (through ionization) CR coefficient.

Table 1: Description of collisional-radiative terms

Appendix E

EFDA-JET special meeting

E.1 Meeting report

ADAS-EU Travel Report

Location:	EFDA-JET Facility, Culham Laboratory, UK.
Date:	26-27 Apr 2012.
ADAS-EU staff:	Nigel Badnell, Martin O'Mullane, Alessandra Giunta, Hugh Summers.
Persons visiting:	Pavel Bogdanovitch (Vilnius), Pascal Quinet(Mons), Patrick Palmeri(Mons).
EFDA/JET staff:	Mathias Groth, Sebastian Brezinsek, Costanza Maggi, Andy Meigs, Kerry Lawson, Mike Stamp,
Purpose:	Design content of ADAS-EU follow-up sub-contracts with Univ. of Vilnius and Univ. of Mons-Hainaut. Discuss progress of tungsten spectral modelling with EFDA-JET team.

Items:

(1) First discussions (26 May a.m.) were with Pavel to plan further calculations using his methods for *ab initio* structure and transition probabilities in the large scale multi-configurational approach with virtual excitations and TROs for low and medium charge states of very heavy systems.

(2) Martin and Hugh wondered about the importance of the 5d-5f promotion in the W^{+2} - W^{+7} iso-nuclear set with open 5d valence shell. Martin's simpler Cowan/Born studies of total radiated power suggest that this transition array would be a main radiator, yet there is no information on 5f levels in the NIST tables and it is excluded from the studies for ADAS-EU by Pascal and Patrick.

(3) Nigel and Hugh conjectured on inclusion of the simple one-electron promotion so that in the structure calculation there would be at most one electron in the 5f shell. Pavel was concerned that the CI of $5d^2$ and $5f^2$ would need to be included, although Nigel and Hugh were prepared to accept the cruder calculation, at least to size up the problem.

(4) Pavel pointed out that multiple f-shell occupancies were not at present included in his structure calculations, but that Gaigalas had the capability to make this extension with him.

(5) It was felt to be feasible to extend the calculations with open 5d shell as done for W^{+2} to further similar systems , perhaps up to W^{+5}, and to include the isoelectronic ions of hafnium, tantalum and rhenium. However computation time suggested that this could only be done in the ADAS-EU time frame with the simpler calculation excluding 5f. Hugh accepted this.

(6) Discussion then moved to lifting the collisional calculation from just the plane-wave Born type, implemented in the initial Vilnius sub-contract. Nigel said that this required transfer of the numerical radial orbitals. Pavel confirmed that he does generate and can provide an orthogonal basis of radial wave functions. With these orbitals available to *autostructure*, Nigel can pursue alignment of the structure calculations and then lift the collisional calculation - first to distorted wave and then to R-matrix.

(7) The mechanics of the transfer would be a matter for Pavel and Nigel.

(8) Hugh felt that he could identify the content of a valuable follow-up sub-contract with Vilnius, relevant to fusion and ADAS-EU from the above and would prepare a document for consideration..

(9) The second set of discussions (26 May p.m.) included Pascal and Patrick and centred on the Mons-Hainaut work. Hugh and Martin wanted to pursue the exploitation of the data transfer pathways established in the initial ADAS-EU sub-contract. With the latter, so far, the refined Cowan structure, coupled with its extension to the collisional regime with plane wave Born, had delivered key ADAS adf04 datasets for W^{+0} , W^{+1} and W^{+2} which are proving very important and exciting for the fusion community.

(10) Martin and Pascal engaged to work out an heavy ion list, from the historic Mons-Hainaut heavy ion evaluations, which would be useful for fusion and for which Cowan structure parameter optimisations were available.

(11) Hugh and Nigel were again enthusiastic to keep moving forward on the lifting of the collisional part of the collaboration. The objective is to enable AUTOSTRUCTURE distorted wave and R-matrix cross-sections from Mons-Hainaut structure inputs.

(12) Nigel pointed out that the alignment of structure calculations by the *autostructure* / *superstructure* procedures and the Cowan procedures had never been done. Hugh was very keen that this should be pursed.

(13) Nigel and Patrick discussed the problems and what needed to be done. Firstly there was the transfer of orbitals to be achieved - demonstrated by a minimal system, such as C^{+3}

with all the Cowan elaborations switched off. The second step would be the addition of special integrals and integral modifiers used by Cowan to *autostructure*. These include scaling, polarization, α, β, γ and T optimizing parameters. Nigel thought that *autostructure* had the infrastructure for everything necessary to achieve this.

(14) Nigel and Patrick engaged to work out the details and felt that Mo^0 would be a good test species for the interchange format.

(15) Hugh was content that there was a good basis for a unique and fusion relevant ADAS-EU extension sub-contract.

(16) Elaborating further discussions took place pair-wise on 27 Apr. to fill out the plans for the sub-contract specifications.

(17) A discussion meeting with a presentation by Martin was held. This was designed so that the ADAS-EU specialists could meet the EFDA-JET user community, so that the relevance and progress of the atomic work could be explained, and so that the fusion community could explain their atomic data utilisation and their key/urgent needs. The meeting was first addressed by Mathias Groth, from the impurity transport modelling area. Mathias explained the various usages.

(18) Sebastian Bresinsek gave a resume of spectral analysis work, especially around influx of tungsten, at JET and Juelich.

(19) Martin then gave a presentation (attached) of some of the outcomes of the ADAS/ADAS-EU effort and the achievements of the sub-contracting specialists present. There was much discussion. The new figures of W^0 photon efficiencies provoked great interest.

(20) The meeting strongly endorsed the pathways that the ADAS-EU team and sub-contractors were pursuing. The impression was that the activities were very well aligned with the fusion needs. The EFDA-JET task force leaders (Mathias and Sebastian) did emphasise the current great importance of aspects such the tungsten influx and encouraged all speed.

H. P. Summers
25 June 2012

University of Strathclyde Glasgow

Status of Tungsten data in ADAS

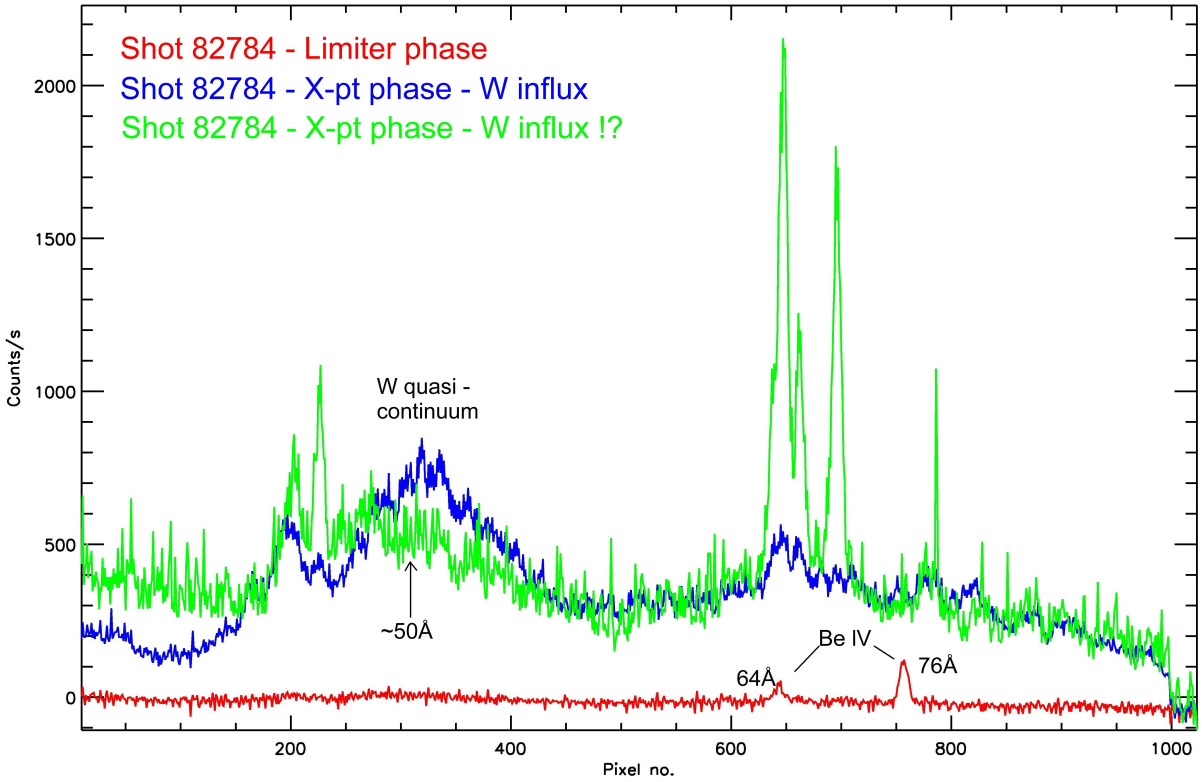
E.2 Tungsten review

Status of Tungsten data in ADAS

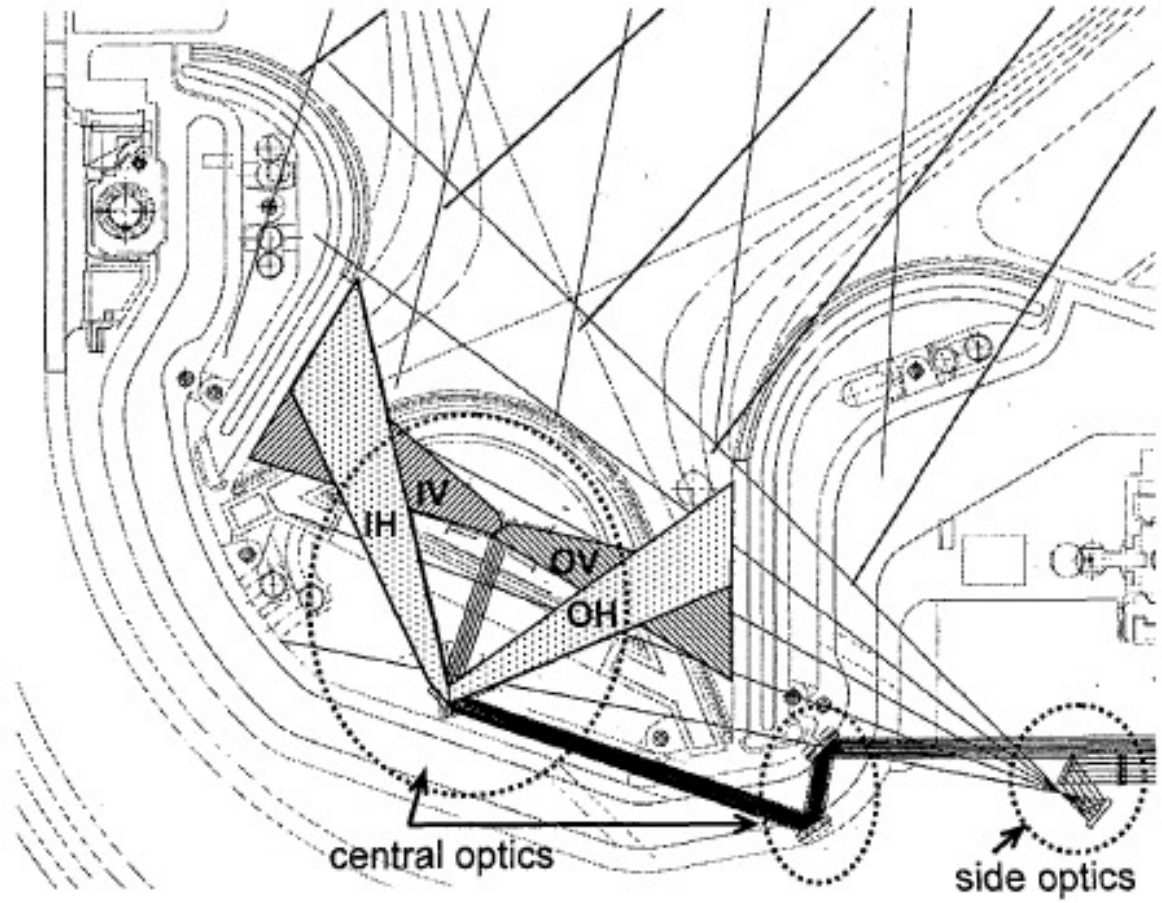
Informal meeting, JET, 27-April-2012

JET's ITER-like wall: ILW

Beryllium plasma facing components with a tungsten divertor.



Proposed divertor spectroscopy for ITER



Areas where atomic data for tungsten is needed

- Neutral and near-neutral species for influx measurements via visible spectgroscopy.
- Strong isolated emission lines in the soft X-ray and VUV from tungsten ion stages with 1–3 optically active electrons arising in the confined plasma.
- Ionisation and recombination coefficients which are density dependent for ionisation (and power) balance calculations.
- Low ionisation stages, $\mathrm{W}^{0} - \mathrm{W}^{+35}$ for divertor and edge modelling.
- Reduction in uncertainity of recombination rates for stages up to W^{+21}.
- Methods to reduce the size and complexity in handling tungsten data.
- Quantification of the influence of active emission from tungsten during neutral beam heating and its contribution to the overall stopping of the beams.

Require *adf04* data for most of these tasks

- Cowan code (`adas8#1`) for baseline production with plane wave Born rates.
- R-matrix sequence data — H, He, Li, F, Ne and Na-like to Kr.
- Other isolated species — all Be, B, some C, O and N.
- `AUTOSTRUCTURE` for complementary baseline — DW accounts for spin changing; input for R-matrix.

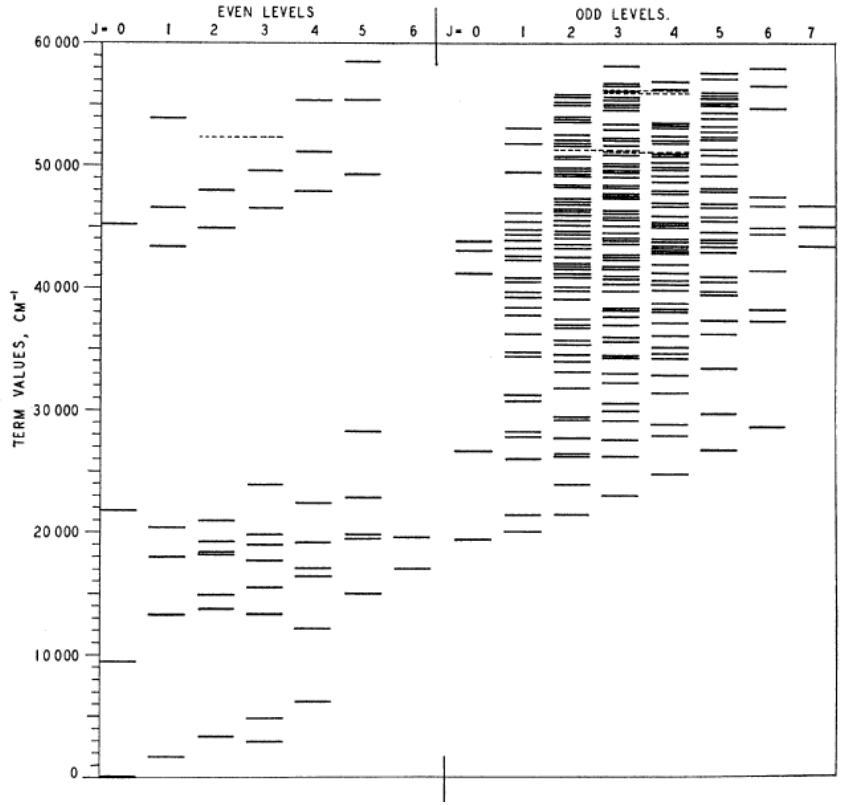
Better structure leads to believable rates

How to improve what we have?

- Mons-Hinaut ASPECT group with improved Cowan.
- Villnius group with massive CI, pure *ab initio* structure.

Harness these efforts as inputs for ADAS collision codes and population modelling. ADAS-EU FP7 has enabled this collaboration.

Consider neutral W



O Laporte and J E Mack, Phys. Rev, 1943

Latest revision: A E Kramida and T Shirai, J Phys Chem Ref Data, 2006

W0 energy levels and our favourite line

			baseline	Mons	NIST
1	4FE 5D4 6S2	(5)2(0.0)	0.0	0.0	0.00
2	4FE 5D4 6S2	(5)2(1.0)	1467.9	1785.2	1670.29
3	4FE 5D5 6S1	(7)0(3.0)	-	2981.7	2951.29
4	4FE 5D4 6S2	(5)2(2.0)	3189.4	3469.8	3325.53
5	4FE 5D4 6S2	(5)2(3.0)	4863.1	4927.4	4830.00
6	4FE 5D4 6S2	(5)2(4.0)	6404.8	6207.7	6219.33
7	4FE 5D4 6S2	(3)1(0.0)	12950.2	9612.9	9528.06
8	4FE 5D4 6S2	(3)5(4.0)	14044.2	12249.8	12161.96
9	4FE 5D4 6S2	(3)1(1.0)	17084.9	13500.8	13307.10
10	4FE 5D4 6S2	(3)4(3.0)	16981.1	13506.3	13348.56

	NIST	U Mons	*adf04*	
E_{ground}	0.00	-88.0	0.0	$5d^4\,6s^2\ ^5D_0$
E_{lower}	2951.29	2893.0	2981.7	$5d^5\,6s\ ^7S_3$
E_{upper}	27889.68	27815.7	27905.5	$5d^4\,6s\,6p\ ^7P_4$
				$5d^5\,6p\ ^7P_4$ (NIST)

W0 — 4009Å and 5224Å identifications

The `adas8#1`/Cowan generated dataset considers the upper level to be $5d^4\,6s\,6p$ with a leading percentage of 67% for ^7P, 22% from other terms in this configuration and 2.62% of $5d^5\,6p\ ^7P$. NIST identifies the upper configuration as $5d^5\,6p\ ^7P$.

Identifications before 1960 and the isotope shift work of Aufmuth (J Phys B, 1988) confirm our classification.

What about the strongest KS8 line?

	NIST	U Mons	*adf04*	
E_{lower}	4830.0	4838	4927.4	$5d^4\,6s^2\ ^5D_3$
E_{upper}	23964.0	23958	24047.8	$5d^4\,6s\,6p\ ^7D_2$

There is no ambiguity in identifying this line but the purity of the upper level, $^7D_2$, is just 44% with 24% due to the the quintet $^5P_2$ indicating that the spin systems are not pure.

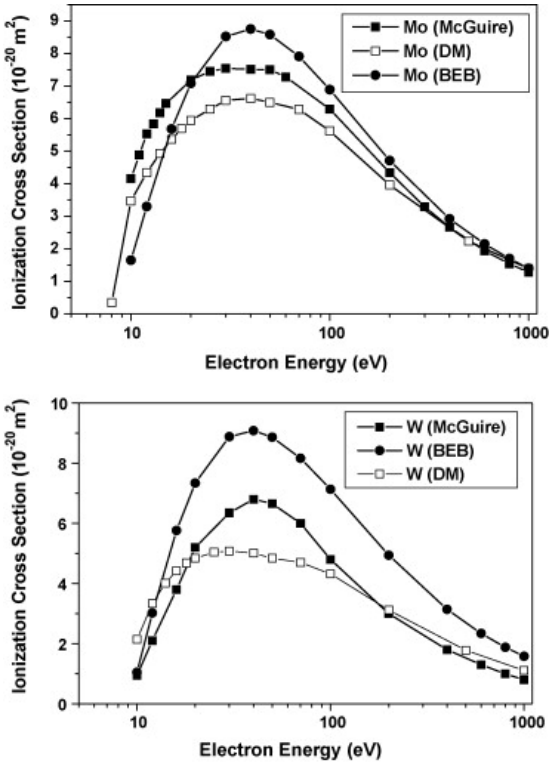
W2+ — emission centered ∼2500Å

				Mons	Villnius	NIST
1	4F14 5S2 5P6 5D4		(5)2(0.0)	0.0	0.00000	0.00
2	4F14 5S2 5P6 5D4		(5)2(1.0)	2291.8	2305.36163	2256.20
3	4F14 5S2 5P6 5D4		(5)2(2.0)	4505.3	4612.69852	4461.19
4	4F14 5S2 5P6 5D4		(5)2(3.0)	6280.7	6506.98415	6277.81
5	4F14 5S2 5P6 5D4		(5)2(4.0)	7615.0	7978.78109	7686.68
6	4F14 5S2 5P6 5D4		(3)1(0.0)	10037.4	10683.80603	9904.30
7	4F14 5S2 5P6 5D3	6S1	(5)3(1.0)	10918.1	12168.55197	10968.54
8	4F14 5S2 5P6 5D3	6S1	(5)3(2.0)	12439.1	13707.06921	12427.09
9	4F14 5S2 5P6 5D4		(3)1(1.0)	12949.8	13735.38143	12881.03
10	4F14 5S2 5P6 5D4		(3)5(4.0)	13803.7	15238.78272	13700.95

Villnius method is just *ab intio*.

Ionisation from neutral W

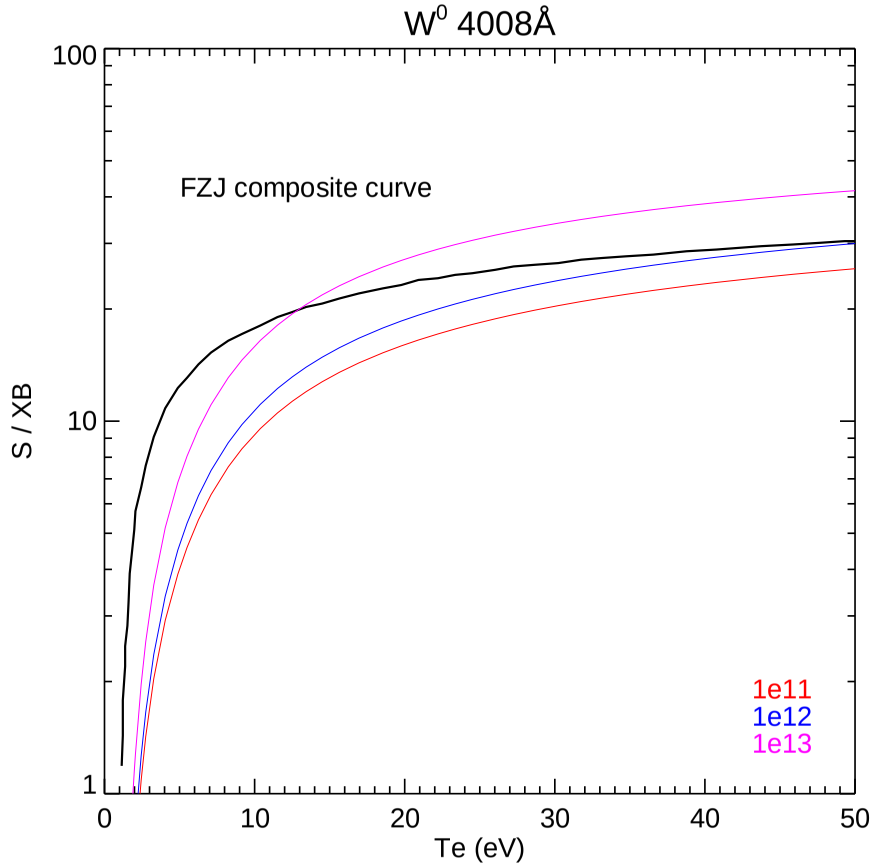
A few to choose from with no great agreement — use range as uncertainty estimate.



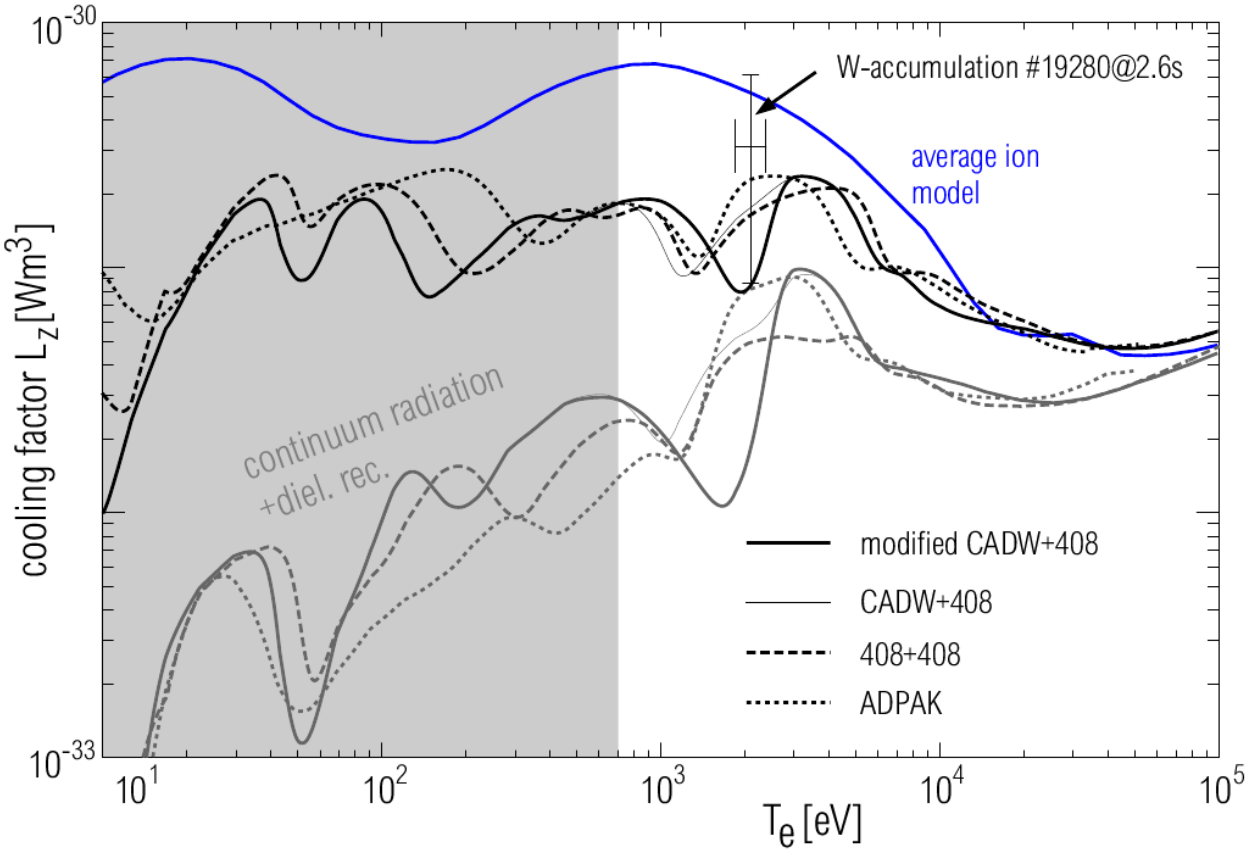
Deutsch et al, Int. J. Mass Spect., 2008

S/XB

If we take Mons *adf04* and CADW *adf07* we get....



Ionisation balance

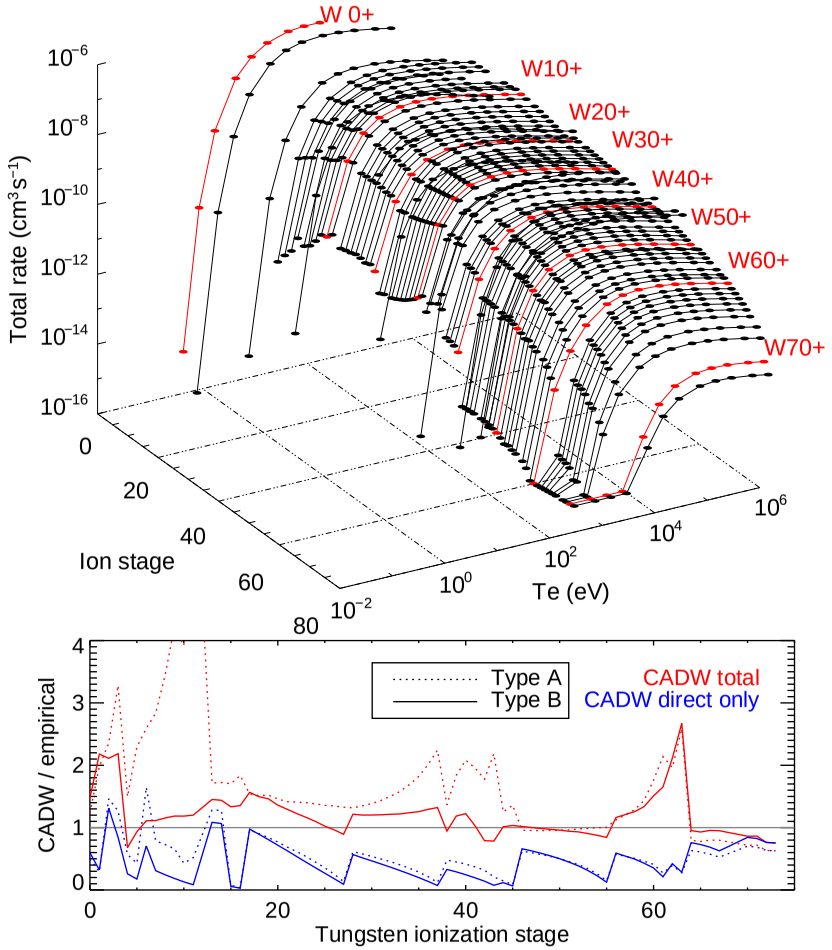


Great uncertainity below 800eV — stages below W^{+28} ($4d^{10}$ ground state).

Ionisation rates

CADW zero-density complete collection — adas8#2.

Loch et al, Phys. Rev. A, 2005



Dielectronic recombination for W^{+20}

Measurement and theory refining rates required for ionisation balance.

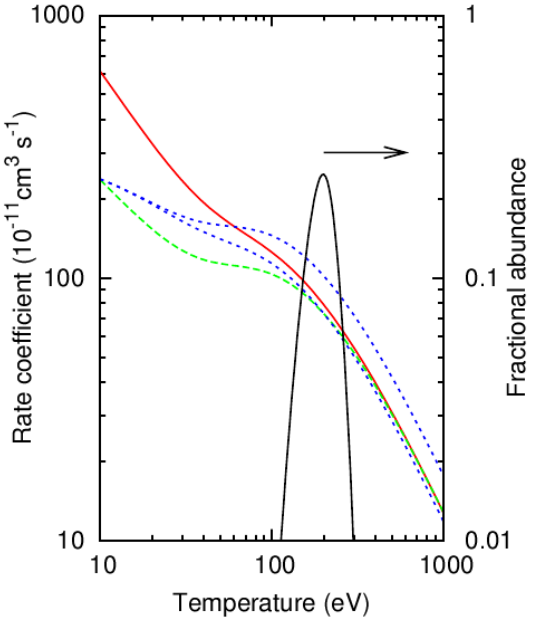


FIG. 7: (Color online) W^{20+} total Maxwellian DR rate coefficients: IC (solid red curve), LS (long-dashed green curve), and CA with-and-without $n = 5$ continuum (short-dashed blue curves). The fractional abundance of W^{20+} in a magnetic fusion plasma is shown also (solid black curve).

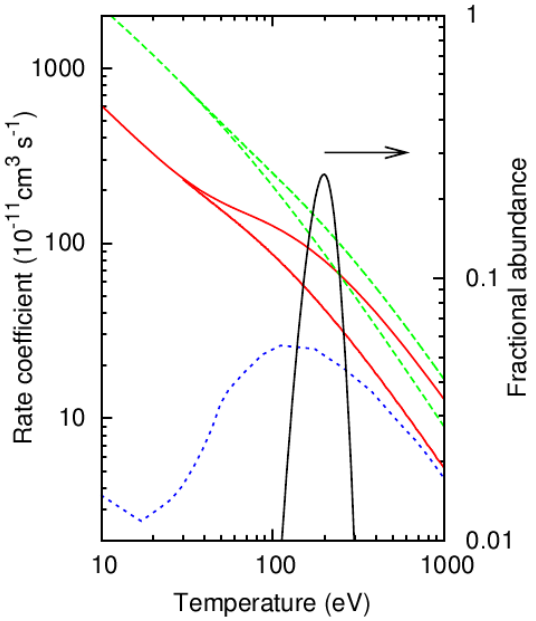


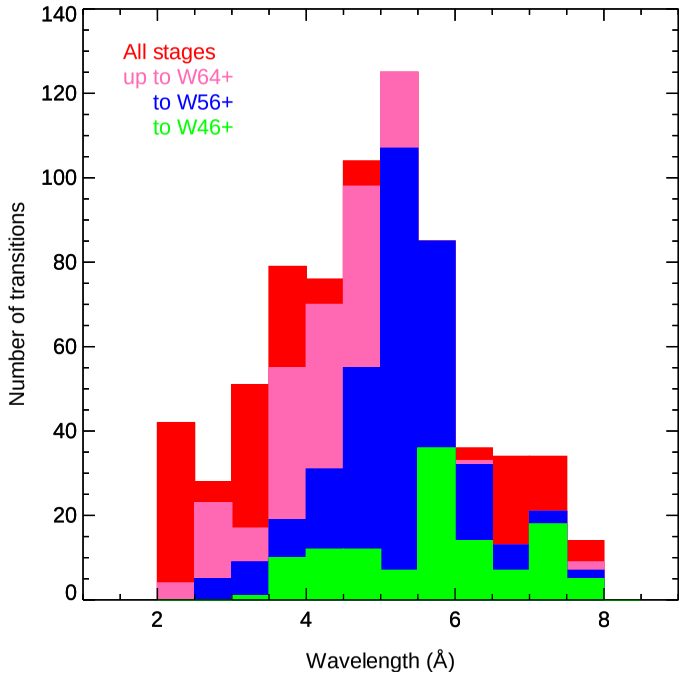
FIG. 8: (Color online) W^{20+} total Maxwellian DR rate coefficients: IC all resonances and to 140 eV only (solid red curves), experiment [7] to 140 eV and with theory top-up for resonances above 140eV (long-dashed green curves), and ADAS [31] (short-dashed blue curve). The fractional abundance of W^{20+} in a magnetic fusion plasma is shown also (solid black curve).

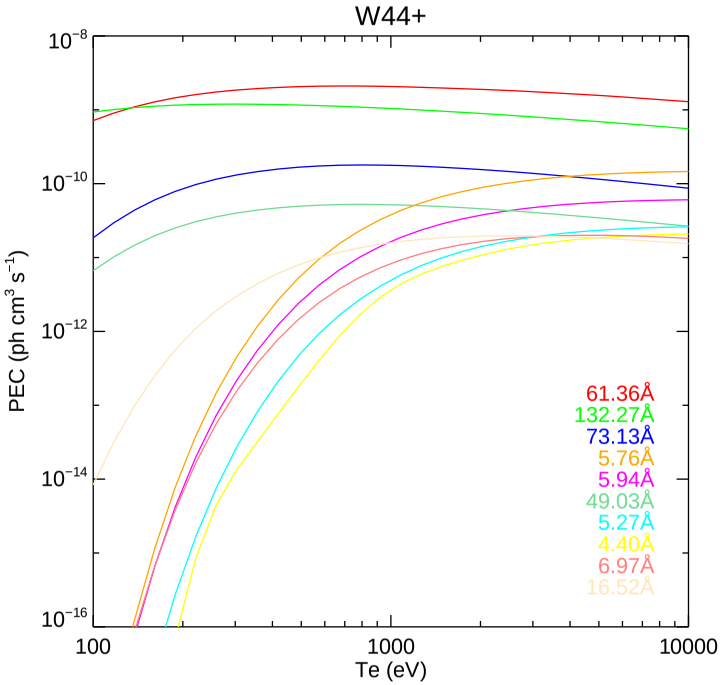
Badnell et al, submitted to Phys. Rev. A

Density dependence of S and α

- Not in CADW ionisation or *adf09* DR rates.
- Comes from GCR model.
- Serious revision of empirical formula used to date.
- Plant `adas316` dependence on S and α.

Tungsten emission in the confined plasma





- W38+ to W73+ contribute lines to the 2–8Å spectral region.
- Strongest lines not necessarily in the X-ray spectrum.
- 708 distinct lines.

Relativistic R-matrix calculations

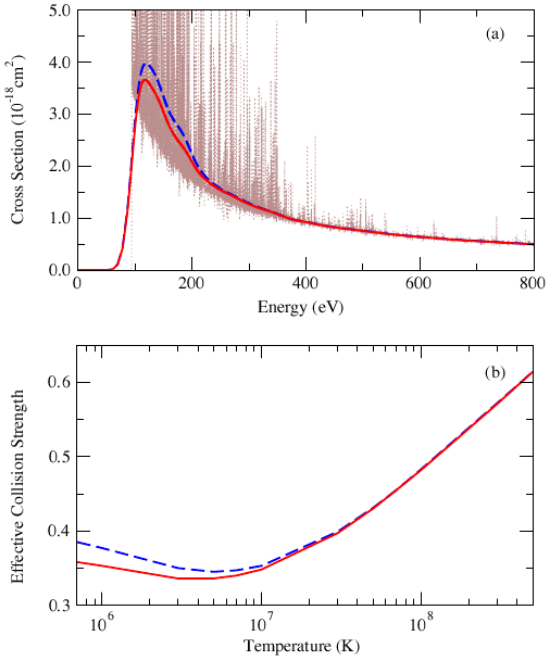


Figure 2. Electron-impact excitation of W^{44+} from the ground state to the $4s4p(1/2, 1/2)_1$ level (level 3). (a) The dotted curve is the damped cross section, the dashed curve is the undamped cross section convoluted with a 30 eV Gaussian, and the solid curve is the damped cross section convoluted with a 30 eV Gaussian. (b) The effective collision strength, where the dashed curve is with no radiation damping and solid curve is with radiation damping.

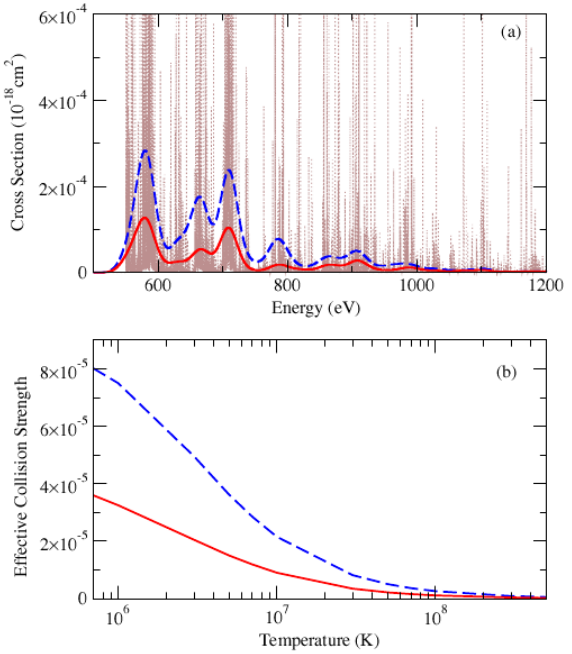


Figure 3. Electron-impact excitation of W^{44+} from the ground state to the $4p4d(3/2, 3/2)_0$ level (level 24). (a) The dotted curve is the damped cross section, the dashed curve is the undamped cross section convoluted with a 30 eV Gaussian, and the solid curve is the damped cross section convoluted with a 30 eV Gaussian. (b) The effective collision strength, where the dashed curve is with no radiation damping and solid curve is with radiation damping.

Apply these techniques to diagnostically significant emitters — Electron Collision Working Party (ECWP) intitiative.

Appendix F

Aachen and Juelich presentations and visits by Dr. Guzman

F.1 PSI conference presentation

P3-089

ADAS Tools for Collisional-Radiative Model for Molecules

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Abstract

New theoretical and computational tools for molecule collisional radiative models are presented. An application to the hydrogen molecule system has been studied. At the same time, a structured database has been created where either fundamental cross sections and rate for individual processes as well as derived data (effective coefficients) have been obtained. Relative populations for vibrational states of ground electronic state of H_2 are presented and compared for the two resolutions considered: electronic transitions where vibronic transitions are summed over electronic states and full vibrational resolution where the vibrational states are considered individually. New reaction rates were calculated by means of impact parameter approximation.

PACS: 52.20.Hv, 34.50.Gb

PSI-20 Keywords: ADAS, Collisional-radiative model, Divertor region, Divertor spectroscopy, Edge plasma, Hydrogen molecules, Molecular assisted recombination, Molecular ions, Vibrational states, Vibrational excitation.

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Computational tools make that process automatic and simplify the data assembly. Rate coefficients versus temperature and density are presented.

Introduction

Molecules desorbed from the wall are present in the edge of tokamak plasmas – they contribute to the neutral density through dissociation and influence divertor physics changing neutral population balance [1]. Experimental measurements in tokamaks show that their densities in the plasma edge can be a significant fraction of neutrals density [2]. Collisional-radiative (CR) coefficients are needed for the interpretation of measurements. Present day simulation codes consider CR coefficients from hydrogen (e.g. [3,4]) and some of the hydrocarbon molecules (e.g. [5]). Under the framework of ADAS-EU project a CR model for molecules is developed. This model will provide the tools for homonuclear diatomic molecule population studies in plasmas and will provide spectroscopic quantities needed for experimental studies. Collisional data and derived spectroscopic data are stored in a comprehensive database so that users can include them in their (plasma modelling) routines. In the next sections the theoretical basis of the collisional radiative model is given, the database structure for H_2 molecular system is discussed and results are presented.

Collisional-Radiative Model for Molecules

Molecules released into the plasma edge of a tokamak will suffer collisions with electrons and ions and can be excited, ionized or dissociated. The continuity equations for the molecular metastables of a diatomic homonuclear molecule can be written as:

$$\frac{dN_\rho}{dt} = N_e S_{\rho k} N_k^{-1} + N_e S_{\rho \nu'} N_{\nu'}^{-1} + C_{\rho j} N_j + C_{\rho\sigma} N_\sigma + N_e r_{\rho\nu} N_\nu^{+1} + \Gamma \tag{1}$$

where C_{xy} are the collisional terms which include all excitation and de-excitation as well as spontaneous and radiative processes from level y to level x and N_x are the level populations. Greek subscript are used for metastable states and latin subscript for ordinary sates. The diagonal C_{xx} coefficients include all the losses due to recombination, ionization, dissociation and excitation from level x. S_{xy} are the ionization rate coefficients from the molecular species with one more electron and r_{xy} are the recombination coefficients from the parent ionized molecule. Γ correspond to the source terms for this molecular species. The continuity equation for the dissociation products (e.g. atoms and ions) is then:

$$\begin{aligned}\frac{dN_\mu^{(A)}}{dt} &= \sum_\sigma N_e D_{\mu\sigma} N_\sigma + \sum_j N_e D_{\mu j} N_j + N_e S_{\mu\mu'} N_{\mu'}^{-1(A)} + \ldots \\ &\ldots + C_{\mu\eta} N_\eta^{(A)} + C_{\mu j''} N_{j''}^{(A)} + N_e r_{\mu\beta} N_\beta^{+1(A)} + \Gamma^{(A)}\end{aligned} \tag{2}$$

Here, terms D_{xy} correspond to dissociative rate coefficients and a summation must be performed over all the molecules which can dissociate from metastables and ordinary states into the dissociated species. The superscript A refers to atomic population.

Assuming quasi-statical equilibrium, it is possible to solve for the ordinary states in function of the metastables [6], obtaining the effective coefficients:

$$\begin{aligned}\frac{dN_\rho}{dt} &= N_e MSCD_{\rho\nu'} N_{\nu'}^{-1} + N_e MQCD_{\rho\sigma} N_\sigma + N_e MACD_{\rho\nu} N_\nu^{+1} + N_e MXCD_{\rho\sigma} N_\sigma + \Gamma \\ \frac{dN_\mu^{(A)}}{dt} &= \sum_\sigma N_e PDCD_{\mu\sigma} N_\sigma + \sum_\nu N_e PXDCD_{\mu\nu} N_\nu + \sum_{\nu'} N_e PXSDCD_{\mu\nu'} N_{\nu'} + \ldots \\ &\ldots + \sum_{\sigma'} N_e DXCD_{\mu\sigma'} N_{\sigma'} + N_e SCD_{\mu\mu'} N_{\mu'}^{-1(A)} + N_e ACD_{\mu\beta} N_\beta^{+1(A)} + \ldots \\ &\ldots + N_e QCD_{\mu\eta} N_\eta^{(A)} + N_e XCD_{\mu\eta'} N_{\eta'}^{(A)} + \Gamma^{(A)}\end{aligned} \tag{3},$$

where the meaning of the collisional radiative terms is given in table 1. These terms depend on both temperature and density and correspond to the effective direct and CR processes.

Quantity	Description
MQCD	Molecular excitation CR coefficient
MSCD	Molecular ionization CR coefficient.
MACD	Molecular recombination CR coefficient.
MXCD	Molecular cross coupling (through ionization) CR coefficient.
PDCD	Partial (from a molecular specie) dissociation CR coefficient.
PXDCD	Partial (from a molecular specie) cross-coupling (through recombination) dissociation CR coefficient.
PXSDCD	Partial (from a molecular specie) double cross-coupling (through molecular recombination and atomic ionization) dissociation CR coefficient.
DXCD	Partial cross-coupling (through atomic ionisation) dissociation CR coefficient.
SCD	Atomic ionization CR coefficient.
ACD	Atomic recombination CR coefficient.
QCD	Atomic excitation CR coefficient.
XCD	Atomic cross-coupling (through ionization) CR coefficient.

Table 1: Description of collisional-radiative terms in equation (3)

Applying the equations (3) to Hydrogen molecule system, it is possible to eliminate most of the cross coupling coefficients due to the negligible presence of molecular and atomic negative ions in the plasma and the practical absence of H_2^+ recombination mechanisms into H_2. The equations for the H_2 system are then:

$$\begin{aligned}
\frac{dN_\rho^{(H_2)}}{dt} &= N_e MQCD_{\rho\sigma} N_\sigma^{(H_2)} + \Gamma^{(H_2)} \\
\frac{dN_\nu^{(H_2^{+1})}}{dt} &= N_e MSCD_{\nu\sigma} N_\sigma^{(H_2)} + N_e MQCD_{\nu\nu} N_\nu^{(H_2^{+1})} + \Gamma^{(H_2^{+1})} \\
\frac{dN_\mu^{(H)}}{dt} &= \sum_{\sigma,\nu} N_e PDCD_{\mu(\sigma,\nu)} N_{(\sigma,\nu)}^{(H_2 H_2^{+1})} + N_e ACD_{\mu\beta} N_\beta^{(H^{+1})} + N_e QCD_{\mu\mu} N_\mu + \Gamma^{(H)} \\
\frac{dN_\beta^{(H^{+1})}}{dt} &= \sum_{\sigma,\nu} N_e PDCD_{\beta(\sigma,\nu)} N_{(\sigma,\nu)}^{(H_2 H_2^{+1})} + \sum_{\sigma,\nu} N_e DXCD_{\beta(\sigma,\nu)} N_{(\sigma,\nu)}^{(H_2 H_2^{+1})} + \ldots \\
&\quad \ldots + N_e SCD_{\beta\mu} N_\mu^{(H)} + N_e QCD_{\beta\beta} N_\beta^{(H^{+1})} + \Gamma^{(H^{+1})}
\end{aligned} \tag{4}$$

where the cross coupling diagonal terms are the losses and are negative terms.

It is now possible to obtain a full equilibrium solution for the population of metastables making the left-hand side members of all equations equal to zero and solving.

ADAS tools and data base.

A series Fortran routines have been created to compute molecular CR coefficients and perform full equilibrium population calculations given plasma conditions of temperature and density. Fundamental data which form the input to the model and the derived CR coefficients are archived in a structured and comprehensive data base that will be available in ADAS [7]. The fundamental data (cross sections and rates) are archived in a specific format file called *mdf02* (*mdf* stands for *molecular data format*). A dedicated routine (ADAS902) produces the Maxwellian rates from these data. The results are output in the specific formats *mdf33* and *mdf34* which store electron impact data and ion impact data respectively. They also make the input of the next main routine: ADAS903. It analyses the collisional matrix and fill the gaps where it is possible. To do so, impact parameter (IP) approximation with a cut-off at close radius [8] is used for the excitation data by means of the ADAS routine EIQIP [7]. For excitation and ionization data, the ECIP approximation [9] which uses binary encounters at close range collisions with IP at long range is available. ADAS903 can utilize the Franck-Condon factors to create data for the two resolutions considered:

1. Electronic resolution where the vibronic transitions are summed over the electronic levels for the ordinary states. Due to the absence of a permanent dipole moment in the homonuclear diatomic molecules, vibronic levels of the metastables are considered as metastables themselves and transitions between them are forbidden.

2. Full vibronic resolution where all the vibronic levels are kept for the calculations. Here Franck-Condon factors are used to split the total cross sections into vibronic states.

The results of ADAS903 are written into the format *mdf04* for electron impact and *mdf14* for ion impact. These formats keep the adequate resolution (electronic or vibrational) of their precursors. They also make the input for the molecular CR model, performed by the routine ADAS904 which calculates the effective coefficients and outputs the populations of the different metastables. The coefficients are archived in the *mdf11* format files. ADAS904 have into account the pre-dissociation and auto-ionization data. The atomic rates are taken from ADAS *adf04* format files [7]. The atomic effective coefficients, which are indistinguishable from the ones obtained with an atomic CR calculation, are taken from ADAS *adf11* formats for the temperature and density required. ADAS904 also accounts for the dissociation due to the spontaneous decay to dissociative states using the Einstein coefficients. Einstein coefficients, Franck-Condon factors and vibrational energies are stored in *mdf00* format files. A series of routines has been created as well to read the different formats, they are called respectively *xxdatm_00*, *xxdatm_02*, *xxdatm_33*, *xxdatm_04* and *xxdatm_11*.

We must note that the Franck-Condon regime is assumed for plasmas containing molecules.

H_2 system collisional data

The H_2 system includes the molecular species and derivatives from H_2. That is, H_2, H_2^+, H_2^-, H, H^+ and H^-. A new compilation of the H_2 system cross section has been used for this work [10]. Most of the input data collections come from a compilation in [10], together with the dissociative attachment from [11] and dissociative ionization rates from [12]. The data compilation have been filtered and chosen from the literature by the authors of [10] to provide recommended sets of data. The problems found are summarized bellow:

- There are only ionization data available from ground state of H_2. Even when ionization from

excited ordinary states is not important in the coronal equilibrium picture, this lack of data would be enough to suppress the density dependence of the effective coefficients. Furthermore, there is no data available for ionization from triplet $c^3\Pi_u$ metastable.

- There are data for dissociative excitation from ground singlet electronic state but as for ionization, there is no data from triplet or excited states. Available pre-dissociation data have been taken from [13] and auto-ionization data from [14]. Basic data such as Franck-Condon factors, A-values and vibrational energies have been taken from [15].
- In the H_2^+ molecular ion, non-dissociative recombination is negligible compared with dissociative recombination so only the latter is accounted for and given in [10]. Only the ground electronic state of H_2^+ is bound and every excitation is dissociative. Vibrationally resolved dissociative excitation is also provided in [10]. Finally, inverse charge exchange processes which suppose the only path back to the neutral species is also archived but not used yet at this stage.

All these gaps have been filled by the calculations of ADAS903 (see previous section). Comparisons with previously theoretical data from [10] gave a difference of a factor ~3 for excitation from ground state to low levels and ~2 for excitation to high states and a two orders of magnitude overestimation of bound-free processes, either ionizative or dissociative. The reason of this is in the nature of the ECIP approximation which does not account for the nuclear movements and the limited size of the molecular core. The influence of this overestimation in the bound-free processes from the non-metastable excited states in the CR model is under study.

Results

First results of the CR model described above for the Hydrogen molecule system are presented here. We have assumed a constant source term of the lowest vibrational state in the

ground electronic state for Hydrogen molecule. Plasma conditions similar to recent experiments [2] have been chosen as a starting point.

A set of 27 electronic states for the H_2 molecule and 3 for the H_2^+ ion have been considered. Of these, 16 are singlets (para-hydrogen states) and 11 triplets (ortho-hydrogen). The dissociative states are the $b^3\Sigma_u^+$ of H_2 and $2p\sigma_u$ and $2p\pi_u$ of H_2^+; the latter two absorb all the excitation from the ionic ground state giving dissociation. Dissociative recombination is assumed at this stage to produce atoms in its ground state. Spontaneous decay to the dissociative triplet *b* is considered and is one of the mechanism which makes dissociation dependent on density [3]. Ionization from H_2^+ is considered as dissociative giving two protons and two electrons as dissociation products. No charge exchange or heavy particle impact processes have been considered at this stage. This particular problem will be studied in the future.

The sum of the effective coefficients for ionization from all vibronic states from the H_2 ground electronic state to all vibronic states of the H_2^+ ground electronic state are presented in fig. 1. Effective ionization has a strong dependence on temperature and increases smoothly with density at the range considered. Ionization processes, unlike in the atomic case, compete with dissociation processes. The sum of effective dissociation coefficients from all vibrational states in the ground state of Hydrogen molecule is plotted in figure 2. From the differences in values we can state that dissociation is the dominant process at the plasma edge temperatures and densities.

The relative population of the 14 vibrational states from ν=1 to ν=14 in the electronic ground state of H_2 normalized to the source term is presented for different temperatures in figures 3 and 4. These relative populations fall steeply for densities higher that 10^{14} cm^{-3} where ionization starts to increase and compete with dissociation and excitation. The main difference between the two temperature cases comes from the low vibrational states ν=1 and ν=2 which

have a higher relative population at lower velocities as can be inferred from the lesser importance of the non-excitative loosing processes (dissociation and ionization).

A fully vibrational calculation at 25 eV has been performed in order to compare with the electronic resolution case. Relative populations for fully vibrational CR are presented in figure 5 in function of densities. As expected, relative population of vibrational states in the ground electronic state are higher than in the electronic resolution case. That can be explained due to the many more states involved in the processes that can decay to the metastables. At the same time, ionization and dissociation become more density dependent due to the same reason making them drop faster than in the electronic resolution case. The definitive mechanism and ultimate causes of this dependence will be matter of future studies.

Conclusions

New theoretical and computational tools for molecule collisional radiative models are presented. An application to the hydrogen molecule system has been studied. Dissociation coefficients present a weak dependence with density and dominate over ionization coefficient in the density range studied. Ionization effective coefficients increase on density making populations fall at electronic densities higher than $10^{14}cm^{-3}$. Populations for the two resolutions considered, electronic and fully vibrational, have been compared obtaining differences due to the bigger completeness of the latter. An structured database that stores fundamental and derived data have been created. From this basis new spectroscopic derived data for molecular bands as Photo-Emission Coefficients and SXD coefficients (Ionization over eXcitation and Dissociation) will be calculated in the future. Predictions about dissociation products and emitted light could be tested with experiments helping to understand the particle balance in divertor and plasma wall interaction physics.

Acknowledgments

The authors would like to thank R. Janev and D. Reiter for providing data and useful discussions. FG would like to acknowledge R. Guirlet and L. Menchero for support and useful discussions.

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Caption of figures.

Figure 1. $H_2(X^1\Sigma_g^+, v=0\text{-}14)$ to $H_2^+(X^2\Sigma, v=0\text{-}18)$ ionization effective coefficients.

Figure 2. $H_2(X^1\Sigma_g^+, v=0\text{-}14)$ to H(1s) dissociation effective coefficients for $n_e = 10^{13}\ cm^{-3}$.

Figure 3. Populations of $H_2(X^1\Sigma_g^+, v=1\text{-}14)$ relative $H_2(X^1\Sigma_g^+, v=0)$ for electronic resolution at T_e= 25 *eV*.

Figure 4. Populations of $H_2(X^1\Sigma_g^+, v=1\text{-}14)$ relative $H_2(X^1\Sigma_g^+, v=0)$ for electronic resolution at T_e= 100 eV.

Figure 5. Populations of $H_2(X^1\Sigma_g^+, v=1\text{-}14)$ relative $H_2(X^1\Sigma_g^+, v=0)$ for fully vibronic resolution at T_e= 25 *eV*.

Figure 1:

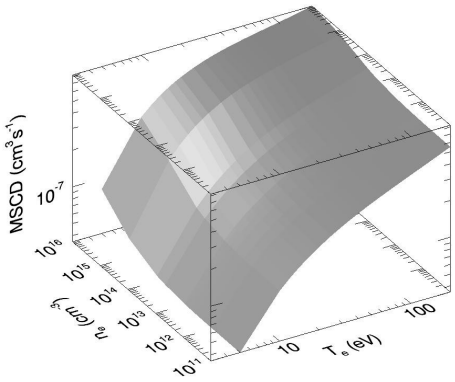


Figure 2:

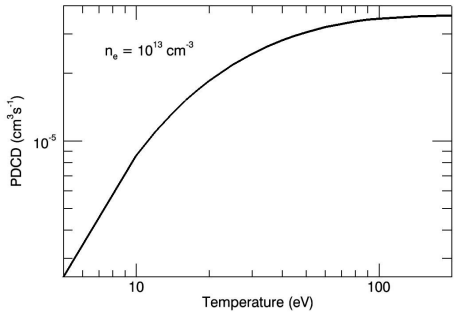


Figure 3:

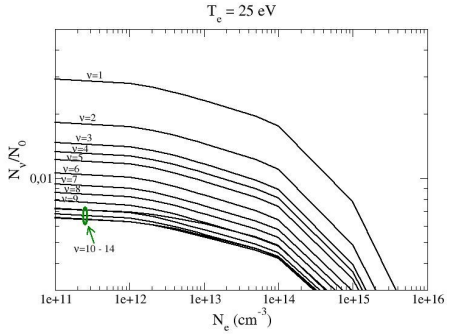


Figure 4:

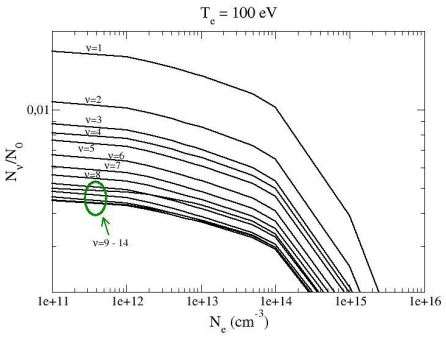
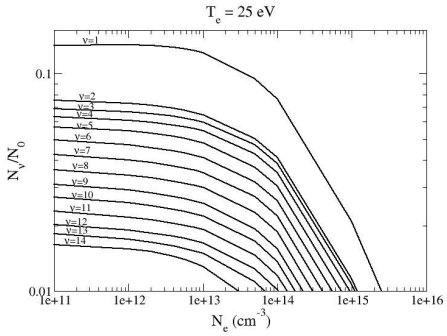


Figure 5:


T_e = 25 eV
v=1
v=2
v=3
v=4
v=5
v=6
v=7
v=8
v=9
v=10
v=11
v=12
v=13
v=14
0.1
0.01
N_v/N_0
1e+11
1e+12
1e+13
1e+14
1e+15
1e+16
N_e (cm^-3)

F.2 Juelich visit report

ADAS-EU Travel Report

Location: Forschungszentrum Juelich, Germany.
Date: 29 May 2012.
ADAS-EU staff: Francisco Guzman
Persons visited: Ratko Janev, Detlev Reiter, Dmitry Borodin and others
Purpose: Work visit to FZJ to present molecular model to modelers in FZJ

Items:

(1) A series of discussions were carried about the extensions and implications of ADAS molecular models and molecular data used in it. They can be separated in two main discussions: a) discussions with D. Reiter and R. Janev about molecular data b) disscusions with FZJ ERO code modelers about implications and possible experiments with ADAS molecular models with Dmitry Borodin.

Discussions about molecular data:

(2) These discussions were maintained with R. Janev and later with D. Reiter.
(3) R. Janev proposed FG to handle RJ and DR the calculations needed in the ADAS903 for completing the collisional matrix. They see it "fair" as an interchange for the molecular data given by them at the starting of the project and that are the grounds of the H model. FG have no objection for that but he replied that now he is busy with other parts of the project and with other ADAS-EU activities as experiments in ASDEX-U or organization of ADAS Workshop and ADAS-EU course. FG thinks that in the end of the year could be a good date to work in that as RJ and DR want the cross sections and not the rates coefficients which are given automatically by ADFAS903. FG does not believe that this will take much time as it is a straightforward modification in IPMRATE routines. RJ wants to obtain scaling laws from these cross sections an publish them in a FZJ internal report.
(4) FG asked RJ about a date to complete his advising contract to ADAS-EU and suggested November that is when both FG and RJ are free of another compromises. RJ wanted for a clarification of the end date of his contract because he thinks it could have finished in April. However he agrees with November.
(5) RJ and DR informed FG that they would like to be referenced to the data they have provided for H2 molecular system with a book ISBN number rather as "private communication", as they are near to publish their book and they have already applied for this number. FG agrees to change this reference in his PSI paper and other forthcoming papers.

ADAS-EU molecular data implications and possible experiments:

(6) A presentation about molecular collisional-radiative model was given to Ratko Janev, Dmitry Borodin, Dmitry Kondratiev and Carolina Björkas. Numerous questions about technical details were answered.
(7) Relevant was the question about how to fulfill the Franck-Condon unitary when calculating the new cross sections. FG answered that that was already checked and that the unitary is automatic when calculating excitation cross sections in vibrational resolution. This is because the IP cross sections depend of dipole moments that are related with Franck-Condon factors so the weighted is automatically done.
(8) Dmitry Borodin was very interested to apply the molecular model to the BeD molecule that is being studied in detail in linear devices as sputtering of Be can be in a big fraction in form of this molecule. He suggested to perform experiments and calculations for it with the ADAS model. We agreed to be in contact when ADAS model is well cross checked and take the data from C. Björkas and Ratko Janev.

F. Guzmán
5 June 2012

Appendix G

IAEA and IM meeting presentations by Dr. O'Mullane

G.1 IAEA-NFRI, 4-7 Sept. 2012: Accommodating uncertainty in ADAS models and data

Accommodating uncertainty in ADAS models and data

Martin O'Mullane, N R Badnell, H P Summers, A Giunta
Department of Physics
University of Strathclyde

and many collaborators at JET, Euratom Associated laboratories,
ITER, NIFS, NFRI, DIII-D, PPPL, Auburn, U Mons, U Giessen, TUW

Outline of talk — a set of questions

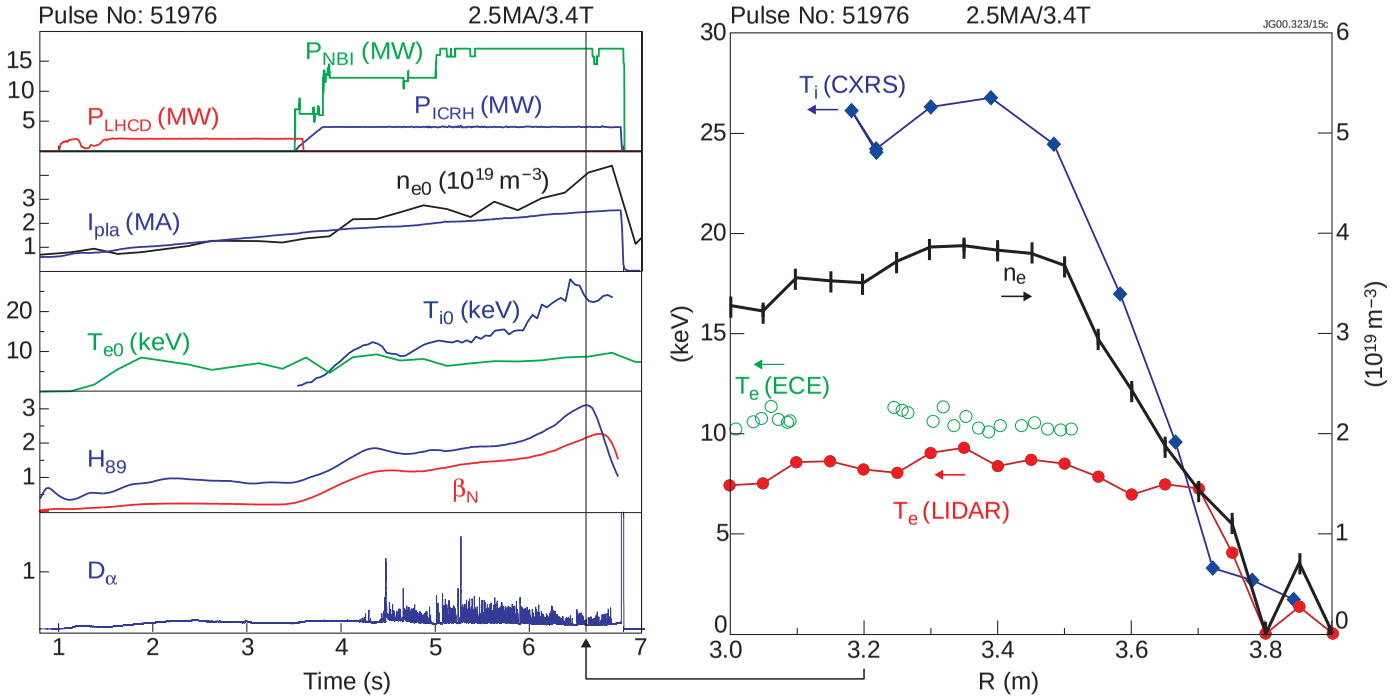
- What is the scope of ADAS?
  - *A set of codes and data designed for spectroscopic and radiated power diagnosis and modelling of hot plasmas.*
- Why the emphasis on codes?
  - *'pure' atomic and molecular quantities are not sufficient by themselves.*
- What data is stored?
  - *Fundamental and derived data for modelling.*
- How to ensure an authoritative and useful set of data?
  - *Data quality, attribution, quantified uncertainty and stable dissemination.*
- What would an ideal ADAS future look like?

Scope of ADAS

- ADAS has focused its efforts in providing atomic data to model and interpret emission from hot, confined plasmas.
- Historical roots are in fusion (JET) and so are the bulk of the users.
- Has also been extensively applied to astrophysics.
- This background lead to the ADAS Project becoming a self-funding consortium of mostly fusion laboratories and its governance is by a steering committee of these members.
- OPEN-ADAS was championed (and funded) by IAEA to make the data more widely available.
- The delivery of this data is via the web but the data is returned as ADAS datasets rather than the more traditional individual cross sections.

Why the emphasis on codes?

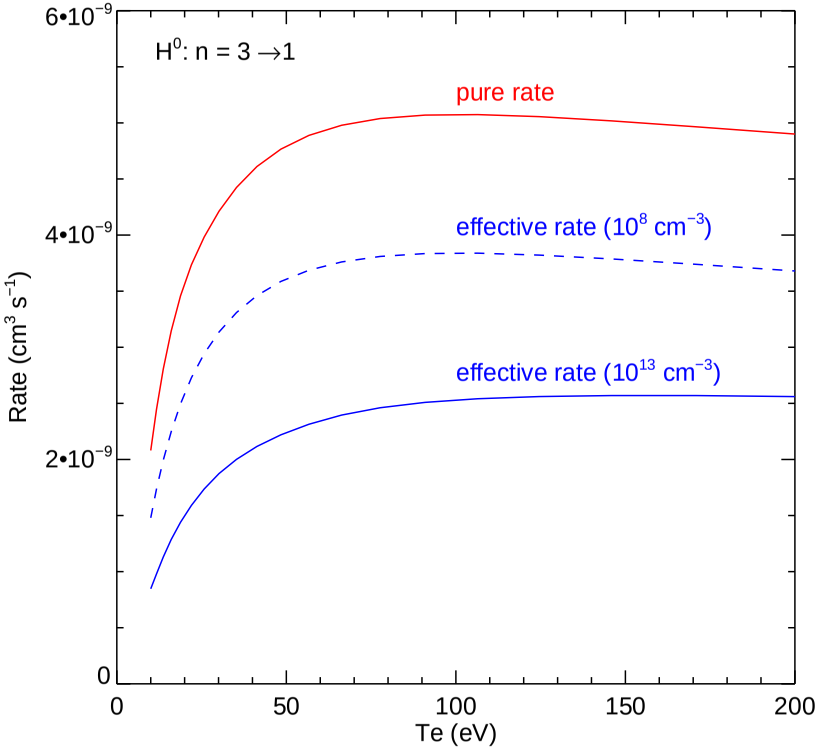
Emission from a tokamak is not representative of an isolated atomic system.



The environment is collisional (high electron density) with a very wide range of electron temperatures.

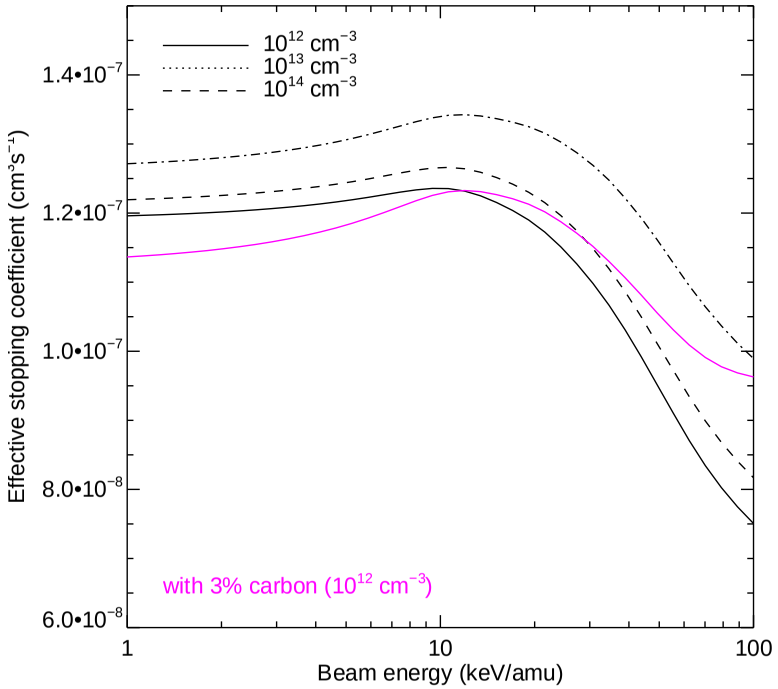
n=3-1 rate of neutral hydrogen

The plasma environment alters the ‘pure’ rate to *effective* rates that we need for modelling.



Stopping a high energy neutral (heating) beam

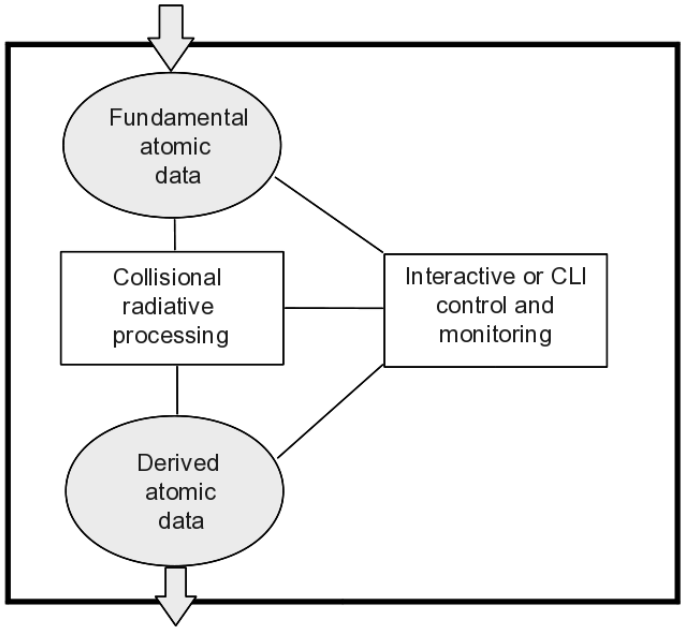
Many coefficients vary with the plasma environment.



But choosing the ‘correct’ model is also essential.

ADAS modelling

Fundamental atomic data must be moderated via population models in order to become useful for diagnostics interpretation and modelling.



But we must ensure that the physics model is correct before worrying about possible uncertainties in the data.

Collisional-radiative population modelling (in brief)

Quasi-static equations for ordinary levels
In term of metastables:

$$\sum_{j=1}^{O} C_{ij} N_j = -\sum_{\sigma=1}^{M} C_{i\sigma} N_\sigma + N_e N_1^+ r_i + N_e N_H q_i^{(CX)} \qquad i = 1,2,..$$

$$C_{ij} = -A_{j\to i} - N_e q_{j\to i}^{(e)} - N_p q_{j\to i}^{(p)} \qquad i \neq j$$

$$C_{ii} = \sum_{j<i} A_{i\to j} + N_e \sum_{j\neq i} q_{i\to j}^{(e)} + N_p \sum_{j\neq i} q_{i\to j}^{(p)} + N_e q_i^{(I)}$$

Invert to give population

$$N_j = -\sum_{i=1}^{O} C_{ji}^{-1} \sum_{\sigma=1}^{M} C_{i\sigma} N_\sigma + \sum_{i=1}^{O} C_{ji}^{-1} r_i N_e N_1^+ + \sum_{i=1}^{O} C_{ji}^{-1} q_i^{(CX)} N_H N_1^+$$

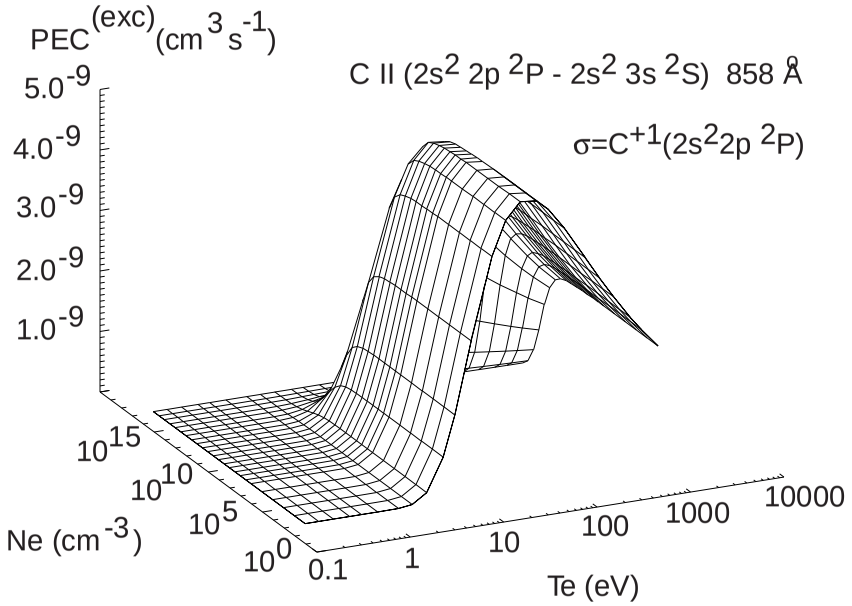
$$\equiv \sum_{\sigma=1}^{M} \mathrm{F}_{j\sigma}^{(exc)} N_e N_\sigma + \mathrm{F}_{j1}^{(rec)} N_e N_1^+ + \mathrm{F}_{j1}^{(CX)} N_H N_1^+$$

$$\varepsilon_{j\to k} = A_{j\to k} \left(\sum_{\sigma=1}^{M} \mathrm{F}_{j\sigma}^{(exc)} N_e N_\sigma + \sum_{\upsilon'=1}^{M_{z+1}} \mathrm{F}_{j\upsilon'}^{(rec)} N_e N_{\upsilon'}^+ \right)$$

Emissivity in a line

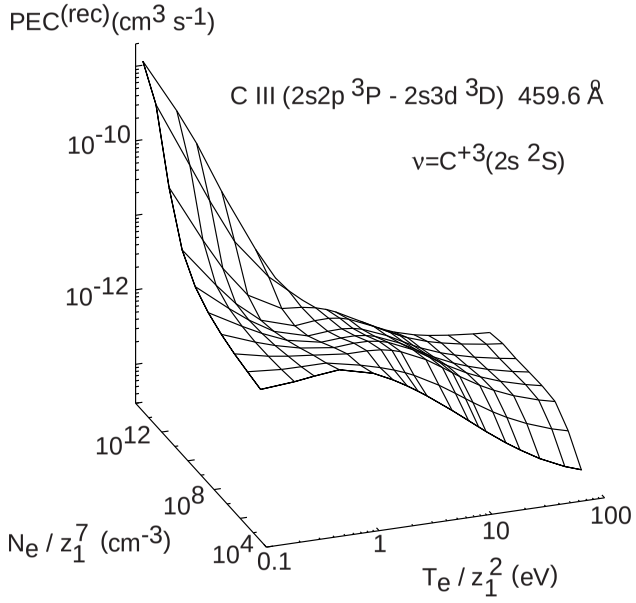
Coefficients are functions of temperature and density

Excitation PEC



- Driven by ground $\mathrm{C}^{+1}\ 2\mathrm{s}^2 2\mathrm{p}\ ^2\mathrm{P}$ population.

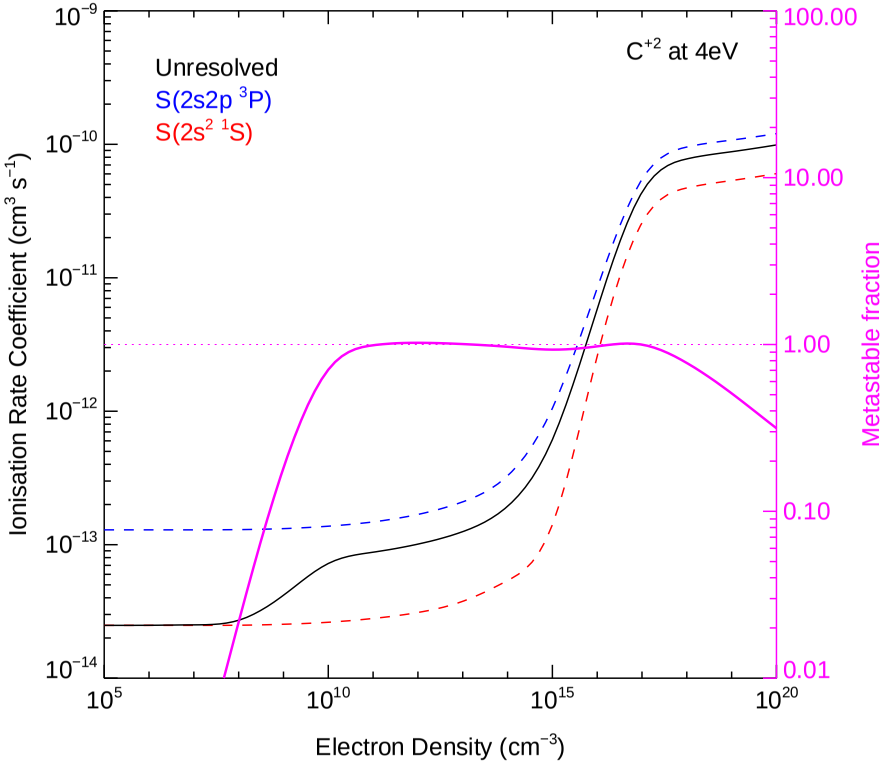
Recombination PEC



- Driven by $\mathrm{C}^{+3}\ 2\mathrm{s}\ ^2\mathrm{S}$ population.
- Note the reduced temperature and density units (for inter-ion comparisons).

And how many depends on the number of metastables

Extra coefficients are required for ionisation balance in the resolved picture



For M_z metastables (incl. ground)

$$\frac{1}{n_e}\frac{\partial N^z_\rho}{\partial t} =$$

$$- \sum_{\gamma=1}^{M_{z+1}} S_{\gamma\rho} N^z_\rho \quad - \sum_{\gamma=1}^{M_{z-1}} \alpha_{\tau\rho} N^z_\rho$$

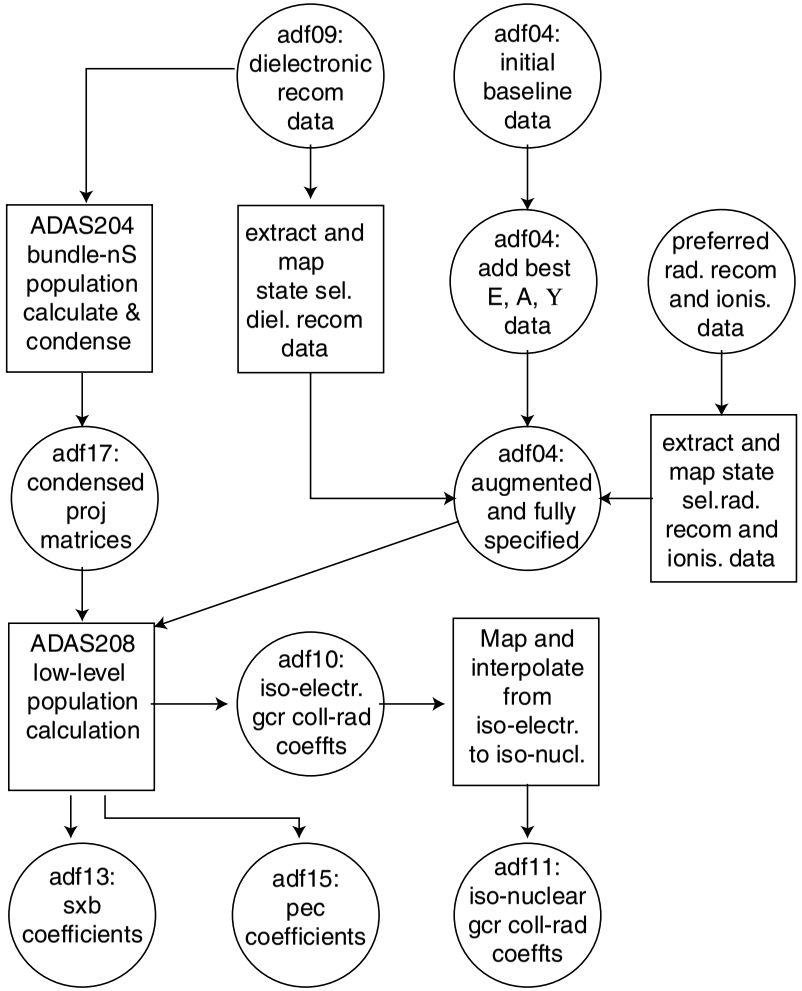
$$+ \sum_{\tau=1}^{M_{z-1}} S_{\rho\tau} N^{z-1}_\tau + \sum_{\gamma=1}^{M_{z+1}} \alpha_{\rho\gamma} N^{z+1}_\gamma$$

$$+ \sum_{\epsilon\neq\gamma}^{M_z} Q_{\rho\epsilon} N^z_\epsilon \quad - \sum_{\epsilon\neq\rho}^{M_z} Q_{\epsilon\rho} N^z_\rho$$

$$+ \sum_{\epsilon>\rho}^{M_z} X_{\rho\epsilon} N^z_\epsilon \quad - \sum_{\epsilon<\rho}^{M_z} X_{\epsilon\rho} N^z_\rho$$

- Q : metastable cross-coupling coefficients (recombined ion).
- X : parent cross-coupling coefficients (via recombined ion)

Workflow to generate derived data



□ : codes and hand-editing / scripting.

◯ : *adf* datasets.

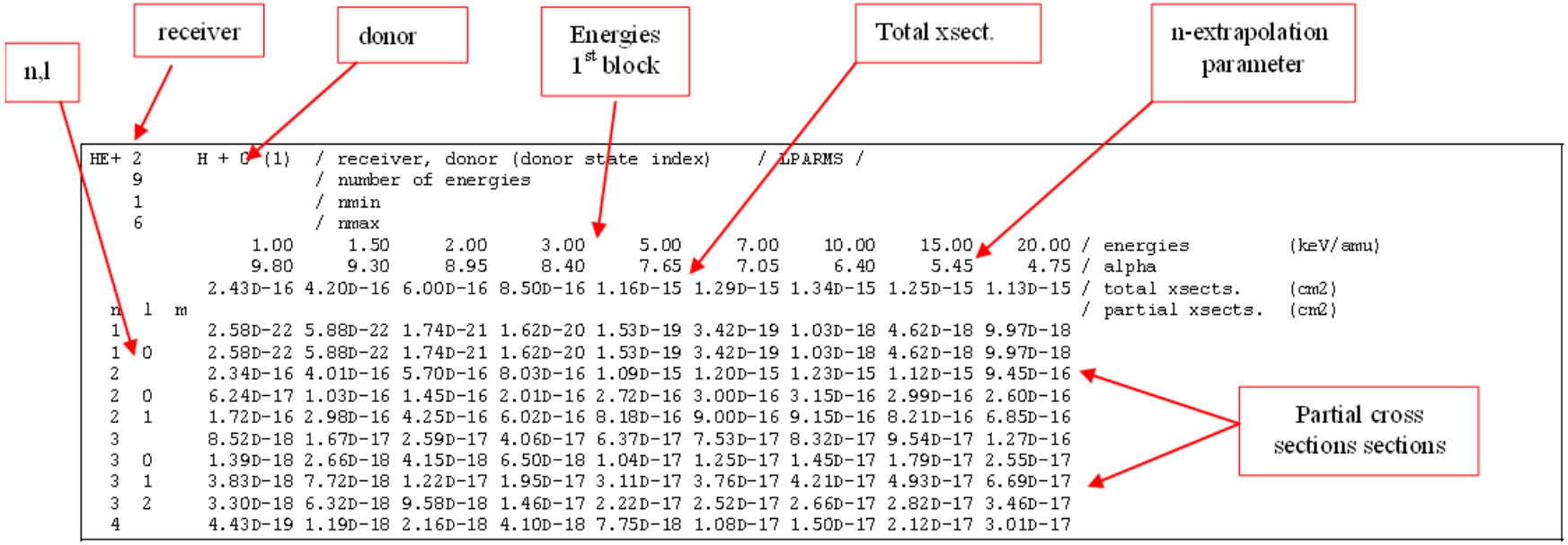
The production of the fundamental data is not shown!

Derived, fundamental and driver data

ADAS data falls into 3 broad classes:

- **Derived data** are data tailored for modelling: electron temperature and density dependent effective emission coefficients, effective ionisation/recombination rates, radiated power, spectral emissivities etc.,
  - Fundamental data processed via population models.
  - Most of these data are ***not*** catalogued in data centres.
- **Fundamental data** are core atomic data necessary for modelling: A-values, cross sections, effective collision strengths etc.,
  - Many sources: collaborators, literature, data centres etc.
  - Many resolutions: from simple to the forefront of computational physics.
- **Driver data** allows for the complete regeneration of all ADAS derived data (and some fundamental data) using the various ADAS codes.
  - unique to ADAS and of no use/interest to non-ADAS users.

ADAS data formats — *adf* — are precisely defined




```
HE+ 2     H + 0 (1)  / receiver, donor (donor state index)     / LPARMS /
   9                 / number of energies
   1                 / nmin
   6                 / nmax
            1.00     1.50     2.00     3.00     5.00     7.00    10.00    15.00    20.00 / energies         (keV/amu)
            9.80     9.30     8.95     8.40     7.65     7.05     6.40     5.45     4.75 / alpha
        2.43D-16 4.20D-16 6.00D-16 8.50D-16 1.16D-15 1.29D-15 1.34D-15 1.25D-15 1.13D-15 / total xsects.    (cm2)
 n  l  m                                                                                 / partial xsects.  (cm2)
 1        2.58D-22 5.88D-22 1.74D-21 1.62D-20 1.53D-19 3.42D-19 1.03D-18 4.62D-18 9.97D-18
 1  0     2.58D-22 5.88D-22 1.74D-21 1.62D-20 1.53D-19 3.42D-19 1.03D-18 4.62D-18 9.97D-18
 2        2.34D-16 4.01D-16 5.70D-16 8.03D-16 1.09D-15 1.20D-15 1.23D-15 1.12D-15 9.45D-16
 2  0     6.24D-17 1.03D-16 1.45D-16 2.01D-16 2.72D-16 3.00D-16 3.15D-16 2.99D-16 2.60D-16
 2  1     1.72D-16 2.98D-16 4.25D-16 6.02D-16 8.18D-16 9.00D-16 9.15D-16 8.21D-16 6.85D-16
 3        8.52D-18 1.67D-17 2.59D-17 4.06D-17 6.37D-17 7.53D-17 8.32D-17 9.54D-17 1.27D-16
 3  0     1.39D-18 2.66D-18 4.15D-18 6.50D-18 1.04D-17 1.25D-17 1.45D-17 1.79D-17 2.55D-17
 3  1     3.83D-18 7.72D-18 1.22D-17 1.95D-17 3.11D-17 3.76D-17 4.21D-17 4.93D-17 6.69D-17
 3  2     3.30D-18 6.32D-18 9.58D-18 1.46D-17 2.22D-17 2.52D-17 2.66D-17 2.82D-17 3.46D-17
 4        4.43D-19 1.19D-18 2.16D-18 4.10D-18 7.75D-18 1.08D-17 1.50D-17 2.12D-17 3.01D-17
```

See http://www.adas.ac.uk/man/appxa-01.pdf

- ADAS codes use *adf* files to interchange information.
- ASCII format with asymptotic behaviour enforced.
- Reading and interrogation codes in fortran, IDL and python.

Much of the ADAS data is disseminated via OPEN-ADAS

OPEN-ADAS

Atomic Data and Analysis Structure

OPEN-ADAS Version 1.2
Report Error
Search

- Freeform search
- Search by wavelength
- Search by ion
- Search by data class
- Documentation
- Download code
- Terminology
- Statistics
- About ADAS
- About OPEN-ADAS
- Removal of login requirement

ADF01 | ADF04 | ADF07 | ADF08 | ADF09 | ADF11 | ADF12 | ADF13 | ADF15 | ADF21 | ADF22

ADF15 File: pec96#c_pjr#c4.dat

Photon Emissivity Coefficients

Ion: C^{4+}
Temperature Range: 1.080 eV → 6460 eV
Density Range 7.810 x 10^{5} cm^{-3} → 7.810 x 10^{19} cm^{-3}
Filename: pec96#c_pjr#c4.dat
Full Path: adf15/pec96#c/pec96#c_pjr#c4.dat

Download Options
Download Data
Documentation
Software libraries

Show comments | Show origins

Wavelength	Transition	Type	Driving Population
32.8Å	$1s1\,5d1\ ^1D_{2.0} \rightarrow 1s2\ ^1S_{0.0}$	Excitation	$1s2\ ^1S_{0.0}$
32.8Å	$1s1\,5p1\ ^3P_{4.0} \rightarrow 1s2\ ^1S_{0.0}$	Excitation	$1s2\ ^1S_{0.0}$
32.8Å	$1s1\,5p1\ ^1P_{1.0} \rightarrow 1s2\ ^1S_{0.0}$	Excitation	$1s2\ ^1S_{0.0}$
32.8Å	$1s1\,5d1\ ^1D_{2.0} \rightarrow 1s2\ ^1S_{0.0}$	Excitation	$1s1\,2s1\ ^3S_{1.0}$
32.8Å	$1s1\,5p1\ ^3P_{4.0} \rightarrow 1s2\ ^1S_{0.0}$	Excitation	$1s1\,2s1\ ^3S_{1.0}$
32.8Å	$1s1\,5p1\ ^1P_{1.0} \rightarrow 1s2\ ^1S_{0.0}$	Excitation	$1s1\,2s1\ ^3S_{1.0}$
32.8Å	$1s1\,5d1\ ^1D_{2.0} \rightarrow 1s2\ ^1S_{0.0}$	Recombination	
32.8Å	$1s1\,5p1\ ^3P_{4.0} \rightarrow 1s2\ ^1S_{0.0}$	Recombination	

Accommodating uncertainty within ADAS

Organizationally it's easy!

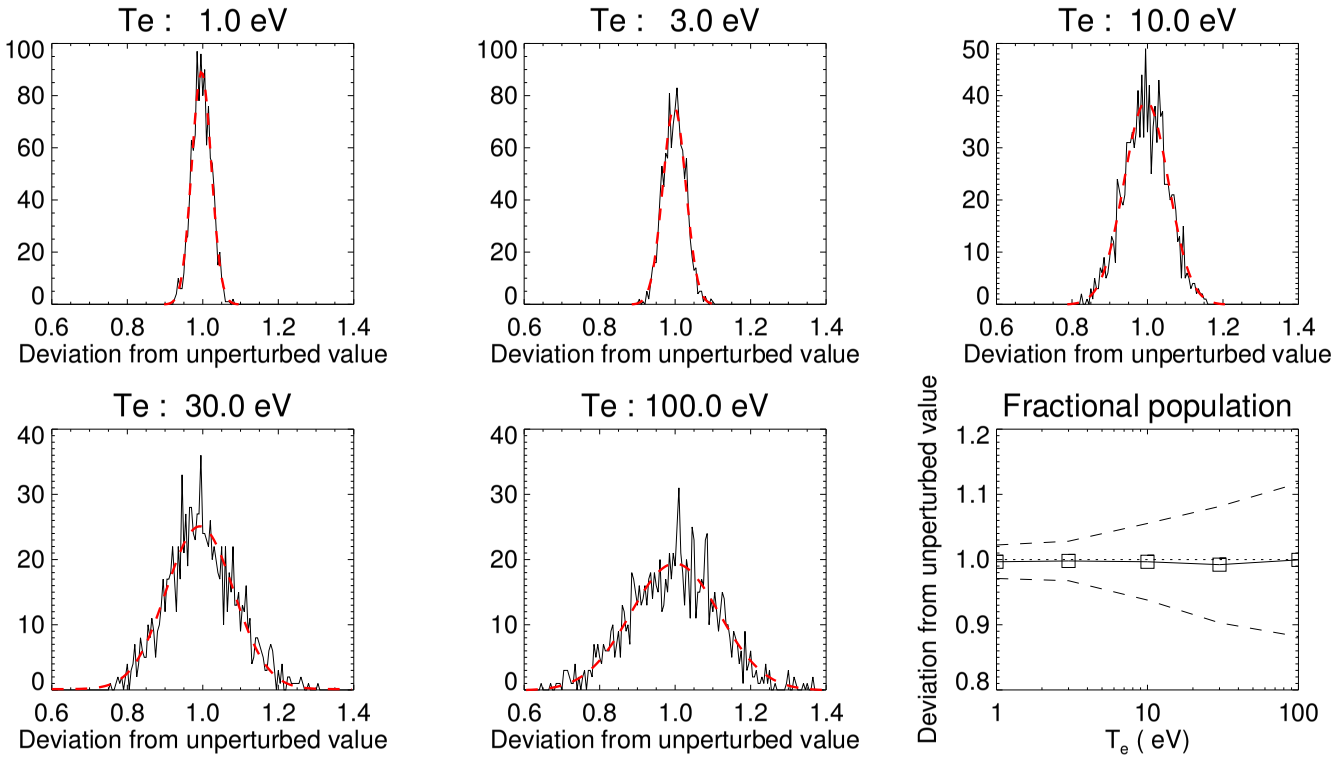
- Simply store a *.err* dataset alongside the data holding *.dat* one.
- Immediate re-use of reading codes and extension of programs to access an error is trivial.

But it is not a simple task

- How do we calculate the error?
- The essential task is to propagate uncertainties in the fundamental input data through the population models.
- How to weight the different inputs — eg how can we assign an error to a projection matrix?

Monte-Carlo is the obvious choice

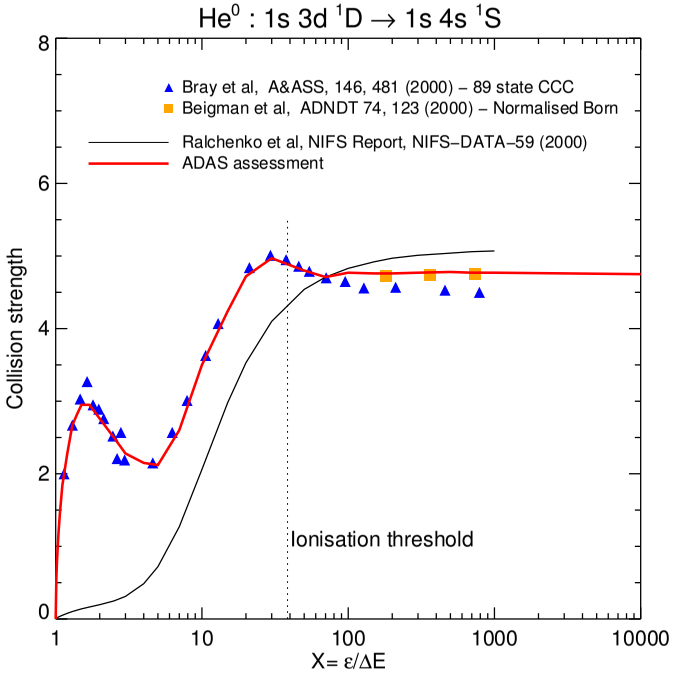
For the $\mathrm{He}^0\ 1s^2\,{}^1S - 1s2p\,{}^1P$ transition with 4000 iterations.



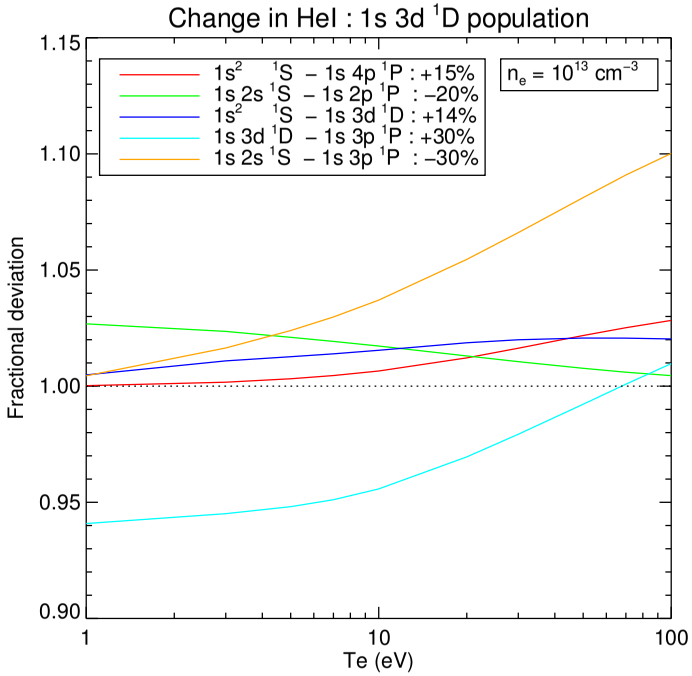
Standard ‘errors’ of between 15%–50% were *ascribed* to each transition.

Ascribing error can be subjective

Differences between approximations can form the basis of the error.



Note that the error in a transition may have little influence on the transition of interest.



Average error of 30%

For a less naïve view

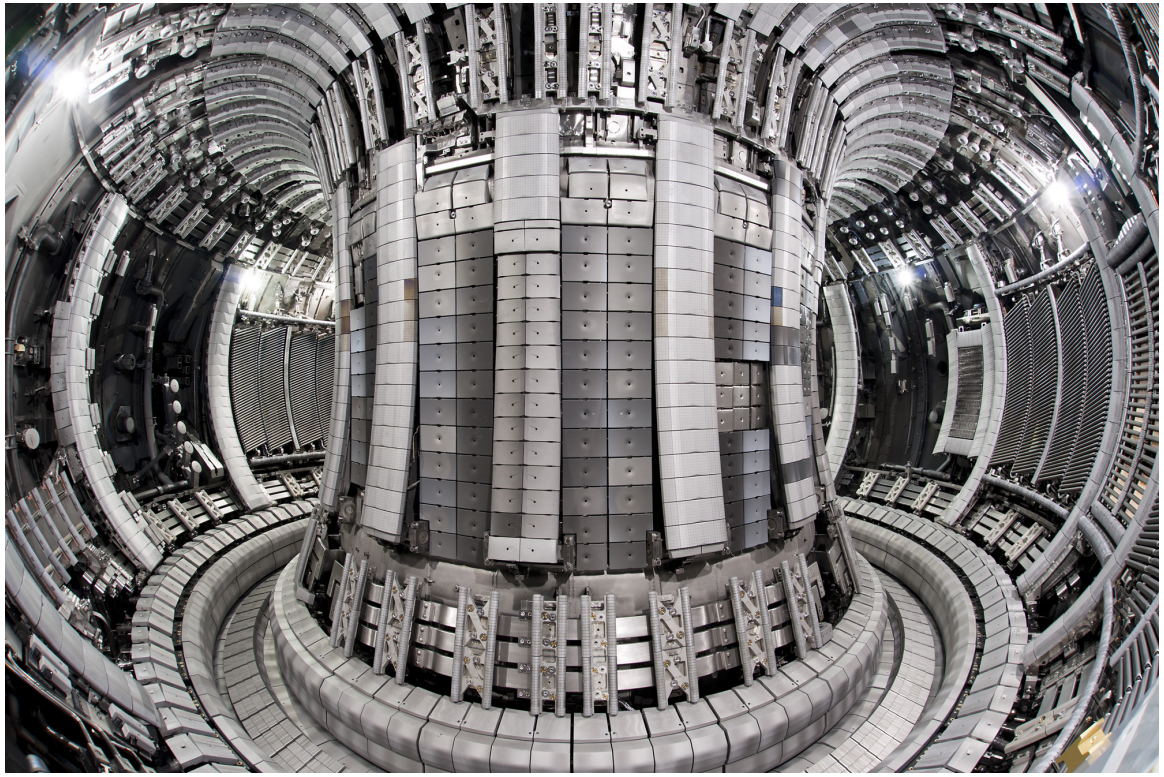
- Just about all fundamental input data comes from *ab initio* codes.
- These are of varying levels of sophistication.
- However all are driven by inputs.
- So are amenable to a sensitivity analysis.
- Propagate this 'objective' uncertainty through the population models.

See:

Connor Ballance's talk for a worked example

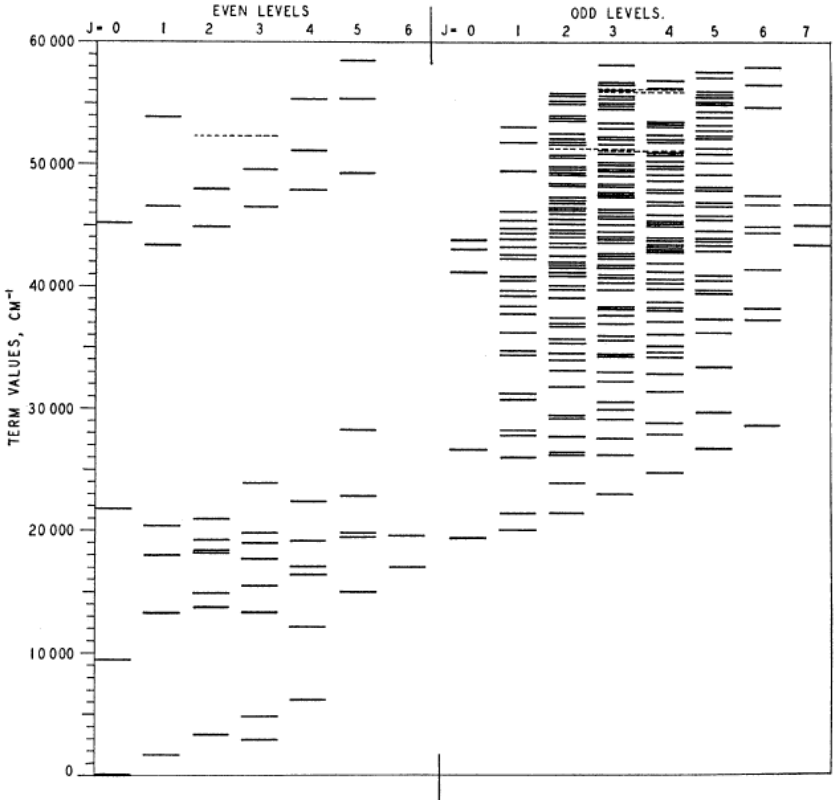
It's too soon for sophisticated errors for some tasks

JET's ITER-like wall: Beryllium lined chamber and tungsten divertor.



What is the emission from W and Be? — And we cannot wait!

Tungsten influx - S/XB ionisation per photon coefficient



O Laporte and J E Mack, Phys. Rev, 1943

Latest revision: A E Kramida and T Shirai, J Phys Chem Ref Data, 2006

WI energy levels and the favoured 4009Å line

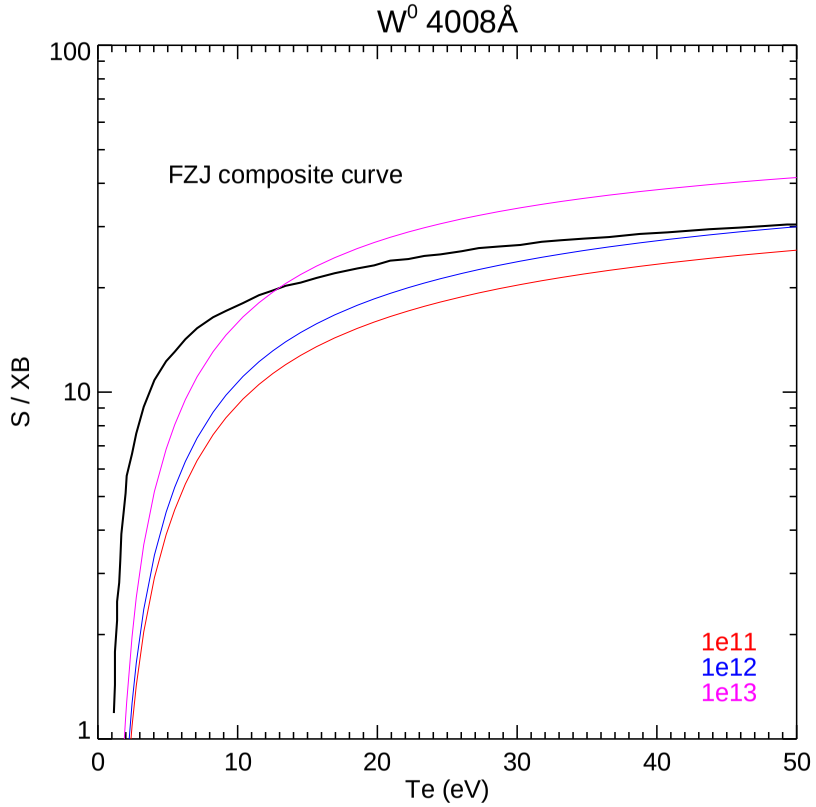
			baseline	Mons	NIST
1	4FE 5D4 6S2	(5)2(0.0)	0.0	0.0	0.00
2	4FE 5D4 6S2	(5)2(1.0)	1467.9	1785.2	1670.29
3	4FE 5D5 6S1	(7)0(3.0)	-	2981.7	2951.29
4	4FE 5D4 6S2	(5)2(2.0)	3189.4	3469.8	3325.53
5	4FE 5D4 6S2	(5)2(3.0)	4863.1	4927.4	4830.00
6	4FE 5D4 6S2	(5)2(4.0)	6404.8	6207.7	6219.33
7	4FE 5D4 6S2	(3)1(0.0)	12950.2	9612.9	9528.06
8	4FE 5D4 6S2	(3)5(4.0)	14044.2	12249.8	12161.96
9	4FE 5D4 6S2	(3)1(1.0)	17084.9	13500.8	13307.10
10	4FE 5D4 6S2	(3)4(3.0)	16981.1	13506.3	13348.56

	NIST	U Mons	*adf04*	
E_{ground}	0.00	-88.0	0.0	$5d^4\,6s^2\ ^5D_0$
E_{lower}	2951.29	2893.0	2981.7	$5d^5\,6s\ ^7S_3$
E_{upper}	27889.68	27815.7	27905.5	$5d^4\,6s\,6p\ ^7P_4$

Good structure and a simple collision model is ‘better’ than a poor structure with a higher quality collision part.

S/XB

Take the Mons *adf04* structure with Born excitation rates, CADW *adf07* ionisation rates to give....



Dielectronic recombination for W^{+20}

Measurement and theory are refining the rates required for ionisation balance.

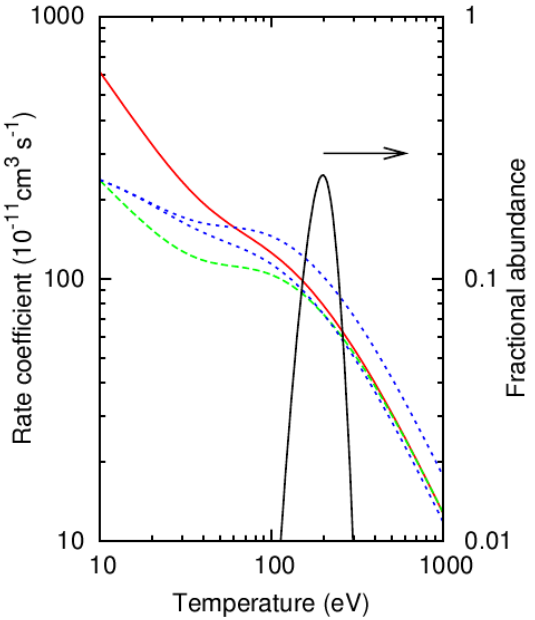


FIG. 7: (Color online) W^{20+} total Maxwellian DR rate coefficients: IC (solid red curve), LS (long-dashed green curve), and CA with-and-without $n = 5$ continuum (short-dashed blue curves). The fractional abundance of W^{20+} in a magnetic fusion plasma is shown also (solid black curve).

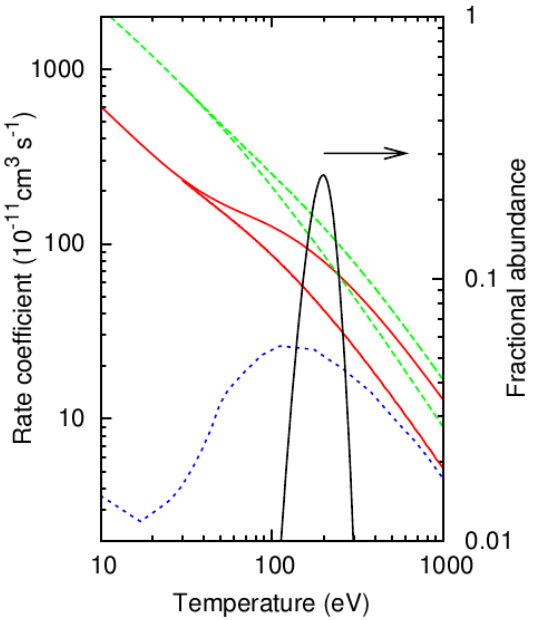


FIG. 8: (Color online) W^{20+} total Maxwellian DR rate coefficients: IC all resonances and to 140 eV only (solid red curves), experiment [7] to 140 eV and with theory top-up for resonances above 140eV (long-dashed green curves), and ADAS [31] (short-dashed blue curve). The fractional abundance of W^{20+} in a magnetic fusion plasma is shown also (solid black curve).

Badnell et al, Phys. Rev. A**85**, 052716 (2012)

An authoritative and useful set of data for fusion should....

- ... have a complete coverage of any elements of interest.
  - Spectroscopic lines, radiated power, influx coefficients, charge exchange emissivities, ionisation balance, E and B field effects, beam stopping data etc.
- ... use well defined data formats which encompass the plasma conditions encountered.
- ... be able to generate quickly baseline quality data for arbitrary elements.
- ... come from a stable source.
- ... have the expectation that the data quality is as good as possible.
- ... be responsive to data needs.
- ... be part of an ongoing research programme.

In this way a system (ADAS in this case) becomes trusted and is accepted as an authoritative source of atomic data.

Ideal ADAS future

Data quality improves —

- Baseline quality undergoes continual uplift.
- More high quality supplementation of diagnostic (and model) significant ionisation stages.
- An error file accompanies each dataset.
- A doi is given to each dataset for fine-grained referencing.
- The physics models are refined with more subtle effects.
- Enhance numerical methods and techniques.
- More people to collaborate and work on improving ADAS.
- Take advantage of world-wide aspect of ITER to form our own collaborations on atomic physics for fusion.

G.2 ITM Innsbruck, 3-7 Dec. 2012: Non-Maxwellian radiated power coefficients for carbon

Non-Maxwellian radiated power coefficients for carbon

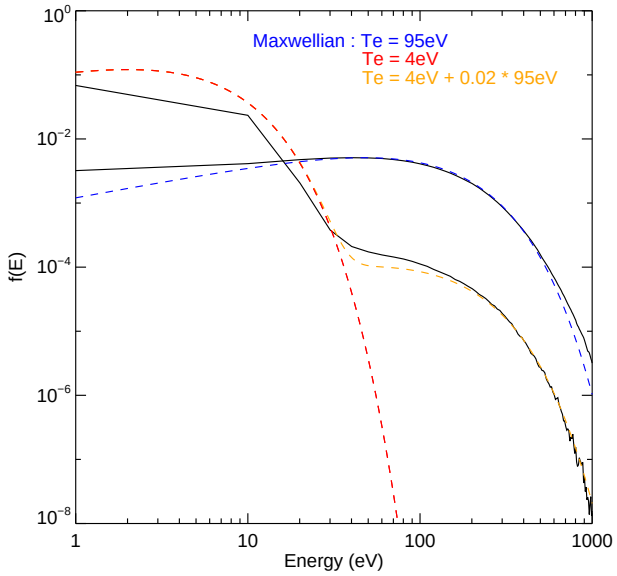
1. New developments in ADAS since the Kudowa code camp (summer 2012) can be used to explore the effect of non-Maxwellian electron energy distribution functions (EEDF) on various coefficients. Here the behaviour of the PLT, the total line power, collisional-radiative coefficient (*adf11/plt*) is examined. Carbon is chosen as the test element.

2. `adas7#1`, an implementation of the AUTOSTRUCTURE (AS) atomic structure and collision code, has been enhanced to generate distorted wave excitation data. This enables a significant improvement of the existing plane wave Born based baselines data, since spin-changing transitions are now calculated.

   adf04 data file for the H-like to Ar-like isoelectronic sequences for all elements between hydrogen and zinc have been calculated with the automation tools of `adas7#3`.

   These data are available in IC and LS resolutions as type 3, Maxwell averaged, and as type 5, AS intermediate format versions. The type 5 files can be post-processed, with an `adas7#3` code, into type 3 and type 4 *adf04* files. Type 4 datasets tabulate upward and downward collision strengths convolved with a supplied EEDF. The up and down versions are required since the symmetry of the Maxwell averaging is lost when forming the excitation and de-excitation rates. Analytical (Kappa and Druyvesteyn) or numerical (stored in *adf37*) EEDFs can be used.

3. Two EEDFs from kinetic code runs (David Tskhakaya):



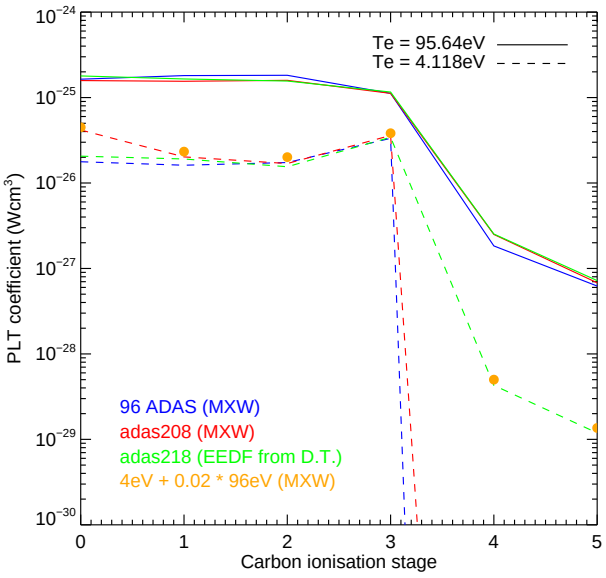
   The low temperature EEDF is characteristic of a region ~ 0.033m from the outer divertor while the higher temperature is from a region ~ 1.4m distant.

   The low temperature EEDF can be approximated by a superposition of two Maxwellians (note – fitted by eye) while the high temperature one is already approaching a Maxwell distribution.

4. `adas218` is a variant of the principal population code in ADAS (`adas208`) which can use type 4 *adf04* data.

5. PLT coefficients, the total radiated power from the sum of all line emission from an ionisation stage, were calculated with the `adas218` collisional-radiative code. Each type 5 *adf04* file was convolved with the numerical EEDF to produce a type 4 dataset. PLTs were also generated with the type 3 Maxwell average datasets to eliminate differences due to factors other than the EEDF chosen. A density of 10^{13}cm^{-3} is used for the comparison.

   The results are (lines drawn as a guide):



   The new baseline data matches the existing central ADAS data well; the discrepancies can be accounted for by the absence of projection in the new calculation and the sensitivity of the neutral stage to differences in the calculation of its atomic structure.

6. It is notable that for the PLT coefficients a superposition of existing Maxwell averaged data is more than sufficient to describe the radiated power in the plasma.

7. The ionisation balance has not been studied. The CADW code in `adas8#2` can be modified to produce a type 1 *adf23* dataset for ionisation cross sections.