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ADAS for fusion in Europe

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

Dissemination report 1

24 June 2010

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

Dissemination report 1

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

Department of Physics, University of Strathclyde, Glasgow, UK

Abstract: *The report reviews dissemination task completion for project months 1-18*

Contents

Preface

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

H P Summers
24 June 2010

Chapter 1

Overview and milestone DSM1

The work package items as specified in the ADAS-EU proposal have been met and the items required for milestone DSM1 achieved. It is noted that an interim report was prepared, made available to the ADAS-EU Governance Committee and verbally explained to them as planned during the 2009 ADAS Workshop (4-7 Oct. 2009 Ringberg Castle, Tegernsee, Germany.

The first ADAS-EU course was very well subscribed and highly successful. Participants from Europe were in the preponderance, but representation was world-wide. IPP Garching is gratefully acknowledged for providing excellent facilities for the course. Details are in chapter 2: section 2.1 and associated appendices.

The pattern of the course has been identified as very helpful for ADAS Project participants outside Europe, but travel to Europe is not possible for large numbers. It has been agreed that Auburn University, Alabama, USA will provide a similar course (called ADAS-US) for American continent participants in early July 2010. This will be taught by ADAS/University of Strathclyde trained scientists in the USA (Dr. Stuart Loch, Dr. Connor Ballance and Dr. Adam Foster) and with the help of ADAS staff (Dr. Martin O'Mullane).

A substantial number of visits to European instutions took place with very positive attitudes and engagement. These were up to the ADAS-EU planning expectation. Details are in chapter 2: section 2.2 and associated appendices.

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 progressing well.

Chapter 2

Work package reports

2.1 Work packages 20-1-1 and 20-2-1

In the ADAS-EU proposal, the annual ADAS-EU course was planned to move in successive years around the fusion laboratories at Fz Juelich, IPP Garching, CEA Cadarache and UKAEA Culham Laboratory. In discussion with Fz Juelich, it was noted that there were insufficient ADAS/IDL enabled workstations available in one location to meet the hands-on requirement of the course. IPP Garching was able to offer the AUG control room area as an alternative together with a convenient meeting room/lecture room for discussions and presentations. Since the annual ADAS Workshop was scheduled to take place at Ringberg Castle, Tegernsee 4-6 Oct. 2009, it was very convenient, and economical for persons wishing to participate in both events, to hold the course at IPP Garching 8-16 Oct. 2009.

The course was widely advertised in association with the ADAS Workshop circulation lists and displayed on the ADAS-EU and ADAS web sites. The first announcement document is attached in Appendix A [1]. The number of external participants was limited to ten by IPP Garching resources leaving headroom for some local IPP participants. The course was oversubscibed. The complete list of participants, including the tutors is attached in Appendix B [1]. The participants were principally from Europe but included persons from as far away as Korea, India and the USA. There were four internal IPP Garching participants.

The principal presenters of the course were the ADAS-EU senior staff, Prof. Hugh Summers, Dr. Martin O'Mullane and Dr. Allan Whiteford. They were supported by shorter presentations from Prof. Nigel Badnell, Department of Physics, Strathclyde University on fundamental atomic structure and collision cross-section calculations and by Dr. Dmitri Borodin, Fz Juelich on application to plasma modelling codes. Prof. Badnell and Dr Borodin each attended for two days of the course in its second week. The working agenda is attached in Appendix A [2]. A pattern evolved of a lecture of 1.5 hours at the beginning of the morning. Further practical instruction in the late morning was followed by hands-on sessions through into the late afternoon. The formal day's work ended with a round table discussion of around one hour. This was an opportunity for each participant to expand on their research interests and allowed the tutors and participants to explore how ADAS could assist.

The complete set of course material are attached in Appendix C [1] - [35]. These materials have been made available on the ADAS-EU web site.

Final shared appraisal of the course at its end was very positive. Participants felt it would be good to have some follow up. A number of scientific engagements did take place at the course which have led to new on-going work.

2.2 Work package 21-1-1 and 21-2-1

There have been six external support visits completed in months 1-18 of ADAS-EU, listed below.

- CIEMAT, Madrid, Spain (14-15 DEc. 2009): see Appendix D[1]

- University Autonoma, Madrid, Spain (16-23 Dec. 2009): see Appendix D[2]
- CEA Cadarache, France (18-22 Jan. 2010): see Appendix D[3]
- CEA Cadarache, France (19-21 Jan. 2010): see Appendix D[4]
- University Mons-Hainaut, Belgium (28-29 Apr. 2010): see Appendix D[5]
- ITER, St Paul-les-Durances, France (7-18 Jun. 2010): see Appendix D[6]

In light of the delay in the employment of the PDRAs, assistance was given in these visits by the ADAS-EU managers - Prof. Hugh Summers and Dr. Martin O'Mullane. It is anticpated that in the next period, the PDRAs will be able to implement external visits and support at the frequency specified in the ADAS-EU contract.

CIEMAT is an Associated laboratory, but not a member of the ADAS Project. A priority was to offer ADAS-EU support to CIEMAT since Dr. Francisco Guzman (PDRA1) is Spanish. The visit was very succesful (see the report in Appendix D[1]). Extended diagnostic exploitation of the helium gas was identified as an item for collaborative support in which ADAS has a strong background.

The Department of Chemistry, University Autonoma (UAM), Madrid is the original home institution of Dr. Francisco Guzman and a sub-contractor with ADAS-EU. There are opportunities for enhanced engagement of UAM with the fusion programme beyond the specific sub-contract. Dr. Francisco Guzman will oversee the sub-contract but will ensure active collaboration also on the range of capabilities at UAM in which he has participated (see the report in Appendix D[2]).

A specific request was made from France, via CEA Cadarache, for assistance from ADAS/ADAS-EU in engaging more atomic physics groups from institutions in France in magnetic confinement fusion and in support of ITER via the French Fusion Research Federation. It was agreed that Prof. Hugh Summers and Dr. Francisco Guzman, representing ADAS-EU, would participate in a special dicussion meeting/workshop to explore possibilities and promote collaborations (see the report in Appendix D[3]). A number of contacts and initial exchanges have taken place following this meeting and it is expected that the engagement will prove fruitful in the longer term.

Dr Francisco Guzman took advantage of the above to also make a visit to the CEA Cadarache spectroscopy and CHRONOS modelling groups. Dr Guzman placement will move to CEA Cadrache in 2011 and this was an opportunity to make a initial survey of the main points of interest with which ADAS-EU engagement would be fruitful (see the report in Appendix D[4]).

The visit to the University of Mons-Hainaut was made by Prof. Hugh Summers, Dr, Martin O'Mullane and Dr. Francisco Guzman. University of Mons-Hainaut is a sub-contractor with ADAS-EU and the purpose of the visit was to accelerate transfer of information on low ionisation stages of tungsten following the identification of this as a key issue for Fz Juelich. This was very succesful in that a software cross-linking with ADAS was enabled (see the report in Appendix D[5]).

Dr Martin O'Mullane made a key first supporting visit to ITER. This was specifically to make calculations for the UV spectrometry design teams in which Korea is the ITER responsible partner. This engagement does represent the hoped for close linking of ADAS-EU with ITER and the associated benefits for Europe at a relatively early stage in the ADAS-EU Project (see the report in Appendix D[6] - not yet in place).

2.3 Work package 26-4-1

The work package task comprises the preparation of this report.

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Appendix A

ADAS-EU course 2009 announcements and agenda

[1] ADAS-EU_course_2009
[2] ADAS-EU_course_agenda_ver2_2009

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THE ADAS-EU COURSE 8-16 OCT. 2009

Guidance on ADAS, atomic calculations and their application to fusion plasma

MAX-PLANCK-INSTITUTE FOR PLASMA PHYSICS,
GARCHING NEAR MUNICH, GERMANY

I enclose preliminary information on the first of the four annual ADAS-EU courses which will take place this year at the Max-Planck-Institute for Plasma Physics, Garching, in the days immediately following the ADAS Workshop. It is an intensive, tailored course for those requiring comprehensive and detailed knowledge of the ADAS Atomic Data and Analysis Structure, atomic calculations associated with it and guidance on their embedding in fusion application. It is assumed that participants on the course are engaged in fusion plasma analysis, diagnostics or models and probably already are at work on applications where ADAS atomic data and modelling inputs might be appropriate. The course, as well as providing lectures and guided tuition, will allow the course tutors and other participants to assist in some of these participant inspired applications. By the end of the course, it is hoped participants will be will be able to act in an advisory capacity on ADAS at their home laboratories.

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 two places reserved for the hosting institution (The Max-Planck-Institute for Plasma Physics, Garching) and four for European Institutions. 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 the Max-Planck-Institut für Plasmaphysik, Boltzmannstr. 2, D-85748 Garching, Germany. It will commence at 9.00 on Thurs. 8 October and finish at 15.00 on Frid. 16 October. It is expected that participants will attend for the full duration of the course. There will be thirteen three-hour working sessions, in the morning and afternoon of each day of the course.

ACCOMMODATION and TRAVEL: Participants are required to make their own accommodation at Garching (see http://englisch.garching.de/ for more information) and their own travel arrangements. The Max-Planck-Institut für Plasmaphysik is served by the Munich U-bahn system http://www.urbanrail.net/eu/muc/muenchen.htm (U6: stop *Forschungszentrum*, one stop on from *Garching* town centre).

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.

COURSE OUTLINE: The course is divided into four parts.

Part 1: Basic and intermediate ADAS use.
Tutors: Dr. M.G. O'Mullane, Dr. Allan Whiteford, Prof. H. P. Summers.
Organisation: Four sessions, each consisting of two, 30 minute lectures, 90 minutes of hands-on tutorial/example work based on example sheets and 30 minutes of coffee/discussion time.

Part 2: ADAS and Atomic Structure and Collision Calculations
Tutors: Dr. M.G. O'Mullane, Dr. Allan Whiteford, Prof. H. P. Summers.
Organisation: Three sessions, each consisting of two, 30 minute lectures, 90 minutes of hands-on tutorial/example work and 30 minutes of coffee/discussion time.

Part 3: Advanced applications in atomic collisions, fusion plasma models and diagnostics
Tutors: Dr. Dmitri Borodin, Dr. Connor Ballance, Dr. Allan Whiteford.
Organisation: Three sessions, each consisting of a 45 minute background lecture, a 30 minute demonstration and 60 minutes of hands-on trial/practice. There will be ~45 minutes of coffee/discussion time.

Part 4: Participant applications
Contributors: All
Organisation: Six 90 minute sessions, each targetting a participant area of interest. ~30 minutes will be available for the participant to introduce and summarise his/her area. The 60 minute discussion will engage all participants and tutors. It will focus on the atomic physics issues. 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 during the course. This part will have a winding-up and future planning session in the final afternoon.

ENQUIRIES: The ADAS-EU course is organized by the University of Strathclyde with the support of the Max-Planck-Institut für Plasmaphysik. Correspondence and general organization will be handled by

Hugh Summers
K1-1-61 JET Facility
Culham Science Centre
Abingdon
Oxfordshire, OX14 3EA
United Kingdom

Email: summers@phys.strath.ac.uk
Phone: +44 (0)1235 46 4459
Fax: +44 (0)1235 46 4535

to whom queries should be sent.

WEBSITE: Important information on the course will be e-mailed to registered participants, but full details about the course will be also be posted at www.adas-fusion.eu/course2009.php .

HPS
15 June 2009

REGISTRATION: Please complete and email the registration slip or notify intentions to Hugh Summers at the email address above as soon as possible.

The ADAS-EU Course 8-16 Oct. 2009 Participant registration

Name:...Institution:...

Address for correspondence:...

....

....Post code:...

Tel:...Email:...

My research area is: ……………………………………………………………………………………..

I do /do not expect to be able to attend for the full duration of the course.

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ADAS-EU COURSE 2009

Course Title:	ADAS and Atomic Calculations for Fusion and Astrophysical Applications
Scheduling:	8 Oct. ‘09 – 16 Oct. ‘09
Lectures:	Introductory one-hour lecture Thu 9 at 10.00; seven 1.5 hour lectures Thu 8 - Fri 16 at 13.30 (normally in two 1/2 hour parts with 1/4 hour of illustrations for each part)
Discussions:	11.00-12.00 Thu 8-Fri 9 – participant problem definition and assessment
	15.00-17.00 Fri 16 – review
Unix sessions:	15.00-17.00 Thu 8-Tue 14 – example classes
	15.00-17.00 Wed 14-Thu 14 – participant problem solving –shared
	09.00-11.00 Fri 9 – participant personal research/ADAS time
	09.00-12.00 Mon 12 – Fri 16 – participant personal research/ADAS time

This is an intensive, restricted entry, tailored course for those requiring comprehensive and detailed knowledge of the ADAS Atomic Data and Analysis Structure and atomic calculations associated with it. Participants after completion of the course will be expected to be able to originate applications for the laboratory fusion plasma and astrophysical plasma regimes, which require ADAS data and modelling inputs. Also, they will be expected to be able to initiate basic atomic structure and collision calculations designed to provide the fundamental data inputs to ADAS needed for their applications. It is intended that course participants will be able to act in an advisory capacity on ADAS at their home laboratories.

The course is divided into two parts. Part 1, led by Prof. H. P. Summers, Dr. A. Whiteford and Dr. M.G. O’Mullane and is focused on ADAS itself. It will comprise 5 lectures in total, the first two concerned with working with the whole of ADAS at a basic level and the second three with advanced modelling and efficient ADAS utilisation aspects.

Part 2 is led by Prof. H. P. Summers , Dr. A. Whiteford, Dr. M.G. O’Mullane, Dr. Dmitri Borodin† and Prof. N. R. Badnell# It will focus on complex atom issues for fusion, high quality electron collision cross-sections and selected application code illustrations from charge exchange spectroscopy and plasma impurity transport modelling. This part may be adjusted according to participant special interests and requests.

The lectures for both parts of the course will have associated hands-on computer example classes exploring the lecture content. It is expected that participants who attend the course will have identified a problem (project) of importance to their personal research which requires ADAS capabilities and which they will wish to work on during the course. Time is allocated to whole class assessment and evaluation of each participant’s project. Additionally a person with ADAS experience suited to each participant’s project will be assigned to help in shared development of that project.

Lectures	1. Introduction – ADAS, IDL, and local setup	HPS/MOM
	2. ADAS tutorial – the interactive system	HPS/MOM
	3. ADAS tutorial – efficient access and use of data and codes.	MOM/ADW
	4. ADAS tutorial – Coll.-rad. modelling for models and spectroscopy	MOM/HPS
	5. ADAS tutorial – CX and beam emission spectroscopy	HPS/ADW
	6. Complex atom modelling	HPS/MOM
	7. Extended ADAS, ERO, CXSFIT	DB/ADW
	8. Electron impact collision calculations	NRB/ADW

† Attending 14-15 Oct.
# Attending 15-16 Oct.

HPS/9 Sep ‘09

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Appendix B

ADAS-EU course 2009 participants

[1] adas-eu_course_participants_2009

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ADAS-EU Course 2009: 8-16 Oct 2009

Participants

Name		Institution	Email
Kiselius	Romas	ITPA Vilnius	romask@itpa.lt
Song	Mi-Young	Korea	mysong@nfri.re.kr
Guirlet	Remy	Cadarache	remy.guirlet@cea.fr
Reinke	Matthew	MIT	mlreinke@MIT.EDU
Jain	Jalaj	Birla, Jaipur	jalajjain83@gmail.com
Liang	Guiyun	Strathclyde	guiyun.liang@strath.ac.uk
Zhang	Daihong	IPP Greifswald	Daihong.Zhang@ipp.mpg.de
Kilbane	Deirdre	UCD, Dublin	deirdre.kilbane@ucd.ie
Gazza	Erica	CNR di Padova	erica.gazza@igi.cnr.it
Igenbergs	Katharina	TUV Vienna	
Sertoli	Marco	IPP Garching	msertoli@ipp.mpg.de
Jauzer	Arthur	IPP Garching	arthur.janzer@ipp.mpg.de
Potzel	Steffen	IPP Garching	steffen.potzel@ipp.mpg.de
Guzman	Francisco	Strathclyde	francisco.guzman@uam.es
Summers	Hugh	Strathclyde	summers@phys.strath.ac.uk
Whiteford	Allan	Strathclyde	allan@phys.strath.ac.uk
O'Mullane	Martin	Strathclyde	Martin.OMullane@jet.uk
Borodin	Dmitri	FZ Juelich	d.borodin@fz-juelich.de
Badnell	Nigel	Strathclyde	badnell@phys.strath.ac.uk

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Appendix C

ADAS-EU course 2009 lecture, task, tutorial and exercise notes

[1] ADAS-EU_lec_1a_2009
[2] ADAS-EU_lec_1a_2009
[3] ADAS-EU_lec_1b_2009
[4] ADAS-EU_lec_2_2009
[5] ADAS-EU_lec_3_2009
[6] ADAS-EU_lec_4_2009
[7] ADAS-EU_lec_4_2009
[8] ADAS-EU_long_writeup_autostructure
[9] ADAS-EU_long_writeup_autostructure_22
[11] ADAS-EU_long_writeup_rmatrix

[12] ADAS-EU_tut_1a_landscape_2009
[13] ADAS-EU_tut_1b_landscape_2009
[14] ADAS-EU_tut_2a_landscape_2009
[15] ADAS-EU_tut_2b_landscape_2009
[16] ADAS-EU_tut_3a_landscape_2009
[17] ADAS-EU_tut_3b_landscape_2009
[18] ADAS-EU_tut_4a_landscape_2009
[19] ADAS-EU_tut_4b_landscape_2009
[20] ADAS-EU_tut_badnell_overview
[21] ADAS-EU_tut_badnell_rmatrix_long
[22] ADAS-EU_tut_badnell_rmatrix_overview
[23] ADAS-EU_tut_borodin_ero
[24] ADAS-EU_tut_omullane_heavyspecies
[25] ADAS-EU_tut_whiteford_cxsfit
[26] ADAS-EU_tut_whiteford_rmatrix_notes1
[27] ADAS-EU_tut_whiteford_rmatrix_notes2
[28] ADAS-EU_tut_whiteford_rmatrix_notes3

[29] ADAS-EU_tut1-ex_2009
[30] ADAS-EU_tut2-ex_2009
[31] ADAS-EU_tut3-ex_2009
[32] ADAS-EU_tut4-ex_2009
[33] ADAS-EU_tasks_balance
[34] ADAS-EU_tasks_beam
[35] ADAS-EU_tasks_cxsfit

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Lecture 1 An introduction to ADAS

The history of the ADAS Project

ADAS had its origin at the JET Joint Undertaking in 1984, when a decision was made to underpin the evolving plasma interpretation and its associated plasma modelling, diagnostic measurements and spectral analysis with an in-house comprehensive theoretical atomic physics capability. It was also recognized that the usual practice of embedding atomic physics development and atomic data in a theoretical plasma physics division was unsound. The relatively crude modelled quantities such as total radiative power generated in typical plasma transport modelling are not adequate for validation of atomic physics data. It is analytic spectroscopy which provides the critical testing and validation and primary need for high grade atomic physics. The JET decision to base theoretical atomic physics in the experimental spectroscopy division and to centralise atomic data for modelling and analysis there was farsighted. Atomic data was exported to the theoretical plasma division from the experimental spectroscopy.

First placement of theoretical atomic physics personnel at JET was in 1984 and the centralised atomic data handling and coding in Experimental Division II commenced in 1985. Programming assistance was provided from 1987 to consolidate codes and data in a robust maintained system to professional standards and the first integrated release of interactive ADAS was in 1989. This was on the (then) large on-site IBM mainframe under the MVS/TSO environment. JET was a European venture and recognized its responsibilities to its EURATOM partners. European scientists from JET returning to their home laboratories sought to have the same ADAS facilities there. Also scientists in the UK and Germany preparing for the new SOHO satellite inquired if ADAS could be provided as ground segment support software. Rutherford Appleton Laboratory funded a preparatory study in 1993 to assess feasibility of conversion of ADAS to UNIX from MVS/TSO. The conversion programme called the ADAS Project was set up as a self-funded activity by five laboratories + JET, managed by Strathclyde University and overseen by a steering committee. The conversion was completed in 1995. The first ADAS workshop was held in 1995 and the Project was perpetuated as an on-going ADAS maintenance and development project. Membership has grown strongly with now both full voting large laboratory members and non-voting smaller university members. At the end of 2009 there are around twenty-five active Project members from all over the world and include most of the main fusion laboratories (see table 1).

Targets of ADAS

In the modern fusion plasma device, a number of different regions are recognized, especially the bulk or core plasma, the edge and divertor plasma and finally the beam penetrated plasma. The high temperature core plasma was the original target of atomic modelling for fusion. Impurity species, especially heavier species which are not fully ionised in the core plasma, are efficient radiators and may prevent achievement of the fusion break-even or ignition criteria. Also they affect the plasma resistivity and hence the distribution of toroidal current flow in tokamak devices. Transport modifies the radial distribution of the ionisation stages of impurity species. Spectral observations are used to infer these transport parameters – an important issue in modern high performance scenarios such as H-mode and ITBs (internal transport barriers). The divertor plasma is markedly different. The plasma is in contact or close to material strike zones which are in turn the principal source of impurities. The divertor must accept the enormous power flow down the scrape-off-layer from the bulk plasma, seek to minimise the release of impurities from the strike zones and retain released impurities in the divertor. The plasma is dynamic and cool. Choice of materials is critical and active control of divertor radiating conditions, by gas injection, is practised. Neutral beams of hydrogen and sometimes helium isotopes provide a main heating procedure for the plasma. The high energy neutrals penetrate the confining magnetic field, ionise through collisions in the core plasma and then thermalise. The beam/plasma zone leads to charge exchange emission and beam emission, both driven primarily by ion collisions. The resulting spectra observations, so-called CXS and BES, are key diagnostic indicators. All these scenarios require substantial atomic modelling and data and are addressed in detail by ADAS.

The ADAS Project has an equivalent involvement in the observation and analysis of astrophysical plasma emission. This is closely linked to spacecraft observatories, especially SOHO, CHANDRA and XMM. Targets of current interest are spectral emission from the solar atmosphere, X-ray emission from cometary and planetary atmospheres and finally VUV, XUV and X-ray line emission from gas clouds and other hot cosmic sources. The ADAS Project has benefited strongly from the mutual interest and shared activity of its members between fusion and astrophysics. Many of the techniques and types of derived data need are similar. However the lack of independent, non-spectroscopic, electron temperature and density diagnostic measurements in astrophysics does require some special methods, such as DEM (differential emission measure analysis), and associated data such as GTEs (contribution functions) which are not used in fusion. The solar astrophysics members have been critical in specifying and orienting the spectral fitting tools of ADAS. Also recent astrophysical observations has stimulated the development of ADAS along new pathways. Some of these are briefly summarised in the following paragraphs.

Participant organisation	**Contact**
JET Facility, UKAEA	K-D Zastrow
IPP-Garching, Germany	K. H. Behringer
KFA-Juelich, Germany	P. Mertens
Oak Ridge-Atom. Data Centre, USA	D. Schultz
Rutherford-Appleton Laboratory, UK	J. Lang
RFX Padua, Italy	M. Valisa
CEA Cadarache, France	R. Guirlet
KTH Stockholm, Sweden	E. Rachlew-Kallne
General Atomics, DIIID, USA	T. Evans
Observatory of Catania, Italy	A. Lanzafame
JAEA, JT60, Japan	H. Kubo
NIFS, LHD, Japan	I. Murakami
CRPP Lausanne, Switzerland	B. Duval
University of Wisconsin, USA	D. den Hartog
University of Toronto, Canada	P. Stangeby
Fraunhofer Institute for Laser Technik/Philips Research Labs, Aachen	T. Kruechen
Auburn University	M. Pindzola
IPR, Gadhinagar, India	P. Vasu
SWIP, Chengdu, China	X. Duan
FOM Rijnhuizen, Netherlands	M. von Hellermann
Kurchatov Institute, Moscow, Russia	A. Tugarinov
Princeton University	D. McCune
ITER	R. Pitts
IAEA, Vienna, Austria (special link)	R. Clark/B. Braams
University of Strathclyde	H. Summers

A number of connections between the fusion and astrophysical plasma scenes are of note and connected with the new and more subtle developments of ADAS. The light element ions such as the carbon ions, seen radiating in the quiet sun spectrum, are similar radiators in the divertors of fusion plasmas, albeit at higher electron densities and with strong influence of wall and recycling sources. Moving away from the divertor strike zones towards the confined plasma, we progress through higher ionisation stages up to the bare nuclei. Moving upward in the solar atmosphere, we see the same progression with the bare nuclei of carbon, nitrogen, oxygen, along with protons and electrons, escaping in the solar wind and within which they are spectroscopically invisible. However, the solar wind does impinge on planetary atmospheres and on ebullient cometary atmospheres. CHANDRA soft x-ray spectral observations of comets show emission from such species (particular K-shell lines). The emission though is complex, with a bremsstrahlung contribution along with spectrum lines which appears to be non-thermal. The proposed mechanism is that the streaming solar wind plasma, encountering the weakly ionised comet atmosphere, provokes a modified two-stream instability which in turn energises the electron distribution. Such a phenomenon is probably quite widely occurring in astrophysics (planetary atmospheres, supernovae remnants etc.) but in different energy regimes. Non-thermal electron distributions but with depleted high energy tails (Druyvesteyn distributions) occur in low pressure discharges and non-thermal distributions with both enhanced and reduced high energy Maxwellian tails are certainly expected in various parts of the fusion plasma. The extension of ADAS to non-Maxwellians is a current focus.

In high temperature plasmas such as flares and core fusion plasma as well as in cosmic sources, we note that species such as argon, calcium, iron and nickel show well-known and distinctive features in the soft x-ray – the so-called 'satellite line' spectra. Analysis considers the set of lines collectively and their differential dependence on electron temperature, electron density, transient ionisation state, ion temperature and impulsive flow velocity. This is the prototype for `special features' which we return to later in the course.

The advance towards a working fusion reactor and the appraisal of plasma facing materials for it means that the avoidance of heavy species in the past, because of their deleterious radiating efficiency in the plasma core has had to be re-appraised. Experiments with thermally resistant materials such as tungsten do indicate encouragingly low penetration into the core plasma. Heavy species in the first and second long periods will not be fully ionised even in ITER core plasmas and so are suitable as markers, detectable spectroscopically. The survey spectrum of a heavy species such as hafnium, ablated into a fusion plasma, in the VUV and XUV is a complex envelope of transition arrays in which the individual lines are largely unresolved. Atomic data and modelling for such species are certainly now necessary, yet the complexity does mean that somewhat different approaches from that used for light elements are required. These matters are currently being addressed by the ADAS Project.

Objectives of integrated modelling

ADAS seeks to provide integrating modelling. This is based on a number of strategic objectives which have become points of principle. These are to separate local atomic tasks from non-local issues, to provide derived atomic data close-linked to experimental spectroscopic data reduction, to provide consistent source function inputs to theoretical plasma modelling and to provide central management of atomic data. In the remainder of the course, it will be shown how ADAS seeks to satisfy these principles.

General principles

The broad mechanism for radiation emission from a hot tenuous plasma is simple. Thermal kinetic energy of electrons in the plasma is transferred by collisions to the internal energy of impurity ions. This energy is then radiated as spectrum line photons which escape from the plasma volume. Similarly ions increase or decrease their charge state by collisions with electrons. In this case the escaping photon may be a continuum one. The picture is often loosely referred to as the 'coronal model'. A detailed quantitative description is complicated because of the need to evaluate individually the many controlling collisional and radiative processes, a task which is compounded by the variety of atoms and ions which participate. The coronal model has been the basis for the description of impurities in fusion plasmas for many years. However in fusion, the progress towards ignition and to higher density plasmas, the use of neutral heating and diagnostic beams and the importance of divertors for impurity control requires a description beyond the coronal approximation. ADAS is centred on generalised collisional-radiative theory. The theory recognises relaxation time-scales of atomic processes and how these relate to plasma relaxation times, metastable states, secondary collisions etc. Attention to these aspects - rigorously specified in generalised collisional-radiative theory - allow an atomic description suitable for modelling the newer areas above (McWhirter & Summers, 1984).

Concerning time constants, the lifetimes of the various states of atoms, ions and electrons in a plasma to radiative or collisional processes vary enormously. Of particular concern for spectroscopic studies are those of translational states of free electrons, atoms and ions and internal excited states (including states of ionisation) of atoms and ions. These lifetimes determine the relaxation times of the various populations, the rank order of which, together with their values relative to observation times and plasma development times determines the modelling approach. The key lifetimes divide into two groups, namely, the intrinsic atomic group comprising metastable radiative decay, τ_m, ordinary excited state radiative decay τ_o and auto-ionising state decay τ_a, and the extrinsic collisional group comprising free electron thermalisation τ_{e-e}, positive ion thermalisation τ_{i-i}, ion-electron equilibration τ_{i-e} and ionisation τ_{ion}. Evidently, the first group are purely atomic parameters while the latter depend on plasma conditions. The intrinsic group are ordered as

$$\tau_a << \tau_o << \tau_m \qquad 1.1$$

Typical values for them are given by

$$\begin{aligned}\tau_m &\sim 10^1/z^8 \quad s\\ \tau_o &\sim 10^{-8}/z^4 \quad s\end{aligned} \qquad 1.2$$

The extrinsic group are ordered as

$$\tau_{ion} >> \tau_{i-e} >> \tau_{i-i} >> \tau_{e-e} \qquad 1.3$$

in general. The intrinsic and extrinsic groups are to be compared with each other and with times for plasma ion diffusion across temperature or density scale lengths, τ_{dif}, the relaxation times of transient plasma phenomena under study, τ_{phen} and instrumental observation sampling times τ_{obs}. For fusion plasmas, usually

$$\tau_{dif} \sim \tau_{ion} \sim \tau_m >> \tau_o >> \tau_{e-e} \qquad 1.5$$

From these time-scales, it may be assumed in most circumstances that the free electrons have a Maxwellian distribution and that the dominant populations of impurities in the plasma are those of the ground and metastable states of the various ions. The dominant populations evolve on time-scales of the order of plasma diffusion time-scales and so should be modelled dynamically, that is in the particle number continuity equations, along with the momentum and energy equations of plasma transport theory. The excited populations of impurities on the other hand may be assumed relaxed with respect to the instantaneous dominant populations, that is they are in a *quasi-equilibrium*. The quasi-equilibrium is determined by local conditions of electron temperature and electron density. So, the atomic modelling may be partially de-coupled from the impurity transport problem into local calculations which provide quasi-equilibrium excited ion populations and emissivities and then effective source coefficients (collisional-radiative coefficients) for dominant populations which must be entered into the transport equations. The solution of the transport equations establishes the spatial and temporal behaviour of the dominant populations which may then be re-associated with the local emissivity calculations, for matching to and analysis of observations.

To make effective use of an atomic modelling system of the above kind, it is helpful to consider the relationship of calculated spectral features to observed features. The starting point is the emission associated with a particular impurity excited level. It is is called a *feature primitive*. It is the set of transition energies and transition probabilities originating from the level. These purely atomic quantities determine positions and relative emissivities of spectrum lines driven by the level population. The level and its population may be a bundled one. All the component lines associated with the bundle constitute the feature primitive in this case, statistical weights alone determining their relative emissivities. No knowledge of the excited state population structure is required to prepare feature primitives. A local quasi-equilibrium population calculation establishes the dependence of the populations of excited levels on each metastable state. In turn this allows combination of feature primitives to form a *feature*. A feature is the set of line positions and local emissivities associated with a metastable and is determined by a local population calculation. A *superfeature* is a set of line of sight integrals of spectral emission. It is obtained by combining features with the line of sight distribution of metastable populations derived from an impurity transport calculation. A superfeature includes line broadening and distortions due to the dynamics of the plasma along the line of sight. It is at the superfeature level that the confrontation of experiment and theory takes place. ADAS may be viewed as providing the tools for

$$\textit{feature primitive} \rightarrow \textit{feature} \rightarrow \textit{superfeature}$$

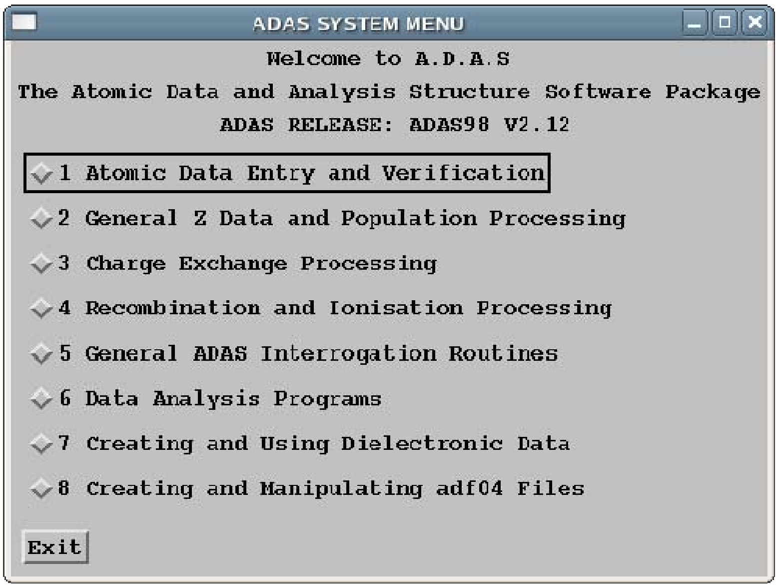
spectral synthesis. Practical implementation and exploitation of these ideas follow in the remainder of the lecture course.

General organisation of ADAS

The Atomic Data and Analysis Structure (ADAS) is an interconnected set of computer codes and data collections for modelling the radiating properties of ions and atoms in plasmas and for assisting in the analysis and interpretation of spectral measurements. The four components of the package are an interactive system, a library of key subroutines, codes and scripts for large scale off-line calculation and a very large database of fundamental and derived atomic data. The interactive part provides immediate display of important fundamental and derived quantities used in analysis together with a substantial capability for preparation of derived data. It also allows exploration of parameter dependencies and diagnostic prediction of atomic population and plasma models. The second part is non-interactive but provides a set of subroutines which can be accessed from the user's own codes to draw in necessary data from the derived ADAS database. The large scale off-line part of ADAS is a new and growing development. ADAS interactive codes are used to define and prepare drivers for the off-line calculations. The latter are normally implemented on and are tuned for massively parallel systems. The database spans most types of data required for fusion and astrophysical application

Interactive ADAS

The various ADAS routines are essentially of three types, namely those which execute atomic modelling calculations, those which are interrogative on the ADAS database (both fundamental and derived parts) and those which produce driver data sets for other large scale codes. The first group may relay substantial quantities of data for further processing or for addition to the derived database.

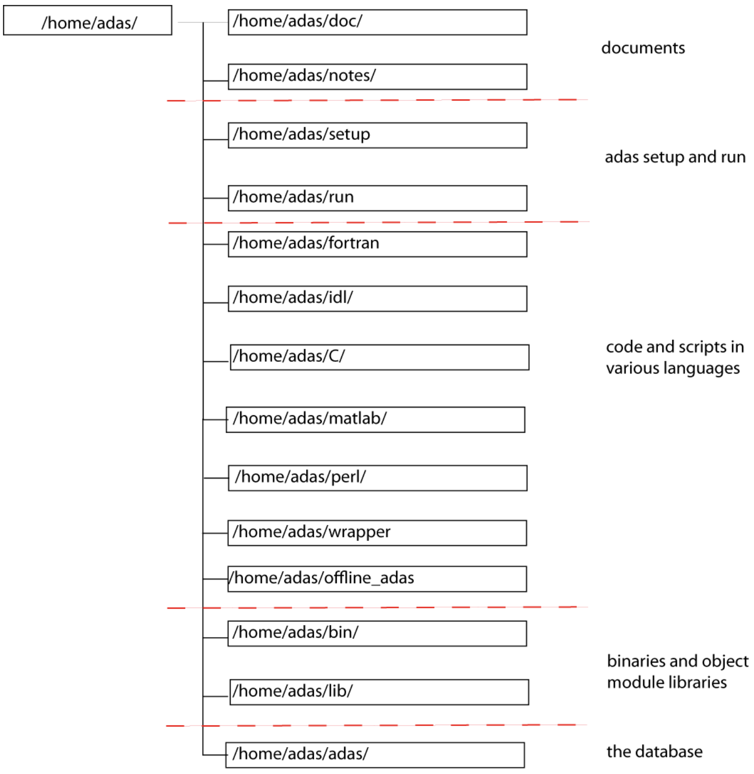


In the interrogative codes, the principle objective has been to allow graphical display of any part of the database. All codes satisfy this quick look and check facility. In ADAS interrogation codes, cubic spline interpolation is performed on the source data from the database. These interpolated values are given as convenient printer tabulations. Atomic modelling codes generally create output data sets as well as normal tabular output. These files are structured according to the requirement of the ADAS data base or for further ADAS programs. It is anticipated that the user will edit these files into standard ADAS named files when establishing a personal database after being satisfied of their correctness.

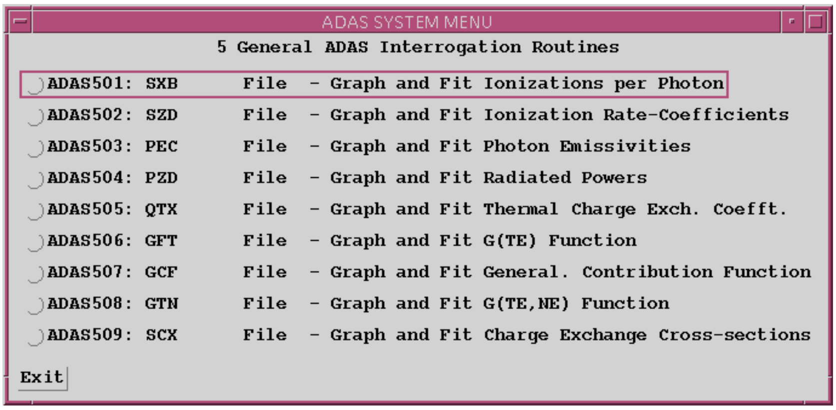
Lecture 1b Computational overview of ADAS

The ADAS suite comprises mainly IDL and FORTRAN code and runs under UNIX. Tested systems include Solaris, DEC, HP, AIX and Linux. Pre-requisites for an installation of ADAS are ~ 5.0Gb disk space; F77 and C compilers; IDL (fully licensed – ADAS will not run in IDL demo mode); a PDF viewer such as Acrobat reader. Installation is carried out and managed by the ADAS manager (Dr. Allan Whiteford). ADAS is usually installed in the /*home* directory of an account with user name '*adas*'.

The ADAS distribution has the directory structure shown below.



The interactive ADAS suite comprises in the region of 85 programs. They are arranged in 8 series reflecting distinct regions of atomic physics purpose. The menu selection for series 5 is shown below.

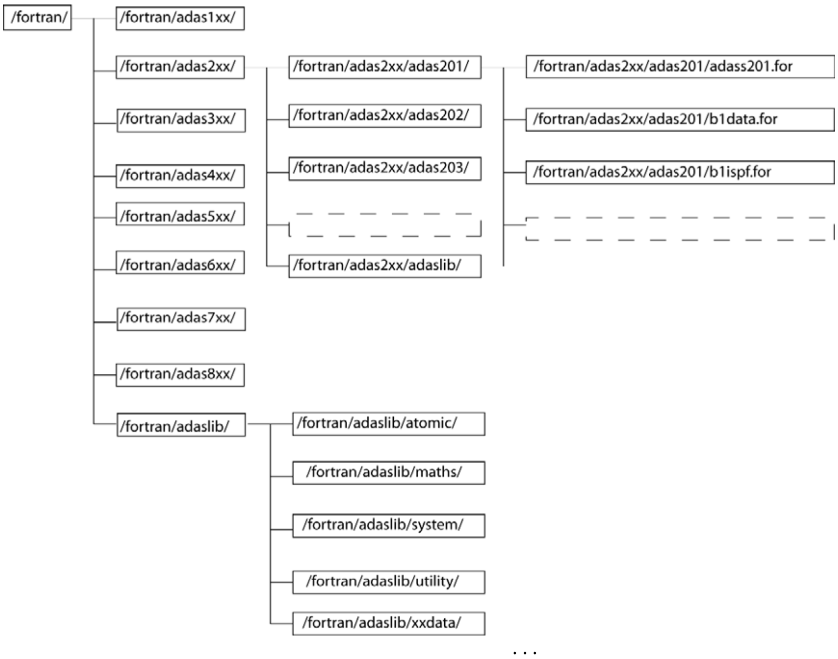


ADAS SYSTEM MENU

5 General ADAS Interrogation Routines

```
○ ADAS501: SXB      File  - Graph and Fit Ionizations per Photon
○ ADAS502: SZD      File  - Graph and Fit Ionization Rate-Coefficients
○ ADAS503: PEC      File  - Graph and Fit Photon Emissivities
○ ADAS504: PZD      File  - Graph and Fit Radiated Powers
○ ADAS505: QTX      File  - Graph and Fit Thermal Charge Exch. Coefft.
○ ADAS506: GFT      File  - Graph and Fit G(TE) Function
○ ADAS507: GCF      File  - Graph and Fit General. Contribution Function
○ ADAS508: GTN      File  - Graph and Fit G(TE,NE) Function
○ ADAS509: SCX      File  - Graph and Fit Charge Exchange Cross-sections
```

The IDL, FORTRAN, C and MATLAB codes and associated sub-routines (>1000) are organized hierarchically according to series and maintained under CVS. /adaslib subdirectories contain subroutines common to codes at their hierarchical level. Series 1 code subroutines names commence with the letter ‘a’ followed by the numerical (hexadecimal) value of the particular code. The structure is shown below in the FORTRAN case.



Note the sub-directories of the top level /fortran/adaslib/ subdirectory according to sub-routine character. Also note the /xxdata/ subdirectory which contains important sub-routines for getting data from the ADAS database int your own FORTRAN programs. The /idl/ subdirectory structure is similar, but note some extras in the top level /idl/adaslib/ sub-directory. There are subdirectories for graphical user interface procedures and read_adf and write_adf procedures which you will find useful. Source IDL code is open, but FORTRAN code is restricted. FORTRAN shared object module libraries are available to user codes.

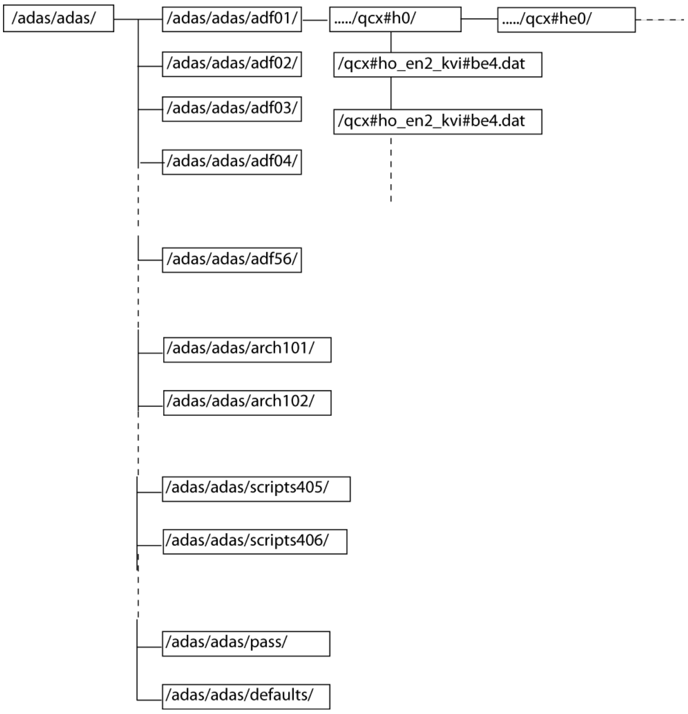
ADAS data

The subdirectory */home/adas/adas/* contains the central ADAS data archive. In also includes sub-directories /*pass* of 'passing files' and /*defaults* of 'defaults' files for use by the user *adas* in testing the distribution. The latter two file categories are also required in each individual ADAS user's file space. The primary data themselves are stored in sub-directories according to ADAS data format number, e.g. *adf04*. There are currently 56 data formats whose layout and organization is precisely specified. These are listed below. It is recommended that each user sets up a personal data space as /home/<uid>/adas/ which parallels the central ADAS structure. ADAS codes are designed to go automatically to the correct ADAS data format either in the central or user space.

adf01	bundle-n and bundle-nl charge exchange cross-sections
adf02	ion impact cross-sections with named participant
adf03	recombination, ionisation and power parameter sets
adf04	resolved specific ion data collections
adf05	general z excitation data collections
adf06	general z recombination/ionisation data collections
adf07	direct resolved electron impact ionisation coefficients
adf08	direct resolved radiative recombination coefficients
adf09	direct resolved dielectronic recombination coefficients
adf10	iso-electronic master files
adf11	iso-nuclear master files
adf12	charge exchange effective emission coefficients
adf13	ionisation per photon coefficients
adf14	thermal charge exchange coefficients
adf15	photon emissivity coefficients
adf16	generalised contribution functions
adf17	condensed projection coefficients
adf18	cross-referencing data
adf19	zero-density radiative power data
adf20	G(Te) functions
adf21	effective beam stopping coefficients
adf22	effective beam emission coefficients
adf23	state selective electron impact ionisation coefficients
adf24	state selective charge transfer cross-sections
adf25	driver data-sets for ADAS204 calculation
adf26	bundle-n populations of excited states in beams
adf27	driver data-sets for ADAS701 calculations
adf28	driver data-sets for ADAS702 post-processing
adf29	driver data sets for ADAS707 calculation
adf30	driver data-sets for ADAS708 post-processing
adf31	feature files for satellite line spectral simulation
adf32	driver data-sets for ADAS802 calculations
adf33	driver data-sets for ADAS803 postprocessing
adf34	driver data-sets for ADAS801 calculations
adf35	spectral filter data
adf36	feature files for series limit spectral simulation
adf37	non-Maxwellian distribution function files
adf38	Seaton - opacity photo-excitation
adf39	Seaton - opacity - photo-ionisation

adf40	envelope feature photon emissivity coefficients
adf41	driver data-sets for offline ADAS8#1 calculations
adf42	driver data-sets for ADAS810 calculations
adf43	GTN photon emissivity functions
adf44	F_GTN envelope feature emissivity functions
adf45	feature files for continuum emission
adf46	BBGP driver datasets for dielectronic recombination
adf47	-
adf48	direct resolved radiative recombination coefficients
adf49	universal z-scaled CXS n and nl resolved xsects
adf50	-
adf51	-
adf52	-
adf53	-
adf54	promotion rules - structure
adf55	promotion rules – dielectronic recombination
adf56	promotion rules - ionisation

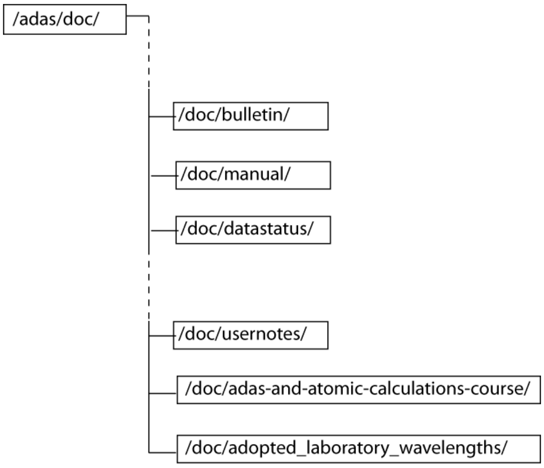
Further layers of sub-directories are assigned as necessary for different species etc. The sub-directory and final data set naming is designed to give some indication of content. The final data sets themselves are all ascii and have the extension *.dat*. The figure below shows the layout.



For central ADAS, sub-directories, *arch101*,…, *scripts405*, … contain only samples. Such data is normally personal to a user.

ADAS documentation

ADAS documentation is now most easily accessed via the web pages from www.adas.ac.uk and on through OPEN-ADAS. The documentation is also present on every ADAS sites in PDF format so is available for viewing electronically and for printing. It is placed in the */.../adas/doc/* directory under several headings. A schematic is shown below.



The principal Unix-IDL-ADAS manual is comprehensive, organised in chapters and sub-chapters connected to the ADAS series and named as */.../adas/doc/manual/chap<i>-<nn>.pdf* where <i> denotes chapter and <nn> denotes the sub-chapter number. It is unfortunately a bit out-of-date now. There are major appendices, in particular appendix B contains full descriptors and current states of the ADAS data formats. Bulletins are currently issued about once per year and are named according to date of issue. They contain information of bug fixes, new data and descriptions of newly added codes.

There are a number of shorter special manuals, which describe particular types of activity within ADAS, such as charge exchange spectroscopy or influx spectroscopy. These are also a bit out of date now. They include

flx-manual	influx spectroscopy
bms-manual	beam emission spectroscopy
cxs-manual	charge exchange spectroscopy
ion1-manual	basic ionisation balance studies
ion2-manual	advanced ionisation balance studies
opac-manual	opacity studies
spec-manual	spectral analysis
cds-manual	atomic modelling for solar analysis

The content of the Datastatus documents, named as */.../adas/doc/datastatus/adf<nn>.pdf* where <nn> is an ADAS data format number, are now present in appendix B of the main user manual. There may be additional files such as data reviews conducted by ADAS participants.

A substantial number of ADAS tutorials have been presented at laboratories in Europe and the USA. The tutorials are named as */…/adas/doc/<lab><yr>-tut/<section>.pdf* where <lab> is a mnemonic for a laboratory and <yr> is a two digit year number. They are divided into sections in which a sub-area is summarised with viewgraphs followed by simple learning exercises with ADAS.
Some of these older tutorial files are 'postscript' .

Initial ADAS user set-up

There are a number of steps which a user must take in order to prepare his/her environment for ADAS properly.

A directory called ‘adas’ must be created in the user’s home directory as */home/<uid>/adas/*. A setup script should then be executed from the newly created directory. The appropriate setup script for a user’s site can be found in the central ADAS file space. The steps at Strathclyde are

```
cd adas
./adas_strathclyde.csh
```

The setup script (a) creates sub-directories with in the user’s *adas*/ directory space; (b) adds entries to the user’s *.cshrc* or *.profile* files to set up the user’s environment for IDL and ADAS; (c) sets the user’s ADASUSER environment variable which is the pathway to the newly created user’s *adas*/ directory.

Important directories are

adas/defaults/ - directory where the user defaults for each ADAS program are stored. The defaults file for an ADAS series code remembers the user entries at the last run of the code.

adas/pass / -directory for storing output files from ADAS codes, called ‘passing files’.

There a number of important entries in the *.cshrc* file. Values at Strathclyde are

setenv ADASUSER /home/<uid>/adas	
source /packages/rsi/idl/bin/idl_setup	sets up default IDL path
source /packages/adas/idl_adas/adas_setup	amends IDL-PATH for ADAS defines ADASCENT – path to central ADAS archive defines ADASFORT – path to FORTRAN executable

Working with interactive ADAS widgets

A number of IDL screens are common to many of the separate ADAS codes in the interactive series. These include the file selection screen on input, the table editor screen used for entry of user values for parameters, graphical input of user data pairs, screens for graphical output, graph display adjustment and graph retention. Code ADAS501 uses these screens and is suitable for practice . The following sub-sections summarize the main features and how to work with these screens. Programs of series 5 make use of data from archived ADAS datasets and initiate an interactive dialogue with the user in three parts, namely, input file selection, entry of user data and disposition of output. Start ADAS501 from the interactive ADAS menus

File selection

The first window has the appearance shown below

1. Data root shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Note that each type of data is stored according to its ADAS data format (*adf* number). Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*, to use this facility.
2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.

3. Available sub-directories are shown in the large file display window. Scroll bars appear if the number of entries exceed the file display window size.
4. Click on a name to select it. The selected name appears in the smaller selection window above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
5. Once a data file is selected, the set of buttons at the bottom of the main window become active.

Data Root: /afs/@cell/u/adas/adas/adf13/

sxb96#c/sxb96#c_pjr#c3.dat

Data File:

```
..
sxb96#c_pjr#c0.dat
sxb96#c_pjr#c1.dat
sxb96#c_pjr#c2.dat
sxb96#c_pjr#c3.dat
sxb96#c_pjr#c4.dat
sxb96#c_pjr#c5.dat
sxb96#c_pju#c0.dat
sxb96#c_pju#c1.dat
sxb96#c_pju#c2.dat
sxb96#c_pju#c3.dat
sxb96#c_pju#c4.dat
sxb96#c_pju#c5.dat
sxb96#c_vsr#c1.dat
sxb96#c_vsr#c2.dat
```

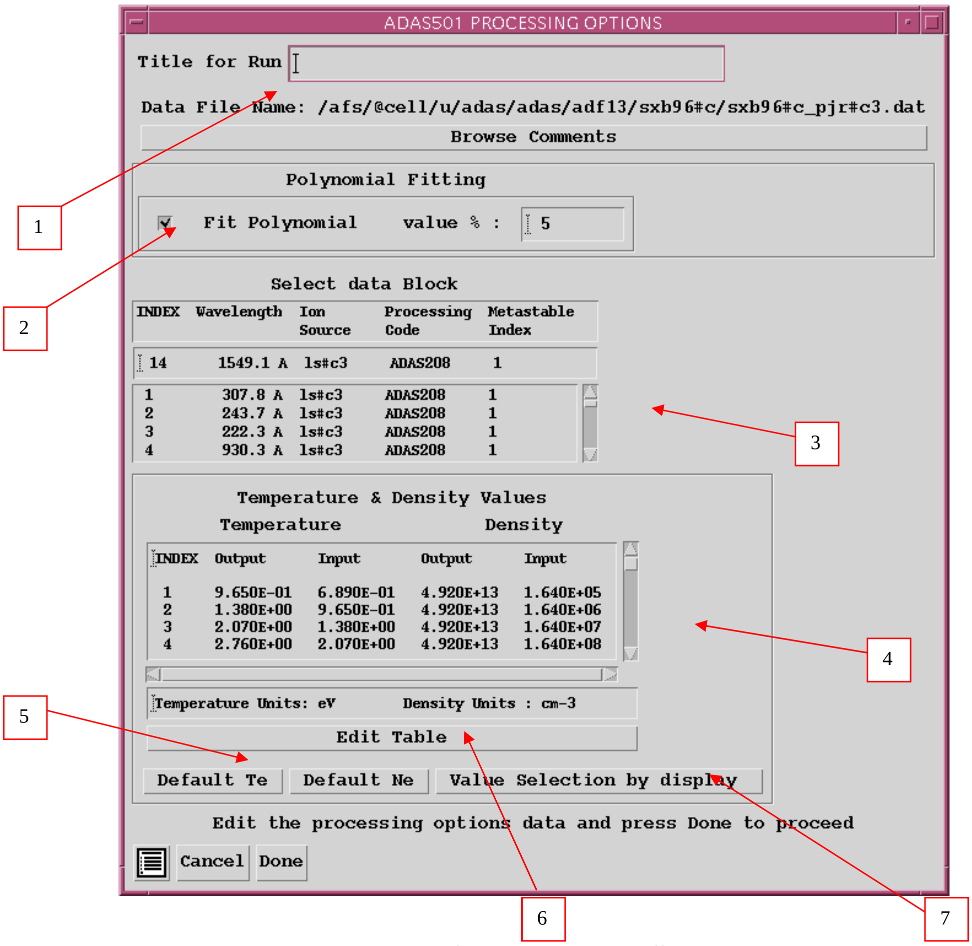
6. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.
7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

Processing options

The next window is called the processing options screen and has the appearance shown below

1. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being analysed is also shown. The button *Browse comments* again allows display of the information field section at the foot of the selected dataset, if it exists.

2. The output data extracted from the datafile, in the case of ADAS501, an ‘emissivity coefficient’, may be fitted with a polynomial. This is as a function of temperature. Clicking the *Fit polynomial* button activates this. The accuracy of the fitting required may be specified in the editable box. The value in the box is editable only if the *Fit Polynomial* button is active.



ADAS501 PROCESSING OPTIONS

Title for Run

Data File Name: /afs/@cell/u/adas/adas/adf13/sxb96#c/sxb96#c_pjr#c3.dat

Polynomial Fitting

☑ Fit Polynomial value % : 5

Select data Block

INDEX	Wavelength	Ion Source	Processing Code	Metastable Index
14	1549.1 A	1s#c3	ADAS208	1
1	307.8 A	1s#c3	ADAS208	1
2	243.7 A	1s#c3	ADAS208	1
3	222.3 A	1s#c3	ADAS208	1
4	930.3 A	1s#c3	ADAS208	1

Temperature & Density Values

	Temperature		Density	
INDEX	Output	Input	Output	Input
1	9.650E-01	6.890E-01	4.920E+13	1.640E+05
2	1.380E+00	9.650E-01	4.920E+13	1.640E+06
3	2.070E+00	1.380E+00	4.920E+13	1.640E+07
4	2.760E+00	2.070E+00	4.920E+13	1.640E+08

Temperature Units: eV Density Units : cm-3

Edit the processing options data and press Done to proceed

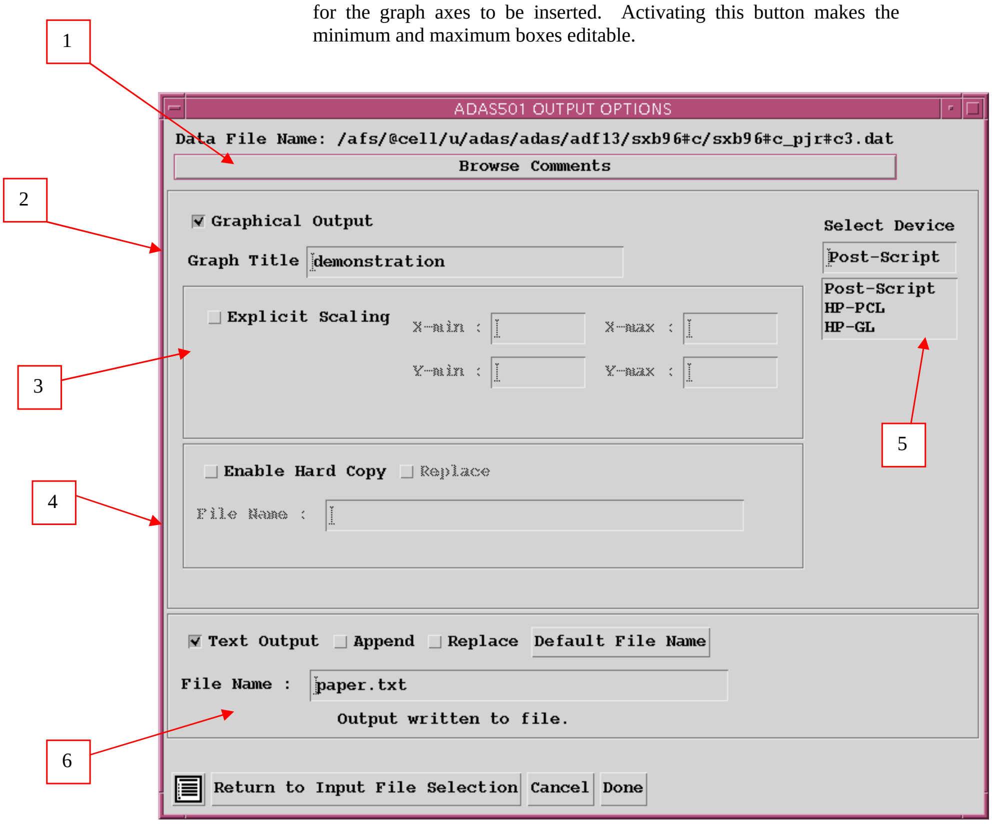
3. Spectrum lines for which emissivity coefficients are available in the data set are displayed in the line list display window. This is a scrollable window using the scroll bar to the right of the window. Click anywhere on the row for a line to select it. The selected line appears in the selection window just above the line list display window.
4. Your settings of electron temperature/electron density pairs (outputs) are shown in the temperature/density display window. The temperature and density values at which the emissivity coefficients are stored in the datafile (inputs) are also shown for information. **Note that you must give temperature/density pairs, ie. the same number of each as for a model.** The underlying datafile has a two-dimensional storage as a function of temperature and density.

5. The program recovers the output temperature/density pairs you used when last executing the program. Pressing the *Default Te* or *Default Ne* buttons insert a default set of temperatures or densities equal to the input values. A choice of particular density or particular temperature respectively from the input sets is allowed on a ‘pop-up’ window.
6. The Temperature & Density Values are editable. Click on the *Edit Table* button if you wish to change the values. A ‘drop-down’ window, the ADAS Table Editor window, appears as shown below:
7. ADAS501 has a more sophisticated graphical method for Te/Ne pair selection. Activate the *Value Selection by Display* button. The detailed operation of the widget is described in Chap1-00 of this user manual.

Output options

The **third window** is called the output options window and has the appearance shown below

1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
2. Graphical display is activated by the *Graphical Output* button. This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph.
3. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.



ADAS501 OUTPUT OPTIONS

Data File Name: /afs/@cell/u/adas/adas/adf13/sxb96#c/sxb96#c_pjr#c3.dat

☑ Graphical Output

Graph Title: demonstration

☐ Explicit Scaling

☐ Enable Hard Copy ☐ Replace

Select Device: Post-Script

☑ Text Output ☐ Append ☐ Replace

File Name : paper.txt

Output written to file.

4. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. If the output graphic file already exits and the *Replace* button has not been activated, a ‘pop-up’ window issues a warning.
5. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.
6. The *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name ‘paper.txt’may be set by pressing the button *Default file name*. A ‘pop-up’ window issues a warning if the file already exists and the *Replace* button has not been activated.
7. The graph is displayed in a following **Graphical Output** window described below.

Graphical output

The final graph display window has some additional controls

1. Printing of the currently displayed graph is activated by the *Print* button.

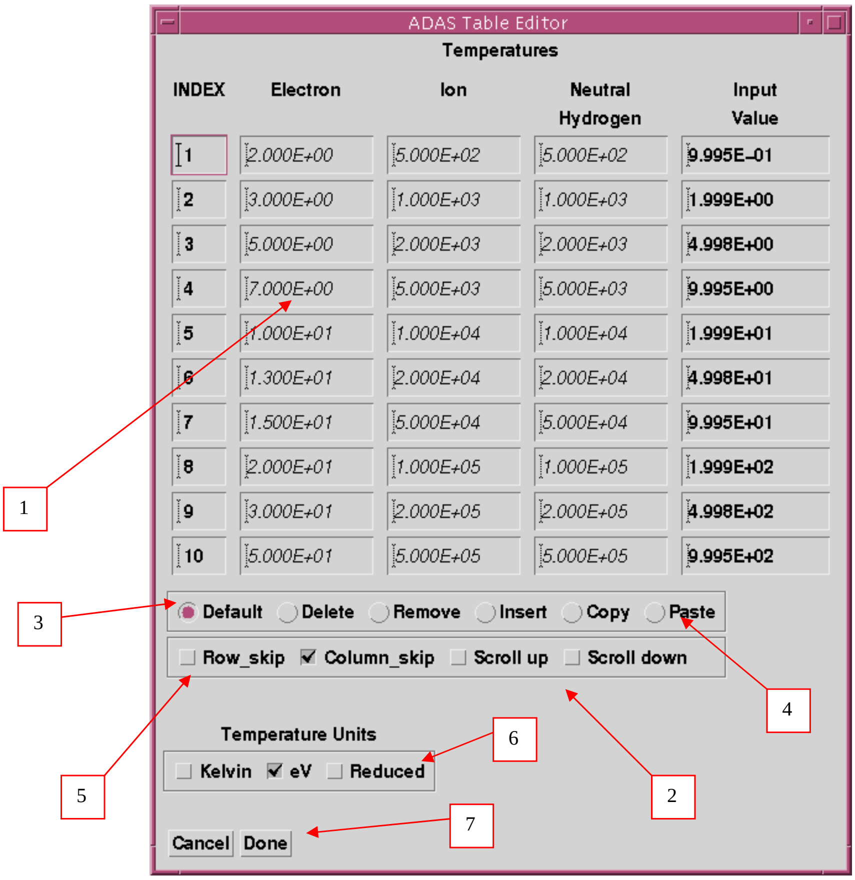
```
IONISATIONS PER PHOTON VS ELECTRON TEMPERATURE : DEMONSTRATION (eV)

ADAS    : ADAS RELEASE: ADAS98 V2.5.5 PROGRAM: ADAS501 V1.14 DATE: 09/07/02 TIME: 15:00
FILE    :/afs/@cell/u/adas/adas/adf13/sxb96#c/sxb96#c_pjr#c3.dat BLK=14; C + 3  WAVELENGTH=   1549.1 A MET=1
MINIMAX : LOGFIT - DEGREE= 7  ACCURACY=  2.24%  END GRADIENT: LOWER=  56.66 UPPER=   0.51
KEY     : (CROSSES - INPUT DATA) (FULL LINE - SPLINE FIT)   (DASH LINE - MINIMAX)

--- EMITTING ION INFORMATION ---

ELEMENT SYMBOL            = C
NUCLEAR CHARGE            = 6
CHARGE STATE              = 3
WAVELENGTH (angstroms)    = 1549.1 A
SPECIFIC ION FILE SOURCE  = ls#c3
PROCESSING CODE           = ADAS208
METASTABLE INDEX          = 1

- ELECTRON TEMPERATURE/DENSITY RELATIONSHIP -

INDEX    TEMPERATURE (eV)    DENSITY (cm-3)
 1        9.650e-01      4.920e+13
 2        1.380e+00      4.920e+13
 3        2.070e+00      4.920e+13
 4        2.760e+00      4.920e+13
 5        4.140e+00      4.920e+13
 6        6.890e+00      4.920e+13
 7        9.650e+00      4.920e+13
 8        1.380e+01      4.920e+13
 9        2.070e+01      4.920e+13
 10       2.760e+01      4.920e+13
 11       4.140e+01      4.920e+13
 12       6.890e+01      4.920e+13
 13       9.650e+01      4.920e+13
 14       1.380e+02      4.920e+13
 15       2.070e+02      4.920e+13
 16       2.760e+02      4.920e+13
 17       4.140e+02      4.920e+13
 18       6.890e+02      4.920e+13
 19       9.650e+02      4.920e+13
 20       1.380e+03      4.920e+13
 21       2.070e+03      4.920e+13
 22       2.760e+03      4.920e+13
 23       4.140e+03      4.920e+13
```

2. Activate the *Adjust* button to pop-up the Graph Adjust window. It's operation is described in Chap1-00 of this user manual.
3. Activate the *Retain* button to pop-up the Multiplot window. This widget permits superposition of graphs from multiple passes through ADAS501 and hence graph comparison. The detailed operation of the widget is described in Chap1-00 of this user manual.

Table Editor

A necessary operation in interactive ADAS is entry of user values into a table. Since this is common to many ADAS programs, a special window has been developed to assist in this task. A typical appearance of the **Table Editor** window is shown below

1. 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.



ADAS Table Editor

Temperatures

INDEX	Electron	Ion	Neutral Hydrogen	Input Value
1	*2.000E+00*	*5.000E+02*	*5.000E+02*	9.995E–01
2	*3.000E+00*	*1.000E+03*	*1.000E+03*	1.999E+00
3	*5.000E+00*	*2.000E+03*	*2.000E+03*	4.998E+00
4	*7.000E+00*	*5.000E+03*	*5.000E+03*	9.995E+00
5	*1.000E+01*	*1.000E+04*	*1.000E+04*	1.999E+01
6	*1.300E+01*	*2.000E+04*	*2.000E+04*	4.998E+01
7	*1.500E+01*	*5.000E+04*	*5.000E+04*	9.995E+01
8	*2.000E+01*	*1.000E+05*	*1.000E+05*	1.999E+02
9	*3.000E+01*	*2.000E+05*	*2.000E+05*	4.998E+02
10	*5.000E+01*	*5.000E+05*	*5.000E+05*	9.995E+02

● Default ○ Delete ○ Remove ○ Insert ○ Copy ○ Paste

☐ Row_skip ☑ Column_skip ☐ Scroll up ☐ Scroll down

Temperature Units

☐ Kelvin ☑ eV ☐ Reduced

2. 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.
3. 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*.
4. The *Copy* and *Paste* round buttons operate for the next immediate action only.
5. 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.
6. 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.
7. 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.

Lecture 2 The interactive system – working with adf04 datasets and population structure

The population equations for the number densities of excited states of an ion in an optically thin thermal plasma are established and solved. Collisions by free Maxwellian electrons drive the excitation. Basic notation for collisional processes is summarised. The ADAS data sources are identified and ADAS code to examine these data outlined. The code to obtain the populations is described and it is shown how the results can be used in line ratio diagnostic prediction. Some preparation is made in additional processes and data format extensions for later parts of the course.

Preliminaries

Basic electron impact excitation reactions and sources in ADAS

The reaction is

$$X_i^{+z}(E_i) + e(\varepsilon_i) \rightarrow X_j^{+z}(E_j) + e(\varepsilon_j)$$

with $\varepsilon_i + E_i = \varepsilon_j + E_j$ where E_i (E_j) is the excitation energy of the state *i* (*j*) denoted by X_i^{+z} (X_j^{+z}) from the lowest level of the ion X^{+z} and ε_i (ε_j) is the energy of the incident (scattered) electron. The reaction is described by a *cross-section* for the process denoted by $\sigma_{i\rightarrow j}(\varepsilon_i)$. The reaction requires $\varepsilon_i \geq \Delta E_{ij} = E_j - E_i$. Introduce the threshold parameter $X = \varepsilon_i / \Delta E_{ij}$, with $X \in [1,\infty]$. In preference to the cross-section, use the symmetric, dimensionless , slowly varying *collision strength* Ω_{ij}. The excitation cross-section $\sigma_{i\rightarrow j}(\varepsilon_i)$, the de-excitation cross-section $\sigma_{i\rightarrow j}(\varepsilon_i)$, and the collision strength Ω_{ij}, are connected by

$$\Omega_{ij} = \omega_i (E_i/I_H)(\sigma_{i\rightarrow j}(\varepsilon_i)/\pi a_0^2) = \omega_j (E_j/I_H)(\sigma_{j\rightarrow i}(\varepsilon_j)/\pi a_0^2)$$

Three distinct types of cross-section are recognised, namely, dipole, non-dipole and spin with distinct asymptotic behaviour.

ADAS is principally, but not exclusively, designed for plasmas in which the free electrons are Maxwellian. The collision strength integrated over a Maxwellian distribution of electron energies at an electron temperatures T_e is called the *rate parameter* or *effective collision strength* and written as γ ('gamma') or Υ ('Upsilon'). It is defined by

$$\Upsilon_{ij} = \int_0^\infty \Omega_{ij}(\varepsilon_j)\exp(-\varepsilon_j/kT_e)\,d(\varepsilon_j/kT_e)$$

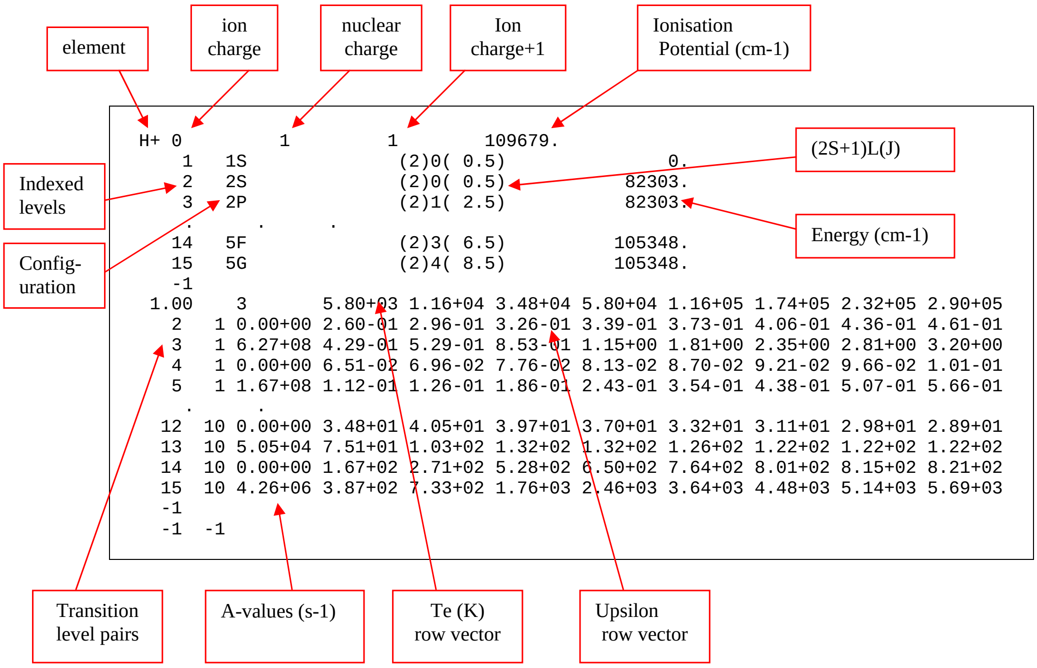
Υ_{ij} is related to the excitation rate coefficient $q_{i\rightarrow j}(T_e)$ and de-excitation rate coefficient $q_{j\rightarrow i}(T_e)$ as

$$q_{j\rightarrow i}(T_e) = \frac{\omega_i}{\omega_j}\exp(\Delta E_{ij}/kT_e)q_{i\rightarrow j}(T_e) = 2\sqrt{\pi}\alpha c a_0^2 \frac{1}{\omega_j}\left[I_H/kT_e\right]^{1/2}\Upsilon_{ij}$$

Burgess C-plots: Burgess & Tully (1992) showed that the whole variation of Υ and T_e can be mapped onto a finite range by introducing a reduced temperature, x, and reduced Upsilon, y, for four types of transition. Also they introduce a parameter C to balance the spread of x-values across its range ([0,1]) . Such mapping gives a compact representation of collision data and is used in ADAS for accurate interpolation, checking of the limiting high temperature behaviour of the rate coefficient.

The adf04 data format

The primary repositories of electron impact collision rate coefficient (Upsilon) data are *adf04* files. Such files are for a specific ion and contain energy level lists, level configuration, term and level classification quantum numbers, level energies. Following the level lists, they contain transition lines, which specify the upper and lower levels of each transition, the A-value for the transition and then a set of Upsilons for the transition as a function of electron temperature. The basic layout is as shown below.



```
H+ 0         1         1        109679.
    1   1S              (2)0( 0.5)               0.
    2   2S              (2)0( 0.5)           82303.
    3   2P              (2)1( 2.5)           82303.
    .      .      .
   14   5F              (2)3( 6.5)          105348.
   15   5G              (2)4( 8.5)          105348.
   -1
 1.00    3       5.80+03 1.16+04 3.48+04 5.80+04 1.16+05 1.74+05 2.32+05 2.90+05
   2   1 0.00+00 2.60-01 2.96-01 3.26-01 3.39-01 3.73-01 4.06-01 4.36-01 4.61-01
   3   1 6.27+08 4.29-01 5.29-01 8.53-01 1.15+00 1.81+00 2.35+00 2.81+00 3.20+00
   4   1 0.00+00 6.51-02 6.96-02 7.76-02 8.13-02 8.70-02 9.21-02 9.66-02 1.01-01
   5   1 1.67+08 1.12-01 1.26-01 1.86-01 2.43-01 3.54-01 4.38-01 5.07-01 5.66-01
    .      .
  12  10 0.00+00 3.48+01 4.05+01 3.97+01 3.70+01 3.32+01 3.11+01 2.98+01 2.89+01
  13  10 5.05+04 7.51+01 1.03+02 1.32+02 1.32+02 1.26+02 1.22+02 1.22+02 1.22+02
  14  10 0.00+00 1.67+02 2.71+02 5.28+02 6.50+02 7.64+02 8.01+02 8.15+02 8.21+02
  15  10 4.26+06 3.87+02 7.33+02 1.76+03 2.46+03 3.64+03 4.48+03 5.14+03 5.69+03
  -1
  -1  -1
```

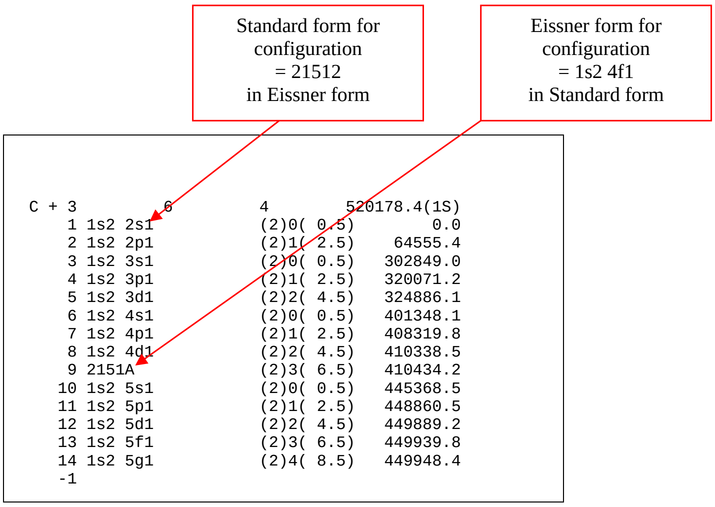
Note that the configuration of a level is the specification of the orbital occupancies as

$$\Gamma_g = n_1 l_1^{\,q_1} n_2 l_2^{\,q_2} ......n_m l_m^{\,q_m} \text{ where } q_i > 0 \text{ for } i = 1,...,m \text{ and } \sum_{i=1}^{m} q_i = N$$

It is helpful to maintain a consistent pattern for configurations for automatic processing of ADF04 files and for matching of energy levels between different datasets.. In ADAS two conventions are use, namely the *Standard form* and *Eissner form*. *Standard form* represents each shell with three characters with a space separating shells in the whole configuration as ' 1s2 2s2 2p1' representing $1s^2 2s^2 2p^1$. For certain calculations, principal quantum numbers greater than 9 may be required and for complex element ion, shell occupancies greater than 9 also may occur. To maintain the three character shell notation, the integers beyond nine are represented alphabetically, that is 10 ≡ 'a', 11 ≡ 'b' etc. Thus in *Standard form*, $2p^6\ 6f^{11}\ 11s^1$ is represented by ' 2p6 6fb bs1'. In *Eissner form*, each orbital, starting from 1s is indexed. The index is an integer up to 9, but continues through the upper case alphabet and then through the lower case alphabet. Thus 1s ≡ '1', 2p ≡ '2', 4f ≡ 'A'. A portion of the conversion table is

Orbital	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f
Eissner	1	2	3	4	5	6	7	8	9	A
Orbital	5s	5p	5d	5f	5g	6s	6p	6d	6f	6g
Eissner	B	C	D	E	F	G	H	I	J	K

The shell occupancy is represented as a two digit integer as 50+q and this precedes the shell index character. Thus again the shell is represented by a three character field but is written with no separation between the fields in the whole configuration. Thus in *Eissner form* $1s^2\ 2s^2\ 2p^6\ 6g^{11}$ is represented by ‘52152256361K’. ADAS works freely with both notations and subroutines in the ADAS library transform from one to the other. *Eissner form* is the preferred form in ADAS series 7 codes since structure calculations there use the *Autostructure* code. Standard form is the preferred form in ADAS series 8 codes since structure calculations there use the *Cowan/O’Mullane* code. *Eissner form* is the most compact and is generally adopted with very complex configurations.



Standard form for
configuration
= 21512
in Eissner form

Eissner form for
configuration
= 1s2 4f1
in Standard form

```
C + 3         6         4        520178.4(1S)
   1 1s2 2s1            (2)0( 0.5)         0.0
   2 1s2 2p1            (2)1( 2.5)     64555.4
   3 1s2 3s1            (2)0( 0.5)    302849.0
   4 1s2 3p1            (2)1( 2.5)    320071.2
   5 1s2 3d1            (2)2( 4.5)    324886.1
   6 1s2 4s1            (2)0( 0.5)    401348.1
   7 1s2 4p1            (2)1( 2.5)    408319.8
   8 1s2 4d1            (2)2( 4.5)    410338.5
   9 2151A              (2)3( 6.5)    410434.2
  10 1s2 5s1            (2)0( 0.5)    445368.5
  11 1s2 5p1            (2)1( 2.5)    448860.5
  12 1s2 5d1            (2)2( 4.5)    449889.2
  13 1s2 5f1            (2)3( 6.5)    449939.8
  14 1s2 5g1            (2)4( 8.5)    449948.4
  -1
```

ADAS201

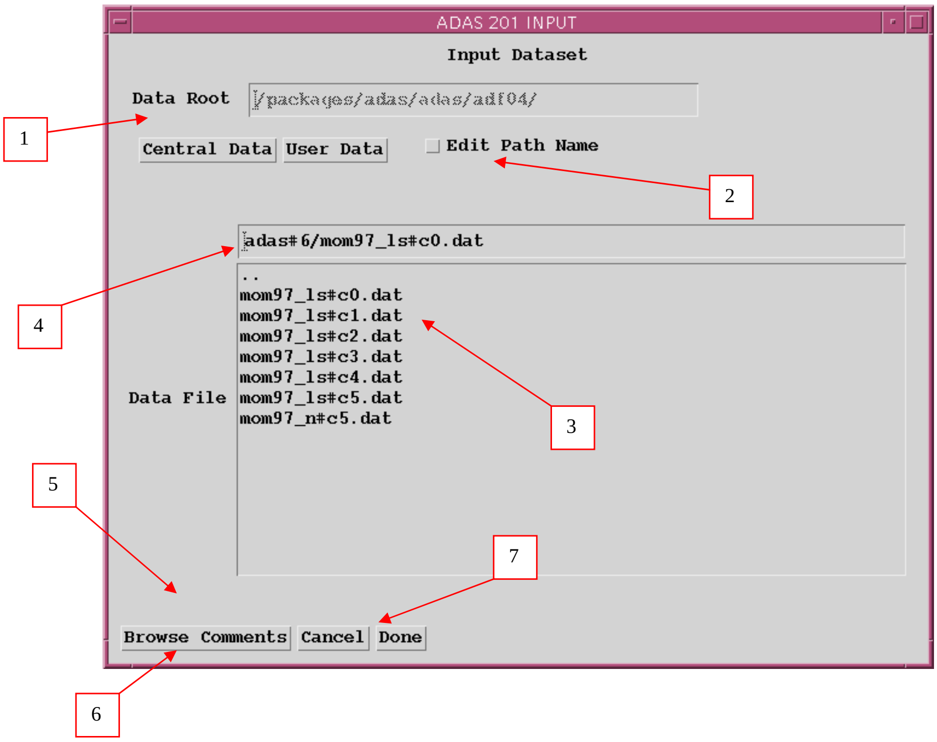
The program interrogates specific ion files of type ADF04. It extracts electron impact rate coefficient data for selected transitions. The data may be interpolated using cubic splines to provide excitation rate coefficients at arbitrarily chosen electron temperatures. A minimax polynomial approximation is also made to the source data. The source and interpolated excitation rate coefficient data are displayed and a tabulation prepared. The tabular and graphical output may be printed and includes the minimax polynomial approximation.

The **file selection window** has the appearance shown below

1. Data root shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type – ADF04 in this case. Note that each type of data is stored according to its ADAS data format (*adf* number). Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas,* to use this facility.
2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
3. Available sub-directories are shown in the large file display window. There are a large number of these, named (a) by iso-electronic sequence (eg. *belike*) (b) by isoelectronic sequence associated with a particular source (eg. *copsm#be*) (c) by iso-nuclear sequence associated with a

particular source (eg. *copmm#16* , where the 16 is the nuclear charge). Scroll bars appear if the number of entries exceed the file display window size.

4. Click on a name to select it. The selected name appears in the smaller selection window above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
5. Once a data file is selected, the set of buttons at the bottom of the main window become active.
6. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.
7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window



Data Root: /packages/adas/adas/adf04/

adas#6/mom97_ls#c0.dat

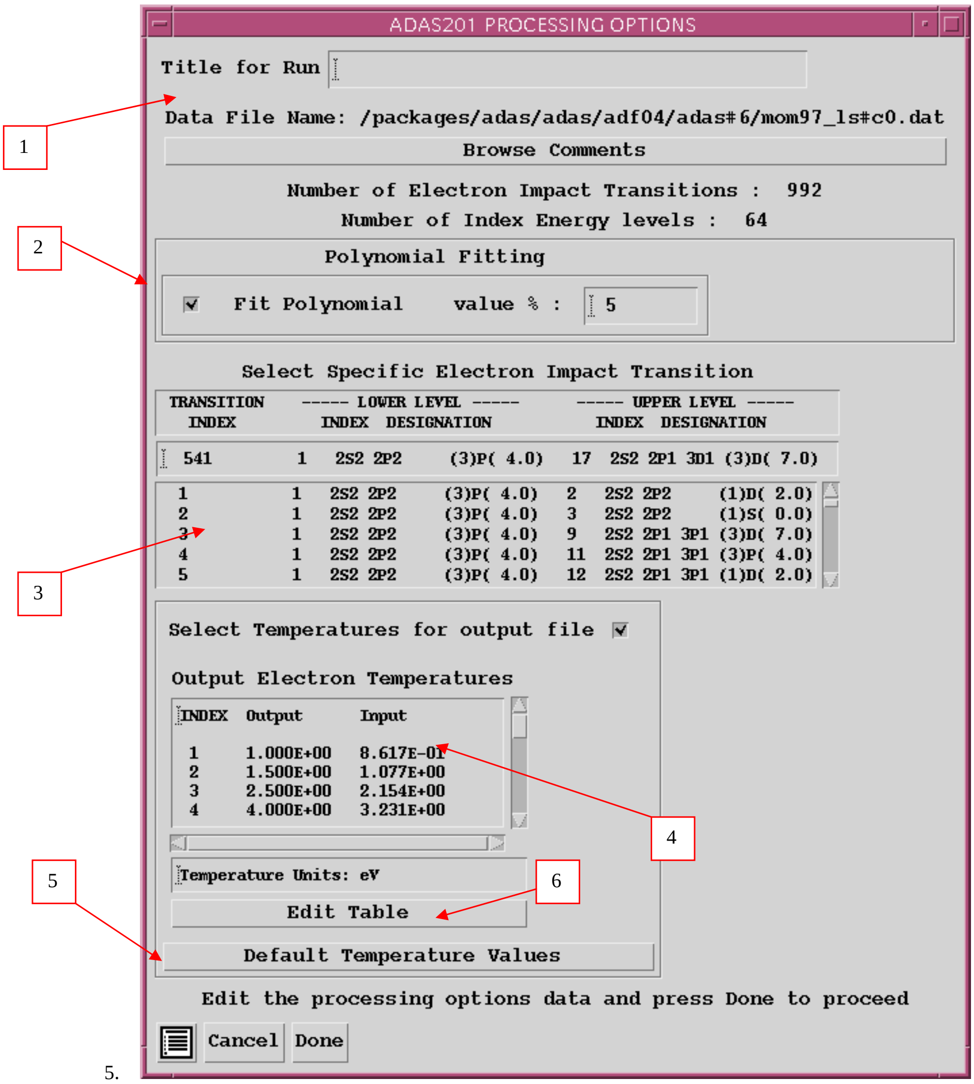
```
..
mom97_ls#c0.dat
mom97_ls#c1.dat
mom97_ls#c2.dat
mom97_ls#c3.dat
mom97_ls#c4.dat
mom97_ls#c5.dat
mom97_n#c5.dat
```

The **processing options window** has the appearance shown below:

1. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being analysed is also shown. The button *Browse comments* again allows display of the information field section at the foot of the selected dataset, if it exists.
2. The output data extracted from the datafile, an ‘excitation rate coefficient’, may be fitted with a polynomial. This is as a function of temperature. Clicking the *Fit Polynomial* button b) activates this. The accuracy of the

fitting required may be specified in the editable box. The value in the box is editable only if the *Fit Polynomial* button is active

3. Transitions for which electron impact excitation data are available in the data set are displayed in the line list display window. This is a scrollable window using the scroll bar to the right of the window. Click anywhere on the row for a line to select it. The selected transition appears in the selection window just above the line list display window.
4. Your settings of electron temperatures (output) are shown in the temperature display window. The temperature values at which the excitation rate coefficients (in fact 'upsilons') are stored in the datafile (input) are also shown for information. The program recovers the output temperatures you used when last executing the program



Title for Run

Data File Name: /packages/adas/adas/adf04/adas#6/mom97_ls#c0.dat

Number of Electron Impact Transitions : 992

Number of Index Energy levels : 64

Polynomial Fitting

☑ Fit Polynomial value % : 5

Select Specific Electron Impact Transition

```
TRANSITION    ----- LOWER LEVEL -----         ----- UPPER LEVEL -----
  INDEX         INDEX  DESIGNATION              INDEX  DESIGNATION

 541            1    2S2 2P2      (3)P( 4.0)   17   2S2 2P1 3D1 (3)D( 7.0)

 1              1    2S2 2P2      (3)P( 4.0)   2    2S2 2P2      (1)D( 2.0)
 2              1    2S2 2P2      (3)P( 4.0)   3    2S2 2P2      (1)S( 0.0)
 3              1    2S2 2P2      (3)P( 4.0)   9    2S2 2P1 3P1  (3)D( 7.0)
 4              1    2S2 2P2      (3)P( 4.0)   11   2S2 2P1 3P1  (3)P( 4.0)
 5              1    2S2 2P2      (3)P( 4.0)   12   2S2 2P1 3P1  (1)D( 2.0)
```

Select Temperatures for output file ☑

Output Electron Temperatures

```
INDEX  Output       Input

 1     1.000E+00    8.617E-01
 2     1.500E+00    1.077E+00
 3     2.500E+00    2.154E+00
 4     4.000E+00    3.231E+00
```

Temperature Units: eV

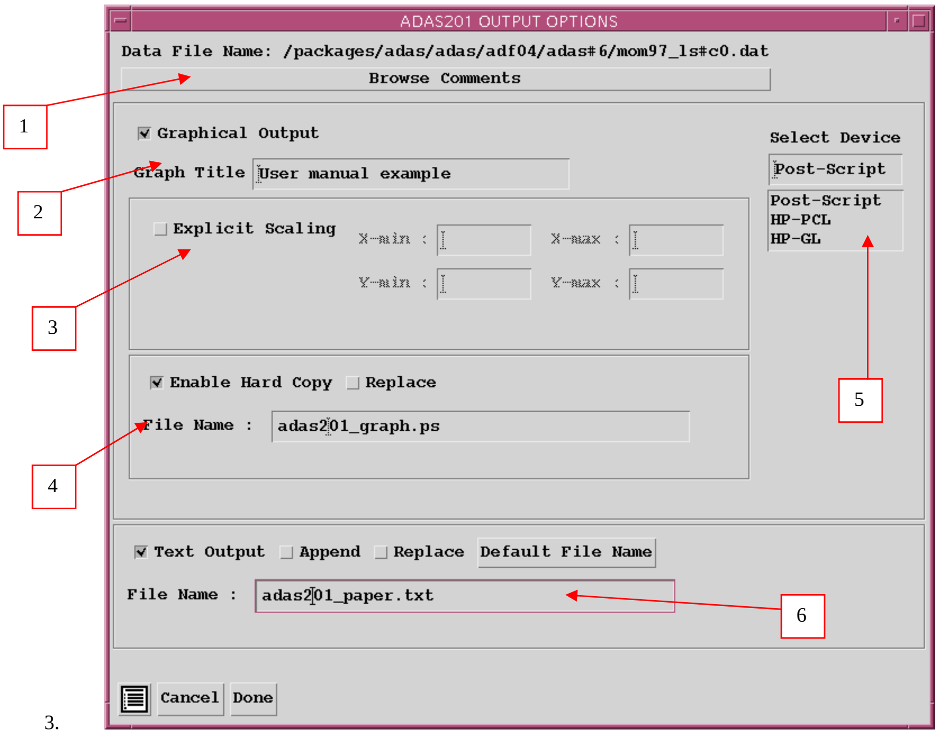
Edit the processing options data and press Done to proceed

5.

5. Pressing th *fault Temperature values* button inserts a default set of temperature al to the input temperatures
6. The Temperature Values are editable. Click on the *Edit Table* button if you wish to change the values. A ‘drop-down’ window, the ADAS Table Editor window: It follows the same pattern of operation as described in bulletin.
7. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

The **output options window** is as shown below

1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
2. Graphical display is activated by the *Graphical Output* button. This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.



Data File Name: /packages/adas/adas/adf04/adas#6/mom97_ls#c0.dat

☑ Graphical Output

Graph Title: User manual example

☐ Explicit Scaling

Select Device: Post-Script

☑ Enable Hard Copy ☐ Replace

File Name : adas201_graph.ps

☑ Text Output ☐ Append ☐ Replace Default File Name

File Name : adas201_paper.txt

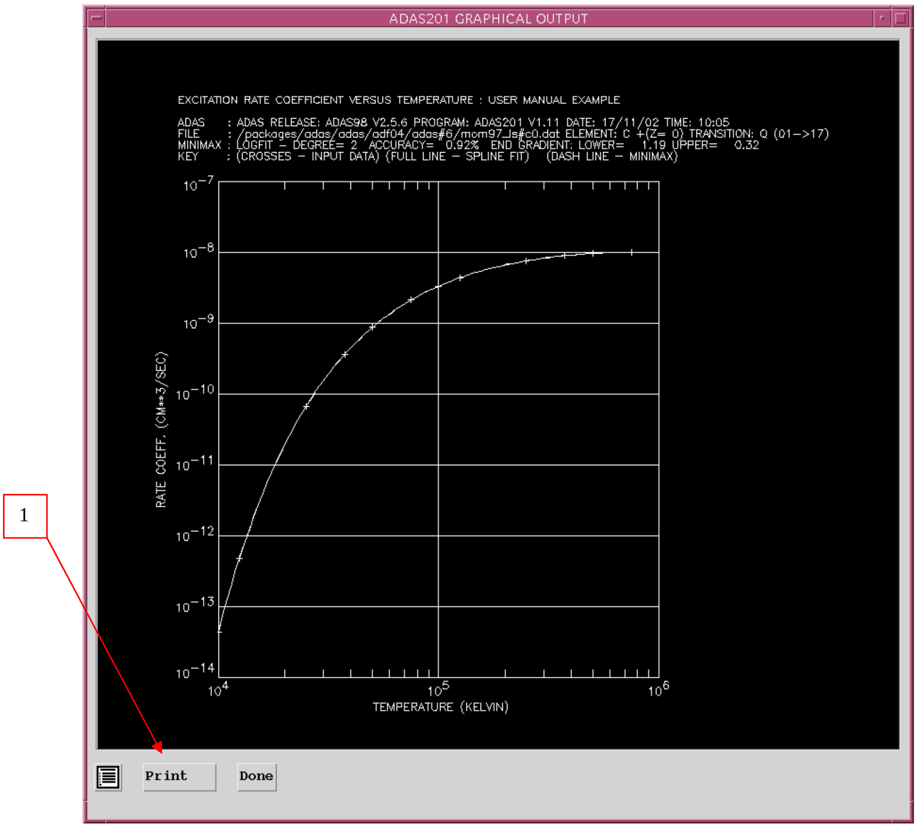
3.

4. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. If the output graphic file already exits and the *Replace* button has not been activated, a ‘pop-up’ window issues a warning.

5. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.
6. The *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name ‘paper.txt’ may be set by pressing the button *Default file name*. A ‘pop-up’ window issues a warning if the file already exists and the *Replace* button has not been activated.

The **Graphical output window** is shown below

1. Printing of the currently displayed graph is activated by the *Print* button.



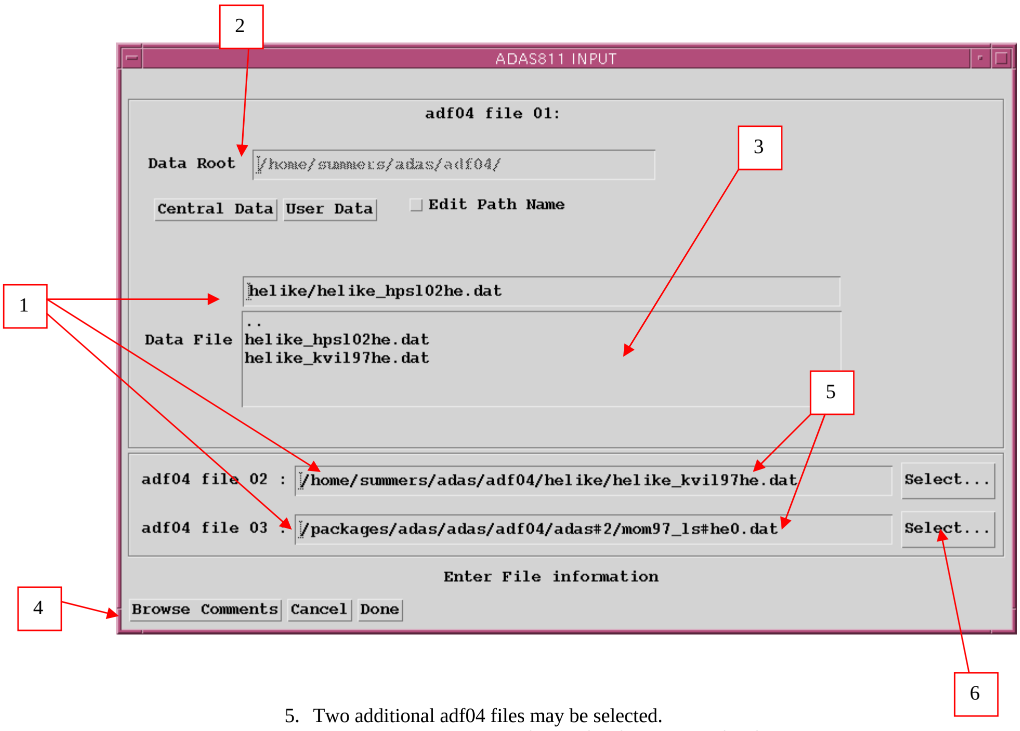
```
EXCITATION RATE COEFFICIENT VERSUS TEMPERATURE : USER MANUAL EXAMPLE

ADAS    : ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS201 V1.11 DATE: 17/11/02 TIME: 10:05
FILE    : /packages/adas/adas/adf04/adas#6/mom97_ls#c0.dat ELEMENT: C +(Z= 0) TRANSITION: Q (01->17)
MINIMAX : LOGFIT - DEGREE= 2  ACCURACY=  0.92%  END GRADIENT: LOWER=   1.19 UPPER=   0.32
KEY     : (CROSSES - INPUT DATA) (FULL LINE - SPLINE FIT)   (DASH LINE - MINIMAX)
```

ADAS811

The code is a new and more sophisticated interrogator and comparator of archived ADAS datasets of format *adf04*. It initiates an interactive dialogue with the user in two parts, namely, input file selection and display/comparison of selected data. There is only graphical output.

The **file selection window** has the appearance shown below

1. Selection of up to three adf04 files is permitted. At least one file, *adf04 file 01*, must be selected.
2. Selection of *adf04 file 01* follows the standard ADAS pattern. Data root shows the full pathway to the appropriate *adf04* data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*, to use this facility. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
3. Available sub-directories are shown in the large file display window. Scroll bars appear if the number of entries exceed the file display window size. Click on a name to select it. The selected name appears in the smaller selection window above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
4. Once *adf04 file 01* is selected, the set of buttons at the bottom of the main window become active. Clicking on the *Browse Comments* button displays the comment line information stored with the *adf04 file 01* datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.



Data Root /home/summers/adas/adf04/

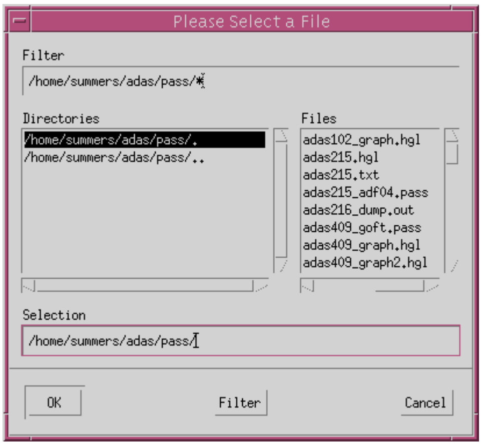
helike/helike_hpsl02he.dat

Data File
..
helike_hpsl02he.dat
helike_kvil97he.dat

adf04 file 02 : /home/summers/adas/adf04/helike/helike_kvil97he.dat

adf04 file 03 : /packages/adas/adas/adf04/adas#2/mom97_ls#he0.dat

5. Two additional adf04 files may be selected.
6. Click the *Select…* button for *adf04 file 02* or *adf04 file 03*. A pop-up Select-a-File widget is presented as shown below. Note that this is a general non-ADAS specific widget, not targetted specifically on *adf04* files. Only comparison of adf04 files is allowed by ADAS811.



Filter
/home/summers/adas/pass/*

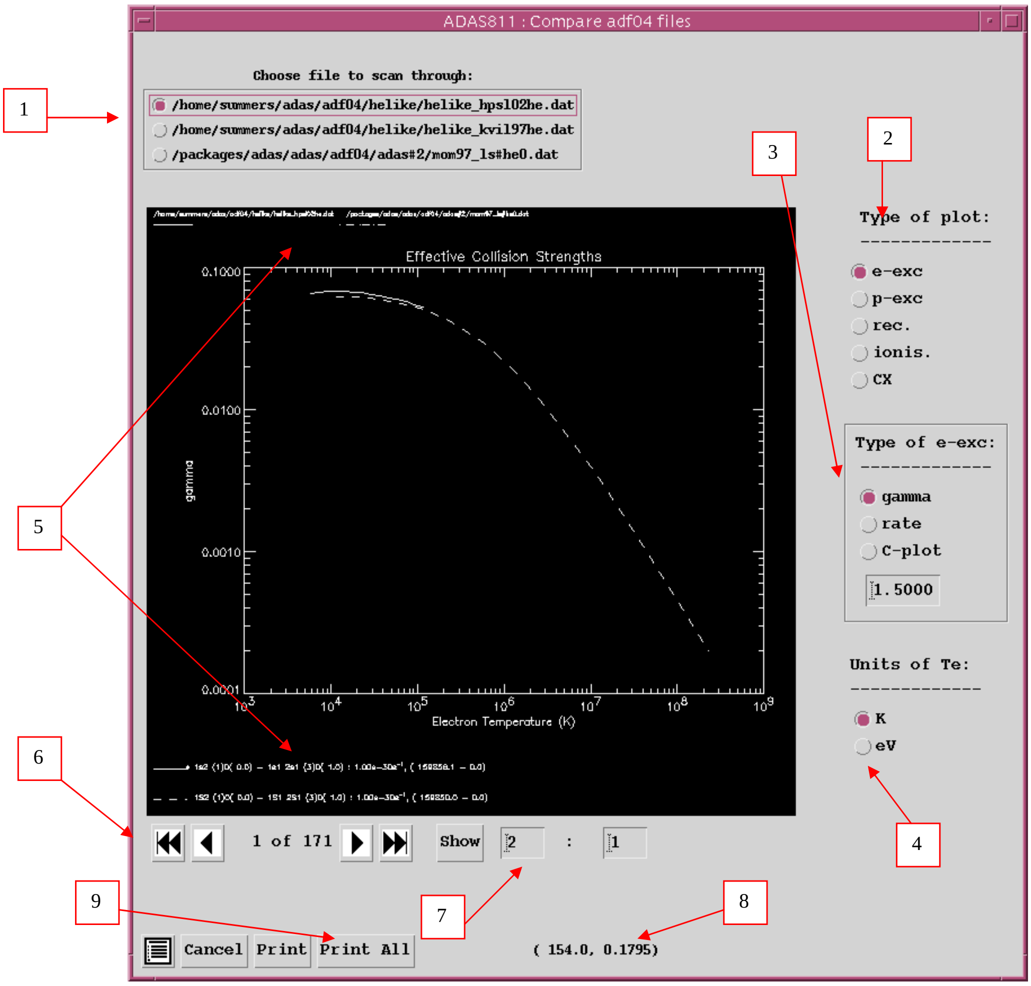
Directories
/home/summers/adas/pass/.
/home/summers/adas/pass/..

Files
adas102_graph.hgl
adas215.hgl
adas215.txt
adas215_adf04.pass
adas216_dump.out
adas409_goft.pass
adas409_graph.hgl
adas409_graph2.hgl

Selection
/home/summers/adas/pass/

The **processing options window** has the appearance shown below

1. more than one file, click the appropriate button for the primary file you wish to scan through. If there is more than one adf04 file, the program will seek to match transitions between them. The matching does depend on standard configuration labelling and formatting in the adf04 files. The graphical display plots the coefficients from each transition from the primary file but plots the same coefficient from the other files only if it is unambigously matched.
2. Five types of rate coefficient can be displayed, namely electron impact excitation, positive ion excitation, recombination, ionisation and charge exchange. Make the appropriate selection.
3. A number of different forms for display of the selected coefficient may be permitted. The choices are displayed are selected by button click.
4. Coefficients are plotted as a function of temperature. The units, K or eV, may be chosen.
5. The legend of the graph plot line appearances is at the top of the graph and the identification of the particular transition given at the bottom.
6. The selected adf04 files are shown at the top of the screen. If there is
7. Tape recorder type controls are provided to move between transitions.
8. The indices of the transition may be typed in explicitly, then click *Show*.
9. Note that the cursor position in graph axis coordinates is given.
10. The button controls allow printing of the current graph , *Print*, or of all the graphs, *Print All*, of the selected type. Be cautious in using *Print All*. The *Escape to Menu* icon is also available for a quick exit to the main ADAS menu. The *Cancel* button returns the user to the input file selection screen.



Choose file to scan through:

● /home/summers/adas/adf04/helike/helike_hps102he.dat
○ /home/summers/adas/adf04/helike/helike_kvi197he.dat
○ /packages/adas/adas/adf04/adas#2/mom97_ls#he0.dat

Type of plot:
● e-exc
○ p-exc
○ rec.
○ ionis.
○ CX

Type of e-exc:
● gamma
○ rate
○ C-plot
1.5000

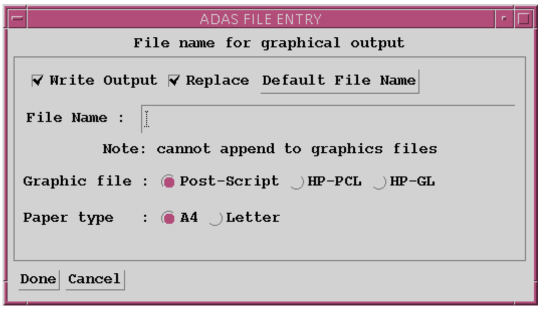
Units of Te:
● K
○ eV

1 of 171

2 : 1

(154.0, 0.1795)

The **graphical file output pop-up** is shown below.



File name for graphical output

☑ Write Output ☑ Replace

File Name :

Note: cannot append to graphics files

Graphic file : ● Post-Script ○ HP-PCL ○ HP-GL

Paper type : ● A4 ○ Letter

Collisional-radiative modelling of populations

Consider ions X^{+z} of the element X. The adjacent ionisation stages are X^{+z+1} and X^{+z-1}. Let the levels of the ion X^{+z} be separated into the *metastable levels* X_ρ^{+z}, indexed by Greek indices, and *excited levels* X_i^{+z}, indexed by Roman indices. The collective name metastable states as used here includes the ground state. The driving mechanisms considered for populating the excited levels X_i^{+z} are excitation from the metastable levels X_ρ^{+z} and recombination from the ground level of the adjacent ion X_1^{+z+1}. The dominant population densities of the ions in the plasma are those of the levels X_ρ^{+z} and X_1^{+z+1}, denoted by N_ρ and N_1^+ respectively. They, or at least their ratios are assumed known from a dynamical ionisation balance. The other dominant population densities in the plasma are the electron density N_e, the proton density N_p and the neutral hydrogen density N_H. The excited populations, denoted by N_i, are assumed to be in a *quasi-static equilibrium* with respect to the dominant populations. The program evaluates the dependence of the excited populations on the dominant populations with this assumption.

Let *M* denote the number of metastable levels and *O* denote the number of excited levels, hereafter called *ordinary* levels. The statistical balance equations take the form

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

where the dominant populations (excluding the electron density) have been taken to the right hand side. The C_{ij} and $C_{i\sigma}$ are elements of the collisional-radiative matrix, r_i is the free electron recombination coefficient directly to the level *i* and $q_i^{(CX)}$ is the charge exchange recombination coefficient from neutral hydrogen to the level *i*. The element C_{ij} of the collisional-radiative matrix is composed as

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

where $A_{j\to i}$, $q_{j\to i}^{(e)}$ and $q_{j\to i}^{(p)}$ are the rate coefficients for spontaneous transition, electron induced collisional transition and proton induced collisional transition respectively.

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

is the total loss rate from level *i*, with $q_i^{(I)}$ the electron impact ionisation rate coefficient.

The solution for the ordinary populations is

$$\begin{aligned} N_j &= -\sum_{i=1}^{O} C_{ji}^{-1} \sum_{\sigma=1}^{M} C_{i\sigma} N_\sigma + \sum_{i=1}^{O} C_{ji}^{-1} r_i N_e N_1^+ \\ &\quad + \sum_{i=1}^{O} C_{ji}^{-1} q_i^{(CX)} N_H N_1^+ \\ &\equiv \sum_{\sigma=1}^{M} \mathcal{F}_{j\sigma}^{(exc)} N_e N_\sigma + \mathcal{F}_{j1}^{(rec)} N_e N_1^+ + \mathcal{F}_{j1}^{(CX)} N_H N_1^+ \end{aligned}$$

where the $\mathcal{F}_{j\sigma}^{(exc)}$, $\mathcal{F}_{j1}^{(rec)}$ and $\mathcal{F}_{j1}^{(CX)}$ are the effective contributions to the excited populations from excitation from the metastables, from free electron capture and from charge exchange recombination from neutral hydrogen respectively. All these coefficients depend on density as well as temperature. The actual population density of an ordinary level may be obtained from them when the dominant population densities are known.

The emissivity coefficients of specific lines are obtained by multiplying the $\mathcal{F}$ s above by the appropriate A-values. They come in the three flavours, (exc), (rec) and (CX) and should be kept distinct in this way for general application. Generalising slightly, there are two kinds of derived coefficients associated with individual spectrum line emission in common use in fusion plasma diagnosis. These are *photon emissivity coefficients* (PEC) and S/XB ratios (SXB). The reciprocals of the latter are also known as *photon efficiencies*. The emissivity in the spectrum line $j \rightarrow k$, allowing for metastables also in the recombining ion is

$$\varepsilon_{j\rightarrow k} = A_{j\rightarrow k}\Big(\sum_{\sigma=1}^{M}\mathsf{F}_{j\sigma}^{(exc)}N_e N_\sigma + \sum_{\upsilon'=1}^{M_{z+1}}\mathsf{F}_{j\upsilon'}^{(rec)}N_e N_{\upsilon'}^{+} +$$

$$\sum_{\upsilon'=1}^{M_{z+1}}\mathsf{F}_{j\upsilon'}^{(CX)}N_H N_{\upsilon'}^{+} + \sum_{\mu'=1}^{M_{z-1}}\mathsf{F}_{j\mu'}^{(ion)}N_e N_{\mu'}^{-}\Big)$$

This allows specification of the *excitation* photon emissivity coefficient

$$\mathsf{PEC}_{\sigma,j\rightarrow k}^{(exc)} = A_{j\rightarrow k}\mathsf{F}_{j\sigma}^{(exc)}$$

the *recombination* photon emissivity coefficient

$$\mathsf{PEC}_{\upsilon',j\rightarrow k}^{(rec)} = A_{j\rightarrow k}\mathsf{F}_{j\upsilon'}^{(rec)}$$

the *charge exchange* photon emissivity coefficient

$$\mathsf{PEC}_{\upsilon',j\rightarrow k}^{(CX)} = A_{j\rightarrow k}\mathsf{F}_{j\upsilon'}^{(CX)}$$

The S/XB are only meaningful for the excitation part of the emissivity and are

$$\mathsf{SXB}_{\sigma,j\rightarrow k} = \sum_{\upsilon=1}^{M_{z+1}}\mathsf{S}_{CD,\sigma\rightarrow\upsilon}/(A_{j\rightarrow k}\mathsf{F}_{j\sigma}^{(exc)})$$

Each of these coefficients is associated with a particular metastable σ, υ' or μ' of the X^{+z}, X^{+z+1} or X^{+z-1} ions respectively. Data format *adf13* encountered in the lecture 2 is the S/XB respository and is interrogated by ADAS501. *adf15* is the repository for the PEC data and is interrogated by ADAS503 in identical manner to ADAS501.

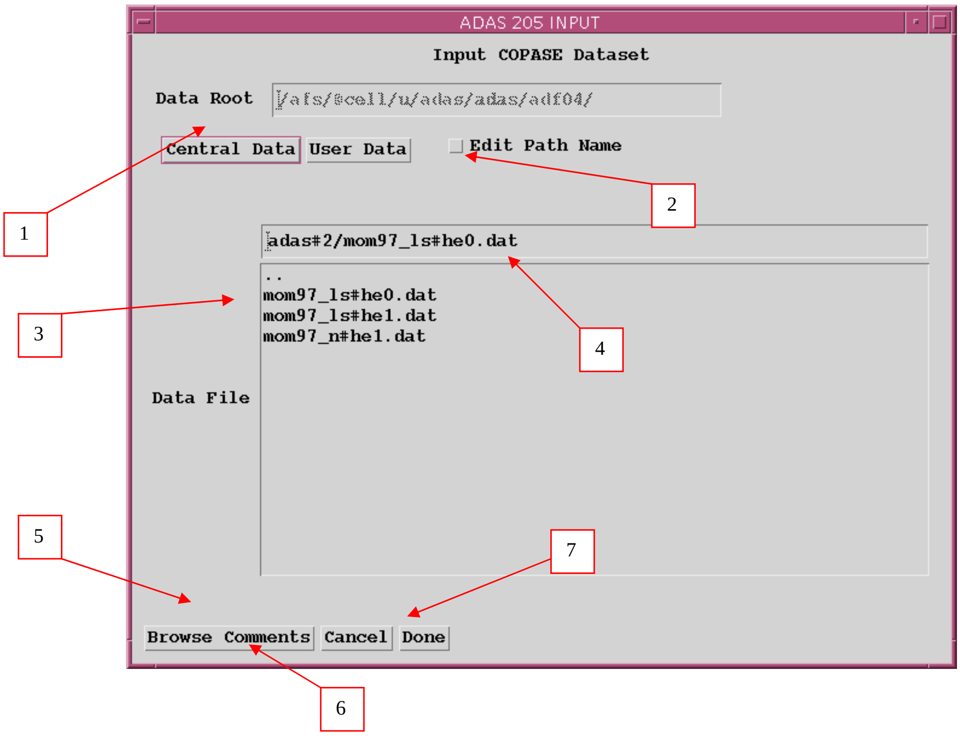
ADAS205

This is the basic code in ADAS for calculating excited state and metastable state populations of a selected ion in a plasma of specified temperatures and densities by drawing on fundamental energy level and rate coefficient data from a specific ion file of type ADF04. It is used principally for displaying the (exc) part of the populations and as a first step in examining diagnostic line ratios.

The **file selection window** has the appearance shown below

1. Data root a) shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. The appropriate ADAS data format for input to this program is ADF04 (‘specific ion files’). Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas,* to use this facility.
2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
3. Available sub-directories are shown in the large file display window b). Scroll bars appear if the number of entries exceed the file display window size.
4. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat.*
5. Once a data file is selected, the set of buttons at the bottom of the main window become active.

6. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.
7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window



Data Root: /afs/@cell/u/adas/adas/adf04/

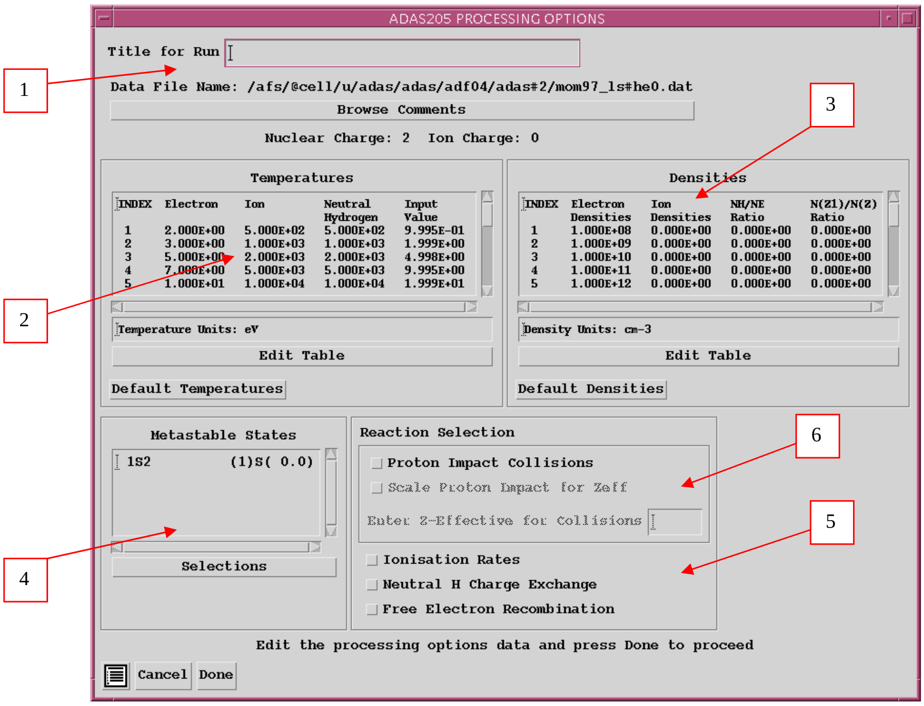
```
adas#2/mom97_ls#he0.dat
```

```
..
mom97_ls#he0.dat
mom97_ls#he1.dat
mom97_n#he1.dat
```

The **processing options window** has the appearance shown below

1. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being analysed is also shown. The button *Browse comments* again allows display of the information field section at the foot of the selected dataset, if it exists.
2. There are three 'pop-up' windows for setting temperatures, densities and for designating metastable levels. For the temperature window, click on the *Edit Table* button to open up the table editor. The editing operations are as described in the Chap1-00. Note that there is a set of input electron temperatures from the selected file. These indicate the safe range of temperatures if extrapolation is to be avoided. Note that altering units (which must be done with the table edit window activated) converts the input values and interprets the output values in the selected units. It **does not convert** output values already typed in. *Default Temperatures* are inserted in the selected units on clicking the appropriate button. Note that the ion and neutral hydrogen temperatures are **only used if** such collisional data is present in the input ADF04 file.

3. The densities table is handled in like manner. Note that in this case there are no input density values. Thus unit changing only affects the interpretation of the output values created by the user. The N_H/N_e and $N(z_1)/N(z)$ **are only used if** neutral hydrogen charge exchange data and free electron recombination data are present in input ADF04 file. These ratio vectors are specified at each electron density so the ratio vectors and electron density vector are of the same length. That is, a model is specified. By contrast the output electron temperatures are independent so that final calculated populations are obtained at points of a two-dimensional electron temperature/electron density grid.
4. The Metastable State *Selections* button pops up a window indexing all the energy levels. Activate the buttons opposite levels which you wish treated as metastables.
5. Various processes, supplementary to the primary electron excitation collisions and bound-bound radiative transitions, are activated as desired by clicking on the appropriate buttons. Note again these only have an effect if such data is present in the ADF04 file except for *Ionisation rates*. This activates ionisation out of excited states and is obtained by an internal calculation of these rates in the ECIP approximation. **Warning**-ionisation should **not** be switched on if you have included auto-ionising levels in your ADF04 dataset but have omitted the details of alternative thresholds etc present in advanced ADF04 files.
6. Proton collisions may be present in the ADF04 file. If so, these rate coefficients may be scaled to represent a mixture of other charged projectiles with a mean Z-effective



Title for Run

Data File Name: /afs/@cell/u/adas/adas/adf04/adas#2/mom97_ls#he0.dat

Nuclear Charge: 2 Ion Charge: 0

INDEX	Electron	Ion	Neutral Hydrogen	Input Value
1	2.000E+00	5.000E+02	5.000E+02	9.995E-01
2	3.000E+00	1.000E+03	1.000E+03	1.999E+00
3	5.000E+00	2.000E+03	2.000E+03	4.998E+00
4	7.000E+00	5.000E+03	5.000E+03	9.995E+00
5	1.000E+01	1.000E+04	1.000E+04	1.999E+01

Temperature Units: eV

INDEX	Electron Densities	Ion Densities	NH/NE Ratio	N(Z1)/N(Z) Ratio
1	1.000E+08	0.000E+00	0.000E+00	0.000E+00
2	1.000E+09	0.000E+00	0.000E+00	0.000E+00
3	1.000E+10	0.000E+00	0.000E+00	0.000E+00
4	1.000E+11	0.000E+00	0.000E+00	0.000E+00
5	1.000E+12	0.000E+00	0.000E+00	0.000E+00

Density Units: cm-3

1S2 (1)S(0.0)

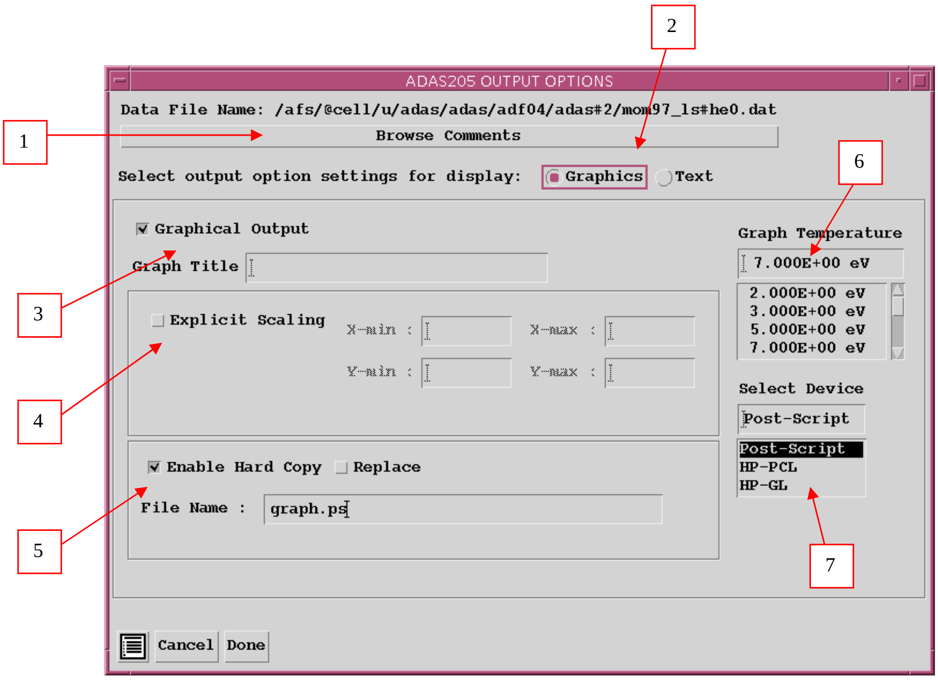
☐ Proton Impact Collisions
☐ Scale Proton Impact for Zeff
Enter Z-Effective for Collisions
☐ Ionisation Rates
☐ Neutral H Charge Exchange
☐ Free Electron Recombination

Edit the processing options data and press Done to proceed

.

The **output graphic options window** has the appearance shown below

1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
2. Click on the *Graphics* or *Text* buttons to toggle between sub-windows for setting up the graphics output or the text file output.
3. Graphical display is activated by the *Graphical Output* button. This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph. By default, graph scaling is adjusted to match the required outputs.
4. Press the *Explicit Scaling* button to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.
5. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. If the output graphic file already exits and the *Replace* button has not been activated, a ‘pop-up’ window issues a warning.
6. Graphical output is at one selected temperature. Make this choice from the list.
7. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.



Data File Name: /afs/@cell/u/adas/adas/adf04/adas#2/mom97_ls#he0.dat

Select output option settings for display: ● Graphics ○ Text

☑ Graphical Output

Graph Title

☐ Explicit Scaling X-min : X-max : Y-min : Y-max :

☑ Enable Hard Copy ☐ Replace

File Name : graph.ps

Graph Temperature 7.000E+00 eV

2.000E+00 eV
3.000E+00 eV
5.000E+00 eV
7.000E+00 eV

Select Device Post-Script

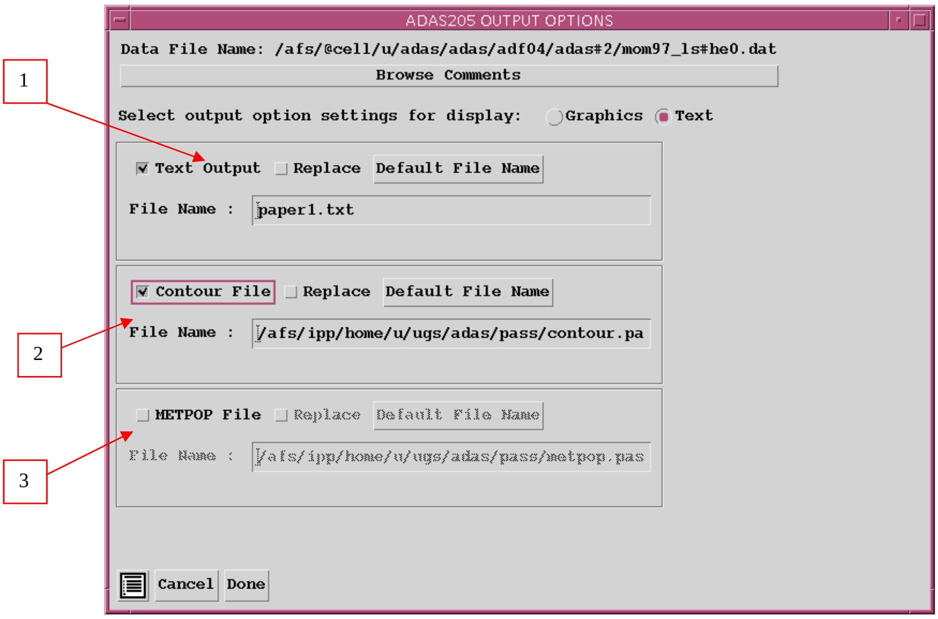
Post-Script
HP-PCL
HP-GL

The **output text options sub-window** has the appearance shown below

1. The *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name ‘paper.txt’ may be set by pressing the button *Default file name*. A ‘pop-up’ window issues a warning if the file already exists and the *Replace* button has not been activated.

2. The *Contour File* button should be activated to write the passing file for use by the diagnostic line ratio program ADAS207. There is no arrangement for permanent storage of such files which reside only in a user's file space and are generally prepared for temporary immediate use. Usually in ADAS such temporary 'passed files' reside in the *pass/* directory. By default ADAS205 sends the contour file to */...../<uid>/adas/pass/contour.pass*
3. The *METPOP File* button should be activated to write a passing file of metastable population fractions. It is of data format ADF11 and can be used in ionisation/recombination applications of ADAS4 series programs. It goes by default into

   /...../<uid>/adas/pass/metpop.pass



ADAS205 OUTPUT OPTIONS

Data File Name: /afs/@cell/u/adas/adas/adf04/adas#2/mom97_ls#he0.dat

Browse Comments

Select output option settings for display: ○ Graphics ● Text

☑ Text Output ☐ Replace Default File Name

File Name : paper1.txt

☑ Contour File ☐ Replace Default File Name

File Name : /afs/ipp/home/u/ugs/adas/pass/contour.pa

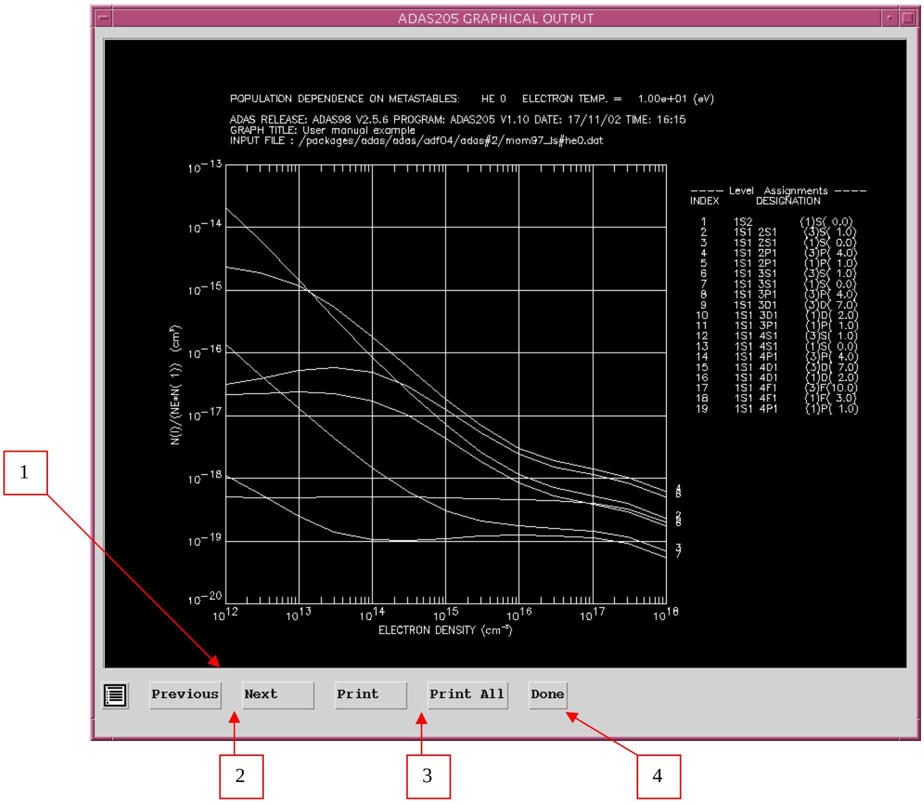
☐ METPOP File ☐ Replace Default File Name

File Name : /afs/ipp/home/u/ugs/adas/pass/metpop.pas

Cancel Done

The **Graphical output window** is shown below

2. The graph has at its foot a *Done* button, and possibly *Next* and *Previous* buttons if there is a sequence of graphs to be displayed. A *Print* and *Print all* button is also present if the *Enable Hard Copy* button on the previous window was activated.
3. Press the *Next* button to show the next graph in a sequence and the *Previous* button to show the previous graph.
4. Press the *Print* button to make a hard copy of the currently displayed picture. Print all makes a hard copy of all the pictures.
5. Pressing the *Done* button restores the previous Output Options window.



```
POPULATION DEPENDENCE ON METASTABLES:    HE 0   ELECTRON TEMP. =   1.00e+01 (eV)

ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS205 V1.10 DATE: 17/11/02 TIME: 16:15
GRAPH TITLE: User manual example
INPUT FILE : /packages/adas/adas/adf04/adas#2/mom97_ls#he0.dat

---- Level  Assignments ----
INDEX        DESIGNATION

  1      1S2           (1)S( 0.0)
  2      1S1  2S1      (3)S( 1.0)
  3      1S1  2S1      (1)S( 0.0)
  4      1S1  2P1      (3)P( 4.0)
  5      1S1  2P1      (1)P( 1.0)
  6      1S1  3S1      (3)S( 1.0)
  7      1S1  3S1      (1)S( 0.0)
  8      1S1  3P1      (3)P( 4.0)
  9      1S1  3D1      (3)D( 7.0)
 10      1S1  3D1      (1)D( 2.0)
 11      1S1  3P1      (1)P( 1.0)
 12      1S1  4S1      (3)S( 1.0)
 13      1S1  4S1      (1)S( 0.0)
 14      1S1  4P1      (3)P( 4.0)
 15      1S1  4D1      (3)D( 7.0)
 16      1S1  4D1      (1)D( 2.0)
 17      1S1  4F1      (3)F(10.0)
 18      1S1  4F1      (1)F( 3.0)
 19      1S1  4P1      (1)P( 1.0)
```

Diagnostic line ratios

Consider emissivities of spectrum lines arising from a single ionisation stage. Ratios of such lines are frequently used as temperature, density or transient state diagnostics in plasmas. The primary advantage of seeking such ratios of lines from a single ionisation stage is that they are independent of the stage to stage ionisation balance (often uncertain). In general it is matter of some investigation to identify the most diagnostically useful ratios. The present program is designed to aid such investigation. A necessary preliminary to evaluating line emissivities is a calculation of populations of excited states of the ion as a function of plasma parameters. In practice, problems of line blending and the spectral resolution of spectrometers mean that it is useful to work with line groups rather than just individual lines. A line group, called a composite assembly in ADAS, is a set of lines conveniently or necessarily measured together. For ‘line ratio’ diagnostics, we deal with two line groups which are built up by the user in the data entry section of the code.
Reall that the solution for the ordinary populations is

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

where the $\mathsf{F}_{j\sigma}^{(exc)}$, $\mathsf{F}_{j1}^{(rec)}$ and $\mathsf{F}_{j1}^{(CX)}$ are the effective contributions to the excited populations from excitation from the metastables, from free electron capture and from charge exchange recombination from neutral hydrogen respectively. Consider now a set of individual lines, or line group, G with upper levels I_G and lower levels J_G. Let $A_{i\to j}$ be the spontaneous emission coefficient for the line $i \to j$. Then the composite emissivity for the line group is

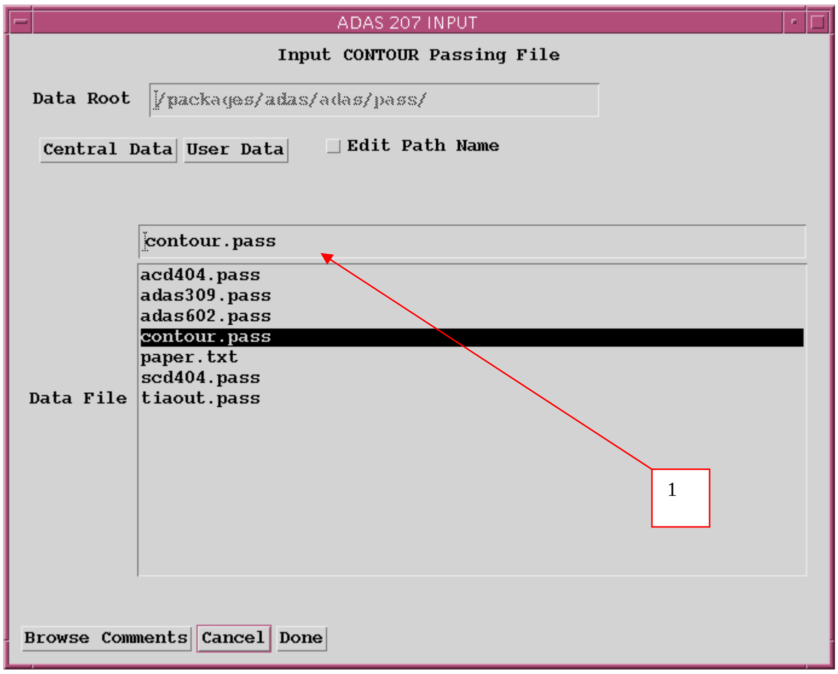
$$\begin{aligned}
\varepsilon_G &= \sum_{j\in J_G, i\in I_G} \varepsilon_{j\to i} = \sum_{j\in J_G, i\in I_G} A_{j\to i} N_j \\
&= \sum_{j\in J_G, i\in I_G} A_{j\to i} \Big(\sum_{\sigma=1}^{M} \mathrm{F}_{j\sigma}^{(exc)} N_e N_\sigma + \mathrm{F}_{j1}^{(rec)} N_e N_1^{+} + \mathrm{F}_{j1}^{(CX)} N_H N_1^{+}\Big) \\
&= N_e N_1 \sum_{j\in J_G, i\in I_G} A_{j\to i} \Big(\sum_{\sigma=1}^{M} \mathrm{F}_{j\sigma}^{(exc)} \frac{N_\sigma}{N_1} + \mathrm{F}_{j1}^{(rec)} \frac{N_1^{+}}{N_1} + \mathrm{F}_{j1}^{(CX)} \frac{N_H}{N_e} \frac{N_1^{+}}{N_1}\Big)
\end{aligned}$$

expressed in terms of the ratios N_σ / N_1, N_1^{+} / N_1 and N_H / N_1. The photon emissivity coefficient for the line group is $\varepsilon_G / N_e N_1$. The coefficient depends on electron density and temperature in general. Ratios of line group emissivities cancel the leading $N_e N_1$ dependence. Modelling diagnostic line ratios involves preparation and operation primarily with a ratio $\varepsilon_{G_1} / \varepsilon_{G_2}$.

ADAS207

The program evaluates and displays line emissivities and their ratios for an ion. It uses a passing file of excited population data from the code ADAS205.

The **file selection window** has the appearance shown below



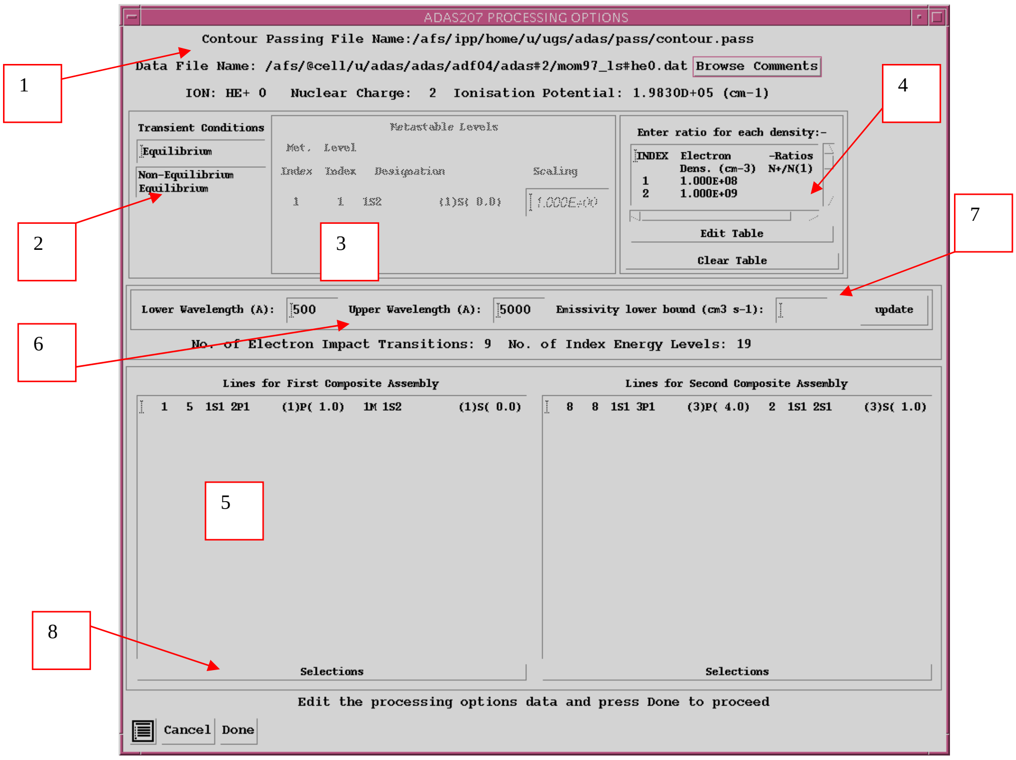
1. The program requires selection of the ‘contour’ data file prepared as output from ADAS205 (see description of ADAS205). There is no arrangement

for central ADAS storage of such files which reside only in a user's file space and are generally prepared for immediate use

.

The **processing options window** has the appearance shown below.

1. It displays information from the *contour file* together with information from the ADF04 file used in the prior ADAS205 program run.



Contour Passing File Name:/afs/ipp/home/u/ugs/adas/pass/contour.pass

Data File Name: /afs/@cell/u/adas/adas/adf04/adas#2/mom97_ls#he0.dat

ION: HE+ 0 Nuclear Charge: 2 Ionisation Potential: 1.9830D+05 (cm-1)

Transient Conditions: Equilibrium

Non-Equilibrium
Equilibrium

Metastable Levels

Met. Index	Level Index	Designation		Scaling
1	1	1S2	(1)S(0.0)	1.000E+00

Enter ratio for each density:-

INDEX	Electron Dens. (cm-3)	-Ratios N+/N(1)
1	1.000E+08	
2	1.000E+09	

Lower Wavelength (A): 500 Upper Wavelength (A): 5000 Emissivity lower bound (cm3 s-1):

No. of Electron Impact Transitions: 9 No. of Index Energy Levels: 19

Lines for First Composite Assembly

```
1    5  1S1 2P1      (1)P( 1.0)   1M 1S2          (1)S( 0.0)
```

Lines for Second Composite Assembly

```
8    8  1S1 3P1      (3)P( 4.0)   2  1S1 2S1      (3)S( 1.0)
```

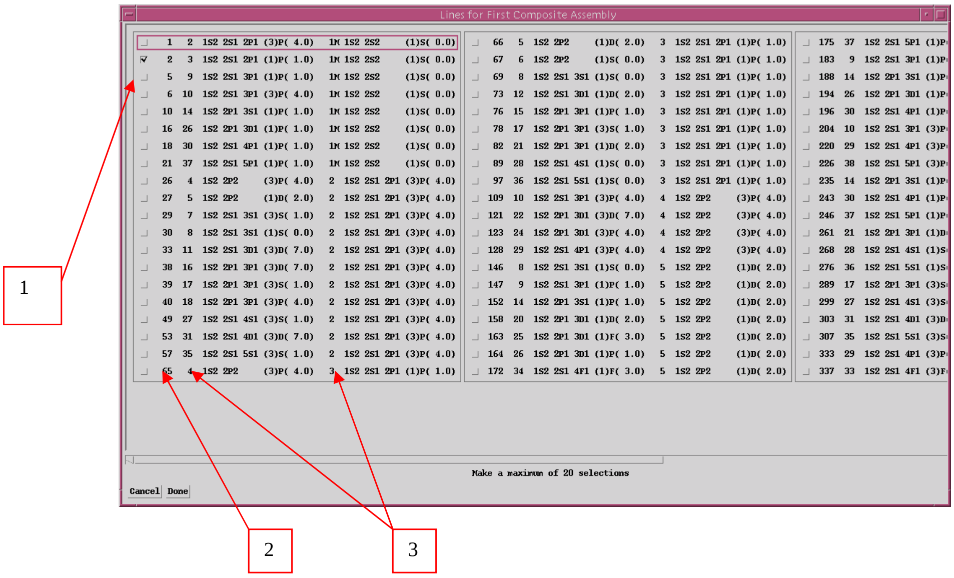
Edit the processing options data and press Done to proceed

2. Select *Non-equilibrium* or *Equilibrium* conditions by clicking the appropriate case in the list. The selection made is shown in the selection window above. Note that a non-equilibrium choice is only meaningful if there is more than one metastable.
3. The metastables selected in the ADAS205 run are shown in the adjacent window. This window becomes active when non-equilibrium conditions are selected. The values to be entered for each metastable is a multiplier on the equilibrium metastable population. Thus 1.00 for each metastable gives the equilibrium case.
4. If recombination contributions to the line emissivities may be present. Thus the ratio of the number densities of the ground state of the un-ionised ion to the ground state of the ionised ion has to be given.
5. A 'line ratio' in the present context is a ratio of a set of lines for the numerator and a set of lines for the denominator, called first and second composite assemblies respectively. The fist composite assembly is shown in the list window. The columns of each row show the transition index and then for the upper and lower levels of the transition, the level index, configuration designation and the outer quantum numbers. These data are taken from the associated ADF04 file.

6. In practice there may be very many available transitions to make up the composite assemblies. This may be restricted to lines only within a selected wavelength range.
7. A minimum value may also be set for the emissivities of lines to be made available.
8. Each line group is assembled by clicking on the appropriate *Selection* button. A new window is presented with all available transitions listed.

The **composite assembly selection window** has the appearance shown below.

1. Clicking on the button alongside a transition allows it to be selected or de-selected.
2. The first number is the transition index in the ADF04 file.
3. The pair of numbers are the upper and lower level indices form the ADF04 file



```
☐   1   2 1S2 2S1 2P1 (3)P( 4.0)   1M 1S2 2S2       (1)S( 0.0)
☑   2   3 1S2 2S1 2P1 (1)P( 1.0)   1M 1S2 2S2       (1)S( 0.0)
☐   5   9 1S2 2S1 3P1 (1)P( 1.0)   1M 1S2 2S2       (1)S( 0.0)
☐   6  10 1S2 2S1 3P1 (3)P( 4.0)   1M 1S2 2S2       (1)S( 0.0)
☐  10  14 1S2 2P1 3S1 (1)P( 1.0)   1M 1S2 2S2       (1)S( 0.0)
☐  16  26 1S2 2P1 3D1 (1)P( 1.0)   1M 1S2 2S2       (1)S( 0.0)
☐  18  30 1S2 2S1 4P1 (1)P( 1.0)   1M 1S2 2S2       (1)S( 0.0)
☐  21  37 1S2 2S1 5P1 (1)P( 1.0)   1M 1S2 2S2       (1)S( 0.0)
☐  26   4 1S2 2P2     (3)P( 4.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  27   5 1S2 2P2     (1)D( 2.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  29   7 1S2 2S1 3S1 (3)S( 1.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  30   8 1S2 2S1 3S1 (1)S( 0.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  33  11 1S2 2S1 3D1 (3)D( 7.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  38  16 1S2 2P1 3P1 (3)D( 7.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  39  17 1S2 2P1 3P1 (3)S( 1.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  40  18 1S2 2P1 3P1 (3)P( 4.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  49  27 1S2 2S1 4S1 (3)S( 1.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  53  31 1S2 2S1 4D1 (3)D( 7.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  57  35 1S2 2S1 5S1 (3)S( 1.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  65   4 1S2 2P2     (3)P( 4.0)   3  1S2 2S1 2P1 (1)P( 1.0)

☐  66   5 1S2 2P2     (1)D( 2.0)   3  1S2 2S1 2P1 (1)P( 1.0)
☐  67   6 1S2 2P2     (1)S( 0.0)   3  1S2 2S1 2P1 (1)P( 1.0)
☐  69   8 1S2 2S1 3S1 (1)S( 0.0)   3  1S2 2S1 2P1 (1)P( 1.0)
☐  73  12 1S2 2S1 3D1 (1)D( 2.0)   3  1S2 2S1 2P1 (1)P( 1.0)
☐  76  15 1S2 2P1 3P1 (1)P( 1.0)   3  1S2 2S1 2P1 (1)P( 1.0)
☐  78  17 1S2 2P1 3P1 (3)S( 1.0)   3  1S2 2S1 2P1 (1)P( 1.0)
☐  82  21 1S2 2P1 3P1 (1)D( 2.0)   3  1S2 2S1 2P1 (1)P( 1.0)
☐  89  28 1S2 2S1 4S1 (1)S( 0.0)   3  1S2 2S1 2P1 (1)P( 1.0)
☐  97  36 1S2 2S1 5S1 (1)S( 0.0)   3  1S2 2S1 2P1 (1)P( 1.0)
☐ 109  10 1S2 2S1 3P1 (3)P( 4.0)   4  1S2 2P2     (3)P( 4.0)
☐ 121  22 1S2 2P1 3D1 (3)D( 7.0)   4  1S2 2P2     (3)P( 4.0)
☐ 123  24 1S2 2P1 3D1 (3)P( 4.0)   4  1S2 2P2     (3)P( 4.0)
☐ 128  29 1S2 2S1 4P1 (3)P( 4.0)   4  1S2 2P2     (3)P( 4.0)
☐ 146   8 1S2 2S1 3S1 (1)S( 0.0)   5  1S2 2P2     (1)D( 2.0)
☐ 147   9 1S2 2S1 3P1 (1)P( 1.0)   5  1S2 2P2     (1)D( 2.0)
☐ 152  14 1S2 2P1 3S1 (1)P( 1.0)   5  1S2 2P2     (1)D( 2.0)
☐ 158  20 1S2 2P1 3D1 (1)D( 2.0)   5  1S2 2P2     (1)D( 2.0)
☐ 163  25 1S2 2P1 3D1 (1)F( 3.0)   5  1S2 2P2     (1)D( 2.0)
☐ 164  26 1S2 2P1 3D1 (1)P( 1.0)   5  1S2 2P2     (1)D( 2.0)
☐ 172  34 1S2 2S1 4F1 (1)F( 3.0)   5  1S2 2P2     (1)D( 2.0)

☐ 175  37  1S2 2S1 5P1 (1)P
☐ 183   9  1S2 2S1 3P1 (1)P
☐ 188  14  1S2 2P1 3S1 (1)P
☐ 194  26  1S2 2P1 3D1 (1)P
☐ 196  30  1S2 2S1 4P1 (1)P
☐ 204  10  1S2 2S1 3P1 (3)P
☐ 220  29  1S2 2S1 4P1 (3)P
☐ 226  38  1S2 2S1 5P1 (3)P
☐ 235  14  1S2 2P1 3S1 (1)P
☐ 243  30  1S2 2S1 4P1 (1)P
☐ 246  37  1S2 2S1 5P1 (1)P
☐ 261  21  1S2 2P1 3P1 (1)D
☐ 268  28  1S2 2S1 4S1 (1)S
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☐ 289  17  1S2 2P1 3P1 (3)S
☐ 299  27  1S2 2S1 4S1 (3)S
☐ 303  31  1S2 2S1 4D1 (3)D
☐ 307  35  1S2 2S1 5S1 (3)S
☐ 333  29  1S2 2S1 4P1 (3)P
☐ 337  33  1S2 2S1 4F1 (3)F

Make a maximum of 20 selections
```
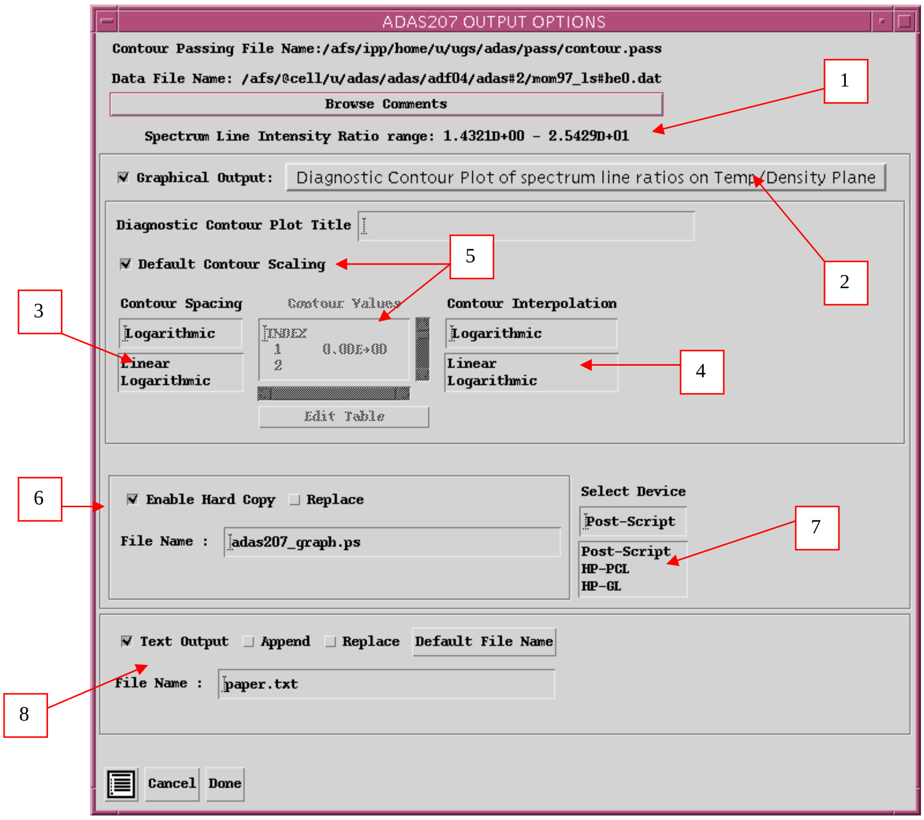

The **output options window** appearance is shown below.

1. The limits of the calculated line group ratio are shown on the output window a). It is important to check this range. Subsequent plots may be selected as logarithmic and it is easy to obtain vanishing line ratios by choice of abnormally low temperatures in the ADAS205 run. In these circumstances meaningless contour plots may be produced.
2. There are three distinct types of plot of the line ratio allowed, namely contours, plots as a function of temperature and plots as a function of density. Click on the appropriate button. The further options selection window changes according to this choice.
3. For the contour plot case, logarithmic or linear choices of contour are permitted. Click on the required type in the lower list window. The chosen type appears in the selection window above.
4. Also the interpolation may be chosen.
5. If *Default contour scaling* is switched off, the table for specifing contour values is activated.

6. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. If the output graphic file already exits and the *Replace* button has not been activated, a ‘pop-up’ window issues a warning.
7. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.
8. The *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name ‘paper.txt’ may be set by pressing the button *Default file name*. A ‘pop-up’ window issues a warning if the file already exists and the *Replace* button has not been activated.


Contour Passing File Name:/afs/ipp/home/u/ugs/adas/pass/contour.pass

Data File Name: /afs/@cell/u/adas/adas/adf04/adas#2/mom97_ls#he0.dat

Spectrum Line Intensity Ratio range: 1.4321D+00 - 2.5429D+01

☑ Graphical Output: Diagnostic Contour Plot of spectrum line ratios on Temp/Density Plane

Diagnostic Contour Plot Title

☑ Default Contour Scaling

Contour Spacing: Logarithmic

Contour Values: INDEX 1 0.00E+00 2

Contour Interpolation: Logarithmic

☑ Enable Hard Copy ☐ Replace

File Name : adas207_graph.ps

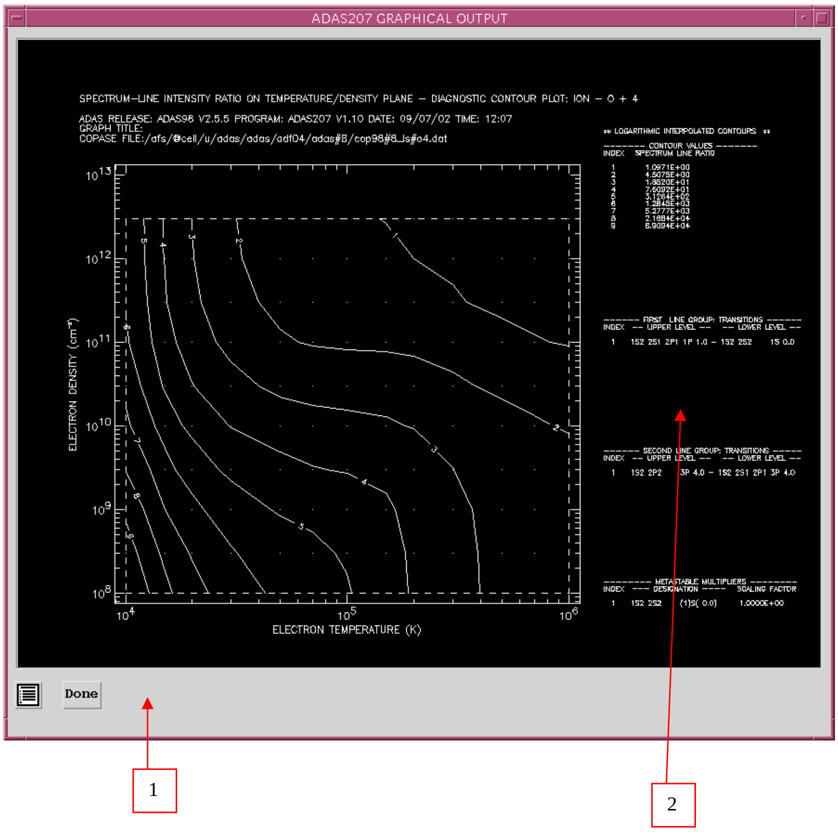
Select Device: Post-Script

☑ Text Output ☐ Append ☐ Replace

File Name : paper.txt

The **Graphical output window** is shown below

1. Printing of the currently displayed graph is activated by the *Print* button.
2. The displayed graph has the usual overall layout, but with supplementary information on the right side listing the line group assemblies and metastable fraction multipliers.



```
SPECTRUM-LINE INTENSITY RATIO ON TEMPERATURE/DENSITY PLANE - DIAGNOSTIC CONTOUR PLOT: ION - O + 4

ADAS RELEASE: ADAS98 V2.5.5 PROGRAM: ADAS207 V1.10 DATE: 09/07/02 TIME: 12:07
GRAPH TITLE:
COPASE FILE:/afs/@cell/u/adas/adas/adf04/adas#8/cop98#8_ls#o4.dat

** LOGARITHMIC INTERPOLATED CONTOURS **

-------- CONTOUR VALUES --------
INDEX   SPECTRUM LINE RATIO

  1        1.0971E+00
  2        4.5075E+00
  3        1.8520E+01
  4        7.6092E+01
  5        3.1284E+02
  6        1.2845E+03
  7        5.2777E+03
  8        2.1684E+04
  9        8.9094E+04

------- FIRST  LINE GROUP: TRANSITIONS -------
INDEX  -- UPPER LEVEL --    -- LOWER LEVEL --

  1    1S2 2S1 2P1 1P 1.0 - 1S2 2S2     1S 0.0

------- SECOND LINE GROUP: TRANSITIONS ------
INDEX  -- UPPER LEVEL --    -- LOWER LEVEL --

  1    1S2 2P2     3P 4.0 - 1S2 2S1 2P1 3P 4.0

--------- METASTABLE MULTIPLIERS ---------
INDEX  --- DESIGNATION ----   SCALING FACTOR

  1    1S2 2S2     (1)S( 0.0)     1.0000E+00
```

The additional processes and the extended adf04 file

At this stage only the basic adf04 file has been introduced. Full generalised collisional radiative (GCR) modelling requires careful attention to other reactions, especially state selective radiative, dielectronic recombination and electron impact ionisation. Also, by some added care and precision in the specifications of the level list in the *adf04* file, a much higher degree of automatic processing is possible and indeed necessary for complex heavy species. Advanced GCR modelling is addressed later in the course, but some preliminaries are mentioned here

Additional processes and their sources in ADAS

Radiative recombination: State selective radiative recombination coefficients, that is which distinguish the initial recombining ion state (ground or possible metastable) and the final recombined ion state, are archived in data format *adf08*. The code ADAS411 interrogates and displays these data in a similar manner to ADAS201 for electron impact excitation data.

Dielectronic recombination: State selective dielectronic recombination coefficients, that is which again distinguish the initial recombining ion state (ground or possible metastable) and the final recombined ion state, are archived in data format *adf09*. The code ADAS410 interrogates and displays these data. The data are very extensive. Dielectronic recombination is required to very highly excited states and so the adf09 tabulations include term and level distinguished data for low levels and bundled nl-shell up to n~12 and bundled n-shell data up to n~1000. The precise organisation depends on whether we are working in ‘term’ resolution or ‘level’ resolution.

Collisional ionisation: State selective electron impact ionisation coefficients, that is which distinguishes the initial ionising ion state (ground, metastable or excited) and the final ionised ion state (ground or metastable), are archived in data formats *adf07* and *adf23*. *adf23* is the principal data class of this type. *adf07* is restricted to ground and metastables only and was created before the more complete data became available. Code ADAS502 interrogates and displays data of format *adf07*. ADAS413 interrogates and displays data of format *adf23*.

Extending the adf04 file

Transition lines denoting other processes: The first character position of a transition line in an *adf04* file is an alphanumeric code (CCODE –see ADAS User manual appxa-04)

CCODE	transition data type code as follows:
	‘ ‘ => unspecified electron impact excitation data
	‘1‘ => dipole electron impact excitation data
	‘2‘ => non-dipole, non-spin change electron impact excitation data
	‘3‘ => spin change electron impact excitation data
	‘p‘ or ‘P’ => positive ion impact excitation data
	‘r‘ or ‘R’ => free electron recombination/capture data
	‘h‘ or ‘H’ => charge exchange recombination data from neutral hydrogen
	‘i‘ or ‘I’ =>electron impact ionisation data from stage below
	‘s‘ or ‘S’ =>electron impact ionisation data to stage above
	‘l‘ or ‘L’ =>unresolved dielectronic satellite line emission data

```
C + 3         6         4        520178.4(1S)   2931440.0(3S)
    1 1s2 2s1           (2)0( 0.5)        0.0   {1}1.000 {2}1.500
    2 1s2 2p1           (2)1( 2.5)    64555.4   {1}1.000
    3 1s2 3s1           (2)0( 0.5)   302849.0   {1}1.000
  .    .      .
   10 1s2 5s1           (2)0( 0.5)   445368.5   {1}1.000
   11 1s2 5p1           (2)1( 2.5)   448860.5   {1}1.000
   12 1s2 5d1           (2)2( 4.5)   449889.2   {1}1.000
   13 1s2 5f1           (2)3( 6.5)   449939.8   {1}1.000
   14 1s2 5g1           (2)4( 8.5)   449948.4   {1}1.000
   -1
  4.0    3       8.00+03 1.60+04 3.20+04 8.00+04 1.60+05 3.20+05 8.00+05 1.60+06 3.20+06 8.00+06 1.60+07
   3   1 1.00-30 5.68-01 5.49-01 5.16-01 4.46-01 3.96-01 3.84-01 3.87-01 3.83-01 3.83-01 3.85-01 3.86-01
   5   1 4.57+05 4.90-01 4.97-01 5.11-01 5.43-01 5.79-01 6.24-01 7.90-01 9.58-01 1.08+00 1.18+00 1.21+00
        .      .       .
  13  12 1.65+02 3.32+03 3.64+03 3.96+03 4.38+03 4.70+03 5.02+03 5.45+03 5.77+03 6.09+03 6.51+03 6.83+03
  14   9 1.09+09 1.59+02 1.64+02 1.74+02 2.06+02 2.53+02 3.22+02 4.48+02 5.63+02 6.89+02 8.69+02 1.01+03
   9   1 1.00-30 9.51-02 9.39-02 9.15-02 8.57-02 7.94-02 7.31-02 6.89-02 6.82-02 6.81-02 6.80-02 6.80-02
R  1  +1         4.33-13 3.08-13 2.19-13 1.41-13 1.01-13 7.39-14 9.62-14 1.34-13 1.09-13 4.80-14 2.13-14
R  2  +1         1.41-12 9.87-13 6.84-13 4.09-13 2.67-13 1.66-13 1.34-13 1.66-13 1.33-13 5.71-14 2.43-14
        .      .
R 13  +2         4.57-10 1.86-10 7.46-11 2.03-11 7.36-12 2.63-12 6.72-13 2.38-13 8.43-14 2.13-14 7.54-15
R 14  +2         9.73-12 3.92-12 1.56-12 4.24-13 1.53-13 5.49-14 1.40-14 4.96-15 1.76-15 4.44-16 1.57-16
S  1  +1         6.19-10 6.73-10 9.77-10 1.44-09 1.87-09 2.31-09 2.80-09 3.00-09 3.03-09 2.79-09 2.46-09
S  1  +2         4.07-11 4.01-11 3.98-11 5.45-11 8.12-11 1.12-10 1.69-10 2.23-10 2.80-10 3.39-10 3.58-10
  -1
  -1  -1
```

Recombination line

Ionisation line

Lecture 3 The ionisation state of ions in a plasma

Preliminaries

Generalised collisional-radiative theory

The basic model for obtaining effective ionisation and recombination rate coefficients in finite density plasmas was established by Bates et al. (1962). The ion in a plasma is viewed as composed of a complete set of levels indexed by i and j and a set of radiative and collisional couplings between them denoted by C_{ij} (an element of the 'collisional-radiative matrix' representing transition from j to i) to which are added direct ionisations from each level of the ion to the next ionisation stage (coefficient $q_i^{(i)}$) and direct recombinations to each level of the ion from the next ionisation stage (coefficient r_i). There is no loss of generality in the present discussion in ignoring other ionisation stages provided couplings to and from them are only via ground states. For each level, there is a total loss rate coefficient for its population denoted by

$$-C_{ii} = \sum_{j\neq i} C_{ji} + N_e q_i^{(i)}$$

The population of any level is determined by the balance of processes populating and depopulating it. Suppose the dominant populations are a recombined ion ground state ($i=1$) and a recombining ion ground state denoted by +. These states alone are assumed significantly populated. Excited level populations (that is N_i for $i>1$) are small in comparison. Then the quasi-equilibrium statistical balance is

$$\tfrac{d}{dt} N_1 = \sum_{j\neq 1} C_{1j} N_j + C_{11} N_1 + N_e N_+ r_1$$

$$0 = \sum_{j\neq 1} C_{ij} N_j + C_{i1} N_1 + N_e N_+ r_i \quad , \quad i = 2,..$$

In matrix form these become

$$\begin{bmatrix} \tfrac{d}{dt} N_1 \\ 0 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{1j} \\ C_{i1} & C_{ij} \end{bmatrix} \begin{bmatrix} N_1 \\ N_j \end{bmatrix} + N_e N_+ \begin{bmatrix} r_1 \\ r_i \end{bmatrix}$$

The populations of the excited levels in quasi-equilibrium, N_j^{eq} are given by

$$N_j^{eq} = -N_e N_+ \sum_{i\neq 1} C_{ji}^{-1} r_i - \sum_{i\neq 1} C_{ji}^{-1} C_{i1} N_1$$

Substitution of equations 1.9 in equation 1.7 for N_1, allows identification of a collisional-dielectronic ionisation coefficient

$$S_{CD} = C_{11} - \sum_{j\neq 1} \sum_{i\neq 1} C_{1j} C_{ji}^{-1} C_{i1}$$

and collisional-dielectronic recombination coefficient

$$\alpha_{CD} = r_1 - \sum_{j\neq 1} \sum_{i\neq 1} C_{1j} C_{ji}^{-1} r_i$$

Physically, the collisional-dielectronic coefficients give the contributions to the effective growth rates for the ground state population due to recombination from and ionisation to the state +, so that the time dependent equation for N_1 becomes

$$d/_{dt}\, N_1 = -N_e S_{CD} N_1 + N_e \alpha_{CD} N_+$$

Some extension is required since populated metastable states can exist and there is no real distinction between them and ground states. We use the term 'metastables' to denote both ground and metastables states and index them by ρ for the recombined ion, and by υ for the recombining ion. Therefore the ion of charge state z has metastable populations $N_\rho^{(z)}$ and the recombining ion population, N^+, must be subdivided into the set $N_{\upsilon}^{(z+1)}$. We sometimes call the recombining ion metastable states 'parent' states. Generalised collisional radiative theory provides effective coefficients which are the extension of those above as:

The ionisation coefficients

$$S_{CD,\sigma\rightarrow\upsilon} = (\mathsf{S}_{\upsilon\sigma} - \sum_{j=1}^{O}\mathsf{S}_{\upsilon j}\sum_{i=1}^{O}\mathsf{C}_{ji}^{-1}\mathsf{C}_{i\sigma})$$

the free electron recombination coefficients

$$\alpha_{CD,\upsilon'\rightarrow\rho} = (\mathsf{R}_{\rho\upsilon'} + \sum_{j=1}^{O}\mathsf{C}_{\rho j}\sum_{i=1}^{O}\mathsf{C}_{ji}^{-1}\mathsf{R}_{i\upsilon'})$$

the charge exchange recombination coefficients

$$C_{CD,\upsilon'\rightarrow\rho} = (\mathsf{Q}_{\rho\upsilon'} + \sum_{j=1}^{O}\mathsf{C}_{\rho j}\sum_{i=1}^{O}\mathsf{C}_{ji}^{-1}\mathsf{Q}_{i\upsilon'})$$

the metastable cross-coupling coefficients

$$X_{CD,\sigma\rightarrow\rho} = (\mathsf{C}_{\rho\sigma} - \sum_{j=1}^{O}\mathsf{C}_{\rho j}\sum_{i=1}^{O}\mathsf{C}_{ji}^{-1}\mathsf{C}_{i\sigma})/N_e$$

and the parent metastable cross-coupling coefficients

$$Q_{CD,\upsilon'\rightarrow\upsilon} = \sum_{j=1}^{O}\mathsf{S}_{\upsilon j}\sum_{i=1}^{O}\mathsf{C}_{ji}^{-1}\mathsf{R}_{i\upsilon'}\;{}_{e}$$

Note the latter coefficients distinguish the parts occurring via recombination from conventional metastable cross-coupling as they are determined in the course of the population structure calculation for the z-times ionised ion. The radiated power loss coefficients are obtained by summing over the population structure. The contribution due to excitation from the metastables of the recombined ion is

$$P_{LT,\sigma} = \sum_{k,j}\Delta E_{kj}A_{j\rightarrow k}\mathsf{F}_{j\sigma}^{(exc)}$$

and there is a corresponding bremsstrahlung, recombination/cascade part

$$P_{RB,\sigma}$$

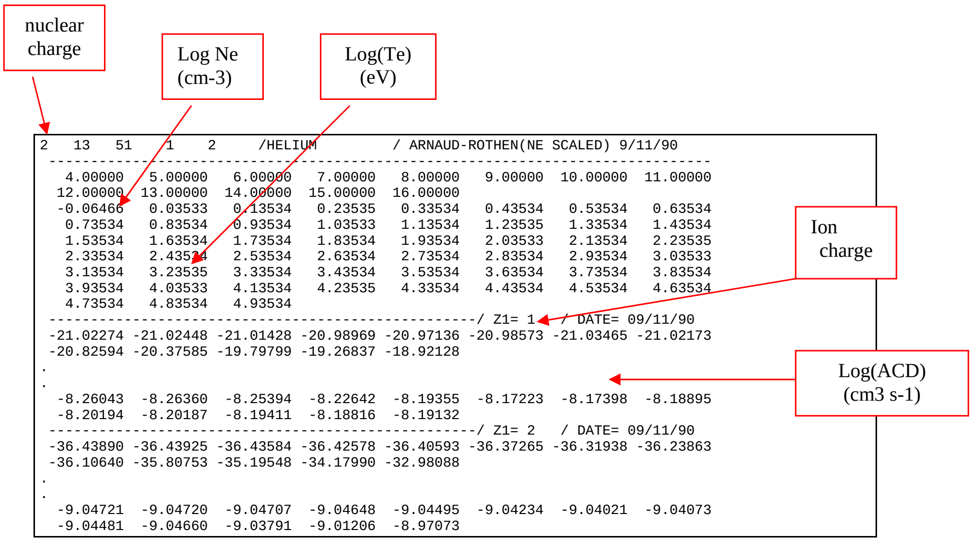
The adf11 data format

The primary repositories of collisional-radiative recombination, ionisation etc. coefficients gathered together by element are *adf11* files sometimes called iso-nuclear master files. The various classes are

Mnemonic	Class	Data prefix
ACD	Coll.-diel. recom. coefft.	R & U (or none)
SCD	Coll.-diel. ionis. coefft.	R & U (or none)
CCD	Coll.-rad. charge exch. coefft.	R & U (or none)
PRB	Coll.-diel. recom./brems. power coefft.	R & U (or none)
PRC	Coll.-rad. charge exch. recom. power coefft.	R & U (or none)
QCD	Coll.-rad. metastable cross coupling coefft.	R
XCD	Coll.-diel. parent meta. cross-coupling coefft.	R
PLT	Coll.-rad. excit. line power coefft.	R & U (or none)
PLS	Coll.-rad. specific line excit. power coefft.	R & U (or none)

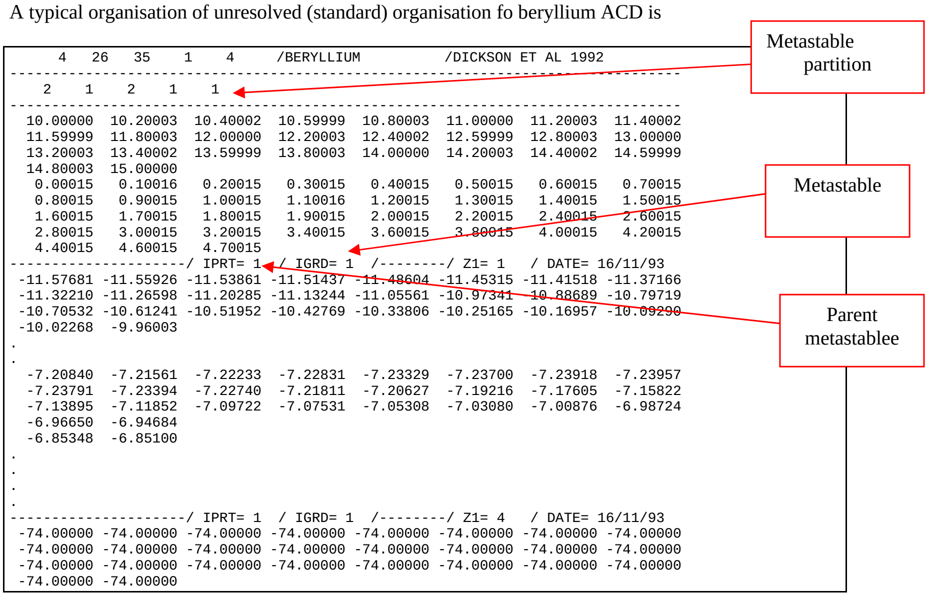
A file is associated with an element and a data class. There are separate files for ordinary and generalised data. The classes of data include the collisional-dielectronic recombination coefficient (ACD), the collisional-dielectronic ionisation coefficient (SCD), the collisional-radiative charge exchange recombination coefficient (CCD), the collisional-dielectronic recombination/cascade / bremsstrahlung radiated power coefficient (PRB), the collisional-radiative charge exchange recombination/cascade power coefficient (PRC), the collisional-radiative metastable cross-coupling coefficient (QCD) and the collisional-dielectronic parent cross-coupling coefficient (XCD), the collisional-radiative excitation total line power coefficient (PLT) and the collisional-radiative excitation specific line power coefficient (PLS). Altogether there are nine classes. The internal organisation of the data is different depending on whether they are stage to stage (data prefix 'U' or no prefix) or metastable resolved (data prefix 'R'). The data classes QCD and XCD do not occur in the stage to stage case. ADF11 data based on different qualities of calculation and of standard and resolved types are assigned a two-digit year number. ‘89’ is standard state-to stage, unreolved baseline data. ‘96’ is high grade partial, metastable resolved data.

A typical organisation of unresolved (standard) organisation for helium ACD is



```
2   13   51    1    2     /HELIUM         / ARNAUD-ROTHEN(NE SCALED) 9/11/90
 ---------------------------------------------------------------------------
   4.00000   5.00000   6.00000   7.00000   8.00000   9.00000  10.00000  11.00000
  12.00000  13.00000  14.00000  15.00000  16.00000
  -0.06466   0.03533   0.13534   0.23535   0.33534   0.43534   0.53534   0.63534
   0.73534   0.83534   0.93534   1.03533   1.13534   1.23535   1.33534   1.43534
   1.53534   1.63534   1.73534   1.83534   1.93534   2.03533   2.13534   2.23535
   2.33534   2.43534   2.53534   2.63534   2.73534   2.83534   2.93534   3.03533
   3.13534   3.23535   3.33534   3.43534   3.53534   3.63534   3.73534   3.83534
   3.93534   4.03533   4.13534   4.23535   4.33534   4.43534   4.53534   4.63534
   4.73534   4.83534   4.93534
 ---------------------------------------------------/ Z1= 1   / DATE= 09/11/90
 -21.02274 -21.02448 -21.01428 -20.98969 -20.97136 -20.98573 -21.03465 -21.02173
 -20.82594 -20.37585 -19.79799 -19.26837 -18.92128
.
.
  -8.26043  -8.26360  -8.25394  -8.22642  -8.19355  -8.17223  -8.17398  -8.18895
  -8.20194  -8.20187  -8.19411  -8.18816  -8.19132
 ---------------------------------------------------/ Z1= 2   / DATE= 09/11/90
 -36.43890 -36.43925 -36.43584 -36.42578 -36.40593 -36.37265 -36.31938 -36.23863
 -36.10640 -35.80753 -35.19548 -34.17990 -32.98088
.
.
  -9.04721  -9.04720  -9.04707  -9.04648  -9.04495  -9.04234  -9.04021  -9.04073
  -9.04481  -9.04660  -9.03791  -9.01206  -8.97073
```

A typical organisation of unresolved (standard) organisation fo beryllium ACD is



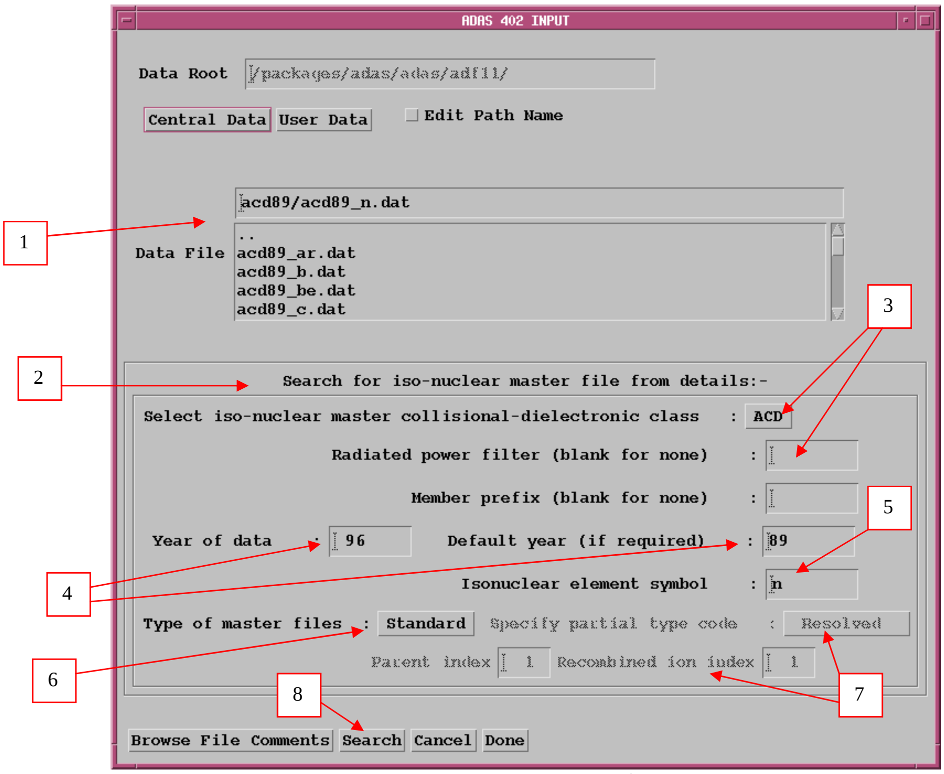
```
      4   26   35    1    4     /BERYLLIUM          /DICKSON ET AL 1992
-------------------------------------------------------------------------------
    2    1    2    1    1
-------------------------------------------------------------------------------
  10.00000  10.20003  10.40002  10.59999  10.80003  11.00000  11.20003  11.40002
  11.59999  11.80003  12.00000  12.20003  12.40002  12.59999  12.80003  13.00000
  13.20003  13.40002  13.59999  13.80003  14.00000  14.20003  14.40002  14.59999
  14.80003  15.00000
   0.00015   0.10016   0.20015   0.30015   0.40015   0.50015   0.60015   0.70015
   0.80015   0.90015   1.00015   1.10016   1.20015   1.30015   1.40015   1.50015
   1.60015   1.70015   1.80015   1.90015   2.00015   2.20015   2.40015   2.60015
   2.80015   3.00015   3.20015   3.40015   3.60015   3.80015   4.00015   4.20015
   4.40015   4.60015   4.70015
---------------------/ IPRT= 1  / IGRD= 1  /--------/ Z1= 1   / DATE= 16/11/93
 -11.57681 -11.55926 -11.53861 -11.51437 -11.48604 -11.45315 -11.41518 -11.37166
 -11.32210 -11.26598 -11.20285 -11.13244 -11.05561 -10.97341 -10.88689 -10.79719
 -10.70532 -10.61241 -10.51952 -10.42769 -10.33806 -10.25165 -10.16957 -10.09290
 -10.02268  -9.96003
.
.
  -7.20840  -7.21561  -7.22233  -7.22831  -7.23329  -7.23700  -7.23918  -7.23957
  -7.23791  -7.23394  -7.22740  -7.21811  -7.20627  -7.19216  -7.17605  -7.15822
  -7.13895  -7.11852  -7.09722  -7.07531  -7.05308  -7.03080  -7.00876  -6.98724
  -6.96650  -6.94684
  -6.85348  -6.85100
.
.
.
.
---------------------/ IPRT= 1  / IGRD= 1  /--------/ Z1= 4   / DATE= 16/11/93
 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000
 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000
 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000
 -74.00000 -74.00000
```

```
.
.
  -9.42566  -9.42504  -9.42431  -9.42348  -9.42260  -9.42169  -9.42080  -9.41994
  -9.41916  -9.41849  -9.41796  -9.41761  -9.41747  -9.41757  -9.41794  -9.41862
  -9.41964  -9.42102  -9.42267  -9.42448  -9.42633  -9.42810  -9.42968  -9.43096
  -9.43182  -9.43215
--------------------------------------------------------------------------------
C
C
C     RATE COEFFICIENTS IN UNITS OF CM**3 S-1
C     ---------------------------------------
C
C     PREPARED USING CODE JETXLE.IONBAL.FORT(WJD404R)
C
C           WILLIAM J. DICKSON   16/11/93
C-------------------------------------------------------------------------------
```

ADAS402

The code interrogates iso-nuclear master files of type ADF11. It extracts collisional radiative coefficients of various classes relevant to plasma modelling stored in iso-nuclear sequence sets. The data may be interpolated using cubic splines to provide the coefficients at a selected charge state of the chosen element and at selected electron temperature/electron density pairs. A minimax polynomial approximation is also made to the data. Interpolated data and some comparative source data are displayed and a tabulation printed. The printed output includes the minimax polynomial approximation.

The **file selection window** is illustrated below. Conventional file selection and selection via a directed search are possible.



Data Root /packages/adas/adas/adf11/

Data File acd89/acd89_n.dat
..
acd89_ar.dat
acd89_b.dat
acd89_be.dat
acd89_c.dat

Search for iso-nuclear master file from details:-

Select iso-nuclear master collisional-dielectronic class : ACD

Radiated power filter (blank for none) :

Member prefix (blank for none) :

Year of data : 96

Default year (if required) : 89

Isonuclear element symbol : n

Type of master files : Standard

Specify partial type code : Resolved

Parent index 1

Recombined ion index 1

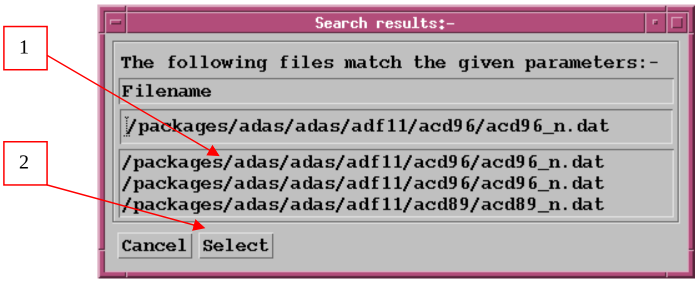
1. Buttons are present to set the data root to that of the *Central data* or to your personal *User data* (provided it is in ADAS organisation. Alternatively the 'data root' may be edit explicitly. Available data sets are shown in the file display window. Selection is made by clicking on the appropriate name, whereupon it appears in the selection window above.
2. There are very many data sets of type *adf11* grouped by year, element and data class. A search strategy is available based on initial identification of an group of files of particular year and type and then conventional selection from the group list.
3. For dataset search, select the iso-nuclear master class first. A drop-down menu is offered. The radiated power data classes (PLT, PRB and PRC) can include the attenuation due to an energy filter. Enter the filter if required. At this stage only a very limited amount of filtered power data has been placed on the workstation database. The naming convention is defined in the *adf11* specification. To allow further distinction of data within the same

year, a prefix can be used within the dataset name structure (eg. *acd93r_<prefix>_o.dat*). Enter this if required at *Member prefix*.

4. Enter the two-digit year number of the data required at *Year of data* . A *Default year* may be entered which will be used if there is no data of the required class in the *Year of data*.
5. Enter the *Iso-nuclear sequence symbol*.
6. There are two primary organisations of adf11 data, Standard (ionisation stage to ionisation stage) and Partial (metastable to metastable). Select the type required in the drop-down menu at *Type of master file*.
7. If Partial is chosen, further selections may be made. Within the Partial type of organisation, true metastable to metastable subdivided data is called Resolved. Stage to stage data can be written into the Partial type of structure and is then called Unresolved. This un-necessary duplication is because of a historical precedent in IBM-ADAS at JET. Select as required in the drop-down menu at *Specify partial type code.* Finally within the Resolved type enter the particular metastable to metastable sought at *Parent index* and *Recombined ion index*. Note that the items selected here are only used when the dataset is opened at the Processing Options stage.
8. Initiate the search for the required dataset sub-list by clicking *Search* .

The **search result window** has the appearance shown above

1. If there is a choice of files, click on the one you wish.
2. Return to the input window by clicking *Select*.



The following files match the given parameters:-

Filename

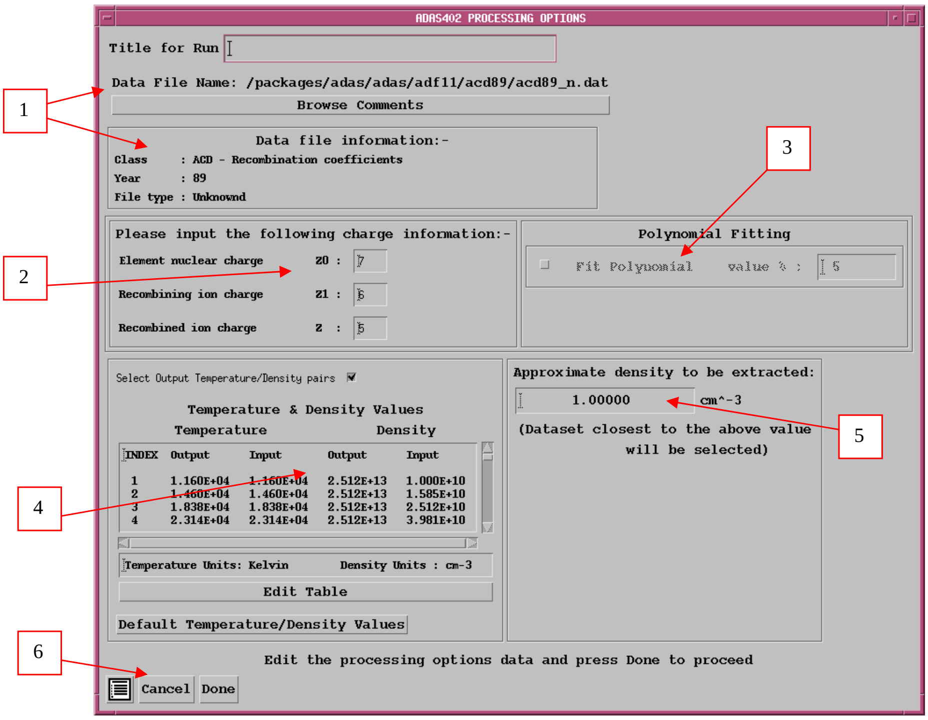
/packages/adas/adas/adf11/acd96/acd96_n.dat

/packages/adas/adas/adf11/acd96/acd96_n.dat
/packages/adas/adas/adf11/acd96/acd96_n.dat
/packages/adas/adas/adf11/acd89/acd89_n.dat

The **processing options window** has the appearance shown below

1. Data file and iso-nuclear sequence information is given.
2. A particular charge state of the iso-nuclear sequence should be selected. This is by entering any one of the three fields, namely, element nuclear charge (nuclear charge number or symbol), recombining ion charge or recombined ion charge
3. The extracted data is interpolated by a cubic spline to the selected ion and user temperature/density pairs for graphical display and tabular output. Additionally a polynomial approximation may obtained by making the appropriate selections.
4. Select temperature and density pairs for data output (Output). The source data is held in two-dimensional arrays, that is as a function of electron temperature and electron density. The source (Input) values are also shown. The table may be edited by clicking on the *Edit Table* button.. The ADAS Table Editor window is then presented with usual set of editing operations available.

5. The displayed graph of the interpolated coefficient as a function of electron temperature also shows some additional curves from the dataset for comparison. These additional curves are drawn directly from the dataset and are not interpolated. Thus they must be at fixed electron density. Specify the *Approximate density to be extracted*. The nearest fixed density in the dataset will be used for the comparative curves.
6. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window. The *Escape to Menu* icon is also available for a quick exit at the bottom left hand corner.



Title for Run

Data File Name: /packages/adas/adas/adf11/acd89/acd89_n.dat

Data file information:-
Class : ACD - Recombination coefficients
Year : 89
File type : Unknownd

Please input the following charge information:-
Element nuclear charge Z0 : 7
Recombining ion charge Z1 : 6
Recombined ion charge Z : 5

Select Output Temperature/Density pairs ☑

Temperature & Density Values

	Temperature		Density	
INDEX	Output	Input	Output	Input
1	1.160E+04	1.160E+04	2.512E+13	1.000E+10
2	1.460E+04	1.460E+04	2.512E+13	1.585E+10
3	1.838E+04	1.838E+04	2.512E+13	2.512E+10
4	2.314E+04	2.314E+04	2.512E+13	3.981E+10

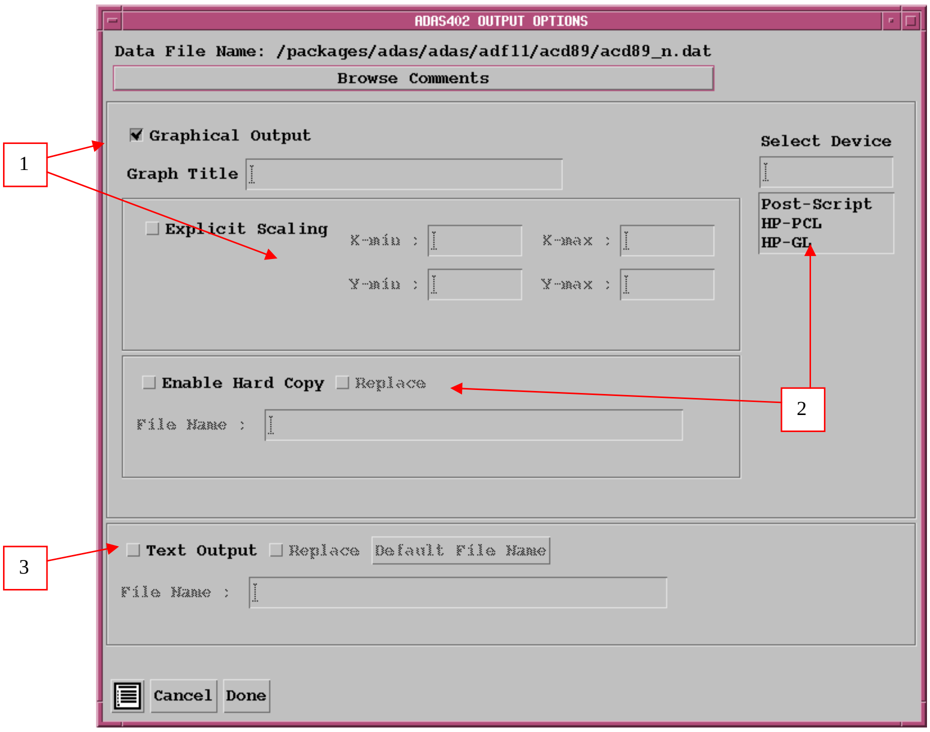
Temperature Units: Kelvin Density Units : cm-3

Approximate density to be extracted: 1.00000 cm^-3
(Dataset closest to the above value will be selected)

Edit the processing options data and press Done to proceed

The **Output options window** is shown below. Broadly it follows the pattern of other ADAS interrogation codes.

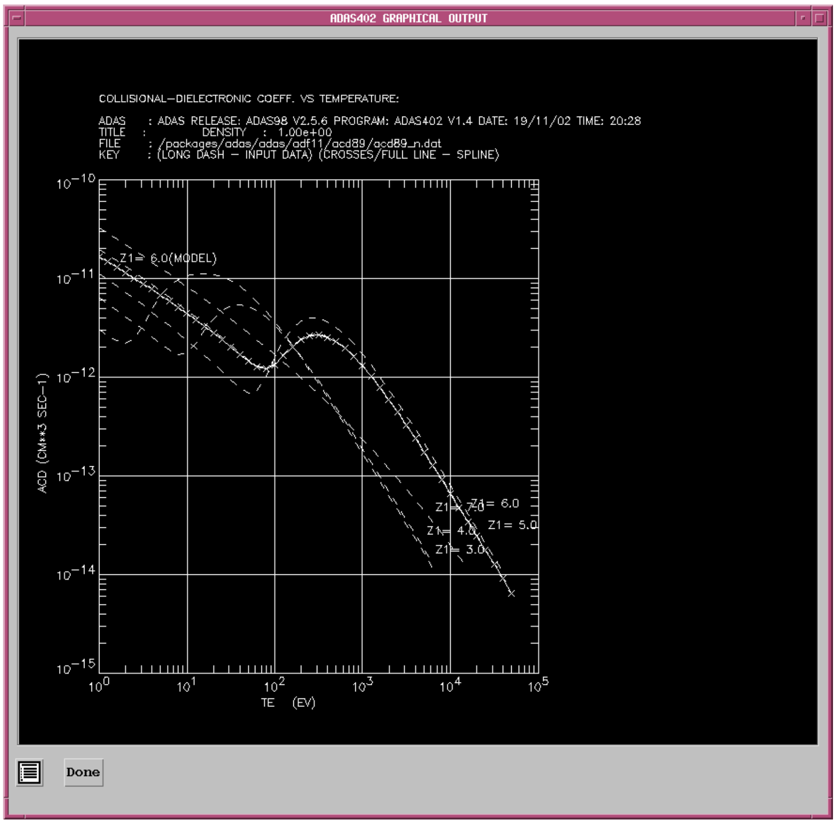
1. Graphical output is enabled by clicking on the button. Default scaling of graphs may be over-ridden by appropriate selections.
2. Hard copy may be enabled and the type of output device selected.
3. As usual a line printer text output file summarising the interrogation may be produced.



Data File Name: /packages/adas/adas/adf11/acd89/acd89_n.dat

☑ Graphical Output

The **graphical output** is as shown below.



```
COLLISIONAL-DIELECTRONIC COEFF. VS TEMPERATURE:

ADAS    : ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS402 V1.4 DATE: 19/11/02 TIME: 20:28
TITLE   :          DENSITY   :  1.00e+00
FILE    : /packages/adas/adas/adf11/acd89/acd89_n.dat
KEY     : (LONG DASH - INPUT DATA) (CROSSES/FULL LINE - SPLINE)
```

ADAS405

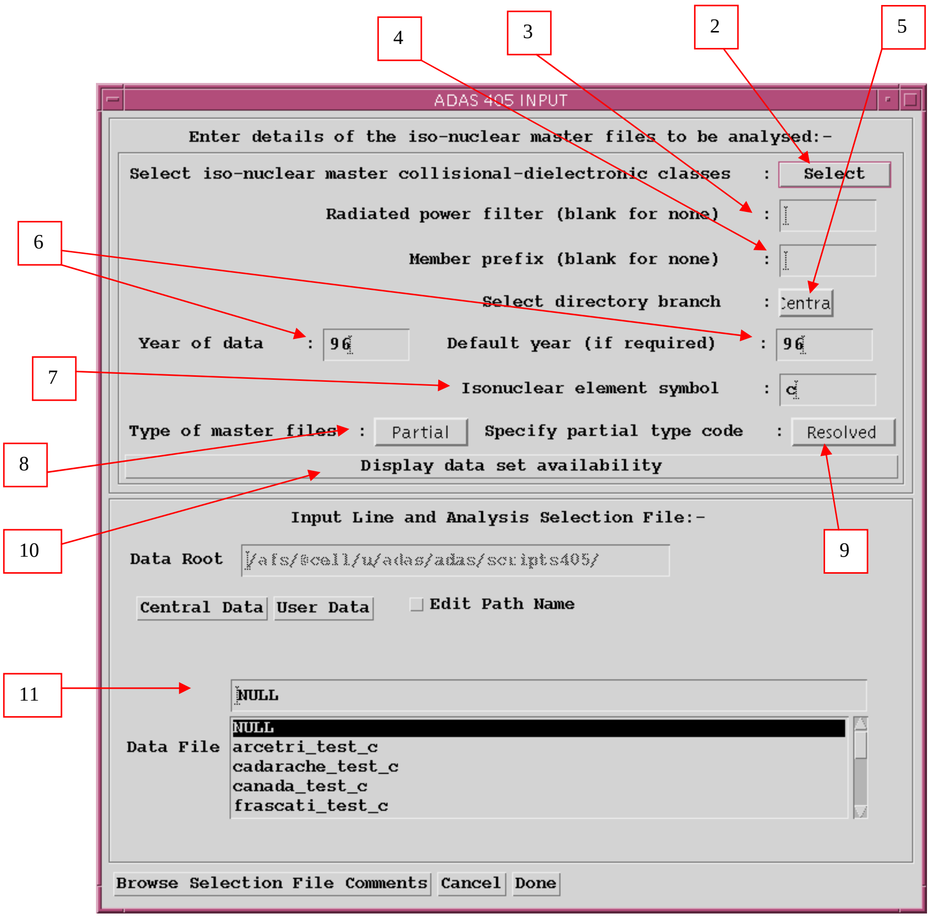
The program calculates the fractional abundances of resolved metastable or unresolved stage populations of the ions of an element in equilibrium in a thermal plasma. It also evaluates the radiated power function and line emission contribution functions . The evaluation of emission functions (and ratios of emission functions between lines of possibly different ions of the same element) is controlled by a ‘script file’. This specifies the composition of the lines required.

The **file selection window** appears first as illustrated below

1. Two types of data file are identified in the file selection, namely, the iso-nuclear master files required for the ionisation balance and power calculations and the script file. The top part of the file selection window is concerned with identifying the master file data required and the lower part with identifying the script file.
2. Click on the *Select* button to drop down a selection list of master file data classes. Activate the buttons at the data classes required for your analysis. It is obligatory to select the ‘*acd*’ and ‘*scd*’ electron impact effective recombination and ionisation data classes since otherwise an ionisation balance cannot proceed. However the other data classes selected are at the

user's choice. This enables investigative studies of the importance of different contributions for example to radiated power.

3. Effective radiated power coefficients ('*prb*', '*plt*' and '*prc*') are often made available both as the whole emitted power and as the power which would pass through certain filters (such as Be/Si windows). The filter is specified either simply as an energy cut-off (eg. *ev2000*) or as filter specification (eg. *ft1235*). These codes appear as an extension in the relevant master file names. Specify the filter choice.
4. Some flexibility for subdivision within a data year is provided by allowing a two character 'member prefix' (eg. '*pj*') which may be present in the final part of a file name (eg. '*/.../acd93r/acd93r_pj#c.dat*').



Enter details of the iso-nuclear master files to be analysed:-

Select iso-nuclear master collisional-dielectronic classes : Select
Radiated power filter (blank for none) :
Member prefix (blank for none) :
Select directory branch : Centra
Year of data : 96
Default year (if required) : 96
Isonuclear element symbol : c
Type of master files : Partial
Specify partial type code : Resolved

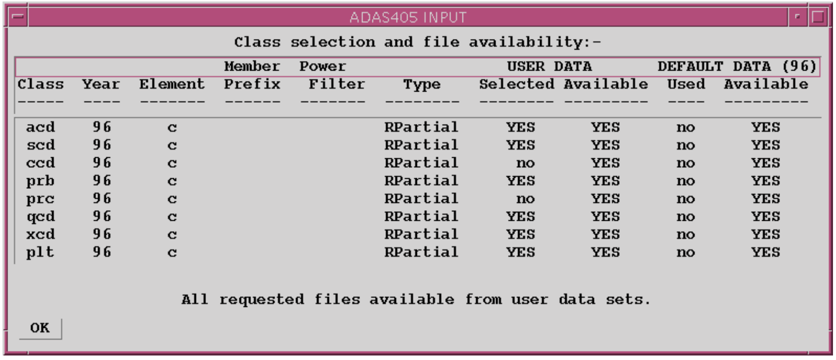
Input Line and Analysis Selection File:-

Data Root /afs/@cell/u/adas/adas/scripts405/
☐ Edit Path Name
NULL
Data File
NULL
arcetri_test_c
cadarache_test_c
canada_test_c
frascati_test_c

5. Select the directory branch, that is the central ADAS or user data area.
6. Select the year of data. In general the two digit year number is used to provide the main groupings of data. Thus '*89*' is the standard, unresolved, JET base line data of low precision but fairly complete. '*93*' is metastable

resolved data, but available only for light elements of primary importance to fusion. Note that a default year must be specified. Often the complete set of data classes for a particular year and type are not available and the capability of filling in from a default (perhaps less accurate but more complete) year is allowed.

7. Specify the element.
8. Specify the type of master file. The distinctions between *standard* and *partial* master file types and *resolved* and *unresolved* types must be clarified. *Standard* data is stage to stage and has a specific layout. *Partial* data distinguishes metastables and has a different layout.
9. Within the partial data layout specify the partial type. .It is possible simply to have each stage represented only by its ground state and therefore to be similar to standard data. However the layout is the partial one. We call such data *partial* but *unresolved*. The usual *partial* data with metastables present is called *resolved*. This distinction and added flexibility are helpful in iso-nuclear master file preparation and archiving.
10. Clicking the *Display data set availability* button at causes display of a file availability summary window as illustrated below. It is important to use this facility since it shows which master files classes sought by the user were not available, where default data files were substituted etc.



Class selection and file availability:-

			Member	Power		USER DATA		DEFAULT DATA (96)	
Class	Year	Element	Prefix	Filter	Type	Selected	Available	Used	Available
acd	96	c			RPartial	YES	YES	no	YES
scd	96	c			RPartial	YES	YES	no	YES
ccd	96	c			RPartial	no	YES	no	YES
prb	96	c			RPartial	YES	YES	no	YES
prc	96	c			RPartial	no	YES	no	YES
qcd	96	c			RPartial	YES	YES	no	YES
xcd	96	c			RPartial	YES	YES	no	YES
plt	96	c			RPartial	YES	YES	no	YES

All requested files available from user data sets.

11. A script file selection may be made. The structure of script file is shown below. We have found it convenient to group script files in a personal ADAS database under a subdirectory classification */scripts405/*. Also, it is possible to bypass contribution function calculation and display by selecting the '*NULL*' script. You may find it helpful to copy the '*NULL*' script from the central ADAS database to your own space. Note that scripts apply to particular cases. Thus the references to emissivity coefficient data in a script applying to metastable resolved will not in general work for unresolved data, indeed will probably crash. We have not built much protection against faulty references into script files at the moment. More protection may be added if this proves a stumbling point for users. You may find it helpful to fetch the *test_c* script from central ADAS for first trials.

A **script file** is illustrated below. Details of the species, number of (composite) lines and line ratios to be obtained are at the head of the file (SPECIES, NLINE, NRATIO). Note that you must follow the positional layout exactly. Emissivity coefficient data are obtained from '*pec*' files of ADAS format ADF15. The number of such files to be searched in the ADAS database are specified at NFILE and the full Unix paths to the files themselves in following lines at PHOTON EMISSIVITY FILE NAMES. The subsequent table identifies the index number of the *pecs* in these files required to build the particular line emission function. The lines are indexed at ILINE, the number of component parts of each line is at NCOMP, the charge of the ion to which the component attaches is at IZION and the components simply indexed at ICOMP. The metastable of the ion to which the component is attached is specified by its ranked index number at IMET (the ground state is 1). INDPH gives the selection index of the component *pec* in the ADF15 file identified at IFILE from the list given earlier. Note the letter qualification on the INDPH index to distinguish electron collision driven *pecs* and charge exchange driven *pecs*. The composite lines may be ratioed as specified by IRATIO, an index number of the ratio; ILINE, the upper composite line of the ratio; JLINE, the lower composite line of the ratio. All other text is for information. Note that a ‘c------’ line is used to separate comments which follow it. Each comment line begins with ‘c’ and we conventionally put in a’c-----’ terminator line for the comments section.

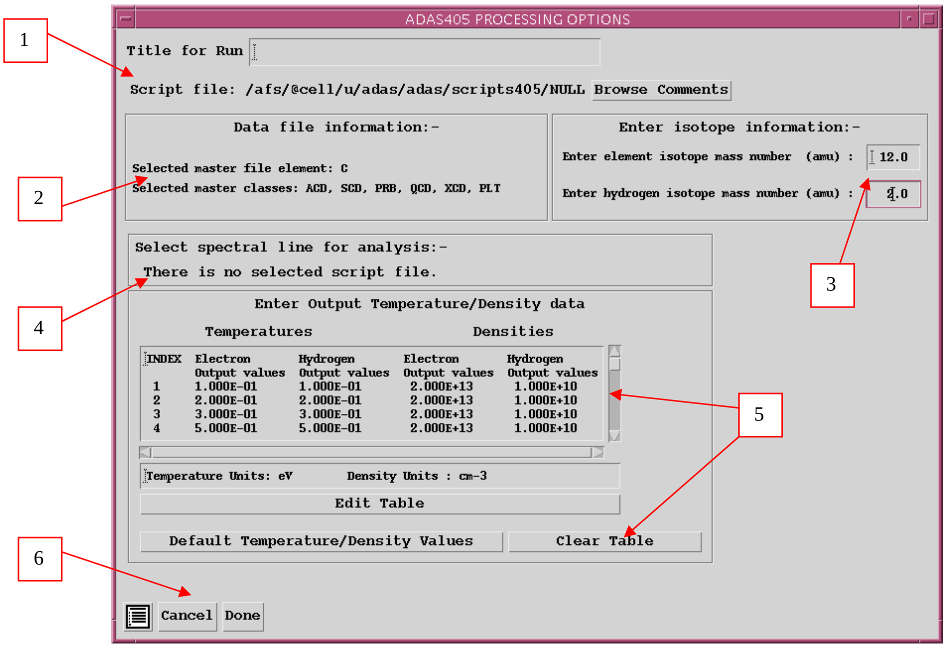
```
SPECIES =  C
NLINE   =  2
NRATIO  =  1
NFILE   =  4
PHOTON EMISSIVITY FILE NAMES = JETSHP.PEC93#C.DATA(PJR#C0)
                               JETSHP.PEC93#C.DATA(PJR#C1)
                               JETSHP.IONELEC.DATA(PEC#C3)
                               JETSHP.IONELEC.DATA(PEC#C4)

 ILINE   NCOMP   IZION   ICOMP   IMET    INDPH   IFILE     TITLE
------------------------------------------------------------------------
   1       4       0       1       1       1E      1       CI      1561A
                   0       2       2      54E      1
                   0       3       3     107E      1
                   0       4       4     160E      1
------------------------------------------------------------------------
   2       2       1       1       1       3E      2       CII      904A
                   1       2       2      25E      2
------------------------------------------------------------------------


 IRATIO  ILINE   JLINE     TITLE
----------------------------------------------------
   1       1       2       CI ( 1561A)/CII (  904A)
----------------------------------------------------
C----------------------------------------------------------------------
C ANALYSIS OF CARBON EMISSION.
C
C   LINES INCLUDED:
C                          1.   CI.     1561A
C                          2.   CII      904A
C
C
C
C----------------------------------------------------------------------
C  CODES:
C         IMET   - Trailing '+'           => IZION+1 metastable
C                  <blank>                => IZION   metastable
C                  trailing '-'           => IZION-1 metastable
C
C         INDPH  - Trailing 'E'or <blank> => Electron coll. driven
C                  Trailing 'H'           => Hydrogen  CX   driven
C
C----------------------------------------------------------------------
```

The **processing options window** has the appearance shown below

1. The script file selected by the user is identified at (a). The *Browse Comments* button displays the comments field at the foot of the script file.
2. Information is presented of the element and master files classes selected in the previous file selection option step.
3. Enter isotope mass numbers for the selected element and background neutral hydrogen in the plasma. This information is only used if charge exchange recombination master file data has been selected.
4. The spectrum lines set up in the script file are shown in the display window. This operates in the same manner as dataset display and selection windows in the input option window of a code such as ADAS205 (see chapter 2). Click on a line to select it. The selected line is shown in the selection window above the display window. Only one line is treated at a time for graphical display. However all lines and line ratios in the script file are computed and tabulated in the output text file.
5. Select temperature and density pairs for data output. The table may be edited by clicking on the *Edit Table* button.. The ADAS Table Editor window is then presented with the same set of editing operations available as

are described in the introductory chapter. Electron temperatures should be monotonic increasing. It has proved helpful to add a *Clear Table* button to remove all entries in the temperature and density output fields.

6. Clicking the *Done* button causes the output options window to be displayed. Remember that *Cancel* takes you back to the previous window.



Title for Run

Script file: /afs/@cell/u/adas/adas/scripts405/NULL

Data file information:-

Selected master file element: C

Selected master classes: ACD, SCD, PRB, QCD, XCD, PLT

Enter isotope information:-

Enter element isotope mass number (amu) : 12.0

Enter hydrogen isotope mass number (amu) : 2.0

Select spectral line for analysis:-

There is no selected script file.

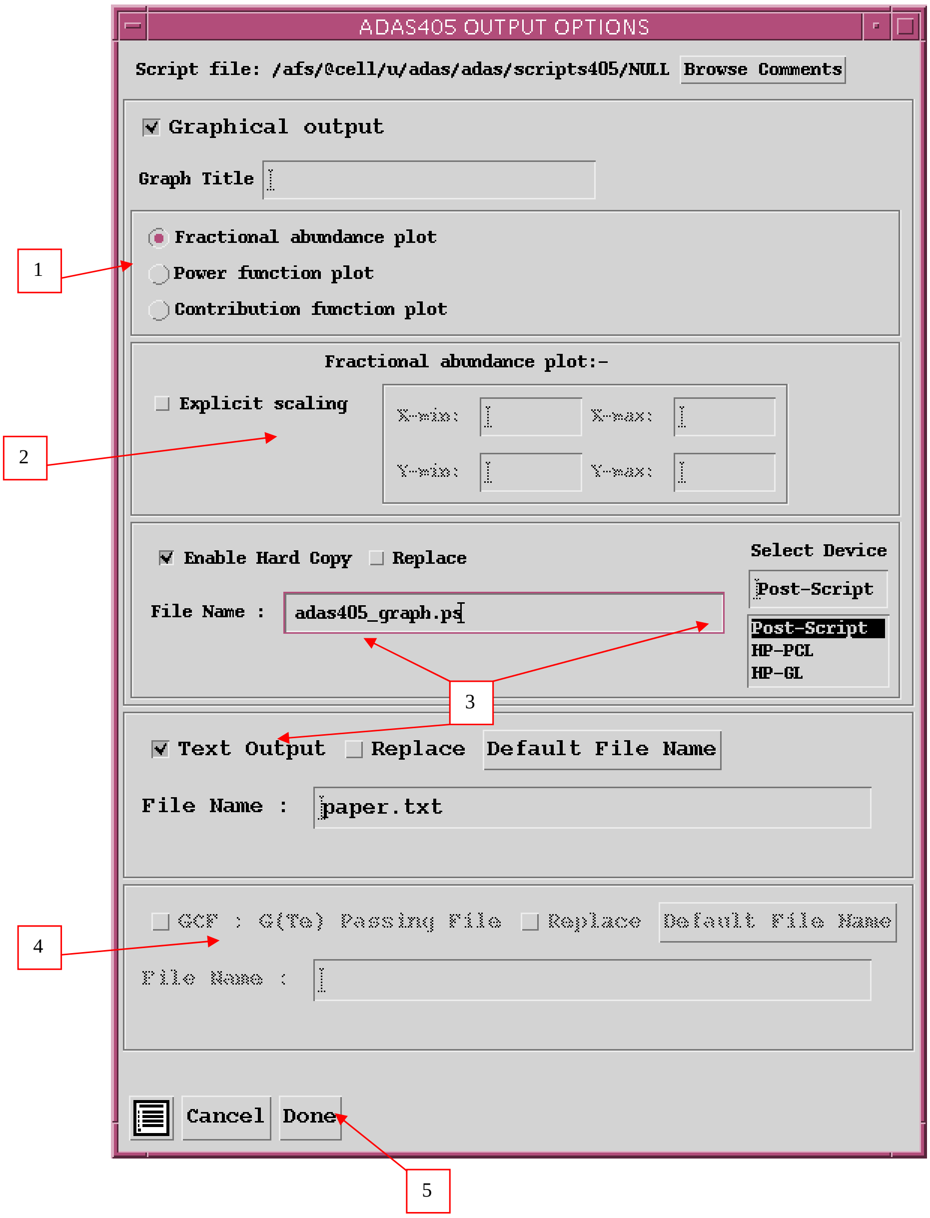
Enter Output Temperature/Density data

	Temperatures		Densities	
INDEX	Electron Output values	Hydrogen Output values	Electron Output values	Hydrogen Output values
1	1.000E-01	1.000E-01	2.000E+13	1.000E+10
2	2.000E-01	2.000E-01	2.000E+13	1.000E+10
3	3.000E-01	3.000E-01	2.000E+13	1.000E+10
4	5.000E-01	5.000E-01	2.000E+13	1.000E+10

Temperature Units: eV Density Units : cm-3

The **output options window** is shown below.

1. It follows the usual pattern except that there is a choice of graphs to display. Thus the fractional abundances, power functions and contribution functions are all of potential interest. Click on the appropriate button . Generally, we find that on the first one or two occasions we wish to see the fractional abundances and powers but then have a more sustained interested in the contribution function shapes and their location in temperature. All the graphs are provided as a function of electron temperature.
2. The sub-window presented depends on the graph choice above. The default scaling may be over-ridden and explicit values for the graph limits entered.
3. Graphical output may enabled in the window together with hard copy device and output file name. This follows the pattern of other ADAS programs. Likewise text output selection is standard.
4. The '*Goft Passing File*' is the name used for the output dataset of calculated contribution functions. It is organised according to an ADAS data format ADF16. The widget is active only if a non NULL script file has been selected on input Specify an output file name. Note that G(Te) functions of type ADF20 (*gft*) are organised differently and have a slightly different definition from the output here of generalised contribution functions of type ADF16 (*gcf*). The expected practice is that ADAS405 will be used either recursively or in distinct runs to examine contribution functions and then decide which to put into the Goft file.
5. An *Append* button has been provided to allow an existing output Goft file to be extended. The *Replace* and *Default file name* buttons have their usual meanings.



Script file: /afs/@cell/u/adas/adas/scripts405/NULL

☑ Graphical output

Graph Title :

● Fractional abundance plot
○ Power function plot
○ Contribution function plot

Fractional abundance plot:-

☐ Explicit scaling X-min: X-max: Y-min: Y-max:

☑ Enable Hard Copy ☐ Replace

Select Device: Post-Script

File Name : adas405_graph.ps

☑ Text Output ☐ Replace

File Name : paper.txt

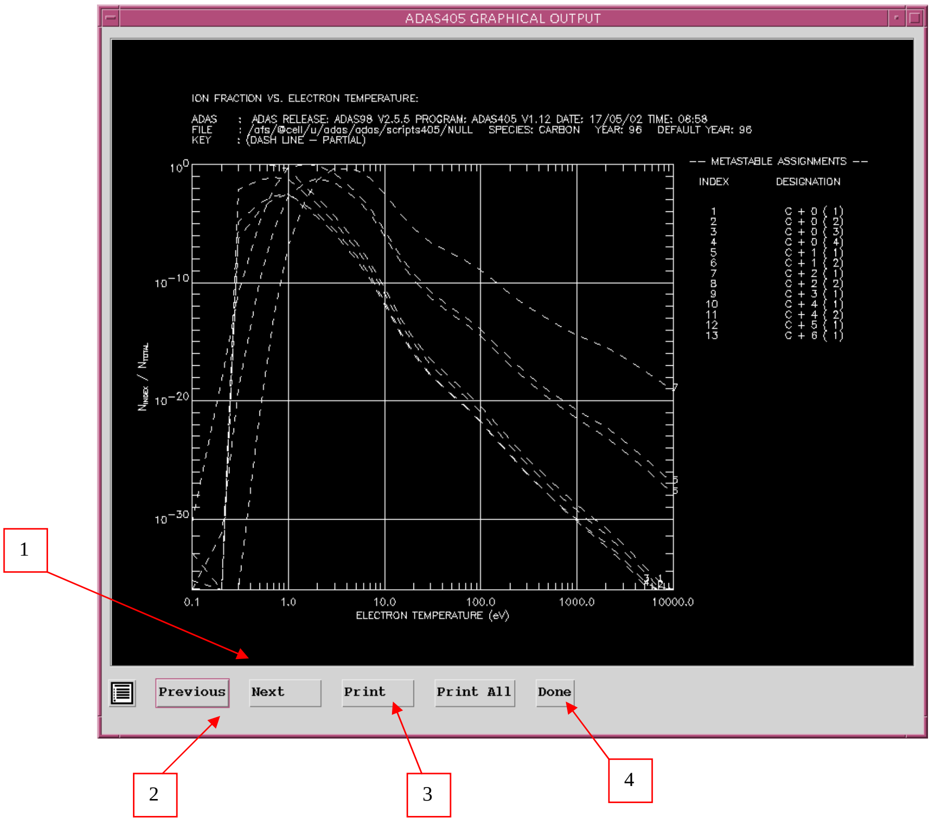
☐ GCF : G(Te) Passing File ☐ Replace

File Name :

The **Graphical output window** is shown below

1. The graph has at its foot a *Done* button, and possibly *Next* and *Previous* buttons if there is a sequence of graphs to be displayed. A *Print* and *Print all* button is also present if the *Enable Hard Copy* button on the previous window was activated.

2. Press the *Next* button to show the next graph in a sequence and the *Previous* button to show the previous graph.
3. Press the *Print* button to make a hard copy of the currently displayed picture. *Print all* makes a hard copy of all the pictures.
4. Pressing the *Done* button restores the previous Output Options window.



```
ION FRACTION VS. ELECTRON TEMPERATURE:

ADAS    :  ADAS RELEASE: ADAS98 V2.5.5 PROGRAM: ADAS405 V1.12 DATE: 17/05/02 TIME: 08:58
FILE    : /afs/@cell/u/adas/adas/scripts405/NULL   SPECIES: CARBON   YEAR: 96   DEFAULT YEAR: 96
KEY     : (DASH LINE - PARTIAL)

-- METASTABLE ASSIGNMENTS --

  INDEX          DESIGNATION

    1             C + 0 ( 1)
    2             C + 0 ( 2)
    3             C + 0 ( 3)
    4             C + 0 ( 4)
    5             C + 1 ( 1)
    6             C + 1 ( 2)
    7             C + 2 ( 1)
    8             C + 2 ( 2)
    9             C + 3 ( 1)
   10             C + 4 ( 1)
   11             C + 4 ( 2)
   12             C + 5 ( 1)
   13             C + 6 ( 1)
```

Generating baseline ionisation, recombination and radiative power data

The main paths for moderate quality automatic ADF04 specific ion file creation available at present is:
COWAN STRUCTURE + BORN rate coefficients
giving files of group name
COPMM#<elem. nucl. charge>.DATA(LS#<ion>).
The specific ion files created by this method has two special features, namely, the electron configuration for each indexed term is given as a symbolic string (called in ADAS the 'Eissner notation') equivalent to

$$n_1 l_1^{\zeta_1} n_2 l_2^{\zeta_2} \ldots\ldots n_m l_m^{\zeta_m}$$

Also, the field for the energies of individual orbitals used in the configurations under study must be present (see appxa-04). These orbital energies are denoted by

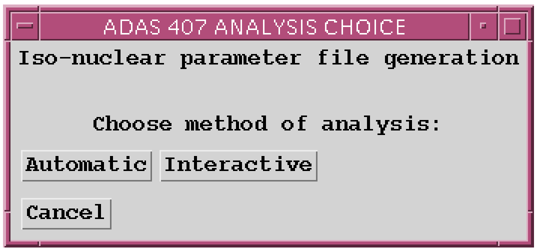
$$\{\varepsilon_k : k = 1,..,m\}$$

Apart from this enhanced rigidity in the use of the optional term naming character field, these files are of the standard ADF04 format.
With this supplementary information, analysis of two such specific ion files corresponding to adjacent ionisation stages z (called the 'ionising' or 'recombined' ion) and $z+1$ (called the 'ionised', 'recombining' or 'parent' ion) allows extraction of a wide range of useful numerical rate coefficient data and parameters of approximate forms for them. ADAS407 is a semi-automatic generator of such parameter sets. ADAS408 uses these parameter sets to generate standard (unresolved, stage to stage) ADF11 files under the year number ‘89’. These baseline data are only of moderate quality but can be created rapidly for any element.

ADAS407

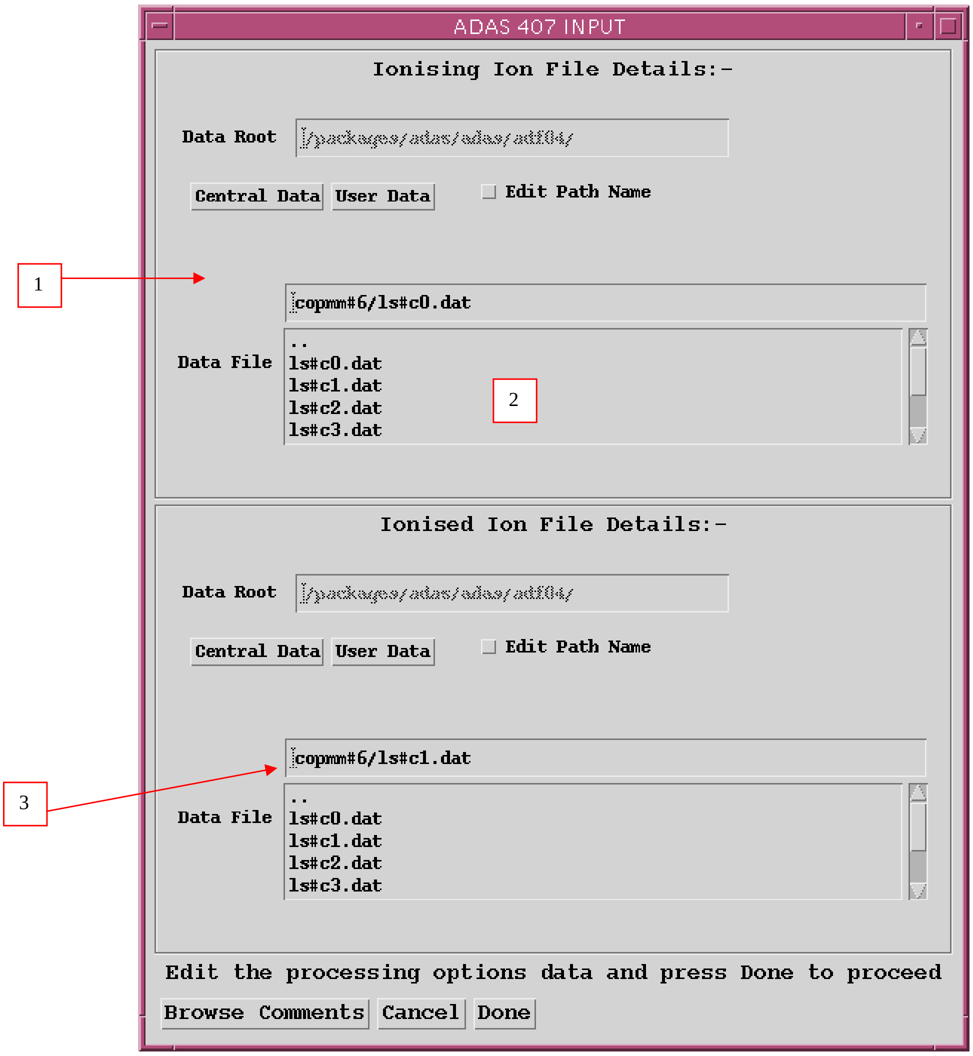
The code analyses specific ion files to obtain moderate accuracy numerical zero density recombination, ionisation and radiated power loss coefficient data. It deduces parameters of approximate forms for these coefficients which may be used to generate standard iso-nuclear master files.

The **analysis choice** window appears first as shown below.



The **file selection window** is shown below. *adf04* is the appropriate format for use by the program ADAS407. ADAS407 requires two such files, namely, for the ‘Ionising Ion’ and the ‘Ionised Ion’. If you wish to use personal data of this type, then as usual it should be held in a similar file structure to central ADAS with your identifier replacing the first *adas*, but in addition it must have the configuration fields in ‘Eissner’ notation and the orbital binding energy fields not empty.

1. The sub-window for the ionising ion is upper one. A Data root path to the correct data type *adf04* appears automatically. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Note that each type of data is stored according to its ADAS data format (*adf* number). Click the *User Data* button to insert the pathway to your own data. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.



ADAS 407 INPUT

Ionising Ion File Details:-

Data Root /packages/adas/adas/adf04/

Data File copmm#6/ls#c0.dat

..
ls#c0.dat
ls#c1.dat
ls#c2.dat
ls#c3.dat

Ionised Ion File Details:-

Data Root /packages/adas/adas/adf04/

Data File copmm#6/ls#c1.dat

..
ls#c0.dat
ls#c1.dat
ls#c2.dat
ls#c3.dat

Edit the processing options data and press Done to proceed

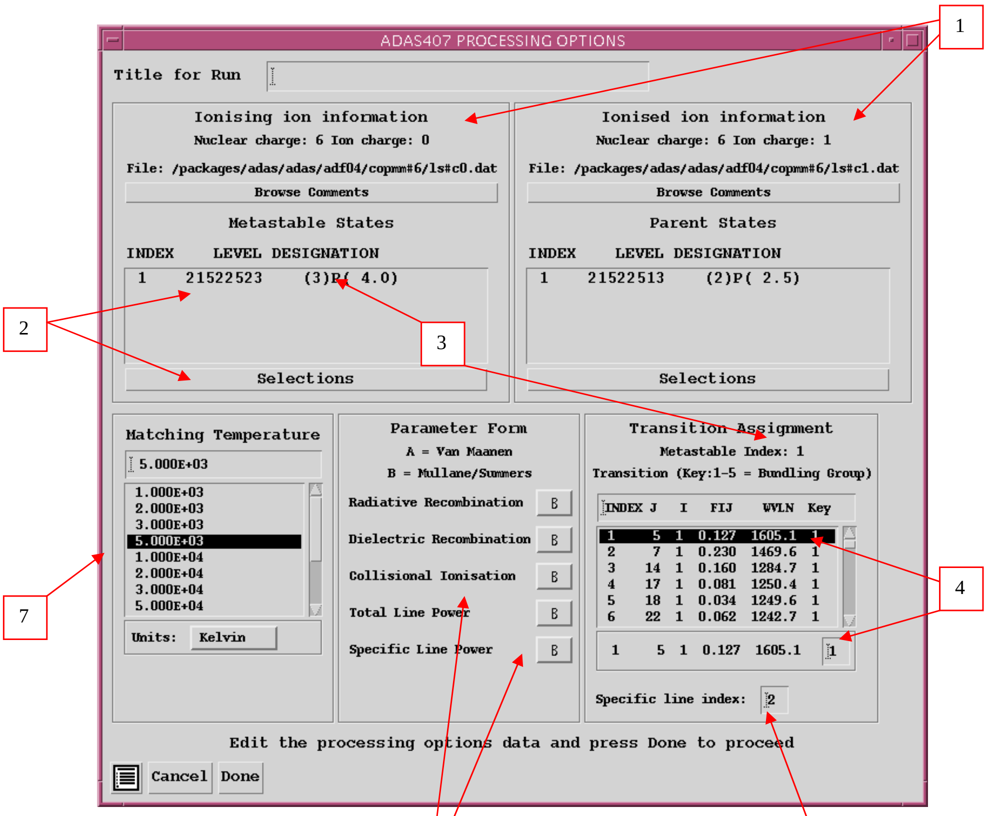
2. Available sub-directories are shown in the large file display window. Click on a name to select it. The selected name appears in the smaller selection window above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual data-files are

presented for selection. Data-files all have the termination *.dat*. Note that data-sets in sub-directories of the form */copss* and */copmm* are the only ones guaranteed to work.

3. When an ionising ion has been chosen, then the corresponding ionised ion has to be chosen . ADAS407 creates the expected file name and displays it if it exists. This name can be over-ridden in the usual manner.

The **processing options window** has the appearance shown below

1. At the top of the window, an arbitrary title may be given for the case being processed. Sub-windows for the ionising and ionised ions appear side by side below this. Summary data of the ions and the files opened are given first. The button *Browse Comments* in each sub-window again allows display of the information field section at the foot of the named ion file, if it exists.



ADAS407 PROCESSING OPTIONS

Title for Run

Ionising ion information
Nuclear charge: 6 Ion charge: 0
File: /packages/adas/adas/adf04/copmm#6/ls#c0.dat

Metastable States

INDEX	LEVEL	DESIGNATION
1	21522523	(3)P(4.0)

Ionised ion information
Nuclear charge: 6 Ion charge: 1
File: /packages/adas/adas/adf04/copmm#6/ls#c1.dat

Parent States

INDEX	LEVEL	DESIGNATION
1	21522513	(2)P(2.5)

Matching Temperature
5.000E+03

1.000E+03
2.000E+03
3.000E+03
5.000E+03
1.000E+04
2.000E+04
3.000E+04
5.000E+04

Units: Kelvin

Parameter Form
A = Van Maanen
B = Mullane/Summers

Radiative Recombination B
Dielectric Recombination B
Collisional Ionisation B
Total Line Power B
Specific Line Power B

Transition Assignment
Metastable Index: 1
Transition (Key:1-5 = Bundling Group)

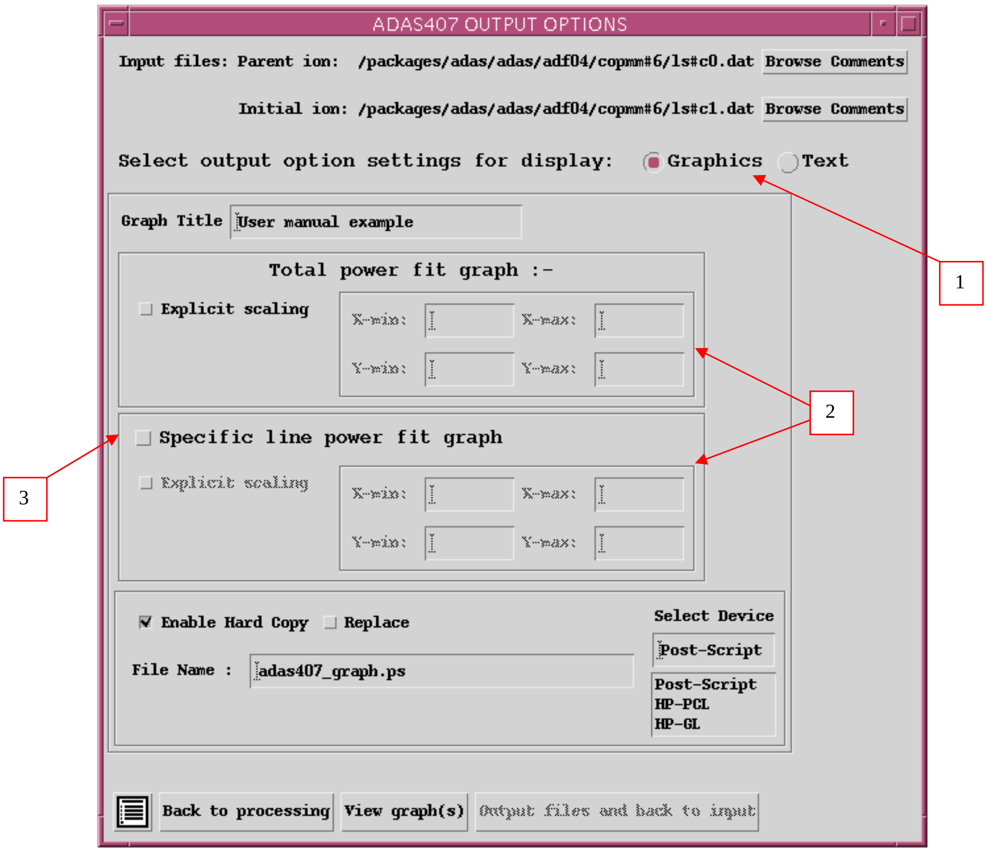
INDEX	J	I	FIJ	WVLN	Key
1	5	1	0.127	1605.1	1
2	7	1	0.230	1469.6	1
3	14	1	0.160	1284.7	1
4	17	1	0.081	1250.4	1
5	18	1	0.034	1249.6	1
6	22	1	0.062	1242.7	1
1	5	1	0.127	1605.1	1

Specific line index: 2

Edit the processing options data and press Done to proceed

2. The states of th ising and ionised ions to be treated as met le must then be decided r the ionising ion, we call these the metast and for the ionised ion, the parents. Click on the *Selection* button to see the full level list available for the ion. Click the toggle button opposite each level you wish switch on (or off) as a metastable. Notice the appearance of the configuration specification part of the level designation. The ‘21522523’ means $1s^2 2s^2 2p^2$ in ‘Eissner notation’ (see the ADAS User Manual for more details).

3. Click on the particular driving metastable of the ionising ion whose associated radiated power loss is to be analysed and displayed. This choice appears in the lower right sub-window,. In this sub-window, below the metastable index information a display window and associated selection window is present. The display window shows all the dipole collisional transitions in the ionising ion *adf04* file linked to selected metastable. The oscillator strength and wavelength of each transition is given.



Input files: Parent ion: /packages/adas/adas/adf04/copmm#6/ls#c0.dat

Initial ion: /packages/adas/adas/adf04/copmm#6/ls#c1.dat

Select output option settings for display: ● Graphics ○ Text

Graph Title: User manual example

Total power fit graph :-

☐ Explicit scaling

☐ Specific line power fit graph

☐ Explicit scaling

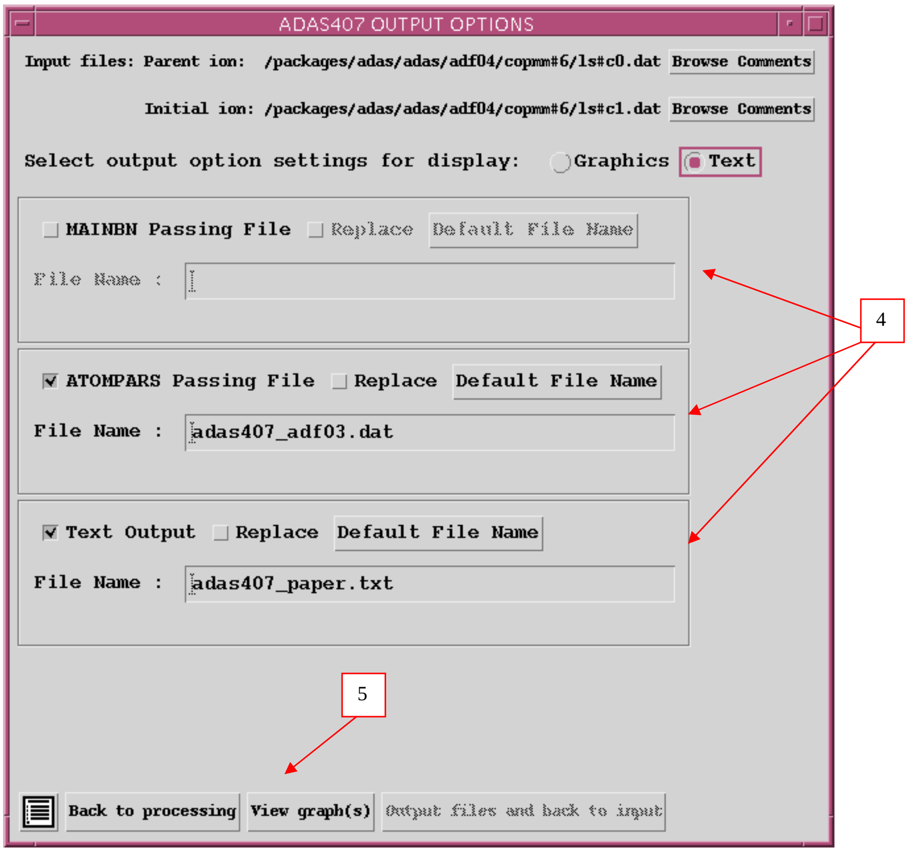
☒ Enable Hard Copy ☐ Replace

File Name : adas407_graph.ps

Select Device: Post-Script

4. ADAS407 seeks to represent the total radiated power driven by the selected metastable by that from up to five effective dipole transitions, called bundling groups. You must associate each transition in the display window with a bundling group. This is usually done by grouping those of similar wavelength. Mostly one or two bundling groups is sufficient. Click on a transition. It appears in the selection window below the display window. Enter the bundling group index in the small editable box at the right side and press *return*. The group index ('Key') appears in the display window along side the transition and the next transition appears in the selection window ready for assignment to a group.
5. The index of a specific line may be entered below the transition selection window. This is a line whose individual contribution to the total line radiated power you wish.

6. The various pieces of information obtainable from the pair of adjacent *adf04* files include the zero density radiative recombination coefficient, zero-density dielectronic recombination coefficient, the direct collisional ionisation coefficient, total zero-density line power radiative loss coefficient and the radiated power coefficient for the one selected transition (cf. 5 above). These are listed in the sub-window . Simple approximate forms are used to obtain these coefficients. For most of the coefficients an 'A' and 'B' choice of approximate forms are available. The 'A' forms have been used quite widely in fusion historically. The 'B' forms are better but may sometimes be unstable in fitting. We are in the process of tightening these up. Click on the selection button to the right of the type of coefficient to drop down the A or B choice menu.



Input files: Parent ion: /packages/adas/adas/adf04/copmm#6/ls#c0.dat

Initial ion: /packages/adas/adas/adf04/copmm#6/ls#c1.dat

Select output option settings for display: ○ Graphics ● Text

☐ MAINBN Passing File ☐ Replace

File Name :

☑ ATOMPARS Passing File ☐ Replace

File Name : adas407_adf03.dat

☑ Text Output ☐ Replace

File Name : adas407_paper.txt

7. For the total zero density line radiated power, the specific ion files allow quite an accurate numerical estimate. Choose an electron temperature in the sub-window at which you wish the approximate form and accurate numerical values to agree.

The **output options window** is shown above. Broadly it follows the pattern of other ADAS interrogation codes. However since a number of graphs and text outputs are possible, the window has been designed to avoid too much complexity on screen.

1. As usual, the input specific ion files under analysis are shown and can be browsed. Two buttons have been added, namely, *Graphics* and *Text*.

Activate *Graphics* and the standard graphical output sub-window appears. Activate *Text* and the standard text file output sub-windows appears instead.

2. In the Graphics case, there are two types of graph, namely, the total radiated power fit graph and the specific line power graph. The former is mandatory and the latter optional.
3. Click the appropriate box if you wish the specific line power fit graph. Default scaling of the chosen graph may be over-ridden by appropriate selections. Below this the usual hard copy may be enabled and a choice of type of output device made.

```
TOTAL LINE POWER COEFFICIENT VERSUS TEMPERATURE: USER MANUAL EXAMPLE

ADAS    : ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS407 V1.11 DATE: 17/11/02 TIME: 12:03
FILE    : /packages/adas/adas/adf04/copmm#6/ls#c0.dat                  ELEM: C + 0  MET: 1  FIT: B
KEY     : (FULL LINE - EXACT) (SHORT DASH - INITIAL)(LONG DASH - SIMPLE) (DOT DASH - OPTIMISED)
```

```
Plot  written to print file.
```

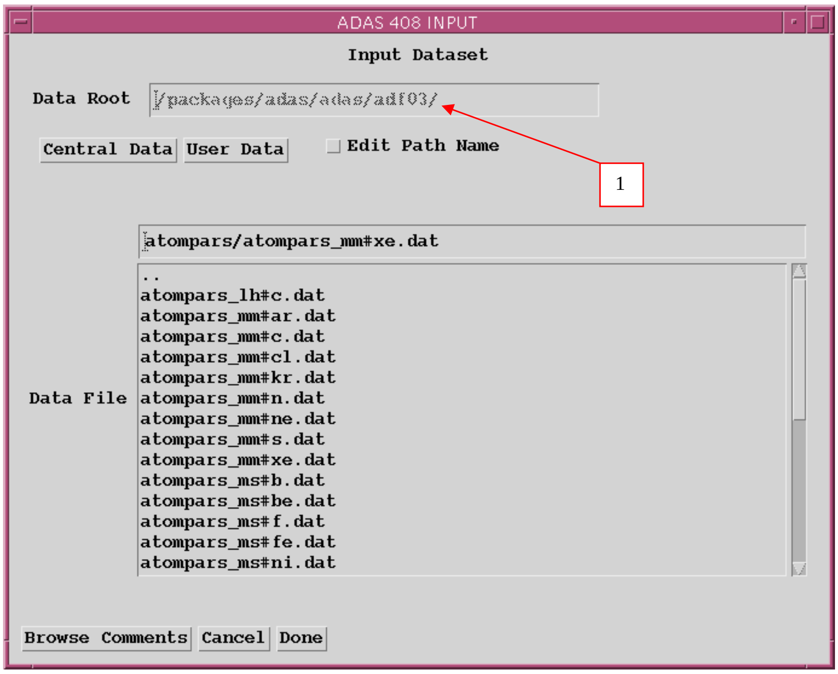
2. In the Text case, three output files are permitted, namely, the standard line printer text output file summarising the interrogation, the 'MAINBN' file at and the 'ATOMPARS' file. These are passing files which are placed by default in your */pass* directory as *mainbn.pass* and *atompars.pass.* The MAINBN file is the driving file for ADAS204. The ATOMPARS file is for use by ADAS408 and is of standard *adf03* type. The usual *Replace* and *Default File Name* buttons are present for all the output files.
5. Various completion buttons are available at d). Click the *View Graph* button to show the graph. *Back to Processing* returns you to the previous window for choice of another transition for analysis. Note that the settings from analyses carried out by you are accumulated. Click the *Output files and back to input* button to write the MAINBN and ATOMPARS passing file and then return to the input options window. In practise, this is the most convenient option since we usually carry on and process all of the ions of an iso-nuclear sequence in succession, assembling thereby a complete ATOMPARS file for an element in one go. The *Exit to Menu* icon takes you directly to the ADAS4 series menu.

ADAS408

The program uses parametric forms for zero density recombination, ionisation and radiated power loss coefficients to prepare standard (unresolved, stage to stage) iso-nuclear master files for a particular element. The iso-nuclear master files may be prepared over arbitrary ranges of electron temperature and electron density

The **file selection window** has the appearance shown below

1. Data root shows the full pathway to the appropriate data sub-directories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. The appropriate ADAS data format for input to this program is *adf03* ('atompars files'). Operation of this file selection window follows the usual pattern.



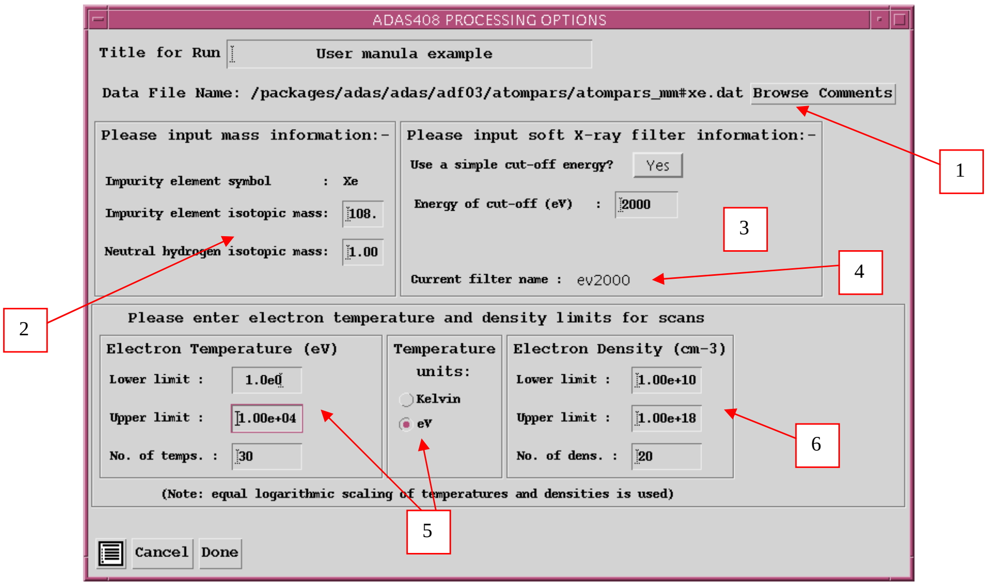
Data Root: /packages/adas/adas/adf03/

☐ Edit Path Name

Data File: atompars/atompars_mm#xe.dat

```
..
atompars_lh#c.dat
atompars_mm#ar.dat
atompars_mm#c.dat
atompars_mm#cl.dat
atompars_mm#kr.dat
atompars_mm#n.dat
atompars_mm#ne.dat
atompars_mm#s.dat
atompars_mm#xe.dat
atompars_ms#b.dat
atompars_ms#be.dat
atompars_ms#f.dat
atompars_ms#fe.dat
atompars_ms#ni.dat
```

The **processing options window** has the appearance shown below



ADAS408 PROCESSING OPTIONS

Title for Run: User manula example

Data File Name: /packages/adas/adas/adf03/atompars/atompars_mm#xe.dat

Please input mass information:-

Impurity element symbol : Xe

Impurity element isotopic mass: 108.

Neutral hydrogen isotopic mass: 1.00

Please input soft X-ray filter information:-

Use a simple cut-off energy? Yes

Energy of cut-off (eV) : 2000

Current filter name : ev2000

Please enter electron temperature and density limits for scans

Electron Temperature (eV)

Lower limit : 1.0e0

Upper limit : 1.00e+04

No. of temps. : 30

Temperature units: ○ Kelvin ● eV

Electron Density (cm-3)

Lower limit : 1.00e+10

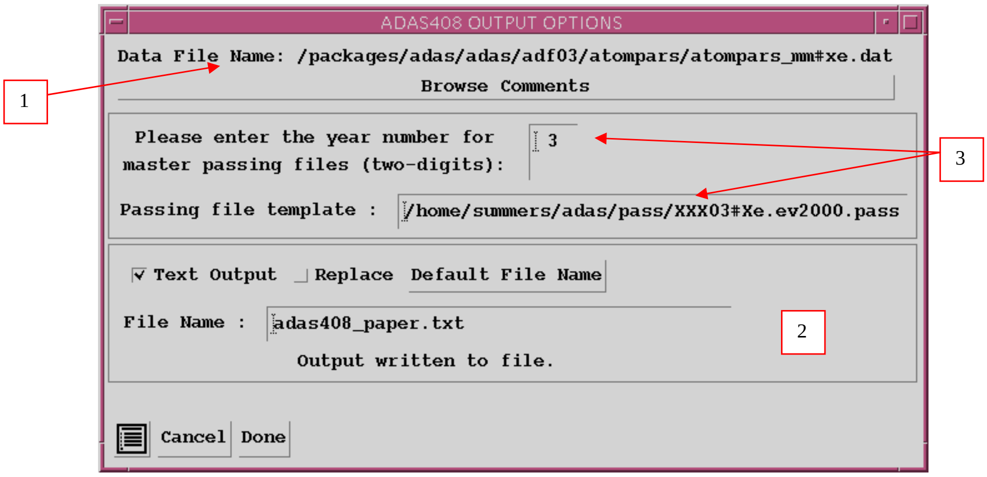
Upper limit : 1.00e+18

No. of dens. : 20

(Note: equal logarithmic scaling of temperatures and densities is used)

1. At the top of the window, an arbitrary title may be given for the case being processed. The name of the data file under analysis is shown. The button *Browse Comments* allows display of the information field section at the foot of the named atompars file, if it exists.
2. Enter the mass number for the actual isotope of the element of the atompars file present in the plasma. For information the element chemical symbol is displayed. Likewise, the mass number of hydrogen isotope constituting the primary plasma species is sought. Type the values in the editable boxes and press return.
3. In the adjacent window, a capability is given for modifying the output file of total radiated line power to include the attenuation through a soft-x-ray filter. Two choices are available, namely, a simple cut-off and a more elaborate representation of the characteristics of beryllium/silica windows. Click in the box to drop down a standard choice menu. In the beryllium/silica case thicknesses must be specified in the following two editable boxes.
4. A suitable 'filter name' is created by ADAS408 which appears as part of the output radiated power file name. In the simple cut-off case, the filter name has the prefix 'ev' followed by the numerical value of the cut-off energy in eV. In the true filter case, the filter name has the prefix 'ft' followed by the first two significant figures of the beryllium and silicon thicknesses.
5. The lower sub-windows allow the plasma electron temperature and electron density for production of the output *adf11* standard master files to be specified. For the temperatures, click on the required temperature units. This choice relates to the units used in the adjacent temperature range selection window. Specify lower temperature limit, upper temperature limit and number of temperatures in the editable boxes. ADAS408 then creates the temperature grid equally spaced in the logarithm. Note that the output files in fact contain the temperatures in eV (see the ADAS User Manual, appxb-11).
6. Similarly specify the electron density limits and number of grid points.

The **output options window** is of restricted form. It only offers the option of an output files.



Data File Name: /packages/adas/adas/adf03/atompars/atompars_mm#xe.dat

Please enter the year number for master passing files (two-digits): 3

Passing file template : /home/summers/adas/pass/XXX03#Xe.ev2000.pass

☑ Text Output ☐ Replace

File Name : adas408_paper.txt

Output written to file.

1. The name of the source atompars file to be used in the bulk generation of *adf11* data is repeated for information.
2. The standard line printer text output file summarising the options selected for ADAS408 is available. The *Replace* and *Default File Name* buttons are present for the text output file as usual.
3. The *adf11* iso-nuclear master file output comprises several files which are placed in your */pass* directory. Collections of *adf11* files are held by year number. Enter a two digit year number for the output. Note that any two digits are acceptable and ‘fictitious’ years can be used for special collections if so desired. Using the year number and the filter name (see 3.2.4 above) a passing file template is created. The ‘XXX’ of the template is replaced by the three letter codes of the iso-nuclear master file classes (‘acd’, ‘scd’ etc.) to create the actual output files. The filter name part of the template only appears in radiated power classes of iso-nuclear master files. Note also the presence of the element chemical symbol in the template. Unfiltered radiated power master files are created as well as the filtered ones. The former do not include a filter name as part of the whole file name.

There is no graphical output option.

Superstages and flexible partitioning

In the generalised-collisional-radiative picture, an element in a plasma is described by the abundances of all the metastables of every ionisation stage, by the effective recombination and ionisation coefficients which link them together and by the emission coefficients which are quasi-static with respect to and driven by these metastables. The complete set of populations, which are then in principle tracked in dynamic transport modelling, is large. However, not all populations are of equal importance and so grouping of populations may be appropriate. This is called a condensation and it reduces the problem to tracking the group populations with their equivalent effective recombination and ionisation coefficients and emission coefficients. The specification of a grouping is called a *partition*.

For example a parent partition with six members may be grouped into two child partition members with $1_c=\{1,2\}$ and $2_c=\{3,4,5,6\}$. We can envisage a particular partition having parent and grandparent partitions and so on in *layers* back to a *root partition*. This is the basic idea, but it can be made more complete and consistent with earlier work in both the *CR* and *GCR* pictures.

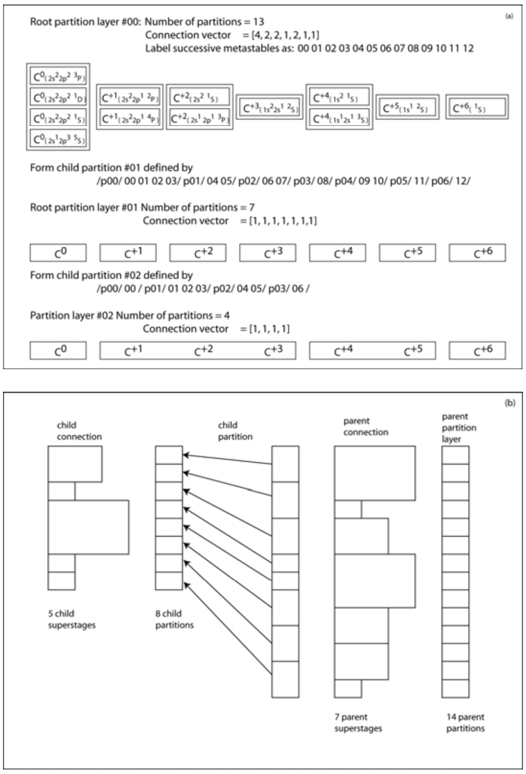


Fig: (a) Metastables of carbon in the resolved *GCR* picture. The child partition grouping to form the stage to stage picture is shown as the boxes enclosing the metastable sets. The connection vector specifies the metastables which are close-coupled. It corresponds in this particular illustration to the child partition grouping. (b) The general partitioning picture with independent child partition groupings and parent connection vector. Note that the child connection vector is determined from the child partition definition and the parent connection vector

Consider the metastables of carbon in the *GCR* picture, as shown schematically in figure-a. The complete set of thirteen metastables (including the bare nucleus) comprise the members of a partition. If the metastables of each ionisation stage are grouped together, then the child partition is composed of members which are the ionisation stages. Then further grandchild partitions can be formed as illustrated. There are really two starting points for partitioning, called the *#00* or *#01* *root partition layers* depending on whether we are in the *GCR* picture of resolved metastables or the unresolved *CR* picture. For computation, a partition is conveniently written as a string, so that the two root partitions layers for carbon appear respectively as

```
        //#00//p00/00/p01/01/p02/02/p03/03/p04/04/
                p05/05/p06/06/p07/07/p08/08/p09/09/
                p10/10/p11/11/p12/12/p13/13/
```

and

```
        //#01//p00/00/p01/01/p02/02/p03/03/p04/04/
```

```
p05/05/p06/06/
```

The child *#01* stage-to-stage partition of carbon for computation from the *#00* root partition is

```
//#01//p00/00 01 02 03/p01/04 05/p02/06 07/
          p03/08/p04/09 10/p5/11/p6/12/
```

It should be noted that the metastables are not all on the same footing. Unlike ionisation stages which are each (usually) only coupled to the two adjacent stages up and down, themetastables are in groups which are close-coupled (for example the first four and the next two and so on). This close coupled grouping is specified by the *connection vector*, a name which will be familiar to those who have worked with ADAS *GCR*} data. The connection vector for carbon in the #00 root partition is (4,2,2,1,2,1,1). The connection vector is similar to a range vector and the range vector for grouping into the *#01* stage-to-stage partition from the *#00* root partition is the connection vector. Introduce a new name *superstage* for the members of a partition which are close coupled as specified by the connection vector. In the special case of the *#01* partition of carbon, the superstages are simply ordinary stages. The connection vector and range vector of a child partition are in the general case independent items. So a child partition can be formed from *#00* root partition which subdivides connected metastables into different child partition members and leaves a non-trivial connection vector for the child partition. This general case is illustrated in figure-b. With light elements, in usual plasma conditions, ionisation is a single electron loss process from ionisation stage. For heavy element ions, multiple electron loss through shake-down and shake-off is more likely. This would result in non-trivial connection vectors and superstages. The heavy element baseline has the root partition layer *#01* and in child partitions, the connection vector is trivially all `ones'.

In practice, superstage condensation (bundling) is influenced by the shell structure of the element. There are two situations of interest at this time. Firstly there is aggressive condensation (bundling) aimed at enabling heavy elements to be handled with the same economy as light elements in sophisticated 2-d or 3-d transport codes. Secondly, there is condensation related to spectroscopy and the occurrence of quasi-continuum. It is in these contexts that the additional classes in the *adf11* data format and those in the *adf15* and *adf40* formats are determined for the child partition in the following two sub-sections.

The natural partition and spectroscopy

Ions with closed shell configurations have an extended region of existence (in electron temperature) in a plasma. They and adjacent alkali-like ions are significant radiators of a resolvable line spectrum of diagnostic value. Sets of ions associated with a partially filled shell, particularly for heavy species, give a complex overlapped spectrum which is difficult to identify and resolve. They are usefully grouped. A map of the fractional variation of ionisation potential $2(I_{z+1} - I_z)/(I_{z+1} + I_z)$ between successive ions of every element, as shown in the figure-a below, highlights the shell structure. We select ions corresponding to peaks and their immediate neighbours as individuals in a partition and group the others. Setting a fraction of the a running mean as a variance for stage individualising allows automatic partitioning. We call this the *natural partition*.

It is useful to be able to preview the natural partition and its approximate implications for the temperature distribution of superstages before executing the substantive generation of a complete ADAS data for a new child partition layer. An IDL procedure accomplishes this:

preview_natural_partition.pro

For example at the IDL command line type

```
IDL> preview_natural_partition,z0=73,plot_type=3,te_min=1,te_max=1e6,te_plot=1000
IDL> preview_natural_partition,z0=73,plot_type=4, partition=all
IDL> preview_natural_partition,z0=73,plot_type=1
IDL> preview_natural_partition,z0=73,plot_type=2
IDL> adas_writefile, file='partition.txt', all=all
```

The text lines of the parent and child partition layers, as required for driver scripts, are written to the screen and the figure is displayed. There are keywords to send the text lines and graphs to files. Plots available are 1: ionisation potential variation, 2: quasi-equilibrium fractions within a superstage, 3: stage-to-stage ionisation balance, 4: superstage ionisation balance. The output temperature used for fractional abundances within a superstage for the plot of type 2 is representative.

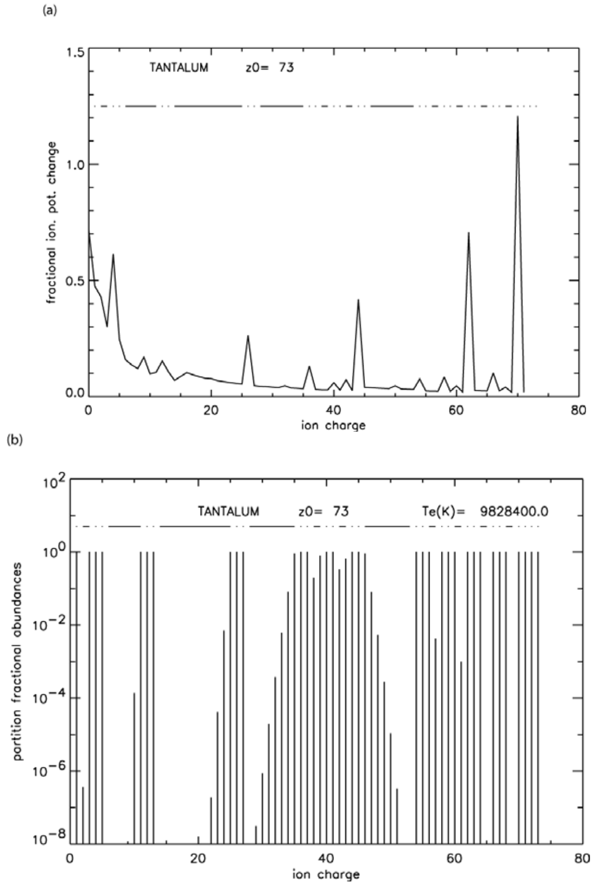


Figure (a) Fractional variation of ionisation potential for the ions of tantalum. The peaks indicate the quantum shell boundaries. The natural partition criterion is set at the 3σ level and the individualised stages and bundles are indicated by dots and bars respectively above the graph. (b) Quasi-equilibrium fractions for each ionisation stage within a bundle with respect to the whole bundle.

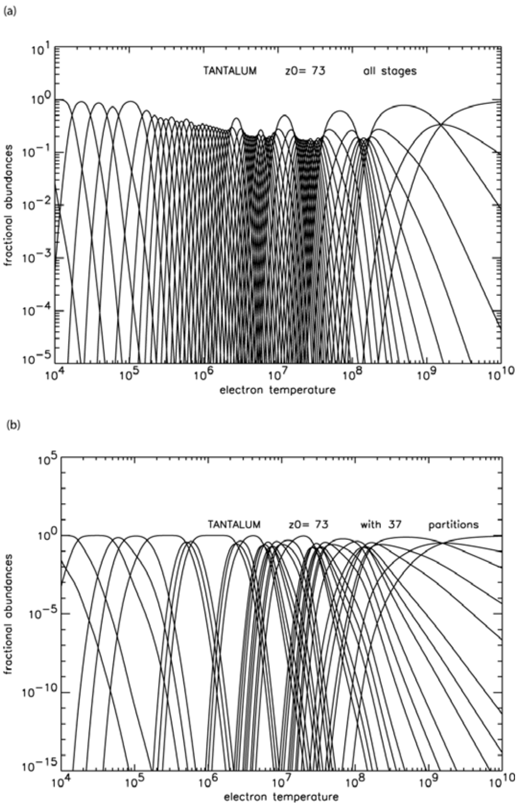


Figure: Ionisation balance for tantalum vs electron temperature. (a) Equilibrium fractional abundances with unresolved individualised stages corresponding to the *# 01* partition. (b) Equilibrium fractional abundances for ionisation stage bundles in the natural partition of the previous figure.

For superstages, photon emissivity coefficients still exist, but they are driven by the superstage. That is the actual emissivity of a line is obtained by multiplying the coefficient by the electron density and the population of the driving superstage. Since a child superstage has implicitly equilibrium ionisation fractional abundances imposed within the parent superstage contributors, the superstage emissivity coefficient is a bit like the astrophysicist's individual spectrum line *contribution functions* – see ADAS405, where they are called *GTN*s. The latter though include full ionisation equilibrium. In cases where superstages are useful there are often huge numbers of spectral lines in a typical observed wavelength range, so it is easiest to deal with the whole spectral interval and introduce so-called feature emissivity coefficients (*adf40*). The latter superpose all the lines in the interval with a broadening function. Feature emissivity coefficients work just the same with superstages. For a spectral interval $\lambda_0 < \lambda < \lambda_1$, written compactly as [0,1], the envelope feature photon emissivity function vector (that is generally a pixellation vector over the spectral interval) is

$$FGTN^{[\#02][0,1](j)} = \sum_{i_0}^{i_1} FGTN^{[\#01][0,1](i)} \left(\frac{N^{[\#01](i)}}{N^{[\#02](j)}} \right)_{eq}$$

where the *FGTN*s are the generalisation of the astrophysicist's individual spectrum line *contribution functions* which we introduced with ADAS405 and called *GTN*s. Recall that a *GTN* is just a photon emissivity coefficient (adf15) multiplied by the equilibrium fractional abundance of the ionisation state in the *CR* picture. **The above superstage PEC and FGTN capabilities are just being finalised in central ADAS – some are missing in release v3.0.**

Superstage condensation and plasma transport models

As discussed earlier, a main advantage of the condensation is in economising complex transport calculations without severe loss of accuracy. However there are some new issues which must be addressed first before superstages are compatible with transport models. A superstage, which is a composite of several ionisation stages has a superstage charge which depends on electron temperature and electron density. It is a collisional-radiative quantity. In fact fluid transport models make use of the ion charge, squared ion charge and ionisation potential in addition to familar quantities such effective ionisation, recombination, radiated power and electron energy loss coefficients. The *adf11* classes must be extended with these extra quantities, which in superstages are all collisional-radiative quantities. In ADAS, these are given the mnemonics *zcd*, *ycd* and *ecd*. ADAS codes and data structures have been adjusted accordingly and there is a revised specification of *adf11*. The definition and computation of *zcd* and *ycd* are straightforward. *ecd* is more subtle. Consider a lowest superstage which is a condensation of low ionisation stages in addition to the first. Then from the point of view of energy conservation, the superstage has a birth energy associated with its appearance in the plasma. In the usual (simplified) ionisation stage picture, a neutral has zero birth energy, which is implicit in the computer codes. For consistency then, there is a 0^{th} block in the *adf11/ecd* dataset which is the birth energy of the lowest superstage. The *#01* root partition has all zeros in this block. In fact this problem is already present in the *GCR* picture, since the energy of metastables of the lowest ionisation stage are usually ignored. A properly formed *ecd* in the *GCR* picture should contain excitation energies from the lowest metatable (the ground state) to higher metastables of the same stage as well as ionisation potentials to the metastables of the next stage. These data are available for selected elements within ADAS under data format *adf00* in data sets of the form

<el.symb.>_ls.dat
<el.symb.>_ic.dat

for *ls* and *ic* cases in addition to the usual unresolved form
<el.symb.>.dat
The FORTRAN subroutine *xxdata_00.for* returns extra information on the metastables, including their configurations. The IDL procedure can also acquire these data if the keyword */ls* or */ic* is appended to the call.

As the historical ADAS *adf11* database does not contain *zcd, ycd* and *ecd*, a PERL script can be supplied to create them as

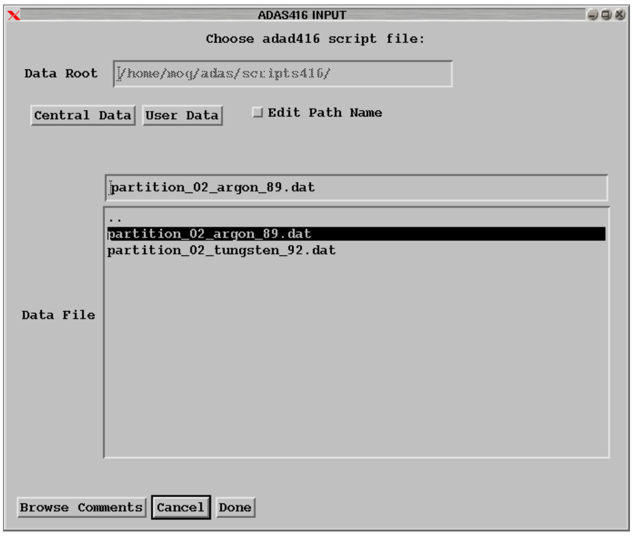
/home/adas/offline_adas/adas4#1/scripts/generate_adf11_classes_10-12.pl

By default this scans the */home/<user>/adas/adf11* subdirectory for the various year numbers and creates matching zcd, ycd and ecd classes for that year number back in */home/<user>/adas/adf11*. It will overwrite *zcd*, *ycd* and *ecd* data already there. Both resolved and unresolved classes are handled and a running commentary is provided on progress and problems encountered. Two arguments may be given in the call to *generate_adf11_classes_10-12.pl* to alter the input subdirectory and the output subdirectory respectively. It is unlikely that you will need this, since ADAS408 can also produce them. It is more a matter for central ADAS with a long history of *adf11* datasets

ADAS416 - Generating the superstage} condensation

The creation of a data for a new child partition is largely automatic. It is in the province of ADAS416. The interactive code, selected from the series 4 menu, follows the usual pattern. It starts with an input screen, which seeks a script for the superstage compression. These are allocated to the /…/<uid> /adas/scripts416 directory. It is expected that the user will have his/her own scripts, the central ADAS ones only being samples, such as shown for argon below. The partition specification starts at the root layer #01 in which each ionization is in it own partition. The layer #02 combines the stages in partitions at the user's wish. The choice of best partitioning is a subject of investigation in association with transport models, however the concept of 'natural partition' is helpful for the spectroscopist. The complete package for superstage compression includes a preview capability in IDL for the original and superstage ionization balance in natural partition, prior to the actual evaluation using ADAS416.

```
argon

89
unresolved

parent pathways
---------------
gcr  :  /home/summers/adas/adf11/***89/***89_ar.dat
pec  :  /home/summers/adas/adf15/pec06#18/ar_01/ic#ar**.dat
f-pec:  /home/summers/adas/adf40/fpec06#18/ar_01/ic#ar**.dat

partition specification
-----------------------
//#02/p00/ 00/p01/ 01/p02/ 02 03 04 05 06/p03/ 07/p04/ 08/
      p05/ 09 10 11 12 13 14/p06/ 15/p07/ 16/p08/ 17/p09/ 18/
//#01/p00/ 00/p01/ 01/p02/ 02/p03/ 03/p04/ 04/p05/ 05/p06/ 06/p07/ 07/p08/ 08/
      p09/ 09/p10/ 10/p11/ 11/p12/ 12/p13/ 13/p14/ 14/p15/ 15/p16/ 16/p17/ 17/
      p18/ 18/
---

child pathways
--------------
gcr  :  /home/summers/adas/adf11/***89/***89_ar_02.dat
pec  :  /home/summers/adas/adf15/pec06#18/ar_02/ic#ar**.dat
f-pec:  /home/summers/adas/adf40/fpec06#18/ar_02/ic#ar**.dat

C-----------------------------------------------------------------------------
C  sample scrip416 file
C
C  Notes:
C         (1) '***' in gcr pathway denotes 'acd', scd' etc
C         (2) '***' in pec, gtn, f-pec and f-gtn pathways denote 'llr', 'pjr'
C                   or pju.
C         (3) '**'  in pec, gtn, f-pec and f-gtn pathways denote partition
C                   member index.  This is the ion charge for the #01 root
C                   partition.  The indexing begins at 00
C         (4) Leave pathways which are not needed as blanks
C         (5) Choices at line 4 are 'resolved' or 'unresolved'
C         (6) Partitions are given in decreasing level order, that is
C             child before parent. This is the same rule as is used in
C             adf11 files with partition blocks and is required by the
C             partition block reader xxrptn.for.
C
C
C  Author:   Hugh Summers
C  Date  :   18 august 2005
C
C-----------------------------------------------------------------------------
```

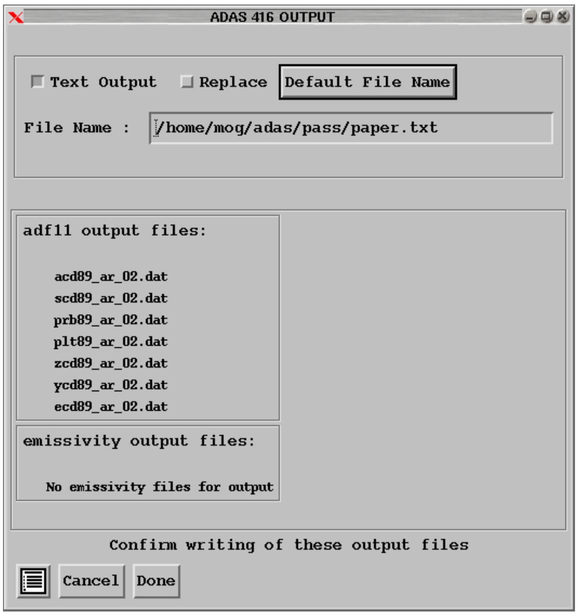


Data Root: /home/mog/adas/scripts416/

partition_02_argon_89.dat

```
..
partition_02_argon_89.dat
partition_02_tungsten_92.dat
```

The input screen is shown below and, following *Done* leads directly to the output screen where the options of wrting the new partition are given. This screen reacts to the available ADF11 files for the parent partition. Note the new classes *zcd*, *ycd* and *ecd* . The output ADF11 files uses an extended specification which includes partition and connection vector information at the head of the file. New ADF11 reading routines are in place in the ADAS libraries to which deal with the extended formatting as well as reading older versions of ADF11.



☐ Text Output ☐ Replace

File Name : /home/mog/adas/pass/paper.txt

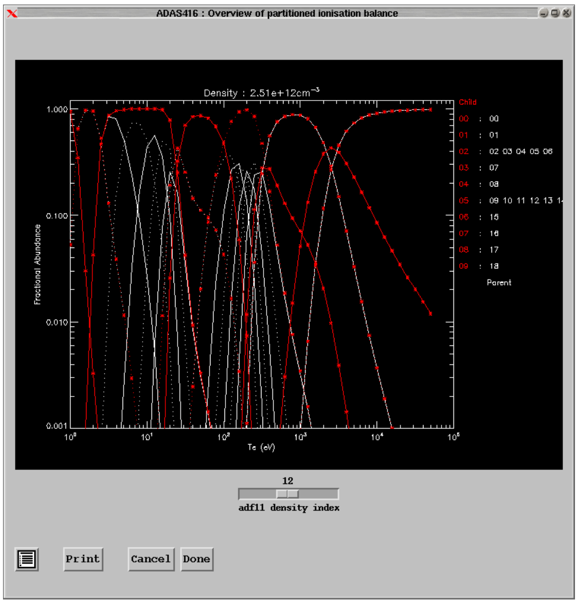
adf11 output files:

acd89_ar_02.dat
scd89_ar_02.dat
prb89_ar_02.dat
plt89_ar_02.dat
zcd89_ar_02.dat
ycd89_ar_02.dat
ecd89_ar_02.dat

emissivity output files:

No emissivity files for output

Confirm writing of these output files



12
adf11 density index

The main calculations are done by a FORTRAN code *adas416.for*, but as usual can be initiated from the IDL command line as \\

```
IDL> z0 = 74
IDL> class_list =  ['acd' 'scd' 'plt' ]
IDL> adas416_script =  '$ADASHOME/adas/scripts416/partition_02_tungsten_1992.dat'
IDL> run_adas416,  z0=z0, adas416_script=adas416_script
```

or

```
IDL> run_adas416,  z0=z0, adas416_script=adas416_script, class_list=class_list
```

or

```
IDL> run_adas416, z0=z0, adas416_script=adas416_script,  class_list=class_list,
                 /adf11_only
```

where the second form restricts the *adf11* classes handled and the third restricts to adf11 data only, omitting adf15 and adf40 processing. This overrides the script driver. Note that the procedure will terminate if the *adf11* classes *acd* and *scd* are not present in the unresolved case (or *acd*, *scd*, *qcd*, *xcd* in the resolved case - that is when the connection vector is non-trivial. The parameter *z0* is merely a check if the script driver does name the element explicitly.

ADAS data format specifications, especially adf11, adf15 and adf40 have been modified to cope with heavy elements and superstage condensation. Updated access codes xxdata_11.for, xxdata_15.for and xxdata_40.for read the new datasets and all older versions transparently to the user.

Lecture 4 Charge exchange and beam emission spectroscopy

Preliminaries

Charge exchange spectroscopy is driven by reactions of the form

$$X^{+z_0} + D^0_{beam}(1) \rightarrow X^{+z_0}(nl) + D^+_{beam}$$

in which an electron is captured from a donor atom in its ground (or an excited) state. The principal application is usually to capture by the bare nuclei of impurity atoms in the plasma from the ground state of deuterium, helium or lithium atoms in fast neutral beams. Subsequently the hydrogen-like impurity ion radiates as

$$X^{+z_0-1}(n'l') \rightarrow X^{+z_0-1}(n''l'') + h\nu$$

Composite spectral line features of the form $n' \rightarrow n''$ are observed made up from unresolved $n'l' \rightarrow n''l''$ multiplet components. Charge exchange line features often involve high principal quantum shells and occur over wide spectral ranges including the visible range. In general the populations of receiver levels are modified by redistributive collisions with plasma ions and electrons and by fields before radiation emission occurs

The programs of series ADAS3 are associated with neutral beams of hydrogen or helium isotopes and there are two streams of modelling. The first stream is concerned with modelling and detailed spectral line emission from hydrogen-like impurity ions in a plasma following charge transfer from fast neutral beams. It commences with a collection of state selective charge transfer cross-section data at n, nl or nlm resolution (type ADF01) spanning an extended region of collision energies and n-shells and in some cases different sources. For interpretation of charge exchange emission lines, effective emission coefficients for relevant spectral lines emitted by the receiver are required. These are archived in ADAS data format ADF12. They require special collisional-radiative population calculations for their evaluation. There are two collisional-radiative processing options, namely for calculations in the *bundle-nl* (ADAS308) or *bundle-nlj* (ADAS306) approximations. The programs ADAS308 and ADAS306 predict data for arbitrary lines at a fixed set of conditions and show extensive detail of the line emission. It is convenient to have available more automatic codes which generate ony tables of ADF12 coefficients over ranges of plasma parameters without the intervening displays. This capability is provided by ADAS309 and ADAS307 for the bundle-nlj and bundle-nl pictures respectively. The latter are termed scanning versions of the codes. The associated codes for interrogation of the fundamental state selective cross-section database and the effective charge exchange emission coefficient database are ADAS301 and ADAS303 respectively.

The ADAS data formats format

The various relevant classes of data are

adf01	bundle-n and bundle-nl charge exchange cross-sections
adf02	ion impact cross-sections with named participant
adf12	charge exchange effective emission coefficients
adf21	effective beam stopping coefficients
adf26	bundle-n populations of excited states in beams

ADF01

For a specified relative collision energy E_i belonging to the tabulation, let the total cross section be $\sigma_{tot}(E_i)$ and the n-shell cross-sections be $\sigma_n(E_i)$. The latter are tabulated for $n_{\min} \le n \le n_{\max}$ for some $n_{\min}$ and $n_{\max}$. For $n \ge n_{\max}$ extrapolation is assumed of the form

$$\sigma_n(E_i) = (n_{\max}/n)^{\beta(E_i)}\,\sigma_{n_{\max}}(E_i)$$

The parameter $\beta(E_i)$ is deduced from $\sigma_{n_{\max}-1}(E_i)$ and $\sigma_{n_{\max}}(E_i)$ and is tabulated in the data set. The $\sigma_n(E_i)$ are normalised to the total cross-section so that, using the extrapolation equation for $n \geq n_{\max}$

$$\sigma_{tot}(E_i) = \sum_{n=n_{\min}}^{\infty} \sigma_n(E_i)$$

Explicit l-subshell cross-sections $\sigma_{nl}(E_i)$ are tabulated for $n_{\min} \leq n \leq n_{\max}$ and $0 \leq l \leq n-1$. In extrapolation there are two cases.

Case 1: No *l* subshell subdivision parameters are given in the ADF01 dataset.. It is assumed that the l distribution for $n > n_{\max}$ is the same as for $n_{\max}$ so that

$$\sigma_{nl}(E_i) = \begin{cases} \sigma_{n_{\max}l}(E_i)(\sigma_n(E_i)/\sigma_{n_{\max}}(E_i)) & for\ l \leq n_{\max}-1 \\ 0 & for\ l \geq n_{\max} \end{cases}$$

4.1.3

Case 2: *l* subshell parameters are given in the the ADF01 dataset. The parameters are obtained as a fit to *l*- subshell cross-section data for a particular n-shell using the program ADAS107. The parameterisation identifies an *l*-type , parameter $ltyp(E_i)$ and an approximate *l* (non integral) at which the cross-section behaviour changes from rising at low *l* to falling at high *l*, parameter $xlcr(E_i)$. The behaviour is then given by

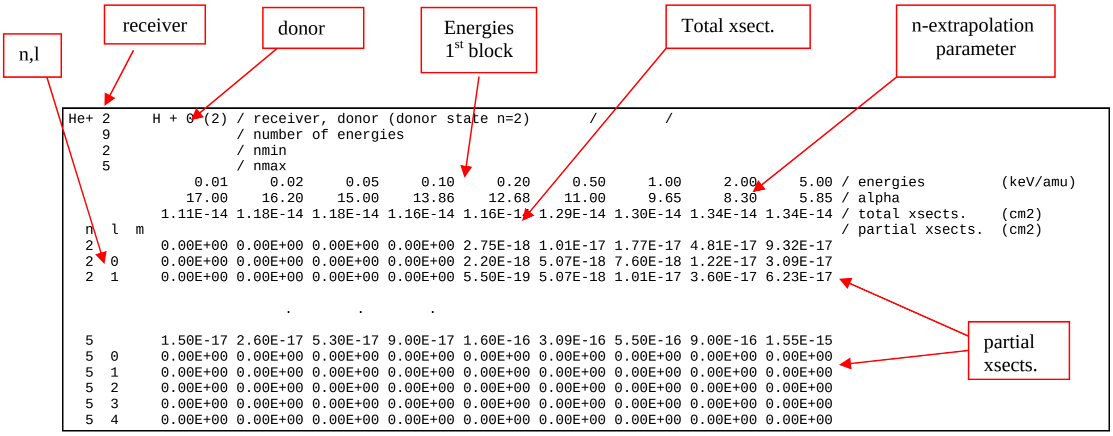
$$\sigma_{nl}(E_i) \sim \begin{cases} (2l+1)^{pl2} & for\ l < xlcr \\ \exp(-(l-xlcr)^{pl3}) & for\ l < xlcr \end{cases}$$

The normalisation

$$\sigma_n(E_i) = \sum_{l=0}^{n-1} \sigma_{nl}(E_i)$$

is maintained while the sharpness of the switching between the two forms varies with the *l*-type. A detailed description is given in ADAS107.

A typical ADF01 organisation is shown for H^0 donor to He^2 receiver

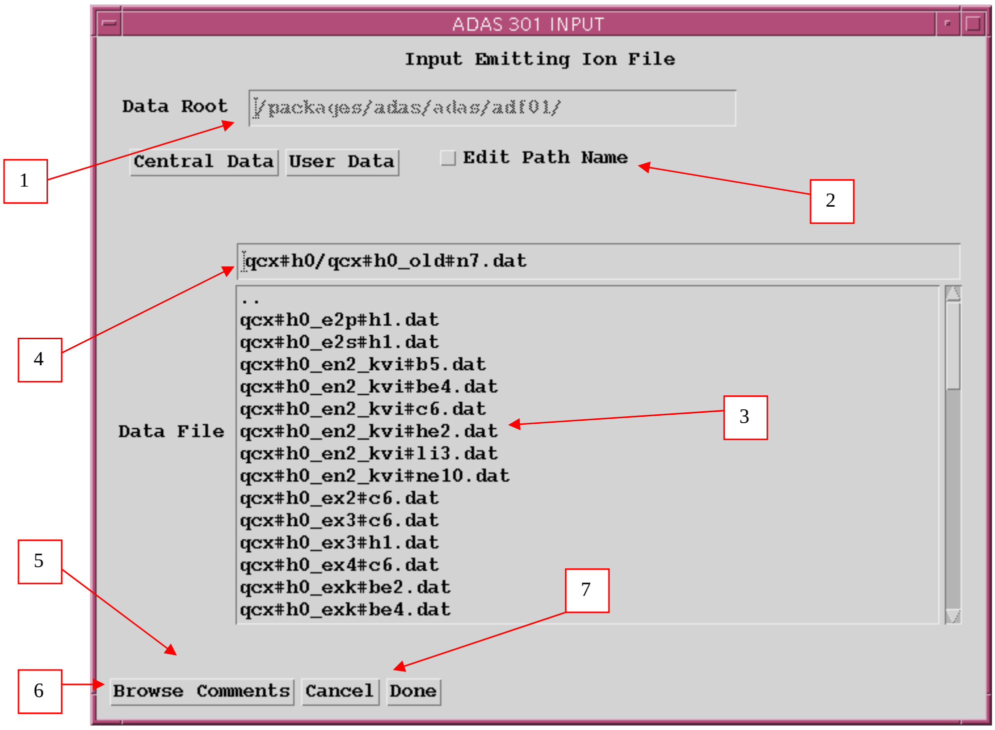


```
He+ 2     H + 0 (2) / receiver, donor (donor state n=2)       /        /
    9               / number of energies
    2               / nmin
    5               / nmax
               0.01     0.02     0.05     0.10     0.20     0.50     1.00     2.00     5.00 / energies         (keV/amu)
              17.00    16.20    15.00    13.86    12.68    11.00     9.65     8.30     5.85 / alpha
           1.11E-14 1.18E-14 1.18E-14 1.16E-14 1.16E-14 1.29E-14 1.30E-14 1.34E-14 1.34E-14 / total xsects.    (cm2)
  n  l  m                                                                                  / partial xsects.  (cm2)
  2        0.00E+00 0.00E+00 0.00E+00 0.00E+00 2.75E-18 1.01E-17 1.77E-17 4.81E-17 9.32E-17
  2  0     0.00E+00 0.00E+00 0.00E+00 0.00E+00 2.20E-18 5.07E-18 7.60E-18 1.22E-17 3.09E-17
  2  1     0.00E+00 0.00E+00 0.00E+00 0.00E+00 5.50E-19 5.07E-18 1.01E-17 3.60E-17 6.23E-17


                          .        .        .


  5        1.50E-17 2.60E-17 5.30E-17 9.00E-17 1.60E-16 3.09E-16 5.50E-16 9.00E-16 1.55E-15
  5  0     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  1     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  2     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  3     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  4     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
```

ADAS301

The code interrogates state selective charge exchange cross-section files of type ADF01. Data may be extracted for capture to a selected n-, nl-or nlm-shell of a hydrogen-like or lithium-like receiving ion depending on the ADF01 file. The data may be interpolated using cubic splines to provide cross-sections at arbitrarily chosen impact energies. A minimax polynomial approximation is also made to the source data. The source and interpolated cross-section data are displayed and a tabulation prepared. The tabular and graphical output may be printed and include the minimax polynomial approximation.

The **file selection window** is shown below.



Data Root: /packages/adas/adas/adf01/

Data File: qcx#h0/qcx#h0_old#n7.dat

```
..
qcx#h0_e2p#h1.dat
qcx#h0_e2s#h1.dat
qcx#h0_en2_kvi#b5.dat
qcx#h0_en2_kvi#be4.dat
qcx#h0_en2_kvi#c6.dat
qcx#h0_en2_kvi#he2.dat
qcx#h0_en2_kvi#li3.dat
qcx#h0_en2_kvi#ne10.dat
qcx#h0_ex2#c6.dat
qcx#h0_ex3#c6.dat
qcx#h0_ex3#h1.dat
qcx#h0_ex4#c6.dat
qcx#h0_exk#be2.dat
qcx#h0_exk#be4.dat
```

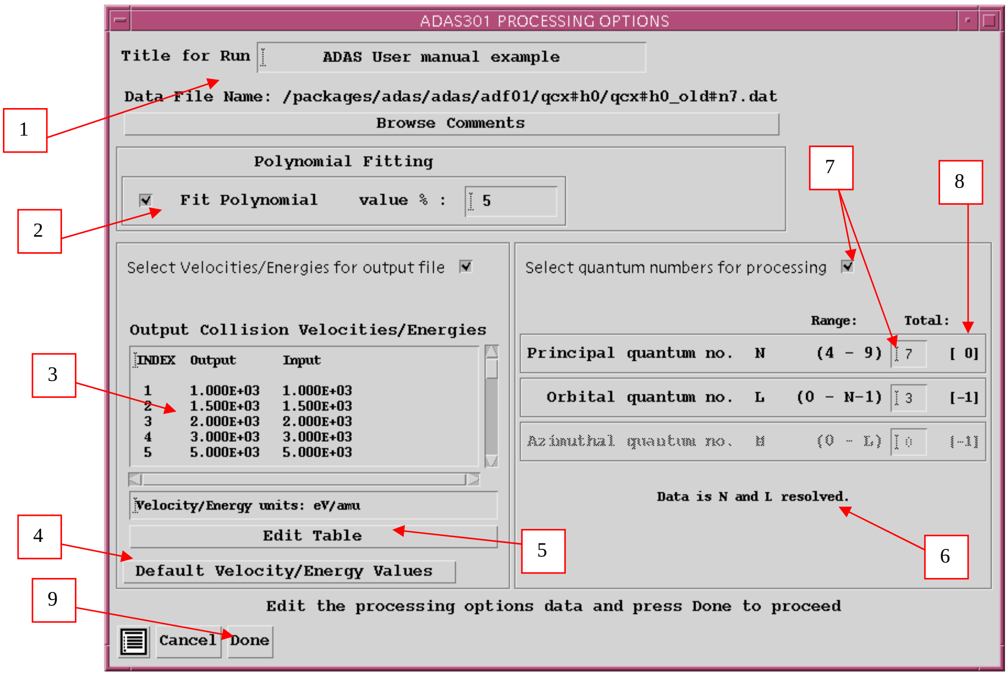
1. Data root shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type – ADF01 in this case. Note that each type of data is stored according to its ADAS data format (*adf* number). Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*, to use this facility.
2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
3. Available sub-directories are shown in the large file display window. There are a large number of these, stored by donor which is usually neutral but not necessarily so (eg. *qcx#h0*). The individual members are identified by the subdirectory name, a code and then fully ionised receiver (eg. qcx#h0*_old#c6.dat*). The data sets generally contain *nl*-resolved cross-section data but *n*-resolved and *nlm*-resolved are handled. Resolution levels must not be mixed in datasets. The codes distinguish different sources.The first letter *o* or the code *old* has been used to indicate that the data has been produced from JET compilations which originally had parametrised *l*-distribution of cross-sections. The nl-resolved data with such code has been reconstituted from them. Data of code *old* is the preferred JET data. Other sources codes include *ory*

(old Ryufuku), *ool* (old Olson), *ofr* (old Fritsch) and *omo* (old molecular orbital). There are new data such as *kvi*.

4. Click on a name to select it. The selected name appears in the smaller selection window above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
5. Once a data file is selected, the set of buttons at the bottom of the main window become active.
6. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.
7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

The **processing options window** has the appearance shown below

1. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being analysed is also shown. The button *Browse Comments* again allows display of the information field section at the foot of the selected dataset, if it exists.
2. The output data extracted from the datafile, a ‘charge exchange cross-section’, may be fitted with a polynomial. This is as a function of relative collision energy per atomic mass unit (eV/amu). Clicking the *Fit Polynomial* button activates this. The accuracy of the fitting required may be specified in the editable box. The value in the box is editable only if the *Fit Polynomial* button is active
3. Your settings of collision velocity/energy (output) are shown in the display window. The velocity/energy values at which the charge exchange coefficients are stored in the datafile (input) are also shown for information. The program recovers the output velocities/energies you used when last executing the program.
4. Pressing the *Default Velocity/Energy values* button inserts a default set of velocities/energies equal to the input velocities/energies
5. The Velocity/Energy values are editable. Click on the *Edit Table* button if you wish to change the values. A ‘drop-down’ window, the ADAS Table Editor window: It follows the same pattern of operation as described in the *18nov-94* bulletin.
6. The specific cross-section data to be extracted is specified by the window to the right. The level or resolution of the data source is shown.
7. Activate the *Select quantun numbers for processing* button to allow new settings of these quantum numbers. The values in the three smaller windowsbecome editable depending also on the resolution of the dataset. Note that the *Range* of the data in the dataset is displayed.
8. There are special codes to be used to obtain summed cross-sections over sub-quantum numbers. These are indicated in brackets under the *Total* column and should be entered into the editable window if required.



ADAS301 PROCESSING OPTIONS

Title for Run: ADAS User manual example

Data File Name: /packages/adas/adas/adf01/qcx#h0/qcx#h0_old#n7.dat

Browse Comments

Polynomial Fitting

☑ Fit Polynomial value % : 5

Select Velocities/Energies for output file ☑

Output Collision Velocities/Energies

INDEX	Output	Input
1	1.000E+03	1.000E+03
2	1.500E+03	1.500E+03
3	2.000E+03	2.000E+03
4	3.000E+03	3.000E+03
5	5.000E+03	5.000E+03

Velocity/Energy units: eV/amu

Edit Table

Default Velocity/Energy Values

Select quantum numbers for processing ☑

	Range:		Total:
Principal quantum no. N	(4 - 9)	7	[0]
Orbital quantum no. L	(0 - N-1)	3	[-1]
Azimuthal quantum no. M	(0 - L)	0	[-1]

Data is N and L resolved.

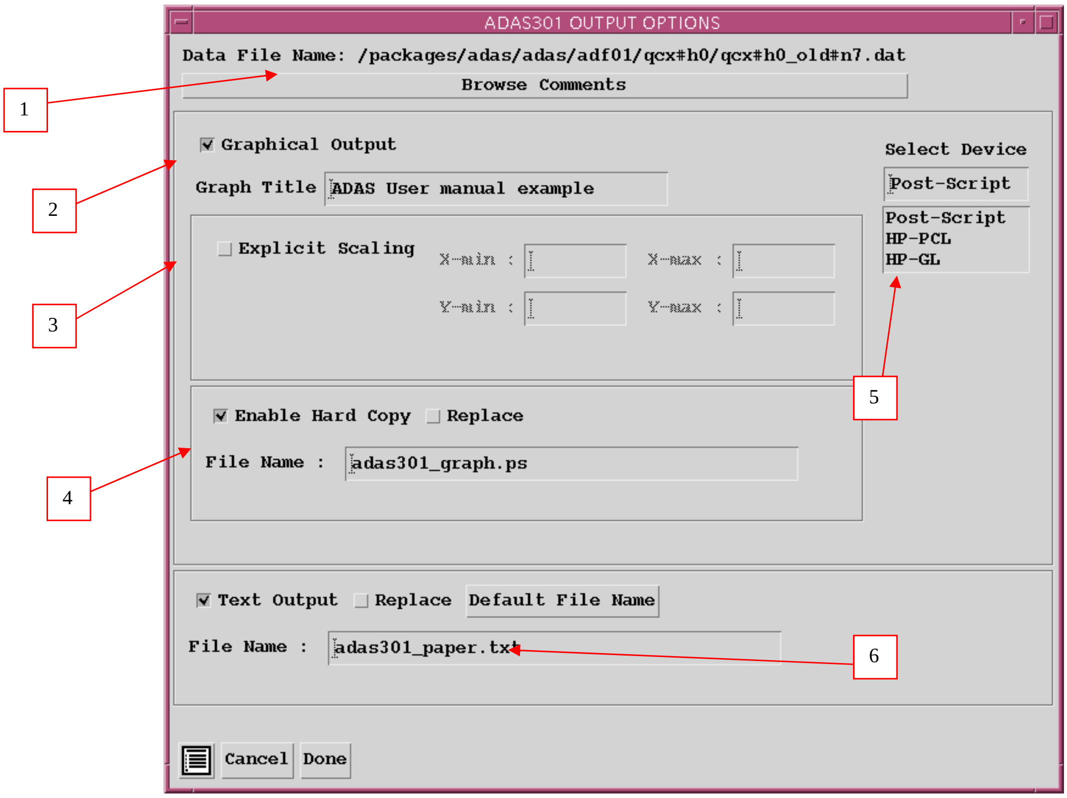
Edit the processing options data and press Done to proceed

Cancel Done

9. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

The **output options window** is shown below

1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
2. Graphical display is activated by the *Graphical Output* button. This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph.
3. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.
4. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. If the output graphic file already exits and the *Replace* button has not been activated, a ‘pop-up’ window issues a warning.
5. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.
6. The *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name ‘paper.txt’ may be set by pressing the button *Default file name*. A ‘pop-up’ window issues a warning if the file already exists and the *Replace* button has not been activated.



Data File Name: /packages/adas/adas/adf01/qcx#h0/qcx#h0_old#n7.dat

☑ Graphical Output

Graph Title ADAS User manual example

Select Device: Post-Script

☐ Explicit Scaling

☑ Enable Hard Copy ☐ Replace

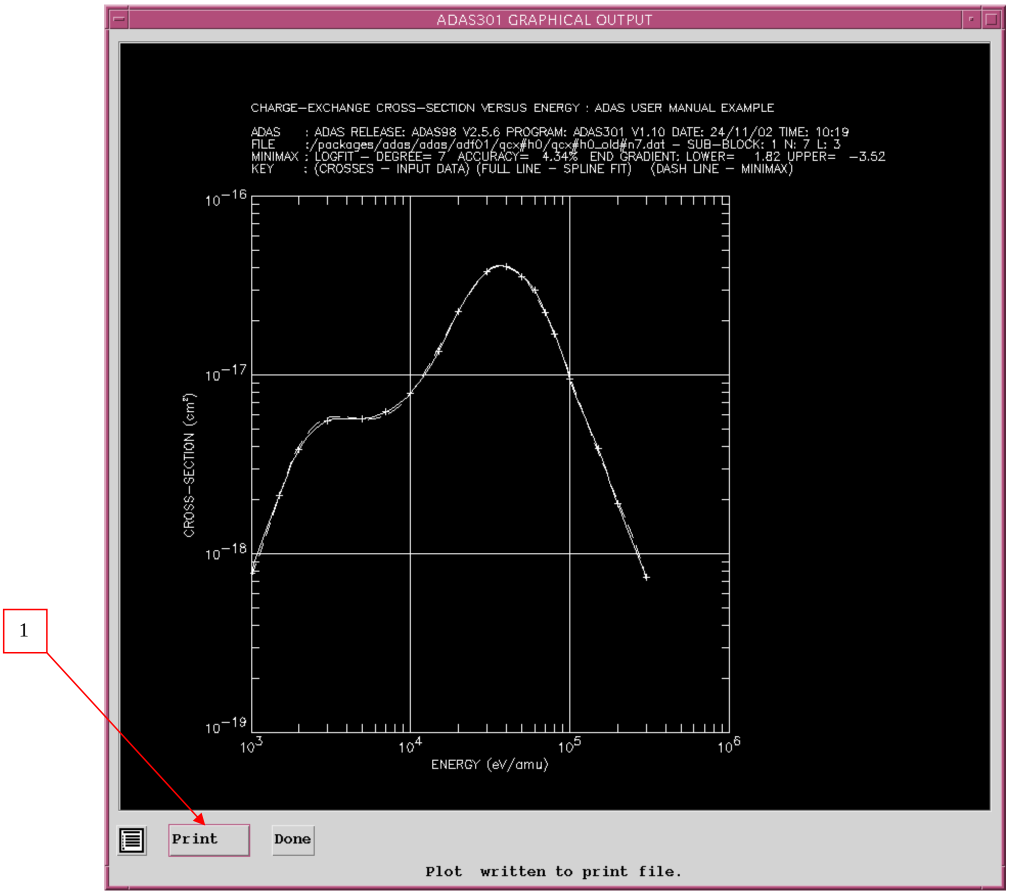
File Name : adas301_graph.ps

☑ Text Output ☐ Replace

File Name : adas301_paper.txt

The **Graphical output window** is shown below

1. Printing of the currently displayed graph is activated by the *Print* button.



```
CHARGE-EXCHANGE CROSS-SECTION VERSUS ENERGY : ADAS USER MANUAL EXAMPLE

ADAS    : ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS301 V1.10 DATE: 24/11/02 TIME: 10:19
FILE    :/packages/adas/adas/adf01/qcx#h0/qcx#h0_old#n7.dat - SUB-BLOCK: 1 N: 7 L: 3
MINIMAX : LOGFIT - DEGREE= 7  ACCURACY=  4.34%  END GRADIENT: LOWER=   1.82 UPPER=  -3.52
KEY     : (CROSSES - INPUT DATA) (FULL LINE - SPLINE FIT)   (DASH LINE - MINIMAX)
```

```
Plot  written to print file.
```

ADF12

Data from files of type ADF12 contain charge exchange effective emission coefficients for principal quantum shell transitions of hydrogen-like impurity ions, $q_{n\to n'}^{(eff)}$, at a reference beam/plasma condition of beam energy $E_u^{(ref)}$, plasma ion density $N_{zeff}^{(ref)}$, plasma ion temperature $T_{zeff}^{(ref)}$, plasma z effective $zeff^{\,(ref)}$ and magnetic field strength $B_{mag}^{(ref)}$. Also they contain the $q_{n\to n'}^{(eff)}$ at varying plasma conditions obtained by keeping all the parameters except one at the reference conditions. These are called one-dimensional scans and there are $q_{n\to n'}^{(eff)}$ sets at the following parameter sets:

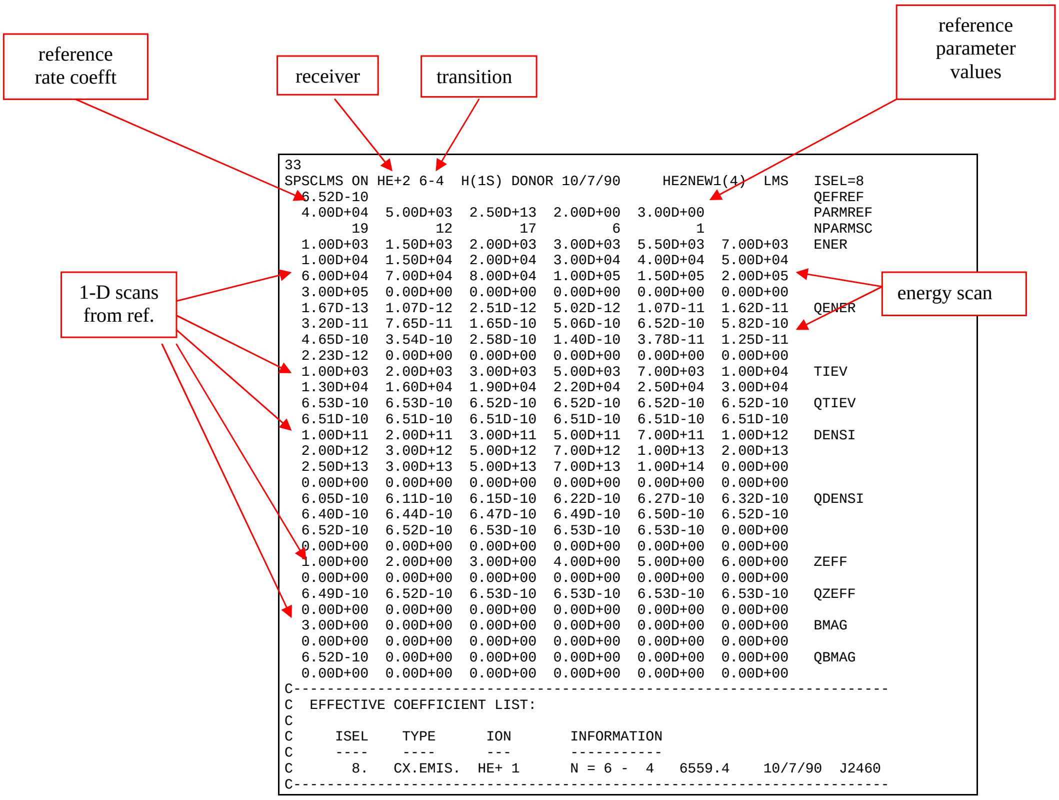
$\{E_{u,i}:i=1,I_E\}, N_{zeff}^{(ref)}, T_{zeff}^{(ref)}, zeff^{\,(ref)}, B^{(ref)}$ with $E_u^{(ref)} \in \{E_{u,i}:i=1,I_E\}$,

$E_u^{(zeff)}, \{N_{zeff}:i=1,I_N\}, T_{zeff}^{(ref)}, zeff^{\,(ref)}, B^{(ref)}$ with $N_{zeff}^{(ref)} \in \{N_{zeff}:i=1,I_N\}$,

$E_u^{(ref)}, N_{zeff}^{(ref)}, \{T_{zeff,i}:i=1,I_T\}, zeff^{\,(ref)}, B^{(ref)}$ with $T_{zeff}^{(ref)} \in \{T_{zeff,i}:i=1,I_T\}$,

$E_u^{(ref)}, N_{zeff}^{(ref)}, T_{zeff}^{(ref)}, \{zeff_i:i=1,I_{zeff}\}, B^{(ref)}$ with $zeff^{\,(ref)} \in \{zeff_i:i=1,I_{zeff}\}$,

$E_u^{(ref)}, N_{zeff}^{(ref)}, T_{zeff}^{(ref)}, zeff^{\,(ref)}, \{B_i:i=1,I_B\}$ with $B^{(ref)} \in \{B_i:i=1,I_B\}$.



```
33
SPSCLMS ON HE+2 6-4  H(1S) DONOR 10/7/90     HE2NEW1(4)  LMS   ISEL=8
  6.52D-10                                                     QEFREF
  4.00D+04  5.00D+03  2.50D+13  2.00D+00  3.00D+00             PARMREF
        19        12        17         6         1             NPARMSC
  1.00D+03  1.50D+03  2.00D+03  3.00D+03  5.50D+03  7.00D+03   ENER
  1.00D+04  1.50D+04  2.00D+04  3.00D+04  4.00D+04  5.00D+04
  6.00D+04  7.00D+04  8.00D+04  1.00D+05  1.50D+05  2.00D+05
  3.00D+05  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  1.67D-13  1.07D-12  2.51D-12  5.02D-12  1.07D-11  1.62D-11   QENER
  3.20D-11  7.65D-11  1.65D-10  5.06D-10  6.52D-10  5.82D-10
  4.65D-10  3.54D-10  2.58D-10  1.40D-10  3.78D-11  1.25D-11
  2.23D-12  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  1.00D+03  2.00D+03  3.00D+03  5.00D+03  7.00D+03  1.00D+04   TIEV
  1.30D+04  1.60D+04  1.90D+04  2.20D+04  2.50D+04  3.00D+04
  6.53D-10  6.53D-10  6.52D-10  6.52D-10  6.52D-10  6.52D-10   QTIEV
  6.51D-10  6.51D-10  6.51D-10  6.51D-10  6.51D-10  6.51D-10
  1.00D+11  2.00D+11  3.00D+11  5.00D+11  7.00D+11  1.00D+12   DENSI
  2.00D+12  3.00D+12  5.00D+12  7.00D+12  1.00D+13  2.00D+13
  2.50D+13  3.00D+13  5.00D+13  7.00D+13  1.00D+14  0.00D+00
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  6.05D-10  6.11D-10  6.15D-10  6.22D-10  6.27D-10  6.32D-10   QDENSI
  6.40D-10  6.44D-10  6.47D-10  6.49D-10  6.50D-10  6.52D-10
  6.52D-10  6.52D-10  6.53D-10  6.53D-10  6.53D-10  0.00D+00
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  1.00D+00  2.00D+00  3.00D+00  4.00D+00  5.00D+00  6.00D+00   ZEFF
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  6.49D-10  6.52D-10  6.53D-10  6.53D-10  6.53D-10  6.53D-10   QZEFF
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  3.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00   BMAG
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  6.52D-10  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00   QBMAG
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
C-----------------------------------------------------------------------
C  EFFECTIVE COEFFICIENT LIST:
C
C     ISEL    TYPE      ION       INFORMATION
C     ----    ----      ---       -----------
C       8.   CX.EMIS.  HE+ 1      N = 6 -  4   6559.4    10/7/90  J2460
C-----------------------------------------------------------------------
```

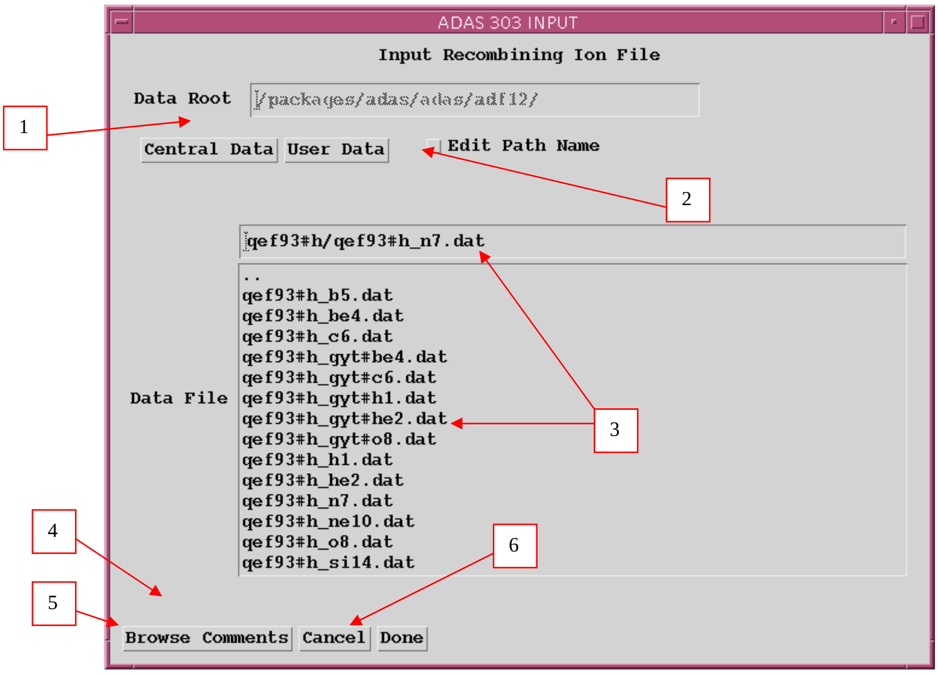
ADAS303

The program interrogates charge exchange spectroscopy effective emission coefficient data sets of type ADF12 associated with a particular neutral donor. The ADF12 data set collections are for the relevant hydrogen-like n-n' spectrum lines grouped according to the recombining ion. The code and data organisation allows the emission coefficient to be obtained (by interpolation using cubic splines) at plasma conditions and at relative collision energies of choice. A minimax polynomial approximation can also be made to the interpolated data. The interpolated data are displayed and a tabulation prepared. The tabular and graphical output may be printed and include the polynomial approximation.

The **file selection window** appears first and has the appearance shown below.

1. Data root shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Note that each type of data is stored according to its ADAS data format (*adf* number). *adf12* is the appropriate format for use by the program ADAS303. Details of the organisation of such data is given in the *appxa-12*. Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*, to use this facility.
2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing

3. Available sub-directories are shown in the large file display window. There are a large number of these. They are stored in sub-directories by donor which is usually neutral but not necessarily so (eg. *qef93#h*). The individual members are identified by the subdirectory name, a code and then fully ionised receiver (eg. *qef93#h_be4.dat*). The data sets generally contain many individual spectrum lines. Scroll bars appear if the number of entries exceed the file display window size. Such data is generally stored by year number (eg. *93*) with the most recent data to be preferred. Click on a name to select it. The selected name appears in the smaller selection window above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
4. Once a data file is selected, the set of buttons at the bottom of the main window become active.
5. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.
6. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window



Data Root: /packages/adas/adas/adf12/

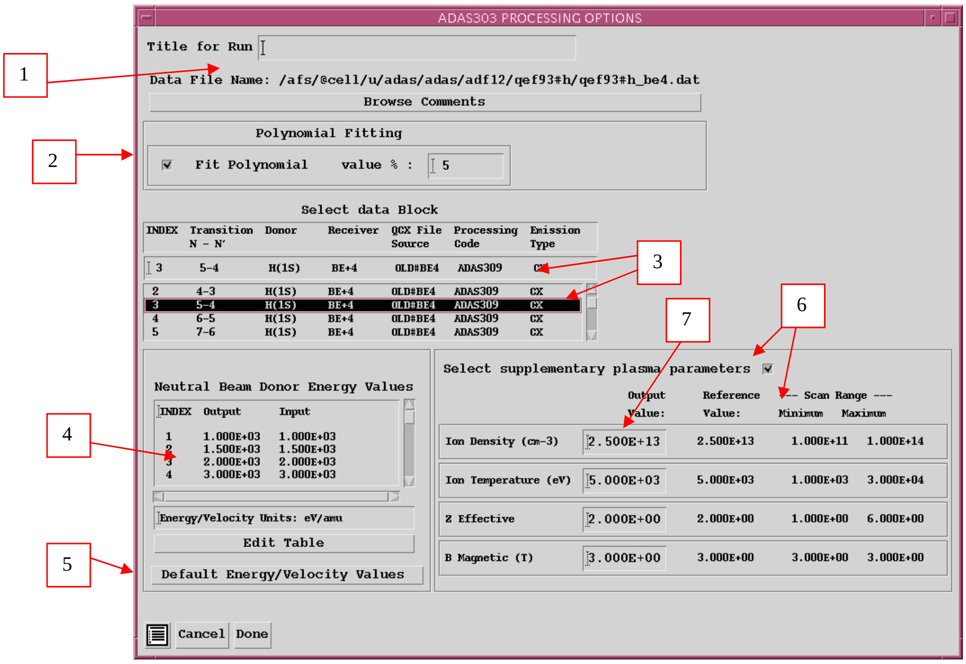
qef93#h/qef93#h_n7.dat

The **processing options window** is shown below:

1. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being analysed is also shown. The button *Browse comments* again allows display of the information field section at the foot of the selected dataset, if it exists.
2. The output data extracted from the datafile may be fitted with a polynomial. Clicking the *Fit Polynomial* button activates this. The accuracy of the fitting required may be specified in the editable box.

The value in the box is editable only if the *Fit Polynomial* button is active.

3. Transitions available in the data set are displayed in the transition list display window. This is a scrollable window using the scroll bar to the right of the window. Click anywhere on the row for a transition to select it. The selected transition appears in the selection window just above the transition list display window.



Title for Run

Data File Name: /afs/@cell/u/adas/adas/adf12/qef93#h/qef93#h_be4.dat

☑ Fit Polynomial value % : 5

INDEX	Transition N – N′	Donor	Receiver	QCX File Source	Processing Code	Emission Type
3	5-4	H(1S)	BE+4	OLD#BE4	ADAS309	CX

2	4-3	H(1S)	BE+4	OLD#BE4	ADAS309	CX
3	5-4	H(1S)	BE+4	OLD#BE4	ADAS309	CX
4	6-5	H(1S)	BE+4	OLD#BE4	ADAS309	CX
5	7-6	H(1S)	BE+4	OLD#BE4	ADAS309	CX

INDEX	Output	Input
1	1.000E+03	1.000E+03
2	1.500E+03	1.500E+03
3	2.000E+03	2.000E+03
4	3.000E+03	3.000E+03

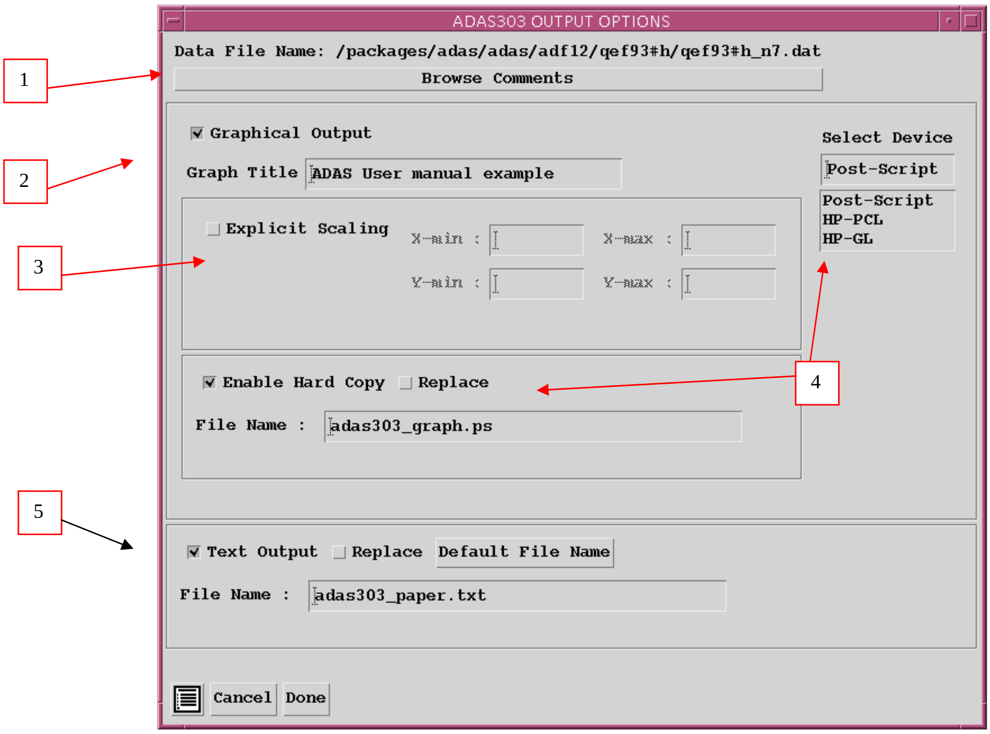
Energy/Velocity Units: eV/amu

	Output Value:	Reference Value:	--- Scan Range --- Minimum	Maximum
Ion Density (cm-3)	2.500E+13	2.500E+13	1.000E+11	1.000E+14
Ion Temperature (eV)	5.000E+03	5.000E+03	1.000E+03	3.000E+04
Z Effective	2.000E+00	2.000E+00	1.000E+00	6.000E+00
B Magnetic (T)	3.000E+00	3.000E+00	3.000E+00	3.000E+00

4. Energies/velocities for the neutral donor are displayed. The particular choice of units in use is shown below the table. Your settings of beam energy/velocity (output) are shown in the display window. The beam energy/velocity values at which the effective emission coefficients are stored in the datafile (input) are also shown for information. Click the *Edit Table* button to drop-down the ADAS Table Editor. Within Table Editor you can select which units to use as well as entering you energy/velocity values for output. Note that final graphed results are of effective emission coefficient versus beam energy (eV/amu).
5. The program recovers the output energies/velocities you used when last executing the program. Pressing the *Default Energy/Velocity values* button inserts a default set of energies/velocities equal to the input values
6. Effective emission coefficients for the ADF12 database are calculated at one-dimensional scans in various plasma parameters relative to a reference set of plasma conditions. Details are given in *appxa-12*. To alter the settings, activate the *Select supplementary plasma parameters* button.
7. The sub-windows become active with the output data entry box in each editable. For information, the reference value of each plasma parameter is given together with the range of the parameter in its one-dimensional scan. Values outside the range should not be entered. For data prepared using processing code ADAS309, the B magnetic field

parameter has no effect, but is simply used for place holding. The scan in *B Magnetic* is of zero length.

The **output options window** is shown below



Data File Name: /packages/adas/adas/adf12/qef93#h/qef93#h_n7.dat

☑ Graphical Output

Graph Title ADAS User manual example

Select Device: Post-Script

☐ Explicit Scaling

☑ Enable Hard Copy ☐ Replace

File Name : adas303_graph.ps

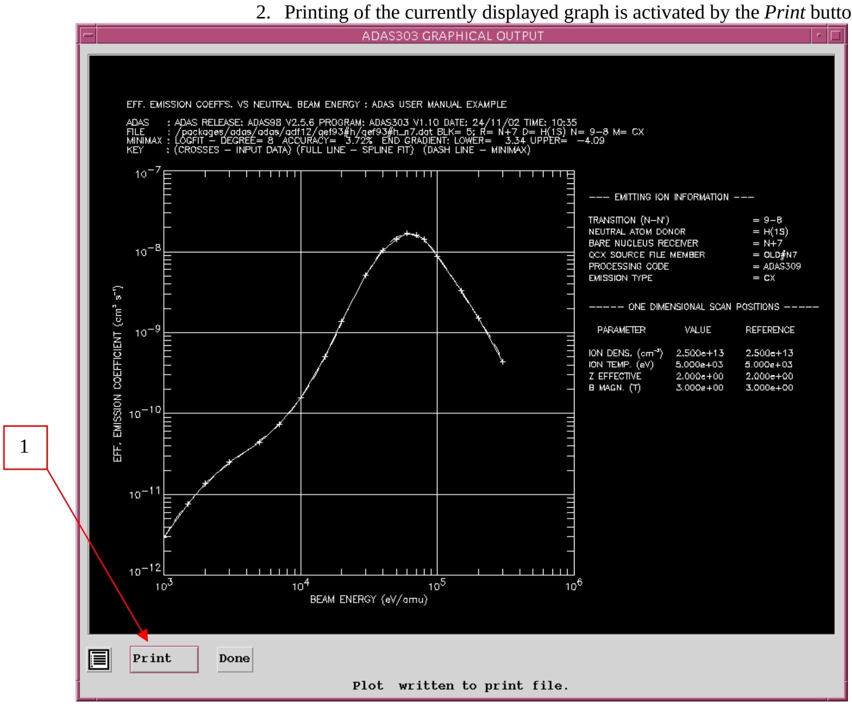
☑ Text Output ☐ Replace

File Name : adas303_paper.txt

7. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
8. Graphical display is activated by the *Graphical Output* button. This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph.
9. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.
10. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. If the output graphic file already exits and the *Replace* button has not been activated, a 'pop-up' window issues a warning. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.
11. The *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name 'paper.txt' may be set by pressing the button *Default file name*. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated.

The **Graphical output window** is shown below

2. Printing of the currently displayed graph is activated by the *Print* button.



```
EFF. EMISSION COEFFS. VS NEUTRAL BEAM ENERGY : ADAS USER MANUAL EXAMPLE

ADAS    : ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS303 V1.10 DATE: 24/11/02 TIME: 10:35
FILE    : /packages/adas/adas/adf12/qef93#h/qef93#h_n7.dat BLK= 5; R= N+7 D= H(1S) N= 9-8 M= CX
MINIMAX : LOGFIT - DEGREE= 8  ACCURACY=  3.72%  END GRADIENT: LOWER=   3.34 UPPER=  -4.09
KEY     : (CROSSES - INPUT DATA) (FULL LINE - SPLINE FIT)  (DASH LINE - MINIMAX)

--- EMITTING ION INFORMATION ---

TRANSITION (N-N')               = 9-8
NEUTRAL ATOM DONOR              = H(1S)
BARE NUCLEUS RECEIVER           = N+7
QCX SOURCE FILE MEMBER          = OLD#N7
PROCESSING CODE                 = ADAS309
EMISSION TYPE                   = CX

----- ONE DIMENSIONAL SCAN POSITIONS -----

 PARAMETER          VALUE        REFERENCE

ION DENS. (cm-3)   2.500e+13     2.500e+13
ION TEMP. (eV)     5.000e+03     5.000e+03
Z EFFECTIVE        2.000e+00     2.000e+00
B MAGN. (T)        3.000e+00     3.000e+00
```

```
Plot  written to print file.
```

Calculating CXS effective emission coefficients

The line-of-sight integrated photon emissivity of a charge exchange driven line may be written as

$$\begin{aligned}
I_{n\to n'}^{(z_0-1)} &= \sum_{l,l'} I_{nl\to n'l'}^{(z_0-1)} \\
&= \int_S \sum_{l,l'} A_{nl\to n'l'} N_{nl}^{(z_0-1)} ds \\
&= \int_S [\sum_{l,l'} A_{nl\to n'l'} (N_{nl}^{(z_0-1)} / N_D N^{(z_0)})] N_D N^{(z_0)} ds \\
&= \int_S [\sum_{l,l'} q_{nl\to n'l'}^{(eff)}] N_D N^{(z_0)} ds \\
&= \int_S q_{n\to n'}^{(eff)} N_D N^{(z_0)} ds \\
&\approx q_{n\to n'}^{(eff)} \int_S N_D N^{(z_0)} ds
\end{aligned}$$

where S is the path length through the neutral beam / plasma intersection along a spectrometer line-of-sight. N_D is the neutral donor number density and $N^{(z_0)}$ is the number density of fully ionised impurity atoms. $q_{n\to n'}^{(eff)}$ is the *effective emission coefficient* for the whole $n \to n'$ principal quantum shell transition and $\int_S N_D N^{(z_0)} ds$ is the *emission measure*. The mean transition energy is

$$\Delta E_{n,n'} = (\sum_{l,l'} \Delta E_{nl,n'l'} q^{(eff)}_{nl\to n'l'}) / q^{(eff)}_{n\to n'}$$

where $\Delta E_{nl,n'l'}$ is the line component transition energy and $q^{(eff)}_{nl\to n'l'}$ is the component effective emission coefficient. The effective emission coefficient $q^{(eff)}_{n\to n'}$ may be calculated theoretically. If it is approximately constant over the emitting volume, then measurement of a charge exchange line intensity $I^{(z_0-1)}_{n\to n'}$ allows deduction of the emission measure $\int_S N_D N^{(z_0)} ds$. If neutral beam attenuation to the observed volume is known or calculable then local impurity density may be inferred.

With the effective emission coefficients calculated theoretically, comparison with one observed charge exchange line intensity allows deduction of the emission measure. Then all other line intensities are predictable. If more than one line intensity is observed, then a mean emission measure may be deduced and some comment may be made on the ratios of experimental to theoretical effective emission coefficients. The organisation of the collisional-radiative modelling in ADAS308 is specifically designed to allow such comparison. The following points and assumptions are made:
(i) From the theoretical point-of-view the direct capture cross-sections to levels are more fundamental quantities for comparison with experiment that the effective emission coefficients.
(ii) The dominant fundamental processes modifying the initial distribution of capture are redistribution within an *n*-shell and radiative cascade in low and moderate density plasmas. Limiting the collisional-radiative theory to these dominant processes allows a compact invertable relationship to be established between column emissivities of charge exchange spectrum lines and direct capture cross-sections.
(ii) It is of most practical value to target experiment / theory comparisons on the *n*-shell distribution of capture (including the *n*-shell decrement) in fusion studies. This may be achieved by imposing theoretical information on the *l* sub-shell distribution of capture.
Consider the monoenergetic direct capture rate coefficients to *nl* sub-levels $q^{(CX)}_{nl}$ from the initial neutral donor state *D⁰(1)* by the fully stripped impurity ion with number density $N^{(z_0)}$, denoted more compactly by N^+.

$$q^{(CX)}_{nl}(E_u) = v\ \sigma^{(CX)}_{nl}(v)$$

where E_u is the relative collision energy per atomic mass unit so that $v = \sqrt{2E_u / m_p}$ is the relative collision speed, with m_p the proton mass and σ the capture cross-section.
It is supposed that

$$q^{(CX)}_{nl}(E_u) = f^{(theor)}_{(n)l} q^{(CX)}_n(E_u)$$

Since no collisional excitation from lower to higher *n*-shells is allowed, the populations of the *lj* sublevels of the principal quantum shell $n' \ge n+1$ may be written as

$$N_{n'l'} = N_D N^+ \sum_{n^{iv} \ge n+1} W_{n'l',n^{iv}} q^{(CX)}_{n^{iv}}$$

Then the equations determining the populations of the sub-shells of the principal quantum shell *n* are

$$\sum_{l''} M_{(n)l,l''} N_{nl''} = N_D N^+ f^{(theor)}_{(n)l} q^{(CX)}_n + \sum_{n' \ge n+1} A_{nl,n'l'} N_{n'l'}$$

so that

$$N_{nlj} = N_D N^+ W_{nlj,n} q^{(CX)}_n + N_D N^+ \sum_{n^{iv} \ge n+1} W_{nlj,n^{iv}} q^{(CX)}_{n^{iv}}$$

with

$$W_{nlj,n} = [\sum_{l''j''} M^{-1}_{(n)lj,l''j''} f^{(theor)}_{(n)l''j''}] q^{(CX)}_n$$

and

$$W_{nlj,n^{iv}} = \sum_{l'',j'',l',j'} M^{-1}_{(n)lj,l''j''} A_{nl''j'',n'l'j'} W_{n'l'j',n^{iv}}$$

The solution can proceed recursively downwards in *n* with compact vector and array storage.
Tabulations of experimental or theoretical state selective charge exchange cross-section data span a range of principal quantum shells $\sigma^{(CX)}_{nlj}(v) : n_0 \le n \le n_1$. Cascade from levels $n > n_1$ may contribute significantly to the populations of lower levels especially at high collision energies when the decrease of the direct charge exchange cross-sections with *n* is slow ($\sigma_n \sim n^{-\alpha}$ and $\alpha \sim 3$). However,

redistribution amongst *lj* sub-levels of the higher *n*-shells is high, approaching statistical in most circumstances. Therefore the cascade solution is initiated at some $n_{\max}$ (~20 typically) for complete *n*-shell populations only (matrices $W^{(high)}$), with subshells implicitly statistically populated, down to n_1 whereupon the *lj* resolved solution (matrices $W^{(low)}$) is commenced.

In general observable spectrum lines are associated with upper principal quantum shells $n \le n_1$. If M_{rep}, lines are identified each with a distinct upper *n*-shells $\bar{n}_{irep} : irep = 1, \ldots, M_{rep}$, then a 'condensation' may be imposed such that

$$q_n^{(CX)} = \sum_{irep=1}^{M_{rep}} L_{n,irep} q_{\bar{n}_{irep}}^{(CX)} \qquad \text{for } n_0 \le n \le n_1$$

and

$$q_n^{(CX)} = (n/n_1)^{\alpha} q_{n_1}^{(CX)} \qquad \text{for } n > n_1$$

giving, after integration along the line-of-sight, a matrix relation

$$\begin{bmatrix} I_{\bar{n}_1 \to \bar{n}_1'} \\ . \\ I_{\bar{n}_{M_{rep}} \to \bar{n}'_{M_{rep}}} \end{bmatrix} = (\int_S N_D N^+ ds) \begin{bmatrix} a_{11}. & . & a_{1M_{rep}} \\ . & . & . \\ a_{M_{rep}1} & . & a_{M_{rep}M_{rep}} \end{bmatrix} \begin{bmatrix} q_{\bar{n}_1}^{(CX)} \\ . \\ q_{\bar{n}_{M_{rep}}}^{(CX)} \end{bmatrix}$$

The coefficients of the matrix are theoretically calculated quantities. The equations may be solved for the the $q_{\bar{n}_i}^{(CX)}$ and the emission measure $\int_S N_D N^+ ds$ subject to the constraint

$$\sum_{irep=1}^{M_{rep}} q_{\bar{n}_{irep}}^{(CX)} = \sum_{irep=1}^{M_{rep}} q_{\bar{n}_{irep}}^{(CX)(theor)}$$

ADAS308

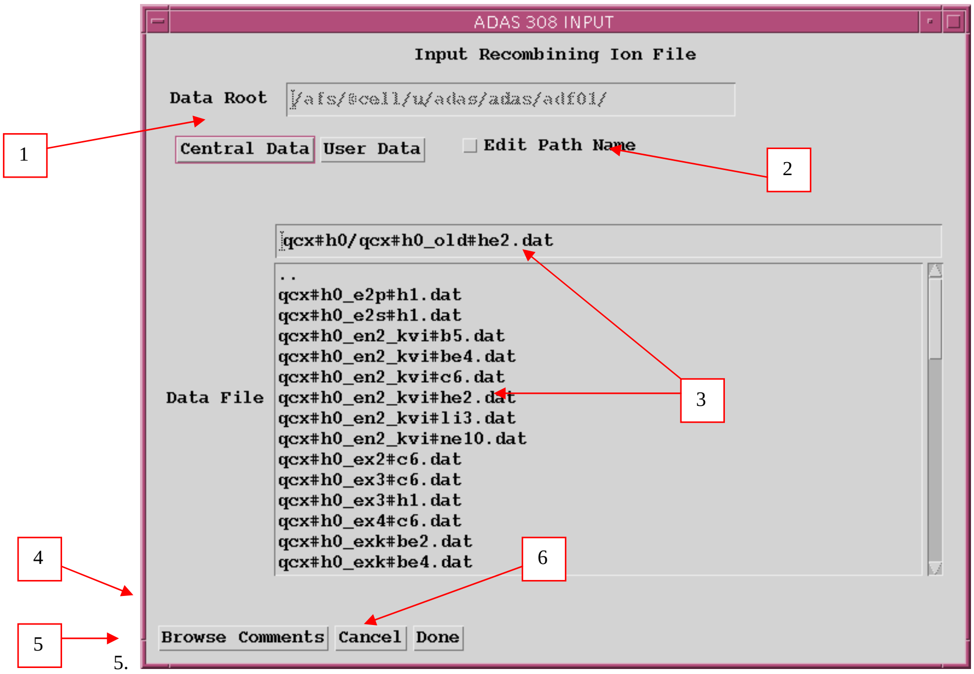
The code analyses *column* (line-of-sight integrated) emissivity observations of charge exchange spectroscopy lines from hydrogenic impurities, occuring through neutral beam / plasma interaction, in terms of emission measure. It predicts the column intensities of spectral components of the charge exchange lines, the Doppler broadened line shapes and effective emission coefficients for arbitrary lines in an l-resolved picture.

The **file selection window** is shown below.

1. Data root shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type – ADF01 in this case. Note that each type of data is stored according to its ADAS data format (*adf* number). Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*, to use this facility.
2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
3. Available sub-directories are shown in the large file display window. Scroll bars appear if the number of entries exceed the file display window size. There are a large number of these. They are stored in sub-directories by donor which is usually neutral but not necessarily so (eg. *qcx#h0*). The individual members are identified by the subdirectory name, a code and then fully ionised receiver (eg. qcx#h0_*old#c6.dat*). The data sets generally contain *nl*-resolved cross-section data but *n*-resolved and *nlm*-resolved are handled. Resolution levels must not be mixed in datasets. The ADF01 file nmaes distinguish different sources. The first letter *o* or the code *old* has been used to indicate that the data has been produced from JET compilations which originally had parametrised *l*-distribution of cross-sections. The nl-

resolved data with such code has been reconstituted from them. Data of code *old* is the preferred JET data. Other sources codes include *ory* (old Ryufuku), *ool* (old Olson), *ofr* (old Fritsch) and *omo* (old molecular orbital). There are newer data such as *kvi*. Additional codes are used for excited donors such as *ex2* for hydrogen n=2. Click on a name to select it. The selected name appears in the smaller selection window above the file display window. Then the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.

4. Once a data file is selected, the set of buttons at the bottom of the main window become active.



Data Root: /afs/@cell/u/adas/adas/adf01/

Data File: qcx#h0/qcx#h0_old#he2.dat

```
..
qcx#h0_e2p#h1.dat
qcx#h0_e2s#h1.dat
qcx#h0_en2_kvi#b5.dat
qcx#h0_en2_kvi#be4.dat
qcx#h0_en2_kvi#c6.dat
qcx#h0_en2_kvi#he2.dat
qcx#h0_en2_kvi#li3.dat
qcx#h0_en2_kvi#ne10.dat
qcx#h0_ex2#c6.dat
qcx#h0_ex3#c6.dat
qcx#h0_ex3#h1.dat
qcx#h0_ex4#c6.dat
qcx#h0_exk#be2.dat
qcx#h0_exk#be4.dat
```

5.

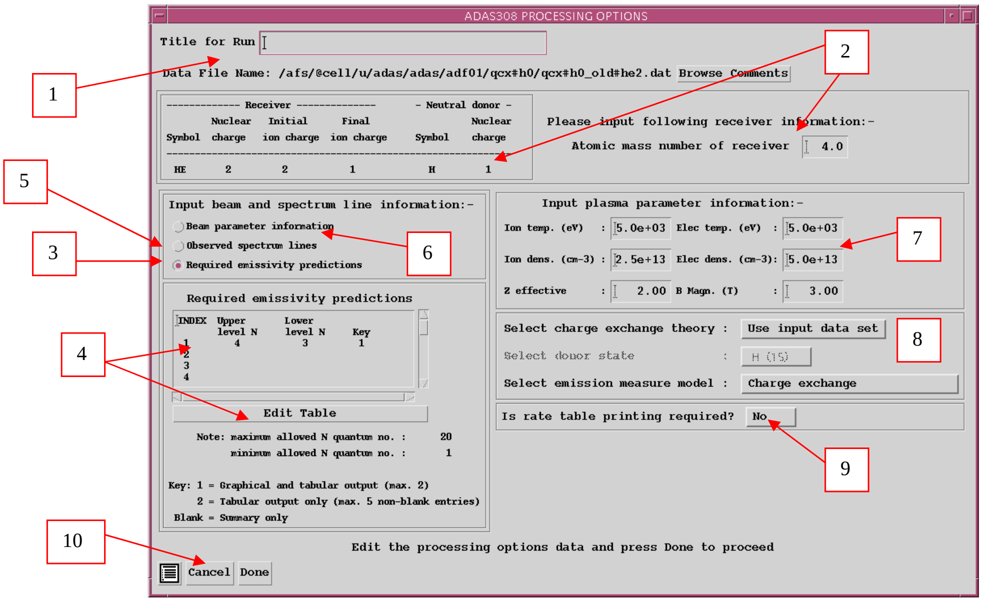
6. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what has gone into the dataset and the attribution of the dataset. The possibility of browsing the comments appears in the subsequent main window also.
7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

The **processing options window** has the appearance shown below

2. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being analysed is also shown. The button *Browse Comments* again allows display of the information field section at the foot of the selected dataset, if it exists.
3. Information is given on the fully ionised impurity receiver and the neutral beam donor. The atomic mass of the receiver must be entered.
4. The specification of beam parameters, details of observed line of sight spectral emissivities to be analysed and emissivities to be predicted are required. Input data of each of these three types may be addressed in

turn by activation of the relevant button. The window below the button list then presents the appropriate table.

5. *The Required emissivity predictions* button is displayed. This activates the predictive part of the code which becomes possible once the observed lines have been analysed in terms of emission measure. Then any set of lines within the N-shell limits may be predicted. The standard output includes the mean wavelength and effective emisison coefficient, but for up to five lines an extended tabulation of line component emissivities may be produced. Graphs may be produced for two selected line. Indicate these selections in the *Key* columnThe table may be edited by clicking on the *Edit Table* button.
6. The *Observed spectrum lines* table allows introduction of a number of observed intensities. It is possible to enter values which do not allow a consistent solution. The code advises of this but it is the responsibility of the user to check that the data is unblended etc. It is also a usual practice to enter just one line, possibly with a fictitious emissivity merely to obtain effective emission coefficients and line component details.
7. The *Beam parameter information* button causes display of the third editable table in the sub-window. Note that no check is made that the various beam energy fractions sum to unity. This is the responsibility of the user.



Title for Run

Data File Name: /afs/@cell/u/adas/adas/adf01/qcx#h0/qcx#h0_old#he2.dat

Receiver Symbol	Receiver Nuclear charge	Receiver Initial ion charge	Receiver Final ion charge	Neutral donor Symbol	Neutral donor Nuclear charge
HE	2	2	1	H	1

Please input following receiver information:-

Atomic mass number of receiver 4.0

Input beam and spectrum line information:-

○ Beam parameter information
○ Observed spectrum lines
● Required emissivity predictions

Required emissivity predictions

INDEX	Upper level N	Lower level N	Key
1	4	3	1
2			
3			
4			

Note: maximum allowed N quantum no. : 20
minimum allowed N quantum no. : 1

Key: 1 = Graphical and tabular output (max. 2)
2 = Tabular output only (max. 5 non-blank entries)
Blank = Summary only

Input plasma parameter information:-

Ion temp. (eV) : 5.0e+03
Elec temp. (eV) : 5.0e+03
Ion dens. (cm-3) : 2.5e+13
Elec dens. (cm-3): 5.0e+13
Z effective : 2.00
B Magn. (T) : 3.00

Select charge exchange theory : Use input data set
Select donor state : H (1S)
Select emission measure model : Charge exchange

Is rate table printing required? No

Edit the processing options data and press Done to proceed

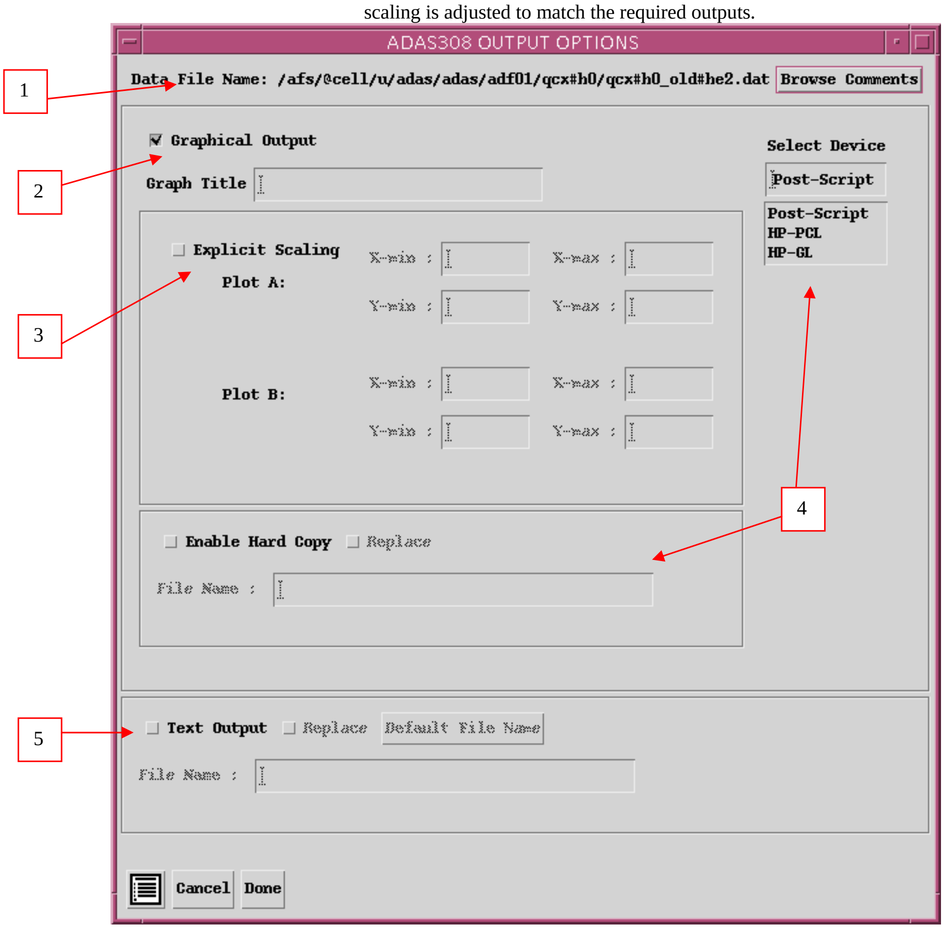
8. Enter the plasma environment parameters. These determine the collisional redistribution of the populations of the recombined plasma ion. For ADAS308, *B Magn*. has no effect, but a value should be entered as a place holder.
9. The final sub-window allows model and theory choices. Details are given in the ADAS Manual. For each type, clicking on the selection window drops down a short menu of choices. Click on the appropriate choice. The ADAS data base source numerical data of type ADF01 is the most usual, that is the *Use input data set* choice button. Note that

the *Select emission measure* model choice includes *Electron impact excitation* as well *as Charge exchange*.

10. Extended information on the rates used in the populaiton modelling may be printed.
11. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

The **Output options window** is shown below. Note that two plots are produced if required. The *Plot A* is the stick diagram of component line-of-sight emissivities. The *Plot B* is of the Doppler broadened profile of the line at the plasma ion temperature.

1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
2. Graphical display is activated by the *Graphical Output* button. This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph. By default, graph scaling is adjusted to match the required outputs.



ADAS308 OUTPUT OPTIONS

Data File Name: /afs/@cell/u/adas/adas/adf01/qcx#h0/qcx#h0_old#he2.dat

☑ Graphical Output

Graph Title :

Select Device: Post-Script

☐ Explicit Scaling

Plot A: X-min : X-max : Y-min : Y-max :

Plot B: X-min : X-max : Y-min : Y-max :

☐ Enable Hard Copy ☐ Replace

File Name :

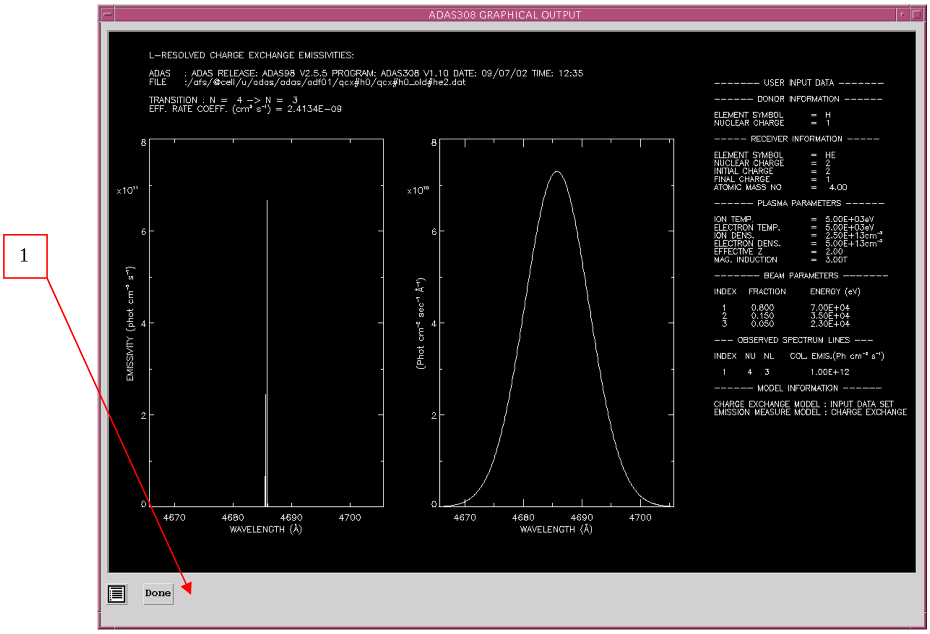
☐ Text Output ☐ Replace

File Name :

3. Press the *Explicit Scaling* button to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable. Plot A axes limits refer to the 'stick diagram and Plot B axes limits to the Doppler broadened profile.
4. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.
5. The *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name 'paper.txt' may be set by pressing the button *Default file name*.

The **Graphical output window** is shown below

3. Printing of the currently displayed graph is activated by the *Print* button.



```
L-RESOLVED CHARGE EXCHANGE EMISSIVITIES:

ADAS   : ADAS RELEASE: ADAS98 V2.5.5 PROGRAM: ADAS308 V1.10 DATE: 09/07/02 TIME: 12:35
FILE   :/afs/@cell/u/adas/adas/adf01/qcx#h0/qcx#h0_old#he2.dat

TRANSITION : N =  4 -> N =  3
EFF. RATE COEFF. (cm^3 s^-1) = 2.4134E-09
```

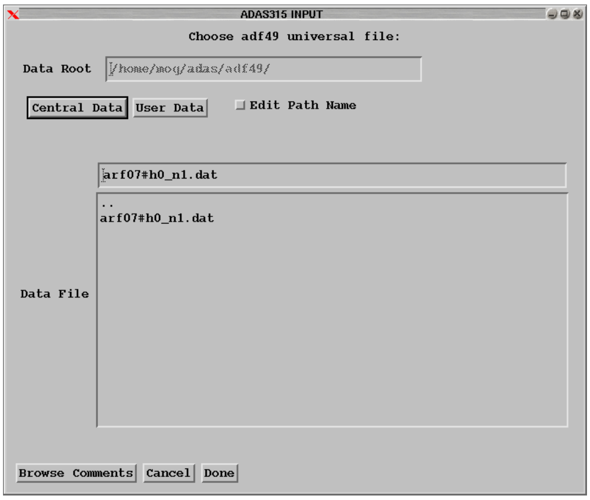
```
-------- USER INPUT DATA --------

------- DONOR INFORMATION -------

ELEMENT SYMBOL        =  H
NUCLEAR CHARGE        =  1

----- RECEIVER INFORMATION -----

ELEMENT SYMBOL        =  HE
NUCLEAR CHARGE        =  2
INITIAL CHARGE        =  2
FINAL CHARGE          =  1
ATOMIC MASS NO        =   4.00

------- PLASMA PARAMETERS -------

ION TEMP.             =  5.00E+03eV
ELECTRON TEMP.        =  5.00E+03eV
ION DENS.             =  2.50E+13cm^-3
ELECTRON DENS.        =  5.00E+13cm^-3
EFFECTIVE Z           =  2.00
MAG. INDUCTION        =  3.00T

-------- BEAM PARAMETERS --------

INDEX   FRACTION      ENERGY (eV)

  1      0.800        7.00E+04
  2      0.150        3.50E+04
  3      0.050        2.30E+04

--- OBSERVED SPECTRUM LINES ---

INDEX  NU  NL    COL. EMIS.(Ph cm^-2 s^-1)

  1     4   3         1.00E+12

------- MODEL INFORMATION -------

CHARGE EXCHANGE MODEL : INPUT DATA SET
EMISSION MEASURE MODEL : CHARGE EXCHANGE
```

Extended CXS capabilities

The charge exchange spectroscopy modelling capabilities of ADAS are still extending. This is largely motivated by the need to cope with heavier receiver ions beyond argon, which may be partially ionized. Attention is drawn to two new codes ADAS315 and ADAS316. Many subroutines have been added or modified to accommodate the new capabilities. The user should check the detailed release notes in item 4. A number of subroutines have modified parameter sets.

ADAS315: Preparation and extraction of universal adf49/adf01 CX cross-section data

This is a straightforward code which creates and ADF01 file for a specific ion of an element from a z-scaleable universal dataset of format ADF49. There are only two datasets of AD49 format corresponding to H(n=1) and H(n=2) donor respectively. The input screen is shown below followed by the output screen. A choice is possible of output energies. It is to be noted that in the level of approximation of the universal ADF49 data and the bundle-n application models, only the residual charge of the recombining ion is relevant. For the high n-shells of importance, the Rydberg electron is effectively in a hydrogenic state in the Coulomb field of the residual charge. The ADF49 datasets are subject to change as more fiducial data becomes available and the opimising of the z-scaling paramterisation is reworked. At this stage ADAS315 and ADAS316 are enabling a first look at the heavy ion CXS.


ADAS315 INPUT

Choose adf49 universal file:

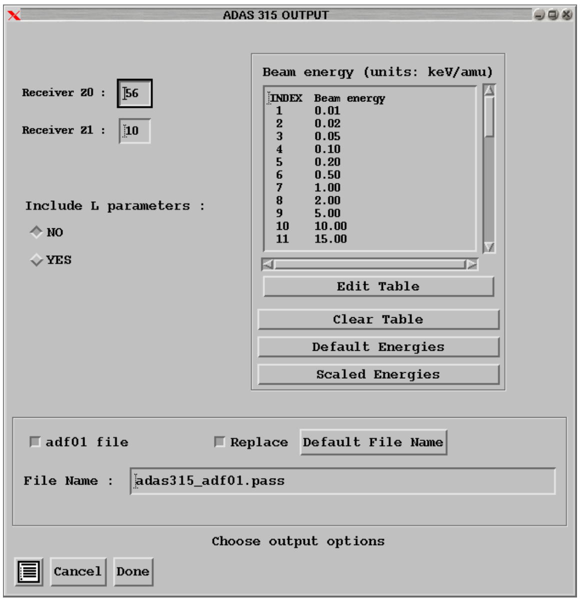
Data Root /home/mog/adas/adf49/

☐ Edit Path Name

Data File arf07#h0_n1.dat

..
arf07#h0_n1.dat

Running ADAS315 (an IDL only) code, available also at the command line, in a script allows output ADF01 files to be generated rapidly for a set of ions of an element.


ADAS 315 OUTPUT

Receiver Z0 : 56

Receiver Z1 : 10

Include L parameters :
◆ NO
◇ YES

Beam energy (units: keV/amu)

INDEX	Beam energy
1	0.01
2	0.02
3	0.05
4	0.10
5	0.20
6	0.50
7	1.00
8	2.00
9	5.00
10	10.00
11	15.00

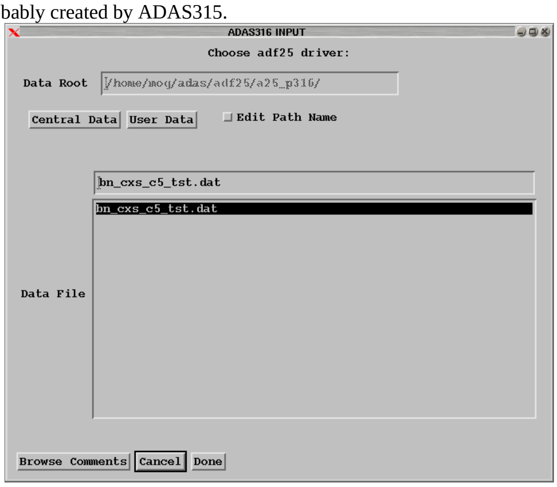
☐ adf01 file ☐ Replace

File Name : adas315_adf01.pass

Choose output options

ADAS316: Charge exchange spectroscopy – process effective coefficients: bundle-n

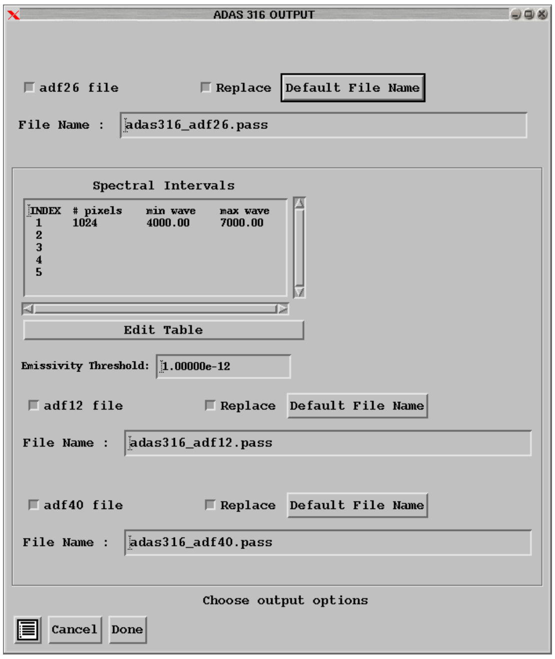
The code calculates charge exchange effective emission coefficients of format ADF12 from and input ADF01 file, probably created by ADAS315.



Data Root /home/mog/adas/adf25/a25_p316/

Data File bn_cxs_c5_tst.dat

The code requires a driver data set and, for bundle-n in ADAS, these have historically been archived in ADF25.



File Name : adas316_adf26.pass

INDEX	# pixels	min wave	max wave
1	1024	4000.00	7000.00
2			
3			
4			
5			

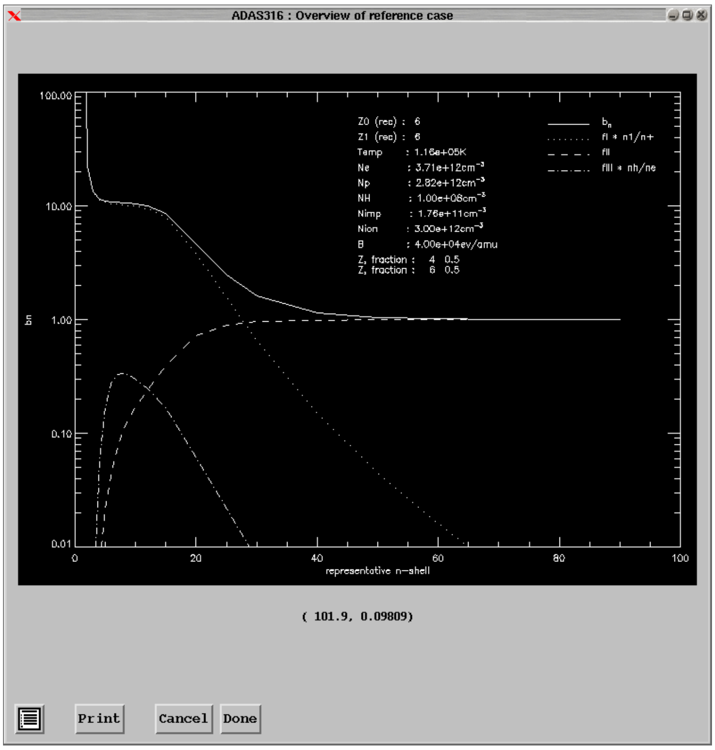
Emissivity Threshold: 1.00000e-12

File Name : adas316_adf12.pass

File Name : adas316_adf40.pass

A new sub-directory /a25_p316 has been assigned and a complete redesign of the driver has been carried out. Also a new read routine exploits the new drivers fully. We would like to move to this type of driver in the future, where there is substantial guidance to the user in the fields and mnemonics used in the driver. The driver allows scans over parameters to be specified. In fact the driver is quite versatile and appropriate to all type of bundle-n calculation . We shall exploit it further for Bremsstrahlung + free-bound continuum iand quasi-continuum high Rydberg line contributions in the future.

The output screen follows a usual pattern. Output ADF26 (the bundle-n population solution), ADF12 (charge exchange effective emission coefficients) and ADF40 (feature emissivity coefficients) may be produced. For heavy species CXS, because of the very large number of transitions between highly excited states, the ADF40 format becomes more useful that ADF12. A graph of the bundle-n-population solution, at the reference plasma parameters (usually at the centroid of the scans) is generated and shown with the free–electron capture and charge exchange capture parts separated – as illustrated below.



Z0 (rec) : 6
Z1 (rec) : 6
Temp : 1.16e+05K
Ne : 3.71e+12cm^{-3}
Np : 2.82e+12cm^{-3}
NH : 1.00e+08cm^{-3}
Nimp : 1.76e+11cm^{-3}
Nion : 3.00e+12cm^{-3}
B : 4.00e+04ev/amu
Z, fraction : 4 0.5
Z, fraction : 6 0.5

Beam stopping and emission

For a neutral beam species A being stopped by fully stripped impurity species and electrons in the plasma, the stopping coefficient is the effective loss rate coefficient of electrons from A . This corresponds closely to the effective ionisation rate coefficient or *collisional-radiative* ionisation coefficient from the ground state of $\mathcal{A}$, where charge transfer losses as well as direct ionisation losses are included. It is usual to write the coefficient in terms of the plasma electron density N_e so that the loss rate is $N_e S_{CR}^{(\mathcal{A})}$.

One can apply almost the same modellelling approach to hydrogen (or helium) atoms in a thermal plasma or to hydrogen atoms in a beam. The practical distinction is made by the assignment of a translational velocity for beam atoms. This velocity is incorporated in the integrals of beam particle / plasma particle cross-sections over the Maxwellian distributions in the thermal plasma. For hydrogen forming part of the thermal plasma, the translational velocity is set to zero. In the latter circumstance, ion impact collision rates are very small compared with electron impact rates. Also recombination (both free-electron capture and charge exchange capture) become significant processes. For the hydrogen atoms in a fast beam, recombination is not relevant and although formally present is ignored in the results. However the translational velocity can make ion impact collisions more important than electron collisions.

For hydrogen or hydrogenic ions in a plasma, the largest collision cross-sections are those for which n=n' and l=l'±1. For these cases the transition energy is nearly zero and the cross-sections are so large for electron and ion densities of relevance for fusion that it is very good approximation to assume relative statistical population for the l-states. Thus for hydrogenic systems only populations of complete n-shells need be evaluated, the *bundle-n* approximation. The equilibrium populations of the n-shells, N_n, are the solution of the statistical balance equations

$$\begin{aligned}
&\sum_{n'>n}[A_{n'\to n} + u(\nu)B_{n'\to n} + N_e q^{(e)}_{n'\to n} + N_e q^{(p)}_{n'\to n}]N_{n'} \\
&+\sum_{n''<n}[u(\nu)B_{n''\to n} + N_e q^{(e)}_{n''\to n} + N_e q^{(p)}_{n''\to n}]N_{n''} \\
&+N_e N_+ \alpha^{(r)}_n + N_e^2 N_+ \alpha^{(3)}_n + N_e N_+ \int u(\nu)B_{\kappa\to n}d\kappa \\
&= \{\sum_{n'>n}[u(\nu)B_{n\to n'} + N_e q^{(e)}_{n\to n'} + N_e q^{(p)}_{n\to n'}] \\
&+ \sum_{n''<n}[A_{n\to n''} + u(\nu)B_{n\to n''} + N_e q^{(e)}_{n\to n''} + N_e q^{(p)}_{n\to n''}] \\
&+\int u(\nu)B_{n\to\kappa}d\kappa + N_e q^{(e)}_{n\to\varepsilon} + N_e q^{(p)}_{n\to\varepsilon}\}N_n
\end{aligned}$$

N_n is the population of the state $X_n^{+z_0-1}$ and N_+ of the parent ion X^{+z_0}. N_e is the free electron density and N_p the free proton density. A and B are the usual Einstein coefficients, $q^{(e)}$ and $q^{(p)}$ denotes collisional rates due to electrons and protons, $\alpha_n^{(r)}$ and $\alpha_n^{(3)}$ denote radiative and three-body recombination and $u(\nu)$ is the energy density of the radiation field. There is one such equation for each value of n from 1 to ∞. The equations may be extended by including reactions for other impurity ions additional to the protons. The radiation field presence in the equations is not of direct relevance to hydrogen population modelling in a fusion plasma, but it can be exploited in a purely technical manner to separate the influence of different driving populations in the collisional-radiative sense.

Population results and preparing tabulations

ADAS 310 is the primary code for evaluating beam stopping and emission coefficients for hydrogen beams. It is too slow in execution for a direct link to inter-pulse experiment analysis and so it is used to prepare tabulations of effective beam stopping and beam emission coefficients for subsequent look-up. The effective coefficients are most sensitive to the beam particle energy and the plasma ion density and less sensitive to plasma ion temperature and Z-effective. Suitable tabulations can therefore be built on a reference set of plasma and beam conditions, a two-dimensional array of coefficients as functions of beam energy and plasma density at the reference conditions of the other parameters and then one-dimensional vectors of the coefficients as functions of each minor parameter at the reference condition of all the other parameters. ADAS310 accepts as input the definition of these scans, establishes an extended list of cases required to achieve these scans and then executes repeated population calculations at each set of plasma conditions in the list. ADAS310 can compute the populations for any mixture of light impurities (hydrogen to neon) in the plasma. It is impractical to deal with all possible mixtures of impurities. It is our usual practice to execute ADAS310 in turn for each light impurity from hydrogen to neon treated as a pure species. The mixed species effective coefficients are constructed from these pure impurity solutions by the theoretical data acquisition routines. The main population output is very complete and in principle contains all information on possible emitted spectrum lines up to very high n-shells together with both ionisation and recombination collisional-radiative coefficients. It is archived as ADAS data format ADF26. ADAS310 can also produce directly the final tabulations of beam stopping coefficient according to ADAS data format ADF21, however this is normally done using the post-processor program ADAS312.

ADAS304 is the interrogation code on the beam stopping coefficient data base ADF21. It also works with the beam emission coefficient data base, which is of identical organisation to the stopping coefficients, and is assigned to ADF22.

In creation of compact interpolable datasets of type ADF21 and ADF22, some simplifications are made. The stopping coefficient data sets for each impurity species are calculated as though that species alone is present in the plasma. For species X^{+z_0}, of nuclear charge z_0, of number density $N^{(z_0)}$, the electron density used in the stopping calculation is $N_e = z_0 N^{(z_0)}$ consistent with charge neutrality. Let the stopping coefficient for the impurity species X^{+z_0} be $S_{CR}^{(\mathrm{A},X)}$ then the loss rate is

$$\begin{aligned} N_e S_{CR}^{(\mathrm{A},X)}(E_B, N^{(z_0)}, T^{(z_0)}) &= N_e S_{CR}^{(\mathrm{A},e)}(E_B, N^{(z_0)}, T^{(z_0)}) \\ &\quad + N^{(z_0)} S_{CR}^{(\mathrm{A},z_0)}(E_B, N^{(z_0)}, T^{(z_0)}) \end{aligned}$$

distinguishing parts driven by excitation from the ground state of $\mathcal{A}$ by electron collisions and by X^{+z_0} ions respectively. The coefficient is

$$\begin{aligned} S_{CR}^{(\mathrm{A},X)}(E_B, N^{(z_0)}, T^{(z_0)}) &= S_{CR}^{(\mathrm{A},e)}(E_B, N^{(z_0)}, T^{(z_0)}) \\ &\quad + (1/z_0) S_{CR}^{(\mathrm{A},z_0)}(E_B, N^{(z_0)}, T^{(z_0)}) \end{aligned}$$

The density dependence of the collisional-radiative coefficient is written in terms of the impurity ion density $N^{(z_0)}$ since ion collisions primarily determine the collisional redistribution..

Consider a set of species $\{X_i^{+z_{0i}} : i = 1,..,I\}$ with fractions $\{f_i : i = 1,..,I\}$, in the plasma causing a composite stopping. The loss rate may be written approximately as

$$\begin{aligned} N_e S_{CR}^{(\mathrm{A})}(E_B, N_I, T_I) &\approx N_e S_{CR}^{(\mathrm{A},e)}(E_B, N_I, T_I) + \\ &\quad \sum_{i=1}^{I} N_i^{(z_{0i})} S_{CR}^{(\mathrm{A},z_{0i})}(E_B, N_I, T_I) \\ &= \sum_{i=1}^{I} N_{e,i} [S_{CR}^{(\mathrm{A}e)}(E_B, N_I, T_I) + \\ &\quad (1/z_{0i}) S_{CR}^{(\mathrm{A}z_{0i})}(E_B, N_I, T_I)] \end{aligned}$$

where

$$N_e = \sum_{i=1}^{I} N_{e,i} = \sum_{i=1}^{I} z_{0i} N^{(z_{0i})} = N_I (\sum_{i=1}^{I} z_{0i} f_i)$$

defines the proportions of the electron density contributed by each impurity species.

From an ion collisional redistribution point of view, in a composite plasma the $\sum_{k=1}^{I} z_{0k}^2 N_k^{(Z_{0k})}$ z-weighted density sum is meaningful so the equivalent density of the single impurity $X_i^{+z_{0i}}$ to correspond to the summed impurity ion density for this purpose is

$$N_i^{(z_{0i}),equiv} = N_I (\sum_{k=1}^{I} z_{0k}^2 f_k) / z_{0i}^2$$

and the equivalent electron density is

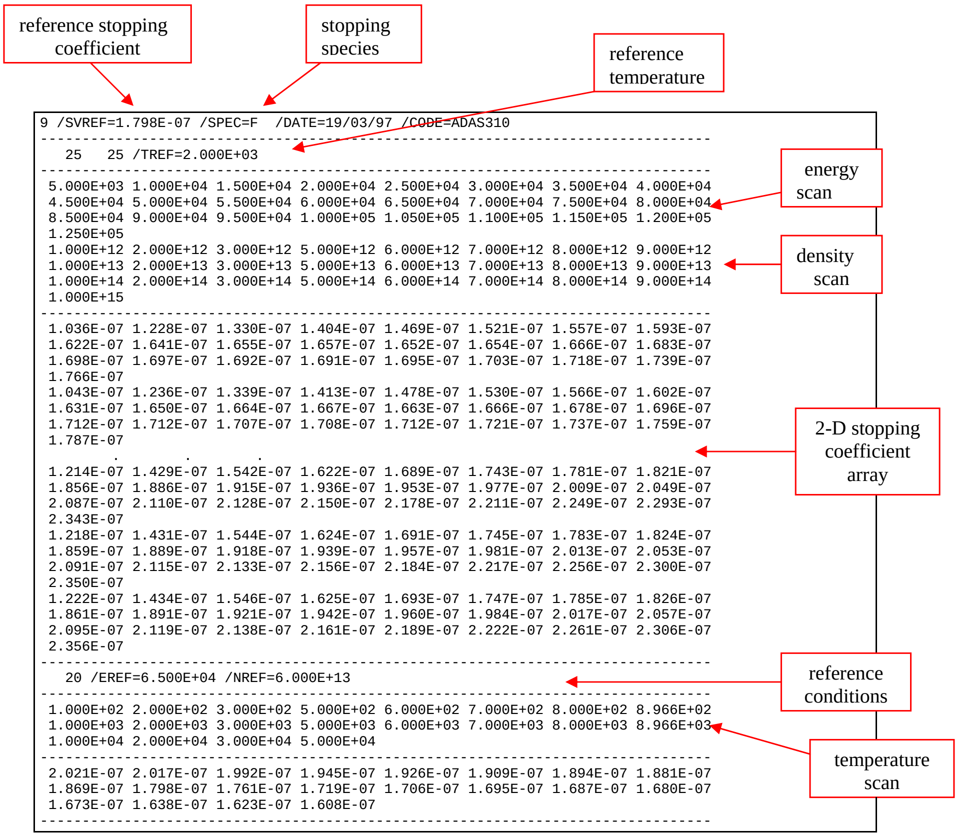
$$N_{ei}^{(z_{0i}),equiv} = \left(\frac{N_e}{\sum_{k=1}^{I} z_{0k} f_k}\right)\left(\sum_{k=1}^{I} z_{0k}^2 f_k\right)/z_{0i}$$

ADAS310 evaluates the stopping & emission coefficients as a function of electron density. The approximate composite stopping coefficient is assembled from the pure species coefficients as

$$S_{CR}^{(\mathrm{A})}(E_B, N_e, T_I) \approx \sum_{i=1}^{I} [z_{0i} f_i S_{CR}^{(\mathrm{A},X_i)}(E_B, N_{ei}^{(z_{0i}),equiv}, T_I)]/(\sum_{k=1}^{I} z_{0k} f_k)$$

The prescription outlined is equally applicable for the storage and handling of beam emission coefficients.

ADF21



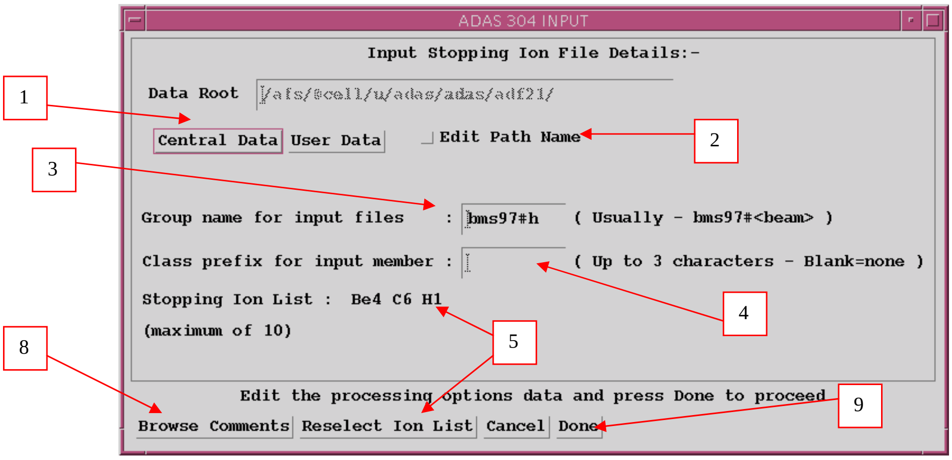
```
9 /SVREF=1.798E-07 /SPEC=F  /DATE=19/03/97 /CODE=ADAS310
--------------------------------------------------------------------------------
   25   25 /TREF=2.000E+03
--------------------------------------------------------------------------------
 5.000E+03 1.000E+04 1.500E+04 2.000E+04 2.500E+04 3.000E+04 3.500E+04 4.000E+04
 4.500E+04 5.000E+04 5.500E+04 6.000E+04 6.500E+04 7.000E+04 7.500E+04 8.000E+04
 8.500E+04 9.000E+04 9.500E+04 1.000E+05 1.050E+05 1.100E+05 1.150E+05 1.200E+05
 1.250E+05
 1.000E+12 2.000E+12 3.000E+12 5.000E+12 6.000E+12 7.000E+12 8.000E+12 9.000E+12
 1.000E+13 2.000E+13 3.000E+13 5.000E+13 6.000E+13 7.000E+13 8.000E+13 9.000E+13
 1.000E+14 2.000E+14 3.000E+14 5.000E+14 6.000E+14 7.000E+14 8.000E+14 9.000E+14
 1.000E+15
--------------------------------------------------------------------------------
 1.036E-07 1.228E-07 1.330E-07 1.404E-07 1.469E-07 1.521E-07 1.557E-07 1.593E-07
 1.622E-07 1.641E-07 1.655E-07 1.657E-07 1.652E-07 1.654E-07 1.666E-07 1.683E-07
 1.698E-07 1.697E-07 1.692E-07 1.691E-07 1.695E-07 1.703E-07 1.718E-07 1.739E-07
 1.766E-07
 1.043E-07 1.236E-07 1.339E-07 1.413E-07 1.478E-07 1.530E-07 1.566E-07 1.602E-07
 1.631E-07 1.650E-07 1.664E-07 1.667E-07 1.663E-07 1.666E-07 1.678E-07 1.696E-07
 1.712E-07 1.712E-07 1.707E-07 1.708E-07 1.712E-07 1.721E-07 1.737E-07 1.759E-07
 1.787E-07
         .        .         .
 1.214E-07 1.429E-07 1.542E-07 1.622E-07 1.689E-07 1.743E-07 1.781E-07 1.821E-07
 1.856E-07 1.886E-07 1.915E-07 1.936E-07 1.953E-07 1.977E-07 2.009E-07 2.049E-07
 2.087E-07 2.110E-07 2.128E-07 2.150E-07 2.178E-07 2.211E-07 2.249E-07 2.293E-07
 2.343E-07
 1.218E-07 1.431E-07 1.544E-07 1.624E-07 1.691E-07 1.745E-07 1.783E-07 1.824E-07
 1.859E-07 1.889E-07 1.918E-07 1.939E-07 1.957E-07 1.981E-07 2.013E-07 2.053E-07
 2.091E-07 2.115E-07 2.133E-07 2.156E-07 2.184E-07 2.217E-07 2.256E-07 2.300E-07
 2.350E-07
 1.222E-07 1.434E-07 1.546E-07 1.625E-07 1.693E-07 1.747E-07 1.785E-07 1.826E-07
 1.861E-07 1.891E-07 1.921E-07 1.942E-07 1.960E-07 1.984E-07 2.017E-07 2.057E-07
 2.095E-07 2.119E-07 2.138E-07 2.161E-07 2.189E-07 2.222E-07 2.261E-07 2.306E-07
 2.356E-07
--------------------------------------------------------------------------------
   20 /EREF=6.500E+04 /NREF=6.000E+13
--------------------------------------------------------------------------------
 1.000E+02 2.000E+02 3.000E+02 5.000E+02 6.000E+02 7.000E+02 8.000E+02 8.966E+02
 1.000E+03 2.000E+03 3.000E+03 5.000E+03 6.000E+03 7.000E+03 8.000E+03 8.966E+03
 1.000E+04 2.000E+04 3.000E+04 5.000E+04
--------------------------------------------------------------------------------
 2.021E-07 2.017E-07 1.992E-07 1.945E-07 1.926E-07 1.909E-07 1.894E-07 1.881E-07
 1.869E-07 1.798E-07 1.761E-07 1.719E-07 1.706E-07 1.695E-07 1.687E-07 1.680E-07
 1.673E-07 1.638E-07 1.623E-07 1.608E-07
--------------------------------------------------------------------------------
```

ADAS304

The code interrogates beam stopping or beam emission coefficient files of type ADF21 or ADF22. Data is extracted for stopping by a composite plasma consisting of a mixture of protons (deuterons) and fully ionised impurities. The data is interpolated using cubic splines at selected beam energy, target density and target temperature triplets. Minimax polynomial fits are made to the interpolated data. The total stopping and partial stopping by each species are given. The beam emission coefficients are handled in a similar manner. The interpolated data are displayed and a tabulation prepared. The tabular and graphical output may be printed and includes the polynomial approximations.

The **file selection window** is shown below. Its operation is a little different from usual.

1. ADF21 is the appropriate format for use by the program ADAS304 (ADAS User Manual, *appxb-21*). A root path to the correct data type ADF21 appears automatically. Your personal data of this type should be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*.



Data Root /afs/@cell/u/adas/adas/adf21/

Group name for input files : bms97#h (Usually - bms97#<beam>)

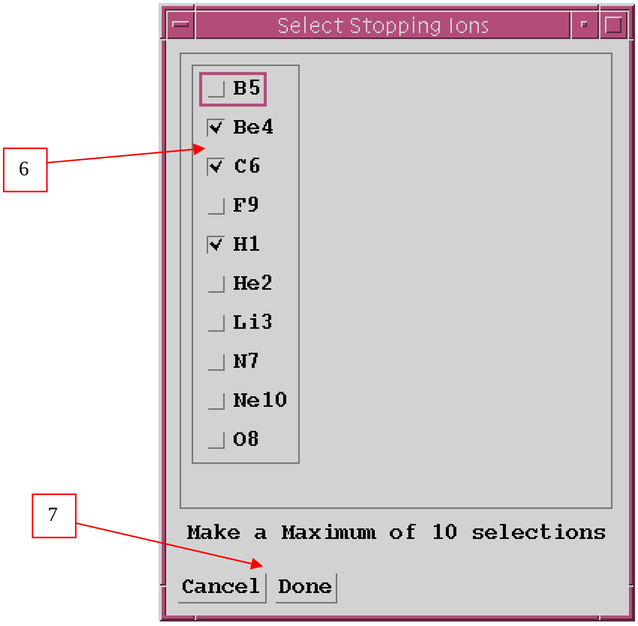
Class prefix for input member : (Up to 3 characters - Blank=none)

Stopping Ion List : Be4 C6 H1

(maximum of 10)

Edit the processing options data and press Done to proceed

2. Buttons are present to set the data root to that of the *Central data* or to your personal *User data* (provided it is in ADAS organisation. Alternatively the ‘data root’ may be edit explicitly.



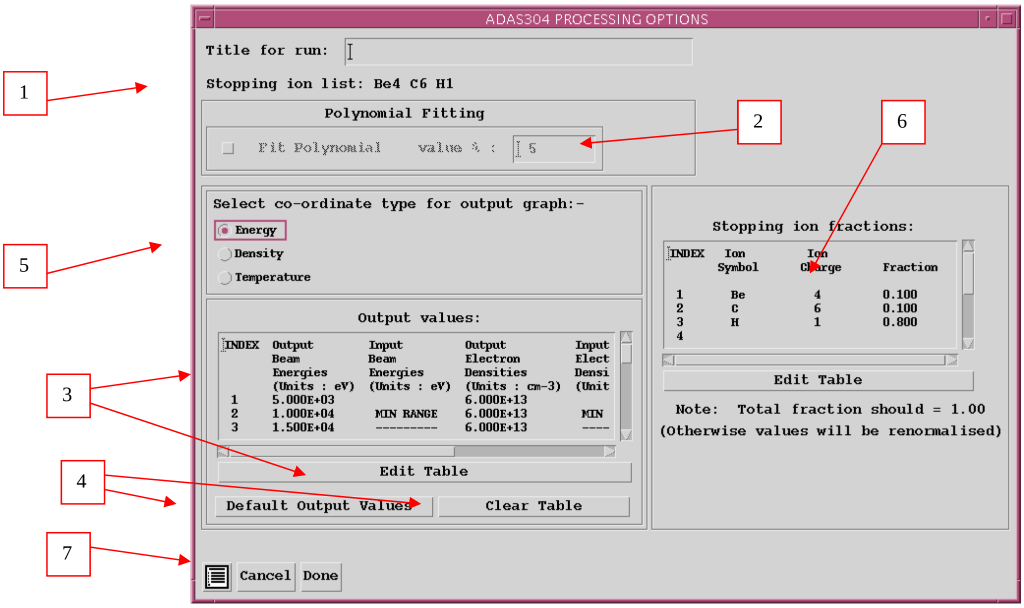
☐ B5
☑ Be4
☑ C6
☐ F9
☑ H1
☐ He2
☐ Li3
☐ N7
☐ Ne10
☐ O8

Make a Maximum of 10 selections

3. A group name for the input files is entered. This is the name of a sub-directory of ADF21 for a particular beam species (usually H or He). The sub-directory contains individual data sets for each impurity contributing to stopping , identified by the element symbol.
4. To increase flexibility in naming a three letter class prefix may be added to the data set name. The primary data in central ADAS has no prefix and so a typical data set name would be */../adas/adas/adf21/bms#h/bms#h_be.dat*.
5. ADAS304 allows you to select all the impurity files you wish easily. Click the *Reselect Ion List* button.
6. The small pop up selection widget appears showing available species. Click the toggle buttons of those you wish to include
7. Click *Done* to restore the main input widget. Your choices are shown at the Stopping Ion List.
8. Clicking on the *Browse Comments* button displays any information stored with the selected data-files. It is important to use this facility to find out what has gone into the data-set and the attribution of the data-set.
9. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window.

The **processing options window** has the appearance shown below

1. The Stopping ion list is repeated for information. The *Browse Comments* button is also provided.



Title for run:

Stopping ion list: Be4 C6 H1

☐ Fit Polynomial value % : 5

● Energy
○ Density
○ Temperature

Output values:

INDEX	Output Beam Energies (Units : eV)	Input Beam Energies (Units : eV)	Output Electron Densities (Units : cm-3)	Input Elect Densi (Unit
1	5.000E+03		6.000E+13	
2	1.000E+04	MIN RANGE	6.000E+13	MIN
3	1.500E+04	---------	6.000E+13	----

Stopping ion fractions:

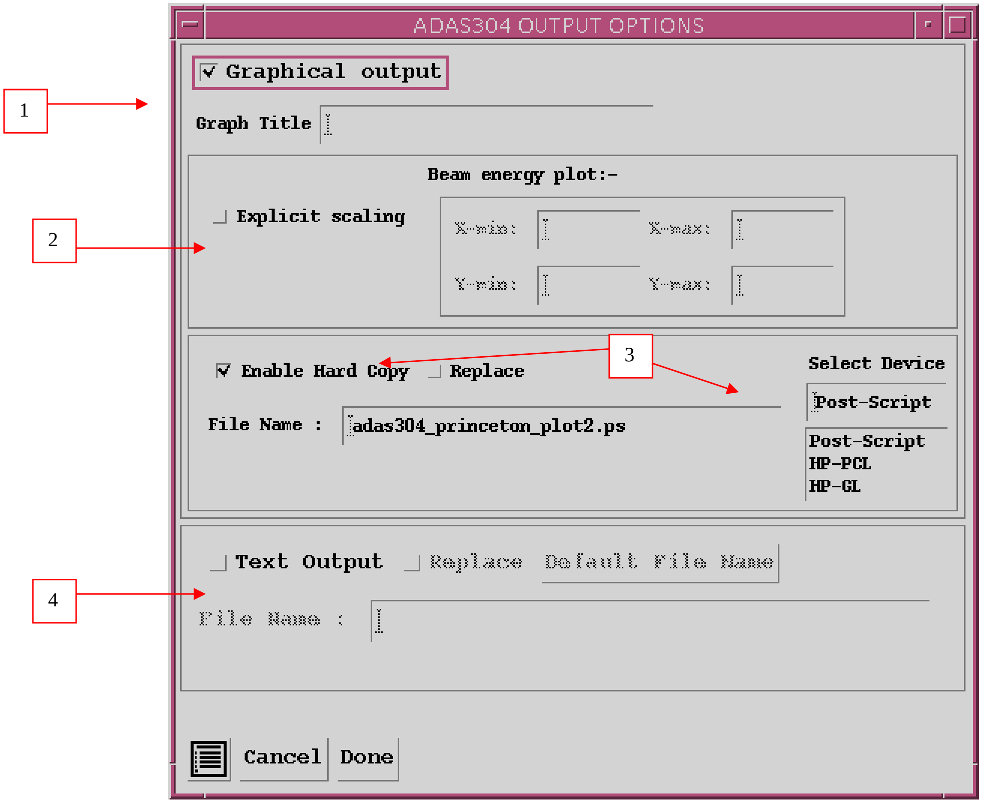
INDEX	Ion Symbol	Ion Charge	Fraction
1	Be	4	0.100
2	C	6	0.100
3	H	1	0.800
4			

Note: Total fraction should = 1.00
(Otherwise values will be renormalised)

2. The extracted data for a selected ion is interpolated by a cubic spline at user selected plasma parameters for graphical display and tabular output. Additionally a polynomial approximation may obtained by making the appropriate selections.
3. The selection of beam energy, density and temperature sets for data output must be made. The source values are held as one-dimensional scans relative to reference values for each impurity separately. The minimum and maximum for each impurity is shown in the Input columns. The table may be edited by clicking on the *Edit Table* button.
4. *Default Output Values* and *Clear Table* buttons are provided.
5. A choice of which parameter of the input model set to use as the x co-ordinate of graphs is given. Click on the required button.
6. The mixture of species contributing to the stopping is assembled at d). This again is an editable table. Click *Edit Table* to pop up the ADAS Table Editor. The required fractions may then be entered. Normalisation to unity takes place.
7. The *Exit to Menu* icon is present in ADAS304. Clicking the *Done* button causes the output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

The **Output options window** is shown below.

12. Graphical display is activated by the *Graphical Output* button. This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph.
13. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.



☑ Graphical output

Graph Title :

☐ Explicit scaling

☑ Enable Hard Copy ☐ Replace

File Name : adas304_princeton_plot2.ps

Select Device: Post-Script

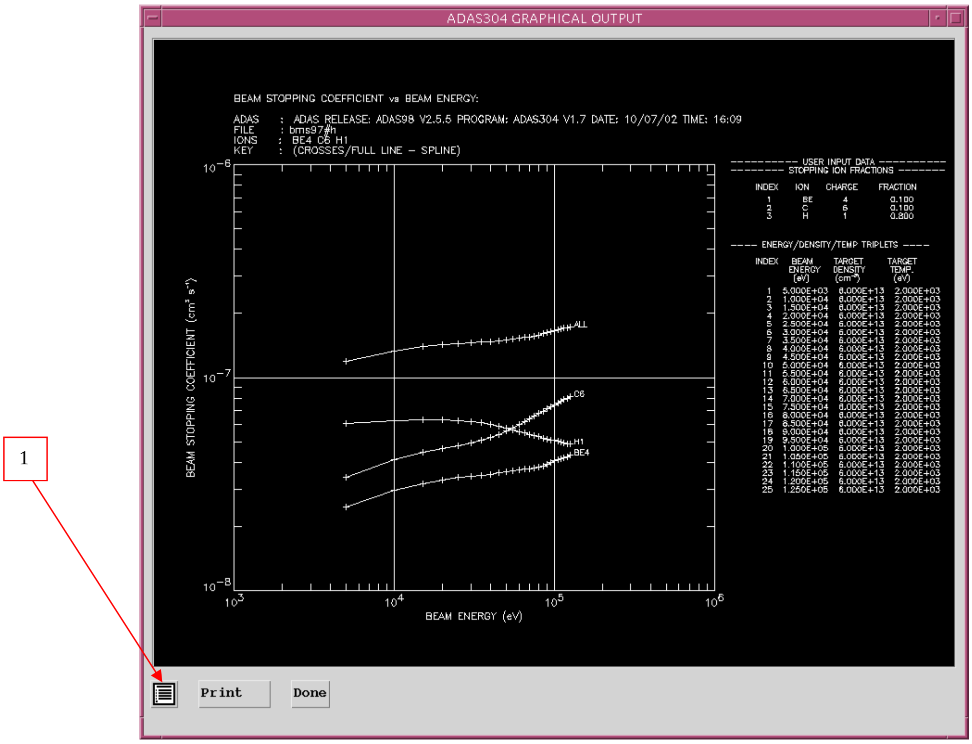
☐ Text Output ☐ Replace Default File Name

File Name :

14. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.
15. The *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name ‘paper.txt’ may be set by pressing the button *Default file name.*

The **Graphical output window** is shown below

4. Printing of the currently displayed graph is activated by the *Print* button.



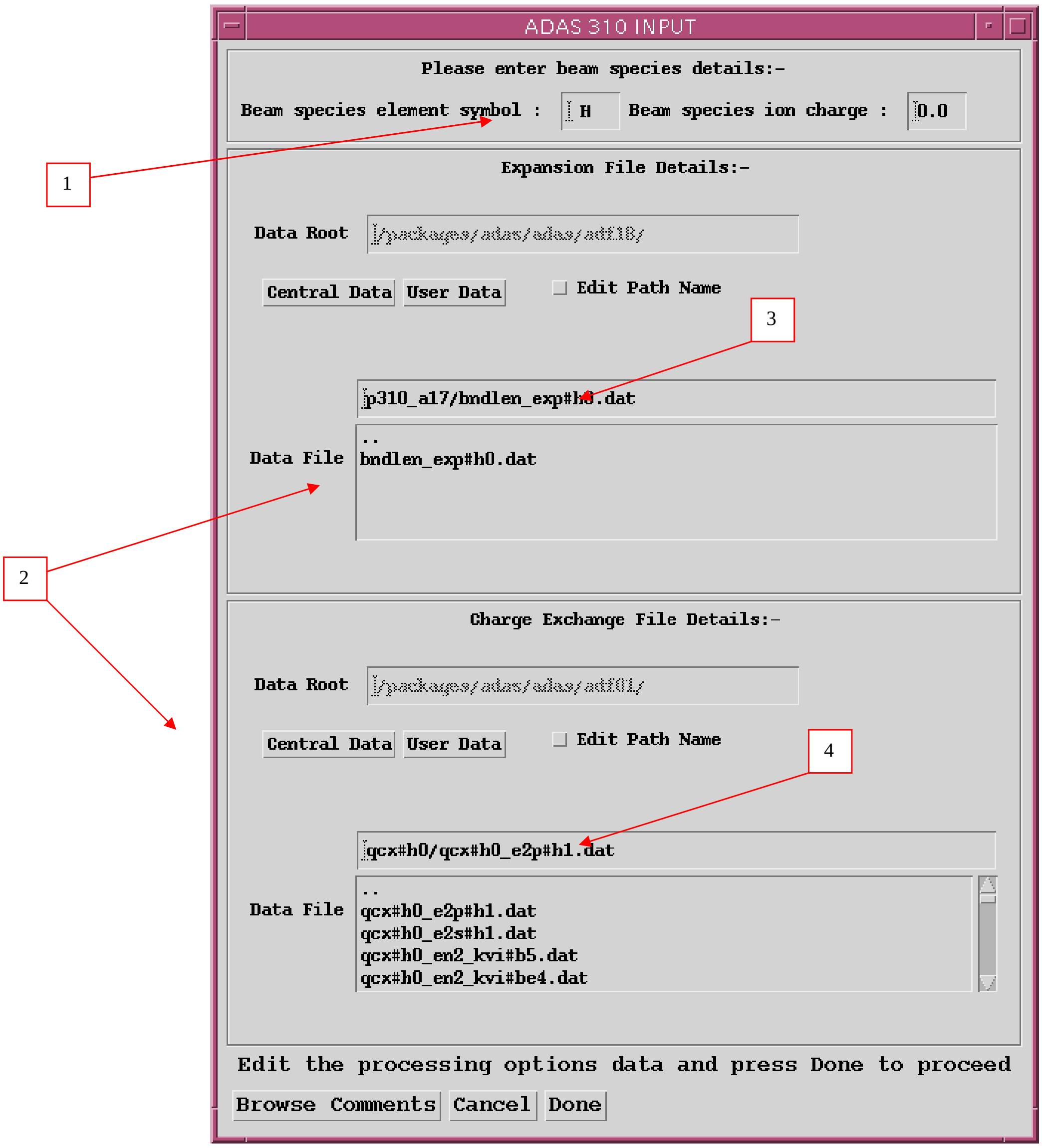
```
BEAM STOPPING COEFFICIENT vs BEAM ENERGY:

ADAS    :  ADAS RELEASE: ADAS98 V2.5.5 PROGRAM: ADAS304 V1.7 DATE: 10/07/02 TIME: 16:09
FILE    : bms97#h
IONS    :  BE4 C6 H1
KEY     :  (CROSSES/FULL LINE - SPLINE)

---------- USER INPUT DATA ----------
-------- STOPPING ION FRACTIONS --------

 INDEX   ION   CHARGE   FRACTION

   1      BE     4       0.100
   2      C      6       0.100
   3      H      1       0.800

---- ENERGY/DENSITY/TEMP TRIPLETS ----

 INDEX   BEAM       TARGET      TARGET
         ENERGY     DENSITY     TEMP.
         (eV)       (cm-3)      (eV)

   1   5.000E+03  6.000E+13  2.000E+03
   2   1.000E+04  6.000E+13  2.000E+03
   3   1.500E+04  6.000E+13  2.000E+03
   4   2.000E+04  6.000E+13  2.000E+03
   5   2.500E+04  6.000E+13  2.000E+03
   6   3.000E+04  6.000E+13  2.000E+03
   7   3.500E+04  6.000E+13  2.000E+03
   8   4.000E+04  6.000E+13  2.000E+03
   9   4.500E+04  6.000E+13  2.000E+03
  10   5.000E+04  6.000E+13  2.000E+03
  11   5.500E+04  6.000E+13  2.000E+03
  12   6.000E+04  6.000E+13  2.000E+03
  13   6.500E+04  6.000E+13  2.000E+03
  14   7.000E+04  6.000E+13  2.000E+03
  15   7.500E+04  6.000E+13  2.000E+03
  16   8.000E+04  6.000E+13  2.000E+03
  17   8.500E+04  6.000E+13  2.000E+03
  18   9.000E+04  6.000E+13  2.000E+03
  19   9.500E+04  6.000E+13  2.000E+03
  20   1.000E+05  6.000E+13  2.000E+03
  21   1.050E+05  6.000E+13  2.000E+03
  22   1.100E+05  6.000E+13  2.000E+03
  23   1.150E+05  6.000E+13  2.000E+03
  24   1.200E+05  6.000E+13  2.000E+03
  25   1.250E+05  6.000E+13  2.000E+03
```

ADAS310

The code calculates the excited population structure, effective ionisation and recombination coefficients of hydrogen atoms or hydrogenic ions in an impure plasma. A very many n-shell bundle-n approximation is used. The hydrogen atoms may be part of the thermal plasma or may be in a beam. The latter case is the only one of relevance for this manual, however the full flexibility of the program has been retained.

The **file selection window** appears first as illustrated below.

1. Enter the beam species (H for hydrogen and its isotopes) and the atomic charge of the beam species. Only data for neutral beam species is present in the central ADAS database at this time.
2. There are two data files to be selected, the expansion file and the charge exchange file. The procedure is the same in both cases.
3. A special ADAS data type *adf18* is used for such 'expansion' and 'cross-referencing' files. They fall into various categories, kept in sub-directories, according to where they map from and to. Thus the sub-directory *a09_a04* contains data sets mapping from the *adf09* data type into the *adf04* data type. We shall deal with the purposes of these in the discussion of advanced population modelling in the next release. For the moment note that *bndlen_exp#h0.dat* is the one needed here and it sits alone as shown in the illustration. Always select it.
4. The charge exchange file is not of importance for neutral beam stopping. The charge exchange data set is required when hydrogen nuclei can act as electron receivers from other species. You will see no effect of your selection here on the beam stopping coefficient but the selection is kept in for the future. Once a charge exchange data file is selected, the set of buttons at the bottom of the main window become active.



Please enter beam species details:-

Beam species element symbol : H
Beam species ion charge : 0.0

Expansion File Details:-

Data Root /packages/adas/adas/adf18/

Data File p310_a17/bndlen_exp#h0.dat

```
..
bndlen_exp#h0.dat
```

Charge Exchange File Details:-

Data Root /packages/adas/adas/adf01/

Data File qcx#h0/qcx#h0_e2p#h1.dat

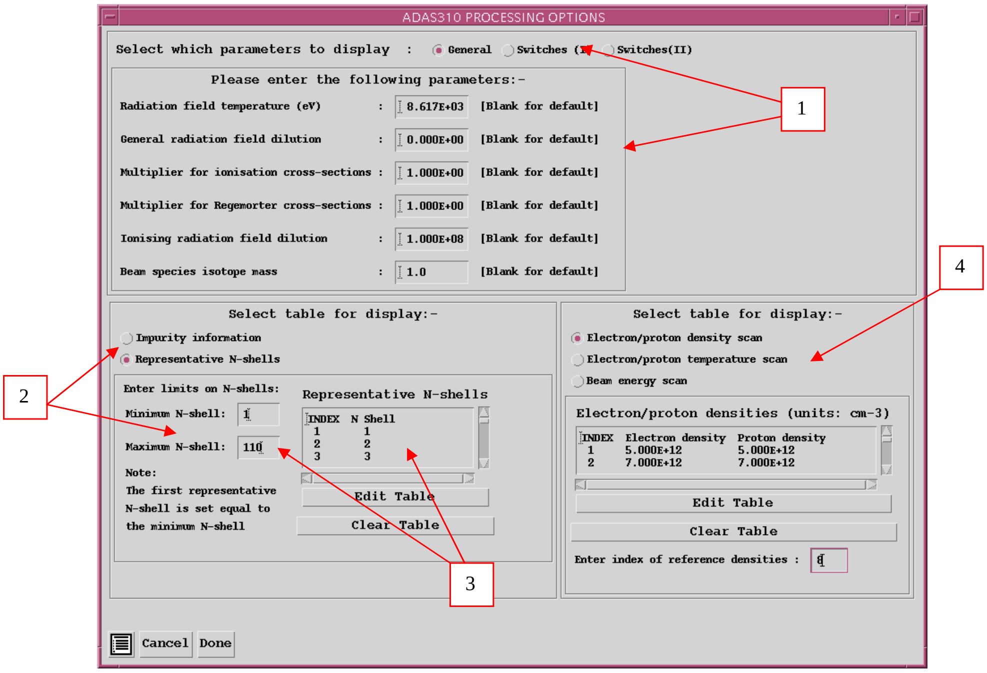
```
..
qcx#h0_e2p#h1.dat
qcx#h0_e2s#h1.dat
qcx#h0_en2_kvi#b5.dat
qcx#h0_en2_kvi#be4.dat
```

Edit the processing options data and press Done to proceed

The **processing options window** has the appearance shown below

1. The various control parameters of the collisional-radiative population calculation are organised into three groups selected in turn by the buttons *General*, *Switches (I)* and *Switches (II)*. These cause the appropriate set of parameters to be displayed in the sub-window immediately below the switches. The default settings for these are reasonable and they can be ignored as long as only beam stopping is the intent. *Switches (I)* allow some

choices to do with electron collision cross-sections and *Switches (II)* allow some choices to do with ion collision cross-sections.



Select which parameters to display : ● General ○ Switches (I) ○ Switches(II)

Please enter the following parameters:-

Radiation field temperature (eV) : 8.617E+03 [Blank for default]
General radiation field dilution : 0.000E+00 [Blank for default]
Multiplier for ionisation cross-sections : 1.000E+00 [Blank for default]
Multiplier for Regemorter cross-sections : 1.000E+00 [Blank for default]
Ionising radiation field dilution : 1.000E+08 [Blank for default]
Beam species isotope mass : 1.0 [Blank for default]

Select table for display:-
○ Impurity information
● Representative N-shells

Enter limits on N-shells:
Minimum N-shell: 1
Maximum N-shell: 110

Note:
The first representative N-shell is set equal to the minimum N-shell

Representative N-shells

INDEX	N Shell
1	1
2	2
3	3

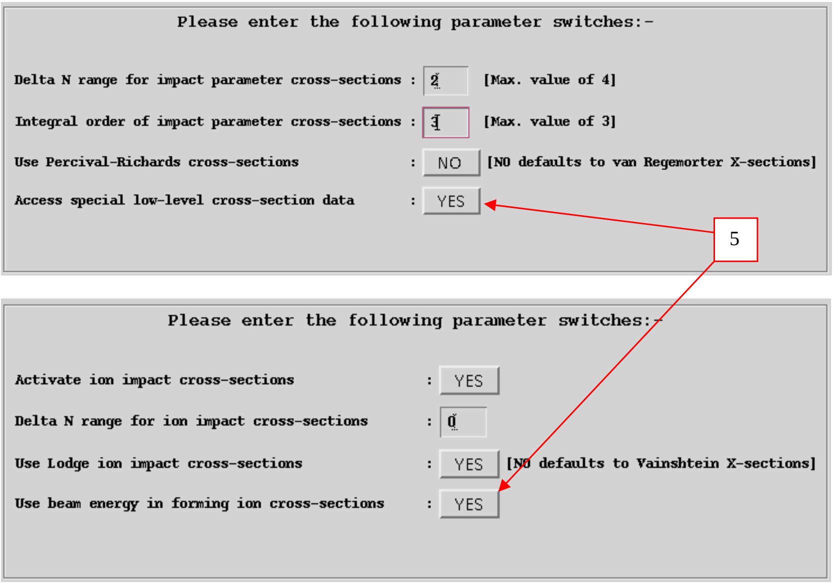
Select table for display:-
● Electron/proton density scan
○ Electron/proton temperature scan
○ Beam energy scan

Electron/proton densities (units: cm-3)

INDEX	Electron density	Proton density
1	5.000E+12	5.000E+12
2	7.000E+12	7.000E+12

Enter index of reference densities : 8

2. Impurity and representative N-shell information is required. Click the *Representative N-shell* buttons to display the appropriate sub-
3. The representative N-shells requires specification of the lowest N-shell, Highest N-shell and a set of sensibly spaced 'representative' N-shells spanning the range. Make sure the lowest is 1 for hydrogen. Make the highest around 110 and use about 20 representative levels. Use all levels up to N=10 and then start to space more widely.
4. A choice of plasma and beam parameters for the scans must be made Click on the appropriate button to work on each scan in turn. Note that you edit in a set of values and then choose one to be the reference value of that parameter. The table may be edited by clicking on the *Edit Table* button.. The ADAS Table Editor window is then presented with the same set of editing operations available as are described in bulletin *nov18-94*. Values should be monotonic increasing. It has proved helpful to add a *Clear Table* button to remove all entries in the output field. When specifying *the Beam energy scan*, note that a neutral hydrogen density in the beam is requested. This is necessary to allow a mathematical separation of the various influences on the neutral hydrogen population structure and is not an experimental beam density. A value of order 10^6 or greater is suitable for the program operation.
5. Details of the switches I and II sub-windows are shown. Make sure that *Access to low level data* is chosen and *Use beam energy informing cross-sections*. It is this latter piece of information that informs the calculation that the neutral hydrogen is in the beam and not in the plasma.
6. In the impurity information sub-window, there are two modes of operation. Single impurity or Multiple impurities. Click the drop-down list button to make your choice.



Please enter the following parameter switches:-

Delta N range for impact parameter cross-sections : 2 [Max. value of 4]

Integral order of impact parameter cross-sections : 3 [Max. value of 3]

Use Percival-Richards cross-sections : NO [NO defaults to van Regemorter X-sections]

Access special low-level cross-section data : YES

Please enter the following parameter switches:-

Activate ion impact cross-sections : YES

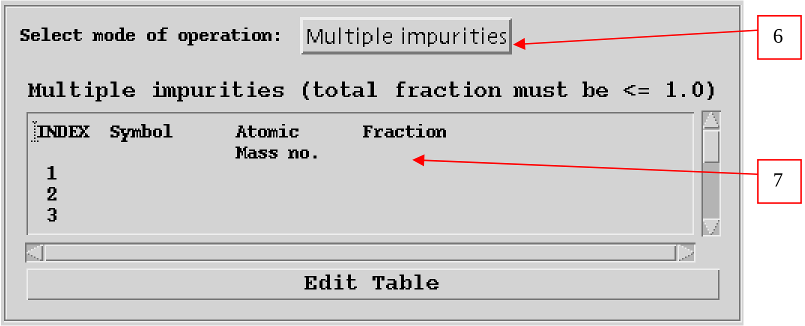
Delta N range for ion impact cross-sections : 0

Use Lodge ion impact cross-sections : YES [NO defaults to Vainshtein X-sections]

Use beam energy in forming ion cross-sections : YES

7. The multiple impurity choice enables us to investigate the influence of an impurity mixture on the stopping with greater precision. Edit in the fractions you wish in the usual manner. Note that the impurity density acts non-linearly in the stopping coefficient and so the linear superposition implied by the use of ADAS304 is imprecise. It is however very fast which is necessary in large scale experimental data analysis.

The single impurity case has only one impurity nucleus in addition to protons present in the plasma. The single impurity case is used to build up such data sets in *adf21*. Note how the impurity and protons fit together (equations 4.10.16 and 4.10.17 in the ADAS User Manual). The proton and electron density choices to be made next influence this.



Select mode of operation: Multiple impurities

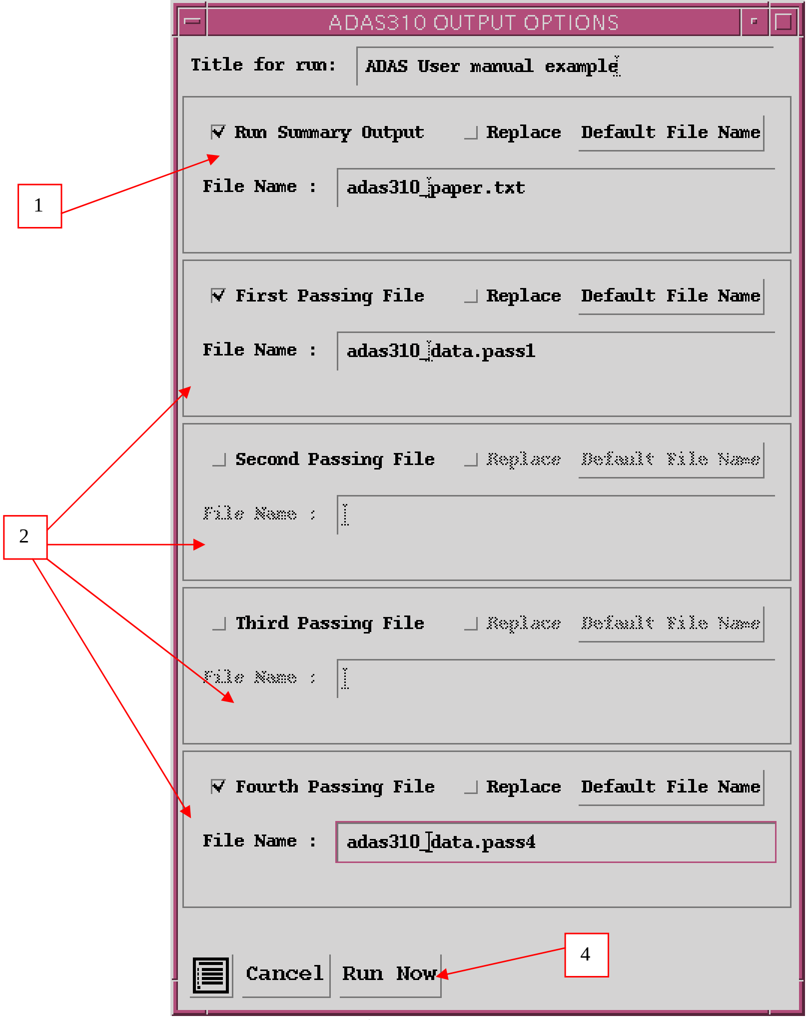
Multiple impurities (total fraction must be <= 1.0)

INDEX	Symbol	Atomic Mass no.	Fraction
1			
2			
3			

The **output options window** is shown below. It follows the usual pattern except that there is no graphical output.

1. The *Run Summary Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Run Summary Output* is on. If the file already exits a choice to *Replace* or *Append* may be made. The default file name ‘paper.txt’ may be set by pressing the button

Default file name. A ‘pop-up’ window issues a warning if the file already exists and the *Append* or *Replace* button has not been activated.



Title for run: ADAS User manual example

☑ Run Summary Output ☐ Replace
File Name : adas310_paper.txt

☑ First Passing File ☐ Replace
File Name : adas310_data.pass1

☐ Second Passing File ☐ Replace
File Name :

☐ Third Passing File ☐ Replace
File Name :

☑ Fourth Passing File ☐ Replace
File Name : adas310_data.pass4

2. Four additional passing files may be produced which are placed in your pass directory. The first passing file is of ADAS data format ADF26 and contains line printer formatted pages of data, one page for each individual population structure case run. The data held on these sheets is very comprehensive. By appropriate choice of the parameters mentioned in the processing section above and choice of input files, hydrogen in all its possible conditions in a fusion plasma can be obtained (beam and non-beam).
3. Click the *Run Now* button to initiate the calculations. These are run in foreground since they are of fairly modest duration. A thermometer widget keeps you informed of the progress of the calculations.

Lecture 4 Charge exchange and beam emission spectroscopy

Preliminaries

Charge exchange spectroscopy is driven by reactions of the form

$$X^{+z_0} + D^0_{beam}(1) \rightarrow X^{+z_0}(nl) + D^+_{beam}$$

in which an electron is captured from a donor atom in its ground (or an excited) state. The principal application is usually to capture by the bare nuclei of impurity atoms in the plasma from the ground state of deuterium, helium or lithium atoms in fast neutral beams. Subsequently the hydrogen-like impurity ion radiates as

$$X^{+z_0-1}(n'l') \rightarrow X^{+z_0-1}(n''l'') + h\nu$$

Composite spectral line features of the form $n' \rightarrow n''$ are observed made up from unresolved $n'l' \rightarrow n''l''$ multiplet components. Charge exchange line features often involve high principal quantum shells and occur over wide spectral ranges including the visible range. In general the populations of receiver levels are modified by redistributive collisions with plasma ions and electrons and by fields before radiation emission occurs

The programs of series ADAS3 are associated with neutral beams of hydrogen or helium isotopes and there are two streams of modelling. The first stream is concerned with modelling and detailed spectral line emission from hydrogen-like impurity ions in a plasma following charge transfer from fast neutral beams. It commences with a collection of state selective charge transfer cross-section data at n, nl or nlm resolution (type ADF01) spanning an extended region of collision energies and n-shells and in some cases different sources. For interpretation of charge exchange emission lines, effective emission coefficients for relevant spectral lines emitted by the receiver are required. These are archived in ADAS data format ADF12. They require special collisional-radiative population calculations for their evaluation. There are two collisional-radiative processing options, namely for calculations in the *bundle-nl* (ADAS308) or *bundle-nlj* (ADAS306) approximations. The programs ADAS308 and ADAS306 predict data for arbitrary lines at a fixed set of conditions and show extensive detail of the line emission. It is convenient to have available more automatic codes which generate ony tables of ADF12 coefficients over ranges of plasma parameters without the intervening displays. This capability is provided by ADAS309 and ADAS307 for the bundle-nlj and bundle-nl pictures respectively. The latter are termed scanning versions of the codes. The associated codes for interrogation of the fundamental state selective cross-section database and the effective charge exchange emission coefficient database are ADAS301 and ADAS303 respectively.

The ADAS data formats format

The various relevant classes of data are

adf01	bundle-n and bundle-nl charge exchange cross-sections
adf02	ion impact cross-sections with named participant
adf12	charge exchange effective emission coefficients
adf21	effective beam stopping coefficients
adf26	bundle-n populations of excited states in beams

ADF01

For a specified relative collision energy E_i belonging to the tabulation, let the total cross section be $\sigma_{tot}(E_i)$ and the n-shell cross-sections be $\sigma_n(E_i)$. The latter are tabulated for $n_{\min} \le n \le n_{\max}$ for some $n_{\min}$ and $n_{\max}$. For $n \ge n_{\max}$ extrapolation is assumed of the form

$$\sigma_n(E_i) = (n_{\max}/n)^{\beta(E_i)}\,\sigma_{n_{\max}}(E_i)$$

The parameter $\beta(E_i)$ is deduced from $\sigma_{n_{\max}-1}(E_i)$ and $\sigma_{n_{\max}}(E_i)$ and is tabulated in the data set. The $\sigma_n(E_i)$ are normalised to the total cross-section so that, using the extrapolation equation for $n \geq n_{\max}$

$$\sigma_{tot}(E_i) = \sum_{n=n_{\min}}^{\infty} \sigma_n(E_i)$$

Explicit l-subshell cross-sections $\sigma_{nl}(E_i)$ are tabulated for $n_{\min} \leq n \leq n_{\max}$ and $0 \leq l \leq n-1$. In extrapolation there are two cases.

Case 1: No *l* subshell subdivision parameters are given in the ADF01 dataset.. It is assumed that the l distribution for $n > n_{\max}$ is the same as for $n_{\max}$ so that

$$\sigma_{nl}(E_i) = \begin{cases} \sigma_{n_{\max}l}(E_i)(\sigma_n(E_i)/\sigma_{n_{\max}}(E_i)) & for\ l \leq n_{\max}-1 \\ 0 & for\ l \geq n_{\max} \end{cases}$$

4.1.3

Case 2: *l* subshell parameters are given in the the ADF01 dataset. The parameters are obtained as a fit to *l*- subshell cross-section data for a particular n-shell using the program ADAS107. The parameterisation identifies an *l*-type , parameter $ltyp(E_i)$ and an approximate *l* (non integral) at which the cross-section behaviour changes from rising at low *l* to falling at high *l*, parameter $xlcr(E_i)$. The behaviour is then given by

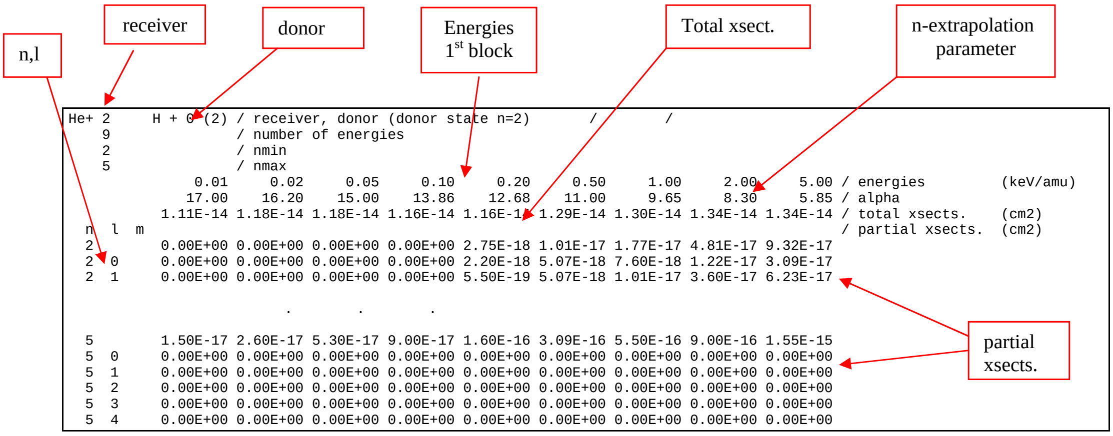
$$\sigma_{nl}(E_i) \sim \begin{cases} (2l+1)^{pl2} & for\ l < xlcr \\ \exp(-(l-xlcr)^{pl3}) & for\ l < xlcr \end{cases}$$

The normalisation

$$\sigma_n(E_i) = \sum_{l=0}^{n-1} \sigma_{nl}(E_i)$$

is maintained while the sharpness of the switching between the two forms varies with the *l*-type. A detailed description is given in ADAS107.

A typical ADF01 organisation is shown for H^0 donor to He^2 receiver

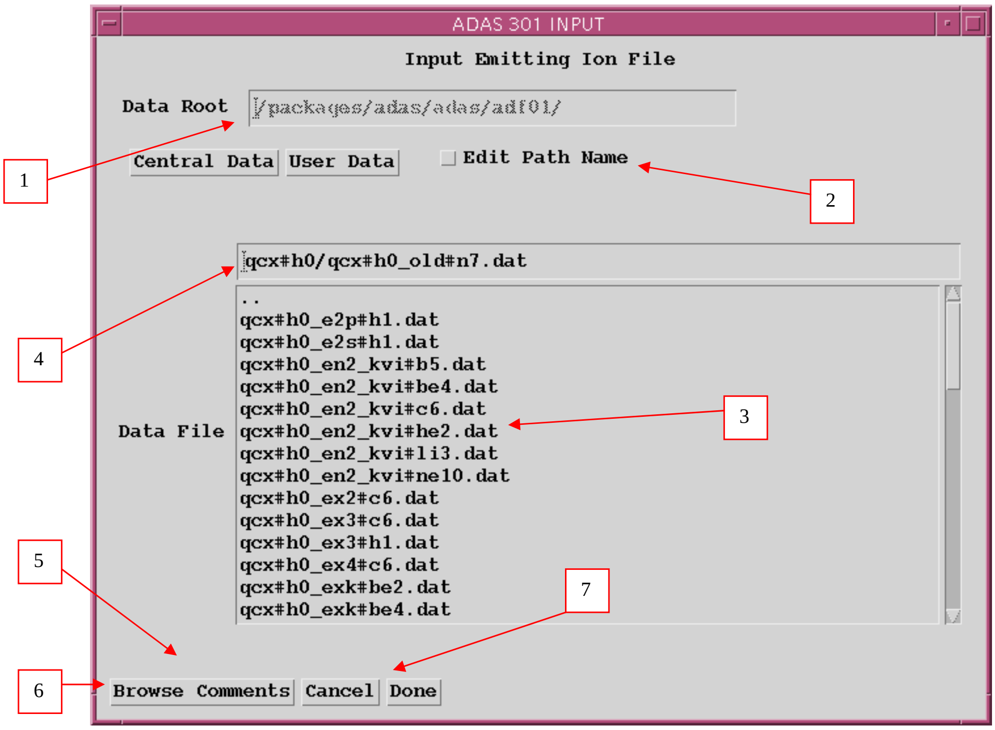


```
He+ 2     H + 0 (2) / receiver, donor (donor state n=2)       /        /
    9               / number of energies
    2               / nmin
    5               / nmax
          0.01     0.02     0.05     0.10     0.20     0.50     1.00     2.00     5.00 / energies         (keV/amu)
         17.00    16.20    15.00    13.86    12.68    11.00     9.65     8.30     5.85 / alpha
      1.11E-14 1.18E-14 1.18E-14 1.16E-14 1.16E-14 1.29E-14 1.30E-14 1.34E-14 1.34E-14 / total xsects.    (cm2)
  n  l  m                                                                              / partial xsects.  (cm2)
  2       0.00E+00 0.00E+00 0.00E+00 0.00E+00 2.75E-18 1.01E-17 1.77E-17 4.81E-17 9.32E-17
  2  0    0.00E+00 0.00E+00 0.00E+00 0.00E+00 2.20E-18 5.07E-18 7.60E-18 1.22E-17 3.09E-17
  2  1    0.00E+00 0.00E+00 0.00E+00 0.00E+00 5.50E-19 5.07E-18 1.01E-17 3.60E-17 6.23E-17

                       .        .        .

  5       1.50E-17 2.60E-17 5.30E-17 9.00E-17 1.60E-16 3.09E-16 5.50E-16 9.00E-16 1.55E-15
  5  0    0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  1    0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  2    0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  3    0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  4    0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
```

ADAS301

The code interrogates state selective charge exchange cross-section files of type ADF01. Data may be extracted for capture to a selected n-, nl-or nlm-shell of a hydrogen-like or lithium-like receiving ion depending on the ADF01 file. The data may be interpolated using cubic splines to provide cross-sections at arbitrarily chosen impact energies. A minimax polynomial approximation is also made to the source data. The source and interpolated cross-section data are displayed and a tabulation prepared. The tabular and graphical output may be printed and include the minimax polynomial approximation.

The **file selection window** is shown below.



Data Root: /packages/adas/adas/adf01/

Data File: qcx#h0/qcx#h0_old#n7.dat

```
..
qcx#h0_e2p#h1.dat
qcx#h0_e2s#h1.dat
qcx#h0_en2_kvi#b5.dat
qcx#h0_en2_kvi#be4.dat
qcx#h0_en2_kvi#c6.dat
qcx#h0_en2_kvi#he2.dat
qcx#h0_en2_kvi#li3.dat
qcx#h0_en2_kvi#ne10.dat
qcx#h0_ex2#c6.dat
qcx#h0_ex3#c6.dat
qcx#h0_ex3#h1.dat
qcx#h0_ex4#c6.dat
qcx#h0_exk#be2.dat
qcx#h0_exk#be4.dat
```

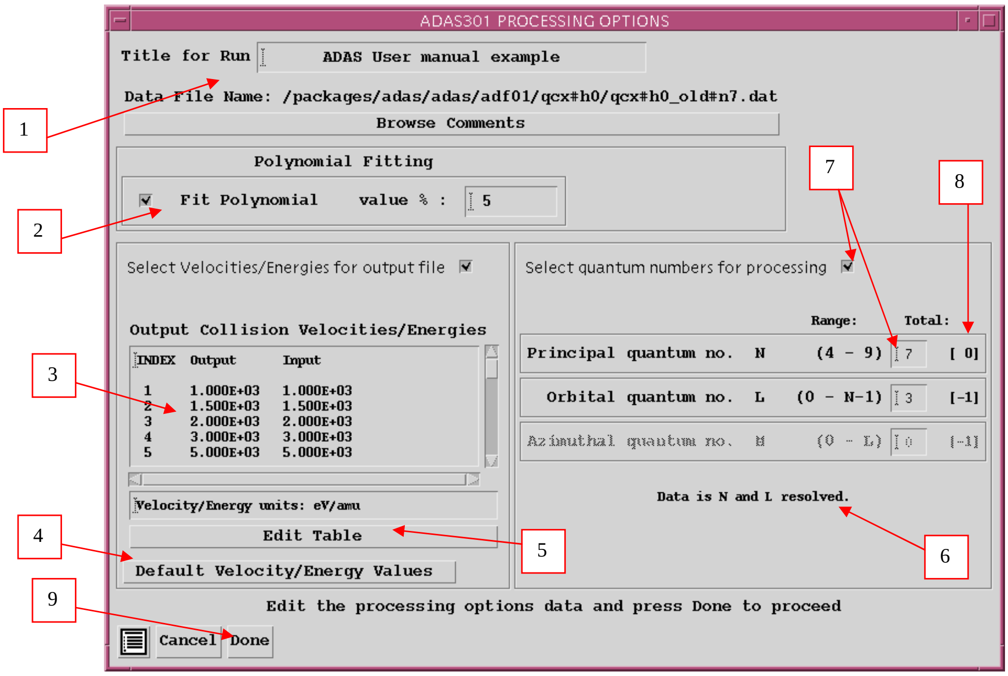
1. Data root shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type – ADF01 in this case. Note that each type of data is stored according to its ADAS data format (*adf* number). Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*, to use this facility.
2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
3. Available sub-directories are shown in the large file display window. There are a large number of these, stored by donor which is usually neutral but not necessarily so (eg. *qcx#h0*). The individual members are identified by the subdirectory name, a code and then fully ionised receiver (eg. qcx#h0_*old#c6.dat*). The data sets generally contain *nl*-resolved cross-section data but *n*-resolved and *nlm*-resolved are handled. Resolution levels must not be mixed in datasets. The codes distinguish different sources.The first letter *o* or the code *old* has been used to indicate that the data has been produced from JET compilations which originally had parametrised *l*-distribution of cross-sections. The nl-resolved data with such code has been reconstituted from them. Data of code *old* is the preferred JET data. Other sources codes include *ory*

(old Ryufuku), *ool* (old Olson), *ofr* (old Fritsch) and *omo* (old molecular orbital). There are new data such as *kvi*.

4. Click on a name to select it. The selected name appears in the smaller selection window above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
5. Once a data file is selected, the set of buttons at the bottom of the main window become active.
6. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.
7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

The **processing options window** has the appearance shown below

1. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being analysed is also shown. The button *Browse Comments* again allows display of the information field section at the foot of the selected dataset, if it exists.
2. The output data extracted from the datafile, a 'charge exchange cross-section', may be fitted with a polynomial. This is as a function of relative collision energy per atomic mass unit (eV/amu). Clicking the *Fit Polynomial* button activates this. The accuracy of the fitting required may be specified in the editable box. The value in the box is editable only if the *Fit Polynomial* button is active
3. Your settings of collision velocity/energy (output) are shown in the display window. The velocity/energy values at which the charge exchange coefficients are stored in the datafile (input) are also shown for information. The program recovers the output velocities/energies you used when last executing the program.
4. Pressing the *Default Velocity/Energy values* button inserts a default set of velocities/energies equal to the input velocities/energies
5. The Velocity/Energy values are editable. Click on the *Edit Table* button if you wish to change the values. A 'drop-down' window, the ADAS Table Editor window: It follows the same pattern of operation as described in the *18nov-94* bulletin.
6. The specific cross-section data to be extracted is specified by the window to the right. The level or resolution of the data source is shown.
7. Activate the *Select quantun numbers for processing* button to allow new settings of these quantum numbers. The values in the three smaller windowsbecome editable depending also on the resolution of the dataset. Note that the *Range* of the data in the dataset is displayed.
8. There are special codes to be used to obtain summed cross-sections over sub-quantum numbers. These are indicated in brackets under the *Total* column and should be entered into the editable window if required.



Title for Run: ADAS User manual example

Data File Name: /packages/adas/adas/adf01/qcx#h0/qcx#h0_old#n7.dat

☑ Fit Polynomial value % : 5

Select Velocities/Energies for output file ☑

Output Collision Velocities/Energies

INDEX	Output	Input
1	1.000E+03	1.000E+03
2	1.500E+03	1.500E+03
3	2.000E+03	2.000E+03
4	3.000E+03	3.000E+03
5	5.000E+03	5.000E+03

Velocity/Energy units: eV/amu

Select quantum numbers for processing ☑

		Range:		Total:
Principal quantum no.	N	(4 - 9)	7	[0]
Orbital quantum no.	L	(0 - N-1)	3	[-1]
Azimuthal quantum no.	M	(0 - L)	0	[-1]

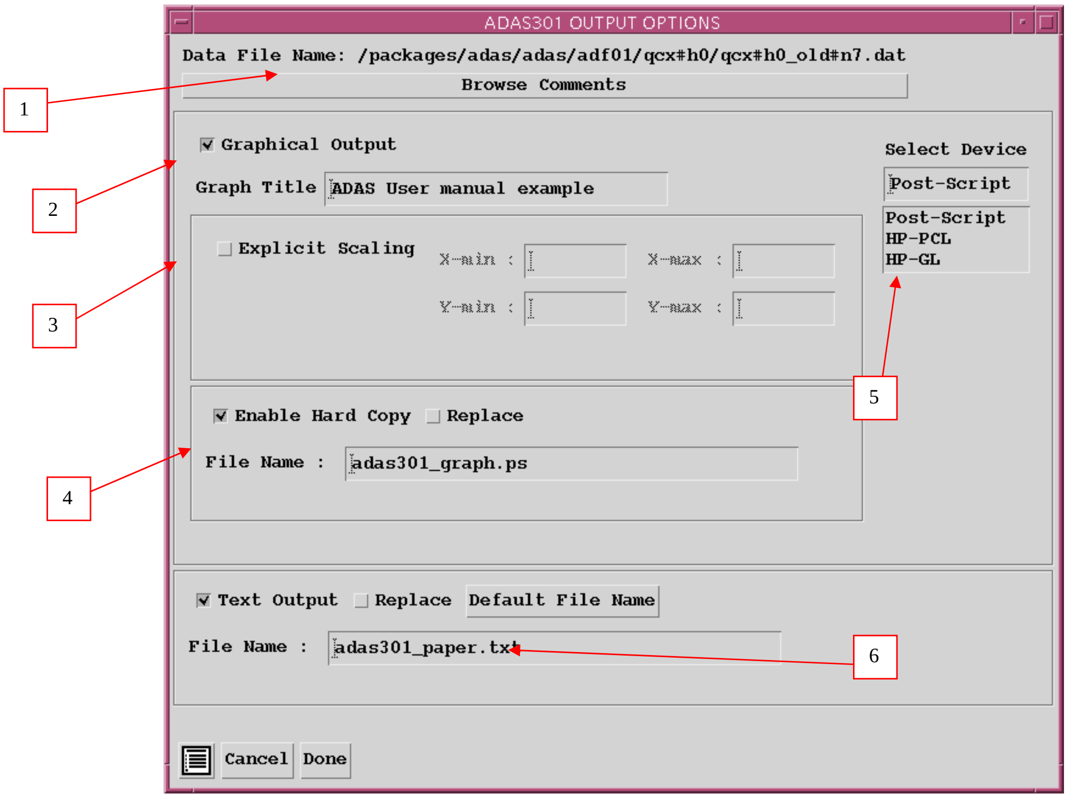
Data is N and L resolved.

Edit the processing options data and press Done to proceed

9. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

The **output options window** is shown below

1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
2. Graphical display is activated by the *Graphical Output* button. This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph.
3. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.
4. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. If the output graphic file already exits and the *Replace* button has not been activated, a ‘pop-up’ window issues a warning.
5. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.
6. The *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name ‘paper.txt’ may be set by pressing the button *Default file name*. A ‘pop-up’ window issues a warning if the file already exists and the *Replace* button has not been activated.


ADAS301 OUTPUT OPTIONS

Data File Name: /packages/adas/adas/adf01/qcx#h0/qcx#h0_old#n7.dat

☑ Graphical Output

Graph Title ADAS User manual example

☐ Explicit Scaling

☑ Enable Hard Copy ☐ Replace

File Name : adas301_graph.ps

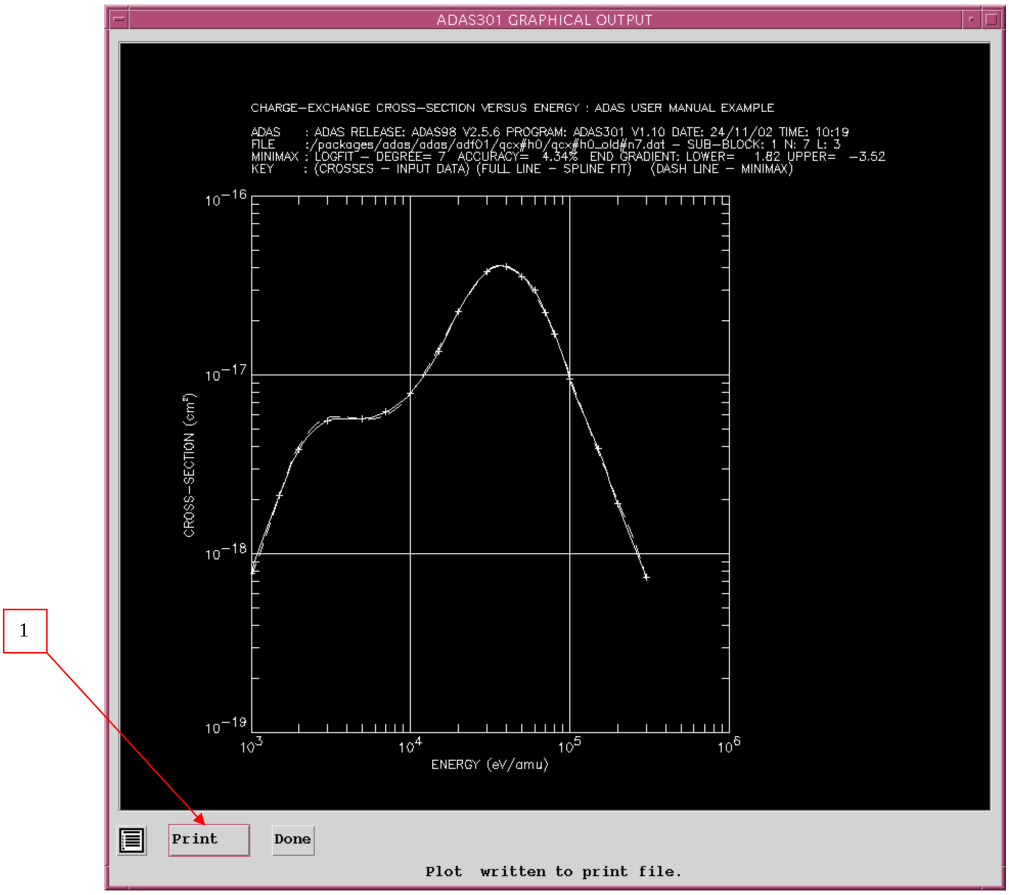
Select Device Post-Script

☑ Text Output ☐ Replace

File Name : adas301_paper.txt

The **Graphical output window** is shown below

1. Printing of the currently displayed graph is activated by the *Print* button.



```
CHARGE-EXCHANGE CROSS-SECTION VERSUS ENERGY : ADAS USER MANUAL EXAMPLE

ADAS    : ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS301 V1.10 DATE: 24/11/02 TIME: 10:19
FILE    :/packages/adas/adas/adf01/qcx#h0/qcx#h0_old#n7.dat - SUB-BLOCK: 1 N: 7 L: 3
MINIMAX : LOGFIT - DEGREE= 7  ACCURACY=  4.34%  END GRADIENT: LOWER=   1.82 UPPER=  -3.52
KEY     : (CROSSES - INPUT DATA) (FULL LINE - SPLINE FIT)   (DASH LINE - MINIMAX)
```

```
Plot  written to print file.
```

ADF12

Data from files of type ADF12 contain charge exchange effective emission coefficients for principal quantum shell transitions of hydrogen-like impurity ions, $q_{n\to n'}^{(eff)}$, at a reference beam/plasma condition of beam energy $E_u^{(ref)}$, plasma ion density $N_{zeff}^{(ref)}$, plasma ion temperature $T_{zeff}^{(ref)}$, plasma z effective $zeff^{\,(ref)}$ and magnetic field strength $B_{mag}^{(ref)}$. Also they contain the $q_{n\to n'}^{(eff)}$ at varying plasma conditions obtained by keeping all the parameters except one at the reference conditions. These are called one-dimensional scans and there are $q_{n\to n'}^{(eff)}$ sets at the following parameter sets:

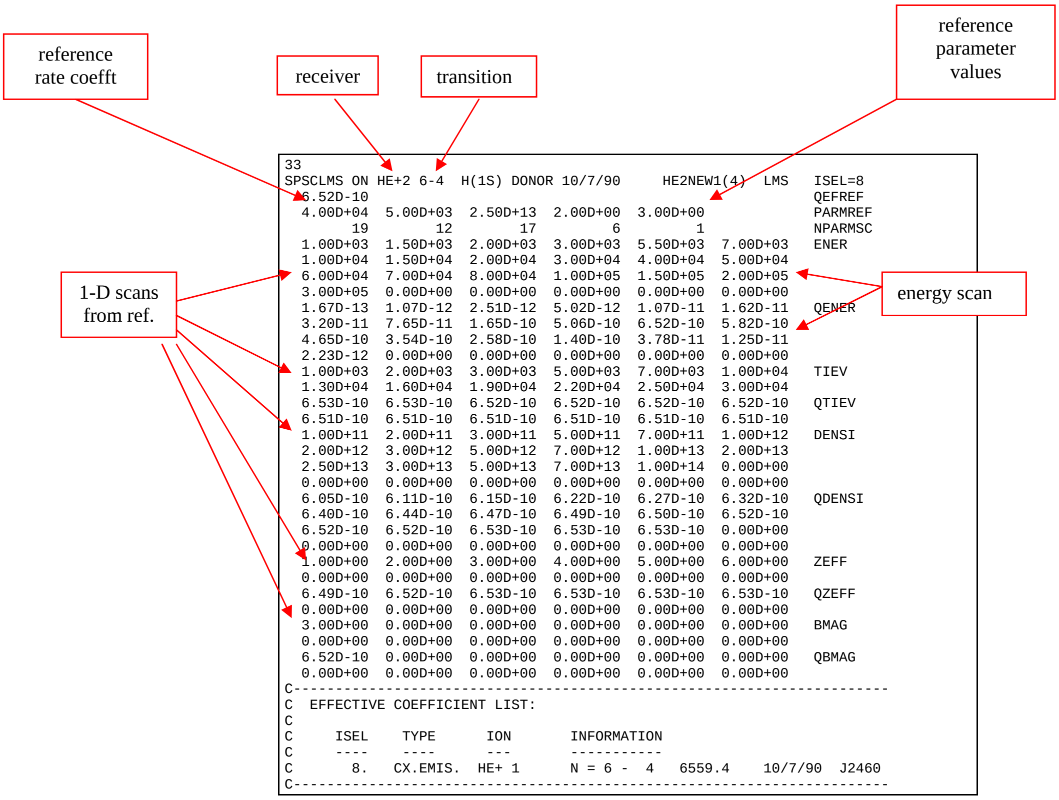
$\{E_{u,i}:i=1,I_E\}, N_{zeff}^{(ref)}, T_{zeff}^{(ref)}, zeff^{\,(ref)}, B^{(ref)}$ with $E_u^{(ref)} \in \{E_{u,i}:i=1,I_E\}$,

$E_u^{(zeff)}, \{N_{zeff}:i=1,I_N\}, T_{zeff}^{(ref)}, zeff^{\,(ref)}, B^{(ref)}$ with $N_{zeff}^{(ref)} \in \{N_{zeff}:i=1,I_N\}$,

$E_u^{(ref)}, N_{zeff}^{(ref)}, \{T_{zeff\,,i}:i=1,I_T\}, zeff^{\,(ref)}, B^{(ref)}$ with $T_{zeff}^{(ref)} \in \{T_{zeff\,,i}:i=1,I_T\}$,

$E_u^{(ref)}, N_{zeff}^{(ref)}, T_{zeff}^{(ref)}, \{zeff_i:i=1,I_{zeff}\}, B^{(ref)}$ with $zeff^{\,(ref)} \in \{zeff_i:i=1,I_{zeff}\}$,

$E_u^{(ref)}, N_{zeff}^{(ref)}, T_{zeff}^{(ref)}, zeff^{\,(ref)}, \{B_i:i=1,I_B\}$ with $B^{(ref)} \in \{B_i:i=1,I_B\}$.



```
33
SPSCLMS ON HE+2 6-4  H(1S) DONOR 10/7/90     HE2NEW1(4)  LMS   ISEL=8
  6.52D-10                                                     QEFREF
  4.00D+04  5.00D+03  2.50D+13  2.00D+00  3.00D+00             PARMREF
        19        12        17         6         1             NPARMSC
  1.00D+03  1.50D+03  2.00D+03  3.00D+03  5.50D+03  7.00D+03   ENER
  1.00D+04  1.50D+04  2.00D+04  3.00D+04  4.00D+04  5.00D+04
  6.00D+04  7.00D+04  8.00D+04  1.00D+05  1.50D+05  2.00D+05
  3.00D+05  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  1.67D-13  1.07D-12  2.51D-12  5.02D-12  1.07D-11  1.62D-11   QENER
  3.20D-11  7.65D-11  1.65D-10  5.06D-10  6.52D-10  5.82D-10
  4.65D-10  3.54D-10  2.58D-10  1.40D-10  3.78D-11  1.25D-11
  2.23D-12  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  1.00D+03  2.00D+03  3.00D+03  5.00D+03  7.00D+03  1.00D+04   TIEV
  1.30D+04  1.60D+04  1.90D+04  2.20D+04  2.50D+04  3.00D+04
  6.53D-10  6.53D-10  6.52D-10  6.52D-10  6.52D-10  6.52D-10   QTIEV
  6.51D-10  6.51D-10  6.51D-10  6.51D-10  6.51D-10  6.51D-10
  1.00D+11  2.00D+11  3.00D+11  5.00D+11  7.00D+11  1.00D+12   DENSI
  2.00D+12  3.00D+12  5.00D+12  7.00D+12  1.00D+13  2.00D+13
  2.50D+13  3.00D+13  5.00D+13  7.00D+13  1.00D+14  0.00D+00
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  6.05D-10  6.11D-10  6.15D-10  6.22D-10  6.27D-10  6.32D-10   QDENSI
  6.40D-10  6.44D-10  6.47D-10  6.49D-10  6.50D-10  6.52D-10
  6.52D-10  6.52D-10  6.53D-10  6.53D-10  6.53D-10  0.00D+00
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  1.00D+00  2.00D+00  3.00D+00  4.00D+00  5.00D+00  6.00D+00   ZEFF
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  6.49D-10  6.52D-10  6.53D-10  6.53D-10  6.53D-10  6.53D-10   QZEFF
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  3.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00   BMAG
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  6.52D-10  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00   QBMAG
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
C-----------------------------------------------------------------------
C  EFFECTIVE COEFFICIENT LIST:
C
C     ISEL    TYPE      ION       INFORMATION
C     ----    ----      ---       -----------
C       8.   CX.EMIS.  HE+ 1      N = 6 -  4   6559.4    10/7/90  J2460
C-----------------------------------------------------------------------
```

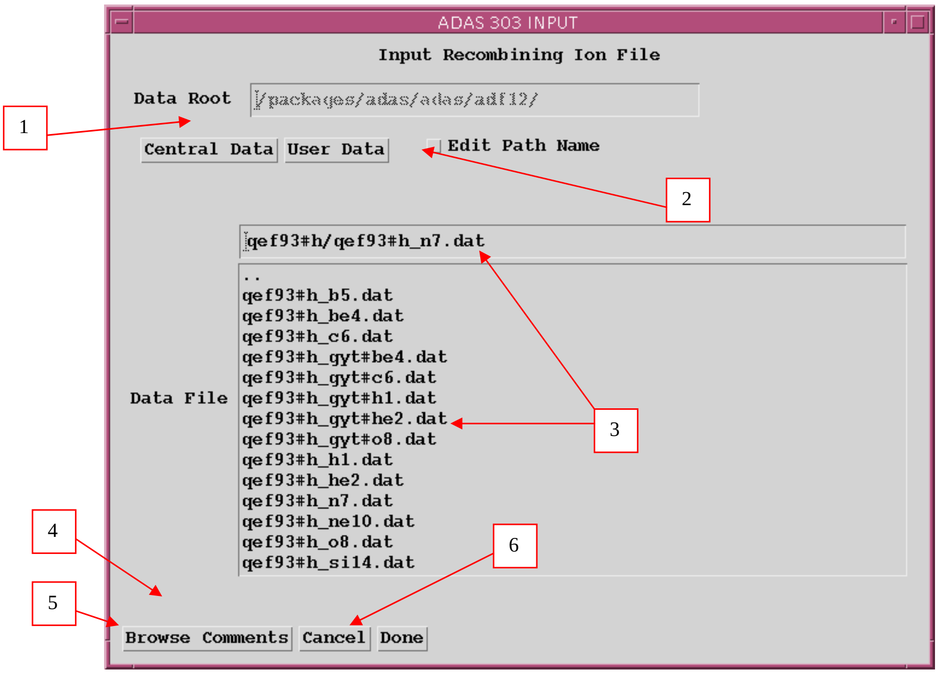
ADAS303

The program interrogates charge exchange spectroscopy effective emission coefficient data sets of type ADF12 associated with a particular neutral donor. The ADF12 data set collections are for the relevant hydrogen-like n-n' spectrum lines grouped according to the recombining ion. The code and data organisation allows the emission coefficient to be obtained (by interpolation using cubic splines) at plasma conditions and at relative collision energies of choice. A minimax polynomial approximation can also be made to the interpolated data. The interpolated data are displayed and a tabulation prepared. The tabular and graphical output may be printed and include the polynomial approximation.

The **file selection window** appears first and has the appearance shown below.

1. Data root shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Note that each type of data is stored according to its ADAS data format (*adf* number). *adf12* is the appropriate format for use by the program ADAS303. Details of the organisation of such data is given in the *appxa-12*. Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*, to use this facility.
2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing

3. Available sub-directories are shown in the large file display window. There are a large number of these. They are stored in sub-directories by donor which is usually neutral but not necessarily so (eg. *qef93#h*). The individual members are identified by the subdirectory name, a code and then fully ionised receiver (eg. *qef93#h_be4.dat*). The data sets generally contain many individual spectrum lines. Scroll bars appear if the number of entries exceed the file display window size. Such data is generally stored by year number (eg. *93*) with the most recent data to be preferred. Click on a name to select it. The selected name appears in the smaller selection window above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
4. Once a data file is selected, the set of buttons at the bottom of the main window become active.
5. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.
6. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window



Data Root /packages/adas/adas/adf12/

Data File qef93#h/qef93#h_n7.dat

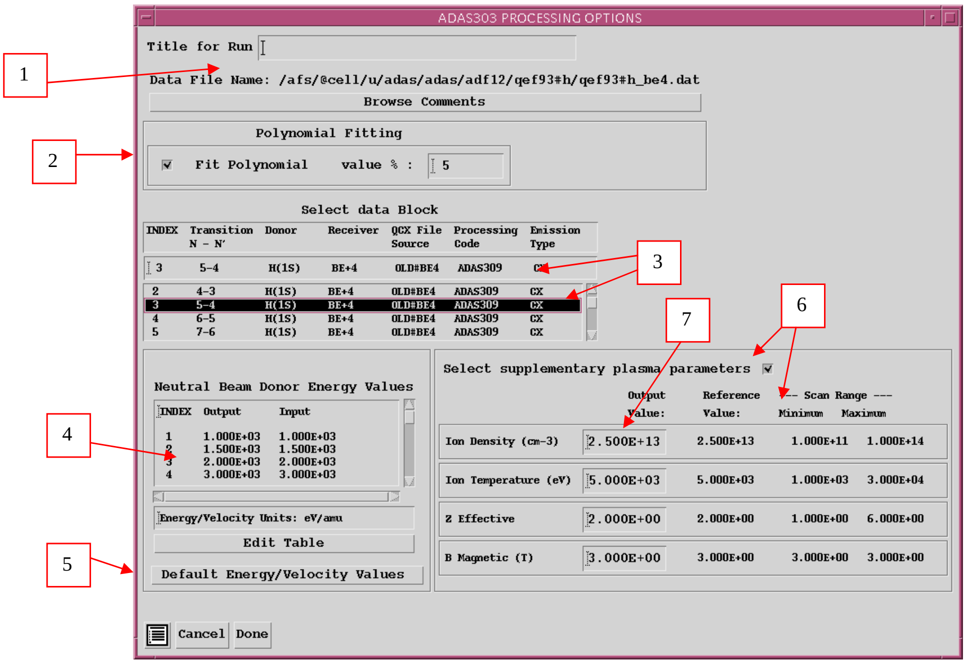
```
..
qef93#h_b5.dat
qef93#h_be4.dat
qef93#h_c6.dat
qef93#h_gyt#be4.dat
qef93#h_gyt#c6.dat
qef93#h_gyt#h1.dat
qef93#h_gyt#he2.dat
qef93#h_gyt#o8.dat
qef93#h_h1.dat
qef93#h_he2.dat
qef93#h_n7.dat
qef93#h_ne10.dat
qef93#h_o8.dat
qef93#h_si14.dat
```

The **processing options window** is shown below:

1. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being analysed is also shown. The button *Browse comments* again allows display of the information field section at the foot of the selected dataset, if it exists.
2. The output data extracted from the datafile may be fitted with a polynomial. Clicking the *Fit Polynomial* button activates this. The accuracy of the fitting required may be specified in the editable box.

The value in the box is editable only if the *Fit Polynomial* button is active.

3. Transitions available in the data set are displayed in the transition list display window. This is a scrollable window using the scroll bar to the right of the window. Click anywhere on the row for a transition to select it. The selected transition appears in the selection window just above the transition list display window.



Title for Run

Data File Name: /afs/@cell/u/adas/adas/adf12/qef93#h/qef93#h_be4.dat

☑ Fit Polynomial value % : 5

INDEX	Transition N – N'	Donor	Receiver	QCX File Source	Processing Code	Emission Type
3	5-4	H(1S)	BE+4	OLD#BE4	ADAS309	CX

2	4-3	H(1S)	BE+4	OLD#BE4	ADAS309	CX
3	5-4	H(1S)	BE+4	OLD#BE4	ADAS309	CX
4	6-5	H(1S)	BE+4	OLD#BE4	ADAS309	CX
5	7-6	H(1S)	BE+4	OLD#BE4	ADAS309	CX

INDEX	Output	Input
1	1.000E+03	1.000E+03
2	1.500E+03	1.500E+03
3	2.000E+03	2.000E+03
4	3.000E+03	3.000E+03

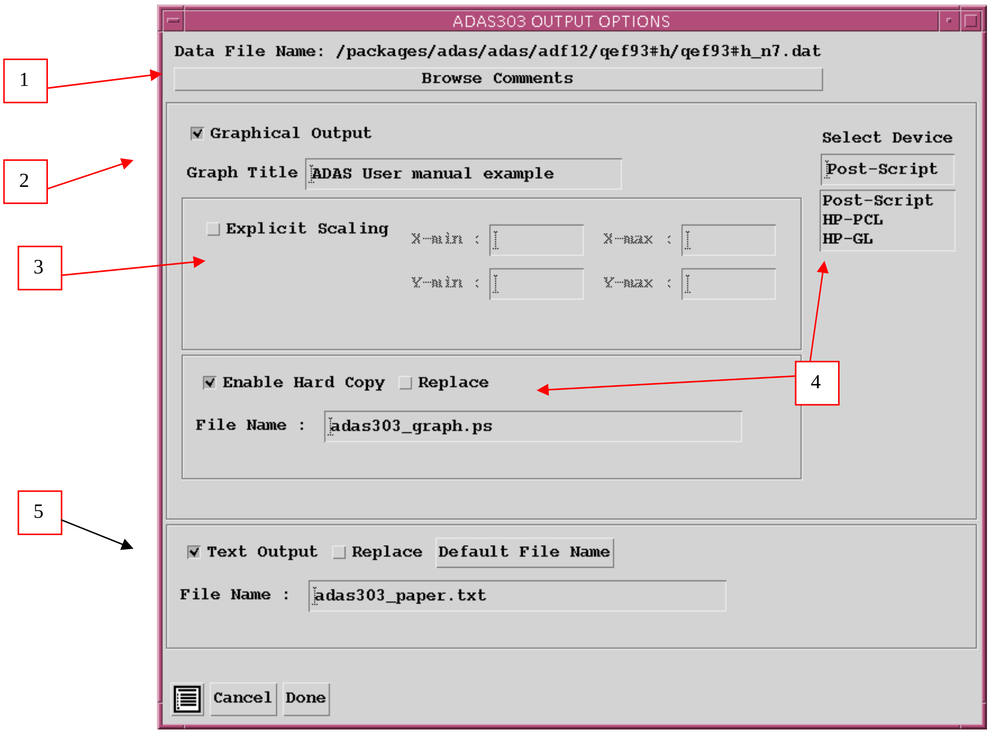
Energy/Velocity Units: eV/amu

	Output Value:	Reference Value:	--- Scan Range --- Minimum	Maximum
Ion Density (cm-3)	2.500E+13	2.500E+13	1.000E+11	1.000E+14
Ion Temperature (eV)	5.000E+03	5.000E+03	1.000E+03	3.000E+04
Z Effective	2.000E+00	2.000E+00	1.000E+00	6.000E+00
B Magnetic (T)	3.000E+00	3.000E+00	3.000E+00	3.000E+00

4. Energies/velocities for the neutral donor are displayed. The particular choice of units in use is shown below the table. Your settings of beam energy/velocity (output) are shown in the display window. The beam energy/velocity values at which the effective emission coefficients are stored in the datafile (input) are also shown for information. Click the *Edit Table* button to drop-down the ADAS Table Editor. Within Table Editor you can select which units to use as well as entering you energy/velocity values for output. Note that final graphed results are of effective emission coefficient versus beam energy (eV/amu).
5. The program recovers the output energies/velocities you used when last executing the program. Pressing the *Default Energy/Velocity values* button inserts a default set of energies/velocities equal to the input values
6. Effective emission coefficients for the ADF12 database are calculated at one-dimensional scans in various plasma parameters relative to a reference set of plasma conditions. Details are given in *appxa-12*. To alter the settings, activate the *Select supplementary plasma parameters* button.
7. The sub-windows become active with the output data entry box in each editable. For information, the reference value of each plasma parameter is given together with the range of the parameter in its one-dimensional scan. Values outside the range should not be entered. For data prepared using processing code ADAS309, the B magnetic field

parameter has no effect, but is simply used for place holding. The scan in *B Magnetic* is of zero length.

The **output options window** is shown below



Data File Name: /packages/adas/adas/adf12/qef93#h/qef93#h_n7.dat

☑ Graphical Output

Graph Title: ADAS User manual example

☐ Explicit Scaling X-min : X-max : Y-min : Y-max :

☑ Enable Hard Copy ☐ Replace

File Name : adas303_graph.ps

Select Device: Post-Script

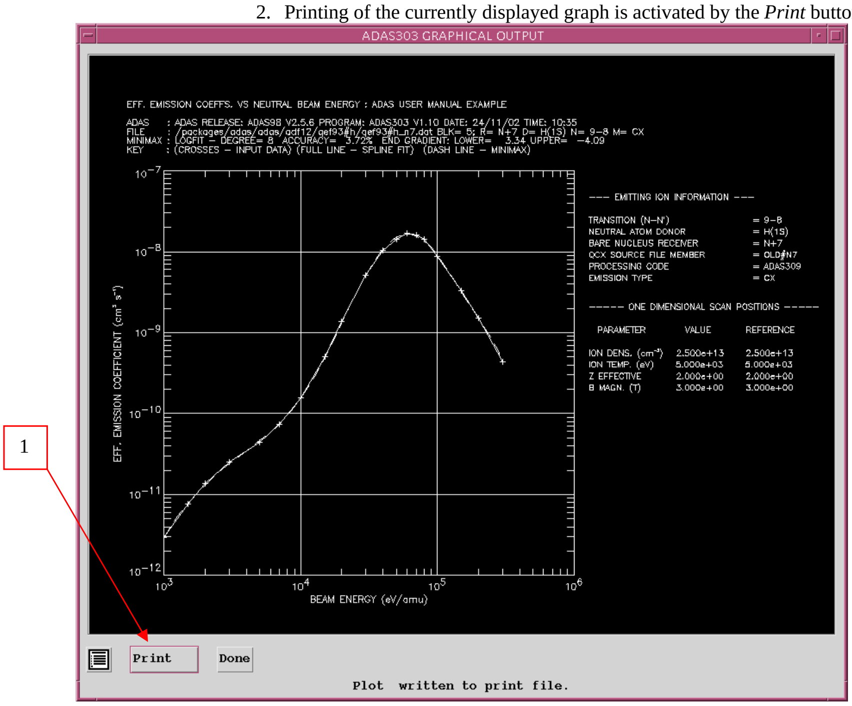
☑ Text Output ☐ Replace

File Name : adas303_paper.txt

7. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
8. Graphical display is activated by the *Graphical Output* button. This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph.
9. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.
10. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. If the output graphic file already exits and the *Replace* button has not been activated, a 'pop-up' window issues a warning. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.
11. The *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name 'paper.txt' may be set by pressing the button *Default file name*. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated.

The **Graphical output window** is shown below

2. Printing of the currently displayed graph is activated by the *Print* button.



```
EFF. EMISSION COEFFS. VS NEUTRAL BEAM ENERGY : ADAS USER MANUAL EXAMPLE

ADAS    : ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS303 V1.10 DATE: 24/11/02 TIME: 10:35
FILE    : /packages/adas/adas/adf12/qef93#h/qef93#h_n7.dat BLK= 5; R= N+7 D= H(1S) N= 9-8 M= CX
MINIMAX : LOGFIT - DEGREE= 8  ACCURACY=  3.72%  END GRADIENT: LOWER=   3.34 UPPER=  -4.09
KEY     : (CROSSES - INPUT DATA) (FULL LINE - SPLINE FIT)  (DASH LINE - MINIMAX)

--- EMITTING ION INFORMATION ---

TRANSITION (N-N')                 = 9-8
NEUTRAL ATOM DONOR                = H(1S)
BARE NUCLEUS RECEIVER             = N+7
QCX SOURCE FILE MEMBER            = OLD#N7
PROCESSING CODE                   = ADAS309
EMISSION TYPE                     = CX

----- ONE DIMENSIONAL SCAN POSITIONS -----

 PARAMETER           VALUE        REFERENCE

ION DENS. (cm^-3)   2.500e+13     2.500e+13
ION TEMP. (eV)      5.000e+03     5.000e+03
Z EFFECTIVE         2.000e+00     2.000e+00
B MAGN. (T)         3.000e+00     3.000e+00
```

Plot written to print file.

Calculating CXS effective emission coefficients

The line-of-sight integrated photon emissivity of a charge exchange driven line may be written as

$$\begin{aligned}
I_{n\to n'}^{(z_0-1)} &= \sum_{l,l'} I_{nl\to n'l'}^{(z_0-1)} \\
&= \int_S \sum_{l,l'} A_{nl\to n'l'} N_{nl}^{(z_0-1)} ds \\
&= \int_S [\sum_{l,l'} A_{nl\to n'l'} (N_{nl}^{(z_0-1)} / N_D N^{(z_0)})] N_D N^{(z_0)} ds \\
&= \int_S [\sum_{l,l'} q_{nl\to n'l'}^{(eff)}] N_D N^{(z_0)} ds \\
&= \int_S q_{n\to n'}^{(eff)} N_D N^{(z_0)} ds \\
&\approx q_{n\to n'}^{(eff)} \int_S N_D N^{(z_0)} ds
\end{aligned}$$

where S is the path length through the neutral beam / plasma intersection along a spectrometer line-of-sight. N_D is the neutral donor number density and $N^{(z_0)}$ is the number density of fully ionised impurity atoms. $q_{n\to n'}^{(eff)}$ is the *effective emission coefficient* for the whole $n \to n'$ principal quantum shell transition and $\int_S N_D N^{(z_0)} ds$ is the *emission measure*. The mean transition energy is

$$\Delta E_{n,n'} = (\sum_{l,l'} \Delta E_{nl,n'l'} q^{(eff)}_{nl\to n'l'}) / q^{(eff)}_{n\to n'}$$

where $\Delta E_{nl,n'l'}$ is the line component transition energy and $q^{(eff)}_{nl\to n'l'}$ is the component effective emission coefficient. The effective emission coefficient $q^{(eff)}_{n\to n'}$ may be calculated theoretically. If it is approximately constant over the emitting volume, then measurement of a charge exchange line intensity $I^{(z_0-1)}_{n\to n'}$ allows deduction of the emission measure $\int_S N_D N^{(z_0)} ds$. If neutral beam attenuation to the observed volume is known or calculable then local impurity density may be inferred.

With the effective emission coefficients calculated theoretically, comparison with one observed charge exchange line intensity allows deduction of the emission measure. Then all other line intensities are predictable. If more than one line intensity is observed, then a mean emission measure may be deduced and some comment may be made on the ratios of experimental to theoretical effective emission coefficients. The organisation of the collisional-radiative modelling in ADAS308 is specifically designed to allow such comparison. The following points and assumptions are made:

(i) From the theoretical point-of-view the direct capture cross-sections to levels are more fundamental quantities for comparison with experiment that the effective emission coefficients.

(ii) The dominant fundamental processes modifying the initial distribution of capture are redistribution within an *n*-shell and radiative cascade in low and moderate density plasmas. Limiting the collisional-radiative theory to these dominant processes allows a compact invertable relationship to be established between column emissivities of charge exchange spectrum lines and direct capture cross-sections.

(ii) It is of most practical value to target experiment / theory comparisons on the *n*-shell distribution of capture (including the *n*-shell decrement) in fusion studies. This may be achieved by imposing theoretical information on the *l* sub-shell distribution of capture.

Consider the monoenergetic direct capture rate coefficients to *nl* sub-levels $q^{(CX)}_{nl}$ from the initial neutral donor state *D⁰(1)* by the fully stripped impurity ion with number density $N^{(z_0)}$, denoted more compactly by N^+.

$$q^{(CX)}_{nl}(E_u) = v\ \sigma^{(CX)}_{nl}(v)$$

where E_u is the relative collision energy per atomic mass unit so that $v = \sqrt{2E_u / m_p}$ is the relative collision speed, with m_p the proton mass and σ the capture cross-section.

It is supposed that

$$q^{(CX)}_{nl}(E_u) = f^{(theor)}_{(n)l} q^{(CX)}_n(E_u)$$

Since no collisional excitation from lower to higher *n*-shells is allowed, the populations of the *lj* sublevels of the principal quantum shell $n' \geq n+1$ may be written as

$$N_{n'l'} = N_D N^+ \sum_{n^{iv}\geq n+1} W_{n'l',n^{iv}} q^{(CX)}_{n^{iv}}$$

Then the equations determining the populations of the sub-shells of the principal quantum shell *n* are

$$\sum_{l''} M_{(n)l,l''} N_{nl''} = N_D N^+ f^{(theor)}_{(n)l} q^{(CX)}_n + \sum_{n'\geq n+1} A_{nl,n'l'} N_{n'l'}$$

so that

$$N_{nlj} = N_D N^+ W_{nlj,n} q^{(CX)}_n + N_D N^+ \sum_{n^{iv}\geq n+1} W_{nlj,n^{iv}} q^{(CX)}_{n^{iv}}$$

with

$$W_{nlj,n} = [\sum_{l''j''} M^{-1}_{(n)lj,l''j''} f^{(theor)}_{(n)l''j''}] q^{(CX)}_n$$

and

$$W_{nlj,n^{iv}} = \sum_{l'',j'',l',j'} M^{-1}_{(n)lj,l''j''} A_{nl''j'',n'l'j'} W_{n'l'j',n^{iv}}$$

The solution can proceed recursively downwards in *n* with compact vector and array storage.

Tabulations of experimental or theoretical state selective charge exchange cross-section data span a range of principal quantum shells $\sigma^{(CX)}_{nlj}(v) : n_0 \leq n \leq n_1$. Cascade from levels $n > n_1$ may contribute significantly to the populations of lower levels especially at high collision energies when the decrease of the direct charge exchange cross-sections with *n* is slow ($\sigma_n \sim n^{-\alpha}$ and $\alpha \sim 3$). However, redistribution amongst *lj* sub-levels of the higher *n*-shells is high, approaching statistical in most circumstances. Therefore the cascade solution is initiated at some $n_{\max}$ (~20 typically) for complete *n*-shell populations only (matrices $W^{(high)}$), with subshells implicitly statistically populated, down to n_1 whereupon the *lj* resolved solution (matrices $W^{(low)}$) is commenced.

In general observable spectrum lines are associated with upper principal quantum shells $n \le n_1$. If M_{rep}, lines are identified each with a distinct upper *n*-shells $\bar{n}_{irep} : irep = 1,\ldots, M_{rep}$, then a 'condensation' may be imposed such that

$$q_n^{(CX)} = \sum_{irep=1}^{M_{rep}} L_{n,irep} q_{\bar{n}_{irep}}^{(CX)} \qquad \text{for } n_0 \le n \le n_1$$

and

$$q_n^{(CX)} = (n/n_1)^{\alpha} q_{n_1}^{(CX)} \qquad \text{for } n > n_1$$

giving, after integration along the line-of-sight, a matrix relation

$$\begin{bmatrix} I_{\bar{n}_1 \to \bar{n}_1'} \\ . \\ I_{\bar{n}_{M_{rep}} \to \bar{n}'_{M_{rep}}} \end{bmatrix} = (\int_S N_D N^+ ds) \begin{bmatrix} a_{11}. & . & a_{1M_{rep}} \\ . & . & . \\ a_{M_{rep}1} & . & a_{M_{rep}M_{rep}} \end{bmatrix} \begin{bmatrix} q_{\bar{n}_1}^{(CX)} \\ . \\ q_{\bar{n}_{M_{rep}}}^{(CX)} \end{bmatrix}$$

The coefficients of the matrix are theoretically calculated quantities. The equations may be solved for the the $q_{\bar{n}_i}^{(CX)}$ and the emission measure $\int_S N_D N^+ ds$ subject to the constraint

$$\sum_{irep=1}^{M_{rep}} q_{\bar{n}_{irep}}^{(CX)} = \sum_{irep=1}^{M_{rep}} q_{\bar{n}_{irep}}^{(CX)(theor)}$$

ADAS308

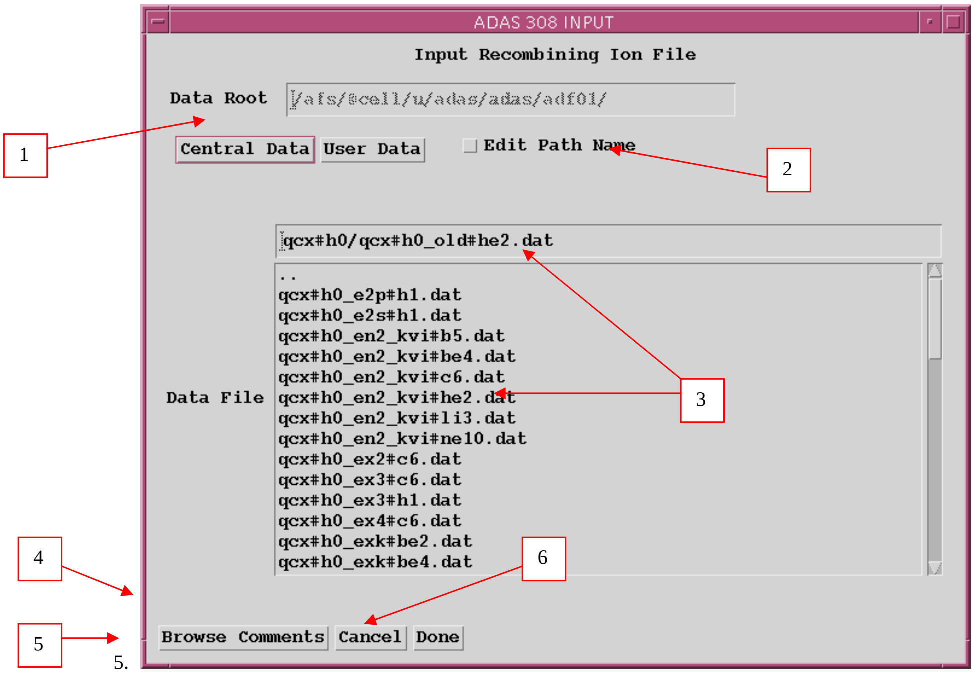
The code analyses *column* (line-of-sight integrated) emissivity observations of charge exchange spectroscopy lines from hydrogenic impurities, occuring through neutral beam / plasma interaction, in terms of emission measure. It predicts the column intensities of spectral components of the charge exchange lines, the Doppler broadened line shapes and effective emission coefficients for arbitrary lines in an l-resolved picture.

The **file selection window** is shown below.

1. Data root shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type – ADF01 in this case. Note that each type of data is stored according to its ADAS data format (*adf* number). Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*, to use this facility.
2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
3. Available sub-directories are shown in the large file display window. Scroll bars appear if the number of entries exceed the file display window size. There are a large number of these. They are stored in sub-directories by donor which is usually neutral but not necessarily so (eg. *qcx#h0*). The individual members are identified by the subdirectory name, a code and then fully ionised receiver (eg. qcx#h0*_old#c6.dat*). The data sets generally contain *nl*-resolved cross-section data but *n*-resolved and *nlm*-resolved are handled. Resolution levels must not be mixed in datasets. The ADF01 file nmaes distinguish different sources. The first letter *o* or the code *old* has been used to indicate that the data has been produced from JET compilations which originally had parametrised *l*-distribution of cross-sections. The nl-

resolved data with such code has been reconstituted from them. Data of code *old* is the preferred JET data. Other sources codes include *ory* (old Ryufuku), *ool* (old Olson), *ofr* (old Fritsch) and *omo* (old molecular orbital). There are newer data such as *kvi*. Additional codes are used for excited donors such as *ex2* for hydrogen n=2. Click on a name to select it. The selected name appears in the smaller selection window above the file display window. Then the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.

4. Once a data file is selected, the set of buttons at the bottom of the main window become active.



Data Root: /afs/@cell/u/adas/adas/adf01/

```
qcx#h0/qcx#h0_old#he2.dat
..
qcx#h0_e2p#h1.dat
qcx#h0_e2s#h1.dat
qcx#h0_en2_kvi#b5.dat
qcx#h0_en2_kvi#be4.dat
qcx#h0_en2_kvi#c6.dat
qcx#h0_en2_kvi#he2.dat
qcx#h0_en2_kvi#li3.dat
qcx#h0_en2_kvi#ne10.dat
qcx#h0_ex2#c6.dat
qcx#h0_ex3#c6.dat
qcx#h0_ex3#h1.dat
qcx#h0_ex4#c6.dat
qcx#h0_exk#be2.dat
qcx#h0_exk#be4.dat
```

5.

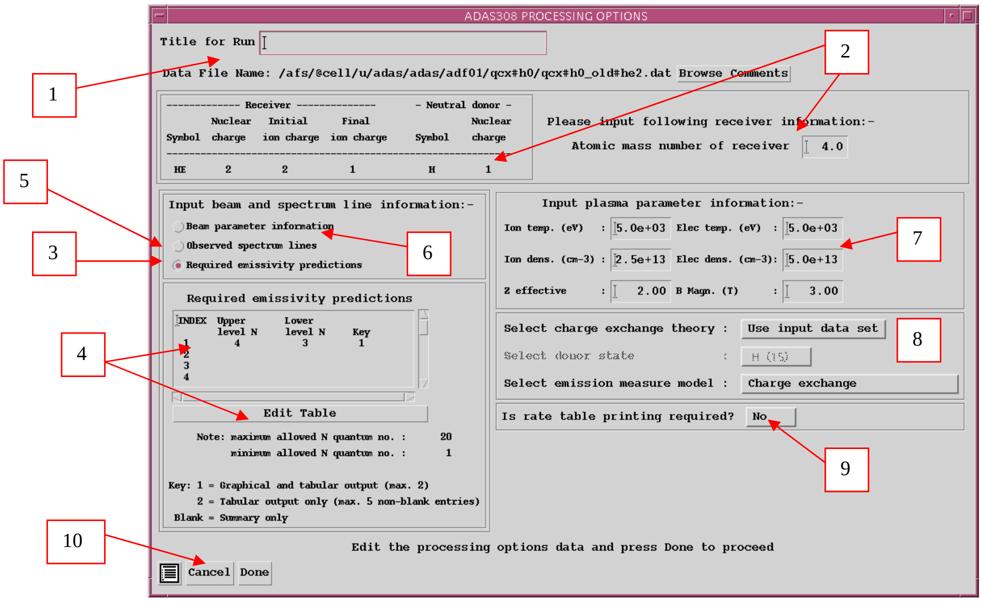
6. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what has gone into the dataset and the attribution of the dataset. The possibility of browsing the comments appears in the subsequent main window also.
7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

The **processing options window** has the appearance shown below

2. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being analysed is also shown. The button *Browse Comments* again allows display of the information field section at the foot of the selected dataset, if it exists.
3. Information is given on the fully ionised impurity receiver and the neutral beam donor. The atomic mass of the receiver must be entered.
4. The specification of beam parameters, details of observed line of sight spectral emissivities to be analysed and emissivities to be predicted are required. Input data of each of these three types may be addressed in

turn by activation of the relevant button. The window below the button list then presents the appropriate table.

5. *The Required emissivity predictions* button is displayed. This activates the predictive part of the code which becomes possible once the observed lines have been analysed in terms of emission measure. Then any set of lines within the N-shell limits may be predicted. The standard output includes the mean wavelength and effective emisison coefficient, but for up to five lines an extended tabulation of line component emissivities may be produced. Graphs may be produced for two selected line. Indicate these selections in the *Key* columnThe table may be edited by clicking on the *Edit Table* button.
6. The *Observed spectrum lines* table allows introduction of a number of observed intensities. It is possible to enter values which do not allow a consistent solution. The code advises of this but it is the responsibility of the user to check that the data is unblended etc. It is also a usual practice to enter just one line, possibly with a fictitious emissivity merely to obtain effective emission coefficients and line component details.
7. The *Beam parameter information* button causes display of the third editable table in the sub-window. Note that no check is made that the various beam energy fractions sum to unity. This is the responsibility of the user.



Title for Run

Data File Name: /afs/@cell/u/adas/adas/adf01/qcx#h0/qcx#h0_old#he2.dat

------------- Receiver	--------------			- Neutral donor -	
	Nuclear	Initial	Final		Nuclear
Symbol	charge	ion charge	ion charge	Symbol	charge
HE	2	2	1	H	1

Please input following receiver information:-

Atomic mass number of receiver 4.0

Input beam and spectrum line information:-

○ Beam parameter information
○ Observed spectrum lines
● Required emissivity predictions

Input plasma parameter information:-

Ion temp. (eV) : 5.0e+03 Elec temp. (eV) : 5.0e+03
Ion dens. (cm-3) : 2.5e+13 Elec dens. (cm-3): 5.0e+13
Z effective : 2.00 B Magn. (T) : 3.00

Select charge exchange theory : Use input data set
Select donor state : H (1S)
Select emission measure model : Charge exchange

Is rate table printing required? No

Required emissivity predictions

INDEX	Upper level N	Lower level N	Key
1	4	3	1
2			
3			
4			

Note: maximum allowed N quantum no. : 20
minimum allowed N quantum no. : 1

Key: 1 = Graphical and tabular output (max. 2)
2 = Tabular output only (max. 5 non-blank entries)
Blank = Summary only

Edit the processing options data and press Done to proceed

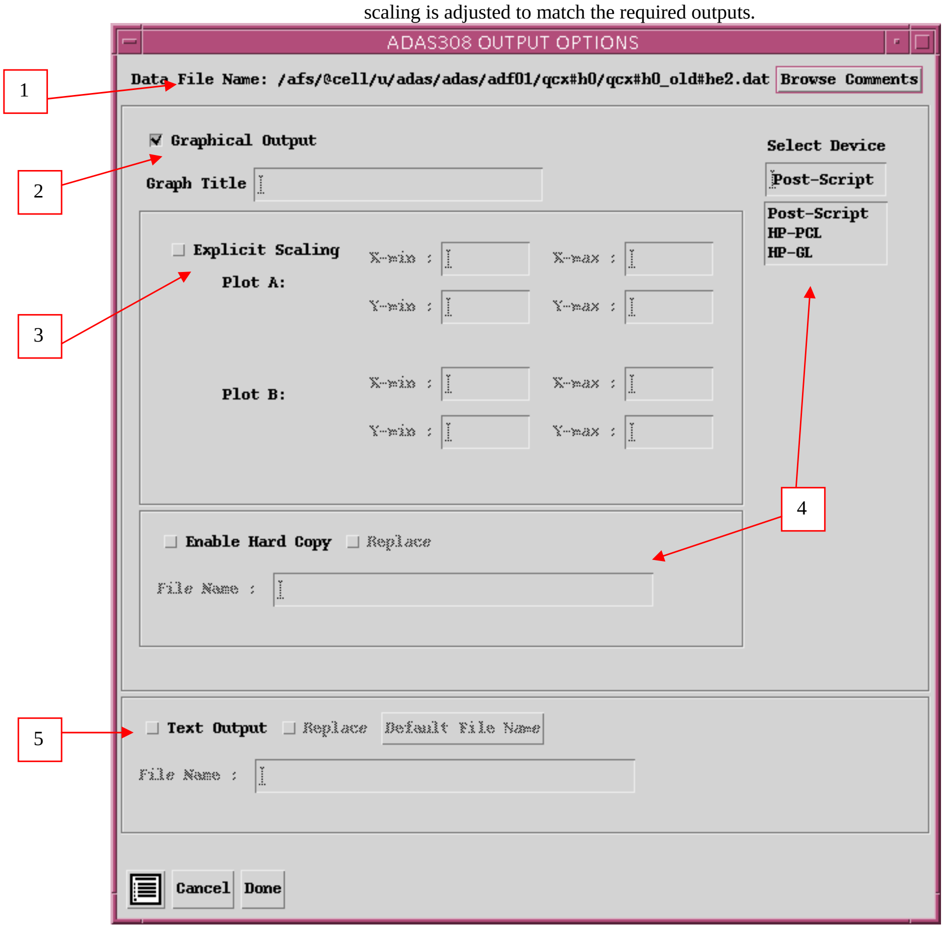
8. Enter the plasma environment parameters. These determine the collisional redistribution of the populations of the recombined plasma ion. For ADAS308, *B Magn*. has no effect, but a value should be entered as a place holder.
9. The final sub-window allows model and theory choices. Details are given in the ADAS Manual. For each type, clicking on the selection window drops down a short menu of choices. Click on the appropriate choice. The ADAS data base source numerical data of type ADF01 is the most usual, that is the *Use input data set* choice button. Note that

the *Select emission measure* model choice includes *Electron impact excitation* as well *as Charge exchange*.

10. Extended information on the rates used in the populaiton modelling may be printed.
11. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

The **Output options window** is shown below. Note that two plots are produced if required. The *Plot A* is the stick diagram of component line-of-sight emissivities. The *Plot B* is of the Doppler broadened profile of the line at the plasma ion temperature.

1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
2. Graphical display is activated by the *Graphical Output* button. This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph. By default, graph scaling is adjusted to match the required outputs.



Data File Name: /afs/@cell/u/adas/adas/adf01/qcx#h0/qcx#h0_old#he2.dat

☑ Graphical Output

Graph Title :

☐ Explicit Scaling

Plot A: X-min : X-max : Y-min : Y-max :

Plot B: X-min : X-max : Y-min : Y-max :

Select Device: Post-Script

☐ Enable Hard Copy ☐ Replace

File Name :

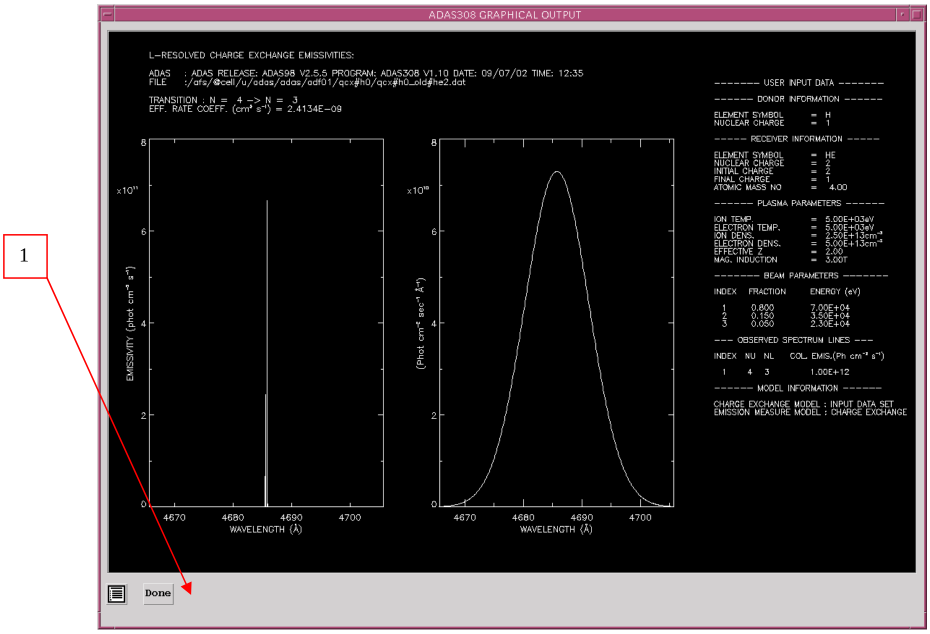
☐ Text Output ☐ Replace Default File Name

File Name :

3. Press the *Explicit Scaling* button to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable. Plot A axes limits refer to the ‘stick diagram and Plot B axes limits to the Doppler broadened profile.
4. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.
5. The *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name ‘paper.txt’ may be set by pressing the button *Default file name*.

The **Graphical output window** is shown below

3. Printing of the currently displayed graph is activated by the *Print* button.



```
L-RESOLVED CHARGE EXCHANGE EMISSIVITIES:

ADAS    : ADAS RELEASE: ADAS98 V2.5.5 PROGRAM: ADAS308 V1.10 DATE: 09/07/02 TIME: 12:35
FILE    :/afs/@cell/u/adas/adas/adf01/qcx#h0/qcx#h0_old#he2.dat

TRANSITION : N =  4 -> N =  3
EFF. RATE COEFF. (cm³ s⁻¹) = 2.4134E-09
```

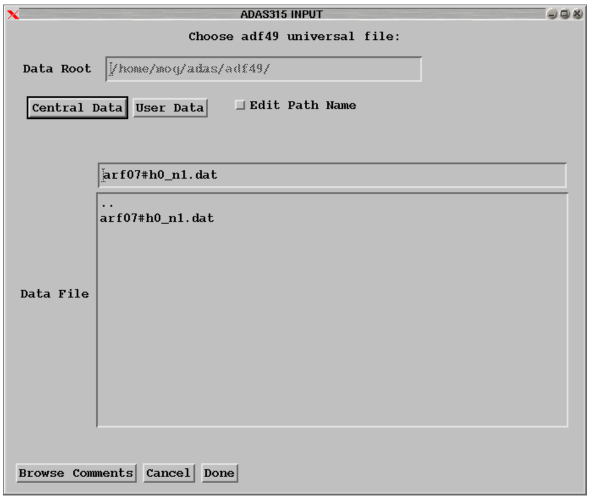
```
-------- USER INPUT DATA --------

------- DONOR INFORMATION -------

ELEMENT SYMBOL       =  H
NUCLEAR CHARGE       =  1

----- RECEIVER INFORMATION -----

ELEMENT SYMBOL       =  HE
NUCLEAR CHARGE       =  2
INITIAL CHARGE       =  2
FINAL CHARGE         =  1
ATOMIC MASS NO       =   4.00

------- PLASMA PARAMETERS -------

ION TEMP.            =  5.00E+03eV
ELECTRON TEMP.       =  5.00E+03eV
ION DENS.            =  2.50E+13cm⁻³
ELECTRON DENS.       =  5.00E+13cm⁻³
EFFECTIVE Z          =  2.00
MAG. INDUCTION       =  3.00T

-------- BEAM PARAMETERS --------

INDEX   FRACTION      ENERGY (eV)

  1      0.800        7.00E+04
  2      0.150        3.50E+04
  3      0.050        2.30E+04

--- OBSERVED SPECTRUM LINES ---

INDEX   NU   NL    COL. EMIS.(Ph cm⁻² s⁻¹)

  1      4    3       1.00E+12

------- MODEL INFORMATION -------

CHARGE EXCHANGE MODEL : INPUT DATA SET
EMISSION MEASURE MODEL : CHARGE EXCHANGE
```

Extended CXS capabilities

The charge exchange spectroscopy modelling capabilities of ADAS are still extending. This is largely motivated by the need to cope with heavier receiver ions beyond argon, which may be partially ionized. Attention is drawn to two new codes ADAS315 and ADAS316. Many subroutines have been added or modified to accommodate the new capabilities. The user should check the detailed release notes in item 4. A number of subroutines have modified parameter sets.

ADAS315: Preparation and extraction of universal adf49/adf01 CX cross-section data

This is a straightforward code which creates and ADF01 file for a specific ion of an element from a z-scaleable universal dataset of format ADF49. There are only two datasets of AD49 format corresponding to H(n=1) and H(n=2) donor respectively. The input screen is shown below followed by the output screen. A choice is possible of output energies. It is to be noted that in the level of approximation of the universal ADF49 data and the bundle-n application models, only the residual charge of the recombining ion is relevant. For the high n-shells of importance, the Rydberg electron is effectively in a hydrogenic state in the Coulomb field of the residual charge. The ADF49 datasets are subject to change as more fiducial data becomes available and the opimising of the z-scaling paramterisation is reworked. At this stage ADAS315 and ADAS316 are enabling a first look at the heavy ion CXS.



ADAS315 INPUT

Choose adf49 universal file:

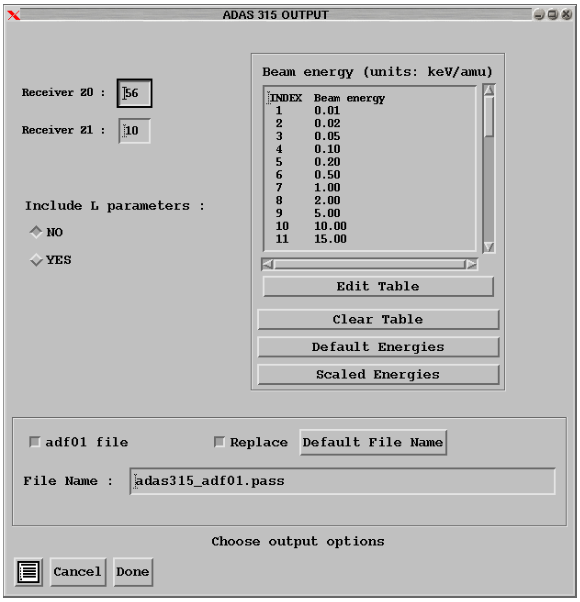
Data Root /home/mog/adas/adf49/

☐ Edit Path Name

Data File arf07#h0_n1.dat

..
arf07#h0_n1.dat

Running ADAS315 (an IDL only) code, available also at the command line, in a script allows output ADF01 files to be generated rapidly for a set of ions of an element.



ADAS 315 OUTPUT

Receiver Z0 : 56

Receiver Z1 : 10

Include L parameters :
◆ NO
◇ YES

Beam energy (units: keV/amu)

INDEX	Beam energy
1	0.01
2	0.02
3	0.05
4	0.10
5	0.20
6	0.50
7	1.00
8	2.00
9	5.00
10	10.00
11	15.00

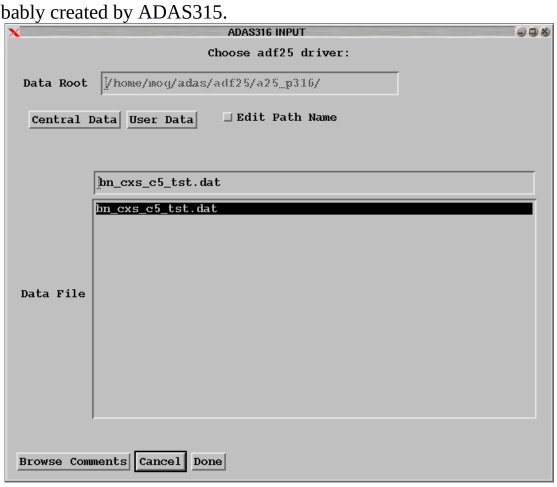
☐ adf01 file ☐ Replace

File Name : adas315_adf01.pass

Choose output options

ADAS316: Charge exchange spectroscopy – process effective coefficients: bundle-n

The code calculates charge exchange effective emission coefficients of format ADF12 from and input ADF01 file, probably created by ADAS315.



Choose adf25 driver:

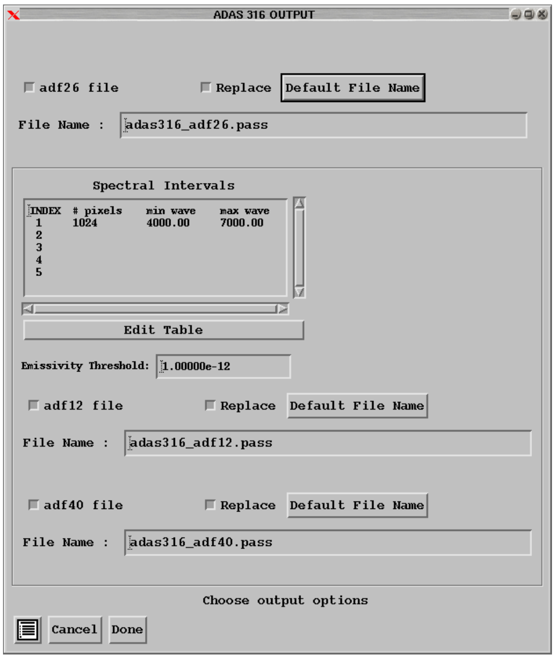
Data Root /home/mog/adas/adf25/a25_p316/

☐ Edit Path Name

Data File bn_cxs_c5_tst.dat

bn_cxs_c5_tst.dat

The code requires a driver data set and, for bundle-n in ADAS, these have historically been archived in ADF25.



☐ adf26 file ☐ Replace

File Name : adas316_adf26.pass

Spectral Intervals

INDEX	# pixels	min wave	max wave
1	1024	4000.00	7000.00
2			
3			
4			
5			

Emissivity Threshold: 1.00000e-12

☐ adf12 file ☐ Replace

File Name : adas316_adf12.pass

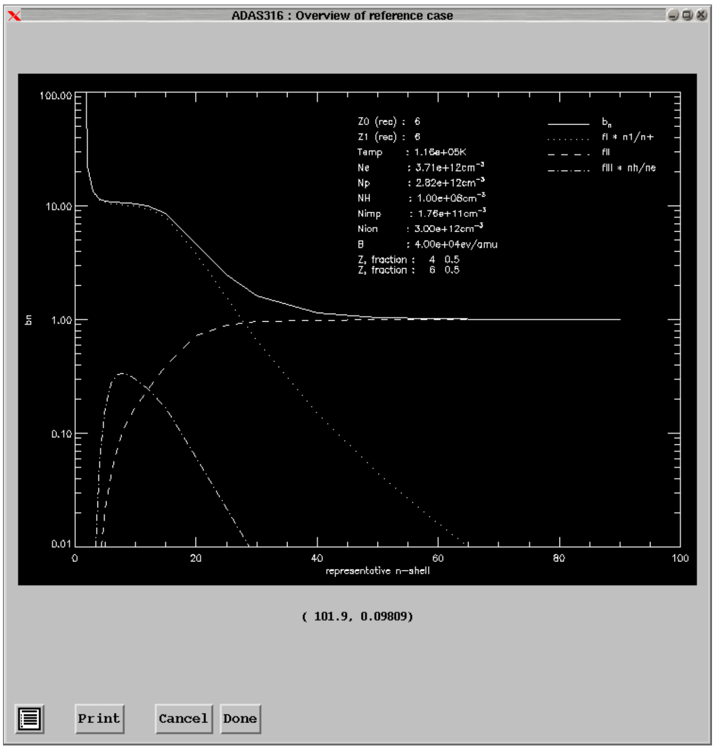
☐ adf40 file ☐ Replace

File Name : adas316_adf40.pass

Choose output options

A new sub-directory /a25_p316 has been assigned and a complete redesign of the driver has been carried out. Also a new read routine exploits the new drivers fully. We would like to move to this type of driver in the future, where there is substantial guidance to the user in the fields and mnemonics used in the driver. The driver allows scans over parameters to be specified. In fact the driver is quite versatile and appropriate to all type of bundle-n calculation . We shall exploit it further for Bremsstrahlung + free-bound continuum iand quasi-continuum high Rydberg line contributions in the future.

The output screen follows a usual pattern. Output ADF26 (the bundle-n population solution), ADF12 (charge exchange effective emission coefficients) and ADF40 (feature emissivity coefficients) may be produced. For heavy species CXS, because of the very large number of transitions between highly excited states, the ADF40 format becomes more useful that ADF12. A graph of the bundle-n-population solution, at the reference plasma parameters (usually at the centroid of the scans) is generated and shown with the free–electron capture and charge exchange capture parts separated – as illustrated below.



```
Z0 (rec) :  6
Z1 (rec) :  6
Temp      : 1.16e+05K
Ne        : 3.71e+12cm-3
Np        : 2.82e+12cm-3
NH        : 1.00e+08cm-3
Nimp      : 1.76e+11cm-3
Nion      : 3.00e+12cm-3
B         : 4.00e+04ev/amu
Z, fraction :   4  0.5
Z, fraction :   6  0.5
```

(101.9, 0.09809)

Beam stopping and emission

For a neutral beam species A being stopped by fully stripped impurity species and electrons in the plasma, the stopping coefficient is the effective loss rate coefficient of electrons from A . This corresponds closely to the effective ionisation rate coefficient or *collisional-radiative* ionisation coefficient from the ground state of $\mathcal{A}$, where charge transfer losses as well as direct ionisation losses are included. It is usual to write the coefficient in terms of the plasma electron density N_e so that the loss rate is $N_e S_{CR}^{(\mathcal{A})}$.

One can apply almost the same modellelling approach to hydrogen (or helium) atoms in a thermal plasma or to hydrogen atoms in a beam. The practical distinction is made by the assignment of a translational velocity for beam atoms. This velocity is incorporated in the integrals of beam particle / plasma particle cross-sections over the Maxwellian distributions in the thermal plasma. For hydrogen forming part of the thermal plasma, the translational velocity is set to zero. In the latter circumstance, ion impact collision rates are very small compared with electron impact rates. Also recombination (both free-electron capture and charge exchange capture) become significant processes. For the hydrogen atoms in a fast beam, recombination is not relevant and although formally present is ignored in the results. However the translational velocity can make ion impact collisions more important than electron collisions.

For hydrogen or hydrogenic ions in a plasma, the largest collision cross-sections are those for which n=n' and l=l'±1. For these cases the transition energy is nearly zero and the cross-sections are so large for electron and ion densities of relevance for fusion that it is very good approximation to assume relative statistical population for the l-states. Thus for hydrogenic systems only populations of complete n-shells need be evaluated, the *bundle-n* approximation. The equilibrium populations of the n-shells, N_n, are the solution of the statistical balance equations

$$\begin{aligned}
&\sum_{n'>n}[A_{n'\to n} + u(\nu)B_{n'\to n} + N_e q_{n'\to n}^{(e)} + N_e q_{n'\to n}^{(p)}]N_{n'} \\
&+\sum_{n''<n}[u(\nu)B_{n''\to n} + N_e q_{n''\to n}^{(e)} + N_e q_{n''\to n}^{(p)}]N_{n''} \\
&+N_e N_+ \alpha_n^{(r)} + N_e^2 N_+ \alpha_n^{(3)} + N_e N_+ \int u(\nu)B_{\kappa\to n}d\kappa \\
&= \{\sum_{n'>n}[u(\nu)B_{n\to n'} + N_e q_{n\to n'}^{(e)} + N_e q_{n\to n'}^{(p)}] \\
&+ \sum_{n''<n}[A_{n\to n''} + u(\nu)B_{n\to n''} + N_e q_{n\to n''}^{(e)} + N_e q_{n\to n''}^{(p)}] \\
&+\int u(\nu)B_{n\to\kappa}d\kappa + N_e q_{n\to\varepsilon}^{(e)} + N_e q_{n\to\varepsilon}^{(p)}\}N_n
\end{aligned}$$

N_n is the population of the state $X_n^{+z_0-1}$ and N_+ of the parent ion X^{+z_0}. N_e is the free electron density and N_p the free proton density. A and B are the usual Einstein coefficients, $q^{(e)}$ and $q^{(p)}$ denotes collisional rates due to electrons and protons, $\alpha_n^{(r)}$ and $\alpha_n^{(3)}$ denote radiative and three-body recombination and $u(\nu)$ is the energy density of the radiation field. There is one such equation for each value of n from 1 to ∞. The equations may be extended by including reactions for other impurity ions additional to the protons. The radiation field presence in the equations is not of direct relevance to hydrogen population modelling in a fusion plasma, but it can be exploited in a purely technical manner to separate the influence of different driving populations in the collisional-radiative sense.

Population results and preparing tabulations

ADAS 310 is the primary code for evaluating beam stopping and emission coefficients for hydrogen beams. It is too slow in execution for a direct link to inter-pulse experiment analysis and so it is used to prepare tabulations of effective beam stopping and beam emission coefficients for subsequent look-up. The effective coefficients are most sensitive to the beam particle energy and the plasma ion density and less sensitive to plasma ion temperature and Z-effective. Suitable tabulations can therefore be built on a reference set of plasma and beam conditions, a two-dimensional array of coefficients as functions of beam energy and plasma density at the reference conditions of the other parameters and then one-dimensional vectors of the coefficients as functions of each minor parameter at the reference condition of all the other parameters. ADAS310 accepts as input the definition of these scans, establishes an extended list of cases required to achieve these scans and then executes repeated population calculations at each set of plasma conditions in the list. ADAS310 can compute the populations for any mixture of light impurities (hydrogen to neon) in the plasma. It is impractical to deal with all possible mixtures of impurities. It is our usual practice to execute ADAS310 in turn for each light impurity from hydrogen to neon treated as a pure species. The mixed species effective coefficients are constructed from these pure impurity solutions by the theoretical data acquisition routines. The main population output is very complete and in principle contains all information on possible emitted spectrum lines up to very high n-shells together with both ionisation and recombination collisional-radiative coefficients. It is archived as ADAS data format ADF26. ADAS310 can also produce directly the final tabulations of beam stopping coefficient according to ADAS data format ADF21, however this is normally done using the post-processor program ADAS312.

ADAS304 is the interrogation code on the beam stopping coefficient data base ADF21. It also works with the beam emission coefficient data base, which is of identical organisation to the stopping coefficients, and is assigned to ADF22.

In creation of compact interpolable datasets of type ADF21 and ADF22, some simplifications are made. The stopping coefficient data sets for each impurity species are calculated as though that species alone is present in the plasma. For species X^{+z_0}, of nuclear charge z_0, of number density $N^{(z_0)}$, the electron density used in the stopping calculation is $N_e = z_0 N^{(z_0)}$ consistent with charge neutrality. Let the stopping coefficient for the impurity species X^{+z_0} be $S_{CR}^{(\mathrm{A},X)}$ then the loss rate is

$$N_e S_{CR}^{(\mathrm{A},X)}(E_B, N^{(z_0)}, T^{(z_0)}) = N_e S_{CR}^{(\mathrm{A},e)}(E_B, N^{(z_0)}, T^{(z_0)}) \\ + N^{(z_0)} S_{CR}^{(\mathrm{A},z_0)}(E_B, N^{(z_0)}, T^{(z_0)})$$

distinguishing parts driven by excitation from the ground state of $\mathcal{A}$ by electron collisions and by X^{+z_0} ions respectively. The coefficient is

$$S_{CR}^{(\mathrm{A},X)}(E_B, N^{(z_0)}, T^{(z_0)}) = S_{CR}^{(\mathrm{A},e)}(E_B, N^{(z_0)}, T^{(z_0)}) \\ +(1/z_0) S_{CR}^{(\mathrm{A},z_0)}(E_B, N^{(z_0)}, T^{(z_0)})$$

The density dependence of the collisional-radiative coefficient is written in terms of the impurity ion density $N^{(z_0)}$ since ion collisions primarily determine the collisional redistribution..

Consider a set of species $\{X_i^{+z_{0i}} : i = 1,..,I\}$ with fractions $\{f_i : i = 1,..,I\}$, in the plasma causing a composite stopping. The loss rate may be written approximately as

$$N_e S_{CR}^{(\mathrm{A})}(E_B, N_I, T_I) \approx N_e S_{CR}^{(\mathrm{A},e)}(E_B, N_I, T_I) + \\ \sum_{i=1}^{I} N_i^{(z_{0i})} S_{CR}^{(\mathrm{A},z_{0i})}(E_B, N_I, T_I) \\ = \sum_{i=1}^{I} N_{e,i} [S_{CR}^{(\mathrm{A}e)}(E_B, N_I, T_I) + \\ (1/z_{0i}) S_{CR}^{(\mathrm{A}z_{0i})}(E_B, N_I, T_I)]$$

where

$$N_e = \sum_{i=1}^{I} N_{e,i} = \sum_{i=1}^{I} z_{0i} N^{(z_{0i})} = N_I (\sum_{i=1}^{I} z_{0i} f_i)$$

defines the proportions of the electron density contributed by each impurity species.

From an ion collisional redistribution point of view, in a composite plasma the $\sum_{k=1}^{I} z_{0k}^2 N_k^{(Z_{0k})}$ z-weighted density sum is meaningful so the equivalent density of the single impurity $X_i^{+z_{0i}}$ to correspond to the summed impurity ion density for this purpose is

$$N_i^{(z_{0i}),equiv} = N_I (\sum_{k=1}^{I} z_{0k}^2 f_k) / z_{0i}^2$$

and the equivalent electron density is

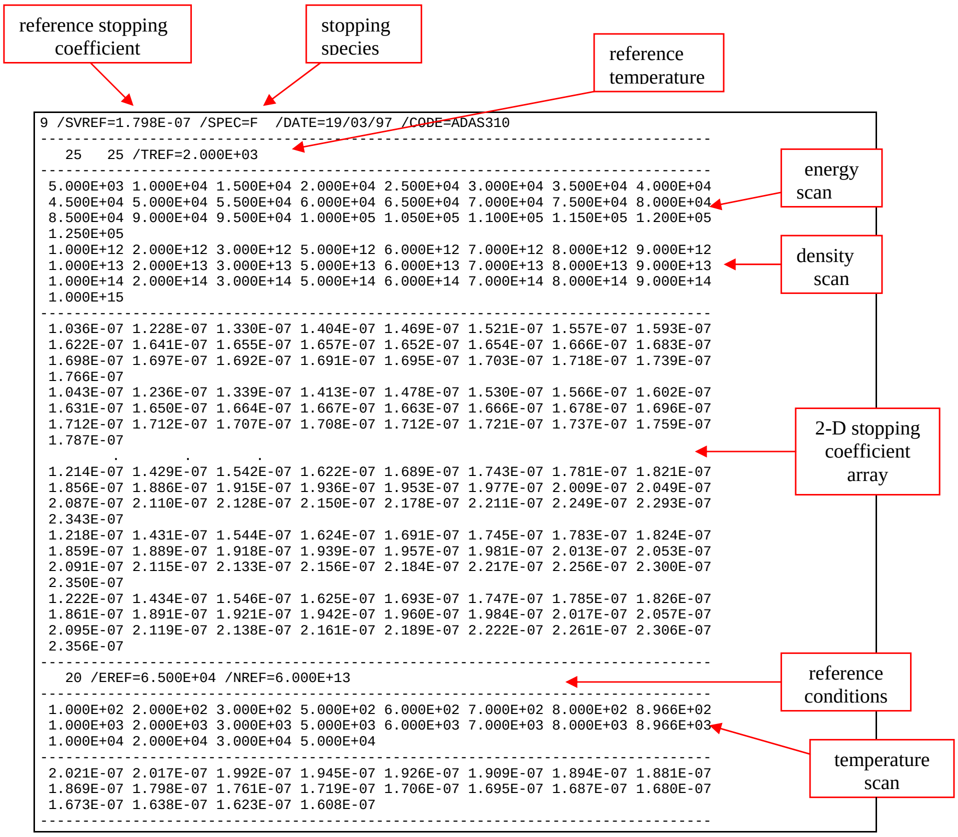
$$N_{ei}^{(z_{0i}),equiv} = \left(\frac{N_e}{\sum\limits_{k=1}^{I} z_{0k} f_k} \right) \left(\sum_{k=1}^{I} z_{0k}^2 f_k \right) / z_{0i}$$

ADAS310 evaluates the stopping & emission coefficients as a function of electron density. The approximate composite stopping coefficient is assembled from the pure species coefficients as

$$S_{CR}^{(A)}(E_B, N_e, T_I) \approx \sum_{i=1}^{I} [z_{0i} f_i S_{CR}^{(A,X_i)}(E_B, N_{ei}^{(z_{0i}),equiv}, T_I)] / (\sum_{k=1}^{I} z_{0k} f_k)$$

The prescription outlined is equally applicable for the storage and handling of beam emission coefficients.

ADF21



```
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 4.500E+04 5.000E+04 5.500E+04 6.000E+04 6.500E+04 7.000E+04 7.500E+04 8.000E+04
 8.500E+04 9.000E+04 9.500E+04 1.000E+05 1.050E+05 1.100E+05 1.150E+05 1.200E+05
 1.250E+05
 1.000E+12 2.000E+12 3.000E+12 5.000E+12 6.000E+12 7.000E+12 8.000E+12 9.000E+12
 1.000E+13 2.000E+13 3.000E+13 5.000E+13 6.000E+13 7.000E+13 8.000E+13 9.000E+13
 1.000E+14 2.000E+14 3.000E+14 5.000E+14 6.000E+14 7.000E+14 8.000E+14 9.000E+14
 1.000E+15
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 1.622E-07 1.641E-07 1.655E-07 1.657E-07 1.652E-07 1.654E-07 1.666E-07 1.683E-07
 1.698E-07 1.697E-07 1.692E-07 1.691E-07 1.695E-07 1.703E-07 1.718E-07 1.739E-07
 1.766E-07
 1.043E-07 1.236E-07 1.339E-07 1.413E-07 1.478E-07 1.530E-07 1.566E-07 1.602E-07
 1.631E-07 1.650E-07 1.664E-07 1.667E-07 1.663E-07 1.666E-07 1.678E-07 1.696E-07
 1.712E-07 1.712E-07 1.707E-07 1.708E-07 1.712E-07 1.721E-07 1.737E-07 1.759E-07
 1.787E-07
         .        .        .
 1.214E-07 1.429E-07 1.542E-07 1.622E-07 1.689E-07 1.743E-07 1.781E-07 1.821E-07
 1.856E-07 1.886E-07 1.915E-07 1.936E-07 1.953E-07 1.977E-07 2.009E-07 2.049E-07
 2.087E-07 2.110E-07 2.128E-07 2.150E-07 2.178E-07 2.211E-07 2.249E-07 2.293E-07
 2.343E-07
 1.218E-07 1.431E-07 1.544E-07 1.624E-07 1.691E-07 1.745E-07 1.783E-07 1.824E-07
 1.859E-07 1.889E-07 1.918E-07 1.939E-07 1.957E-07 1.981E-07 2.013E-07 2.053E-07
 2.091E-07 2.115E-07 2.133E-07 2.156E-07 2.184E-07 2.217E-07 2.256E-07 2.300E-07
 2.350E-07
 1.222E-07 1.434E-07 1.546E-07 1.625E-07 1.693E-07 1.747E-07 1.785E-07 1.826E-07
 1.861E-07 1.891E-07 1.921E-07 1.942E-07 1.960E-07 1.984E-07 2.017E-07 2.057E-07
 2.095E-07 2.119E-07 2.138E-07 2.161E-07 2.189E-07 2.222E-07 2.261E-07 2.306E-07
 2.356E-07
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 1.000E+03 2.000E+03 3.000E+03 5.000E+03 6.000E+03 7.000E+03 8.000E+03 8.966E+03
 1.000E+04 2.000E+04 3.000E+04 5.000E+04
--------------------------------------------------------------------------------
 2.021E-07 2.017E-07 1.992E-07 1.945E-07 1.926E-07 1.909E-07 1.894E-07 1.881E-07
 1.869E-07 1.798E-07 1.761E-07 1.719E-07 1.706E-07 1.695E-07 1.687E-07 1.680E-07
 1.673E-07 1.638E-07 1.623E-07 1.608E-07
--------------------------------------------------------------------------------
```
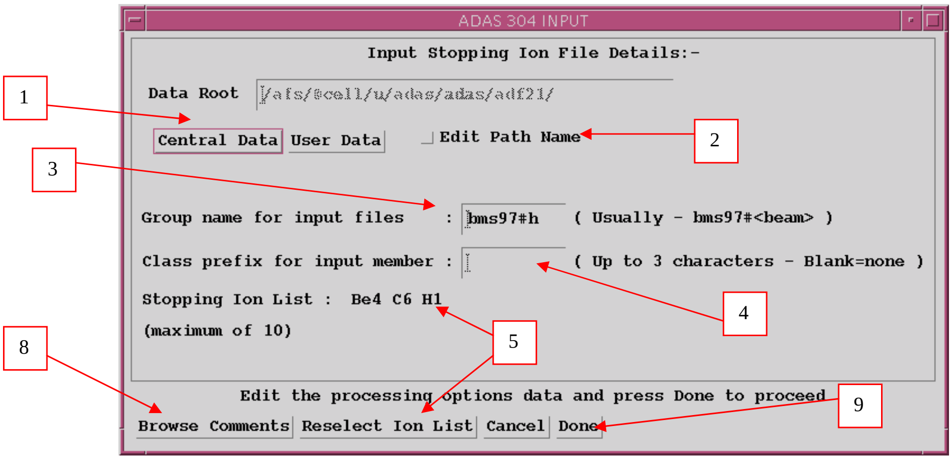

ADAS304

The code interrogates beam stopping or beam emission coefficient files of type ADF21 or ADF22. Data is extracted for stopping by a composite plasma consisting of a mixture of protons (deuterons) and fully ionised impurities. The data is interpolated using cubic splines at selected beam energy, target density and target temperature triplets. Minimax polynomial fits are made to the interpolated data. The total stopping and partial stopping by each species are given. The beam emission coefficients are handled in a similar manner. The interpolated data are displayed and a tabulation prepared. The tabular and graphical output may be printed and includes the polynomial approximations.

The **file selection window** is shown below. Its operation is a little different from usual.

1. ADF21 is the appropriate format for use by the program ADAS304 (ADAS User Manual, *appxb-21*). A root path to the correct data type ADF21 appears automatically. Your personal data of this type should be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas.*



Data Root /afs/@cell/u/adas/adas/adf21/

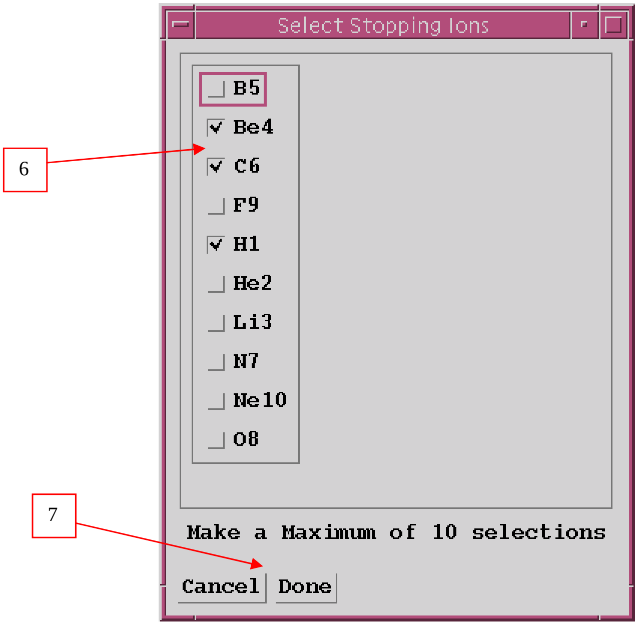
Group name for input files : bms97#h (Usually - bms97#<beam>)

Class prefix for input member : (Up to 3 characters - Blank=none)

Stopping Ion List : Be4 C6 H1

(maximum of 10)

2. Buttons are present to set the data root to that of the *Central data* or to your personal *User data* (provided it is in ADAS organisation. Alternatively the 'data root' may be edit explicitly.



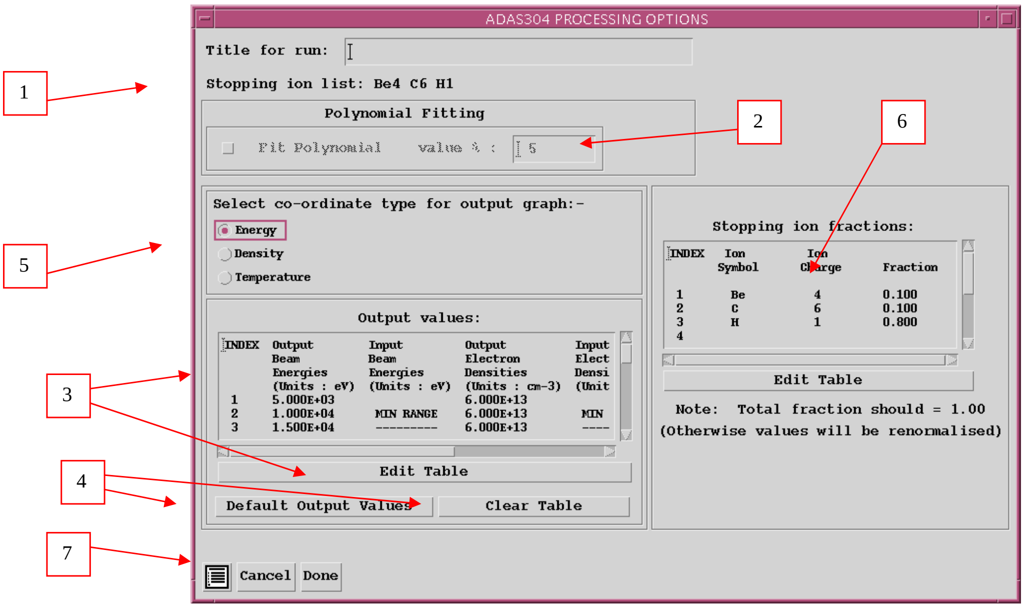
☐ B5
☑ Be4
☑ C6
☐ F9
☑ H1
☐ He2
☐ Li3
☐ N7
☐ Ne10
☐ O8

Make a Maximum of 10 selections

3. A group name for the input files is entered. This is the name of a sub-directory of ADF21 for a particular beam species (usually H or He). The sub-directory contains individual data sets for each impurity contributing to stopping , identified by the element symbol.
4. To increase flexibility in naming a three letter class prefix may be added to the data set name. The primary data in central ADAS has no prefix and so a typical data set name would be */../adas/adas/adf21/bms#h/bms#h_be.dat*.
5. ADAS304 allows you to select all the impurity files you wish easily. Click the *Reselect Ion List* button.
6. The small pop up selection widget appears showing available species. Click the toggle buttons of those you wish to include
7. Click *Done* to restore the main input widget. Your choices are shown at the Stopping Ion List.
8. Clicking on the *Browse Comments* button displays any information stored with the selected data-files. It is important to use this facility to find out what has gone into the data-set and the attribution of the data-set.
9. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window.

The **processing options window** has the appearance shown below

1. The Stopping ion list is repeated for information. The *Browse Comments* button is also provided.



Title for run:

Stopping ion list: Be4 C6 H1

Polynomial Fitting

☐ Fit Polynomial value % : 5

Select co-ordinate type for output graph:-

● Energy
○ Density
○ Temperature

Output values:

INDEX	Output Beam Energies (Units : eV)	Input Beam Energies (Units : eV)	Output Electron Densities (Units : cm-3)	Input Elect Densi (Unit
1	5.000E+03		6.000E+13	
2	1.000E+04	MIN RANGE	6.000E+13	MIN
3	1.500E+04	---------	6.000E+13	----

Stopping ion fractions:

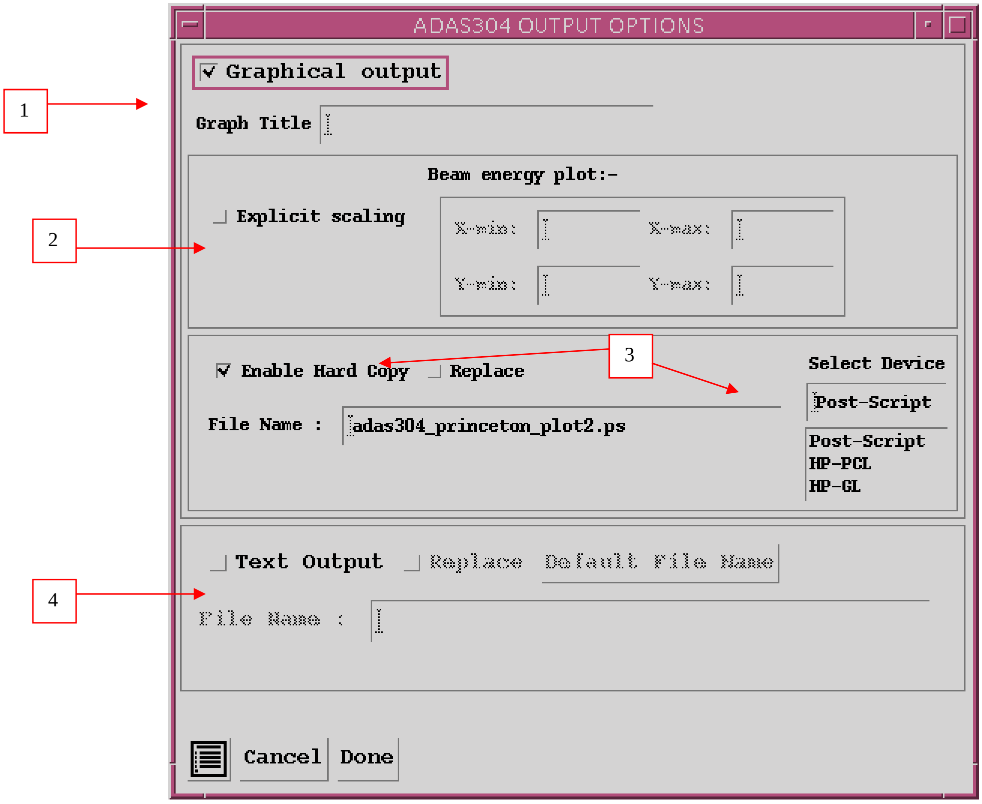
INDEX	Ion Symbol	Ion Charge	Fraction
1	Be	4	0.100
2	C	6	0.100
3	H	1	0.800
4			

Note: Total fraction should = 1.00
(Otherwise values will be renormalised)

2. The extracted data for a selected ion is interpolated by a cubic spline at user selected plasma parameters for graphical display and tabular output. Additionally a polynomial approximation may obtained by making the appropriate selections.
3. The selection of beam energy, density and temperature sets for data output must be made. The source values are held as one-dimensional scans relative to reference values for each impurity separately. The minimum and maximum for each impurity is shown in the Input columns. The table may be edited by clicking on the *Edit Table* button.
4. *Default Output Values* and *Clear Table* buttons are provided.
5. A choice of which parameter of the input model set to use as the x co-ordinate of graphs is given. Click on the required button.
6. The mixture of species contributing to the stopping is assembled at d). This again is an editable table. Click *Edit Table* to pop up the ADAS Table Editor. The required fractions may then be entered. Normalisation to unity takes place.
7. The *Exit to Menu* icon is present in ADAS304. Clicking the *Done* button causes the output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

The **Output options window** is shown below.

12. Graphical display is activated by the *Graphical Output* button. This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph.
13. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.



☑ Graphical output

Graph Title :

☑ Enable Hard Copy ☐ Replace

File Name : adas304_princeton_plot2.ps

Select Device : Post-Script

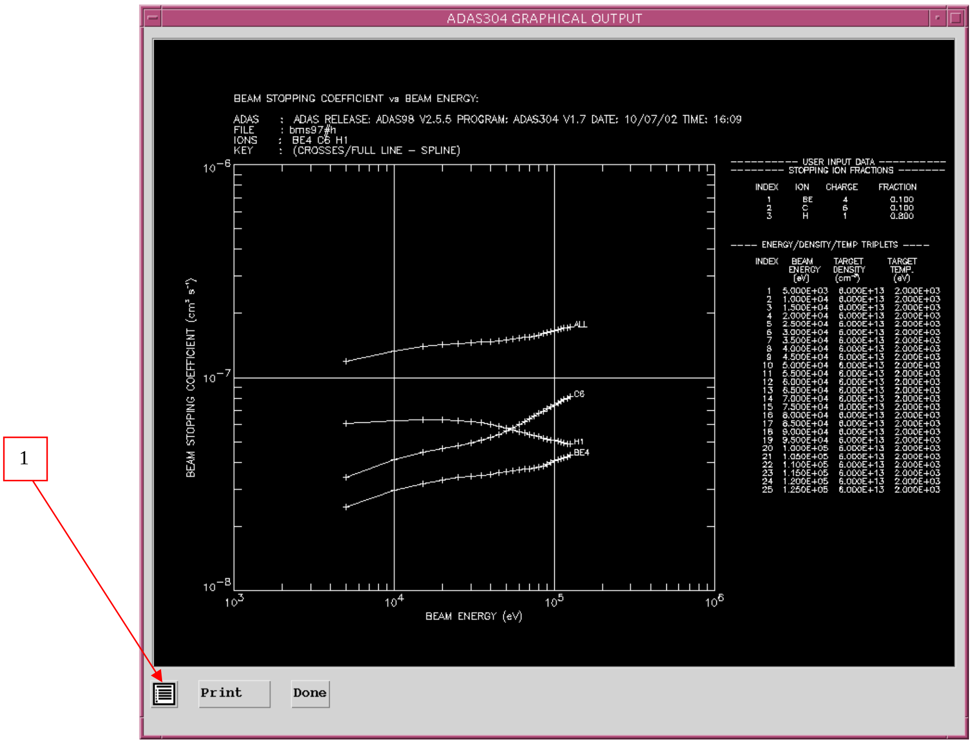
☐ Text Output

File Name :

14. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.
15. The *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name 'paper.txt' may be set by pressing the button *Default file name.*

The **Graphical output window** is shown below

4. Printing of the currently displayed graph is activated by the *Print* button.



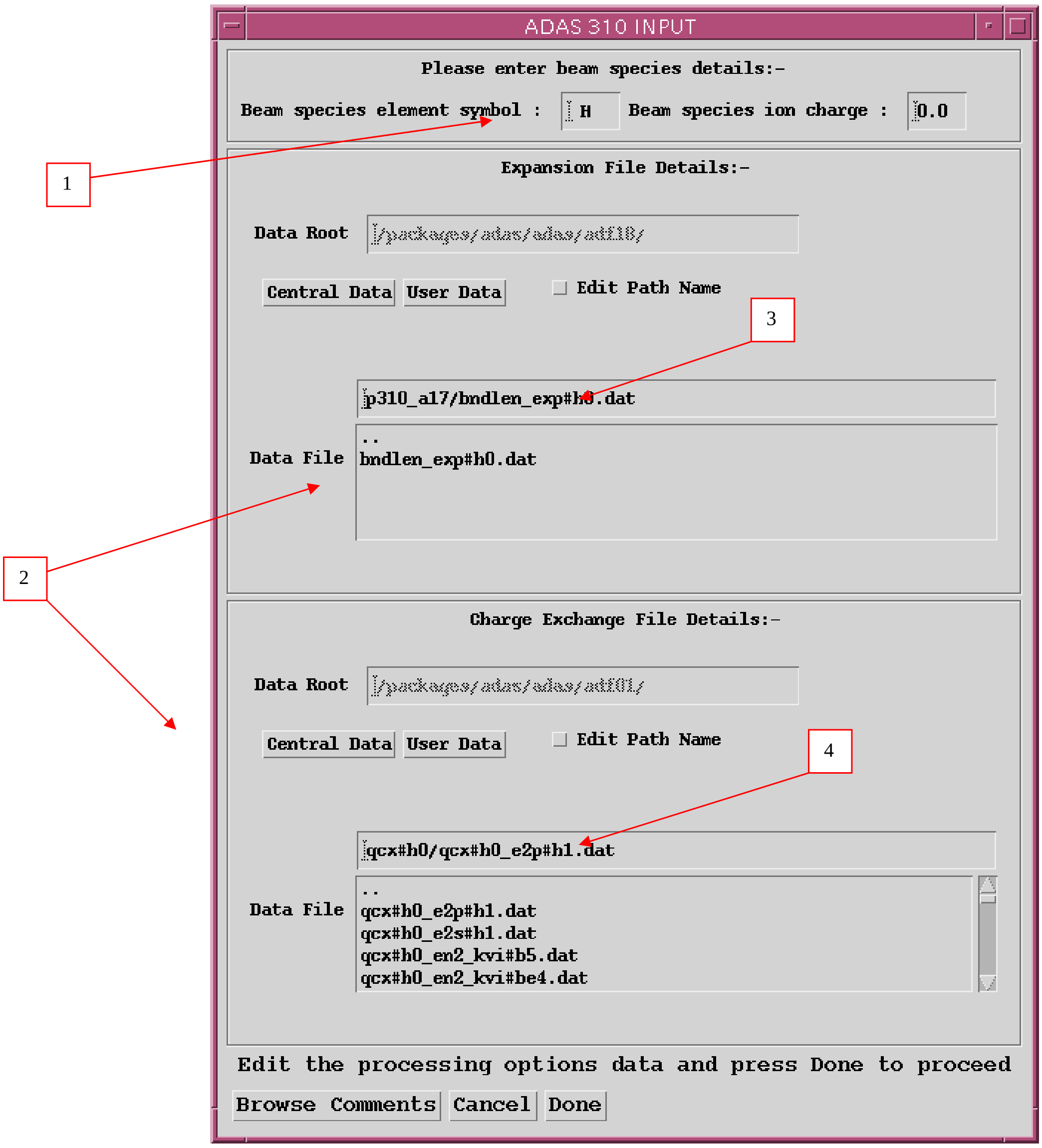
```
BEAM STOPPING COEFFICIENT vs BEAM ENERGY:

ADAS    :  ADAS RELEASE: ADAS98 V2.5.5 PROGRAM: ADAS304 V1.7 DATE: 10/07/02 TIME: 16:09
FILE    : bms97#h
IONS    :  BE4 C6 H1
KEY     :  (CROSSES/FULL LINE - SPLINE)

---------- USER INPUT DATA ----------
-------- STOPPING ION FRACTIONS --------

  INDEX    ION    CHARGE     FRACTION

    1       BE      4          0.100
    2       C       6          0.100
    3       H       1          0.800

---- ENERGY/DENSITY/TEMP TRIPLETS ----

  INDEX    BEAM      TARGET      TARGET
          ENERGY    DENSITY      TEMP.
           (eV)     (cm^-3)      (eV)

     1  5.000E+03  6.000E+13  2.000E+03
     2  1.000E+04  6.000E+13  2.000E+03
     3  1.500E+04  6.000E+13  2.000E+03
     4  2.000E+04  6.000E+13  2.000E+03
     5  2.500E+04  6.000E+13  2.000E+03
     6  3.000E+04  6.000E+13  2.000E+03
     7  3.500E+04  6.000E+13  2.000E+03
     8  4.000E+04  6.000E+13  2.000E+03
     9  4.500E+04  6.000E+13  2.000E+03
    10  5.000E+04  6.000E+13  2.000E+03
    11  5.500E+04  6.000E+13  2.000E+03
    12  6.000E+04  6.000E+13  2.000E+03
    13  6.500E+04  6.000E+13  2.000E+03
    14  7.000E+04  6.000E+13  2.000E+03
    15  7.500E+04  6.000E+13  2.000E+03
    16  8.000E+04  6.000E+13  2.000E+03
    17  8.500E+04  6.000E+13  2.000E+03
    18  9.000E+04  6.000E+13  2.000E+03
    19  9.500E+04  6.000E+13  2.000E+03
    20  1.000E+05  6.000E+13  2.000E+03
    21  1.050E+05  6.000E+13  2.000E+03
    22  1.100E+05  6.000E+13  2.000E+03
    23  1.150E+05  6.000E+13  2.000E+03
    24  1.200E+05  6.000E+13  2.000E+03
    25  1.250E+05  6.000E+13  2.000E+03
```

ADAS310

The code calculates the excited population structure, effective ionisation and recombination coefficients of hydrogen atoms or hydrogenic ions in an impure plasma. A very many n-shell bundle-n approximation is used. The hydrogen atoms may be part of the thermal plasma or may be in a beam. The latter case is the only one of relevance for this manual, however the full flexibility of the program has been retained.

The **file selection window** appears first as illustrated below.

1. Enter the beam species (H for hydrogen and its isotopes) and the atomic charge of the beam species. Only data for neutral beam species is present in the central ADAS database at this time.
2. There are two data files to be selected, the expansion file and the charge exchange file. The procedure is the same in both cases.
3. A special ADAS data type *adf18* is used for such ‘expansion’ and ‘cross-referencing’ files. They fall into various categories, kept in sub-directories, according to where they map from and to. Thus the sub-directory *a09_a04* contains data sets mapping from the *adf09* data type into the *adf04* data type. We shall deal with the purposes of these in the discussion of advanced population modelling in the next release. For the moment note that *bndlen_exp#h0.dat* is the one needed here and it sits alone as shown in the illustration. Always select it.
4. The charge exchange file is not of importance for neutral beam stopping. The charge exchange data set is required when hydrogen nuclei can act as electron receivers from other species. You will see no effect of your selection here on the beam stopping coefficient but the selection is kept in for the future. Once a charge exchange data file is selected, the set of buttons at the bottom of the main window become active.



Please enter beam species details:-

Beam species element symbol : H

Beam species ion charge : 0.0

Expansion File Details:-

Data Root /packages/adas/adas/adf10/

Data File p310_a17/bndlen_exp#h0.dat

..
bndlen_exp#h0.dat

Charge Exchange File Details:-

Data Root /packages/adas/adas/adf01/

Data File qcx#h0/qcx#h0_e2p#h1.dat

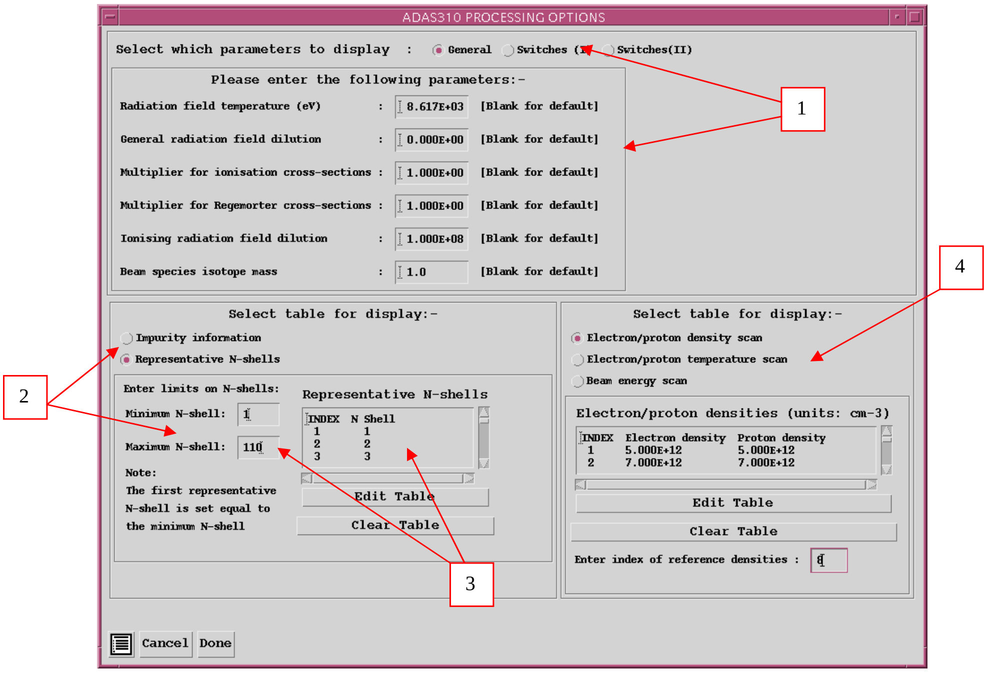
..
qcx#h0_e2p#h1.dat
qcx#h0_e2s#h1.dat
qcx#h0_en2_kvi#b5.dat
qcx#h0_en2_kvi#be4.dat

Edit the processing options data and press Done to proceed

The **processing options window** has the appearance shown below

1. The various control parameters of the collisional-radiative population calculation are organised into three groups selected in turn by the buttons *General*, *Switches (I)* and *Switches (II)*. These cause the appropriate set of parameters to be displayed in the sub-window immediately below the switches. The default settings for these are reasonable and they can be ignored as long as only beam stopping is the intent. *Switches (I)* allow some

choices to do with electron collision cross-sections and *Switches (II)* allow some choices to do with ion collision cross-sections.



Select which parameters to display : ● General ○ Switches (I) ○ Switches(II)

Please enter the following parameters:-

Radiation field temperature (eV) : 8.617E+03 [Blank for default]

General radiation field dilution : 0.000E+00 [Blank for default]

Multiplier for ionisation cross-sections : 1.000E+00 [Blank for default]

Multiplier for Regemorter cross-sections : 1.000E+00 [Blank for default]

Ionising radiation field dilution : 1.000E+08 [Blank for default]

Beam species isotope mass : 1.0 [Blank for default]

Select table for display:-

○ Impurity information

● Representative N-shells

Enter limits on N-shells:

Minimum N-shell: 1

Maximum N-shell: 110

Note:
The first representative N-shell is set equal to the minimum N-shell

Representative N-shells

INDEX	N Shell
1	1
2	2
3	3

Select table for display:-

● Electron/proton density scan

○ Electron/proton temperature scan

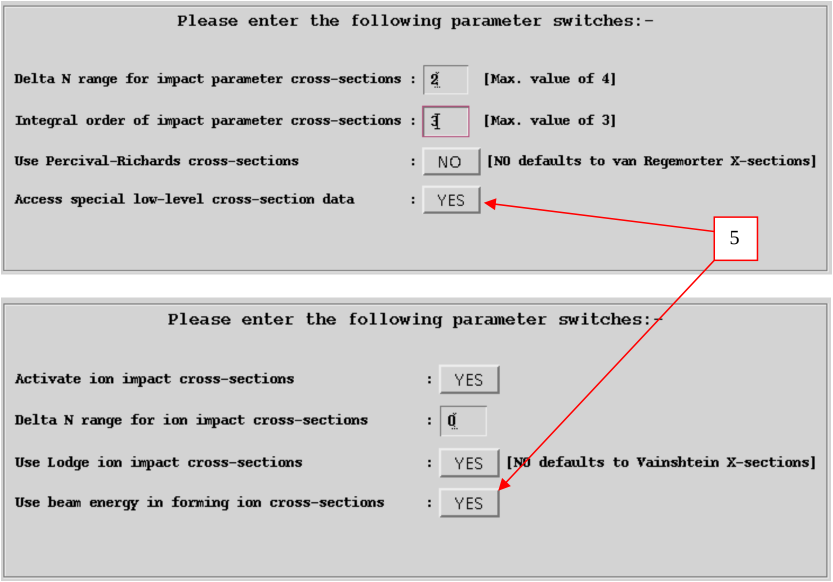
○ Beam energy scan

Electron/proton densities (units: cm-3)

INDEX	Electron density	Proton density
1	5.000E+12	5.000E+12
2	7.000E+12	7.000E+12

Enter index of reference densities : 8

2. Impurity and representative N-shell information is required. Click the *Representative N-shell* buttons to display the appropriate sub-
3. The representative N-shells requires specification of the lowest N-shell, Highest N-shell and a set of sensibly spaced 'representative' N-shells spanning the range. Make sure the lowest is 1 for hydrogen. Make the highest around 110 and use about 20 representative levels. Use all levels up to N=10 and then start to space more widely.
4. A choice of plasma and beam parameters for the scans must be made Click on the appropriate button to work on each scan in turn. Note that you edit in a set of values and then choose one to be the reference value of that parameter. The table may be edited by clicking on the *Edit Table* button.. The ADAS Table Editor window is then presented with the same set of editing operations available as are described in bulletin *nov18-94*. Values should be monotonic increasing. It has proved helpful to add a *Clear Table* button to remove all entries in the output field. When specifying *the Beam energy scan*, note that a neutral hydrogen density in the beam is requested. This is necessary to allow a mathematical separation of the various influences on the neutral hydrogen population structure and is not an experimental beam density. A value of order 10^6 or greater is suitable for the program operation.
5. Details of the switches I and II sub-windows are shown. Make sure that *Access to low level data* is chosen and *Use beam energy informing cross-sections*. It is this latter piece of information that informs the calculation that the neutral hydrogen is in the beam and not in the plasma.
6. In the impurity information sub-window, there are two modes of operation. Single impurity or Multiple impurities. Click the drop-down list button to make your choice.



Please enter the following parameter switches:-

Delta N range for impact parameter cross-sections : 2 [Max. value of 4]

Integral order of impact parameter cross-sections : 3 [Max. value of 3]

Use Percival-Richards cross-sections : NO [NO defaults to van Regemorter X-sections]

Access special low-level cross-section data : YES

Please enter the following parameter switches:-

Activate ion impact cross-sections : YES

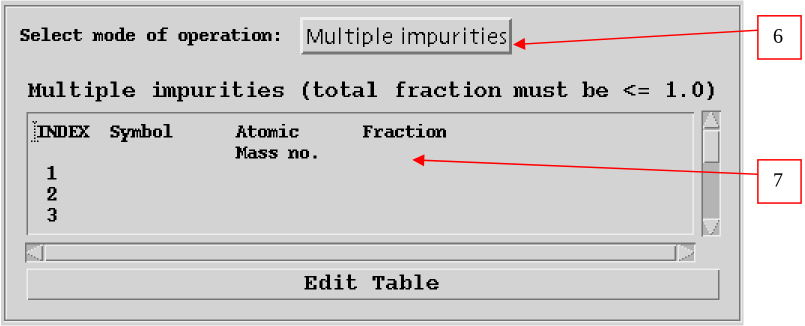
Delta N range for ion impact cross-sections : 0

Use Lodge ion impact cross-sections : YES [NO defaults to Vainshtein X-sections]

Use beam energy in forming ion cross-sections : YES

7. The multiple impurity choice enables us to investigate the influence of an impurity mixture on the stopping with greater precision. Edit in the fractions you wish in the usual manner. Note that the impurity density acts non-linearly in the stopping coefficient and so the linear superposition implied by the use of ADAS304 is imprecise. It is however very fast which is necessary in large scale experimental data analysis.

The single impurity case has only one impurity nucleus in addition to protons present in the plasma. The single impurity case is used to build up such data sets in *adf21*. Note how the impurity and protons fit together (equations 4.10.16 and 4.10.17 in the ADAS User Manual). The proton and electron density choices to be made next influence this.



Select mode of operation: Multiple impurities

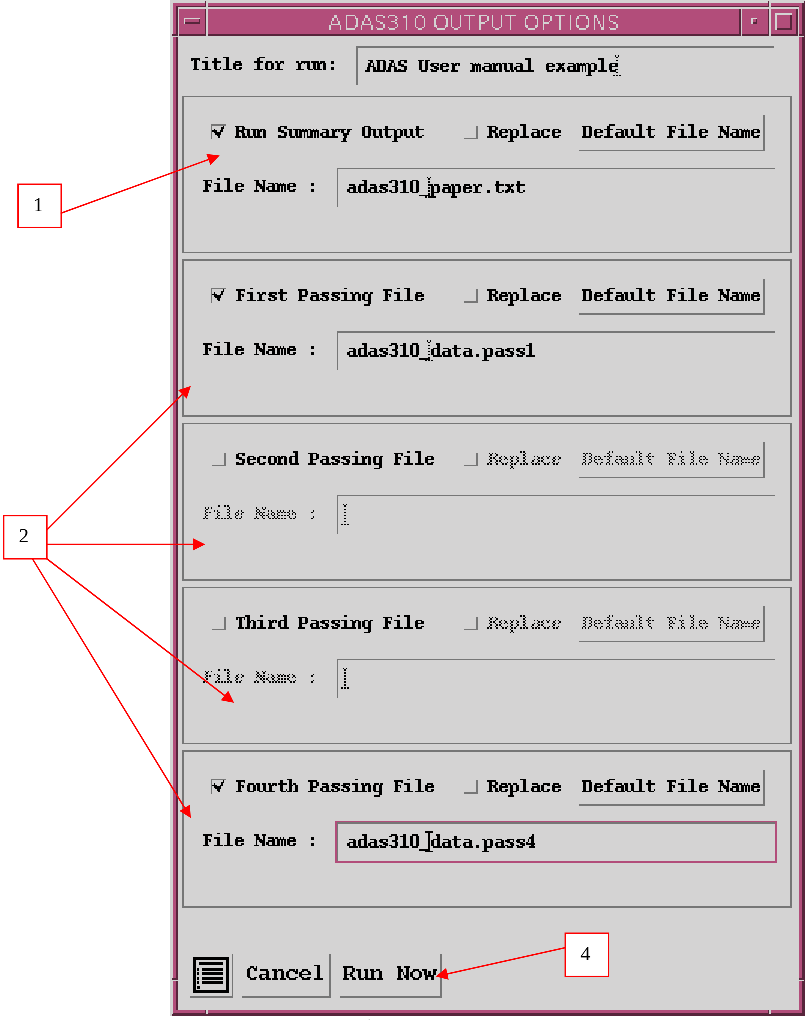
Multiple impurities (total fraction must be <= 1.0)

INDEX	Symbol	Atomic Mass no.	Fraction
1			
2			
3			

The **output options window** is shown below. It follows the usual pattern except that there is no graphical output.

1. The *Run Summary Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Run Summary Output* is on. If the file already exits a choice to *Replace* or *Append* may be made. The default file name ‘paper.txt’ may be set by pressing the button

Default file name. A ‘pop-up’ window issues a warning if the file already exists and the *Append* or *Replace* button has not been activated.



Title for run: ADAS User manual example

☑ Run Summary Output ☐ Replace
File Name : adas310_paper.txt

☑ First Passing File ☐ Replace
File Name : adas310_data.pass1

☐ Second Passing File ☐ Replace
File Name :

☐ Third Passing File ☐ Replace
File Name :

☑ Fourth Passing File ☐ Replace
File Name : adas310_data.pass4

2. Four additional passing files may be produced which are placed in your pass directory. The first passing file is of ADAS data format ADF26 and contains line printer formatted pages of data, one page for each individual population structure case run. The data held on these sheets is very comprehensive. By appropriate choice of the parameters mentioned in the processing section above and choice of input files, hydrogen in all its possible conditions in a fusion plasma can be obtained (beam and non-beam).
3. Click the *Run Now* button to initiate the calculations. These are run in fore-ground since they are of fairly modest duration. A thermometer widget keeps you informed of the progress of the calculations.

N. R. Badnell

AUTOSTRUCTURE

(21.16)

14/10/09

This write-up, codes and installation instructions are available via the WWW from http://amdpp.phys.strath.ac.uk/autos .

1. Introduction

Historically, AUTOSTRUCTURE (AS) was developed from SUPERSTRUCTURE (SS). The theory behind SS is described by Eissner, Jones, & Nussbaumer in their Computer Physics Communications paper CPC8,270-306 (1974). Further significant development was undertaken by Storey. SS deals with bound state problems: energy levels and radiative rates (E_k & M_k).
AS deals with collisions as well: autoionization rates, photoionization cross sections, for example. The original theory may be found in J.Phys.B19, 3827-35 (1986).

Here is a simple guide to get you going. It is not exhaustive. In general, if you want to do something not described here, and it is physically possible, then it is likely that it is already possible/coded but just not detailed here.

2. Energy levels & Radiative rates

All input described is free-formatted and NAMELISTed, EXCEPT for the first 4 characters of line 1 which flag the input style.
Here, we focus on A.S. (There is also S.S. which enables configurations to be input fixed-format using the Eissner notation, no details.)

So,

A.S. Starts the file and the rest of the line is for comment.

Next we have the "algebra" NAMELIST: e.g.

```
 &SALGEB  MXCONF=3 MXVORB=3  &END
```

is the minimal input where MXCONF is the number of target configurations and MXVORB is the number of distinct (valence) electron orbitals which describe them. For example, Be-like C4+ described by 1s^2 2s^2, 1s^2 2s 2p and 1s^2 2p^2 :

```
 1 0  2 0  2 1
  2    2    0
  2    1    1
  2    0    2
```

Recall, the input is free-formatted. The MXVORB nl-orbital quantum numbers are listed before the MXVORB occupation numbers for the MXCONF configurations.

Finally, we have the "radial" NAMELIST SMINIM in which we define the nuclear charge NZION:

```
 &SMINIM NZION=6  &END
```

for Carbon.

In total, we now have:

Example 1.

```
A.S. Be-like C structure - energies
 &SALGEB MXCONF=3 MXVORB=3  &END
 1 0  2 0  2 1
  2    2    0
  2    1    1
  2    0    2
 &SMINIM NZION=6  &END
```

This is the minimal input and it will give term energies in LS-coupling:
You should obtain (see INSTALL for compilation & execution details):

```
  I         T        K*CM  2S+1 L    CF     WEIGHTS        (EI-E1)/RY     E1/RY =    -72
.851752
  1         5           0.    1 0    1       0.000          0.000000
  2         3       53615.   -3 1    2       0.000          0.488573
  3         4      110474.   -1 1    2       0.000          1.006710
  4         2      138472.    3 1    3       0.000          1.261854
  5         1      154159.    1 2    3       0.000          1.404803
  6         6      191335.    1 0    3       0.000          1.743577
```

(This is just the end of the UNIT6 output file, default name "olg".)
Further, more machine friendly, files are also created holding similar
data, viz. TERMS and ols.

Now, you want more? For example, what about intermediate coupling and
radiative rates? CUP specifies the coupling scheme (default was ’LS’)
and RAD specifies the type of radiation (default was ’ ’, i.e. none).

So,

Example 2.

```
A.S. Be-like C structure - energies + radiative rates
 &SALGEB CUP=’IC’ RAD=’E1’ MXCONF=3 MXVORB=3  &END
 1 0  2 0  2 1
  2    2    0
  2    1    1
  2    0    2
 &SMINIM NZION=6  &END
```

gives intermediate coupling and electric dipole radiative rates.

Here is an excerpt from the end of the olg file:

```
  K        LV         T        K*CM     2*S+1  L   2J   CF         (EK-E1)/RY     E1/RY
 =   -72.87735575
  1         8         5           0.      1    0    0    1         0.00000000
  2        10         3       53644.     -3    1    0    2         0.48884302
  3         5         3       53686.     -3    1    2    2         0.48921840
  4         3         3       53768.     -3    1    4    2         0.48997080
  5         6         4      110586.     -1    1    2    2         1.00773259
  6         7         2      138633.      3    1    0    3         1.26331372
  7         4         2      138674.      3    1    2    3         1.26369176
  8         2         2      138756.      3    1    4    3         1.26444164
  9         1         1      154402.      1    2    4    3         1.40701910
 10         9         6      191560.      1    0    0    3         1.74562283
.
.

 E1-DATA   K  KP           A(EK)*SEC           S               G*F         ...
```

```
  1        3   1          2.068E+02       0.000002         3.227E-07      ...
  2        5   1          2.414E+09       2.643179         8.879E-01
  3        6   3          1.669E+09       1.343586         3.467E-01
  4        6   5          3.229E+02       0.000007         6.155E-07
  5        7   2         -5.579E+08      -1.343584        -3.470E-01
  6        7   3         -4.178E+08      -1.007687        -2.601E-01
  7        7   4          6.943E+08       1.679481         4.331E-01
.
.
```

There is more data to the right of A(EK) the radiative rate, S the line strength and G*F the symmetric oscillator strength.

Negative "rates" are just flagging the sign of the matrix element before it was squared.
(Some applications require the (sign of) the matrix element itself.)

To do some type of collision problem, e.g. photoionization, we would need to set the RUN variable (default ' ', structure). But, before we do that, here is a listing of the commonly used SALGEB NAMELIST variables and commonly used settings, which may or may not mean anything to you (yet).

SALGEB:

```
RUN='  ', default. Allows calculation of energies (LS or IC), radiative
          rates (if RAD set) and autoionization rates (if continuum
          present - see optional input below).
   ='PI', will calculate (non-resonant) photoionization as well,
          if continuum present.
   ='DR','RR','PE','RE'. All expect one or more Rydberg orbitals
          to be defined (see below) and will read the optional namelist DRR
          to define the nl values of the Rydberg series to be run over.
    'DR'  calculates energies, radiative and autoionization rates.
    'RR'  calculates non-resonant "radiative recombination" (in the form of PI).
    'PE'  only differs from 'DR' in its use of default atomic structure - both
          default to the initial state, which is the final state of the other.
          In these cases, if no radiation is specified, E1 will be switched on.
    'RE'  differs from option 'DR' only via no radiation being a valid option.

CUP='LS'  for non-relativistic LS-coupling, default.
   ='LSM' or 'MVD' for LS-coupling including mass-velocity and Darwin operators.
   ='IC'  for intermediate coupling (gives non-relativistic LS results as well).
   ='ICM' for intermediate coupling (with LS results as per 'LSM'/'MVD').
   ='ICR' for IC using kappa-averaged relativistic wavefunctions i.e. mass-velocity
          and Darwin operators are included in the solution of the radial equations.

RAD='  ' or 'NO'  for no radiative data, default (unless RUN='DR' etc).
   ='E1' or 'YES' for electric dipole radiation.
   ='E2' or 'M1' for electric quadrupole and magnetic dipole, plus above.
   ='E3' or 'M2' for electric octupole and magnetic quadrupole, plus above.
   = 'ALL' for all possible radiative data currently available, inc M1+BP corrections.
   ='DIM1' a dimension check only, for an 'E1' run.
   ='DIM2' a dimension check only, for an 'E2' run.

BORN='INF' evaluates infinite energy limit Born collision strengths.
    ='YES' evaluates finite energy Born collision strengths (Type-1 adf04).
    ='NO' does not, default (unless RAD='ALL', then defaults to 'INF'.)

KORB1.AND.KORB2 .OR. KCOR1.AND.KCOR2 denote closed shells (use one or other)
     e.g. KCOR1=1 KCOR2=3 denotes a Ne-like core (assuming standard order).
     This also defines any core model potential generated for R-matrix, the
     effective charge is written in place of the duplicate radial mesh points.
```

```
KUTSS controls valence-valence two-body fine-structure interactions.
   =-1 None, default.
   =-9 All.
     |KUTSS| .gt. 1 includes the interactions for the first |KUTSS|
     configurations, KUTSS positive neglects the interaction between
     distinct configurations.

KUTSO controls the evaluation of the generalized spin-orbit parameter.
   = 0 All.
   < 0 includes interactions between the first -KUTSO configurations
       and within a configuration for the remainder, default=-1.
   > 0 includes interactions within a configuration for the first
       KUTSO configurations and neglects all for the remainder.

KUTOO controls the evaluation of the two-body non-fine-structure
      interactions viz. contact spin-spin, two-body Darwin and
      orbit-orbit (NOT available for non-relativistic LS).
   = 0 or -1 neglected, default.
   else all included (excepting 88(O-O),99(CSSD) & 98 reserved).

BASIS ='   ' uses a unique orbital basis. Each configuration uses the
        same orbitals. Default.
      ='RLX' uses a relaxed orbital basis. Each configuration uses its
        own set of orbitals and overlaps are neglected.

NAST, number of distinct SLp terms (listed following if .gt. 0 as 2S+1 L p)
     generated from the configuration list, can be used with care in IC.
     If .eq. 0 all possible terms are generated, default.

KCUT = 0 all configurations are treated as spectroscopic, default.
     > 0 configuration numbers greater than KCUT are treated as "correlation"
         and terms are only generated from them if they also exist in the
         spectroscopic list. Correlation terms are ignored when forming
         the energy functional during optimization and no transition
         probabilities (autoionization or radiative) are calculated for them.

MSTART controls the restart facility that is useful for large isoelectronic
       runs where it is desirable to calculate the angular algebra once only.
      = 0 does nothing, default.
      = 1 writes the angular algebra to file RESTART.
      = 5 reads the angular from file RESTART.
     (= 2,3,4 continue an angular algebra calculation that did not complete.)

MXVORB is the number of distinct valence orbitals required to describe the
       configurations.
       > 0 their nl definitions are read next.
       < 0 standard order is assumed for -MXVORB orbitals.
       No default, 0 not allowed.

MXCONF is the number of (base) configurations. Occupation nos are specified
       for the |MXVORB| orbitals, after any nl definition.
       No default, must be >0.

Optionally, promotion rules can be applied to base configurations to easily
obtain a large configuration interaction basis (CI):

ICFG = 0 (default) just applies above MXVORB, MXCONF.
     = 1 Reads RMX STG2 style global (MNAL, MXAL) min and max occupations nos,
         before config occupation nos, for |MXVORB| orbitals, and NXCITE
         promotions at the end of the config line.
     = 2 Reads MNAL,MXAL before each base config.
     =-1 Read (possibly modified) CONFIG.DAT produced by ICFG>0 run.
(ICFG .ne. 0 redefines MXCONF internally!)
```

NXTRA, LXTRA, IFILL (for ICFG.ne.0) extends the nl definition to n=NXTRA, l=LXTRA
in standard order AND assumes MNAL(I,M)=0, MXAL(I,M)=IFILL, for
orbitals I > |MXVORB|, and base config. M occupation 0; i.e. only READ
such info for I <= |MXVORB| now. Then, MXVORB is redefined internally!

The above approach can be extended to describe a collision problem just by specifying target configs and a RUN switch (and, maybe, some N+1 bound configs).

If RUN.ne.' ' and no continuum orbitals are specified on the (optional) orbital redefinition line then it is assumed that the MXCONF N-electron target configs have been specified (as above) and N+1 electron target+continuum configs are internally generated by adding LCON continuum orbitals to each target config. Depending on RUN, a Rydberg orbital is also added. Any KCUT input is relative to the MXCONF N-electron configs, it is adjusted internally to match the resultant N+1 electron target+continuum configs (which are ordered for KCUT).

If explicit bound orbital N+1 electron configs are needed (e.g. DR) then

MXCCF > 0 reads bound N+1 configs in same fashion as N-electron configs, and after them.
< 0 determines all possible based on adding a base orbital to all N-electron configs.
= 0 (default) no explicit bound N+1 electron configs.

Note: N+1 ICFG is determined from ICFG/10 (N-electron ICFG is actually MOD(ICFG,10).)
Ditto IFILL.

KCUTCC is the equivalent of KCUT, but for the MXCCF N+1 configs and is specified relative to MXCCF, i.e. is independent of the MXCONF N-electron configs.

Note: configs with both a Rydberg and continuum (which result from a core re-arrangement autoionization) can also be handled, and KCUTI - see Example 8. below.

****

Let's next look at the SMINIM NAMELIST. The radial equations use a "model" potential to describe the affect of the atomic electrons upon each other. The default is the Thoma-Fermi-Dirac-Amaldi (see the CPC paper for details). To provide "optimization", NLAM adjustable scaling parameters (lambdas) are introduced on the potential's radial coordinate - one for each nl-orbital. A weighted-sum of INCLUD eigenenergies is minimized to determine the optimum structure by varying NVAR of the scaling parameters. For example: we include all 6 terms in the sum to be minimized. We read-in NLAM=3 initial scaling parameters of value 1.0 and we vary two of them corresponding to the 2s and 2p (orbitals 2 and 3):

Example 3.

```
A.S. Be-like C structure
 &SALGEB CUP='LS' MXVORB=3 MXCONF=3  &END
 1 0  2 0  2 1
  2    2    0
  2    1    1
  2    0    2
 &SMINIM NZION=6 INCLUD=6 NLAM=3 NVAR=2  &END
  1.0 1.0 1.0
       2   3
```

To obtain (in the olg file)

```
 MINIMIZATION RESULT OF VARIATIONAL PARAMETERS:   1.23224   1.16141
```

and new energies

```
 I         T        K*CM  2S+1 L   CF     WEIGHTS        (EI-E1)/RY     E1/RY =    -72.
892998
 1         5          0.    1 0    1       1.000          0.000000
 2         3      53749.   -3 1    2       1.000          0.489799
 3         4     112734.   -1 1    2       1.000          1.027305
 4         2     139697.    3 1    3       1.000          1.273012
 5         1     156276.    1 2    3       1.000          1.424089
 6         6     195549.    1 0    3       1.000          1.781974
```

which may, or may not, be an improvement on those obtained previously.

Note, the non-zero WEIGHTS show which terms were INCLUDed in the energy sum, and their weighting.

Again, here is a listing of the commonly used SMINIM NAMELIST variables and commonly used settings, which may or may not mean anything to you (yet).

```
SMINIM:
-------

NZION = Nuclear charge (no default).
      .gt. 0 radial functions are calculated in an nl-dependent TFDA potential.
             The orbitals are Schmidt orthogonalized, by default.
      .lt. 0 radial functions are calculated in an nl-dependent Hartree potential
             evaluated with Slater-Type-Orbitals.
             The orbitals are NOT Schmidt orthogonalized, by default.

INCLUD .eq. 0 no variational procedure, default.
       .gt. 0 include lowest INCLUD terms (LS), weighted over fine-structure (IC),
              in energy-sum to be minimized.
       .lt. 0 include -INCLUD terms (weighted over f.s.) in energy sum, the T-index
              labels and weighting factors follow next (before lambdas, see below).
              Note: the T-index is required, not the I-index. This is output
              in olg on the term (f.s. weighted) energy list from a trial run.
       See Note 2 on ISHFTLS/IC (below) regarding minimizing the difference
       with observed energies.

NLAM  is the number of (lambda) scaling parameters. Both TFDA and STO
      Hartree potentials contain a radial scaling parameter.
    = 0 all lambda’s equal unity.
      If NLAM is less than the number of orbitals then the last
      scaling parameter read will be used for the remaining orbitals.

NVAR  is the number of variational parameters.

Note 1:
      If BASIS=’RLX’ in SALGEB, then NLAM/NVAR refer to the number of sets
      of parameters to be read, which are preceded by the configuration
      number and the number of parameters in the set. Values for
      (common) closed-shell orbitals are denoted by a configuration of zero.
      The scaling parameter for a continuum orbital (see below) follows that
      of the last (global occupied) bound orbital.

Note 2:
      The scaling/variational parameters are normally positive numbers
      around 1. This gives a "physical" orbital. Pseudo-orbitals are
      generated with negative lambdas. The default is a screened
      hydrogenic potential of charge |lambda*NZION|. However, if.....


ORTHOG=’YES’ impose Schmidt orthogonalization, overriding NZION default.
       ’NO’ do not impose Schmidt orthogonalization, overriding NZION default.
       ’LPS’ then orthogonal Laguerre pseudo-states are generated for that nl.
```

```
       The -lambda is then the scaling parameter associated with the Laguerre
       orbital, with the Z dependence factored out so that lambda=-1 is usual.
       (Negative lambda without 'LPS' uses screened hydrogenic z=|NZION*lambda|.)

MCFMX: Case of STO Hartree/X potentials. MCFMX configuration numbers are read,
       one for each orbital. The Hartree potential, for each orbital, uses
       the occupation numbers from the specified configuration. If the number
       of orbitals is .gt. MCFMX the last configuration is used for the
       remaining orbitals. The orbital must exist in the flagged configuration.

MEXPOT = 0 (default) the STO potential is Hartree.
       = 1 a local exchange term is added to the Hartree potential.

PRINT='FORM' (default) usual detailed formatted output for a structure
              run. Energy/Rate files for DR/RE run are formatted.
     ='UNFORM' limited writes to UNIT6 and Energy/Rate files for DR/RE
               are unformatted.

RADOUT='YES' produces a radial file (radout) suitable for LS/BP R-matrix stg1r.
      ='NO' doesn't (default).

MAXE  is the maximum scattering energy in Rydbergs. Useful for non-resonant
      processes to ensure an optimal radial mesh is set-up, not too fine (slow)
      and not too coarse (inaccurate, or later failure).

ISHFTLS (ISHFTIC) .eq. 0, no shifts (default).
 .eq. 1 Read term (level) numbers and energy corrections from file SHFTLS
        (SHFTIC) preceded by the number of state/energy pairs to be read and
        the energy units used (as IP of H). Can be used together in an IC run,
        then LS energy shifts are applied as term energy corrections to H(IC)
        and the IC shifts as a (further) correction to the diagonal of H(IC),
        before diagonalization. If applying both to H(IC) then they are best
        determined consistently through iteration, see next option.
        The term(level) numbers are the algebraic T (LV) numbers, not the energy
        ordered.
 .gt. 1 then assumes observed energies, relative to the ground (averaged-over
        fine-structure for terms) NOT corrections, are input and then ISHFTLS OR
        ISHFTIC iterations of H(IC) are carried-out. ISHFTLS iterations are
        applied as term energy corrections (TEC) to H(IC). The FINAL TECs can
        then be input in SHFTLS with ISHFTLS=1 and THEN (optionally) ISHFTIC
        iterations can be applied as level energy corrections (LEC) to the diagonal
        of H(IC) before diagonalization. The FINAL LECs can then be input in SHFTIC
        with ISHFTIC=1 to regenerate the final structure without iteration.
 .lt. 0 no iterations (as .eq. 1) but assumes input observed energies (as .gt. 1).
        Note, the IC shifts are applied AFTER diagonalization now (as they must be),
        and so they can be used to achieve exact level positioning.

Note 1: the LS term energies are shifted by whatever term energy corrections are
        present, which may not be optimal for LS of course if IC is the focus.

Note 2: if INCLUD.ne.0 then the usual variation of scaling parameters operates but
        the functional being minimized is the difference between theory and observed.
        This requires the absolute theoretical ground state energy, in addition to
        the observed energies relative to the ground. The actual (non-zero) value of
        ISHFTLS/IC is irrelevant now (no iteration is carried-out if .gt. 0 and
        corrections are not assumed even for .eq. 1).


If kappa-averaged relativistic radial functions are in use (CUP='ICR') then
there are a number of options which apply solely to this case:

IREL = 1 neglects small component, and renormalizes large component to unity (default).
     = 2 includes small component estimate.

INUKE=-1 Point nucleus.
```

```
     = 0 Uniformly charged finite nucleus (with default atomic mass ATM=2.5*Z).
     = 1 Approximation to Fermi distribution viz. U_6 charge distribution of
         Bogdanovich & Rancova Lithuanian J. Phys. v42, 257 (2002). Default.

IBREIT= 0 "usual" Breit interaction (long wavelength approx), default.
      =-1 Generalized Breit interaction (non-zero exchange photon energy).
      = 1 applies generalized to Coulomb, as per Moller interaction.

QED = 0 No QED corrections, default.
    = 1 Include vacuum polarization and self-energy contributions to level energies.
    =-1 Include on term energies, as well.

IRTARD = 0 Full retardation off, default.
       = 1 Full retardation on. Needed for high-energy photoionization, then
           requires small component on (IREL=2).
```

THIS ENDS THE MINIMUM INPUT.

* * *

OPTIONAL INPUT

3. Autoionization and photoionization:

Let’s introduce a continuum electron, which may be produced following autoionization or photoionization. We now have two sets of configurations: firstly, N-electron target configurations to which a continuum electron is coupled; secondly, (N+1)-electron bound orbital configurations (often confusingly called correlation configurations) whose energy levels may either be true bound or lie above the ionization limit (i.e. autoionizing). For example, consider the KLL Li-like resonances autoionizing to the He-like ground state. We have MXCONF=1 (electron) target configurations, viz. 1s^2, and (here) MXCCF=3 (N+1)-electron autoionizing configurations, viz. 1s 2s^2, 1s 2s 2p, 1s 2p^2. A typical dataset would then be of the form (the blank line separating the MXCONF and MXCCF configuration occupation numbers is optional, just to guide the eye):

Example 4.

```
A.S. KLL Li-like -> He-like + e-
 &SALGEB CUP='LS' RAD='  '  MXVORB=3 MXCONF=1 MXCCF=3 &END
 1 0  2 0  2 1
  2    0    0

  1    2    0
  1    1    1
  1    0    2
 &SMINIM NZION=26  &END
 &SRADCON MENG=4 &END
 300 320 340 360
```

The non zero-value for MXCCF is enough for the code to recognize that the MXCONF target configurations need to be coupled to a continuum electron. (Internally, continuum orbitals are flagged by n=90-99, usually 90.)
It then requires the namelist SRADCON to be present where the user tells the code which MENG continuum energies to use for interpolation purposes.

Autoionization rates are written on-the-fly interspersed with the H diagonalization output in olg (continuum configurations are flagged negative):

```
   T,2S+1L (P)  H(ZZ)/2RY   EIGEN-H/2RY   CF NI  NO   MATRIX <GSL!CASL>  AND  H(Z)/2RY-
TRIANGLE.
    NA  W   T  TP        AA*SEC      ECONT(A.U)       E-I(A.U)
   1  2  2  0    -505.76600   -489.838238 -3  1   1   1.0000  0.0000 15.9278
   2  2  2  0    -506.21711   -490.237970  6  1   2   0.0000  1.0000 -0.0304 15.9791
      10   1   2     -1.533E+14       169.6003      -659.8382
     1
   3  4  1  0    -506.21711   -491.139116  6  2   1   1.0000 15.0780
   4  4  1  1    -506.31938   -492.862636  5  1   1   1.0000 13.4567
   5  2  1  0    -506.21711   -489.969377  6  3   1   1.0000 16.2477
   6  2  1  1    -505.76600   -489.838238 -2  1   1   1.0000  0.0000  0.0000 15.9278
   7  2  1  1    -506.31938   -490.904473  5  2   2   0.0000  0.7467 -0.6651 -0.0145 15
.1472
   8  2  1  1    -506.31938   -491.509723  5  3   3   0.0000  0.6651  0.7467  0.0205 -0
.3006 15.0774
        6   6   7     -9.919E+13       168.9338      -659.8382
        6   6   8      5.404E+12       168.3285      -659.8382
     2
   9  2  0  0    -505.76600   -489.838238 -1  1   1   1.0000  0.0000  0.0000 15.9278
  10  2  0  0    -506.42165   -493.271597  4  1   2   0.0000  0.9480 -0.3184 -0.0235 13
.5788
  11  2  0  0    -506.21711   -489.042327  6  4   3   0.0000  0.3184  0.9480  0.0195  1
.2766 16.7460
        2   9  10     -1.359E+14       166.5666      -659.8382
        2   9  11      1.968E+13       170.7959      -659.8382
     2
```

Negative rates again just flag the sign of the matrix element before it was squared.

The ols file now contains the autoionization rates, in a form useful for further processing.

Further details on the NAMELIST SRADCON entries:

SRADCON:

MENG is the number of interpolation energies (in Rydbergs). MENG energies
     follow and the continuum orbitals are calculated at those energies.
     If .lt. 0, only the range need be specified and the -MENG interpolation
     energies will be chosen internally.

EMIN, EMAX specify the energy range (in Rydbergs).
      When in doubt, set EMIN to zero and EMAX to the maximum core excitation
      energy, e.g., that of 1s^2 to 1s2p in Exampole 4.

If none of the above are set then the code *attempts* to determine suitable energies internally.

For autoionization, the code looks for a TERMS/LEVELS file from a previous structure run. This should include the core de-/excitations for the autoionizing transitions under study. (For the He-like + e- example above, 1s2s and/or 1s2p should be added to 1s^2 target to produce a usable TERMS/LEVELS file.)

For photoionization, it chooses a wide logarithmic energy range suitable for forming recombination coefficients. Indeed, the user should "choose" this option for rate coefficient determination. For photoionization cross sections as the end requirement, such a range is likely to be to wide and too coarsely tabulated. In this instance, MENG,EMIN,EMAX should be set to give the required energy range and density of energy points.

ECORLS/ECORIC is an optional correction energy (Ryd) added to all target continuum. If negative, this lowers all target states relative to the autoionizing states. This ensures that autoionization data exists for low-lying autoionizing states. It may be discarded later, in a post-processor, by further application of observed energies. Default=0.

Here is an example of outer-shell photoionization: 1s^2 2s and 1s^2 2p to 1s^2

Example 5.

```
A.S. PI of Li-like -> He-like + e-
 &SALGEB RUN=’PI’ CUP=’LS’ RAD=’  ’  MXVORB=3 MXCONF=1 MXCCF=2 &END
 1 0  2 0  2 1
  2    0    0

  2    1    0
  2    0    1
 &SMINIM NZION=26  &END
 &SRADCON MENG=-15  EMIN=0. EMAX=1500. &END
```

Note that it is necessary to set RUN now. While autoionization rates are automatically computed by default, photoionization must be requested.
You will also see from your output that E1 radiation has been switched-on.
RAD=’E1’ alone would just have given bound radiative rates without RUN=’PI’ as well.

```
   E1-DATA  I  IP      A(EK)*SEC   ...
    1       2   1      1.658E+09   ...
    2      -3   2     -2.337E-20
    3      -4   1     -2.469E-20
    4      -5   2      8.207E-22
```

Detailed PI cross sections now appear in the opls file. (Only a single energy PI cross section is written in place of a radiative rate in the olg file, and is flagged by a negative term index I.)

```
  NV=    2  LV=   -1       K
 15 E(RYD)   Z=26    N= 3     LS-Coupling           EIONMIN=       0.000000
    0.00000E+00    6.86104E-01    1.84295E+00    3.79350E+00    7.08234E+00
    1.26277E+01    2.19777E+01    3.77427E+01    6.43243E+01    1.09144E+02
    1.84713E+02    3.12132E+02    5.26973E+02    8.89218E+02    1.50000E+03
        I-S            C-S          PHOTO-IONIZATION DATA       Z=26   N= 3
   CF    T    W   CF    T   EO       P/CM2         E-I(RYD)      E-C(RYD)
    5    3    6   -3    1    1   -2.33701E-20   -1465.056299   -1319.676409
   -2.33701E-20   -2.30374E-20   -2.24901E-20   -2.16049E-20   -2.02115E-20
   -1.81142E-20   -1.51728E-20   -1.14709E-20   -7.49090E-21   -4.03266E-21
   -1.72397E-21   -5.76008E-22   -1.51826E-22   -3.24475E-23   -5.81412E-24
    4    5    2   -2    2    1   -2.46915E-20   -1468.495610   -1319.676409
   -2.46915E-20   -2.44624E-20   -2.40828E-20   -2.34612E-20   -2.24629E-20
   -2.09097E-20   -1.86130E-20   -1.54720E-20   -1.16447E-20   -7.66581E-21
   -4.28161E-21   -1.99417E-21   -7.74833E-22   -2.54968E-22   -7.26467E-23
    5    3    6   -1    4    1    8.20745E-22   -1465.056299   -1319.676409
    8.20745E-22    8.11736E-22    7.96843E-22    7.72547E-22    7.33773E-22
    6.74070E-22    5.87243E-22    4.71603E-22    3.36321E-22    2.04000E-22
    1.01004E-22    3.96388E-23    1.22026E-23    2.97772E-24    5.92108E-25
```

Negative cross sections again just flag the sign of the matrix element before it was squared.

4. Dielectronic & Radiative recombination, resonant-excitation etc.
****

In principle, we have already discussed how to calculate atomic data for these processes viz. autoionization and radiative rates, as well as photoionization cross sections. However, what characterizes DR, RR & RE etc is that a large number of Rydberg states can contribute and to run each configuration manually is impractical. If the user sets RUN='DR', 'RR', 'RE' or 'PE' ('PE' flags photo-excitation autoionization, i.e. inverse DR, and like 'RE' it is mainly a convenience to the user to use these alternative flags) then the NAMELIST DRR is read to define the Rydberg nl-values that AS will loop-over. (Internally, Rydberg orbitals are flagged by n=80-89, usually 80.)

For example, DR of Li-like Carbon:

Example 6.

```
A.S. DR of Li-like Carbon
 &SALGEB RUN='DR' CUP='LS' MXVORB=2 MXCONF=2 MXCCF=3 KCOR1=1 KCOR2=1 &END
 2 0  2 1
  1    0
  0    1

  2    0
  1    1
  0    2
 &DRR  NMIN=3 NMAX=15 JND=14 LMIN=0 LMAX=7 &END
16   20   25   35   45   55   70  100  140  200  300  450  700  999
 &SMINIM  NZION=6 PRINT='FORM' &END
 &SRADCON MENG=-15  EMIN=0 EMAX=2 &END
```

Note, we have taken the opportunity to remove explicit specification of the closed-shell 1s^2 core via use of KCOR1, KCOR2 instead, and we will omit mention of it now. So, we have target 2s and 2p configurations. In addition to coupling on a continuum electron, the RUN='DR' flag ensures a Rydberg electron is also coupled to the same target configurations. The nl-values of this Rydberg electron are specified in the DRR NAMELIST viz. NMIN, NMAX, LMIN,LMAX. We also read-in (free-format, subsequently) JND additional n-values so as to span high Rydberg states efficiently.

We also have MXCCF Be-like correlation configurations 2s^2, 2s 2p and 2p^2 which allow for outer-electron radiation in the DR process. Outer-electron radiation to higher excited states outside of the core is usually post-processed in (hydrogenically).

SRADCON specifies the continuum interpolation energies again.

The full DRR specification is:

DRR

NMIN, NMAX: Loop the valence orbital over n=NMIN to NMAX incrementing n by 1.

JND = 0, default.
JND .gt. 0, then JND additional n-values are read following the namelist.
      AS inserts an additional n-value between each input value to aid
      interpolation and numerical integration over n in user-supplied
      post-processing routines.

NRAD =1000, default. In DR runs the radiation from high-n is negligible
      and the effect of the Rydberg orbital on the core is small.
      So, for n.gt.NRAD no new radiative rates are calculated.
      The default value is to always to compute radiative data.

LMIN, LMAX: Loop the valence orbital over l=LMIN to LMAX incrementing l by 1.

LCON is the number of l-values for the continuum orbitals.
Let lc denoted the continuum angular momenta and lv the Rydberg angular momentum. Then the internal assignment is
lc=lv-(LCON-1)/2, lv-(LCON-1)/2 +1, ... , lv+LCON/2.
Generally, LCON should be set to 2*LAMAX+1, where LAMAX is the largest target multipole transition required. Thus, LCON=3 for dipole, and =5 for quadrupole core transitions as well.
Default: is 2* max_target orbital l, plus 1.

The corresponding RR example is similar, but simpler:

Example 7.

```
A.S. RR of Li-like Carbon
 &SALGEB RUN='RR' CUP='LS' MXVORB=2 MXCONF=2 KCOR1=1 KCOR2=1 &END
 2 0  2 1
  1    0
  0    1
 &DRR  NMIN=3 NMAX=15 JND=14 LMIN=0 LMAX=3 &END
16   20   25   35   45   55   70  100  140  200  300  450  700  999
 &SMINIM  NZION=6 PRINT='UNFORM' MAXE=40 &END
 &SRADCON EMAX=40 &END
```

The RUN='RR' flag switches-on photoionization (which is converted to recombination via detailed balance during post-processing). No (N+1)-bound configurations are required since we are dealing with a one-body operator. The l-range is reduced since it is more efficient to post-process high-l (very high for low temperatures) hydrogenically. Unlike 'DR', we do not have to specify any energy details if the goal is a recombination rate coefficient, then it is best to let the code choose them. Here, we have artificially restricted the upper range via EMAX otherwise we may need a larger radial dimension, set by MAXB1. Also, because the scattering energies can be large for non-resonant processes, it can be necessary to specify the maximum scattering energy MAXE in SMINIM also, where the radial array is set-up. Here, it is being used to stop the mesh being set too fine!

Note the use of the PRINT='UNFORM' option so as to output unformatted files olsu and oplsu, both for speed and accuracy, but not user friendly.

The final example in this section is that of inner-shell dielectronic recombination. We now have to handle the situation of core-rearrangement autoionization which leaves a Rydberg orbital in the N-electron target configurations. Thus, we must specify it in the MXVORB orbital list which defines the target configurations. Here, we recall that such an orbital is flagged internally by having n=80 (its l-value is irrelevant).

So, consider:

Example 8.

```
A.S. Inner-shell DR of Li-like C.
 &SALGEB RUN='DR' CUP='LS' MXVORB=4 MXCONF=6 MXCCF=3 &END
 1 0  2 0  2 1 80 1
  2    1    0    0
  2    0    1    0
  1    2    0    0
  1    1    1    0
  1    0    2    0

  2    0    0    1
```

```
  2    2    0    0
  2    1    1    0
  2    0    2    0

 &DRR  NMIN=3 NMAX=10 LMIN=0 LMAX=5 &END
 &SMINIM  NZION=6 &END
 &SRADCON MENG=-15  EMIN=0 EMAX=25 &END
```

Here, our 6th target configuration contains the Rydberg orbital. There can be as many such configurations as we like, but they must all be listed after all of the regular target configurations. (Again, the blank line is irrelevant and is to guide the eye only.)

The regular subset of target configurations are treated as in the outer-shell case: (N+1)-electron configurations are formed by coupling on a Rydberg electron as well as angular momentum adjusting continuum orbitals. The new subset which already contains a Rydberg orbital just gives rise to (N+1)-electron configurations with fixed angular momentum continuum orbitals, since this autoionization is independent of the l-varying Rydberg orbital. Internally, the fixed angular momentum continuum are flagged by n=99, adjustable by n=90-98.

```
****************************************************************************
----------------------------------------------------------------------------
```

REMAINING OPTIONAL INPUT

The final optional NAMELIST input concerns orbital replacement, i.e. where one wants to use radial wavefunction determined from some alternative external source such Fischer's MCHF code or Hibbert's CIV3 code. A subset of the MXVORB orbitals is flagged for replacement by setting their n-values in the range 70-79. The NAMELIST SRADWIN is then read, which specifies how the "external" orbitals are to be input.

SRADWIN

```
KEY=- 9, default. Assumes that the external input file (radwin) is in
         Opacity/Iron/RmaX/APAP Project format (approx. the old IMPACT format).
   =-10, UNIT5 read of free-formatted STO/Clementi orbital input as per
         R-matrix STG2, from UNIT5 input file.
```

An example (neutral Chromium):

Example 9.

```
A.S.  Neutral Cr
 &SALGEB  RUN='  ' RAD='E1' CUP='LS' MXVORB=7 MXCONF=8
          KCOR1=1 KCOR2=-5 NAST=2  &END
 71 0 72 0 72 1 73 0 73 1 73 2 74 0 74 1 74 2 74 3 75 0 75 1
 4 0 1 1 0 0 0
 4 1 0 1 0 0 0
 5 0 1 0 0 0 0
 4 1 1 0 0 0 0
 4 1 0 0 0 0 1
 4 0 1 0 0 1 0
 5 1 0 0 0 0 0
 4 0 0 0 0 1 1
 5 0 0
 5 1 1
```

```
 &SMINIM  NZION=24  &END
 &SRADWIN  &END
```

NOTE the use of negative KCOR2 to read ALL nl definitions (as we must if we want to replace the core orbitals as well as the valence) but valence occupation numbers only for the configurations.

Note: All of the orbitals are tagged for replacement so SMINIM requires little input. The version of Fischers code used produces OP format. Although the use of 71 0 72 0 is suggestive of 1s and 2s replacement (and helpful) it should be noted that the 1st orbital (71 0) will be replaced by the first s-orbital in the file radwin. We could have written 72 0 71 0 and the same result would be obtained, if somewhat confusing - the 1s orbital (assuming it was infront of the 2s on radwin) would be in 72 0.

Finally, we used NAST to restrict the number of terms to be generated from the listed configurations for neutral Chromium, which would be large otherwise.

Another example illustrates using Clementi/STO orbitals from CIV3:

Example 10.

```
A.S. Be+ using STO input from Berrington et al JPB30, 4973 (1997)
 &SALGEB MXVORB=10 MXCONF=12 &END
   1 0 2 0 2 1 3 0 73 1 3 2 74 0 74 1 74 2 74 3
 2     1 8*0
 2 1*0 1 7*0
 2 2*0 1 6*0
 2 3*0 1 5*0
 2 4*0 1 4*0
 2 5*0 1 3*0
 2 6*0 1 2*0
 2 7*0 1 1*0
 2 8*0 1
 1 2 0 7*0
 1 1 1 7*0
 1 0 2 7*0
 &SMINIM  NZION=4  &END
 &SRADWIN KEY=-10 &END
 4                                                  "1sbar"
 1 2 3 4
 0.971825    1.004046   1.737171   1.374292
 4.5503412 -25.1391755 10.0594491 12.5146482
 2                                                  "1pbar"
 2 3
 2.021253   1.212317
 7.9481978 -0.7926990
 3                                                  "2pbar"
 2 3 4
 1.32       1.32      1.32
 8.1450302 -9.0962054 2.0607677
 2                                                  "1dbar"
 3 4
 1.4889106  0.8167585
 1.1371840 -0.6610356
 2                                                  "1fbar"
 4 5
 1.894808   0.551422
 1.0009988 -0.1575788
```

Here, the 1s,2s,2p,3s and 3d are (spectroscopic) internal orbitals.
The "4s", "3p", "4p", "4d", "4f" are (pseudo) external orbitals.

```
****************************************************************************
----------------------------------------------------------------------------
```

MISCELLANEOUS EXAMPLES.

Here, I’ll place some examples that might be of interest.

Example 11.

A.S. Generate all Be-like CFs nln’l’ up to n=5. Use MXVORB<0 for standard order.

```
 &SALGEB KCOR1=1 KCOR2=1 MXVORB=-14 MXCONF=1 ICFG=1 &END
 14*0                !minimum occupation nos
 14*2                !maximum occupation nos
 2 13*0  2           !base config and no. of promotions
 &SMINIM NZION=26 &END
```

This illustrates basic usage of promotional rules. See SALGEB input.

Example 12.

A.S. Generate a B-like Laguerre pseudo-state expansion to 10d

```
 &SALGEB CUP=’LS’ KCOR1=1 KCOR2=1 MXVORB=2 NXTRA=10 LXTRA=2 MXCONF=2 ICFG=1 &END
 2 0 2 1
 0 0               !minimum occupation nos
 2 2               !maximum occupation nos
 2 1  1            !base config and no. of promotions
 1 2  1            !base config and no. of promotions
 &SMINIM NZION=6 NLAM=4 ORTHOG=’LPS’ RADOUT=’YES’ &END
1. 1. 1. -1.       !1s,2s,2p spect. 3s upwards Laguerre.
```

For a small RMPS calculation.

Example 13.

A.S. Produce support files for an R-matrix stgicf calculation: OMGINF, adf04.

```
 &SALGEB CUP=’IC’ MXVORB=3 MXCONF=3 RAD=’ALL’ KUTSO=0 &END !KUTSO for R-matrix
 1 0  2 0  2 1
  2    2    0
  2    1    1
  2    0    2
 &SMINIM NZION=6 ESKPL=1. ESKPH=1.1 ECORR=1.3 &END !Flags correlation by energy
```

Correlation TERMS/LEVELS lie between ESKPL,ESKPH and above ECORR.
KUSTO=0 corresponds to R-matrix usage.

```
_______________________________________________________________________


EEEEEEEEEEEEEEEEENNNNNNNNNNNNNNNNNNNNNNNNNNDDDDDDDDDDDDDDDDDDDDD
       E                     N                      D
```

POST-PROCESSING

```
                              ***************
```

The AUTOSTRUCTURE code produces large amounts of LS and IC data that is written to the files ’ols(u)’ and ’oic(u)’, and ’opls(u)’ and ’opic(u)’ for photoionization. In general, this cannot be processed by hand. The transition probabilities are normally combined in many different ways depending on the resonant process that you wish to study. Similarly, photoionization cross sections can be reduced to a more manageable form, e.g. totals. Historically, there was a single general post-processor MDRCS (current incarnation the mdrcs13.f code) which covered any and all applications. More specialized and structured codes evolved from this viz. the ADAS post-processors for DR, RR, PE and PI. They deal with one specific process and have evolved themselves so that they are often somewhat more accurate than the general one as such development has not been ported back to the historic general code. Some obscure requirements can still only be dealt with by the general code.

ADASDR POST-PROCESSOR
****

The program ’adasdr.f’ reads standard AUTOSTRUCTURE output files and processes them specifically to form (final-state resolved) ADAS ADF09 files for the modelling of dielectronic recombination. See the ADAS web pages (http://www.adas.ac.uk) for information about ADAS, its capabilities and detailed documentation, including precise specification of the ADF09 format. The series 7 codes are ADAS implementations of AUTOSTRUCTURE (701) and adasdr (702), these are basically just the standalone codes with an IDL wrapper for people familiar with working in the ADAS IDL environment.

Formatted data from AUTOSTRUCTURE is expected in file ’o1’ and unformatted data in file ’o1u’. The file ’o1’ is checked first. In addition to the ADF09 output, to file ’adf09’, the (UNIT6) output to ’adasout’ contains a terse summary of DR cross sections as a function of Rydberg nl, to be studied for convergence, and an estimate of the total rate coefficient from each initial metastable for the core excitation being processed.

The UNIT5 data is free-formatted and namelisted, as follows:

The first four characters of line 1 MUST be /LS/ or /IC/ so as to denote the type of data being processed. This generates 1998 style adf09 files (to recover 1993 style (LS) use / /). The rest of line 1 is for comment.

Namelist ONE

COREX=’n-m’ selects the core transition n->m to be processed, where n and m are the initial and final principal quantum numbers. The l-values need not and must not be specified i.e. ’n-m’ is 3 characters. The default is ’   ’, no restriction on core excitations. Thus, COREX should be specified. ADAS expects separate ADF09 files for each core excitation.

NTAR1=Number of initial (metastable) target states.

NTAR2=Number of final resolved parent states.

The values of (2S+1) L p (case /LS/) or 2J p 2S+1 L (case /IC/, where p, S and L are for labelling purposes only in adf09 - p is the parity) follow free-formatted, after Namelist TWO, for the NTAR2 parent states. (The files TERMS and LEVELS produced following a suitable target run with AUTOSTRUCTURE should provide this data.) This input data is compulsory.

Namelist TWO

```
NECOR=0 (default) does nothing.
     >0, read NECOR calculated then experimental energies (in Rydbergs)
         relative to the ground. They follow the statistical weight info.
```

Example 1. Be-like target, term-resolved.

```
/LS/ Be-like target, 2->2 core excitations.
 &ONE NTAR1=2 NTAR2=6 COREX='2-2'  &END
 &TWO  &END
 1 0 0    1    1          0.000000
 3 1 1    2    1          0.489799
 1 1 1    2    2          1.027305
 3 1 0    3    2          1.273012
 1 2 0    3    1          1.424089
 1 0 0    3    3          1.781974
 0 0 0    0    0        -72.892998
```

The input after &TWO is taken directly from the TERMS file.
The calculated (C2+) energies listed here will be checked internally against those in the rate file.

Example 2. Li-like target, level-resolved.

```
/IC/ Li-like target, 2s->2p core excitations.
 &ONE NTAR1=1 NTAR2=3 COREX='2-2'  &END
 &TWO NECOR=3  &END
 1 0   2 0
 1 1  -2 1
 3 1  -2 1
0.0 0.594108 0.595113       These are the calculated (core) energies for C3+.
0.0 0.587621 0.588603       These are the observed. This text is not read.
```

If energies are read alongside the symmetry info, as in Example 1, then the calculated energies MUST NOT be listed afterwards, just the observed.

ADASRR POST-PROCESSOR

The program 'adasrr.f' reads standard AUTOSTRUCTURE output files and processes them specifically to form (final-state resolved) ADAS ADF48 files for the modelling of radiative recombination. It is similar in spirit to ADASDR and its minimum input is just NTAR1 and NTAR2 (and stat. weight info) as described for ADASDR. (There is no COREX or NECOR now.)

ADASPE/PI POST-PROCESSORS

The programs 'adaspe.f' and 'adaspi.f' read standard AUTOSTRUCTURE output files and process them specifically to form (final-state resolved) ADAS ADF38 and ADF39 files for the modelling of photoexcitation-autoionization and (direct) photoionization. These ADFXX files are also used by Mike Seaton's OP codes. They can also produce R-matrix style X-files: XPEPAR, XPETOT, XDPIPAR, XDIPTOT and the resonant "PE" files can be added to their corresponding direct "DPI" files using the ’xpeppi.f’ code.

The NAMELISTed input is similar to that for ADASDR, but simpler.

ADASPE: Reads the same ’on’ or ’onu’ AUTOSTRUCTURE files (n=1,2,3,4 etc) as ADASDR.

ADASPI: In addition, reads photoionization files ’opn’ or ’opnu’. The ’on’ files must match the ’opn’ files obtained from the same AUTOSTRUCTURE run.

The first four characters of line 1 MUST be /LS/ or /IC/ so as to denote the type of data being processed. The rest of line 1 is for comment.

We refer to the initial state as the one that the photon impacts on and final state that of the residual ion that the ejected electron "sees".

Namelist ONE

NTAR=Number of (final) electron "target" states for which symmetry info is read.

Unlike ADASDR/RR, NTAR is for labelling info only in the adf38/39 files.

The values of (2S+1) L p (case /LS/) or 2J p 2S+1 L (case /IC/, where p, S and L are for labelling purposes only in adf38/39 - p is the parity) follow free-formatted, after Namelist TWO, for the NTAR final "target" states. (The files TERMS and LEVELS produced following a suitable target run with AUTOSTRUCTURE can provide this data.)

The above is the standard (minimal) input for OP work, i.e. all possible data produced on adf38/39. It can be restricted though:

NTARP, NTART restrict the number of electron targets resolved for partial data, and which go into any total sum. They are independent of each other, and of NTAR. So, the amount of partial data resolved can be restricted without affecting any totals.

IRSLMX is the max no. of initial photon targets, default all. (Strictly speaking, it is the adf38/39 IRSL index label, which may not be energy ordered if multiple opn files are processed...)

ADASPE only options:

JRSLMX is as IRSLMX but for upper photon states.

RAD=’YES’ includes radiation damping. This includes damping to autoionizing states, which is not included by standard R-matrix. Default.
= ’NO’ omits radiation damping.

PABS=’YES’ then photoabsorption cross sections are written.
= ’NO’ then "photoionization" is written, default.

Namelist TWO

None normally, for adf38/39 production.

An alternative scheme involves producing R-matrix style X-files. This is controlled by the EWDITH and related parameters (see ONE).

EWIDTH .gt.0 then PI cross sections and (energy-averaged) PE cross sections are convoluted with a Gaussian of FWHM of EWIDTH Rydbergs and written to the partial XDPIPAR, XPEPAR and total XDIPTOT, XPETOT files.

EMIN, EMAX are the range of photon energies for which cross sections are convoluted.

NBIN is the number of energy bins, between EMIN and EMAX, for energy-averaged PE cross sections (ADASPE only).

The IRSLMX and NTAR defaults are different here viz. IRSLMX=1, and NTAR *does* restrict the X-file writes.

Finally, the program ’xpeppi.f’ will add the resonance and direct files together.

POST-PROCESSOR (General)

****

The post-processor ’mdrcs13.f’ can be used to study many resonant processes, maybe combined with direct backgrounds. *** If you just want to produce ADF09/48/38/39 files for ADAS then use instead the programs adasdr/rr/pe/pi detailed previously.

The UNIT5 data is all free-formatted and namelisted. The basic most commonly used variables are detailed below. There are many other options, some quite esoteric, which are available for manipulating the raw AUTOSTRUCTURE data. Information on these can be found in the comment cards towards the beginning of the code under the headings NAMELIST-ONE, NAMELIST-TWO and NAMELIST-THREE.

Formatted data from AUTOSTRUCTURE is expected in file ’o1’ and unformatted data in file ’o1u’. The file ’o1’ is checked first.
Non-resonant backgrounds can be added by simply making a suitable file available as the file ’ombg’. "Standard" R-matrix ’omega’ and ’omegdr’ files are acceptable.

Namelist ONE

\------------

RUN=’DR’ Process for photon emission (dielectronic recombination) default.
   =’RE’ Process for electron emission (resonant excitation).

NTAR1=Number of initial (populated) target states.
NTAR2=Number of final resolved states for RE (not used for DR).

The values of (2S+1) L or 0 2J+1 follow free-formatted after Namelist TWO for the NTAR1 initial states. This is the minimal target info required. Suitable data is produced in the TERMS/LEVELS files by structure runs. They contain more info e.g. energy levels, which can be used by the ADASXX post-processors.

NCUT=Rydberg principal quantum number cut-off of AUTOSTRUCTURE data (default all).
LCUT=Rydberg angular momentum cut-off of AUTOSTRUCTURE data (default all).

UNITS=1.0 Rydberg energy units (default).
     =13.606 Electron-volt energy units.

IPRINT=0,-1,-2,-3 Print-level, increasing values give a more detailed printout.
      =-1 is the default and the best first choice.

```
NC<=0 (default) binned cross sections are written to the file 'ocs'.
   =1  Processing very large rate files can be time consuming. By setting
       NC=1 the binned cross sections can be read-back from 'ocs' and then
       convoluted. Thus one can vary the convolution without having to
       re-process the raw data each time.


Namelist TWO
------------

EMIN=Minimum continuum energy (in UNITS) for which rates are both processed
     and plotted.
EMAX=Maximum, ditto.

NBIN=Number of bin energies (number of bins=NBIN-1). The bin width,
     (EMAX-EMIN)/(NBIN-1) should be smaller than the convolution width
     and larger than the natural width of the resonances.

EWIDTH>0 Convolute the (bin) energy-averaged cross sections with a Gaussian
         of FWHM EWIDTH UNITS.
      =-0.5 (actually any non-integer negative number) convolute with a
        Maxwellian distribution.
      =0.0 Convolute with a cooler distribution, the characteristic
       temperatures are given by:

TPAR and TPER in UNITS.

NR1>0 is the lowest final-state principal quantum number for a radiating
      Rydberg electron that was NOT included in the AUTOSTRUCTURE run.
      For example, dn=0 DR in highly-charged ions may allow the rydberg
      electron to stabilize to quite a high n-value that would be impractical
      and time consuming to include in an AUTOSTRUCTURE run. These rates
      are generated hydrogenically within the post-processor (very fast).
      Default, no rydberg electron radiation added.

NECOR=0 (default) does nothing.
     >0 read NECOR calculated then experimental energies (in UNITS) relative
        to the ground. They follow the statistical weight information.


Namelist THREE
--------------

None normally, historic graphing input.



EEEEEEEEEEEEEEEEENNNNNNNNNNNNNNNNNNNNNNNDDDDDDDDDDDDDDDDDDDDDDDD
       E                     N                      D
```

This is a development Write-Up for AS v22.x, which will eventually be merged with the regular WRITEUP file.

New for v22.x:

RUN='DE' Direct electron-impact Excitation, colloquially "DW" but DR, RR
         etc are also DW, of course, hence the more precise 'DE'.

Collision strengths (between terms) can be calculated in LS-coupling and level-resolved (TBD) in Breit-Pauli jK-coupling. Each coupling input (via SALGEB) is described next, followed by the common input for scattered energies (via SRADCON). In particular, collision strengths are calculated at the same set of *final scattered* energies for ALL transitions, e.g. zero gives all threshold collision strengths. Slater integrals etc. are interpolated at the appropriate initial scattering energy.

NAMELIST SALGEB

CUP='LS', and its variants, generate collision algebra in LS-coupling
          over a range of L given by

MINLT, MAXLT = min and max total L (both parities) for
MINST, MAXST = min and max total S.

It is not necessary to set MIN/MAXST (default, all).
It is not necessary, but possibly desirable, to set MIN/MAXLT (default 0-30).

Exchange is neglected for L greater than (you should not need to change it)

MAXLX= max total L for which exchange is included.
       Default is twice the max exchange multipole included, where

MXLAMX= max exchange multipole.
        Default is twice the max orbital ang. mom. plus 1.

Thereafter, the problem is solved for a single target spin-system, as per NX RM, and the total spin is flagged in the same fashion. (In some cases MAXLX may be slightly larger as there is also the requirement that the full channel expansion be "open".)

Top-up is automatically included at

LRGLAM=MAXLT (but can be reduced/switched-off by the user for testing.)

In addition, collisional two-body non-fine-structure is controlled by

KUTOOX= 1 includes orbit-orbit etc in the same fashion as the target KUTOO.
      =-1 off (default).

KUTOOX is independent of KUTOO, but some off/on combinations are more meaningful than others.

In addition to target symmetries being restrictable by the usual NAST/KCUT parameters (see WRITEUP), the (N+1)-electron SLp symmetries can be restricted by

INAST .gt. 0, read INAST symmetries of the form 2S+1 L p (p=0,1)
              after the config. spec. and any NAST input.
              By default, top-up is OFF (LRGLAM is set .lt.0) now.

(Recall, NAST refers to target symmetries, not states, so a target SLp need only be listed once to include all such. This is in contrast to R-matrix usage where it refers to states/terms and a given term must be listed many times.)

Finally, excitations can be restricted by

NMETA= the number of ground plus metastable TERMS for which excitation
       algbera/data is computed between themselves and to ALL excited states,
       i.e., transitions between excited states are omitted.
       The NMETA terms are the energetically lowest ones.
       Default is the highest term from which, and for all lower,
       no E1 radiation exists.

****

CUP='jK' or 'IC', and its variants (will) generate collision data in Breit-Pauli
          jK-coupling over a range of 2J given by

MINJT, MAXJT = min and max 2J (both parities).

It is not necessary, but possibly desirable, to set MIN/MAXJT (default, min/max allowed by MIN/MAXLT). If MIN/MAXJT is set then it is not necessary to set MIN/MAXLT.

In addition, generation of collisional two-body fine-structure (2fs) algebra in an LSJ representation is controlled by (and *has* been coded)

KUTSSX=-1 off (default)
      =-9 all possible
      = 1 first target config only.
      = etc. all values have the same interpretation as the target KUTSS.

KUTSSX is independent of KUTSS, but some off/on combinations are more meaningful than others.

Since 2fs is likely only to be important for weak transitions, and it is time consuming, generating it over the full J-range is not desirable and so

MAXJFS=the max 2J for which two-body fine-structure is included.
       (The min value is just MINJT.)

It is not necessary, but possibly desirable, to set MAXJFS.
If KUTSSX is "on" then, if not set, MAXJFS defaults to the max allowed by MAXLX.

The (N+1)-electron Jp symmetries can be restricted by

INASTJ .gt. 0, read INASTJ symmetries of the for 2J p (p=0,1)
               after any INAST input.

If you accidently restrict SLp so that a symmetry required by your requested Jp is missing then the code will flag this and, currently, aborts.

If you use NMETA (terms) then, like ICFT RM, it is likely desirable to include an extra term or two so that the dominant spin-orbit mixing is accounted-for.

It is likely that an NMETAJ will be introduced at some stage.
(It has no meaning until re-coupling from LSJ to jK.)

NAMELIST SRADCON

While no input is required, the user will possibly want to set their own final scattered energies (all energies are in unscaled Rydbergs):

MENG .eq. 0 (default) uses 0, DE/3, DE, 3*DE (& 8*DE if MAXLT.gt.35)

```
            where DE=max(ionization potential, highest term energy)
     .gt. 0 reads MENG final scattered energies following the NAMELIST.
     .lt. 0 internally sets -MENG energies between a user specified range:
```

EMIN, EMAX the minimum & maximum scattered energies.

In general, additional interpolation energies will be required as the scattered energies are likely too coarsely spaced (the code automatically handles the fact that the largest initial scattering energy required is the maximum final scattered energy plus the maximum excitation energy, by adding additional suitable points.)

There are several ways to specify additional interpolation energies:

```
  | ***The best choice is still to be determined by experience and so options    |
  | and recommendations are subject to change, "best" being the smallest and     |
  | most accurate interpolation basis. Since an arbitrary set of energies can be |
  | handled, if you have an improved "algorithm" it can easily be incorporated.  !
```

Systems with a small set of well defined excitation energies can be dealt with formally by reading

```
NDE .gt. 0 excitation energies, to be read after the scattered energies.
    .eq. 0 default, none, unless MENG=0, then uses internally generated ones.
```

Then, the code adds interpolation energies at all (initial scattering) energies defined by adding all excitation energies to all final scattered energies. Zero is automatically added/needed, so do not specify.
This approach becomes increasingly time-consuming for "large" NDE & MENG, so keep MENG as small as possible - we are talking non-resonant DW after all.

The user can also specify interpolation energies more directly via

```
MENGI .gt. 0 reads MENGI interpolation energies following the scattered energies.
      .lt. 0 inserts -MENGI energies between each scattered energy.
             Running -1 followed by -2 enables one to gauge interpolation errors.
      .eq. 0 (default) none here.
```

Finally, it can be useful to set the maximum scattering energy, via MAXE, in SMINIM so as to ensure a suitably fine radial mesh is generated to support the continuum.
Also in SMINIM, setting JPRINT.gt.0 gives increasingly more detailed output (=1-4)
Default JPRINT=-1 (corresponds to PRINT='FORM' while -3 corresponds to 'UNFORM'.)

NRB 16/09/09

R-Matrix
****

These Classic R-matrix and related codes do not correspond exactly to any published or unpublished R-matrix codes. However, they do contain features not found in the Belfast/UCL codes which you may find of use. The Belfast (inner-region) codes have been published in Computer Physiscs Communications (CPC v92 p290 1995 - BP/LS exchange and v62 p76 1992 - LS non-exchange) and are availablevia the WWW from http://www.cpc.cs.qub.ac.uk/cpc/ under catalogue numbers ADCP and ACGP. The UCL/Belfast (outer region) codes remain unpublished.

WARNING: DO NOT MIX these R-matrix codes with any others!

N. R. Badnell 06/05/09

oooooooooooooooooooooooooooooooooooooo

INNER REGION CODES
****

Familiarity at least with the latest (non-CPC) NAMELIST/free-format input, and operation, would be helpful but it is not essential.

To use the local executables you should add /home/badnell/rmatrix/x to your path - and have an account on a local machine!

Prior to running any R-matrix codes you should have generated previously a 'radial' file (called 'radout' by AUTOSTRUCTURE) that will be used by R-matrix to re-generate your previously determined atomic structure. If you haven't done this then go back and read the AUTOSTRUCTURE file WRITEUP.

A suitable dataset for C2+ is:

```
123456789 21522 21512513 21523
                10 20 21
 &SALGEB  RUN='  ' RAD='NO' CUP='LS' TITLE='C2+ test' KORB1=0 KORB2=0  &END
 &SMINIM  NZION=6 INCLUD=0 PRINT='FORM' NLAM=3 NVAR=0 RADOUT='YES'   &END
 1.3678 1.2308 1.1670
```

Then copy or move the file 'radout' to 'radial'.

The (local) full exchange executables for non-relativistic (see 1. here) and Breit-Pauli (see 2. below) operation are:

```
stg1r.x  stg2r.x  (stgjk1.x) stg3r.x
```

on SUNs, replace .x with .xsg on the SG machines.

1. Non-relativistic (LS-coupling) operation.
----

stgjk1.x is omitted during an LS run (this is the RECUPD code).

The file containing the UNIT5 input detailed below is specified by the redirect "<", e.g. stg1r.x <dstg1 and the UNIT6 output automatically goes to a file called 'routnr' where n will be 1,2,3 etc.

STG1: read bound orbitals (from file 'radial'), generate continuum basis
**** orbitals and evaluate all possible bound-bound, bound-continuum and
      continuum-continuum integrals that could be required.

STG1 Input

The first four characters of line 1 MUST BE: S.S. unless you know better.

Then the namelist STG1A input:

None normally, but

```
ISMITN = 1 Use new orthogonalization method with pseudo-state expansion.
       = 0 Default, use original recurrence relation (unstable).
```

Then the namelist STG1B input:

MAXLA = maximum N-electron (atomic) angular momentum.

MAXLT = maximum (N+1)-electron (total) angular momentum.

MAXC = maximum number of continuum basis orbitals per angular momentum.

MAXE (optional) if specified, is the maximum scattering energy in Rydbergs for your problem. If the MAXC you have specified is too small, an estimate of the value required is printed and execution halts.

Note, for a given MAXC, the maximum scattering energy for which accurate collision strengths can be calculated is one half the maximum eigen-energy of the continuum basis orbitals (approximately).

ISMIT(I)=nl, denotes which, if any, of your nl orbitals are non-spectroscopic.
       e.g. ISMIT(1)=40 ISMIT(2)=41 labels the 4s and 4p orbitals as pseudo.
Alternatively, use NMIN, NMAX, LMIN, LMAX to give a range of nl-values.
Or, if you set NMAX.LT.NMIN then specify NPS(l)=n where l=pseudo a.m. and n is the max (pseudo) principal quantum number for that l. The min is given by NMIN of course.

Example: C2+

```
S.S.  C2+ TARGET 1 CPC TEST
 &STG1A  &END
 &STG1B  MAXLA=2 MAXLT=8 MAXC=25 MAXE=4  &END
```

+++
To use STO orbital specification, instead of a radial file but everything else as above, then replace S.S. by STO- and set NZED, NELC, MAXORB in STG1B with MAXORB as per STG2 (next).
+++

```
STG2: Evaluate N- and (N+1)-electron angular algebra. Form N- and (N+1)-electron
****  Hamiltonians. Diagonalize N-electron Hamiltonian to regenerate the
      target eigen-energies (and eigen-vectors).
```

STG2 Input

The first four characters of line 1 MUST BE: S.S. unless you know better.

Then the namelist STG2A input:

None, normally.

Then the namelist STG2B input:

MAXORB = maximum number of orbitals that will be used to define the target configurations. Their nl values follow the namelist.

NELC = number of target electrons.

```
NAST = number of target terms, specified as 2S+1 L p after the namelists (S.S.),
                               specified as L 2S+1 p after the namelists (STO-).

INAST = number of total SLp symmetries, specified as 2S+1 L p after the
        namelist. Set p=0 for even parity and p=1 for odd parity.

If INAST = 0  then

MINLT = minimum total L.

MAXLT = maximum total L.

MINST = minimum total 2S+1.

MAXST = maximum total 2S+1.

SLp’s will be generated internally for this range, both parities.

endif
```

The target configurations are specified via orbital occupation numbers. It is possible to allow promotions from a basic configuration subject to an overall minimum and maximum occupation constraint.

The (N+1)-electron configurations, which are added to compensate for the enforced orthogonality of the continuum orbitals to the bound orbitals, are specified in a similar manner.

You must specify at least those (N+1)-electron configurations that arise from adding any of the bound orbitals to an N-electron configuration that gives rise to a term that is specified by NAST.
If you specify (N+1)-electron configurations that arise from adding a bound orbital to a configuration that includes a term not specified by NAST then you may run into problems with pseudo-resonances (no details!).

The simplest, safest solution for the non-expert is to use N-electron configurations that are purely CC (i.e. all terms are specified by NAST) or purely CI (i.e. containing no terms specified by NAST). You then use the MAXORB orbitals to form all possible (N+1)-electron configurations from the CC N-electron configurations BUT NOT from the CI configurations.

Now would seem like a good time for an example: C2+ again

```
S.S.  C2+ TARGET 1 CPC TEST
 &STG2A    &END
 &STG2B MAXORB=3 NELC=4 NAST=6 INAST=0 MINLT=0 MAXLT=8 MINST=2 MAXST=4 &END
 1 0 2 0 2 1
 3
  2  0  0
  2  2  2
  2  2  0    0
  2  1  1    0
  2  0  2    0
   1   0   0
   1   0   0
   3   1   1
   1   1   1
   3   1   0
   1   2   0
 3
  2  0  1
  2  2  3
  2  2  1    0
  2  1  2    0
```

```
  2  0  3    0
```

Note, the input is all free-formatted.

a)Following the namelists, the three nl orbitals are specified.

b)Then the number of target configurations is specified, 3.

c)Then the minimum and maximum occupation numbers of the target configurations are specified, these constrain possible configurations allowed by promotions from a basic configuration.

d)Then the 3 target configurations themselves are specified, the final zero denotes that no promotions are allowed from these 3 basic configurations, they are the only configurations required.

e)The NAST=6 target terms are then specified. While it is natural to list them by energy order it is infact computationally much more efficient to group them by symmetries, as has been done for the singlet S even, so that the angular algebra is solved-for only once per target symmetry.

f) Then b), c) & d) are repeated, this time for the (N+1)-electron configurations. If INAST were non-zero then e) would also be repeated.

STG3 (sometimes known as STGH): Diagonalize (N+1)-electron Hamiltonian.
****

STG3 Input

The first four characters of line 1 MUST BE: S.S. unless you know better.

Then the namelist STG3A input:

None, normally.

Then the namelist STG3B input:

```
INAST = 0 (default) then all (N+1)-electron symmetries specified in STG2 are
          looped-over.
      > 0 then specify the SLp's to be used, this is a much slower operation
          and should only be used if really needed.

NAST = 0 (default) do nothing.
     > 0 Read NAST experimental energies in Rydbergs relative to the ground.
         Adjustments are then made to the diagonal of the continuum-continuum
         part of the Hamiltonian.
```

Example: C2+ yet again

```
S.S.  C2+ TARGET 1 CPC TEST
 &STG3A  &END
 &STG3B INAST=0 NAST=6 &END
0.0000 1.6632 0.4775 0.9327 1.2526 1.3293
```

Note, the energies are free-formatted and are input in the order that the terms were listed in STG2 (after any re-ordering), or the levels were listed in recupd/stgjk.

----

2. Breit-Pauli operation

This is not too different from the non-relativistic operation.
Remember to execute stgjk1.x (aka RECUPD) after stg2r.x.

In addition to the input described for non-relativistic operation, for

STG1:
****
Add to namelist STG1A, RELOP='YES'

STG2:
****
Add to namelist STG2A, RELOP='YES'

Note, the N-electron Hamiltonian is not diagonalized now and the CC expansion is forced (expanded) to be the same as the CI expansion.
Also, ensure MAXLT is set large enough (.GE.J+MAX(S)) so that all possible matrix elements required for subsequent recoupling are present.

```
STGJK: (aka RECUPD) Recouple N- and (N+1)-electron Hamiltonians. Diagonalize
*****  N-electron Hamiltonian to regenerate the target eigen-energies (and
       eigen-vectors).
```

STGJK Input

The first four characters of line 1 MUST BE: S.S. unless you know better.

Then the namelist STGJA input:

None, normally.

Then the namelist STGJB input:

JNAST = number of target levels, specified as 2J p after the namelist.

IJNAST = number of total Jp symmetries, specified as 2J p after the namelist.

If IJNAST = 0 then

J2MIN = minimum total 2*J.

J2MAX = maximum total 2*J.

Jp's will be generated internally for this range, both parities.

endif

Example: C2+ ad nauseum

```
S.S.  C2+ TARGET 1 CPC TEST
 &STGJA  &END
 &STGJB JNAST=10 IJNAST=0 J2MIN=1 J2MAX=5 &END
 0  0      1S
 0  1      3P
 2  1      3P
 4  1      3P
 2  1      1P
 0  0      3P
 2  0      3P
 4  0      3P
 4  0      1D
 0  0      1S
```

Note, the "term" label after the target levels is for identification purposes only.
(Aside, is there any efficiency in grouping like levels together?)

STG3 and the outer region codes now follow as for non-relativistic operation except that we are dealing with levels rather than terms. Any reference to L is replaced by 2J and any reference to 2S+1 L p by 0 2J p.

In addition, TERM COUPLING COEFFICIENTS can be obtained as well by setting RELOP='TCC' in STG2A, they are actually output to TCCDW.DAT by STGJK.
In this instance STG2 evaluates the N-electron Hamiltonian twice.
Firstly to evaluate the LS e-energies and e-vectors, INCLUDING Mass-Velocity and Darwin terms. So to make a meaningful comparison between TCC and LS results the LS results should include Mass-Velocity and Darwin terms. This can be achieved by running STG1 with RELOP='YES' or 'MVD' and STG2 with RELOP='MVD', then STG3 etc. as in a non-relativistic run. STGJK is ONLY needed when the spin-orbit interaction has been switched-on via RELOP='YES' or 'TCC' in STG2.
Secondly, STG2 evaluates the N-electron B.P. Hamiltonian including the spin-orbit interaction ready for recoupling and diagonalization by STGJK.
The TCCs are in addition to a full Breit-Pauli run. If only TCCs are required, e.g. from a large LS calculation, then set RELOP='TCC' and IDWOUT=2 in stg1r/stg2r/stgjk for maximum efficiency (stgjk=recupd).

----

3. Photoionization operation

The non-relativistic operation follows 1., and Breit-Pauli follows 2.
EXCEPT that one MUST use the local executable stgjk2.x, which has the photoionization memory switched-on (MZIPH=2).

In addition to the input described in 1. and 2., for

STG1:
*****
Add to namelist STG1A, RAD='YES'

STG2:
*****
Add to namelist STG2A, RAD='YES'
(In Breit-Pauli mode the (N+1)-e symmetries MUST be grouped by parity, even then odd.)

STGJK: (For level-level)
******
Add to namelist STGJA, RAD='YES'

Also, the target levels MUST be grouped by parity.

STG3:
*****
Add to namelist STG3A, RAD='YES'

Note, STG3 generates the dipole matrix elements in the files Dnm.

The outer region codes STGB and STGF should be run next, generating the Bnm and Fnm files for the bound and free matrix elements.
Finally, PREBF and STGBF generate the photoionization cross sections.
See the outer region code descriptions below.

---

4. Non-exchange (non-relativistic) code operation

The non-exchange (non-relativistic ONLY) executables are (see 4. here)

stg1nx.x stg2nx.x stg3nx.x

The 3 stages are:

STG1NX (aka NXANG): which calculates the angular algebra.
******
STG2NX (aka NXRAD): which calculates the basis orbitals and radial integrals.
******
STG3NX (aka NXHAM): which diagonalizes the N- and (N+1)-electron Hamiltonians.
******

We run the NX codes as a continuation of the exchange codes. Thus, the files named NX1.DAT and NX2.DAT, generated automatically during an exchange run, must be present. They are used by all 3 stages. All 3 stages read the unit5 file called ’dstgnx’ which is of the form:

```
CONTinuation run.
 &STGNX  MINLT=9 MAXLT=12  &END
```

The first 4 characters of line 1 must be CONT.

Then,
MINLT = minimum total angular momentum (generally = exchange code MAXLT+1).
MAXLT = maximum total angular momentum (I have tested up to 80).

In addition, the (exchange) STG3 dataset must also be present and named ’dstg3’. Only the observed energies are read from this file. If only calculated energies are used then only a generic file needs to be present.

The UNIT6 output files are ’routmnx’ with m=1,2,3.

A standard H.DAT file is produced for use by an outer-region code (see below).

oooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooo

OUTER REGION CODES

FREE

They read the H.DAT file generated by STG3(NX) and calculate collision strengths at a user supplied set of energies and write them to an OMEGA file. Note, all input energies are z**2 scaled in the residual charge, if z>0.

oooooooooooooooooo

STGF: Seaton’s perturbative treatment of the long-range coupling potentials.
**** Now extended to handle neutrals (NRB).

Local executable stgf.x

STGF Input

```
----------

Namelist STGF

IQDT = 0 Default, standard STGF operation.
     = 1 MQDT operation via the unphysical S-matrix.
     = 2 MQDT operation via the unphysical K-matrix.

IMODE= 0 Write unphysical K/S-matrix to JBIN file. Default.
     = 1 Read unphysical K/S-matrix from JBIN file.
     =-1 Single pass interpolation of coarse mesh (see IEQ) onto
         the "usual" fine mesh.

IPRKM= 0 Do not write unphysical K/S-matrix to file k/smtls.dat. Default.
     = 4 Write unphysical K/S-matrix to file k/smtls.dat for stgicf.
         By default, these files are split by symmetry viz. k/smtls001,
         k/smtls002, k/smtls003 etc.

IMESH defines the type of energy mesh and subsequent namelist to be read.
     = 1  Constant spacing in energy dE.
     = 2  Constant spacing in effective quantum number dn.
     = 3  An arbitrary set of user-supplied energies.

IEQ controls how often the MQDT K-/S-matrix is calculated.
     = -1 The MQDT K-/S-matrix is calculated at every energy (default).
     >  0 then calculated at IEQ linearly spaced energies across the
          energy range defined by MESH. This is single pass operation.
          (see note: below)

PERT = 'NO' Neglect long-range coupling potentials (fast operation).
     = 'YES' Include long-range coupling potentials (factor 5-10 slower).

LRGLAM >=0 Maximum L-value (or 2*J) from STG3, partial wave sum will be
           topped-up with an estimate for LRGLAM to infinity.
       < 0 (default) No top-up.

IBIGE = 0 default, does nothing.
      = 1 append infinite energy scaled collision strength to the file OMEGA.

IPRINT defines the print level, -2 is lowest level and +3 the highest.

IRAD = 0 (default) collision strengths only.
     = 1 write the Fnm files for photoionization, as well.
     = 2 ditto, but no computation of collision strengths.

IOPT1 = 1 (default) all SLp cases.
      = 2 specify cases, (2S+1) L p or 0 2J p after energies (see next).
          Terminate with -1 -1 -1.


Namelist MESH1

MXE = the number of energy mesh points.

E0 = the first (scaled) energy point.

EINCR = the (scaled) energy increment.

or

Namelist MESH2

DQN = effective quantum number step

QNMAX = maximum effective quantum number of resonances to be resolved.
```

EMIN = minimum total energy.

EMAX = maximum total energy.

DEOPEN = interval in (EMIN,EMAX) for all channels open.

or

Namelist MESH3

```
MXE = the number of user supplied (scaled) energies in Rydbergs, relative
      to the ground state, which are read free-formatted after this namelist.
```

```
Note, I tend to use MESH1, with a "small" EINCR through the resonance region
****  (˜5000 points) and a "large" EINCR where all channels are open (˜10
      points). But, in MQDT mode (IQDT=1 or 2) the following approach should be
      used (with IEQ=-1, default):
      Run with a coarse energy mesh first (IMODE=0, default).
      Then re-run with a fine energy mesh (set IMODE=1).
      For production runs a single pass (IMODE=-1) is more efficient, making
      use of IEQ>0.
```

Example: Note only one of the MESH namelist’s is read, that specified by IMESH.

```
 &STGF  IMESH=1 PERT=’YES’ LRGLAM=8 IPRINT=-1 &END
 &MESH1 MXE=600 E0=0.1193 EINCR=0.0005 &END

 &MESH2 DQN=0.001 QNMAX=6.0 EMIN=0.1193 EMAX=0.2331 DEOPEN=0.0 &END
 &MESH3 MXE=5 &END
 0.45 0.50 0.60 0.80 1.00
```

It is IMPORTANT that you test that the resonances are sufficiently well resolved and that any that are not resolved are eliminated!

ooooooooooooooooooo

```
STGICF: Term-couple (unphysical) LS-coupling K-matrices to form intermediate
******  coupled collision strengths, following a STGF run.
```

Local executable: stgicf.x

STGICF Input

The first line is used for user comments, then

Namelist STGIC

```
IMODE = 0 generate (write) jK or ic data (K-matrices and channel info) on the
          original (coarse) STGF energy mesh. Reads unphysical LS K-matrices
          generated by STGF run with IQDT=200 and IPRKM=4, following a normal
          STG1/STG2/STG3 run with RELOP=’MVD’. Default.
      = 1 read previously generated (IMODE=0) jK/ic data and calculate collision
          strengths on a fine energy mesh (input via namelist /MESH1/ as STGF).
      =-1 single pass operation combining IMODE=0 and 1 without any disk I/O
          other than reading the STGF generated datafiles and writing to OMEGA.

ITCC = 0 pure jK-coupling.
     = 1 intermediate coupling (default) requires
         TCCDW.DAT from STG1/STG2/STGJK run with RELOP=’TCC’ and IDWOUT=2.

IBIGE = 0 default, does nothing.
```

```
      = 1 read LS dipole line strengths (generated by STGF with IBIGE=1) to
          append infinite energy scaled collision strength to the file OMEGA.

INOEXCH = 0 default, does nothing.
        = 1 non-exchange run, supplementing prior exchange run. Use IMODE=0,
            since no resonances present, only the coarse energy mesh is needed.
            Expects JMNTWO to be set, discussed next.

JMNTWO = twice the minimum value of J (total) to be included in the non-
         exchange run, following on from the last J of the exchange run.
       = -1 default, but must be set if INOEXCH=1.

LRGLAM = -1 default, does nothing.
       >= 0 applies Burgess dipole top-up at 2*J=2*LRGL2=LRGLAM.
          Normally, just set LRGLAM=999 (say) to top-up as code resets it to
          the largest appropriate 2*J-value available.
          In addition, the non-dipole transitions are topped-up assuming a
          geometric series.


Example: Single (stgicf) pass in the resonance region.

STGF data

 &STGF  IQDT=2 IMESH=1 PERT='YES' IPRKM=4 &END
 &MESH1 MXE=101 E0=.01 EINCR=.00025 &END

STGICF data

C  This line is for comments
 &STGIC ITCC=1 IMODE=-1 INOEXCH=0 &END
 &MESH1 MXE=2001 E0=0.01 EINCR=0.0000125 &END



See also the file stgicfadas.txt which gives a step-by-step guide to the
practical usage of stgicf.


                    ooooooooooooooooooooooooooooo

BOUND
*****
Read the H.DAT file generated by STG3 and calculate bound-state
eigen-energies and eigen-vectors for the (N+1)-electron ion.

                          oooooooooooooooooo


STGB: Seaton's perturbative treatment of the long-range coupling potentials.
****  Now extended to handle (electron+) neutrals.

Local executable stgb.x

STGB Input
----------

Namelist STGB

IPRINT defines the print level, 0  is the lowest and 3 the highest.

IPERT = 0 (default) Neglect long-range coupling potentials.
      = 1 Include long-range coupling potentials, not normally necessary.

IOPT2 = 1 (default) Scan for bound states.
```

```
      = 2 Read estimates of bound-state energy.

IRAD = 0 (default) Bound state energies only.
     = 1 Write e-vectors to Bnm files for photoionization.
```

Then read (2S+1) L p or 0 2J p and scan range and step in terms of effective quantum number or energy estimates, depending on IOPT2. Terminate with -1 -1 -1.

Example: Fe25+

```
 &STGB IOPT2=1 IRAD=1 IPERT=0 IPRINT=0 &END
 0 0 1
0.5 5.5 0.025
 0 0 0
0.5 5.5 0.025
 0 2 1
0.5 5.5 0.025
 0 2 0
0.5 5.5 0.025
 0 4 1
0.5 5.5 0.025
 0 4 0
0.5 5.5 0.025
-1 -1 -1
```

ooooooooooooooooooooooooooooo

BOUND-FREE
****

Read the Dnm files generated by STG3, Bnm by STGB and Fnm by STGF and then calculate photoionization cross sections. Run PREBF first then STGBF.

oooooooooooooooooo

STGBF: Seaton’s perturbative treatment of the long-range coupling potentials.
***** Now extended to handle (electron+) neutrals.

Local executables prebf.x, stgbf.x

PREBF Input

Namelist PREBF

```
IPRINT = 0 Default.
         1 For more detailed printout

IBUT = 0 Default, no Buttle correction to orbital.
       1 Orbital Buttle correction included.
```

WARNING: This simple input relies on the end-of-file to terminate gracefully so do NOT leave or insert any extra lines of data besides this NAMELIST PREBF else an attempt to read it will result in almost certain failure (if you are lucky, if unlucky.....)

STGBF Input

Namelist STGBF

IPRINT=-2   Cross section for leaving the residual

```
               ion in each of the target states, use for DR/RR.
       -1      No printing of cross sections, levels
               above ionization limit skipped. Used for production runS,
        0      Total cross sections to a final SLP (default).
        1      Files opened, qdt onset.
        2      Partial cross section to each channel.
        3      Beta and x-sectn to each target state.

IBUT = 0 Default, no Buttle correction to orbital.
       1 Orbital Buttle correction included.

If STGF has been run in MQDT mode (IQDT=1 or 2) then also

MXE, E0, EINCR - meaning as per STGF - but now to define a new fine mesh.

EWIDTH > 0.0 Preconvolute TOTAL photoionization/recombination data with
              this (z-scaled) width.

WARNING: This simple input relies on the end-of-file to terminate gracefully
         so do NOT leave or insert any extra lines of data besides this
         NAMELIST STGBF else an attempt to read it will result in almost
         certain failure (if you are lucky, if unlucky.....)

                    ooooooooooooooooooooooooooooo

BOUND-BOUND
***********
Read the Dnm files generated by STG3 and Bnm by STGB and then calculate
radiative data.

                          oooooooooooooooooo


STGBB: For positive ions only, Seaton’s perturbative treatment of the long-range
*****  coupling potentials.

Local executables stgbb.x

STGBB Input
-----------

Namelist STGBB

IPRINT =-1 Default, write f-values to file FVALUE,
         1 and write line strengths to UNIT6 as well,
         0 and write f-values to UNIT6 as well.

IBUT = 0 Default, no Buttle correction to orbital.
       1 Orbital Buttle correction included.

Then read pairs of terms (2S+1) L p or levels 0 2J p for which radiative
data is required. Terminate with -1 -1 -1 -1 -1 -1, or end-of-file.

             ooooooooooooooooooooooooooooooooooooooooooo


RADIATION + AUGER DAMPING
*************************
Read the H.DAT and Dnm files generated by STG3 and Bnm by STGB.

                          oooooooooooooooooo

STGFDAMP: A radiation+Auger damped version of STGF. Note, Type-I damping only
********* can be obtained from STGF with IRDEC=1 (and NDRMET>0 for OMEGDR).
```

Local executable stgfdamp.x

STGFDAMP Input

Namelist STGF

All variables present in STGF plus switches to turn radiation+Auger damping on (=1) or off (=0).

```
NTYP1   = 1 (Core electron) radiation damping to non-STGB states, default.

NTYP2I  = 1 In-the-box damping to STGB states, default.
            Requires dipole matrices to these states as in a normal (undamped)
            photoionization calculation with STGBF i.e. RAD='YES' in stg1/2/3

NTYP2OR = 1 Outer electron radiative stabilization to non-STGB states, default.

NTYP2OF = 1 Radiative recombination to non-STGB states.
        =-1 Not set. Default, since NDRMET=0 by default.

NMIN    =   lowest principal quantum number n to apply NTYP2OR/F.
            Default=-1, not set. Attempts to determine it from B00 but if
            NTYP2I=0 (and NTYP2OR/F=1) it must be set by the user.
            It should be 1 greater than the largest stgb n-value.
```

In non-MQDT mode, sufficient recombined states must be generated via STGB so that the in-the-box damping of the omitted states is negligible. Outer region damping is done via a complex energy and theta function.

In MQDT mode, only those final states formed by bound orbitals input from STG1 should be generated via STGB - they have been projected out of the continuum basis. All other final states are taken into account (both inner and outer region damping) via a complex energy in MQDT.

```
NDRMET >0  Determine DR from the first NDRMET metastables, output to OMEGDR.
           Note: this switches on elastic transitions and which are now
           present in the OMEGA file.
       =0  None (default).
```

oooooooooooooooooooo

```
STGICFDAMP: Term-couple (unphysical) LS-coupling damped K/S-matrices to form
**********  intermediate coupled collision strengths, following a STGFDAMP run.
```

Local executable: stgicfdamp.x

STGICFDAMP Input

The first line is used for user comments, then

Namelist STGIC

All input variables from stgicf plus:

```
NTYP1 = 1 Include Type-1 (inner electron) damping (default). Note, Type-2
          (outer-electron) damping would have been included back in the
          stgfdamp run and is built into the now complex K-matrix.

NDRMET> 0  Determine DR from the first NDRMET metastables, output to OMEGDR.
           Note: this switches on elastic transitions and which are now
           present in the OMEGA file.
```

```
      = 0  None (default).

IQDT  = 0  Looks for a K-matrix file from a stgfdamp run. If not found it
           looks for an S-matrix file instead.
      = 1  Look for S-matrix file smtls.dat only and stop if not found.
      = 2  Look for K-matrix file z/kmtls.dat only and stop if not found.

Note extension to INOEXCH variable:

INOEXCH > 0 Read complex K-matrices on zkmtls.dat from a STGFDAMP NX run.
        < 0 Read real K-matrices on kmtls.dat from a STGF NX run.
        = 0 Read complex K-matrices on zkmtls.dat from a STGFDAMP exchange
            run, default.

                          oooooooooooooooooo


STGBF0DAMP: A radiation+Auger damped photoionization code - initial
**********  states MUST be fully contained within the R-matrix box.

Local executable stgbf0damp.x

STGBF0DAMP Input
----------------

Namelist STGF

All variables present in STGFDAMP plus switches to specify the initial
states to photionize from.

IPHOTO = Number of electron continua to photoionize to. Default = 1.
         (Zero gives no photoionization.)

NPISYM = Number of STGB symmetries to photoionize from. Default = 1.
         (Taken in the order they specified in the STGB run.)

NPIEB  = Number of STGB energies per symmetry to photoionize from. Default=1.
         (Taken in the order they were determined in the STGB run.)



                    ooooooooooooooooooooooooooooo


                           Utility Codes
                           *************

ADASEX: Produce ADAS adf04 file (LS-resolved). Minimal input - see code.
******

ADASEXJ: Produce ADAS adf04 file (IC-resolved). Minimal input - see code.
*******

**2ASCI and ASCI2**: Programs to convert files from binary to ASCI and
******************** vice versa. Not the most elegent way to port between
                     machines, but it works...

OMADD: Add two OMEGA files together. Typically a fine meshed exchange one
****** including resonances and a coarse meshed non-exchange. The latter is
       interpolated onto the former. In addition, it can analyse resonance
       resolution and eliminate unresolved resonances. Can also be used to
       compare two OMEGA files - one with top-up and one without and produce
       detailed diagnostics on the top-up contribution, both dipole and
       non-dipole. Default operation (adding) requires no input. See code
       for options for other operations.
```

```
OMGMRG: Merge two OMEGA files, calculated at different energies.
******

OM2OMU, OMU2OM: Convert between formatted and unformated omega files.
***************

OMORDER: Re-order and/or reduce target states and associated omegas.
********

XTRCT: Simple interactive code to extract a collision strength for an
****** input transition, at all energies, from an OMEGA file - suitable
       for viewing with GNUPLOT.
       See the code for particular form of desired I/O.

STGG: Graphics program for R-matrix omega file.
****

 Local executable stgg.x

 STGG Input
 ----------

 Although there are many options, you can infact get a sensible plot without
 setting any of them at all. Only the most commonly used parameters are
 described below, see the beginning of the source code stgg.f for them all.

 Namelist STGG

 NGRAPH -- number of transitions to be graphed
           > 0 collision strengths
           < 0 cross sections
 EWIDTH --  convolute with a Gaussian of width EWIDTH, if > 0.
 UNITS -- 1.0 for Ry or 13.606 for eV
 NPUB -- set equal to 1 to get publication quality graph
 NPLOT -- plot this transition number only
 ESCL -- energy scale interval for plot in UNITS (see below also).
 EMN -- minimum energy for plot in UNITS, relative to ENAT(1).
        maybe increased internally if ESCL=0.
 EMX -- maximum energy for plot in UNITS, relative to ENAT(1).
        maybe decreased internally if ESCL=0.
***NOTE: transitions from excited-states have energies relative to
         ENAT(i) not ENAT(1). to get "nice" EMN & EMX here set
         ESCL.lt.0, the input EMN & EMX are then assumed to be
         relative to ENAT(i) (i.e. fixed) so will only be "nice"
         for that particular ENAT(i).
 SSCL -- cross section scale interval (see below also).
 SGMN -- minimum collision strength or cross section in Mb for plot.
         if SSCL=0, SGMN maybe decreased internally.
 SGMX -- maximum collision strength or cross section in Mb for plot.
         if SSCL=0, SGMX maybe increased internally.
 YMULT -- if an omega is greater than a factor YMULT larger than
          the ones one energy step lower & higher, reset to the
          smaller one. default 1.0e24 - no reset.


OOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOO


                              Distorted-Wave
                              **************

LS
**
The LS distorted-wave code (local executable stgdwls.x, run after stg1r.x and
```

stg2r.x) reads target eigen-energies and eigen-vectors from a file MIXDW.DAT and collision algebra from a file ALGDWU.DAT, both written by STG2 of the EXCHANGE codes, FOR ALL L. It then evaluates continuum distorted-waves and continuum-continuum (reactance) matrix elements and writes collision strengths in the standard form to the file OMEGDW. Note, for large cases the local executable stg2rdw.x should be used in place of stg2r.x.

STG1 Input

In namelist STG1A, specify

```
IDWOUT= 0 (default) for CC only.
      = 1 for CC and DW.
      = 2 for DW only, recommended (fast).
```

All other variables are as before (see 1.). However, if IDWOUT=2, only MAXLA needs to be specified and the other variables are ignored.

Example: N,

```
S.S.
 &STG1A IDWOUT=2  &END
 &STG1B MAXLA=4  &END
```

STG2 Input

In namelist STG2A, IDWOUT, same meaning as above, is specified along with ISORT which is discussed below.

In namelist STG2B, in addition to the variables descibed above (see 1.) for STG2 input, NMETA and (optionally) IMETA(N) are specified where,

NMETA is the number of (initial) metastables (including the ground) from which collision data is required. If

```
ISORT= 0 the first NMETA target terms listed (see 1.) are the metastables. This
         is only useful if the terms are energy-ordered, which is inefficient
         for large cases.
     =-1 the NMETA metastables are defined by IMETA(N)=1 where N is the position
         in the input term list, which maybe symmetry or energy-ordered.
     = 1 the term list is sorted into symmetry-order and the lowest energy term
         of the first NMETA symmetry groups is taken to be metastable. This
         can be overridden by IMETA(N)=1 where N is the term position in the
         SORTED list. HOWEVER, the term list is expanded to explicitly include
         all correlation terms of the same symmetry that were in the original
         term list.
```

The specification of the N-electron configurations and term list follows as before (see 1.).

BUT, there is NO specification of (N+1)-electrons configurations since the Distorted-Wave code uses non-orthogonal continuum orbitals and evaluates exchange-overlap integrals instead. This is important if you use INAST>0 since the (N+1)-electron SLp symmetries now follow directly the target terms. If INAST=0 then nothing is read after the target terms and the above discussion can be ignored.

```
LNOEX = the highest L for which all exchange multipoles are calculated.
        Default = 10.
```

Example: (partial) N,

S.S.

```
 &STG2A IDWOUT=2 ISORT=-1 &END
 &STG2B  MAXORB=6 NELC=7 NAST=34 NMETA=3 IMETA(1)=1 IMETA(3)=1 IMETA(6)=1
    INAST=0 MINLT=0 MAXLT=8 MINST=1 MAXST=5  &END
 1 0 2 0 2 1 3 0 3 1 3 2
 6
  2   0   2   0   0   0
  2   2   5   1   1   1
  2   2   3   0   0   0    0
  2   1   4   0   0   0    0
  2   0   5   0   0   0    0
  2   2   2   1   0   0    0
  2   2   2   0   1   0    0
  2   2   2   0   0   1    0
  4 0 1
  4 0 1
  2 2 1
  2 2 1
  2 2 1
  2 1 1
  2 1 1
  2 1 1
  2 1 1
  2 1 1
  4 1 0
  4 1 0
  4 1 0
  2 1 0
  2 1 0
  2 1 0
  2 1 0
  2 0 1
.
.
.
.
etc.
```

```
STGDW Input
-----------
In namelist STGDW, specify

INAST = the number of SLp symmetries. The first INAST symmetries generated in
        STG2 are included, see also LTOP and LCUT below for alternative ways to
        read a subset of the collision algebra.
        Default = 999, all symmetries present.

MXE = the number of user supplied UNSCALED energies in Rydbergs relative to the
      ground state which are read free-formatted after this namelist.
      MUST be specified > 0.

NMETA <= the number of metastables specified in STG2, the first NMETA STG2
         metastables are used.
         Default = the value of NMETA specified in STG2.

NAST = Number of observed energies (Ry) to be read AFTER the MXE scattering
       energies, relative to the ground and in the same order as listed
       in the STG2 data (or in the MIXDW.DAT file). Default = 0, none.

ELAS='NO' (default) no elastic data calculated.
    ='YES', elastic collision strengths calculated and written to file OMEGDW.

IPERT = 0 neglect contribution from long-range integrals outside of
          the atom - similar in spirit to PERT in the STGF outer-region code.
      = 1 (default) include full long-range contribution. See LRANGE next:
```

LRANGE = 0 (default) evaluate long-range integrals (if IPERT=1) to the end of the continuum mesh.
       = 1 Add-in the contribution from beyond the end of the mesh, particularly slow for a small mesh, elsewise just slow.

IPRTM defines the print level, -1 the lowest and +1 the highest. Default=0.

LTOP = Highest total L for which explicit data is to be used. The contribution from LTOP+1 to Infinity is then calculated assuming a geometric series in L.
Default LTOP=999, no "top-up".

LCUT = Exclude contribution from L>LCUT. Only useful if "top-up" (LTOP) is not used since specification of LTOP imposes an LCUT in practice.
Default = 999, no cut.

NTHRSH = 0 (default) use only the input MXE energies.
       = 1 calculate every threshold collision strength. This can be useful for ions since we tend to use a very coarse energy mesh, the collision strengths can be splined subsequently.
DO NOT USE FOR NEUTRALS since you know already that the collision strength is zero then.

LNOEX = Highest L for which exchange is included (if indeed present). Much better to use LNOEX in STG2 to save calculating and writing it in the first place.
Default = 999, all exchange present included.

IDFOT = 0 Default.
      = 1 Reserved output for differential code not discussed here.
      = 2 Reserved output for differential code not discussed here.
      = 3 Write reactance (K-) matrix elements to ’rmtls’ for STGDWIC.

NUNIT = 0 Default. Non-unitarized. Fast.
      = 1 Unitarized. requires NMETA=NAST in STG2. Slow.

Example: N,

```
 &STGDW  INAST=54 MXE=5 NTHRSH=0 NMETA=3 ELAS='YES' IPERT=0 IPRTM=-1 LTOP=8 &END
1.0
1.5
2.0
3.0
4.0
```

Note, INAST=54 corresponds to the number of symmetries generated by the STG2 specification MINLT=0 MAXLT=8 MINST=1 MAXST=5 (both parities).

The same results could have been obtained with a reduced namelist viz.

```
  &STGDW MXE=5 ELAS='YES' LTOP=8  &END
```

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IC
**

The IC distorted-wave code (local executable stgdwic.x) again reads MIXDW.DAT as well as term coupling coefficients from TCCDW.DAT and reactance matrix elements, newly generated by STGDW, from the file ’RMTLS.DAT’.
The TCC’s are generated most efficiently for a DW-only run by setting IDWOUT=2 and RELOP=’TCC’ when running through STG1, STG2 and STGJK, see 2.
Note, this is a separate run from that which generated the LS collision algebra.

```
STGDWIC Input
-------------
To be done


                    ooooooooooooooooooooooooooooo


GRAPHICS: The R-matrix graphics program STGG (executable stgg.x) can be used
********  to generate simple DW plots, although it is geared-up to handling a
          dense energy mesh of resonant collision strengths. Do not try and
          convolute with a Gaussian. Note, you must move 'OMEGDW' to 'OMEGA'
          if no R-matrix OMEGA file exists.

OOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOO
```

-

1a. An overview of the ADAS Project

- A little history
- An integrated approach to modelling radiating properties of plasmas
- The Atomic Data and Analysis Structure

JET and ADAS

- The commitment to atomic physics at JET.
- Theoretical atomic physics based in the experimental spectroscopy division
- Data centralisation for modelling and analysis
- Responsibility to EURATOM partners
- Access to JET atomic data

The establishment of the ADAS Project

- Theoretical atomic physics support commenced at JET - 1984
- Centralised atomic data and coding under EDII, JET - 1985
- First IBM/TSO interactive ADAS release - 1989
- UNIX conversion preparatory study - 1993
- Start of ADAS project managed by Strathclyde University - 1993
- ADAS UNIX/IDL conversion - 1993/95
- 1st ADAS annual Workshop - 1995
- Start of ADAS project on going maintenance - 1996
- First non-voting university members (TUV) - 1997

The ADAS Project

- Project, self-funded by participants

Participant organisation	Contact
JET Facility/UKAEA Culham Laboratory	K-D Zastrow
IPP-Garching, Germany	K. H. Behringer
KFA-Juelich, Germany	P. Mertens
Oak Ridge-Atom. Data Centre, USA	D. Schultz
Rutherford-Appleton Laboratory, UK	J. Lang
RFX Padua, Italy	M. Valisa
CEA Cadarache, France	R. Guirlet
KTH Stockholm, Sweden	E. Rachlew-Kallne
General Atomics, DIIID, USA	T. Evans
Observatory of Catania, Italy	A. Lanzafame
JAEA, JT60, Japan	H. Kubo
NIFS, LHD, Japan	I. Murakami
CRPP Lausanne, Switzerland	B. Duval
University of Wisconsin, USA	D. den Hartog
University of Toronto, Canada	P. Stangeby
Fraunhofer Institute for Laser Technik/Philips Research Labs, Aachen	T. Kruechen
Auburn University, USA	M. Pindzola
IPR, Gadhinagar, India	P. Vasu
SWIP, Chengdu, China	X. Duan
Birla Institute, Jaipur, India	R. Prakash
FOM Rijnhuizen, Netherlands	M. von Hellermann
Armagh Observatory, Armagh, Northern Ireland	G. Doyle
Kurchatov Institute, Moscow, Russia	A. Tugarinnov
Princeton University	D. McCune
ITER	R. Pitts
IAEA, Vienna, Austria (in process)	R. Clark/B. Braams
University of Strathclyde	H. P. Summers

ADAS-EU

- European Framework 7: support action – provided by the University of Strathclyde.
- Commenced 1 Jan 2009 for four years.
- Provide atomic physics support for fusion associated laboratories throughout Europe.
- Main themes: heavy species, charge exchange spectroscopy, beam emission spectroscopy, hydrogen molecules, special features
- On-site ADAS-EU staff at selected main European laboratories.
- Sponsorship of an annual ADAS training course.

Targets of ADAS

- Fusion Plasma
  - » Bulk plasma
  - » Edge divertor plasma
  - » Beam penetrated plasma

- Astrophysical Plasma
  - » Spectral emission from the solar atmosphere
  - » X-ray emission from cometary and planetary atmospheres
  - » VUV, XUV and X-ray line emission from gas clouds and other hot cosmic sources

Objectives of integrated atomic modelling

- Separating the local atomic tasks
- Provision of derived data close-linked to experimental spectroscopic data reduction
- Provision of consistent source function inputs to theoretical plasma modelling
- Central management of atomic data

Collisional radiative modelling

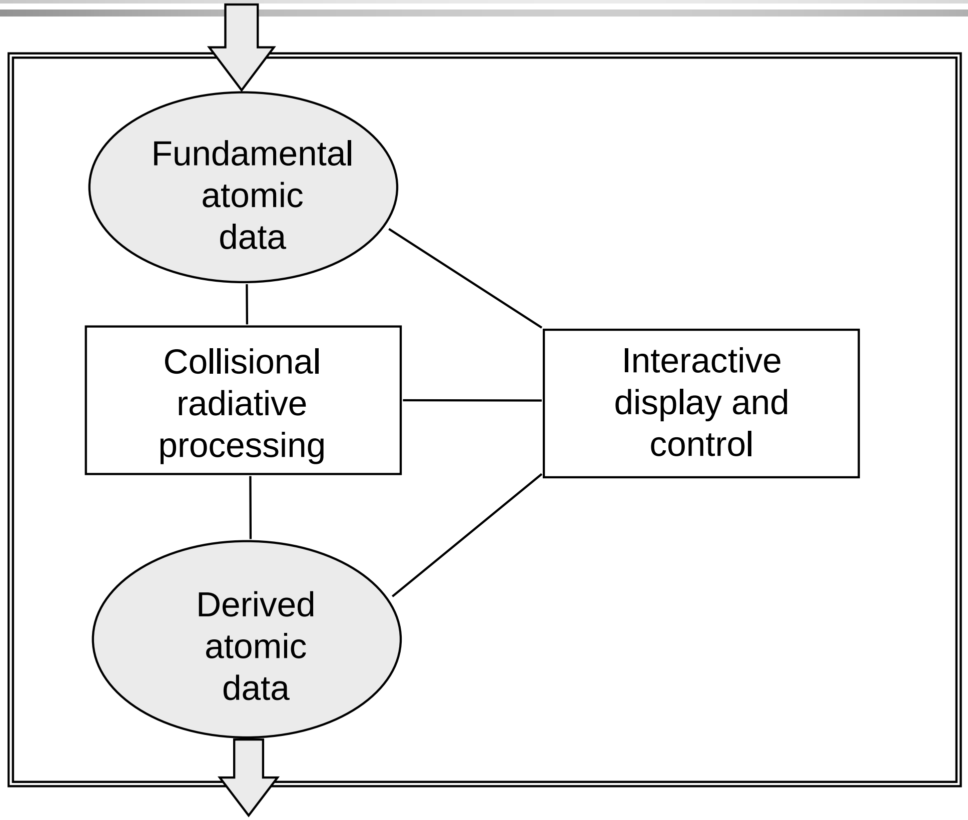
- Fundamental and derived atomic data
  - » Finite density plasma

- Atomic time constants
  - » Dynamic and quasi-static separation

- Local and non-local properties
  - » Features and superfeatures

- ADAS uses generalised collisional-radiative modelling

ADAS modelling schematic



Fundamental atomic data

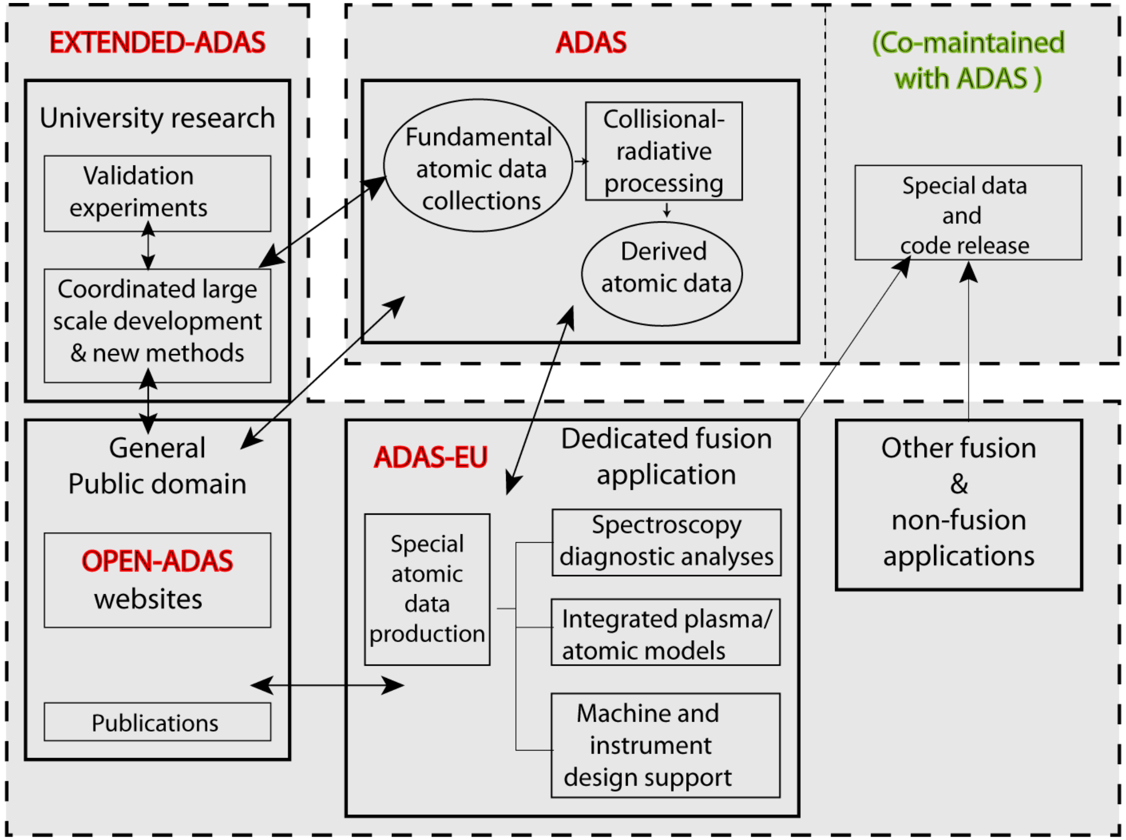
Collisional radiative processing

Interactive display and control

Derived atomic data

models and experiment analysis

The ADAS family and relationships



EXTENDED-ADAS

University research

Validation experiments

Coordinated large scale development & new methods

ADAS

Fundamental atomic data collections

Collisional-radiative processing

Derived atomic data

(Co-maintained with ADAS)

Special data and code release

General Public domain

OPEN-ADAS websites

Publications

ADAS-EU

Dedicated fusion application

Special atomic data production

Spectroscopy diagnostic analyses

Integrated plasma/ atomic models

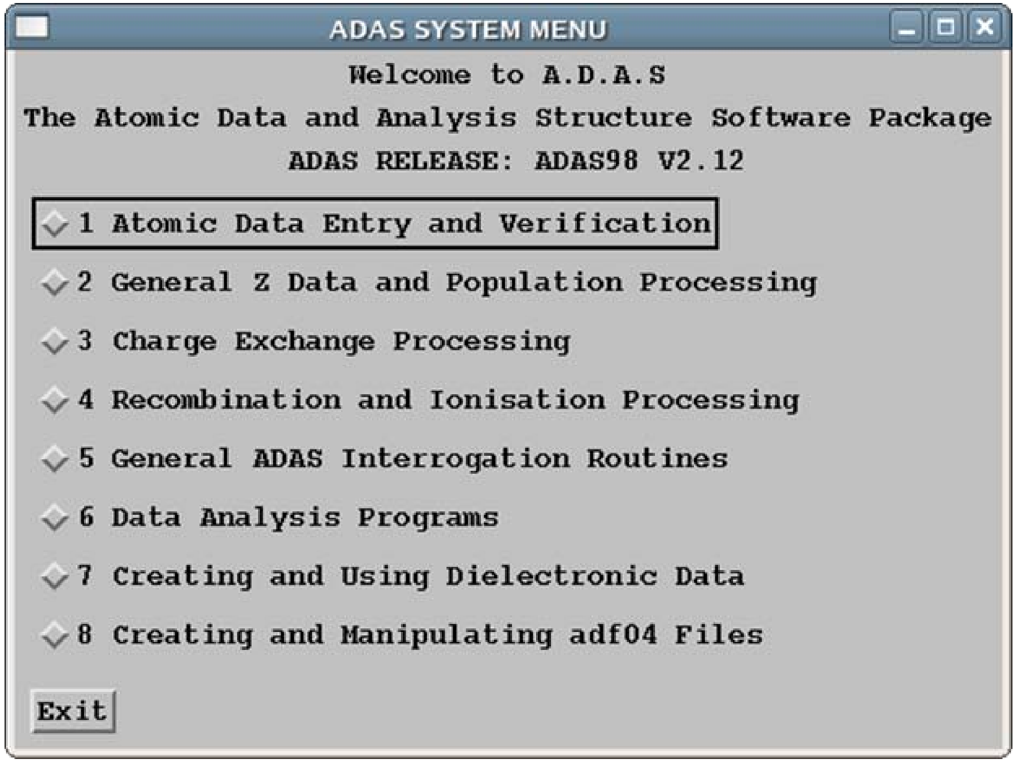
Machine and instrument design support

Other fusion & non-fusion applications

ADAS

- The interactive user interface
    - » ADAS series
- The fundamental and derived databases
    - » ADAS data formats
- The application interface
    - » ADAS Fortran and IDL subroutine libraries
- Offline-ADAS
- Documentation

ADAS main menu



Welcome to A.D.A.S

The Atomic Data and Analysis Structure Software Package

ADAS RELEASE: ADAS98 V2.12

1b. Computational overview of ADAS

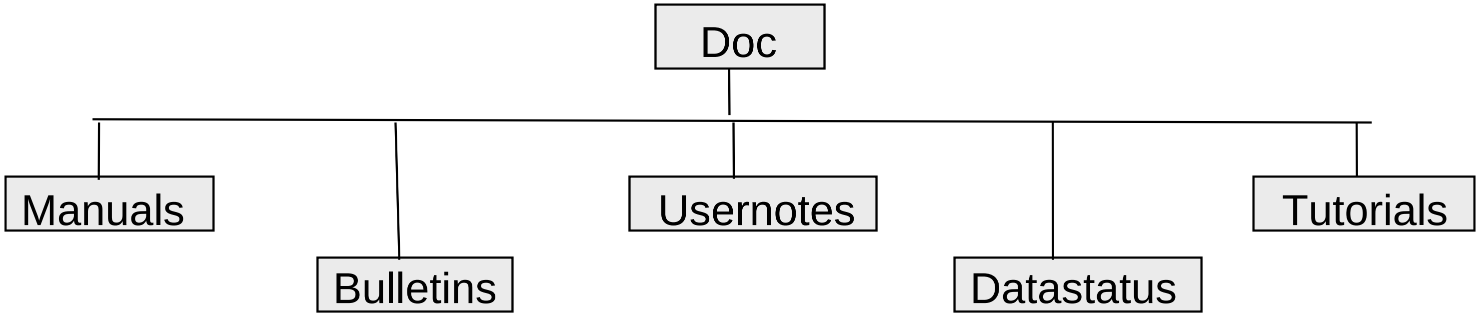
- Introduction
  - » Supported systems and language details
  - » Overall organization
- Initial setup of ADAS
  - » Establishing the local IDL/ADAS environment
  - » Standard user space organization and setup
- Some components of ADAS
  - » The code part of ADAS
  - » The database and adf numbers
  - » The documentation
- Learning to use ADAS online
  - » ADAS501
  - » using common widgets

ADAS

- The interactive user interface
  - » ADAS series
- The fundamental and derived databases
  - » ADAS data formats
- The application interface
  - » Large ADAS FORTRAN and IDL subroutine libraries
  - » Small C, MATLAB and PERL libraries
- Offline-ADAS
- Documentation

Documentation

- Documentation is accessible on the world-wide-web
  - » *http://www.adas.ac.uk*
  - » Also present on all local ADAS work-stations
  - » */<path>/adas/doc/*
- The main user manual - ver 2.5.6 - is in
  - » */<path>/adas/doc/manual/*



Doc

Manuals

Bulletins

Usernotes

Datastatus

Tutorials

ADAS series

Interactive codes are grouped in series. Currently ~ 85 codes.

- Atomic data entry and verification
- Population processing
- Charge exchange processing
- Recombination, ionisation processing
- General interrogation programs
- Data analysis and spectral fitting
- Creating and using dielectronic data
- Structure and excitation calculations

ADAS code disposition

- The codes and sub-routines (>1000) are organised hierarchically and maintained under SCCS in
  - »
```
/<path>/adas/idl          /adaslib
                          /adas1xx      /adaslib
                                        /adas101
                                         . . .
                          /adas2xx      /adaslib
                                        /adas201
                           . . .
             /fortran     /adaslib
                          /adas1xx      /adaslib
                                        /adas101
                                         . . .
```
- Source IDL code is open, but FORTRAN code is restricted. FORTRAN shared object module libraries are available to user codes.
  - »
```
/<path>/adas/lib /libadaslib.a
                 /libadas1xx.a
                  . . .
```

Database

- Fundamental and derived data. Currently ~ 6 Gbyte.
- The various classes of ADAS data have precisely specified organisation called ADAS data formats or ‘ADFs’ for short (eg. *ADF14*). There are ~ 56 different classes.
- Some key ADF’s for fusion application
  - » *ADF04* : specific ion data
  - » *ADF11* : coll.-rad. ionis. & recom. coefficients.
  - » *ADF13* : ionisation per photon ratios
  - » *ADF15* : emissivity coefficients
  - » ADF40 : envelope feature photon emiss. coefficients.

ADAS data disposition

- The data are organised by data format and maintained under CVS in
  - »

```
/<path>/adas/adas      /adf01   /<sub-dir1>
                                /<sub-dir2>
                                 . . .
                       /adf02   /<sub-dir1>
                                /<sub-dir2>
                                 . . .
```

- Sub-directory naming is not standardised but
  - » All final data sets have the extension ‘*.dat*’
  - » Year numbers are frequently used. In ADAS directories, year numbers mark the introduction of a method. It does not necessarily mean year of calculation.
  - » Preferred data is often distinguished by the name ‘*adas’.* Initials may be used to identify a particular data compiler.
  - » All data sets must have a final comment block identifying at minimum the producer, date and updates

The interactive ADAS user

- An ADAS user requires a UID on a work- station with access to the ADAS and IDL servers.
- ADAS expects a number of directories to be present in the user file space, including
    - » The ‘defaults’ directory which remembers the settings and values from the previous use of each code

      /<path>/<UID>/adas/defaults
    - » The ‘pass’ directory to which ADAS created data sets are routed

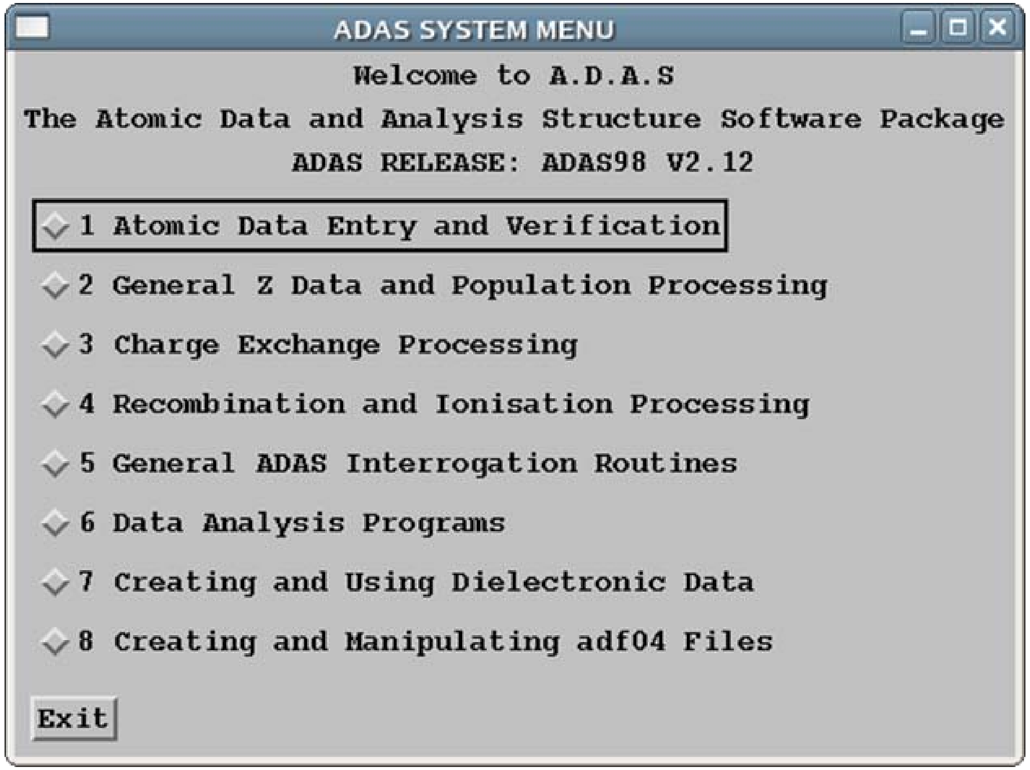
      /<path>/<UID>/adas/pass
- A start-up script is available to set pathways, environments and directories required by the ADAS user.
- It is helpful to maintain data sets in structures matching central ADAS as

  /<path>/<UID>/adas/adf01/…/

ADAS on-line

- Move to your '*/pass*' directory.
- Initiate ADAS on a unix workstation or a linux personal computer by typing '*adas'.*
- An interactive session begins starting with program selection from menus
- Each program interacts with the user via a variety of screens, normally including 'input', 'processing' and 'output' screens.

ADAS main menu

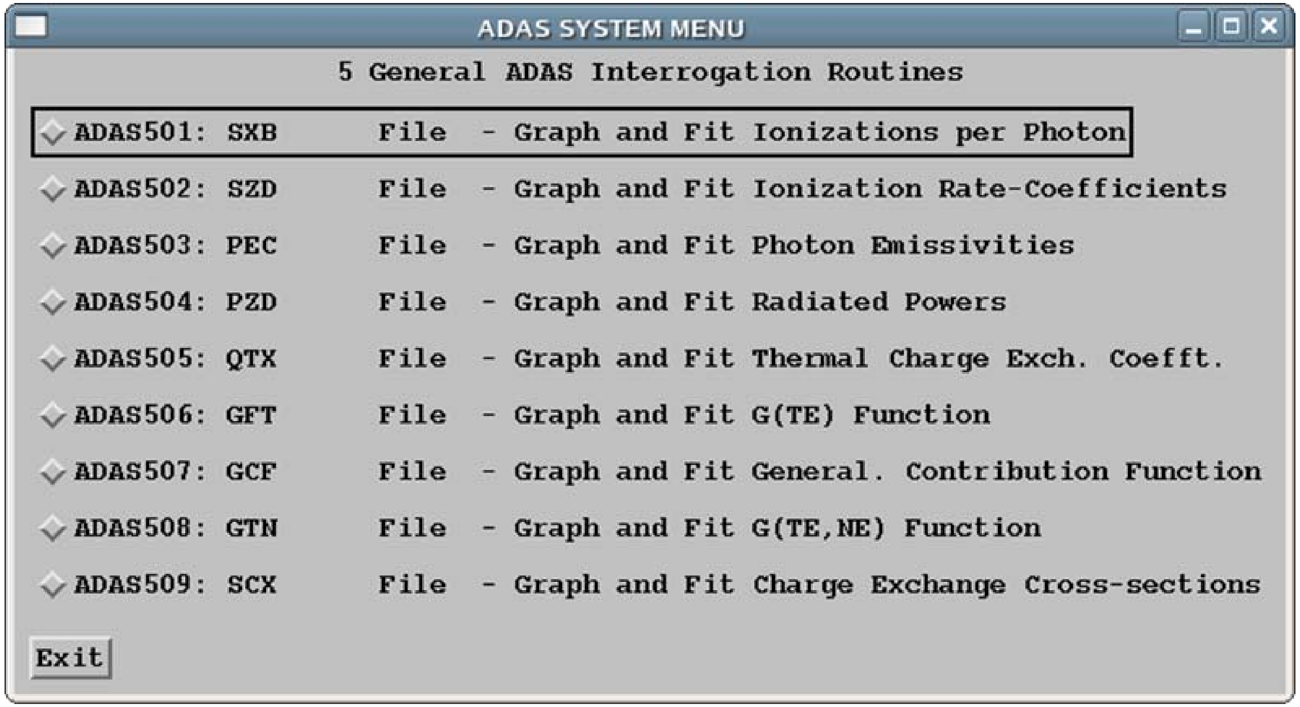


Welcome to A.D.A.S

The Atomic Data and Analysis Structure Software Package

ADAS RELEASE: ADAS98 V2.12

ADAS series 5 menu



ADAS SYSTEM MENU

5 General ADAS Interrogation Routines

◇ ADAS501: SXB File - Graph and Fit Ionizations per Photon
◇ ADAS502: SZD File - Graph and Fit Ionization Rate-Coefficients
◇ ADAS503: PEC File - Graph and Fit Photon Emissivities
◇ ADAS504: PZD File - Graph and Fit Radiated Powers
◇ ADAS505: QTX File - Graph and Fit Thermal Charge Exch. Coefft.
◇ ADAS506: GFT File - Graph and Fit G(TE) Function
◇ ADAS507: GCF File - Graph and Fit General. Contribution Function
◇ ADAS508: GTN File - Graph and Fit G(TE,NE) Function
◇ ADAS509: SCX File - Graph and Fit Charge Exchange Cross-sections

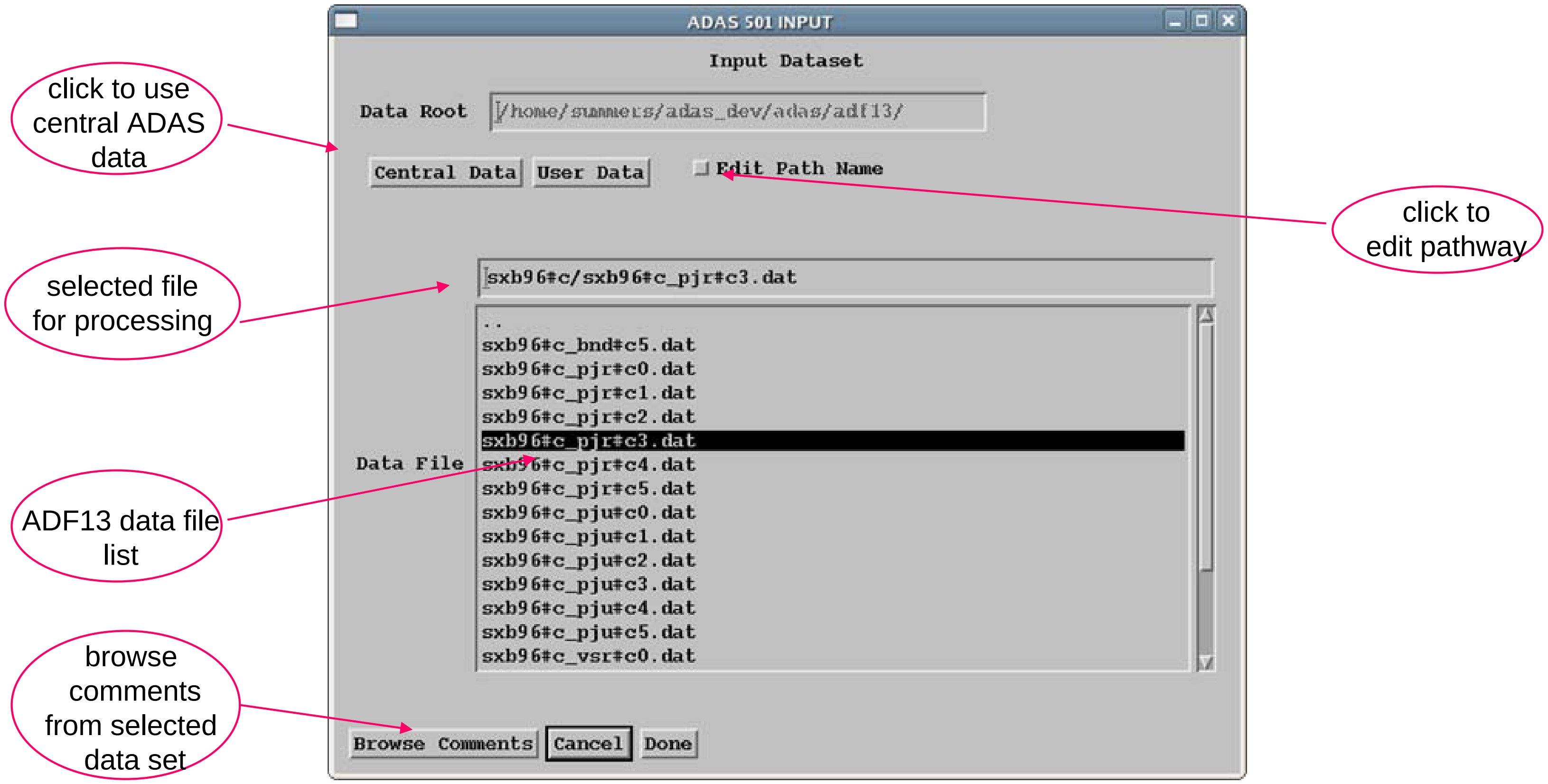
ADAS501 - a typical interrogation code

- Datasets of class ADF13 contain ionisation per photon ratios (SXB data) as a function of Te and Ne.
- The code ADAS501 interrogates ADF13 data sets at a temperature/density model of your choice.
- ADAS501 has a standard sequential three screen structure, namely *file selection*, *processing options* & *output options* screens

ADAS501 (contd.)

- File selection
  - » The path to central ADAS data of the correct class (*ADF13*) is selected by button press.
  - » A display screen shows available files which are selected by clicking on them.
  - » Files have the *.dat* extension otherwise they are directories.
  - » *Done* means go to next screen, *Cancel* means return to the previous screen.
  - » On many screens there is a small ikon button along side *Cancel* allowing *Exit and Return to Menu*.

ADAS501 input



Data Root /home/summers/adas_dev/adas/adf13/

sxb96#c/sxb96#c_pjr#c3.dat

Data File

```
..
sxb96#c_bnd#c5.dat
sxb96#c_pjr#c0.dat
sxb96#c_pjr#c1.dat
sxb96#c_pjr#c2.dat
sxb96#c_pjr#c3.dat
sxb96#c_pjr#c4.dat
sxb96#c_pjr#c5.dat
sxb96#c_pju#c0.dat
sxb96#c_pju#c1.dat
sxb96#c_pju#c2.dat
sxb96#c_pju#c3.dat
sxb96#c_pju#c4.dat
sxb96#c_pju#c5.dat
sxb96#c_vsr#c0.dat
```

click to use central ADAS data

click to edit pathway

selected file for processing

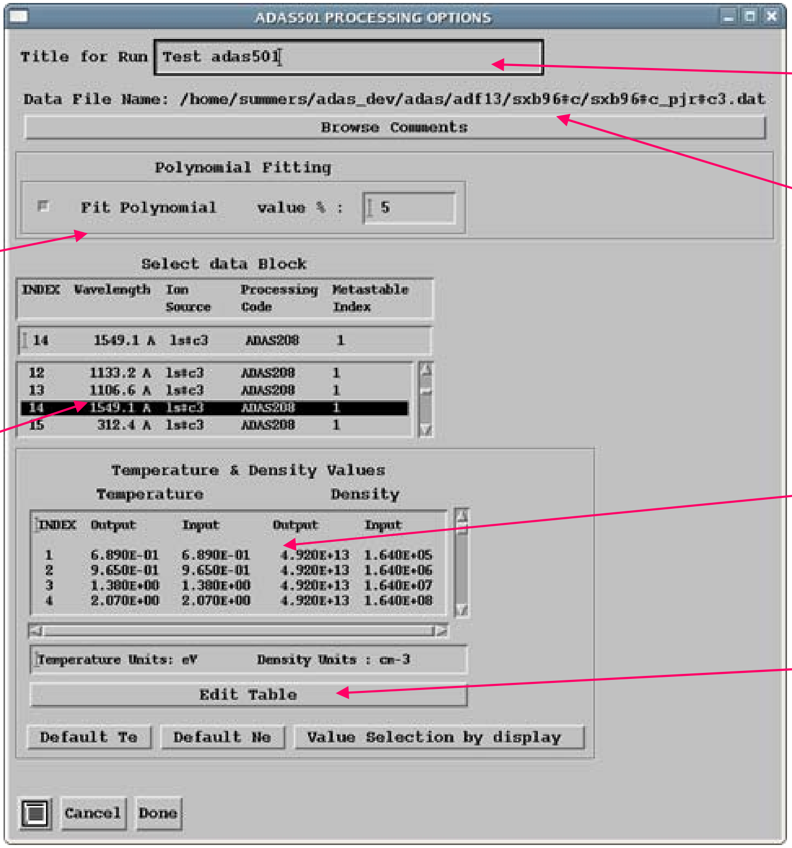
ADF13 data file list

browse comments from selected data set

ADAS501 (contd.)

- Processing options
  - » First select the spectrum line required.
  - » Then the choice of temperature and density pairs must be entered.
  - » The ‘Table Editor’ widget is activated by button press to allow this.
  - » Using the editor takes a little practice.
  - » An advanced graphical method for Te/Ne pair selection may be used

ADAS501 Processing



Title for Run: Test adas501

Data File Name: /home/summers/adas_dev/adas/adf13/sxb96#c/sxb96#c_pjr#c3.dat

Polynomial Fitting

☐ Fit Polynomial value % : 5

Select data Block

INDEX	Wavelength	Ion Source	Processing Code	Metastable Index
14	1549.1 A	ls#c3	ADAS208	1
12	1133.2 A	ls#c3	ADAS208	1
13	1106.6 A	ls#c3	ADAS208	1
14	1549.1 A	ls#c3	ADAS208	1
15	312.4 A	ls#c3	ADAS208	1

Temperature & Density Values

	Temperature		Density	
INDEX	Output	Input	Output	Input
1	6.890E-01	6.890E-01	4.920E+13	1.640E+05
2	9.650E-01	9.650E-01	4.920E+13	1.640E+06
3	1.380E+00	1.380E+00	4.920E+13	1.640E+07
4	2.070E+00	2.070E+00	4.920E+13	1.640E+08

Temperature Units: eV Density Units : cm-3

your title
to appear on
graphs & tables

selected
data set

make
polynomial
fit to data

select line
for analysis

enter
Te/Ne pairs
for output

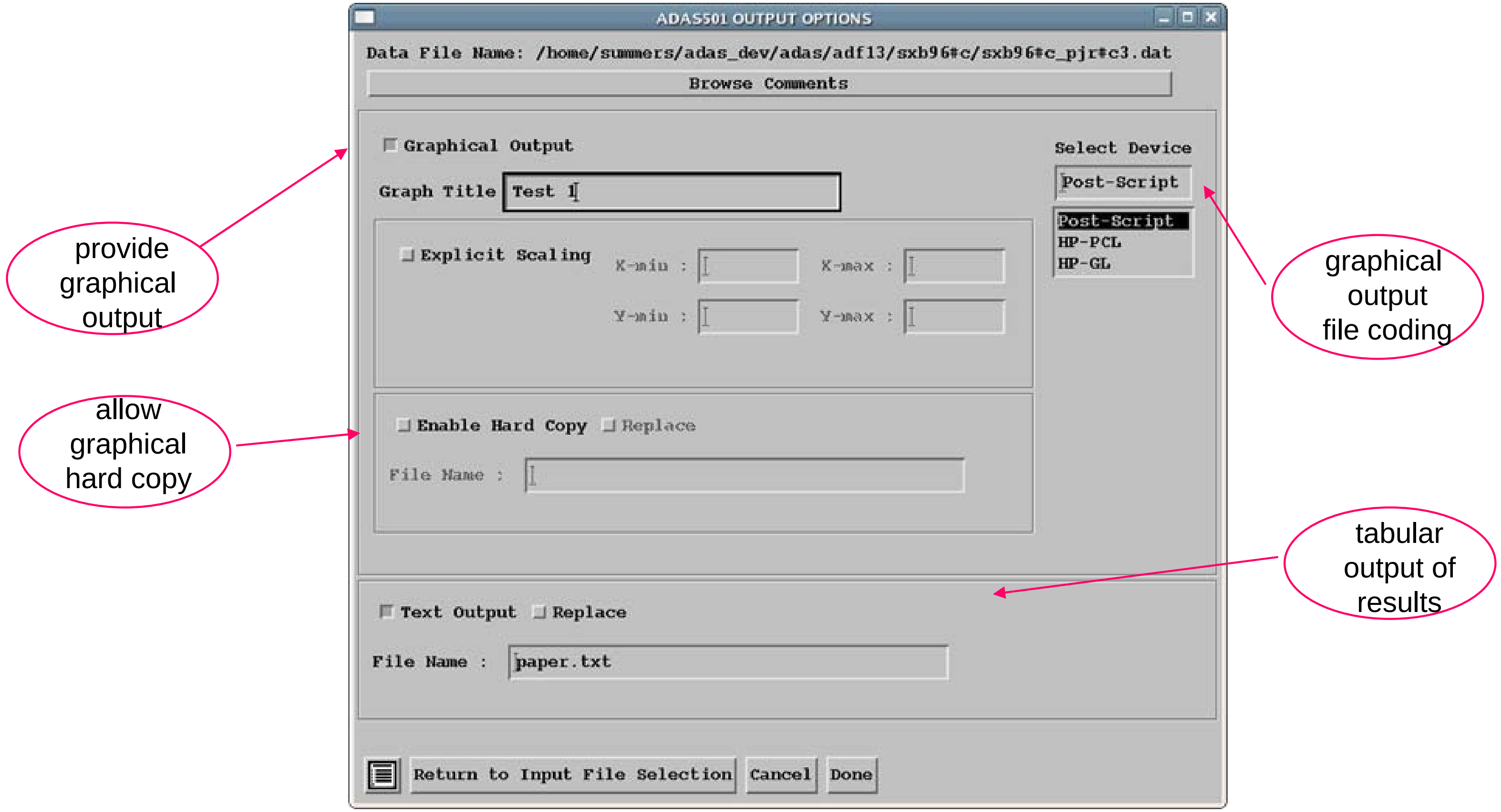
edit table

set default
output values

ADAS501 (contd.)

- Output options
  - » Graphical display is of SXB as a function of temperature at temp/density pairs.
  - » Graphical hard copy and a listing summary of the extracted and fitted data are available.
  - » Automatic or explicit scaling may be chosen.
  - » The displayed graph can be adjusted and/or retained by further controls.
  - » Retain and Adjust require a little practice.

ADAS501 Output



Data File Name: /home/summers/adas_dev/adas/adf13/sxb96#c/sxb96#c_pjr#c3.dat

☐ Graphical Output

Graph Title Test 1

☐ Explicit Scaling X-min : X-max : Y-min : Y-max :

☐ Enable Hard Copy ☐ Replace

File Name :

☐ Text Output ☐ Replace

File Name : paper.txt

Select Device: Post-Script

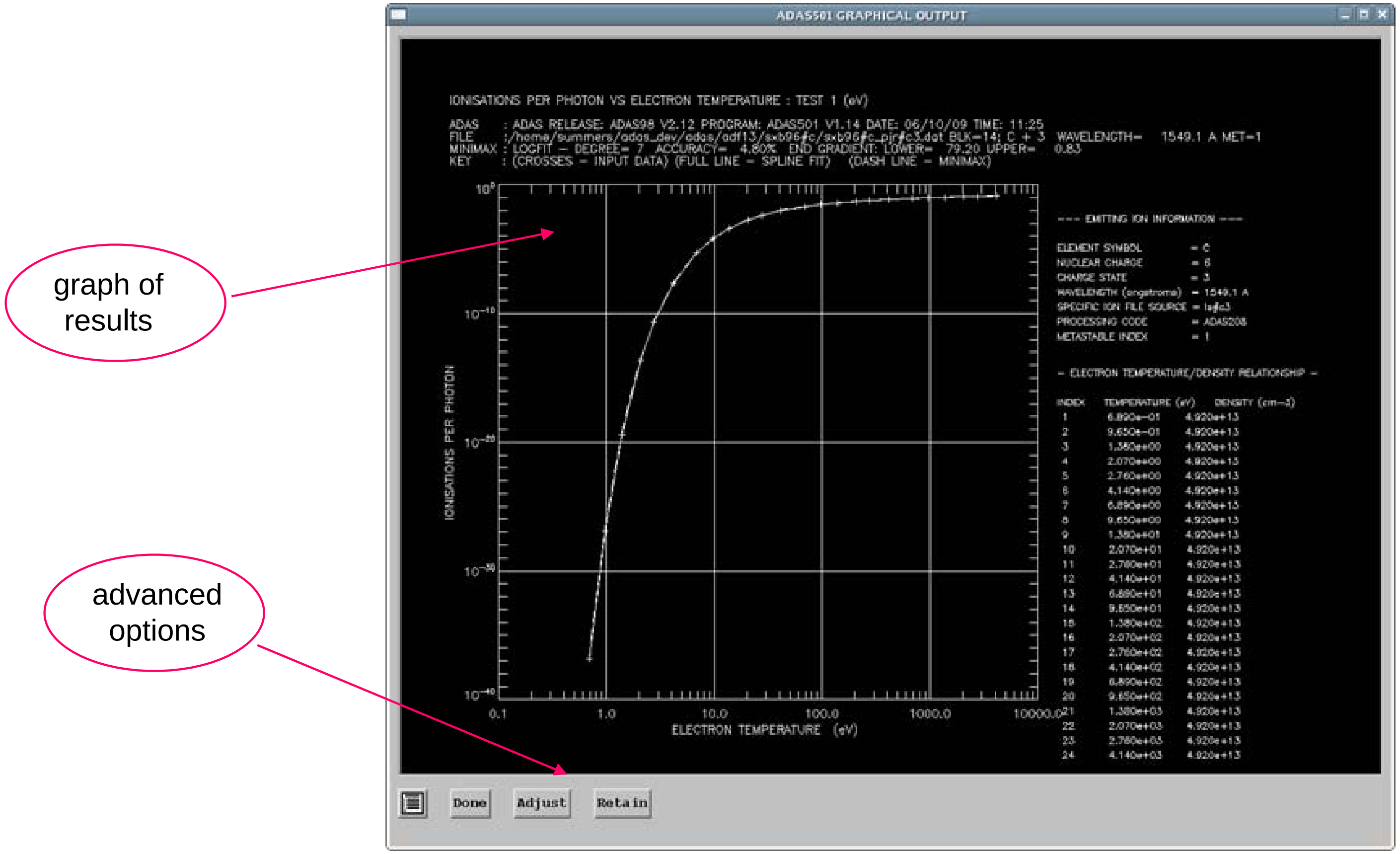
provide graphical output

allow graphical hard copy

graphical output file coding

tabular output of results

ADAS501 Graph

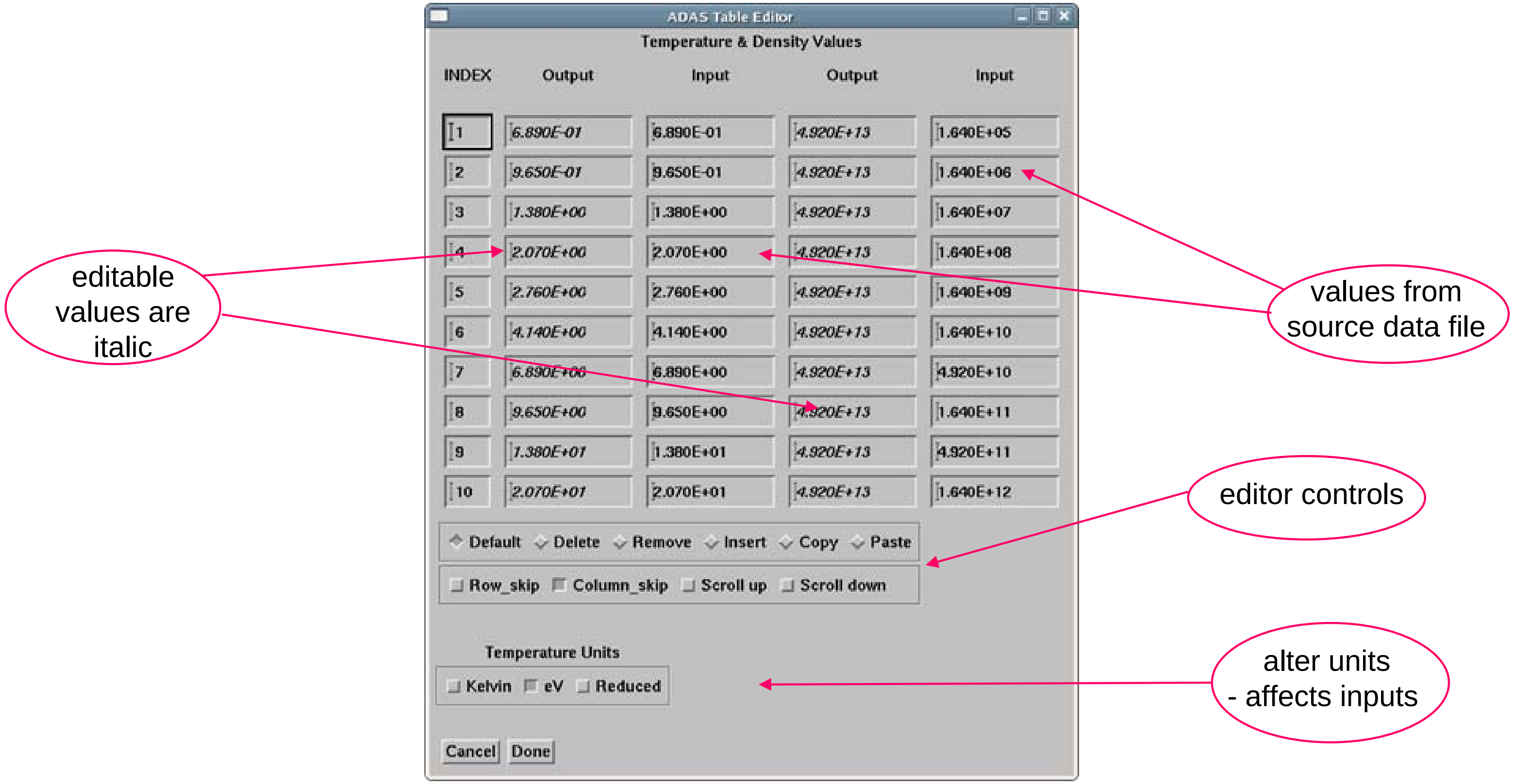


```
IONISATIONS PER PHOTON VS ELECTRON TEMPERATURE : TEST 1 (eV)

ADAS    : ADAS RELEASE: ADAS98 V2.12 PROGRAM: ADAS501 V1.14 DATE: 06/10/09 TIME: 11:25
FILE    :/home/summers/adas_dev/adas/adf13/sxb96#c/sxb96#c_pjr#c3.dat BLK=14; C + 3  WAVELENGTH=   1549.1 A MET=1
MINIMAX : LOGFIT - DEGREE= 7  ACCURACY=  4.80%  END GRADIENT: LOWER=  79.20 UPPER=   0.83
KEY     : (CROSSES - INPUT DATA) (FULL LINE - SPLINE FIT)   (DASH LINE - MINIMAX)

--- EMITTING ION INFORMATION ---

ELEMENT SYMBOL            = C
NUCLEAR CHARGE            = 6
CHARGE STATE              = 3
WAVELENGTH (angstroms)    = 1549.1 A
SPECIFIC ION FILE SOURCE  = ls#c3
PROCESSING CODE           = ADAS208
METASTABLE INDEX          = 1

- ELECTRON TEMPERATURE/DENSITY RELATIONSHIP -

INDEX   TEMPERATURE (eV)   DENSITY (cm-3)
  1       6.890e-01        4.920e+13
  2       9.650e-01        4.920e+13
  3       1.380e+00        4.920e+13
  4       2.070e+00        4.920e+13
  5       2.760e+00        4.920e+13
  6       4.140e+00        4.920e+13
  7       6.890e+00        4.920e+13
  8       9.650e+00        4.920e+13
  9       1.380e+01        4.920e+13
 10       2.070e+01        4.920e+13
 11       2.760e+01        4.920e+13
 12       4.140e+01        4.920e+13
 13       6.890e+01        4.920e+13
 14       9.650e+01        4.920e+13
 15       1.380e+02        4.920e+13
 16       2.070e+02        4.920e+13
 17       2.760e+02        4.920e+13
 18       4.140e+02        4.920e+13
 19       6.890e+02        4.920e+13
 20       9.650e+02        4.920e+13
 21       1.380e+03        4.920e+13
 22       2.070e+03        4.920e+13
 23       2.760e+03        4.920e+13
 24       4.140e+03        4.920e+13
```

graph of results

advanced options

Table editor



ADAS Table Editor

Temperature & Density Values

INDEX	Output	Input	Output	Input
1	*6.890E-01*	6.890E-01	*4.920E+13*	1.640E+05
2	*9.650E-01*	9.650E-01	*4.920E+13*	1.640E+06
3	*1.380E+00*	1.380E+00	*4.920E+13*	1.640E+07
4	*2.070E+00*	2.070E+00	*4.920E+13*	1.640E+08
5	*2.760E+00*	2.760E+00	*4.920E+13*	1.640E+09
6	*4.140E+00*	4.140E+00	*4.920E+13*	1.640E+10
7	*6.890E+00*	6.890E+00	*4.920E+13*	4.920E+10
8	*9.650E+00*	9.650E+00	*4.920E+13*	1.640E+11
9	*1.380E+01*	1.380E+01	*4.920E+13*	4.920E+11
10	*2.070E+01*	2.070E+01	*4.920E+13*	1.640E+12

editable values are italic

values from source data file

editor controls

alter units - affects inputs

2a. The interactive system - working with adf04 datasets

- Preliminaries
  - Electron impact cross-sections and rate coefficients
  - The ADF04 file format
  - Interrogating adf04 collisional excitation data using ADAS201 and ADAS811

Electron impact cross-sections and rates

The excitation reaction $X_i^{+z}(E_i) + e(\varepsilon_i) \rightarrow X_j^{+z}(E_j) + e(\varepsilon_j)$

is described by an excitation cross-section $\sigma_{i\rightarrow j}(\varepsilon_i)$

More useful for tabulation is the collision strength Ω_{ij} with independent variable

$X = \varepsilon_i / \Delta E_{ij}$ with $X \in [1, \infty]$

$$\Omega_{ij} = \omega_i (E_i / I_H)(\sigma_{i\rightarrow j}(\varepsilon_i) / \pi a_0^2) = \omega_j (E_j / I_H)(\sigma_{j\rightarrow i}(\varepsilon_j) / \pi a_0^2)$$

ADAS principally deals with Maxwell averaged rate coefficients $q_{i\rightarrow j}(T_e)$

Υ_{ij} $\quad \Upsilon_{ij} = \int_0^\infty \Omega_{ij}(\varepsilon_j) \exp(-\varepsilon_j / kT_e) \, d(\varepsilon_j / kT_e)$

Electron impact cross-sections and rates (contd.)

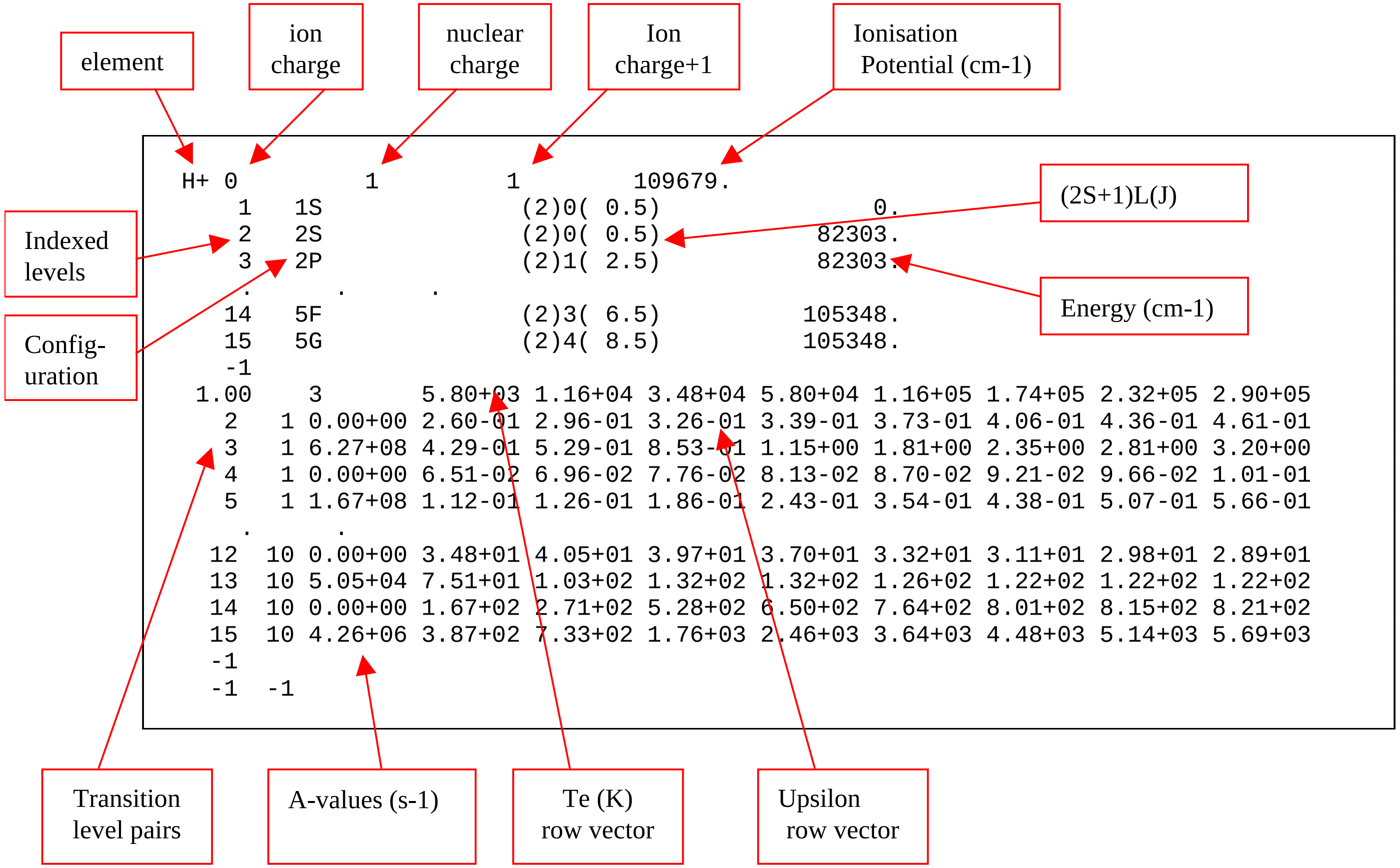
More useful for tabulation is the Maxwell averaged collision strength $\Upsilon_{ij}(T_e)$

$$\Upsilon_{ij} = \int_0^{\infty} \Omega_{ij}(\varepsilon_j) \exp(-\varepsilon_j / kT_e) \, d(\varepsilon_j / kT_e)$$

$$q_{j\to i}(T_e) = \frac{\omega_i}{\omega_j} \exp(\Delta E_{ij} / kT_e) q_{i\to j}(T_e) = 2\sqrt{\pi}\alpha \, c a_0^2 \frac{1}{\omega_j} \left[I_H / kT_e \right]^{1/2} \Upsilon_{ij}$$

The ADAS adf04 format is used to archive sets of energy level lists, A-values and Maxwell averaged collision strengths for an ion sufficient to allow a population calculation.

The basic adf04 file



element

ion charge

nuclear charge

Ion charge+1

Ionisation Potential (cm-1)

Indexed levels

Config-uration

(2S+1)L(J)

Energy (cm-1)

```
H+ 0         1         1        109679.
    1   1S             (2)0( 0.5)               0.
    2   2S             (2)0( 0.5)           82303.
    3   2P             (2)1( 2.5)           82303.
    .      .      .
   14   5F             (2)3( 6.5)          105348.
   15   5G             (2)4( 8.5)          105348.
   -1
 1.00     3       5.80+03 1.16+04 3.48+04 5.80+04 1.16+05 1.74+05 2.32+05 2.90+05
   2    1 0.00+00 2.60-01 2.96-01 3.26-01 3.39-01 3.73-01 4.06-01 4.36-01 4.61-01
   3    1 6.27+08 4.29-01 5.29-01 8.53-01 1.15+00 1.81+00 2.35+00 2.81+00 3.20+00
   4    1 0.00+00 6.51-02 6.96-02 7.76-02 8.13-02 8.70-02 9.21-02 9.66-02 1.01-01
   5    1 1.67+08 1.12-01 1.26-01 1.86-01 2.43-01 3.54-01 4.38-01 5.07-01 5.66-01
    .      .
  12   10 0.00+00 3.48+01 4.05+01 3.97+01 3.70+01 3.32+01 3.11+01 2.98+01 2.89+01
  13   10 5.05+04 7.51+01 1.03+02 1.32+02 1.32+02 1.26+02 1.22+02 1.22+02 1.22+02
  14   10 0.00+00 1.67+02 2.71+02 5.28+02 6.50+02 7.64+02 8.01+02 8.15+02 8.21+02
  15   10 4.26+06 3.87+02 7.33+02 1.76+03 2.46+03 3.64+03 4.48+03 5.14+03 5.69+03
  -1
  -1   -1
```

Transition level pairs

A-values (s-1)

Te (K) row vector

Upsilon row vector

Configuration specification

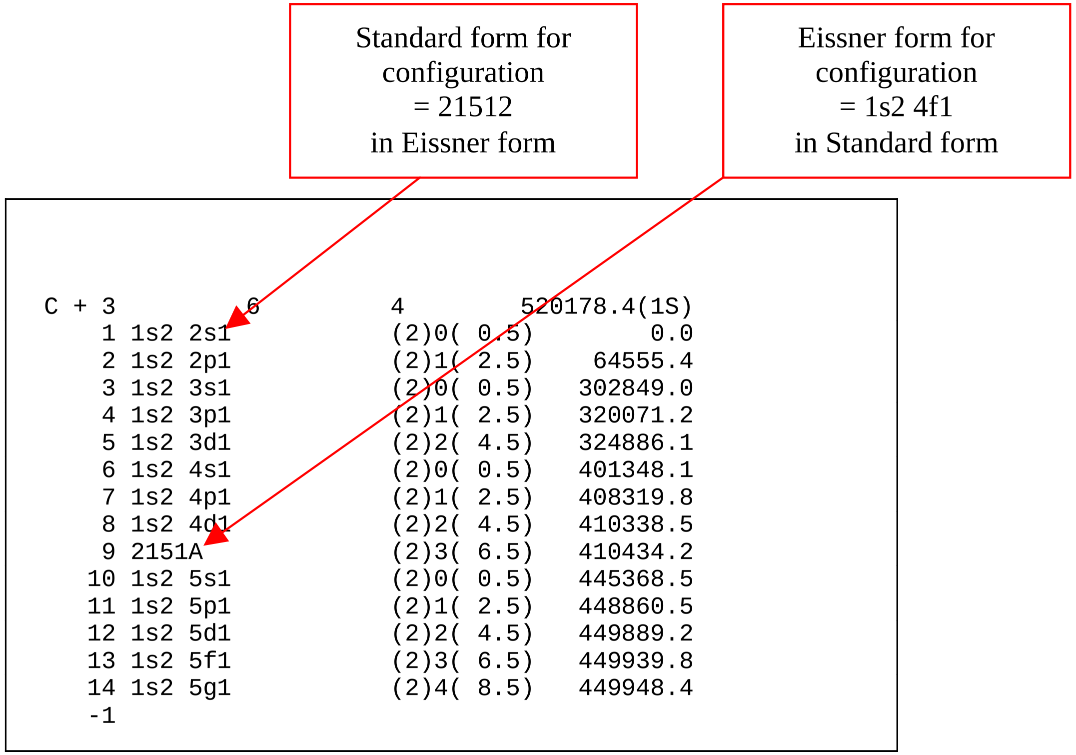
$$\Gamma = n_1 l_1^{\,q_1} n_2 l_2^{\,q_2} \ldots\ldots n_m l_m^{\,q_m}$$

$$\text{where } q_i > 0 \text{ for } i = 1,\ldots,m \text{ and } \sum_{i=1}^{m} q_i = N$$

ADAS prefers Standard and Eissner configuration representations in ADF04 files for automatic processing and matching of levels between different data sets.

Configuration	Standard form	Eissner form
$1s^2 2s^2 2p^4$	1s2 2s2 2p4	21522543
$1s^2 2s^2 2p^6 6f^{11}$	1s2 2s2 2p6 6fb	2152254361J

The basic adf04 file

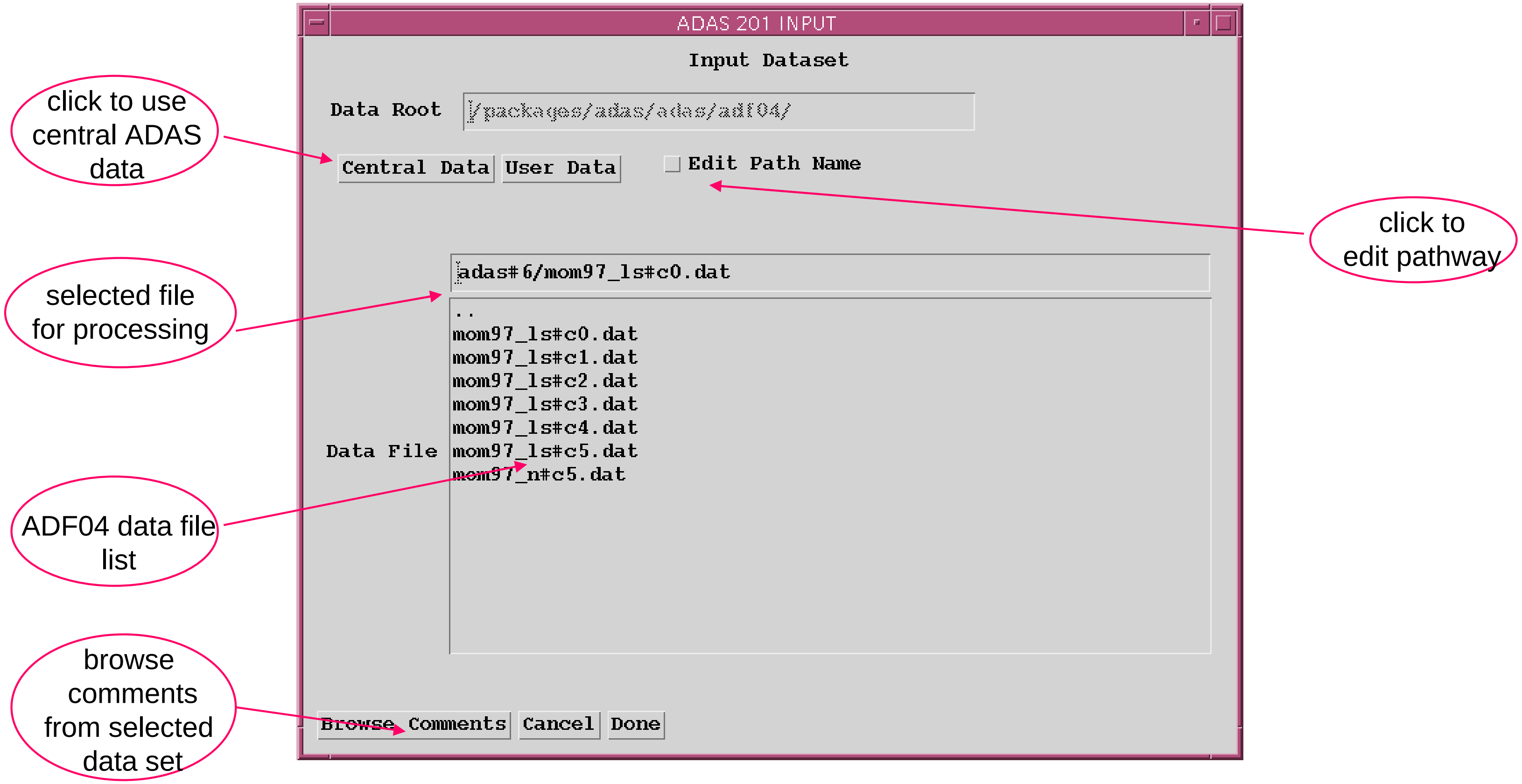


Standard form for
configuration
= 21512
in Eissner form

Eissner form for
configuration
= 1s2 4f1
in Standard form

```
C + 3         6         4        520178.4(1S)
    1 1s2 2s1           (2)0( 0.5)        0.0
    2 1s2 2p1           (2)1( 2.5)    64555.4
    3 1s2 3s1           (2)0( 0.5)   302849.0
    4 1s2 3p1           (2)1( 2.5)   320071.2
    5 1s2 3d1           (2)2( 4.5)   324886.1
    6 1s2 4s1           (2)0( 0.5)   401348.1
    7 1s2 4p1           (2)1( 2.5)   408319.8
    8 1s2 4d1           (2)2( 4.5)   410338.5
    9 2151A             (2)3( 6.5)   410434.2
   10 1s2 5s1           (2)0( 0.5)   445368.5
   11 1s2 5p1           (2)1( 2.5)   448860.5
   12 1s2 5d1           (2)2( 4.5)   449889.2
   13 1s2 5f1           (2)3( 6.5)   449939.8
   14 1s2 5g1           (2)4( 8.5)   449948.4
   -1
```

ADAS201 input



Data Root /packages/adas/adas/adf04/

Data File adas#6/mom97_ls#c0.dat

```
..
mom97_ls#c0.dat
mom97_ls#c1.dat
mom97_ls#c2.dat
mom97_ls#c3.dat
mom97_ls#c4.dat
mom97_ls#c5.dat
mom97_n#c5.dat
```

click to use central ADAS data

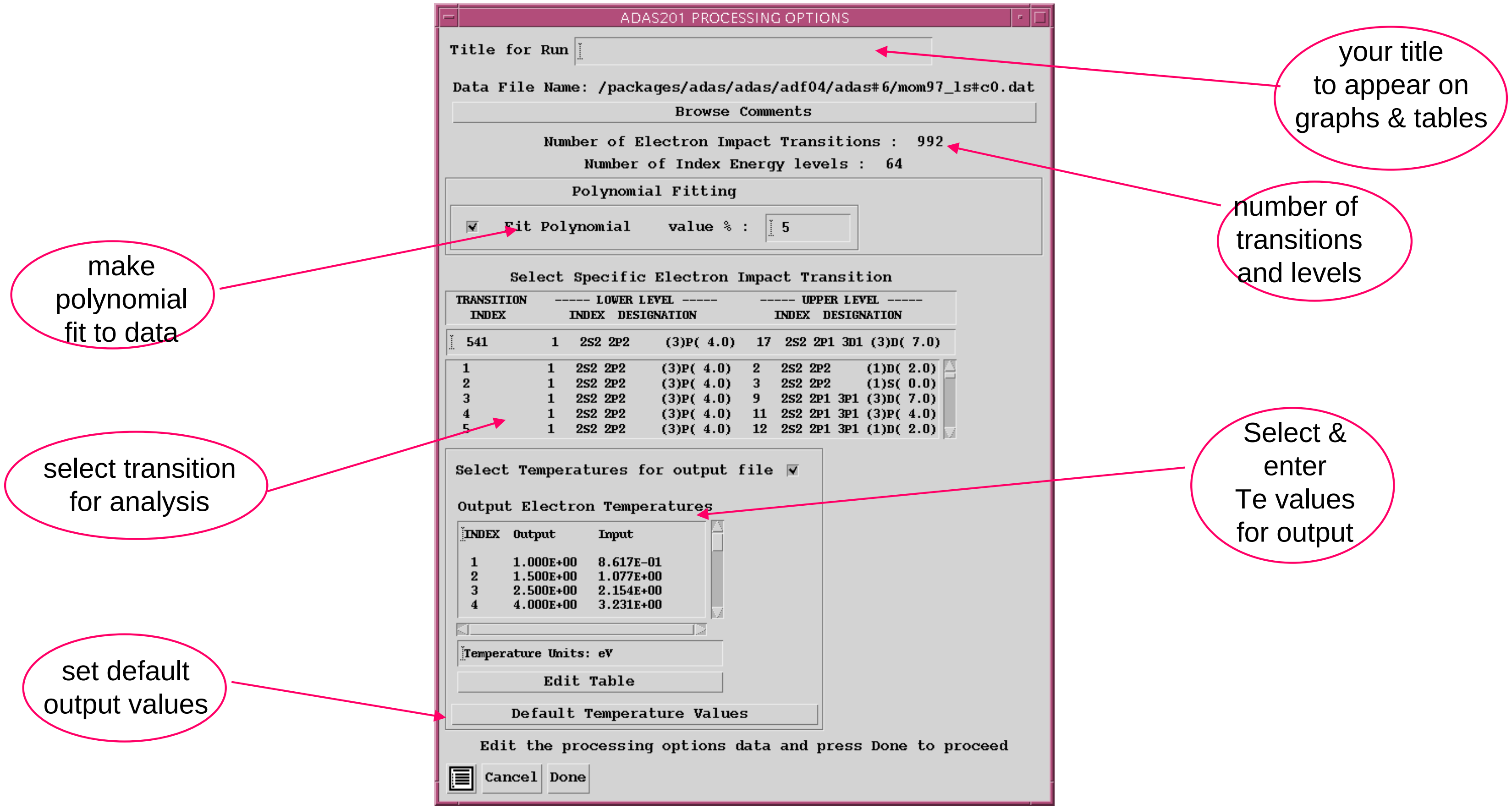
selected file for processing

ADF04 data file list

browse comments from selected data set

click to edit pathway

ADAS201 Processing



Title for Run

Data File Name: /packages/adas/adas/adf04/adas#6/mom97_ls#c0.dat

Number of Electron Impact Transitions : 992
Number of Index Energy levels : 64

Polynomial Fitting

☑ Fit Polynomial value % : 5

Select Specific Electron Impact Transition

TRANSITION INDEX	LOWER LEVEL INDEX	LOWER LEVEL DESIGNATION		UPPER LEVEL INDEX	UPPER LEVEL DESIGNATION	
541	1	2S2 2P2	(3)P(4.0)	17	2S2 2P1 3D1	(3)D(7.0)
1	1	2S2 2P2	(3)P(4.0)	2	2S2 2P2	(1)D(2.0)
2	1	2S2 2P2	(3)P(4.0)	3	2S2 2P2	(1)S(0.0)
3	1	2S2 2P2	(3)P(4.0)	9	2S2 2P1 3P1	(3)D(7.0)
4	1	2S2 2P2	(3)P(4.0)	11	2S2 2P1 3P1	(3)P(4.0)
5	1	2S2 2P2	(3)P(4.0)	12	2S2 2P1 3P1	(1)D(2.0)

Select Temperatures for output file ☑

Output Electron Temperatures

INDEX	Output	Input
1	1.000E+00	8.617E-01
2	1.500E+00	1.077E+00
3	2.500E+00	2.154E+00
4	4.000E+00	3.231E+00

Temperature Units: eV

Edit the processing options data and press Done to proceed

your title to appear on graphs & tables

number of transitions and levels

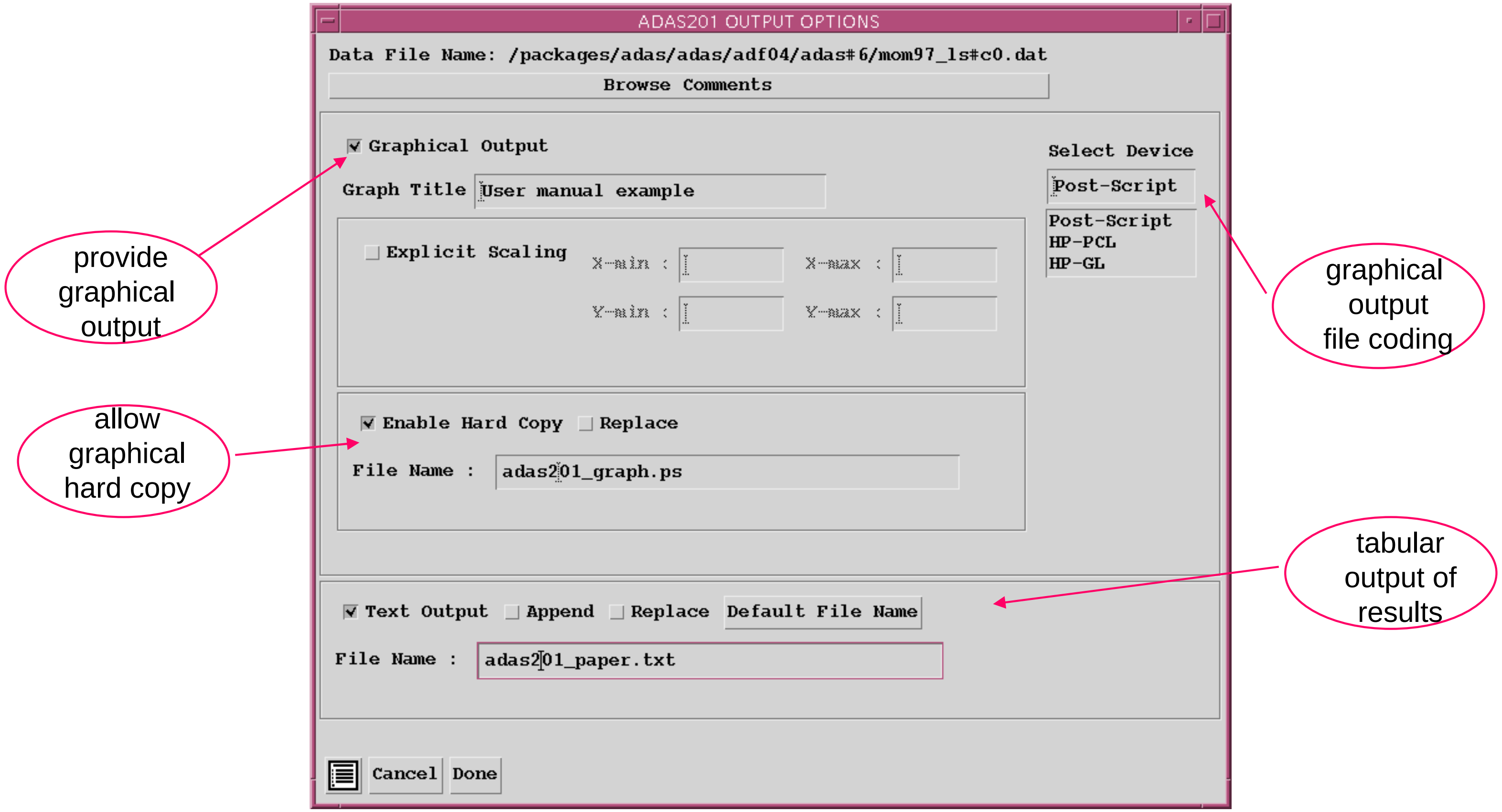
make polynomial fit to data

select transition for analysis

Select & enter Te values for output

set default output values

ADAS201 Output



ADAS201 OUTPUT OPTIONS

Data File Name: /packages/adas/adas/adf04/adas#6/mom97_ls#c0.dat

☑ Graphical Output

Graph Title: User manual example

☐ Explicit Scaling

☑ Enable Hard Copy ☐ Replace

File Name : adas201_graph.ps

Select Device: Post-Script

☑ Text Output ☐ Append ☐ Replace

File Name : adas201_paper.txt

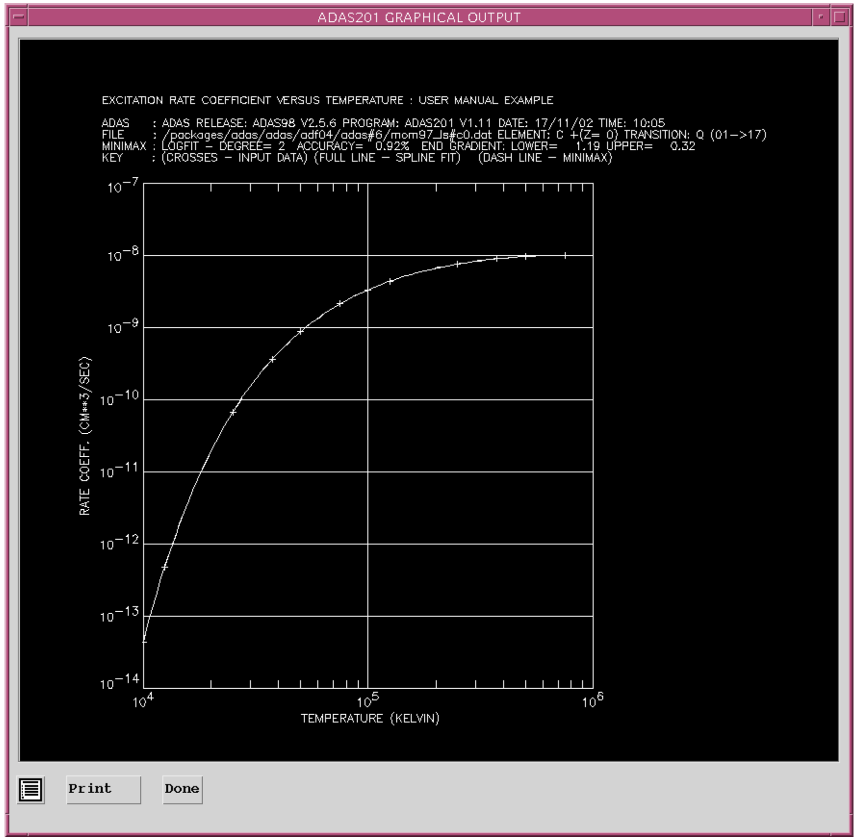
provide graphical output

allow graphical hard copy

graphical output file coding

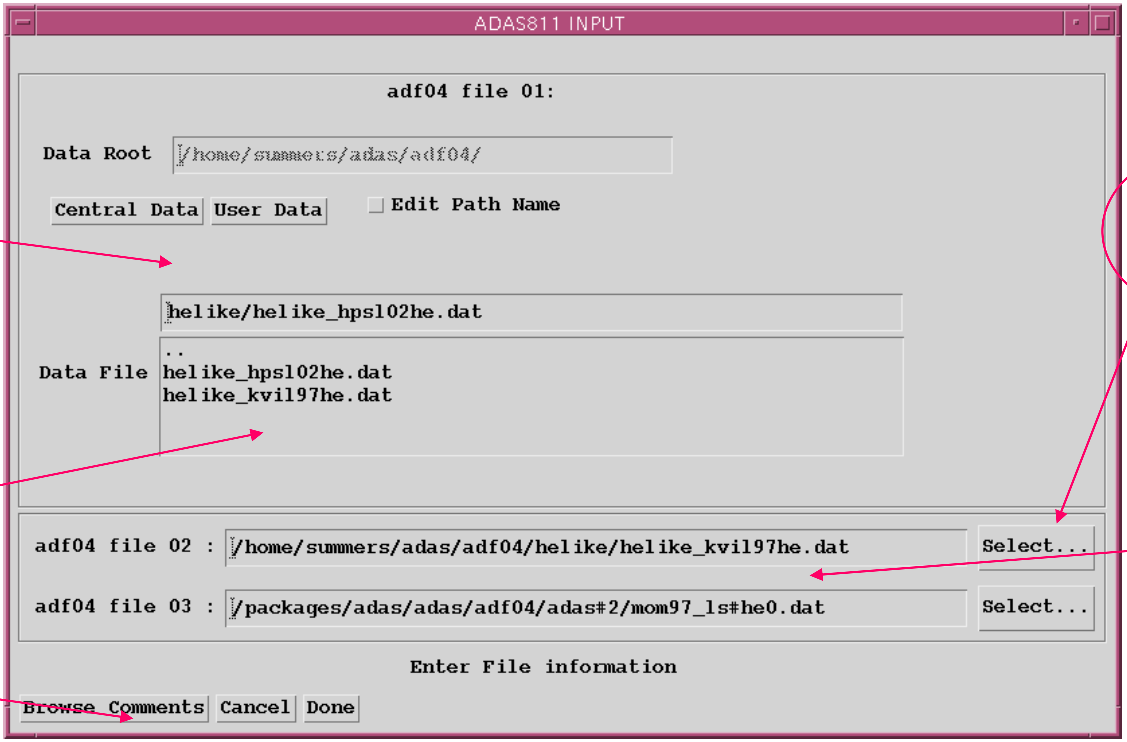
tabular output of results

ADAS201 Graph



```
EXCITATION RATE COEFFICIENT VERSUS TEMPERATURE : USER MANUAL EXAMPLE

ADAS    : ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS201 V1.11 DATE: 17/11/02 TIME: 10:05
FILE    : /packages/adas/adas/adf04/adas#6/mom97_ls#c0.dat ELEMENT: C +(Z= 0) TRANSITION: Q (01->17)
MINIMAX : LOGFIT - DEGREE= 2  ACCURACY=  0.92%  END GRADIENT: LOWER=   1.19 UPPER=   0.32
KEY     : (CROSSES - INPUT DATA) (FULL LINE - SPLINE FIT)   (DASH LINE - MINIMAX)
```

ADAS811 input



adf04 file 01:

Data Root: /home/summers/adas/adf04/

helike/helike_hpsl02he.dat

Data File:
..
helike_hpsl02he.dat
helike_kvil97he.dat

adf04 file 02 : /home/summers/adas/adf04/helike/helike_kvil97he.dat

adf04 file 03 : /packages/adas/adas/adf04/adas#2/mom97_ls#he0.dat

Enter File information

Select first file

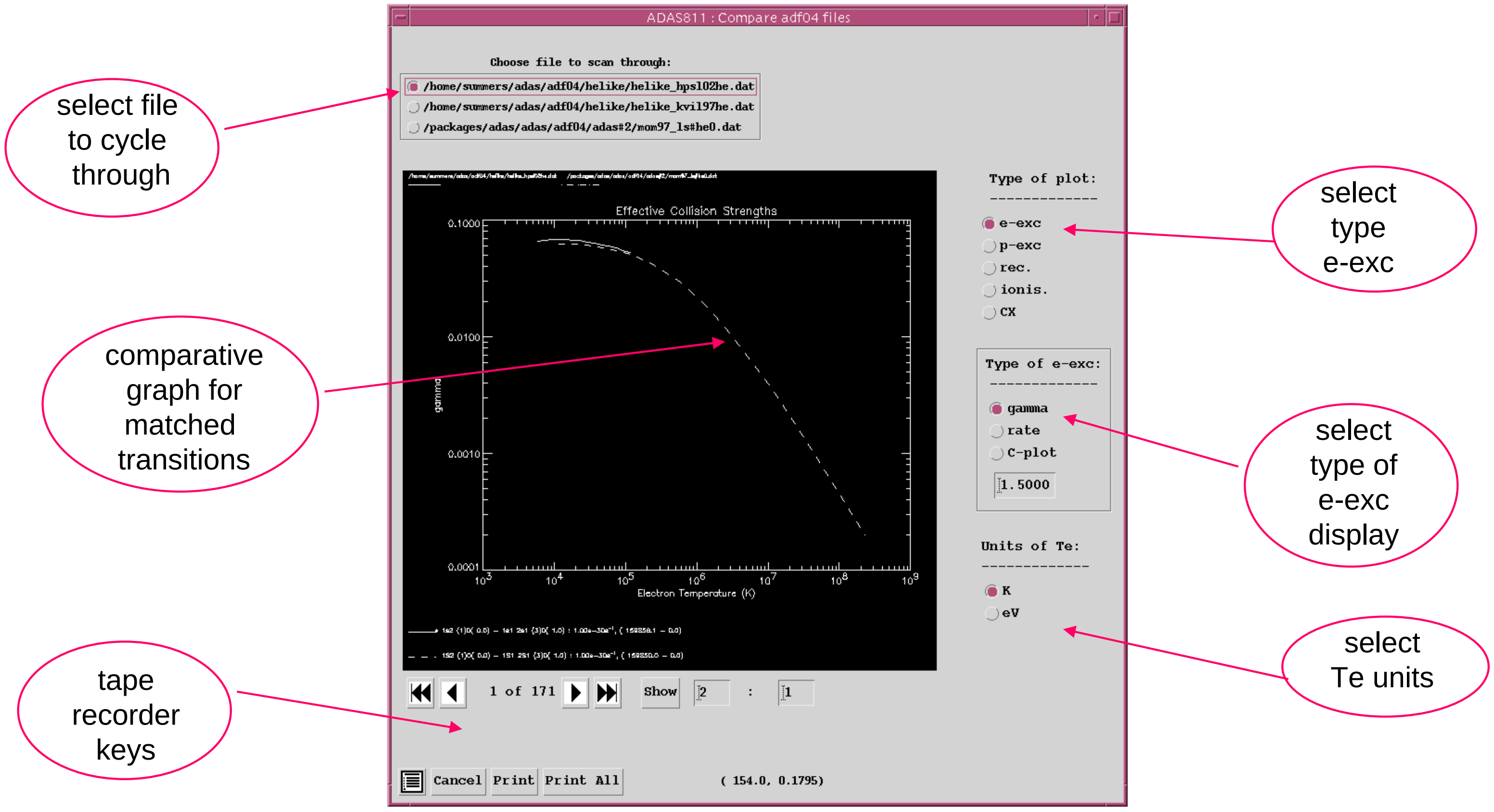
ADF04 data file list

browse comments from first data set

Click to show file chooser pop-up

Second and third files

ADAS811 Processing



ADAS811 : Compare adf04 files

Choose file to scan through:

- ● /home/summers/adas/adf04/helike/helike_hps102he.dat
- ○ /home/summers/adas/adf04/helike/helike_kvi197he.dat
- ○ /packages/adas/adas/adf04/adas#2/mom97_ls#he0.dat

Type of plot:

- ● e-exc
- ○ p-exc
- ○ rec.
- ○ ionis.
- ○ CX

Type of e-exc:

- ● gamma
- ○ rate
- ○ C-plot

1.5000

Units of Te:

- ● K
- ○ eV

1 of 171

Show 2 : 1

(154.0, 0.1795)

select file to cycle through

comparative graph for matched transitions

tape recorder keys

select type e-exc

select type of e-exc display

select Te units

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

Populations calculation (contd.)

Distinguish metastable levels X_{ρ}^{+z} indexed by Greek letters
and ordinary levels X_{i}^{+z} indexed by Roman letters

Write the quasi-static equations for the ordinary levels populations in terms of the metastable populations as:

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

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

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

Populations calculation (contd.)

Solution for the ordinary populations is

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

$$+ \sum_{i=1}^{O} C_{ji}^{-1} q_i^{(CX)} N_H N_1^+$$

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

Populations calculation (contd.)

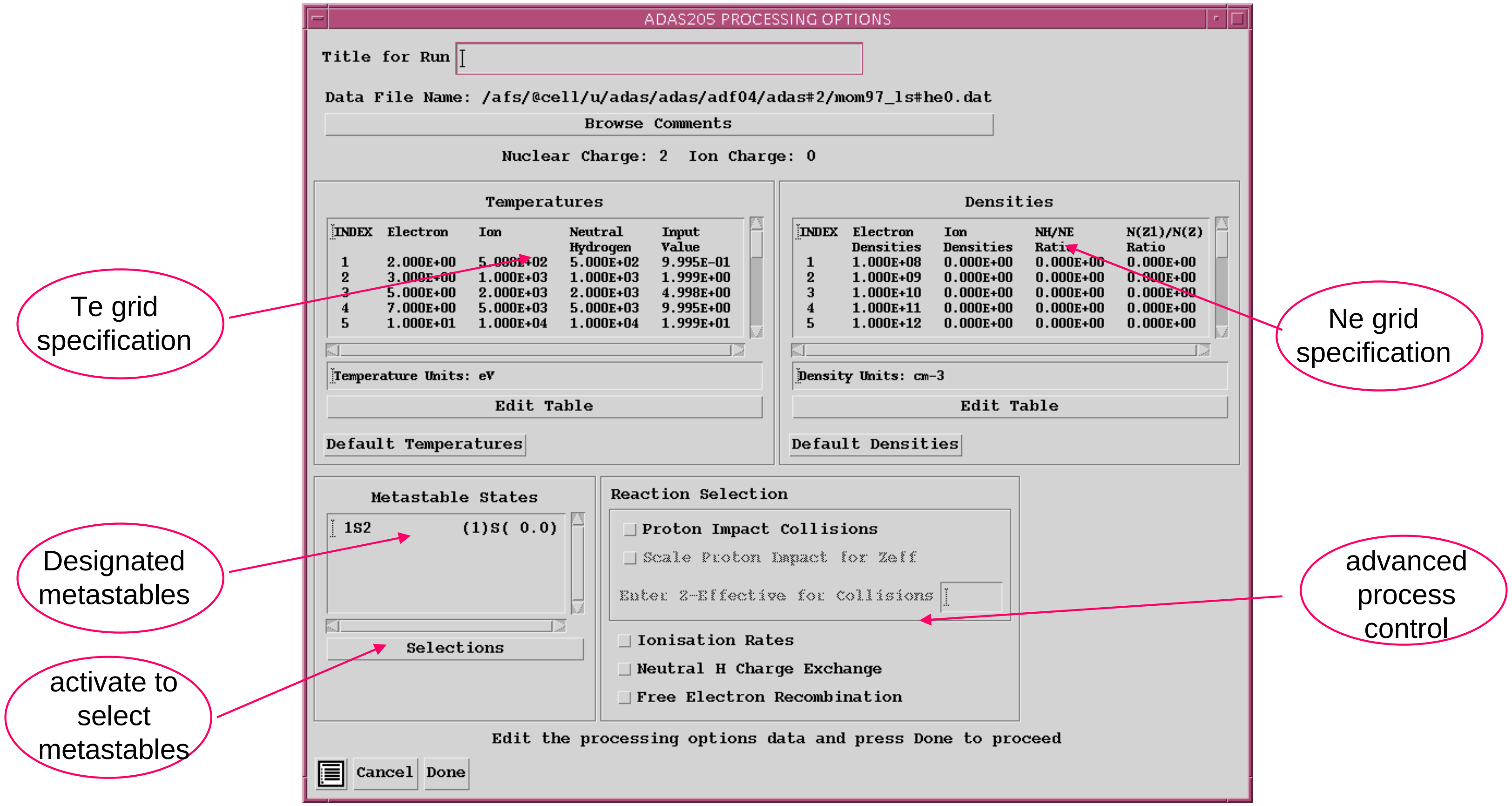
Spectrum line emissivities are

$$\varepsilon_{j\to k} = A_{j\to k}\Big(\sum_{\sigma=1}^{M} \mathsf{F}_{j\sigma}^{(exc)} N_e N_\sigma + \sum_{\upsilon'=1}^{M_{z+1}} \mathsf{F}_{j\upsilon'}^{(rec)} N_e N_{\upsilon'}^{+} + \sum_{\upsilon'=1}^{M_{z+1}} \mathsf{F}_{j\upsilon'}^{(CX)} N_H N_{\upsilon'}^{+} + \sum_{\mu'=1}^{M_{z-1}} \mathsf{F}_{j\mu'}^{(ion)} N_e N_{\mu'}^{-}\Big)$$

Identify excitation and recombination photon emissivity coefficients as

$$\boxed{\mathrm{PEC}_{\sigma,j\to k}^{(exc)} = A_{j\to k}\mathsf{F}_{j\sigma}^{(exc)}} \qquad \mathrm{PEC}_{\upsilon',j\to k}^{(rec)} = A_{j\to k}\mathsf{F}_{j\upsilon'}^{(rec)}$$

ADAS205 processing



Title for Run

Data File Name: /afs/@cell/u/adas/adas/adf04/adas#2/mom97_ls#he0.dat

Nuclear Charge: 2 Ion Charge: 0

Temperatures

INDEX	Electron	Ion	Neutral Hydrogen	Input Value
1	2.000E+00	5.000E+02	5.000E+02	9.995E-01
2	3.000E+00	1.000E+03	1.000E+03	1.999E+00
3	5.000E+00	2.000E+03	2.000E+03	4.998E+00
4	7.000E+00	5.000E+03	5.000E+03	9.995E+00
5	1.000E+01	1.000E+04	1.000E+04	1.999E+01

Temperature Units: eV

Densities

INDEX	Electron Densities	Ion Densities	NH/NE Ratio	N(Z1)/N(Z) Ratio
1	1.000E+08	0.000E+00	0.000E+00	0.000E+00
2	1.000E+09	0.000E+00	0.000E+00	0.000E+00
3	1.000E+10	0.000E+00	0.000E+00	0.000E+00
4	1.000E+11	0.000E+00	0.000E+00	0.000E+00
5	1.000E+12	0.000E+00	0.000E+00	0.000E+00

Density Units: cm-3

Metastable States

1S2 (1)S(0.0)

Reaction Selection

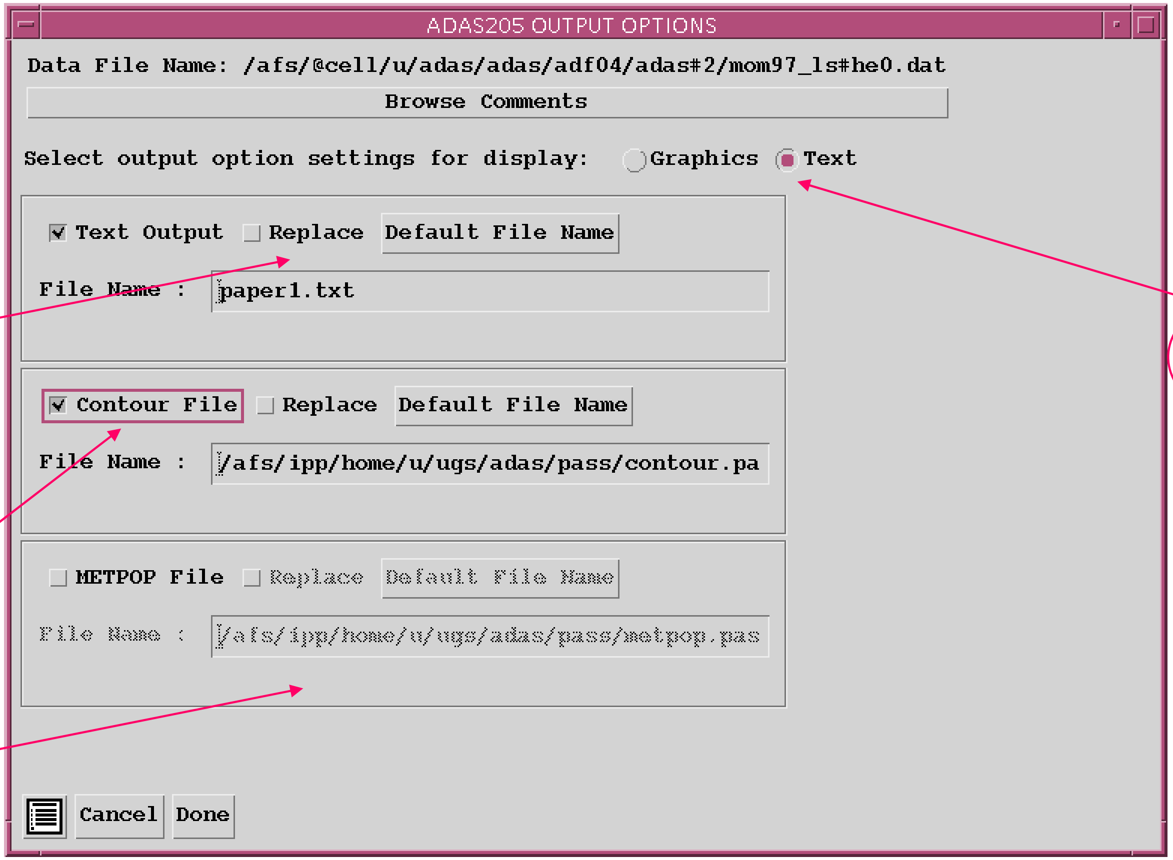
☐ Proton Impact Collisions
☐ Scale Proton Impact for Zeff
Enter Z-Effective for Collisions
☐ Ionisation Rates
☐ Neutral H Charge Exchange
☐ Free Electron Recombination

Edit the processing options data and press Done to proceed

Populations and line ratio studies (contd.)

- Output options
  - » Graphical display of the $\mathsf{F}_{j\sigma}^{(exc)}$ as a function of density is allowed.
  - » An output file of the $\mathsf{F}_{j\sigma}^{(exc)}$, called the ‘contour’ pass file, can be generated. This file must be created to allow the next step of looking a line ratios.

ADAS205 output - text



Data File Name: /afs/@cell/u/adas/adas/adf04/adas#2/mom97_ls#he0.dat

Select output option settings for display: ○ Graphics ● Text

☑ Text Output ☐ Replace

File Name : paper1.txt

☑ Contour File ☐ Replace

File Name : /afs/ipp/home/u/ugs/adas/pass/contour.pa

☐ METPOP File ☐ Replace

File Name : /afs/ipp/home/u/ugs/adas/pass/metpop.pas

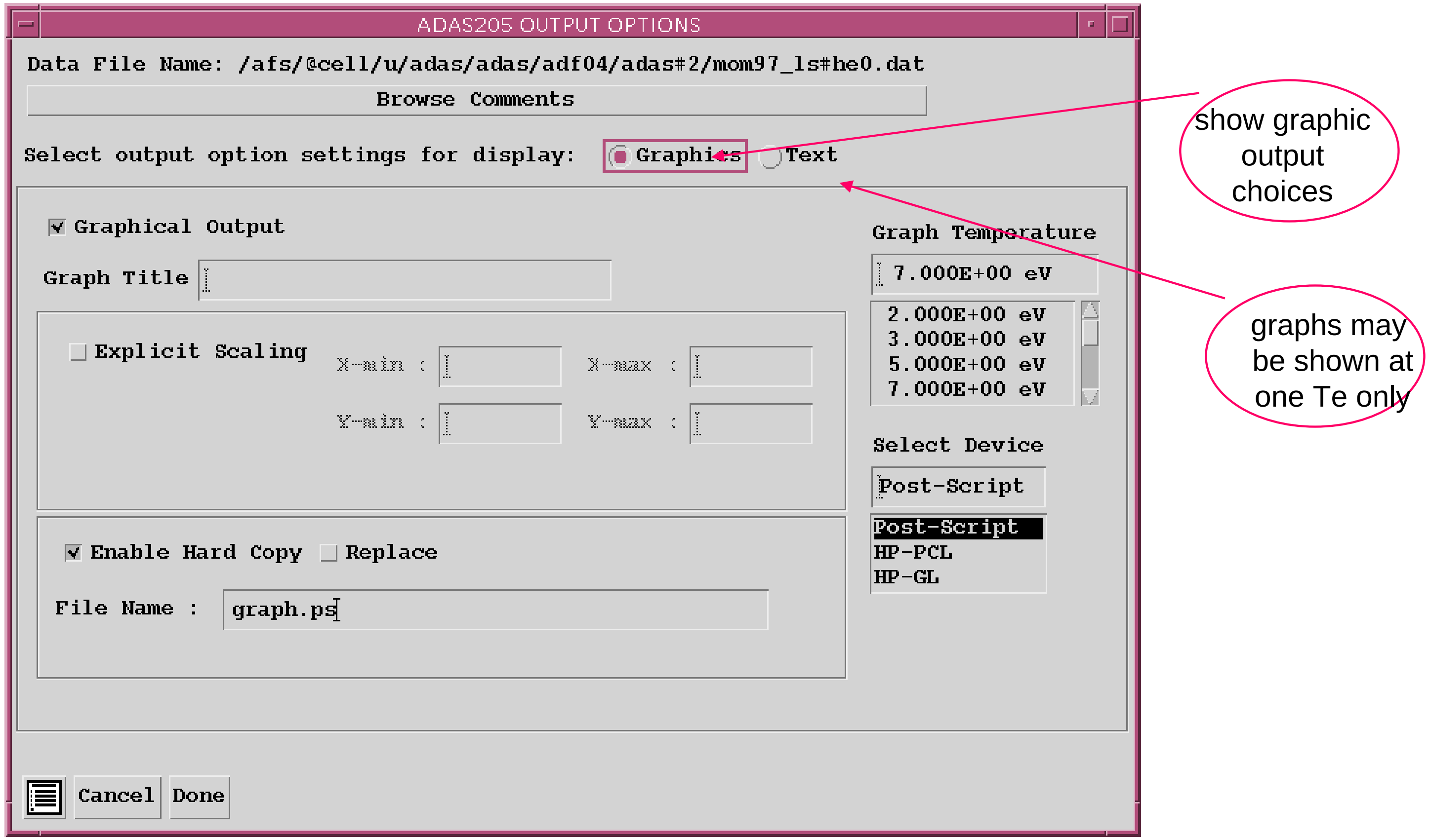
ADF11 classes selected

output file required for ratio studies

graph of results

show text output choices

ADAS205 output - graphics



Data File Name: /afs/@cell/u/adas/adas/adf04/adas#2/mom97_ls#he0.dat

Select output option settings for display: ● Graphics ○ Text

☑ Graphical Output

Graph Title :

☐ Explicit Scaling

X-min :
X-max :
Y-min :
Y-max :

☑ Enable Hard Copy ☐ Replace

File Name : graph.ps

Graph Temperature

7.000E+00 eV

2.000E+00 eV
3.000E+00 eV
5.000E+00 eV
7.000E+00 eV

Select Device

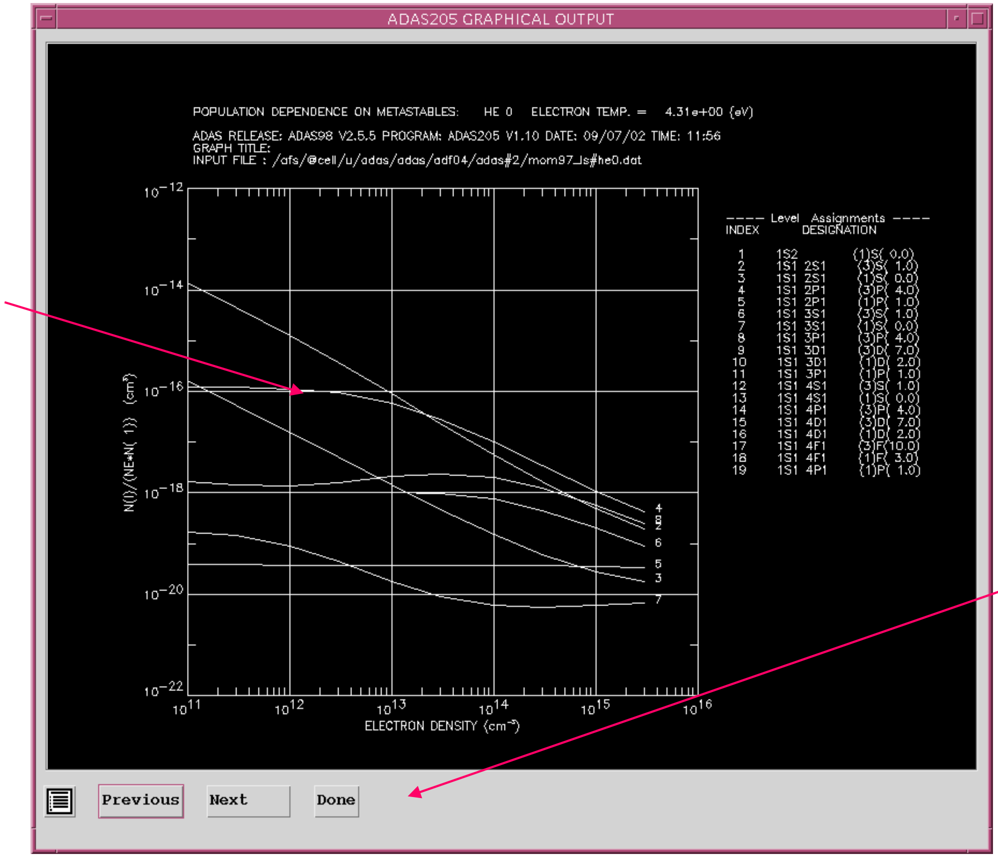
Post-Script

Post-Script
HP-PCL
HP-GL

show graphic output choices

graphs may be shown at one Te only

ADAS205 graph



```
POPULATION DEPENDENCE ON METASTABLES:    HE 0   ELECTRON TEMP. =   4.31e+00 (eV)

ADAS RELEASE: ADAS98 V2.5.5 PROGRAM: ADAS205 V1.10 DATE: 09/07/02 TIME: 11:56
GRAPH TITLE:
INPUT FILE : /afs/@cell/u/adas/adas/adf04/adas#2/mom97_ls#he0.dat
```

```
---- Level  Assignments ----
INDEX        DESIGNATION

  1     1S2          (1)S( 0.0)
  2     1S1  2S1     (3)S( 1.0)
  3     1S1  2S1     (1)S( 0.0)
  4     1S1  2P1     (3)P( 4.0)
  5     1S1  2P1     (1)P( 1.0)
  6     1S1  3S1     (3)S( 1.0)
  7     1S1  3S1     (1)S( 0.0)
  8     1S1  3P1     (3)P( 4.0)
  9     1S1  3D1     (3)D( 7.0)
 10     1S1  3D1     (1)D( 2.0)
 11     1S1  3P1     (1)P( 1.0)
 12     1S1  4S1     (3)S( 1.0)
 13     1S1  4S1     (1)S( 0.0)
 14     1S1  4P1     (3)P( 4.0)
 15     1S1  4D1     (3)D( 7.0)
 16     1S1  4D1     (1)D( 2.0)
 17     1S1  4F1     (3)F(10.0)
 18     1S1  4F1     (1)F( 3.0)
 19     1S1  4P1     (1)P( 1.0)
```

excited population graph

Print button is present if graphic file chosen

Setting up lines

- Code ADAS207 is the diagnostic analysis program which allows study of line ratios.

- It needs the ‘contour’ pass file of populations. It also fetches the specific ion file, of type ADF04, which was used in the population calculation.

Setting up lines (contd.)

The program in deals with two line assemblies which from the numerator and denominator of the line ratio.

The composite emissivity for a line assembly is written as

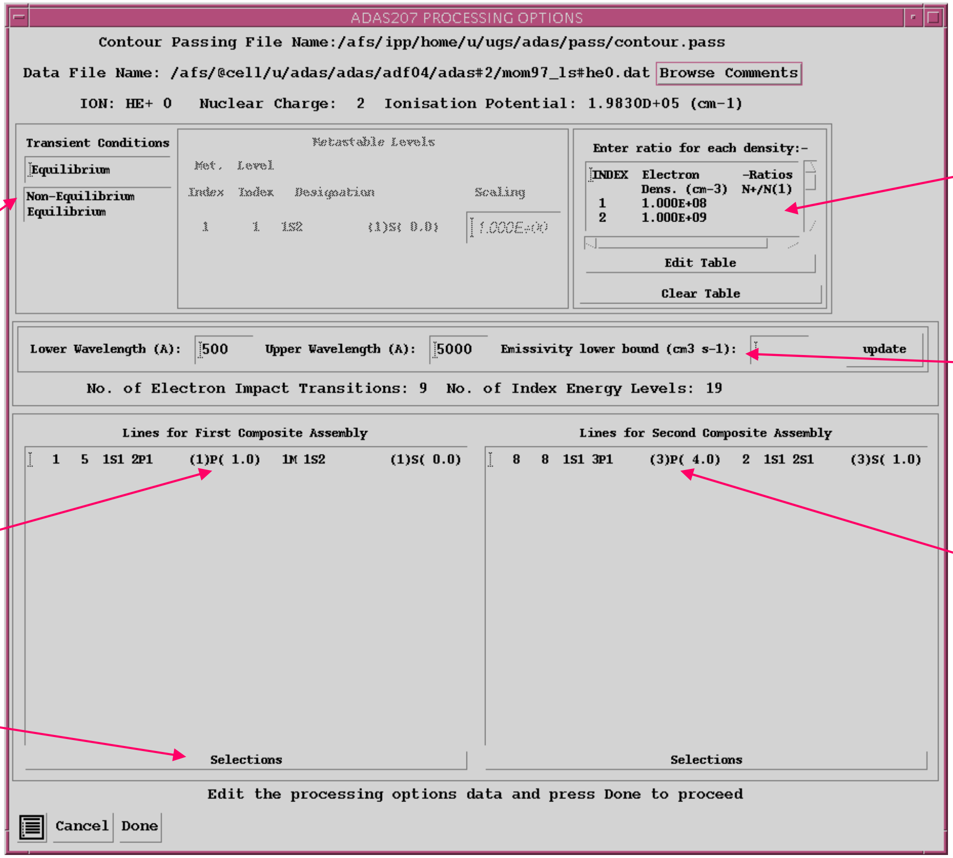
$$\varepsilon_G = \sum_{j\in J_G, i\in I_G} \varepsilon_{j\to i} = \sum_{j\in J_G, i\in I_G} A_{j\to i} N_j$$

$$= \sum_{j\in J_G, i\in I_G} A_{j\to i} (\sum_{\sigma=1}^{M} \mathsf{F}_{j\sigma}^{(exc)} N_e N_\sigma + \mathsf{F}_{j1}^{(rec)} N_e N_1^+ + \mathsf{F}_{j1}^{(CX)} N_H N_1^+)$$

$$= N_e N_1 \sum_{j\in J_G, i\in I_G} A_{j\to i} (\sum_{\sigma=1}^{M} \mathsf{F}_{j\sigma}^{(exc)} \frac{N_\sigma}{N_1} + \mathsf{F}_{j1}^{(rec)} \frac{N_1^+}{N_1} + \mathsf{F}_{j1}^{(CX)} \frac{N_H}{N_e} \frac{N_1^+}{N_1})$$

Diagnostic line ratio modelling deals with $\varepsilon_{G_1} / \varepsilon_{G_2}$

ADAS207 processing



Contour Passing File Name:/afs/ipp/home/u/ugs/adas/pass/contour.pass

Data File Name: /afs/@cell/u/adas/adas/adf04/adas#2/mom97_ls#he0.dat

ION: HE+ 0   Nuclear Charge: 2   Ionisation Potential: 1.9830D+05 (cm-1)

Transient Conditions

- Equilibrium
- Non-Equilibrium Equilibrium

Metastable Levels

Met. Index	Level Index	Designation		Scaling
1	1	1S2	(1)S(0.0)	1.000E+00

Enter ratio for each density:-

INDEX	Electron Dens. (cm-3)	-Ratios N+/N(1)
1	1.000E+08	
2	1.000E+09	

Lower Wavelength (A): 500   Upper Wavelength (A): 5000   Emissivity lower bound (cm3 s-1):

No. of Electron Impact Transitions: 9   No. of Index Energy Levels: 19

Lines for First Composite Assembly

```
1   5  1S1 2P1    (1)P( 1.0)   1M 1S2          (1)S( 0.0)
```

Lines for Second Composite Assembly

```
8   8  1S1 3P1    (3)P( 4.0)   2  1S1 2S1      (3)S( 1.0)
```

Edit the processing options data and press Done to proceed

advanced use with metastables

lines in numerator of ratio

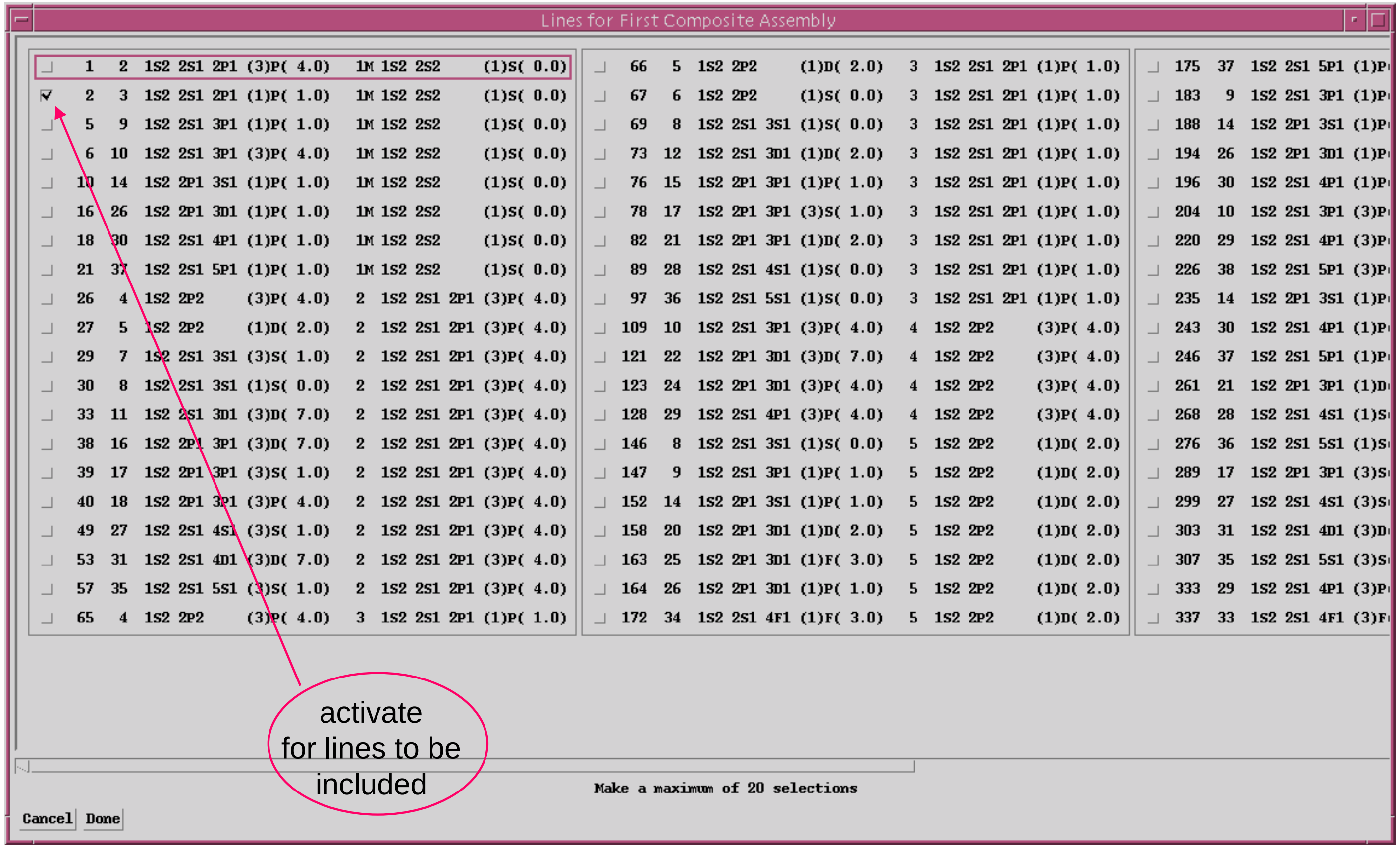
show line selection list

advanced use for recombination

restrict the choice of lines

lines in denominator of ratio

ADAS207 line assembly



```
☐   1   2  1S2 2S1 2P1 (3)P( 4.0)   1M 1S2 2S2      (1)S( 0.0)
☑   2   3  1S2 2S1 2P1 (1)P( 1.0)   1M 1S2 2S2      (1)S( 0.0)
☐   5   9  1S2 2S1 3P1 (1)P( 1.0)   1M 1S2 2S2      (1)S( 0.0)
☐   6  10  1S2 2S1 3P1 (3)P( 4.0)   1M 1S2 2S2      (1)S( 0.0)
☐  10  14  1S2 2P1 3S1 (1)P( 1.0)   1M 1S2 2S2      (1)S( 0.0)
☐  16  26  1S2 2P1 3D1 (1)P( 1.0)   1M 1S2 2S2      (1)S( 0.0)
☐  18  30  1S2 2S1 4P1 (1)P( 1.0)   1M 1S2 2S2      (1)S( 0.0)
☐  21  37  1S2 2S1 5P1 (1)P( 1.0)   1M 1S2 2S2      (1)S( 0.0)
☐  26   4  1S2 2P2     (3)P( 4.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  27   5  1S2 2P2     (1)D( 2.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  29   7  1S2 2S1 3S1 (3)S( 1.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  30   8  1S2 2S1 3S1 (1)S( 0.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  33  11  1S2 2S1 3D1 (3)D( 7.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  38  16  1S2 2P1 3P1 (3)D( 7.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  39  17  1S2 2P1 3P1 (3)S( 1.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  40  18  1S2 2P1 3P1 (3)P( 4.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  49  27  1S2 2S1 4S1 (3)S( 1.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  53  31  1S2 2S1 4D1 (3)D( 7.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  57  35  1S2 2S1 5S1 (3)S( 1.0)   2  1S2 2S1 2P1 (3)P( 4.0)
☐  65   4  1S2 2P2     (3)P( 4.0)   3  1S2 2S1 2P1 (1)P( 1.0)
```

```
☐  66   5  1S2 2P2     (1)D( 2.0)   3  1S2 2S1 2P1 (1)P( 1.0)
☐  67   6  1S2 2P2     (1)S( 0.0)   3  1S2 2S1 2P1 (1)P( 1.0)
☐  69   8  1S2 2S1 3S1 (1)S( 0.0)   3  1S2 2S1 2P1 (1)P( 1.0)
☐  73  12  1S2 2S1 3D1 (1)D( 2.0)   3  1S2 2S1 2P1 (1)P( 1.0)
☐  76  15  1S2 2P1 3P1 (1)P( 1.0)   3  1S2 2S1 2P1 (1)P( 1.0)
☐  78  17  1S2 2P1 3P1 (3)S( 1.0)   3  1S2 2S1 2P1 (1)P( 1.0)
☐  82  21  1S2 2P1 3P1 (1)D( 2.0)   3  1S2 2S1 2P1 (1)P( 1.0)
☐  89  28  1S2 2S1 4S1 (1)S( 0.0)   3  1S2 2S1 2P1 (1)P( 1.0)
☐  97  36  1S2 2S1 5S1 (1)S( 0.0)   3  1S2 2S1 2P1 (1)P( 1.0)
☐ 109  10  1S2 2S1 3P1 (3)P( 4.0)   4  1S2 2P2     (3)P( 4.0)
☐ 121  22  1S2 2P1 3D1 (3)D( 7.0)   4  1S2 2P2     (3)P( 4.0)
☐ 123  24  1S2 2P1 3D1 (3)P( 4.0)   4  1S2 2P2     (3)P( 4.0)
☐ 128  29  1S2 2S1 4P1 (3)P( 4.0)   4  1S2 2P2     (3)P( 4.0)
☐ 146   8  1S2 2S1 3S1 (1)S( 0.0)   5  1S2 2P2     (1)D( 2.0)
☐ 147   9  1S2 2S1 3P1 (1)P( 1.0)   5  1S2 2P2     (1)D( 2.0)
☐ 152  14  1S2 2P1 3S1 (1)P( 1.0)   5  1S2 2P2     (1)D( 2.0)
☐ 158  20  1S2 2P1 3D1 (1)D( 2.0)   5  1S2 2P2     (1)D( 2.0)
☐ 163  25  1S2 2P1 3D1 (1)F( 3.0)   5  1S2 2P2     (1)D( 2.0)
☐ 164  26  1S2 2P1 3D1 (1)P( 1.0)   5  1S2 2P2     (1)D( 2.0)
☐ 172  34  1S2 2S1 4F1 (1)F( 3.0)   5  1S2 2P2     (1)D( 2.0)
```

```
☐ 175  37  1S2 2S1 5P1 (1)P
☐ 183   9  1S2 2S1 3P1 (1)P
☐ 188  14  1S2 2P1 3S1 (1)P
☐ 194  26  1S2 2P1 3D1 (1)P
☐ 196  30  1S2 2S1 4P1 (1)P
☐ 204  10  1S2 2S1 3P1 (3)P
☐ 220  29  1S2 2S1 4P1 (3)P
☐ 226  38  1S2 2S1 5P1 (3)P
☐ 235  14  1S2 2P1 3S1 (1)P
☐ 243  30  1S2 2S1 4P1 (1)P
☐ 246  37  1S2 2S1 5P1 (1)P
☐ 261  21  1S2 2P1 3P1 (1)D
☐ 268  28  1S2 2S1 4S1 (1)S
☐ 276  36  1S2 2S1 5S1 (1)S
☐ 289  17  1S2 2P1 3P1 (3)S
☐ 299  27  1S2 2S1 4S1 (3)S
☐ 303  31  1S2 2S1 4D1 (3)D
☐ 307  35  1S2 2S1 5S1 (3)S
☐ 333  29  1S2 2S1 4P1 (3)P
☐ 337  33  1S2 2S1 4F1 (3)F
```

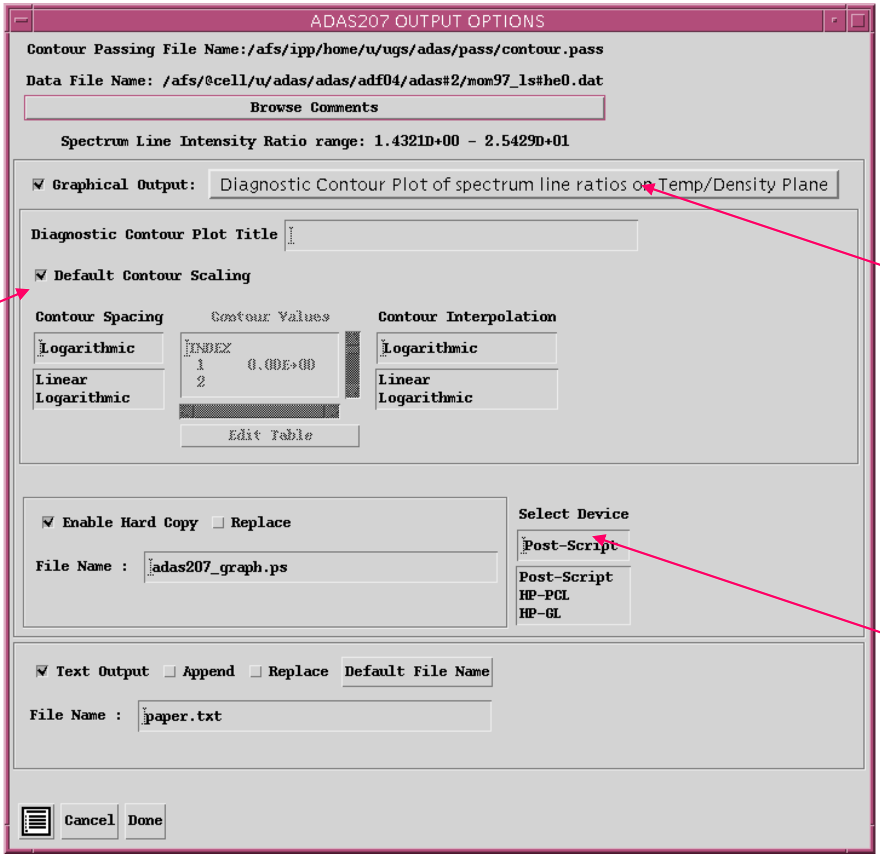
Make a maximum of 20 selections

activate for lines to be included

Displaying line ratios

- Output options
  - » The type of display of the ratio of line assemblies may be chosen.
  - » The contour form on the Te/Ne plane seems to be the favourite.
  - » Crosses on the graph mark the tabular points at which the populations were explicitly evaluated.
  - » The extensive range of controls on the plot scales and contour lines should be used to refine the diagnostic plot.

ADAS207 output



ADAS207 OUTPUT OPTIONS

Contour Passing File Name:/afs/ipp/home/u/ugs/adas/pass/contour.pass

Data File Name: /afs/@cell/u/adas/adas/adf04/adas#2/mom97_ls#he0.dat

Spectrum Line Intensity Ratio range: 1.4321D+00 - 2.5429D+01

☑ Graphical Output: Diagnostic Contour Plot of spectrum line ratios on Temp/Density Plane

Diagnostic Contour Plot Title

☑ Default Contour Scaling

Contour Spacing: Logarithmic

Contour Values

INDEX	
1	0.00E+00
2	

Contour Interpolation: Logarithmic

☑ Enable Hard Copy ☐ Replace

File Name : adas207_graph.ps

Select Device: Post-Script

☑ Text Output ☐ Append ☐ Replace

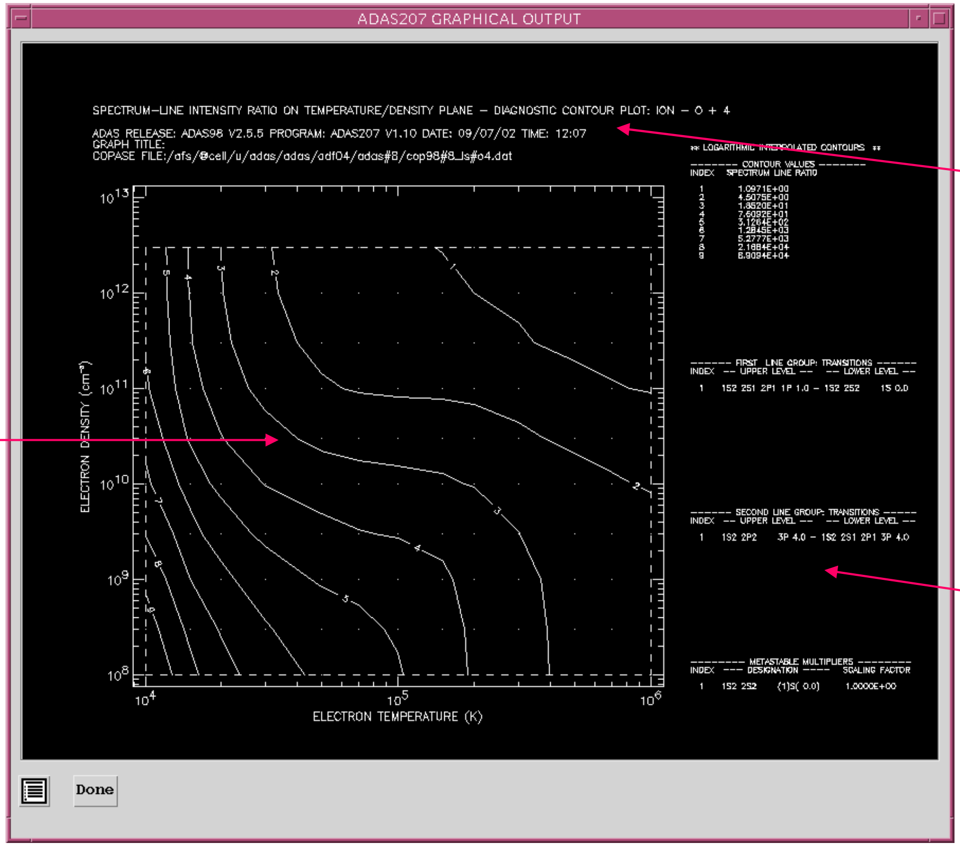
File Name : paper.txt

controls on contour plotting

select type of plot

usual graph and text output choices

ADAS207 graph



```
SPECTRUM-LINE INTENSITY RATIO ON TEMPERATURE/DENSITY PLANE - DIAGNOSTIC CONTOUR PLOT: ION - O + 4

ADAS RELEASE: ADAS98 V2.5.5 PROGRAM: ADAS207 V1.10 DATE: 09/07/02 TIME: 12:07
GRAPH TITLE:
COPASE FILE:/afs/@cell/u/adas/adas/adf04/adas#8/cop98#8_ls#o4.dat

** LOGARITHMIC INTERPOLATED CONTOURS **

-------- CONTOUR VALUES --------
INDEX    SPECTRUM LINE RATIO

  1          1.0971E+00
  2          4.5075E+00
  3          1.8520E+01
  4          7.6092E+01
  5          3.1264E+02
  6          1.2845E+03
  7          5.2777E+03
  8          2.1684E+04
  9          8.9094E+04

------- FIRST  LINE GROUP: TRANSITIONS -------
INDEX  -- UPPER LEVEL --    -- LOWER LEVEL --

  1    1S2 2S1  2P1  1P 1.0 - 1S2 2S2     1S 0.0

------- SECOND LINE GROUP: TRANSITIONS ------
INDEX  -- UPPER LEVEL --    -- LOWER LEVEL --

  1    1S2 2P2      3P 4.0 - 1S2 2S1 2P1 3P 4.0

---------- METASTABLE MULTIPLIERS ----------
INDEX  --- DESIGNATION -----    SCALING FACTOR

  1    1S2 2S2      (1)S( 0.0)       1.0000E+00
```

final line ratio contours

unique record of case studied

details of graph presented

3a. The ionisation state of ions in a plasma – part 1

- 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

Effective ionisation and recombination

- Collisional-radiative modelling
  - Full modelling for the populations of an ion also gives the collisional-radiative ionisation and recombination coefficients.

  - In basic CR modelling, the coeffts. give stage to stage connections. In GCR modelling, the coeffts. give connections between metastables within and across ionisation stages.

  - The data format ADF11 is assigned to Maxwell averaged, Te and Ne dependent CR and GCR coeffts.

Collisional-radiative theory

Then the quasi-equilibrium statistical balance is

$$\tfrac{d}{dt} N_1 = \sum_{j\neq 1} C_{1j} N_j + C_{11} N_1 + N_e N_+ r_1$$

$$0 = \sum_{j\neq 1} C_{ij} N_j + C_{i1} N_1 + N_e N_+ r_i \quad , \quad i = 2,..$$

In matrix form these become

$$\begin{bmatrix} \frac{d}{dt} N_1 \\ 0 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{1j} \\ C_{i1} & C_{ij} \end{bmatrix} \begin{bmatrix} N_1 \\ N_j \end{bmatrix} + N_e N_+ \begin{bmatrix} r_1 \\ r_i \end{bmatrix}$$

The populations of the excited levels in quasi-equilibrium, N_j^{eq} are given by

$$N_j^{eq} = -N_e N_+ \sum_{i\neq 1} C_{ji}^{-1} r_i - \sum_{i\neq 1} C_{ji}^{-1} C_{i1} N_1$$

Collisional-radiative theory (contd.)

Collisional-dielectronic ionisation coefficient

$$S_{CD} = C_{11} - \sum_{j\neq 1}\sum_{i\neq 1} C_{1j} C_{ji}^{-1} C_{i1}$$

and collisional-dielectronic recombination coefficient

$$\alpha_{CD} = r_1 - \sum_{j\neq 1}\sum_{i\neq 1} C_{1j} C_{ji}^{-1} r_i$$

$${}^{d}\!/_{dt}\, N_1 = -N_e S_{CD} N_1 + N_e \alpha_{CD} N_+$$

Collisional-radiative theory (generalised)

The ionisation coefficients

$$S_{CD,\sigma\to\upsilon} = (\mathsf{S}_{\upsilon\sigma} - \sum_{j=1}^{O}\mathsf{S}_{\upsilon j}\sum_{i=1}^{O}\mathsf{C}_{ji}^{-1}\mathsf{C}_{i\sigma})$$

the free electron recombination coefficients

$$\alpha_{CD,\upsilon'\to\rho} = (\mathsf{R}_{\rho\upsilon'} + \sum_{j=1}^{O}\mathsf{C}_{\rho j}\sum_{i=1}^{O}\mathsf{C}_{ji}^{-1}\mathsf{R}_{i\upsilon'})$$

the charge exchange recombination coefficients

$$C_{CD,\upsilon'\to\rho} = (\mathsf{Q}_{\rho\upsilon'} + \sum_{j=1}^{O}\mathsf{C}_{\rho j}\sum_{i=1}^{O}\mathsf{C}_{ji}^{-1}\mathsf{Q}_{i\upsilon'})$$

the metastable cross-coupling coefficients

$$X_{CD,\sigma\to\rho} = (\mathsf{C}_{\rho\sigma} - \sum_{j=1}^{O}\mathsf{C}_{\rho j}\sum_{i=1}^{O}\mathsf{C}_{ji}^{-1}\mathsf{C}_{i\sigma}) / N_e$$

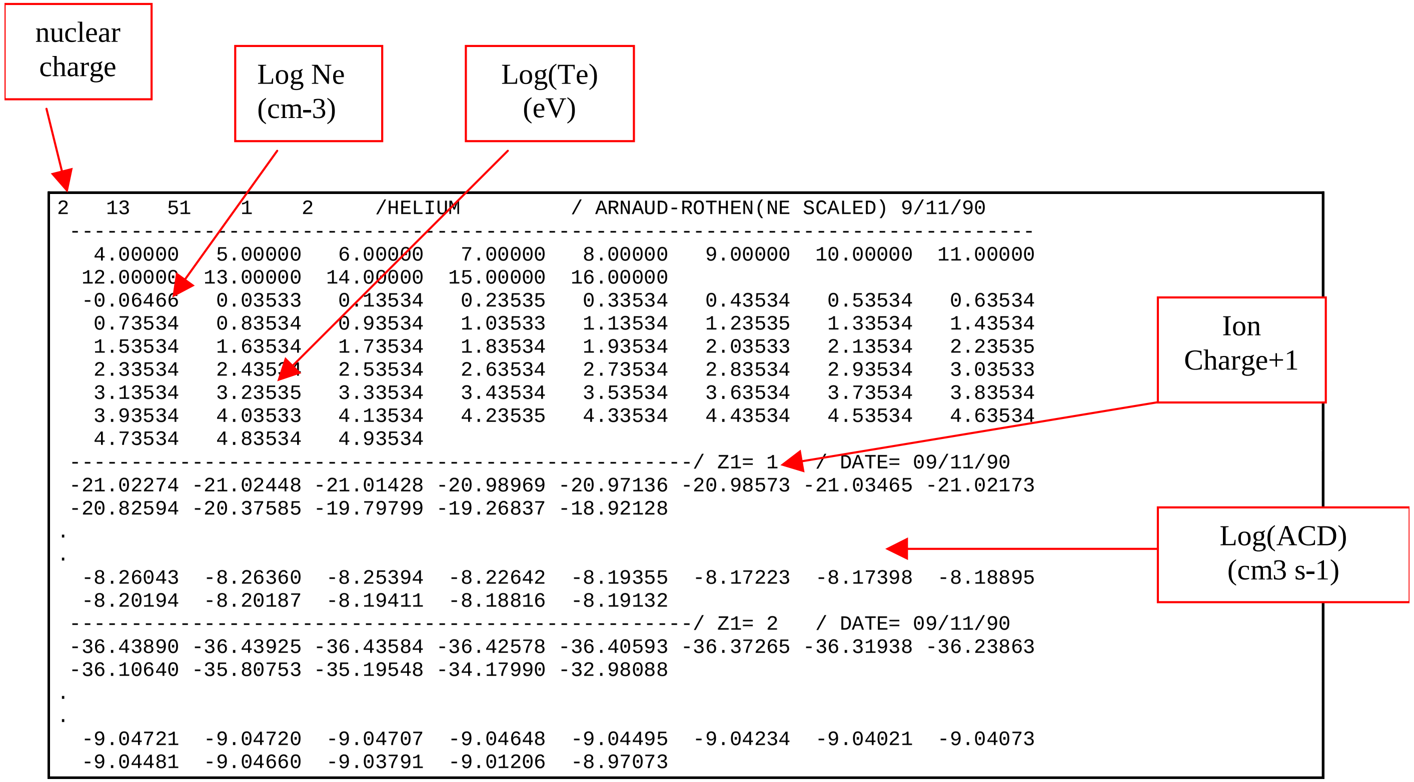
and the parent metastable cross-coupling coefficients

$$Q_{CD,\upsilon'\to\upsilon} = \sum_{j=1}^{O}\mathsf{S}_{\upsilon j}\sum_{i=1}^{O}\mathsf{C}_{ji}^{-1}\mathsf{R}_{i\upsilon'}{}_{e}$$

ADF11 iso-nuclear master file classes

Mnemonic	Class	Data prefix
ACD	Coll.-diel. recom. coefft.	R & U (or none)
SCD	Coll.-diel. ionis. coefft.	R & U (or none)
CCD	Coll.-rad. charge exch. coefft.	R & U (or none)
PRB	Coll.-diel. recom./brems. power coefft.	R & U (or none)
PRC	Coll.-rad. charge exch. recom. power coefft.	R & U (or none)
QCD	Coll.-rad. metastable cross coupling coefft.	R
XCD	Coll.-diel. parent meta. cross-coupling coefft.	R
PLT	Coll.-rad. excit. line power coefft.	R & U (or none)
PLS	Coll.-rad. specific line excit. power coefft.	R & U (or none)

ADF11 iso-nuclear master file layout (standard- unresolved)



nuclear charge

Log Ne (cm-3)

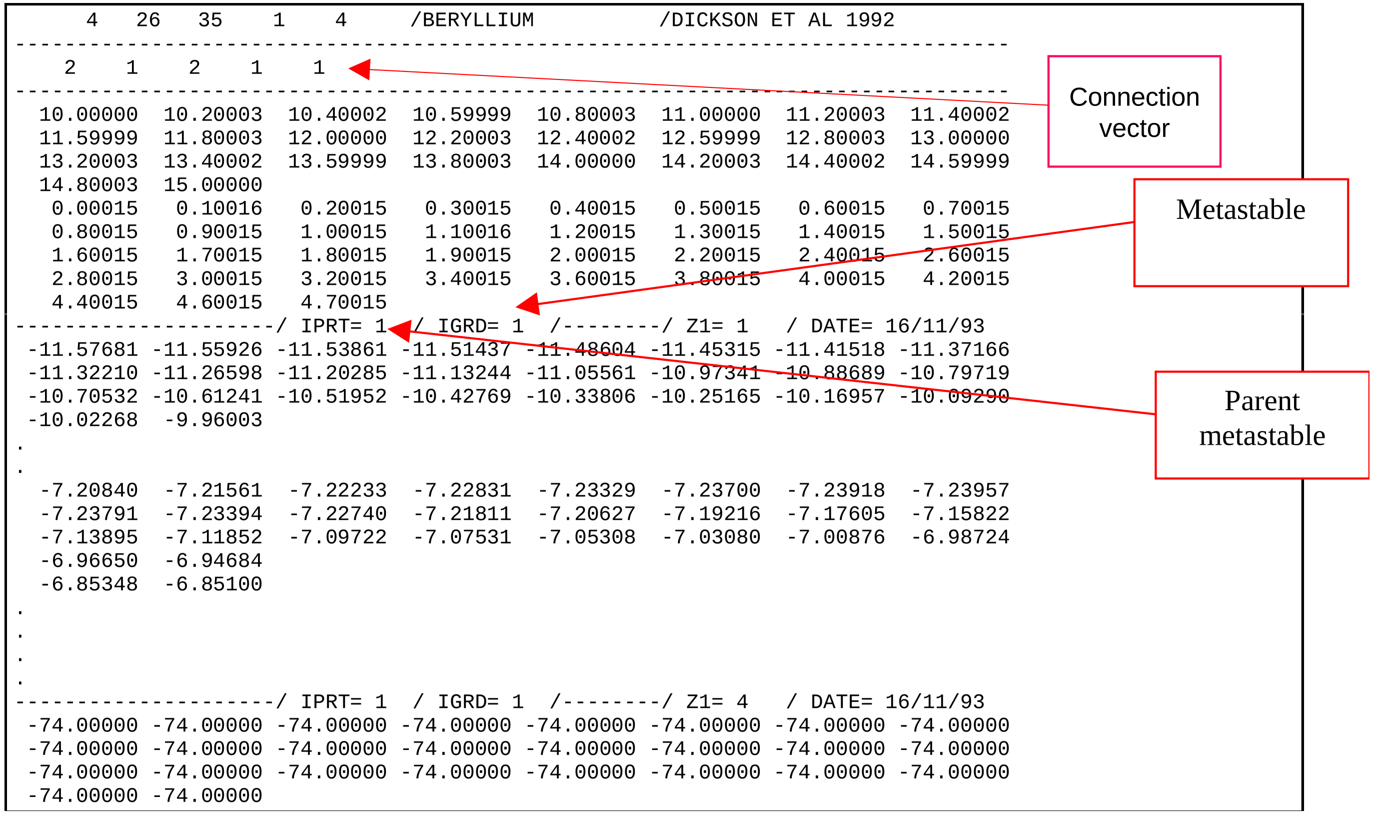
Log(Te) (eV)

Ion Charge+1

Log(ACD) (cm3 s-1)

```
2   13   51    1    2      /HELIUM         / ARNAUD-ROTHEN(NE SCALED) 9/11/90
 -------------------------------------------------------------------------------
   4.00000   5.00000   6.00000   7.00000   8.00000   9.00000  10.00000  11.00000
  12.00000  13.00000  14.00000  15.00000  16.00000
  -0.06466   0.03533   0.13534   0.23535   0.33534   0.43534   0.53534   0.63534
   0.73534   0.83534   0.93534   1.03533   1.13534   1.23535   1.33534   1.43534
   1.53534   1.63534   1.73534   1.83534   1.93534   2.03533   2.13534   2.23535
   2.33534   2.43534   2.53534   2.63534   2.73534   2.83534   2.93534   3.03533
   3.13534   3.23535   3.33534   3.43534   3.53534   3.63534   3.73534   3.83534
   3.93534   4.03533   4.13534   4.23535   4.33534   4.43534   4.53534   4.63534
   4.73534   4.83534   4.93534
 ---------------------------------------------------/ Z1= 1   / DATE= 09/11/90
 -21.02274 -21.02448 -21.01428 -20.98969 -20.97136 -20.98573 -21.03465 -21.02173
 -20.82594 -20.37585 -19.79799 -19.26837 -18.92128
.
.
  -8.26043  -8.26360  -8.25394  -8.22642  -8.19355  -8.17223  -8.17398  -8.18895
  -8.20194  -8.20187  -8.19411  -8.18816  -8.19132
 ---------------------------------------------------/ Z1= 2   / DATE= 09/11/90
 -36.43890 -36.43925 -36.43584 -36.42578 -36.40593 -36.37265 -36.31938 -36.23863
 -36.10640 -35.80753 -35.19548 -34.17990 -32.98088
.
.
  -9.04721  -9.04720  -9.04707  -9.04648  -9.04495  -9.04234  -9.04021  -9.04073
  -9.04481  -9.04660  -9.03791  -9.01206  -8.97073
```

ADF11 iso-nuclear master file layout (partial- resolved)

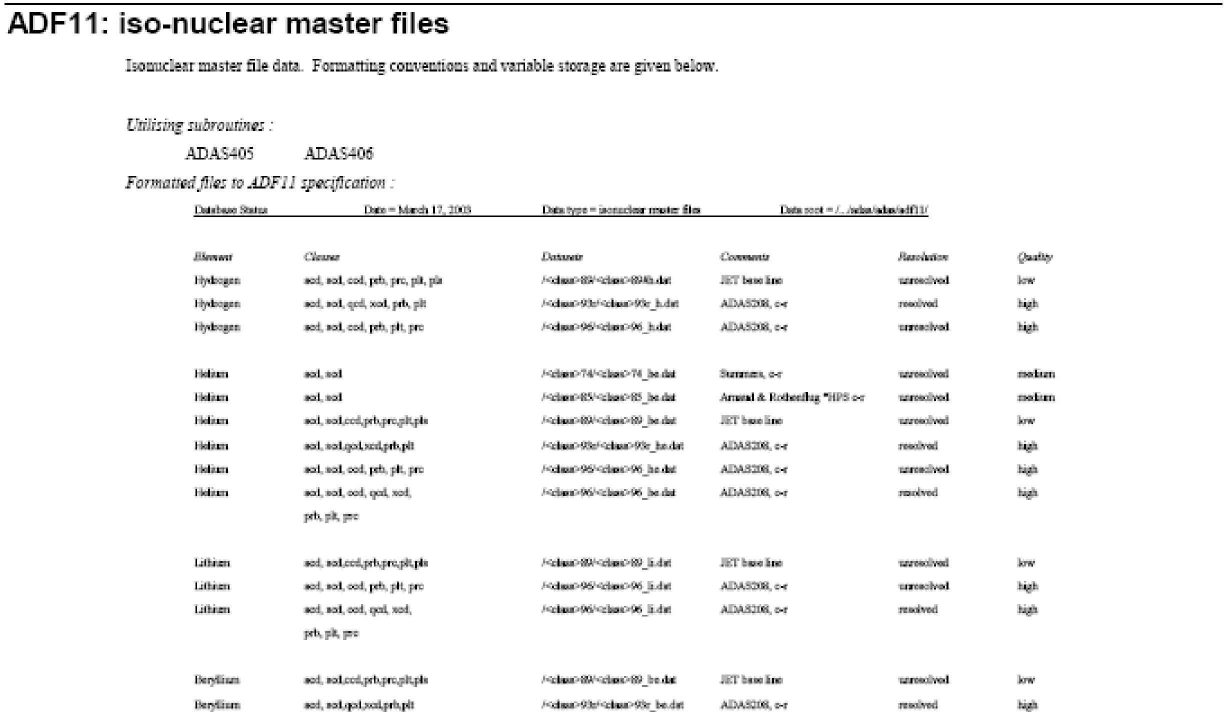


```
    4   26   35    1    4     /BERYLLIUM          /DICKSON ET AL 1992
--------------------------------------------------------------------------------
   2    1    2    1    1
--------------------------------------------------------------------------------
  10.00000  10.20003  10.40002  10.59999  10.80003  11.00000  11.20003  11.40002
  11.59999  11.80003  12.00000  12.20003  12.40002  12.59999  12.80003  13.00000
  13.20003  13.40002  13.59999  13.80003  14.00000  14.20003  14.40002  14.59999
  14.80003  15.00000
   0.00015   0.10016   0.20015   0.30015   0.40015   0.50015   0.60015   0.70015
   0.80015   0.90015   1.00015   1.10016   1.20015   1.30015   1.40015   1.50015
   1.60015   1.70015   1.80015   1.90015   2.00015   2.20015   2.40015   2.60015
   2.80015   3.00015   3.20015   3.40015   3.60015   3.80015   4.00015   4.20015
   4.40015   4.60015   4.70015
---------------------/ IPRT= 1  / IGRD= 1  /--------/ Z1= 1   / DATE= 16/11/93
 -11.57681 -11.55926 -11.53861 -11.51437 -11.48604 -11.45315 -11.41518 -11.37166
 -11.32210 -11.26598 -11.20285 -11.13244 -11.05561 -10.97341 -10.88689 -10.79719
 -10.70532 -10.61241 -10.51952 -10.42769 -10.33806 -10.25165 -10.16957 -10.09290
 -10.02268  -9.96003
.
.
  -7.20840  -7.21561  -7.22233  -7.22831  -7.23329  -7.23700  -7.23918  -7.23957
  -7.23791  -7.23394  -7.22740  -7.21811  -7.20627  -7.19216  -7.17605  -7.15822
  -7.13895  -7.11852  -7.09722  -7.07531  -7.05308  -7.03080  -7.00876  -6.98724
  -6.96650  -6.94684
  -6.85348  -6.85100
.
.
.
.
---------------------/ IPRT= 1  / IGRD= 1  /--------/ Z1= 4   / DATE= 16/11/93
 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000
 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000
 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000
 -74.00000 -74.00000
```

ADF11 (contd.)

- ADF11 year numbers
    - » baseline CR data are assigned the ‘89’ year number. They are stage to stage data and available for very many elements.
    - » GCR data on the restricted Te/Ne grid are assigned the ‘93’ year number. They are LS-coupled, metastable resolved data for selected light elements.
    - » GCR data on the extended Te/Ne grid are assigned the ‘96’ year number. They are LS-coupled, metastable resolved data for selected light elements. CR data ‘condensed’ from the GCR data is also provided.
    - » Other approximations, eg. Arnaud/Rothenflug. are available but sub-categories are generally incomplete.

appxa-11.pdf



ADF11: iso-nuclear master files

Isonuclear master file data. Formatting conventions and variable storage are given below.

Utilising subroutines :

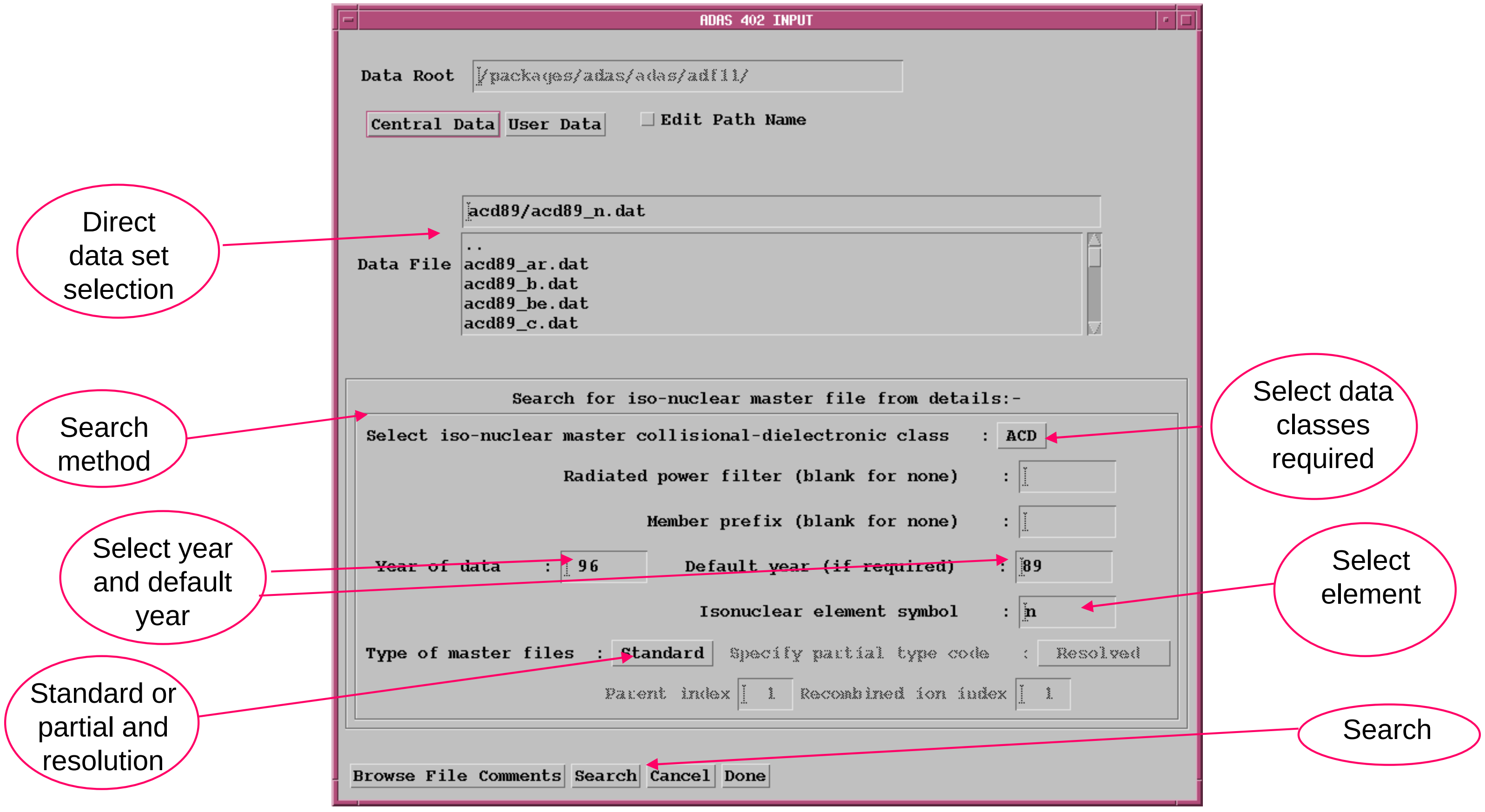
ADAS405 ADAS406

Formatted files to ADF11 specification :

Database Status Date = March 17, 2003 Data type = isonuclear master files Data root = /…/adas/adas/adf11/

Element	*Classes*	*Datasets*	*Comments*	*Resolution*	*Quality*
Hydrogen	acd, scd, ccd, prb, prc, plt, pls	/<class>89/<class>89#h.dat	JET base line	unresolved	low
Hydrogen	acd, scd, qcd, xcd, prb, plt	/<class>93r/<class>93r_h.dat	ADAS208, c-r	resolved	high
Hydrogen	acd, scd, ccd, prb, plt, prc	/<class>96/<class>96_h.dat	ADAS208, c-r	unresolved	high
Helium	acd, scd	/<class>74/<class>74_he.dat	Summers, c-r	unresolved	medium
Helium	acd, scd	/<class>85/<class>85_he.dat	Arnaud & Rothenflug *HPS c-r	unresolved	medium
Helium	acd, scd,ccd,prb,prc,plt,pls	/<class>89/<class>89_he.dat	JET base line	unresolved	low
Helium	acd, scd,qcd,xcd,prb,plt	/<class>93r/<class>93r_he.dat	ADAS208, c-r	resolved	high
Helium	acd, scd, ccd, prb, plt, prc	/<class>96/<class>96_he.dat	ADAS208, c-r	unresolved	high
Helium	acd, scd, ccd, qcd, xcd, prb, plt, prc	/<class>96/<class>96_he.dat	ADAS208, c-r	resolved	high
Lithium	acd, scd,ccd,prb,prc,plt,pls	/<class>89/<class>89_li.dat	JET base line	unresolved	low
Lithium	acd, scd, ccd, prb, plt, prc	/<class>96/<class>96_li.dat	ADAS208, c-r	unresolved	high
Lithium	acd, scd, ccd, qcd, xcd, prb, plt, prc	/<class>96/<class>96_li.dat	ADAS208, c-r	resolved	high
Beryllium	acd, scd,ccd,prb,prc,plt,pls	/<class>89/<class>89_be.dat	JET base line	unresolved	low
Beryllium	acd, scd,qcd,xcd,prb,plt	/<class>93r/<class>93r_be.dat	ADAS208, c-r	resolved	high

ADAS402 Input



ADAS 402 INPUT

Data Root /packages/adas/adas/adf11/

Central Data | User Data | ☐ Edit Path Name

Data File acd89/acd89_n.dat

..
acd89_ar.dat
acd89_b.dat
acd89_be.dat
acd89_c.dat

Search for iso-nuclear master file from details:-

Select iso-nuclear master collisional-dielectronic class : ACD

Radiated power filter (blank for none) :

Member prefix (blank for none) :

Year of data : 96

Default year (if required) : 89

Isonuclear element symbol : n

Type of master files : Standard

Specify partial type code : Resolved

Parent index 1

Recombined ion index 1

Direct data set selection

Search method

Select year and default year

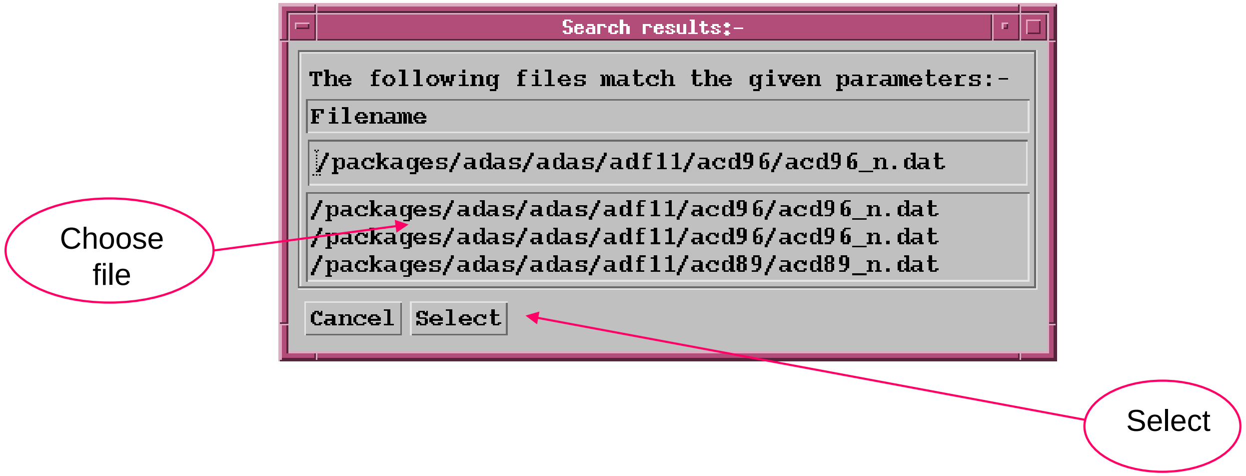
Standard or partial and resolution

Select data classes required

Select element

Search

ADAS402 Search



The following files match the given parameters:-

Filename

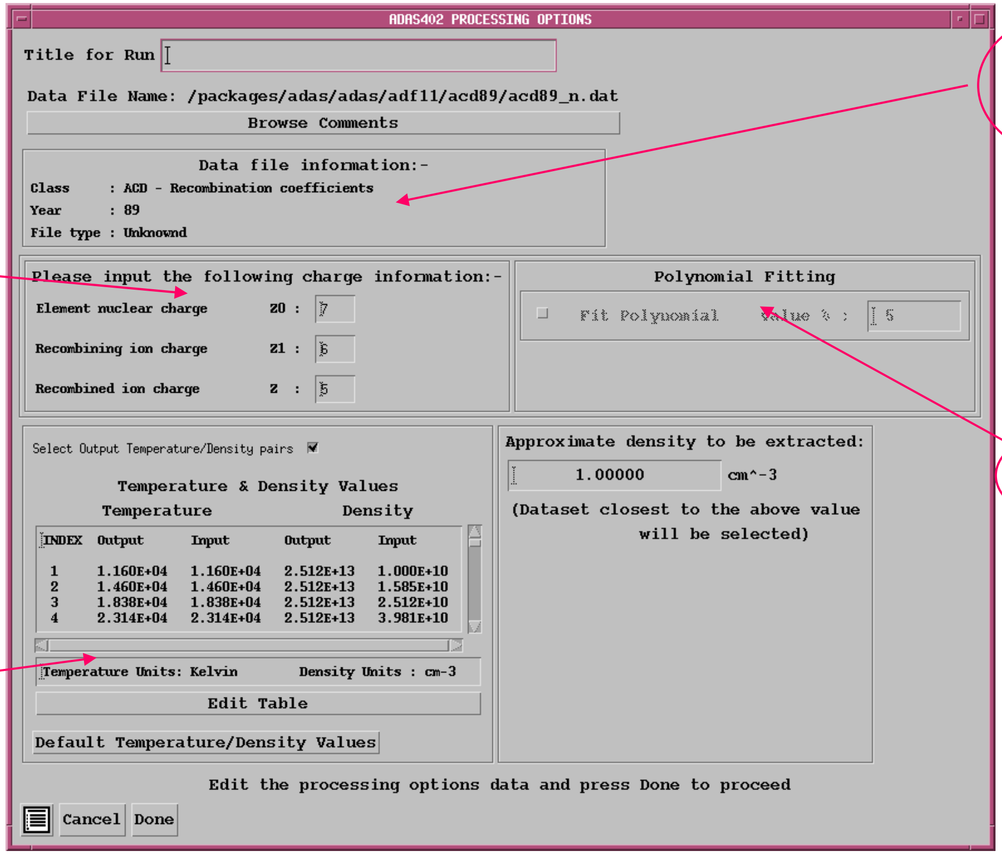
```
/packages/adas/adas/adf11/acd96/acd96_n.dat
```

```
/packages/adas/adas/adf11/acd96/acd96_n.dat
/packages/adas/adas/adf11/acd96/acd96_n.dat
/packages/adas/adas/adf11/acd89/acd89_n.dat
```

Choose file

Select

ADAS402 Processing



Title for Run

Data File Name: /packages/adas/adas/adf11/acd89/acd89_n.dat

Data file information:-

Class : ACD - Recombination coefficients
Year : 89
File type : Unknownd

Please input the following charge information:-

Element nuclear charge Z0 : 7
Recombining ion charge Z1 : 6
Recombined ion charge Z : 5

Polynomial Fitting

☐ Fit Polynomial Value % : 5

Select Output Temperature/Density pairs ☑

Temperature & Density Values

INDEX	Temperature Output	Temperature Input	Density Output	Density Input
1	1.160E+04	1.160E+04	2.512E+13	1.000E+10
2	1.460E+04	1.460E+04	2.512E+13	1.585E+10
3	1.838E+04	1.838E+04	2.512E+13	2.512E+10
4	2.314E+04	2.314E+04	2.512E+13	3.981E+10

Temperature Units: Kelvin Density Units : cm-3

Approximate density to be extracted:

1.00000 cm^-3

(Dataset closest to the above value will be selected)

Edit the processing options data and press Done to proceed

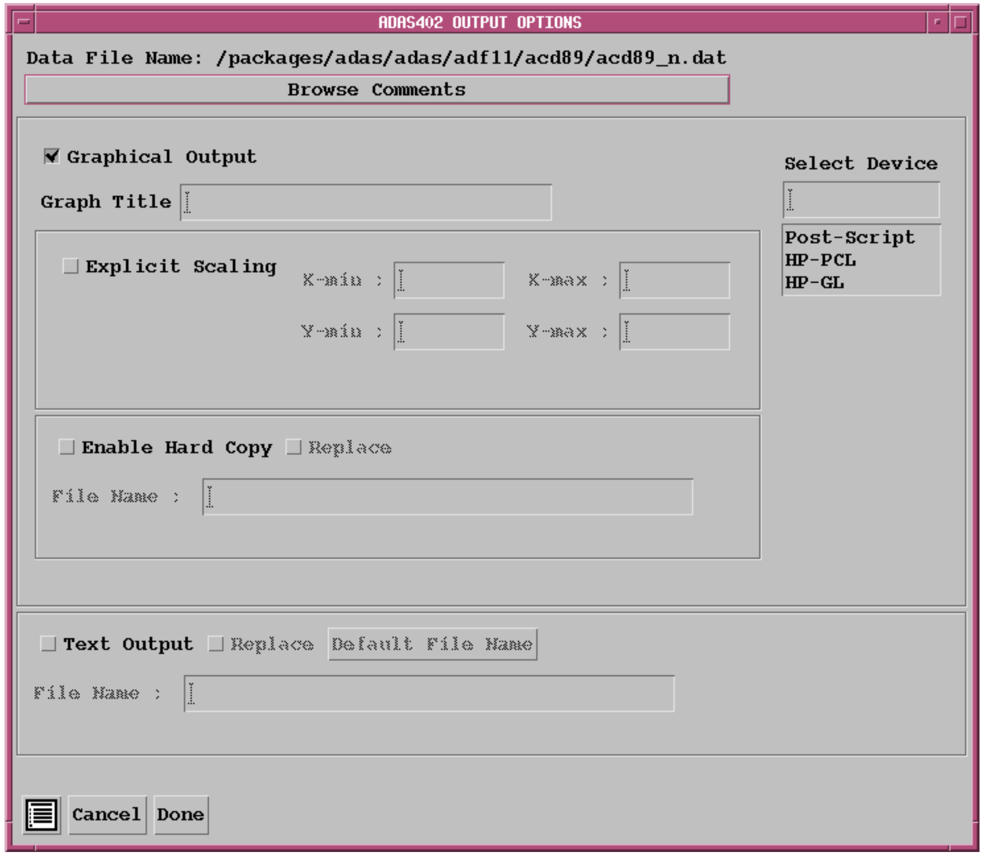
Data class selected

ion required

Polynomial fit

Specify Te/Ne pair values

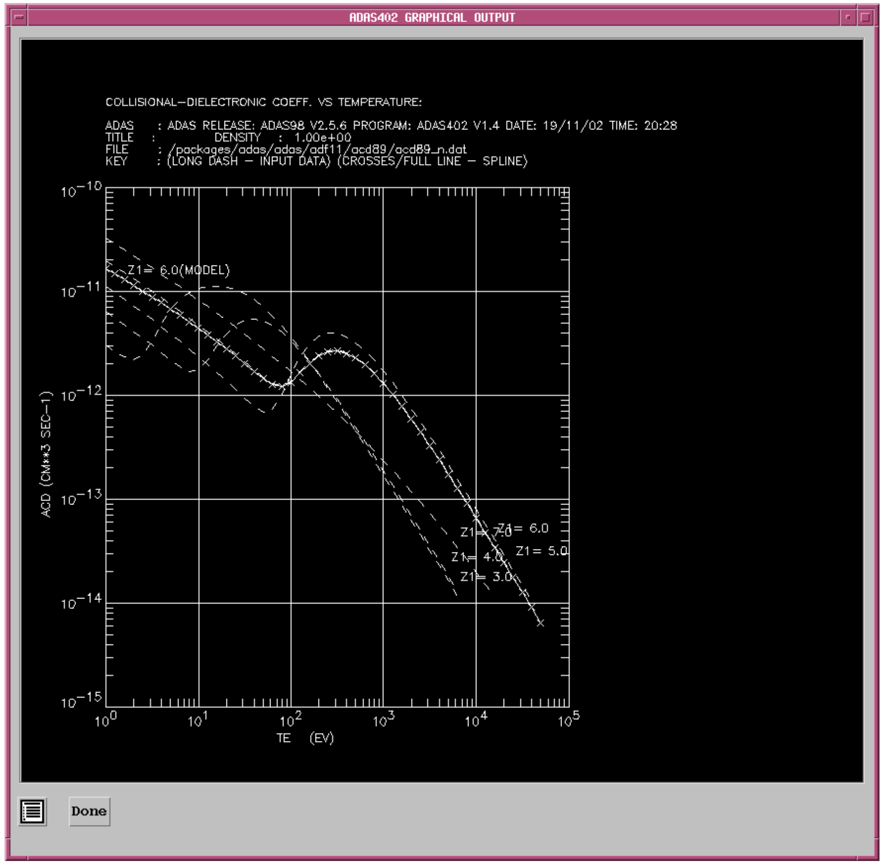
ADAS402 Output



Data File Name: /packages/adas/adas/adf11/acd89/acd89_n.dat

☑ Graphical Output

ADAS402 Graph

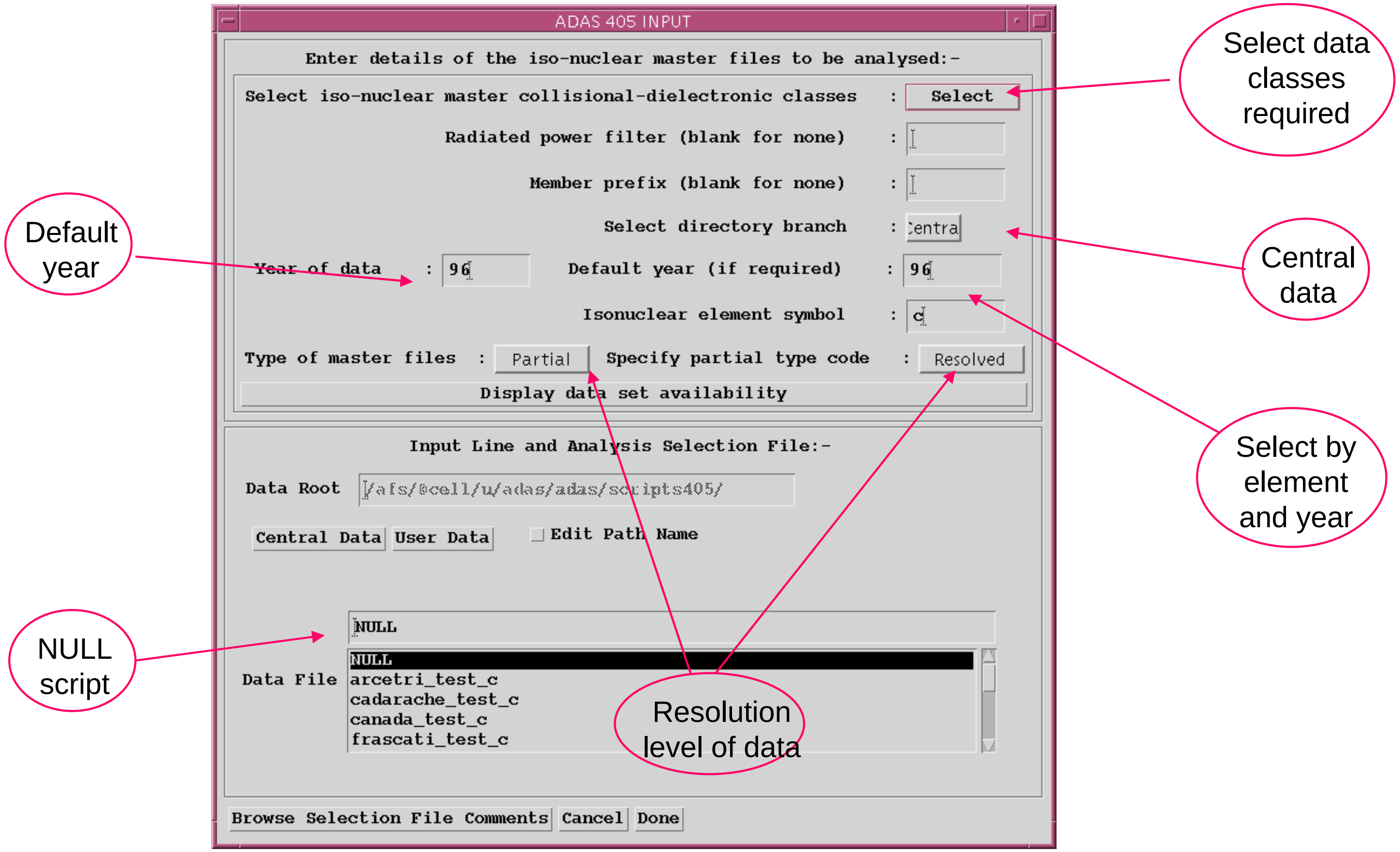


```
COLLISIONAL-DIELECTRONIC COEFF. VS TEMPERATURE:

ADAS    : ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS402 V1.4 DATE: 19/11/02 TIME: 20:28
TITLE   :          DENSITY   :  1.00e+00
FILE    : /packages/adas/adas/adf11/acd89/acd89_n.dat
KEY     : (LONG DASH - INPUT DATA) (CROSSES/FULL LINE - SPLINE)
```

Equilibrium ionisation balance

- The ionisation balance is often a weakness in the theoretical input.
- Code ADAS405 is provided for examining and contrasting ionisation balances as a function of Te and Ne.
- It has also capability for examining radiated power and the ingredients of G(Te(h),Ne(h)) functions

ADAS405 Input



ADAS 405 INPUT

Enter details of the iso-nuclear master files to be analysed:-

Select iso-nuclear master collisional-dielectronic classes : Select

Radiated power filter (blank for none) :

Member prefix (blank for none) :

Select directory branch : Centra

Year of data : 96

Default year (if required) : 96

Isonuclear element symbol : c

Type of master files : Partial

Specify partial type code : Resolved

Display data set availability

Input Line and Analysis Selection File:-

Data Root /afs/@cell/u/adas/adas/scripts405/

Central Data | User Data | ☐ Edit Path Name

Data File NULL

NULL
arcetri_test_c
cadarache_test_c
canada_test_c
frascati_test_c

Browse Selection File Comments | Cancel | Done

Select data classes required

Central data

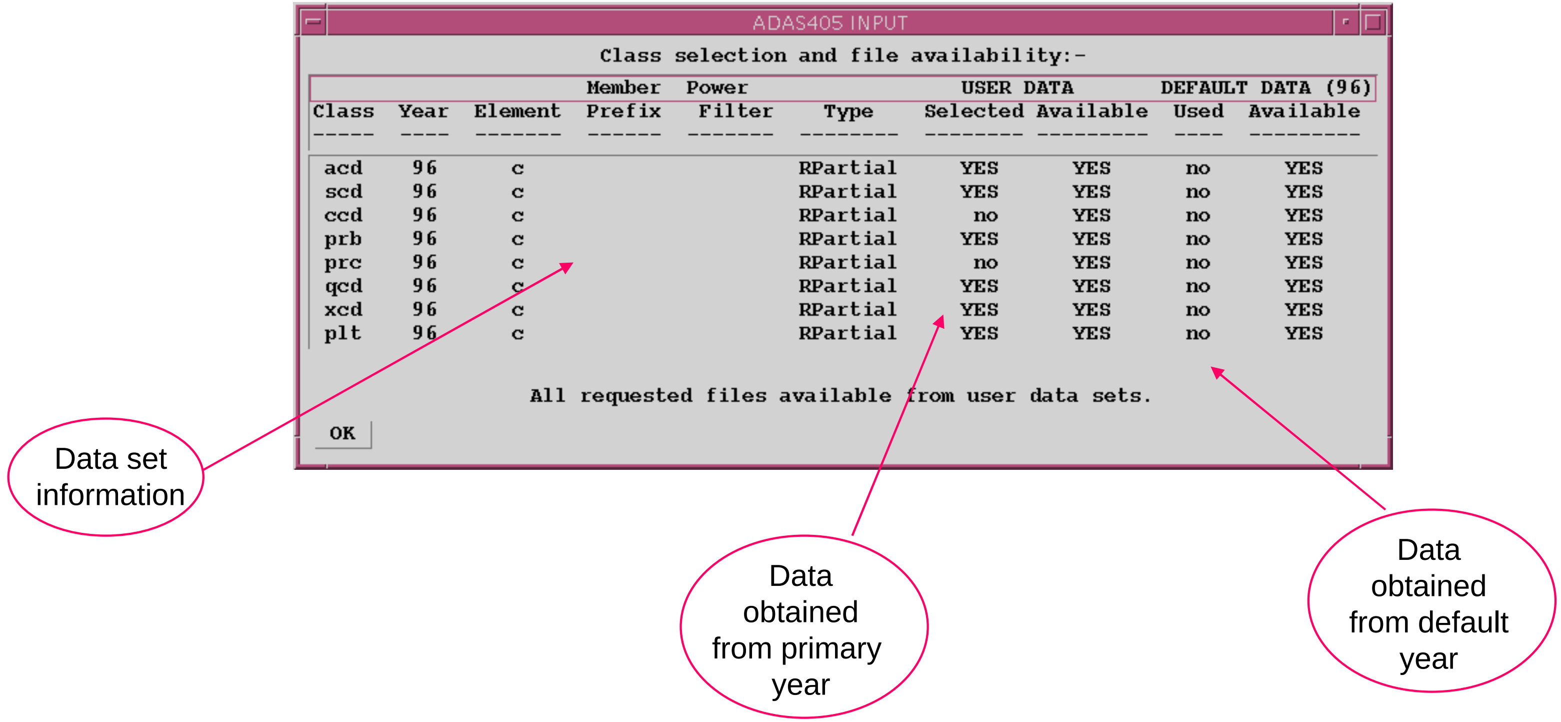
Select by element and year

Default year

NULL script

Resolution level of data

Availability of ADF11 data



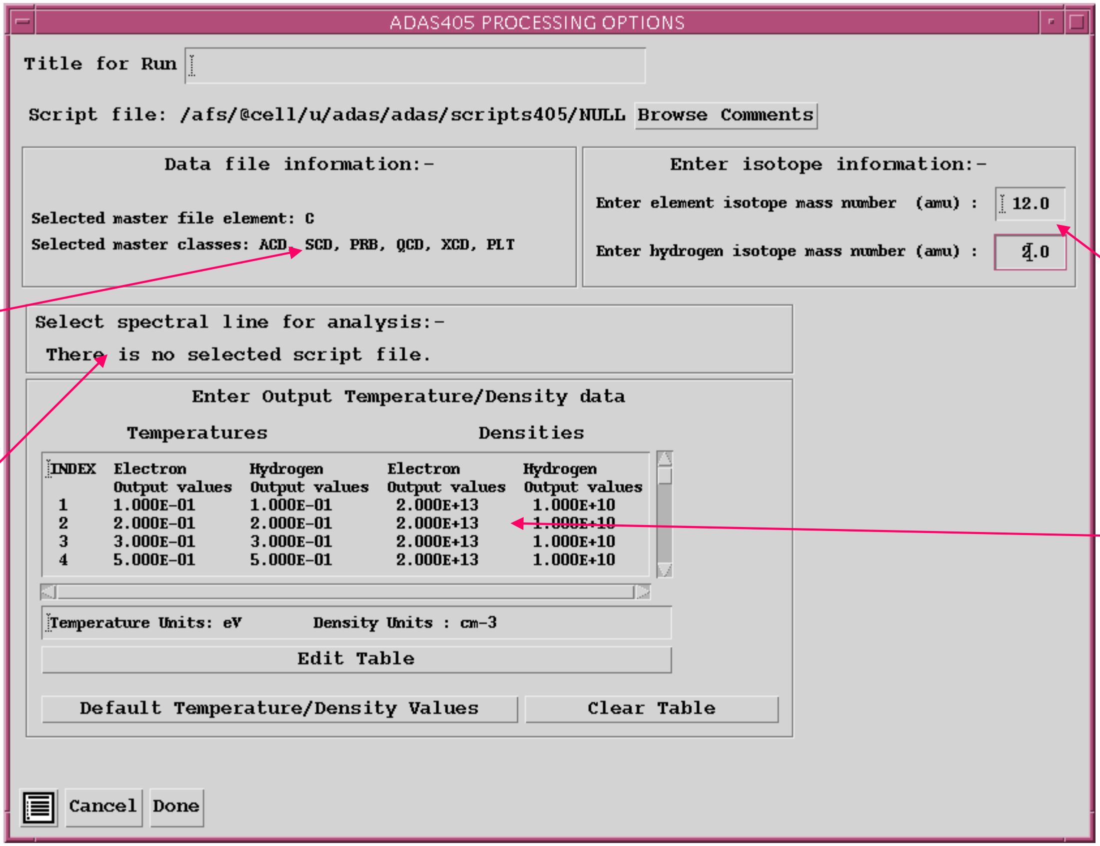
```
                  Class selection and file availability:-
                      Member  Power              USER DATA        DEFAULT DATA (96)
Class  Year  Element  Prefix  Filter    Type    Selected Available  Used  Available
-----  ----  -------  ------  -------  --------  -------- ---------  ----  ---------
 acd    96      c                      RPartial    YES      YES       no      YES
 scd    96      c                      RPartial    YES      YES       no      YES
 ccd    96      c                      RPartial     no      YES       no      YES
 prb    96      c                      RPartial    YES      YES       no      YES
 prc    96      c                      RPartial     no      YES       no      YES
 qcd    96      c                      RPartial    YES      YES       no      YES
 xcd    96      c                      RPartial    YES      YES       no      YES
 plt    96      c                      RPartial    YES      YES       no      YES

            All requested files available from user data sets.
```

Data set information

Data obtained from primary year

Data obtained from default year

ADAS405 processing



Title for Run

Script file: /afs/@cell/u/adas/adas/scripts405/NULL

Data file information:-

Selected master file element: C

Selected master classes: ACD, SCD, PRB, QCD, XCD, PLT

Enter isotope information:-

Enter element isotope mass number (amu) : 12.0

Enter hydrogen isotope mass number (amu) : 2.0

Select spectral line for analysis:-

There is no selected script file.

Enter Output Temperature/Density data

INDEX	Temperatures Electron Output values	 Hydrogen Output values	Densities Electron Output values	 Hydrogen Output values
1	1.000E-01	1.000E-01	2.000E+13	1.000E+10
2	2.000E-01	2.000E-01	2.000E+13	1.000E+10
3	3.000E-01	3.000E-01	2.000E+13	1.000E+10
4	5.000E-01	5.000E-01	2.000E+13	1.000E+10

Temperature Units: eV Density Units : cm-3

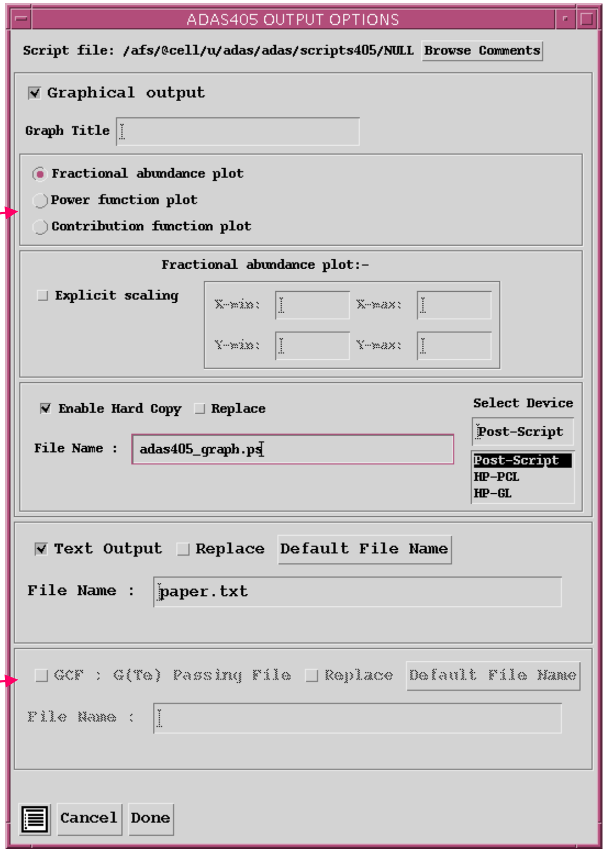
ADF11 classes selected

No script file present- no lines for selection

Set element parameters

Select Te and Ne pairs

ADAS405 Output



Script file: /afs/@cell/u/adas/adas/scripts405/NULL

☑ Graphical output

Graph Title

● Fractional abundance plot
○ Power function plot
○ Contribution function plot

Fractional abundance plot:-

☐ Explicit scaling   X-min: X-max: Y-min: Y-max:

☑ Enable Hard Copy ☐ Replace

File Name : adas405_graph.ps

Select Device: Post-Script

☑ Text Output ☐ Replace

File Name : paper.txt

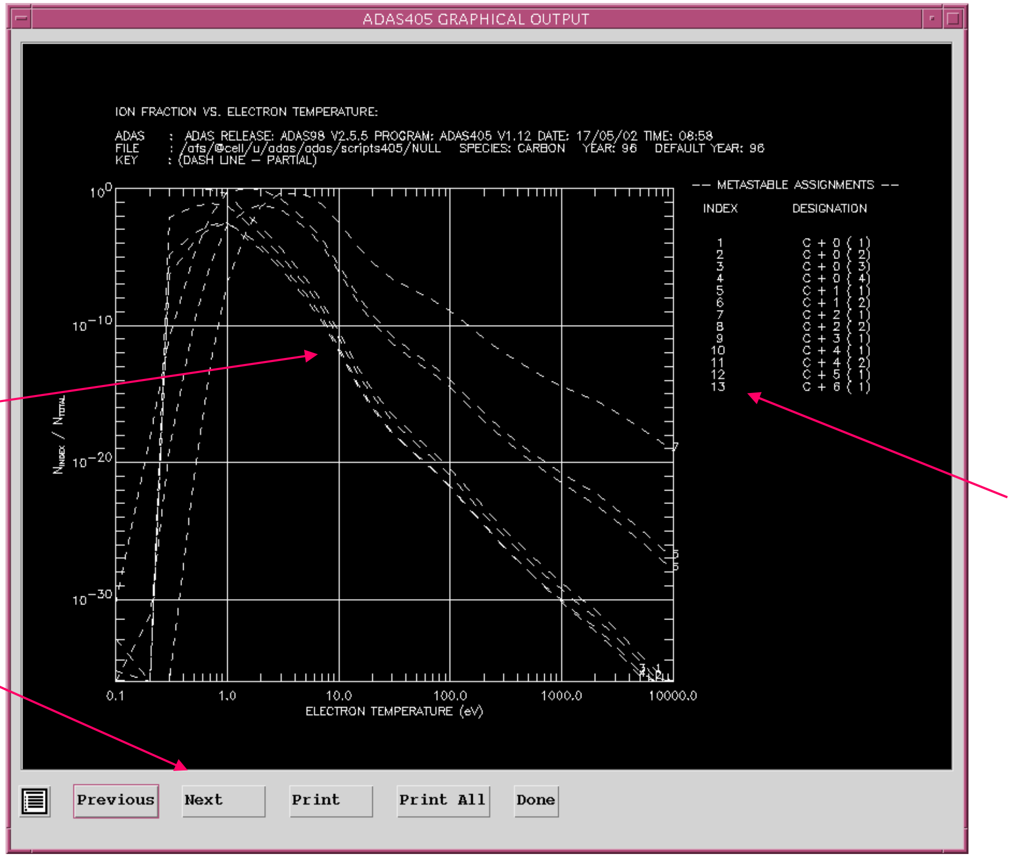
☐ GCF : G(Te) Passing File ☐ Replace

File Name :

Choice of graphs

No GCF output since no script

ADAS405 fractional abundance graph



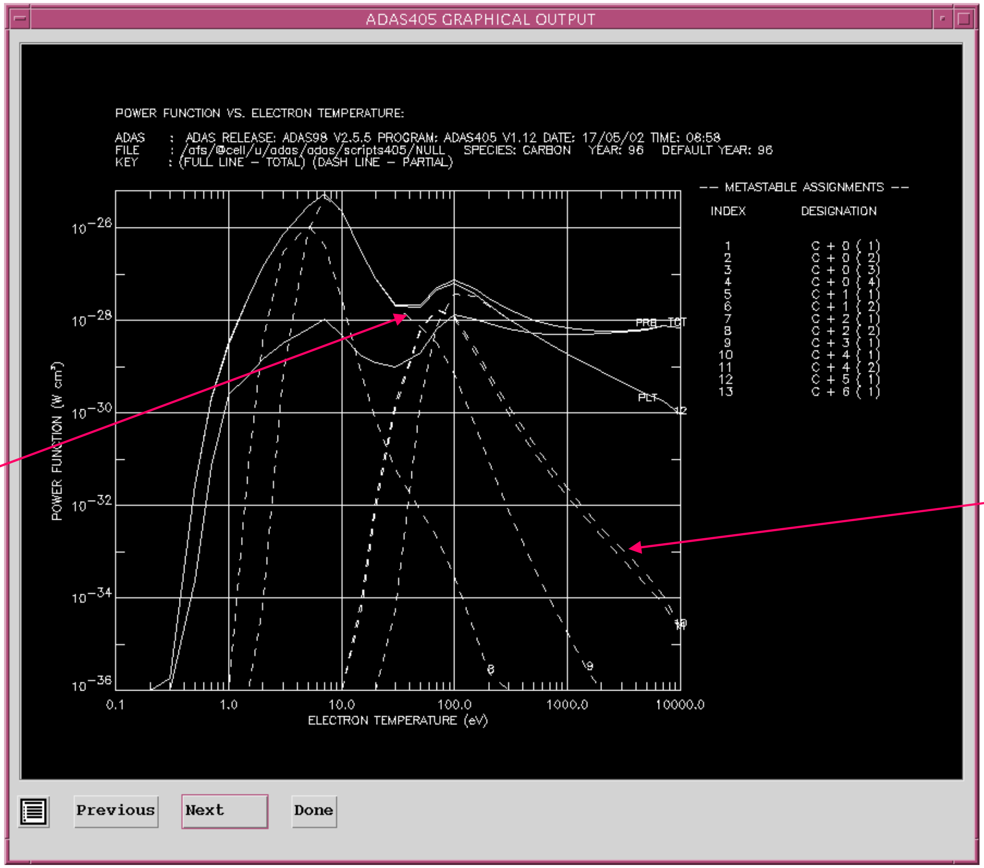
```
ION FRACTION VS. ELECTRON TEMPERATURE:

ADAS    :  ADAS RELEASE: ADAS98 V2.5.5 PROGRAM: ADAS405 V1.12 DATE: 17/05/02 TIME: 08:58
FILE    : /afs/@cell/u/adas/adas/scripts405/NULL   SPECIES: CARBON   YEAR: 96   DEFAULT YEAR: 96
KEY     : (DASH LINE - PARTIAL)

-- METASTABLE ASSIGNMENTS --

 INDEX        DESIGNATION

   1           C + 0 ( 1)
   2           C + 0 ( 2)
   3           C + 0 ( 3)
   4           C + 0 ( 4)
   5           C + 1 ( 1)
   6           C + 1 ( 2)
   7           C + 2 ( 1)
   8           C + 2 ( 2)
   9           C + 3 ( 1)
  10           C + 4 ( 1)
  11           C + 4 ( 2)
  12           C + 5 ( 1)
  13           C + 6 ( 1)
```

Fractional abundances - seven curves / screen

Page through graphs

Index - note metastable resolved case

ADAS405 power graph



```
POWER FUNCTION VS. ELECTRON TEMPERATURE:

ADAS    :  ADAS RELEASE: ADAS98 V2.5.5 PROGRAM: ADAS405 V1.12 DATE: 17/05/02 TIME: 08:58
FILE    : /afs/@cell/u/adas/adas/scripts405/NULL   SPECIES: CARBON   YEAR: 96   DEFAULT YEAR: 96
KEY     : (FULL LINE - TOTAL) (DASH LINE - PARTIAL)
```

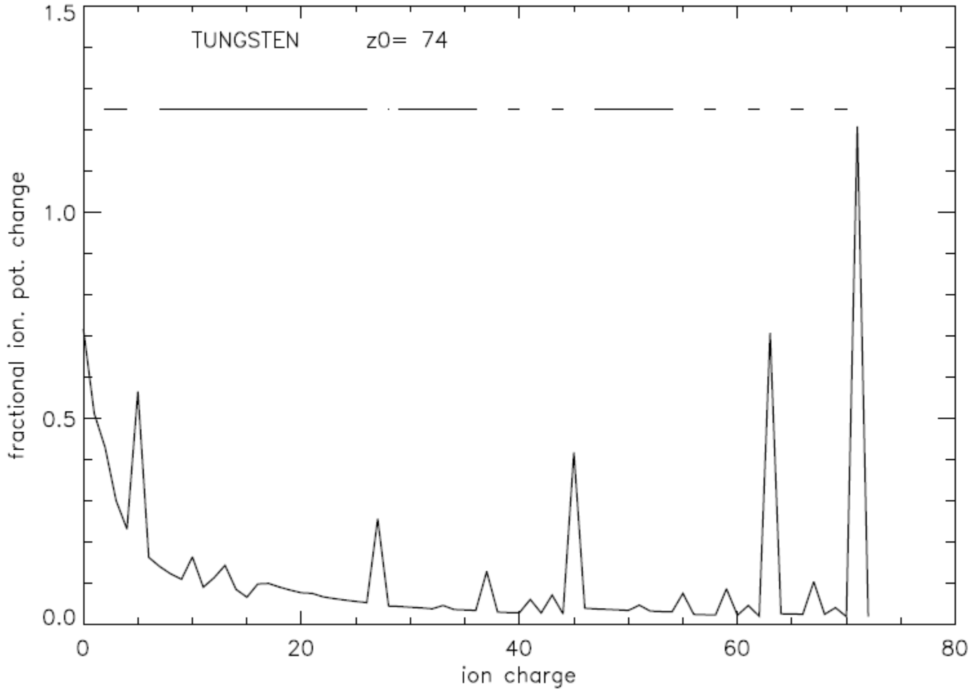
```
-- METASTABLE ASSIGNMENTS --

 INDEX        DESIGNATION

   1          C + 0 ( 1)
   2          C + 0 ( 2)
   3          C + 0 ( 3)
   4          C + 0 ( 4)
   5          C + 1 ( 1)
   6          C + 1 ( 2)
   7          C + 2 ( 1)
   8          C + 2 ( 2)
   9          C + 3 ( 1)
  10          C + 4 ( 1)
  11          C + 4 ( 2)
  12          C + 5 ( 1)
  13          C + 6 ( 1)
```

Total power and components

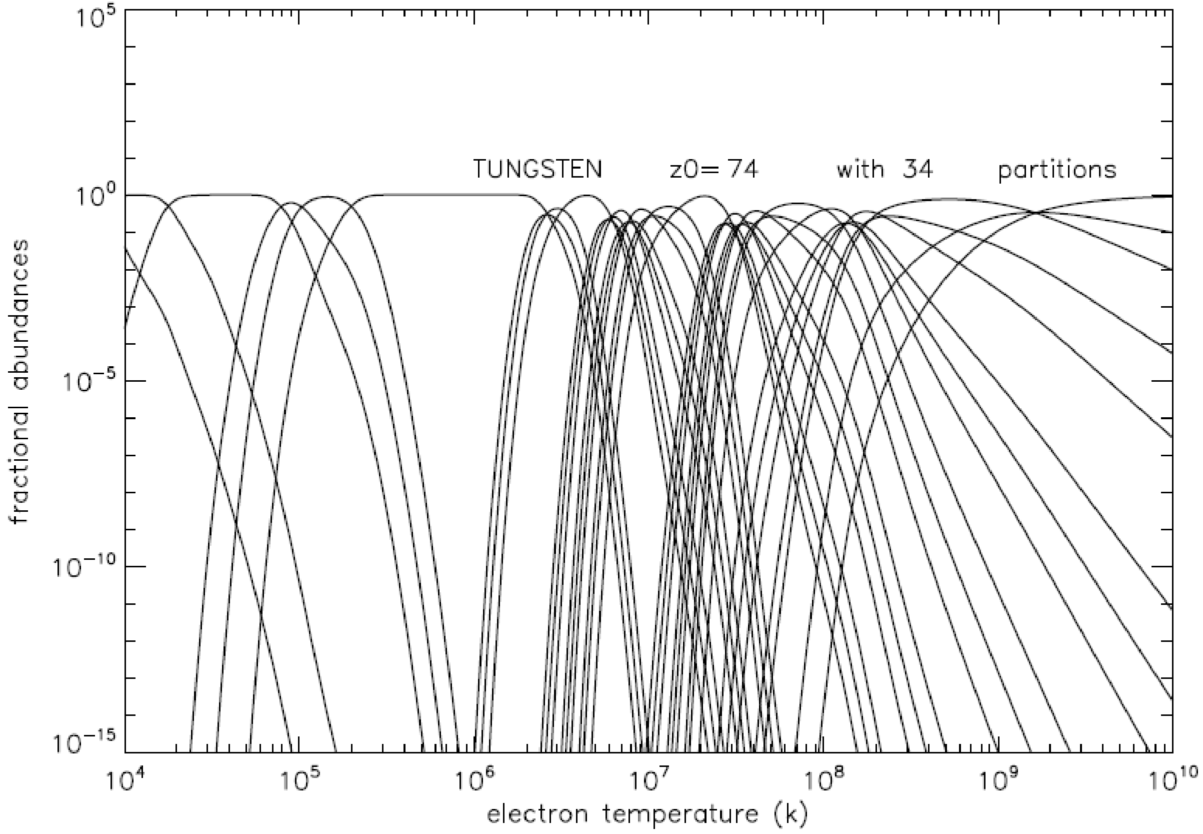
Metastable contributions to total

Superstages and partitions

- Another IDL procedure: *preview_natural_partition.pro*



Natural partition ionisation balance for tungsten

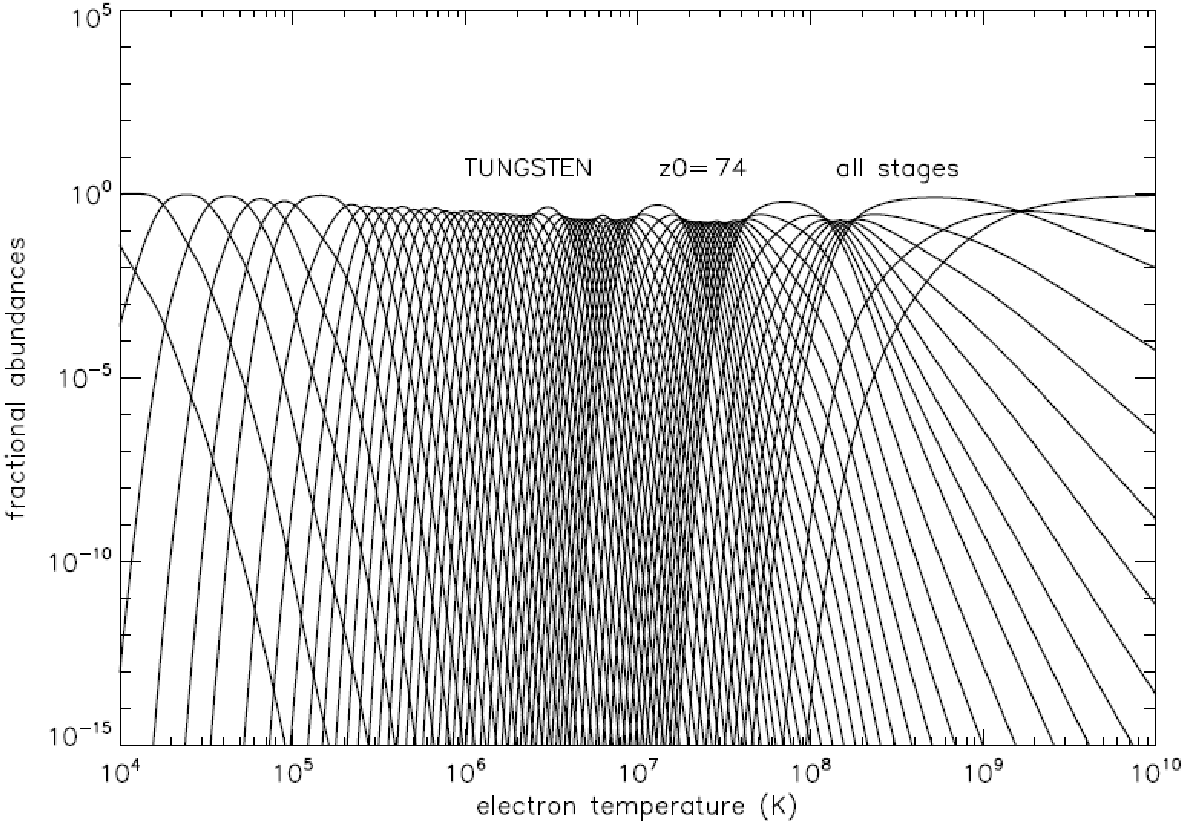


3b. The ionisation state of ions in a plasma – part 2

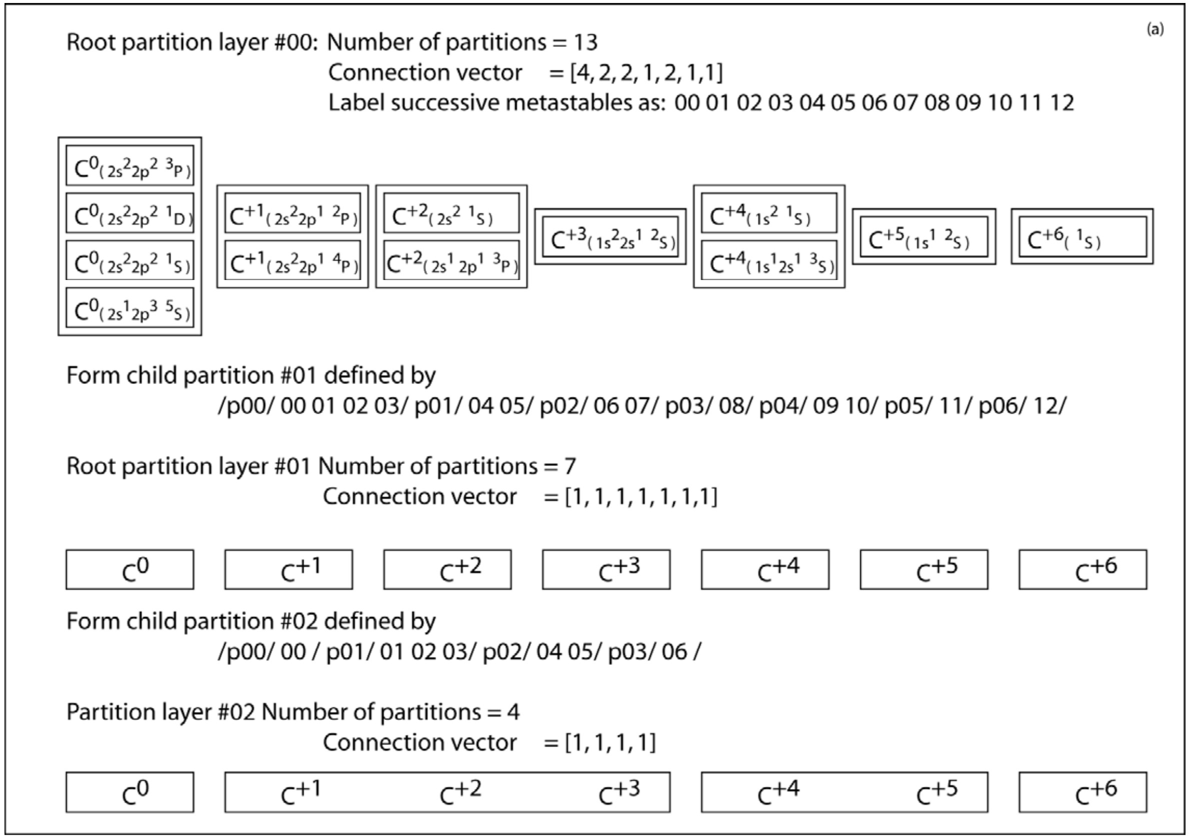
- Superstage compression
  - » Extension of the ADF11 data classes
  - » The root partitions and specification of a new partition
  - » ADAS416

- 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

Stage to stage (unresolved root partition) ionisation balance for tungsten



Main ideas based on carbon as an illustration



(a)

Root partition layer #00: Number of partitions = 13
Connection vector = [4, 2, 2, 1, 2, 1, 1]
Label successive metastables as: 00 01 02 03 04 05 06 07 08 09 10 11 12

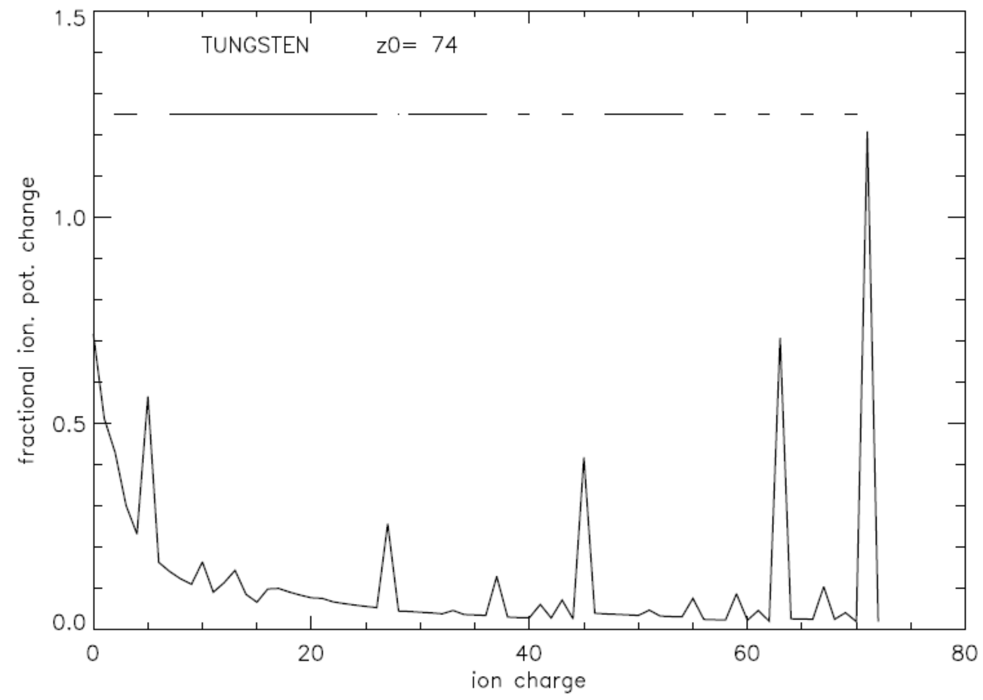
Form child partition #01 defined by
/p00/ 00 01 02 03/ p01/ 04 05/ p02/ 06 07/ p03/ 08/ p04/ 09 10/ p05/ 11/ p06/ 12/

Root partition layer #01 Number of partitions = 7
Connection vector = [1, 1, 1, 1, 1, 1, 1]

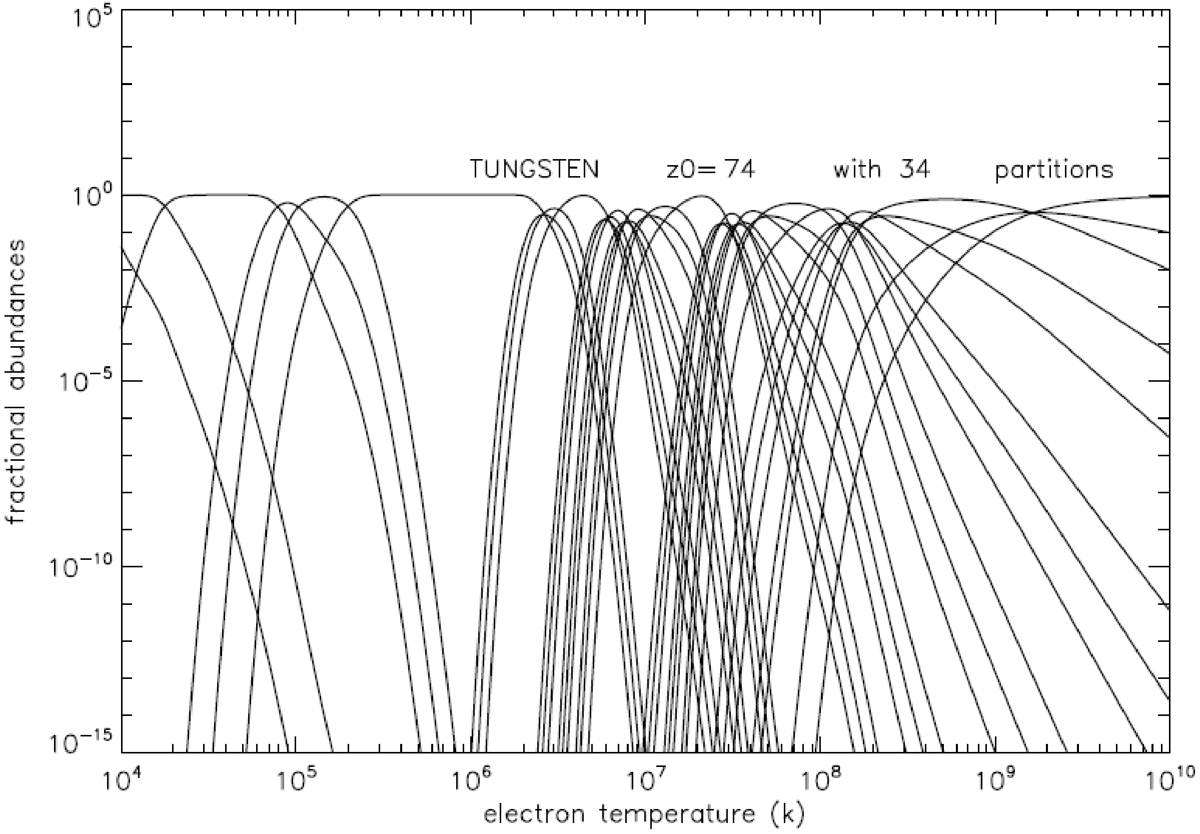
Form child partition #02 defined by
/p00/ 00 / p01/ 01 02 03/ p02/ 04 05/ p03/ 06 /

Partition layer #02 Number of partitions = 4
Connection vector = [1, 1, 1, 1]

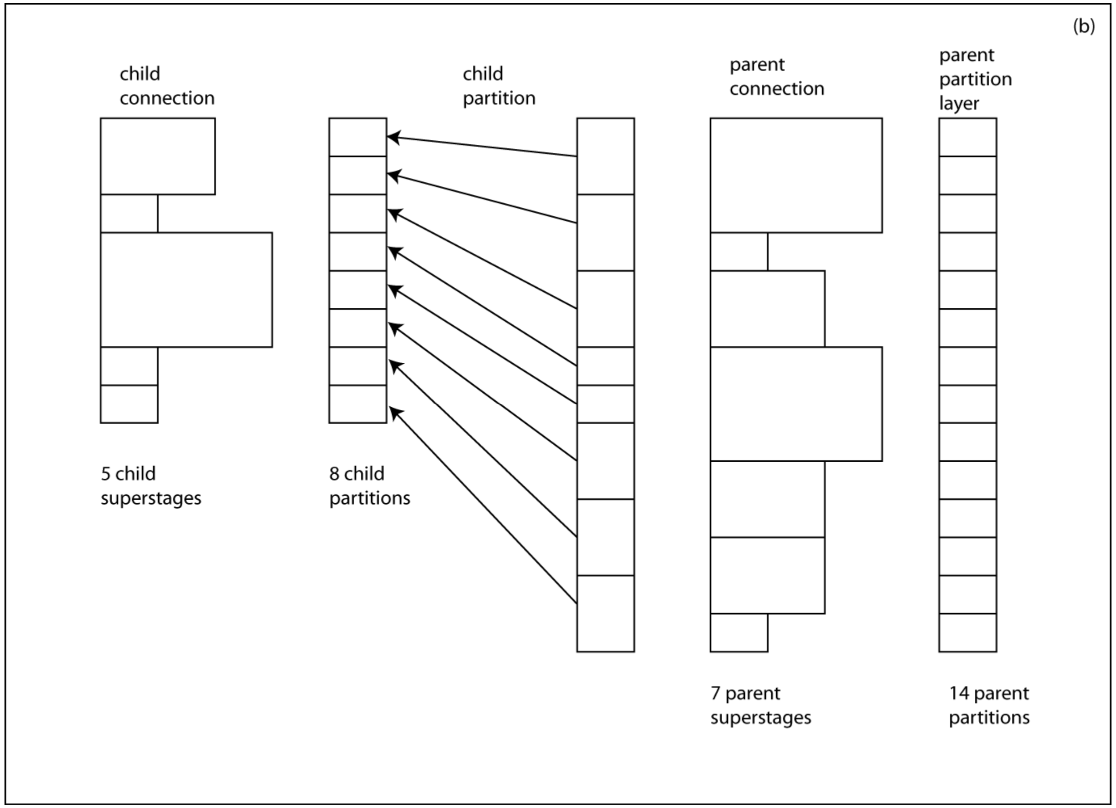
Superstages and partitions



Natural partition ionisation balance for tungsten



Partitioning



adf11 tungsten acd

an unresolved - #01 partition level

```
 74     8   24     1    6     /TUNGSTEN      /ACD /GCR PROJECT
--------------------------------------------------------------------------------
//#02/p00/ 00 01/
      p01/ 02 03 04 05/
      p02/ 06 07 08 09 10 11 12/
      p03/ 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27/
      p04/ 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45/
      p05/ 46 47 48 49 50 51 52 53 54 55/
      p06/ 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74/
//#01/p00/ 00/p01/ 01/p02/ 02/p03/ 03/p04/ 04/p05/ 05/p06/ 06/p07/ 07/
      p08/ 08/p09/ 09/p10/ 10/p11/ 11/p12/ 12/p13/ 13/p14/ 14/p15/ 15/
      p16/ 16/p17/ 17/p18/ 18/p19/ 19/p20/ 20/p21/ 21/p22/ 22/p23/ 23/
      p24/ 24/p25/ 25/p26/ 26/p27/ 27/p28/ 28/p29/ 29/p30/ 30/p31/ 31/
      p32/ 32/p33/ 33/p34/ 34/p35/ 35/p36/ 36/p37/ 37/p38/ 38/p39/ 39/
      p40/ 40/p41/ 41/p42/ 42/p43/ 43/p44/ 44/p45/ 45/p46/ 46/p47/ 47/
      p48/ 48/p49/ 49/p50/ 50/p51/ 51/p52/ 52/p53/ 53/p54/ 54/p55/ 55/
      p56/ 56/p57/ 57/p58/ 58/p59/ 59/p60/ 60/p61/ 61/p62/ 62/p63/ 63/
      p64/ 64/p65/ 65/p66/ 66/p67/ 67/p68/ 68/p69/ 69/p70/ 70/p71/ 71/
      p72/ 72/p73/ 73/p74/ 74/
--------------------------------------------------------------------------------
  10.00000  10.67128  11.34256  12.01384  12.68513  13.35641  14.02769  14.69897
  -0.30103  -0.13086   0.03930   0.20947   0.37963   0.54980   0.71996   0.89013
   1.06030   1.23046   1.40063   1.57079   1.74096   1.91113   2.08129   2.25146
   2.42162   2.59179   2.76195   2.93212   3.10229   3.27245   3.44262   3.61278
---------------------/ ISPP= 1  / ISPB= 1  /--------/ S1= 1   / DATE= 12:09:05
 -11.64510 -11.66588 -11.69610 -11.71692 -11.74369 -11.74369 -12.74277 -12.74277
```

partition
specification

unresolved child
partition level
#02

adf11 format class extensions

class index		type content
1	acd	effective recombination coefficients
2	scd	effective ionisation coefficients
3	ccd	CX recombination coeffts
4	prb	recomb/brems power coeffts
5	prc	CX power coeffts
6*	qcd	base meta. coupl. coeffts
7*	xcd	parent metastable coupling coeffts
8	plt	low level line power coeffts
9	pls	representative line power coefficient
10	zcd	effective charge
11	ycd	effective squared charge
12	ecd	effective ionisation potential

* Only present with metastable resolved cases (1996 data)

Useful codes and procedures

- *preview_natural_partition.pro*

- *xxdata_11.for*, *xxdata_11.pro* and *read_adf11.pro* are all able to read the extended data classes and the partition information in the data sets

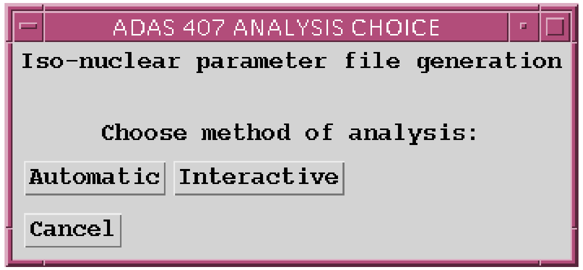
- The interactive series 4 code ADAS416 implements superstage compression and outputs a complete set of new (compressed) ADF11 datasets. See also

  run_adas416.pro

Preparing baseline ADF11 data

- The most basic ADAS calculation of stage to stage ADF11 datasets for an element uses codes ADAS407 and ADAS408.
- ADAS407 processes mass produced ADF04 files for an element, extracting approximate form parameters (ADF03).
- ADAS408 uses ADF03 parameters to generate the ADF11 datasets.

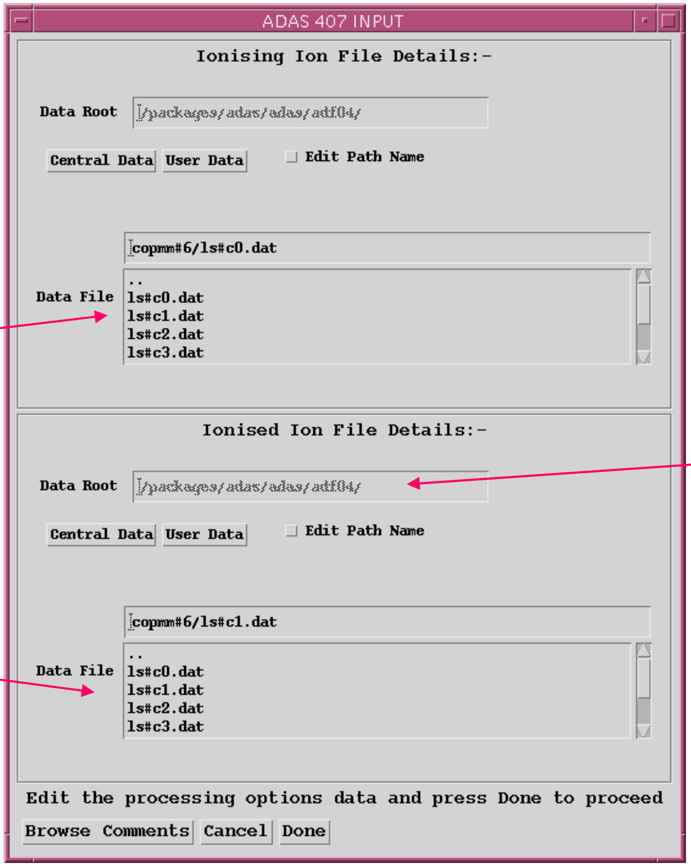
ADAS407 Analysis Choice



Iso-nuclear parameter file generation

Choose method of analysis:

ADAS407 Input



Ionising Ion File Details:-

Data Root /packages/adas/adas/adf04/

Data File copmm#6/ls#c0.dat

```
..
ls#c0.dat
ls#c1.dat
ls#c2.dat
ls#c3.dat
```

Ionised Ion File Details:-

Data Root /packages/adas/adas/adf04/

Data File copmm#6/ls#c1.dat

```
..
ls#c0.dat
ls#c1.dat
ls#c2.dat
ls#c3.dat
```

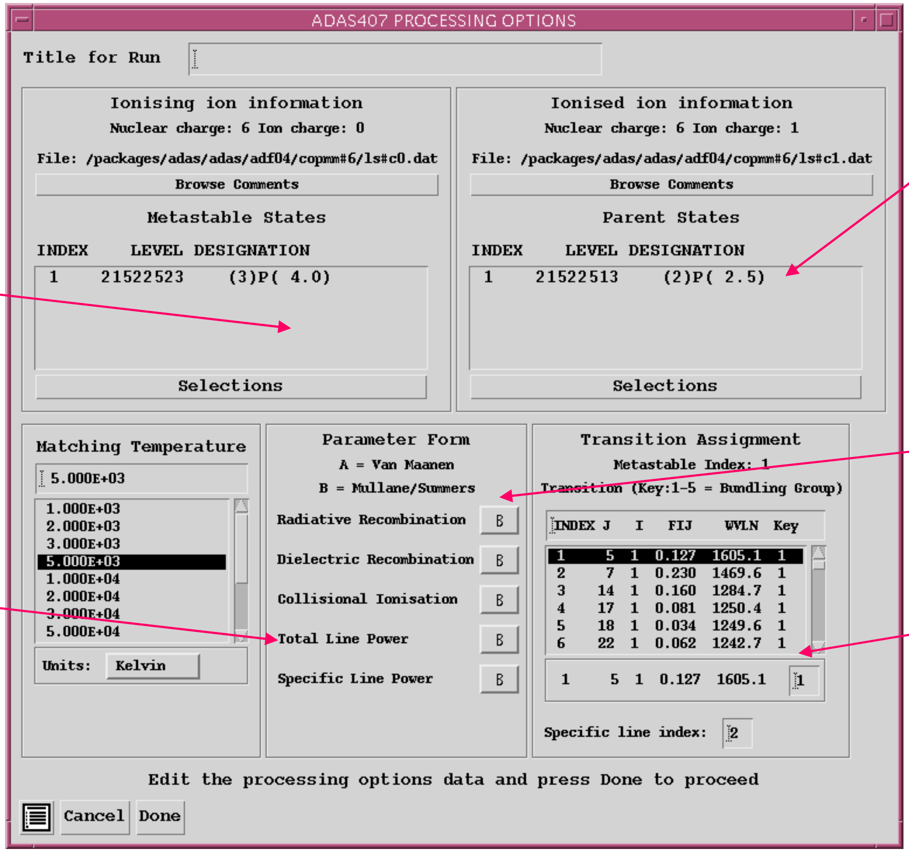
Edit the processing options data and press Done to proceed

Choose adf04 file of ionising ion

file name set automatically copss or copmm type

Choose adf04 file of ionised stage

ADAS407 Processing



Title for Run

Ionising ion information

Nuclear charge: 6 Ion charge: 0

File: /packages/adas/adas/adf04/copmm#6/ls#c0.dat

Metastable States

INDEX	LEVEL	DESIGNATION
1	21522523	(3)P(4.0)

Ionised ion information

Nuclear charge: 6 Ion charge: 1

File: /packages/adas/adas/adf04/copmm#6/ls#c1.dat

Parent States

INDEX	LEVEL	DESIGNATION
1	21522513	(2)P(2.5)

Matching Temperature

5.000E+03

1.000E+03
2.000E+03
3.000E+03
5.000E+03
1.000E+04
2.000E+04
3.000E+04
5.000E+04

Units: Kelvin

Parameter Form

A = Van Maanen
B = Mullane/Summers

Radiative Recombination B
Dielectric Recombination B
Collisional Ionisation B
Total Line Power B
Specific Line Power B

Transition Assignment

Metastable Index: 1

Transition (Key:1-5 = Bundling Group)

INDEX	J	I	FIJ	WVLN	Key
1	5	1	0.127	1605.1	1
2	7	1	0.230	1469.6	1
3	14	1	0.160	1284.7	1
4	17	1	0.081	1250.4	1
5	18	1	0.034	1249.6	1
6	22	1	0.062	1242.7	1
1	5	1	0.127	1605.1	1

Specific line index: 2

Edit the processing options data and press Done to proceed

Specify metastables of ionising ion (just ground for baseline)

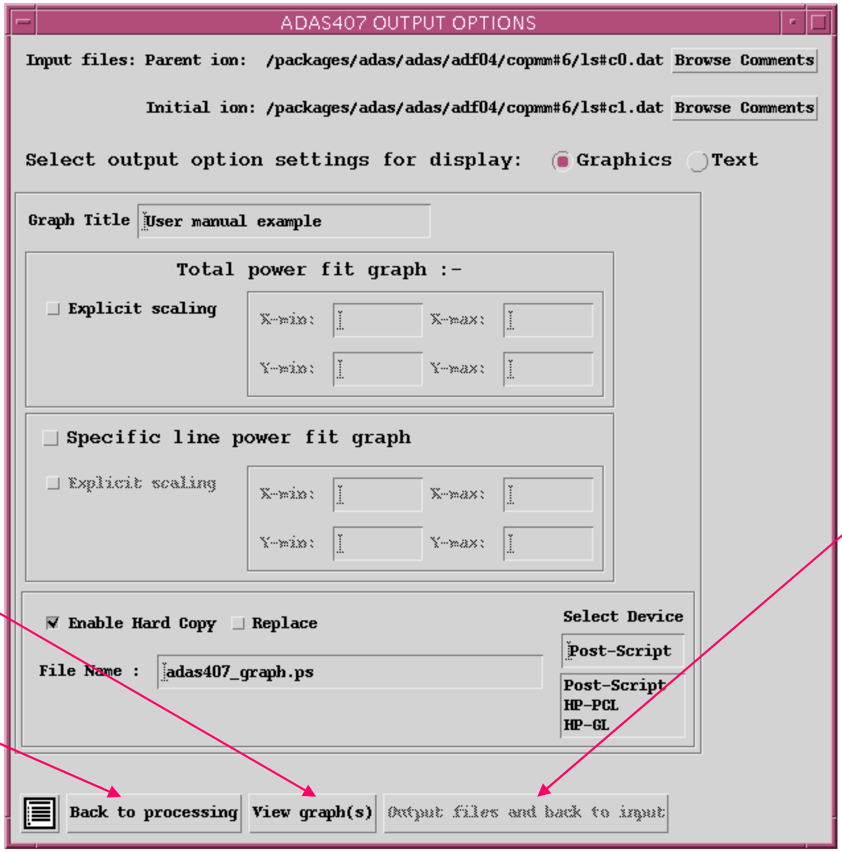
Specify metastables of ionised ion (just ground for baseline)

Select approx. forms

Set matching Te for power approx. fitting to exact power

Assign transitions to groups for approx. form fit.

ADAS407 Output-graphics



Input files: Parent ion: /packages/adas/adas/adf04/copmm#6/ls#c0.dat

Initial ion: /packages/adas/adas/adf04/copmm#6/ls#c1.dat

Select output option settings for display: ● Graphics ○ Text

Graph Title: User manual example

☐ Explicit scaling

☐ Specific line power fit graph

☐ Explicit scaling

☑ Enable Hard Copy ☐ Replace

File Name : adas407_graph.ps

Select Device: Post-Script

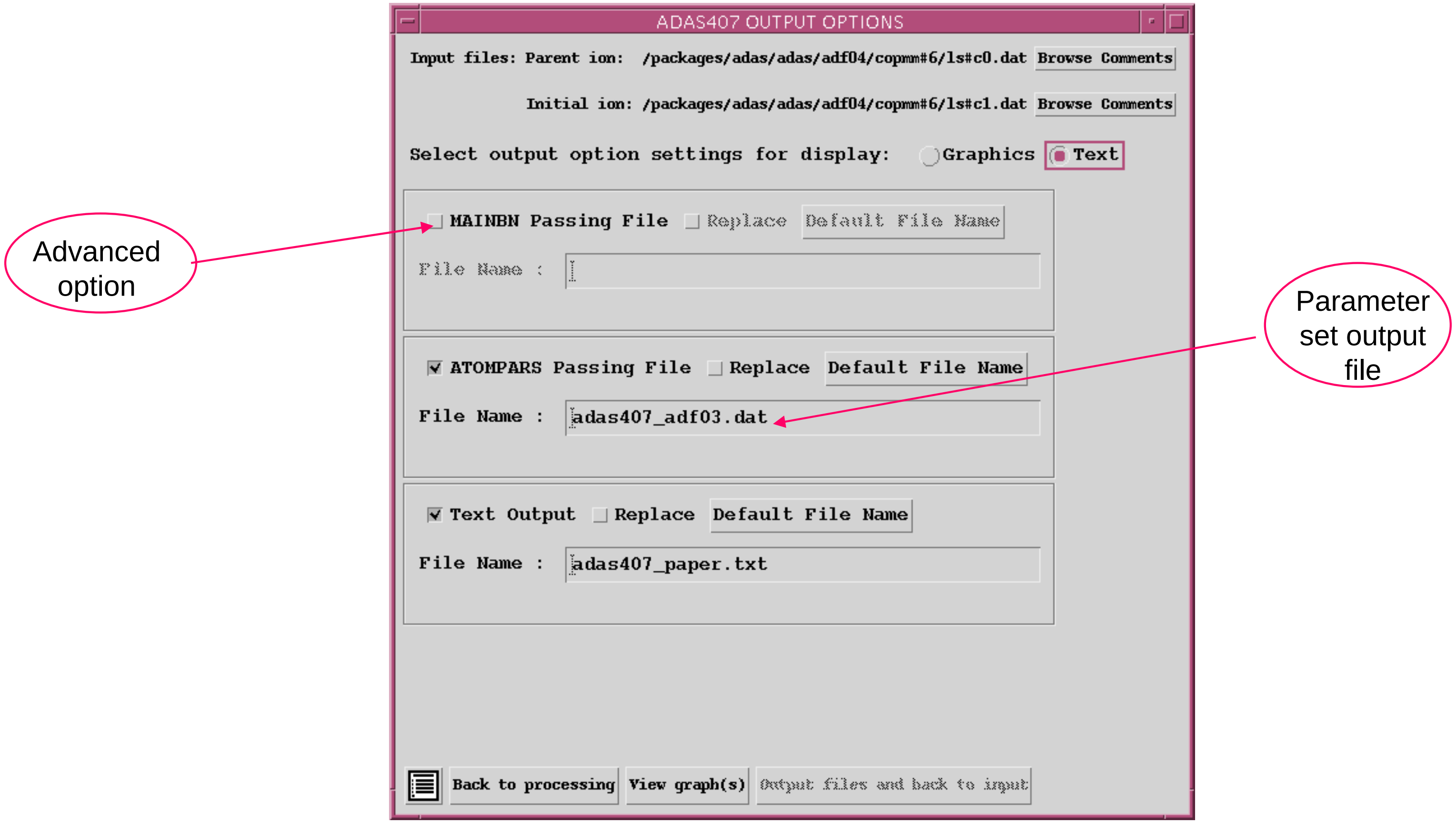
Post-Script
HP-PCL
HP-GL

View graphs

View and reprocess to adjust fit

Finish up

ADAS407 Output - text



Input files: Parent ion: /packages/adas/adas/adf04/copmm#6/ls#c0.dat

Initial ion: /packages/adas/adas/adf04/copmm#6/ls#c1.dat

Select output option settings for display: ○ Graphics ● Text

☐ MAINBN Passing File ☐ Replace

File Name :

☑ ATOMPARS Passing File ☐ Replace

File Name : adas407_adf03.dat

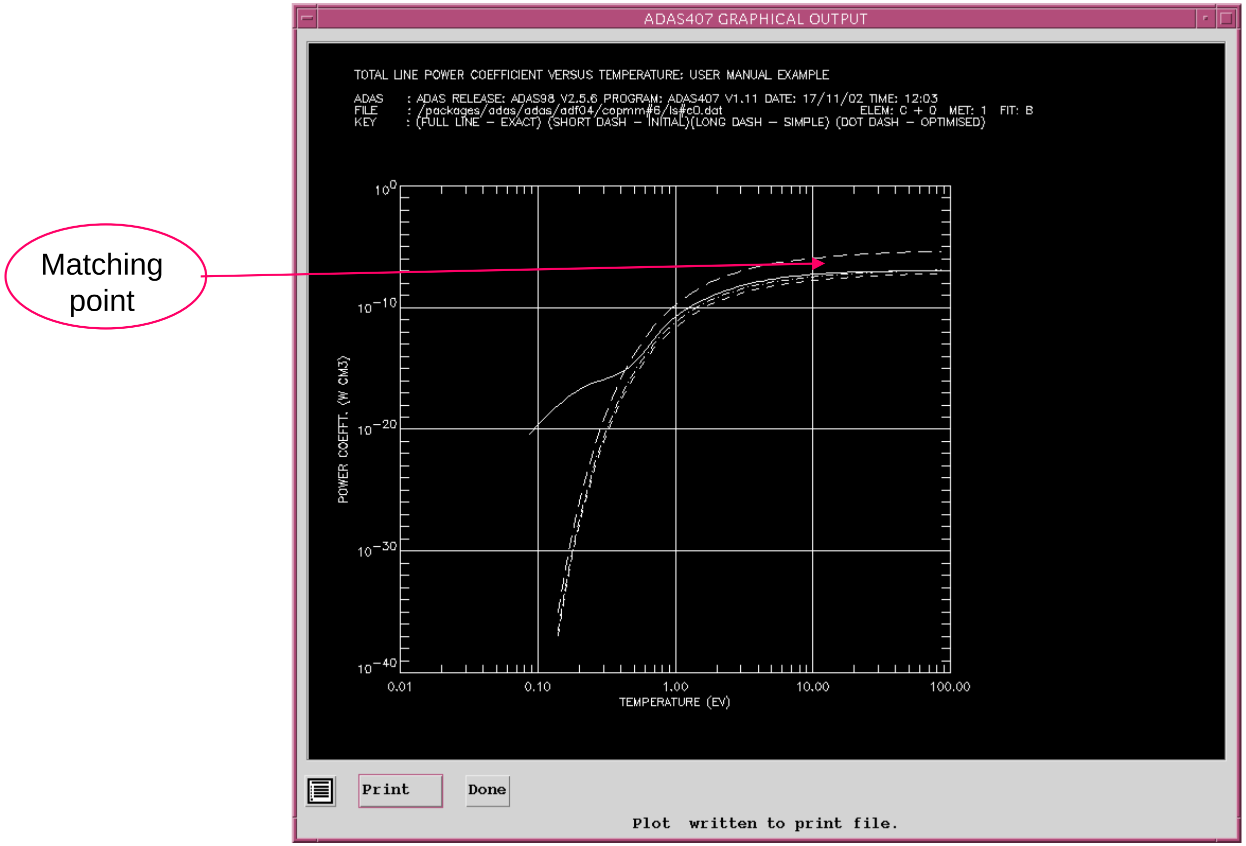
☑ Text Output ☐ Replace

File Name : adas407_paper.txt

Advanced option

Parameter set output file

ADAS407 Graph



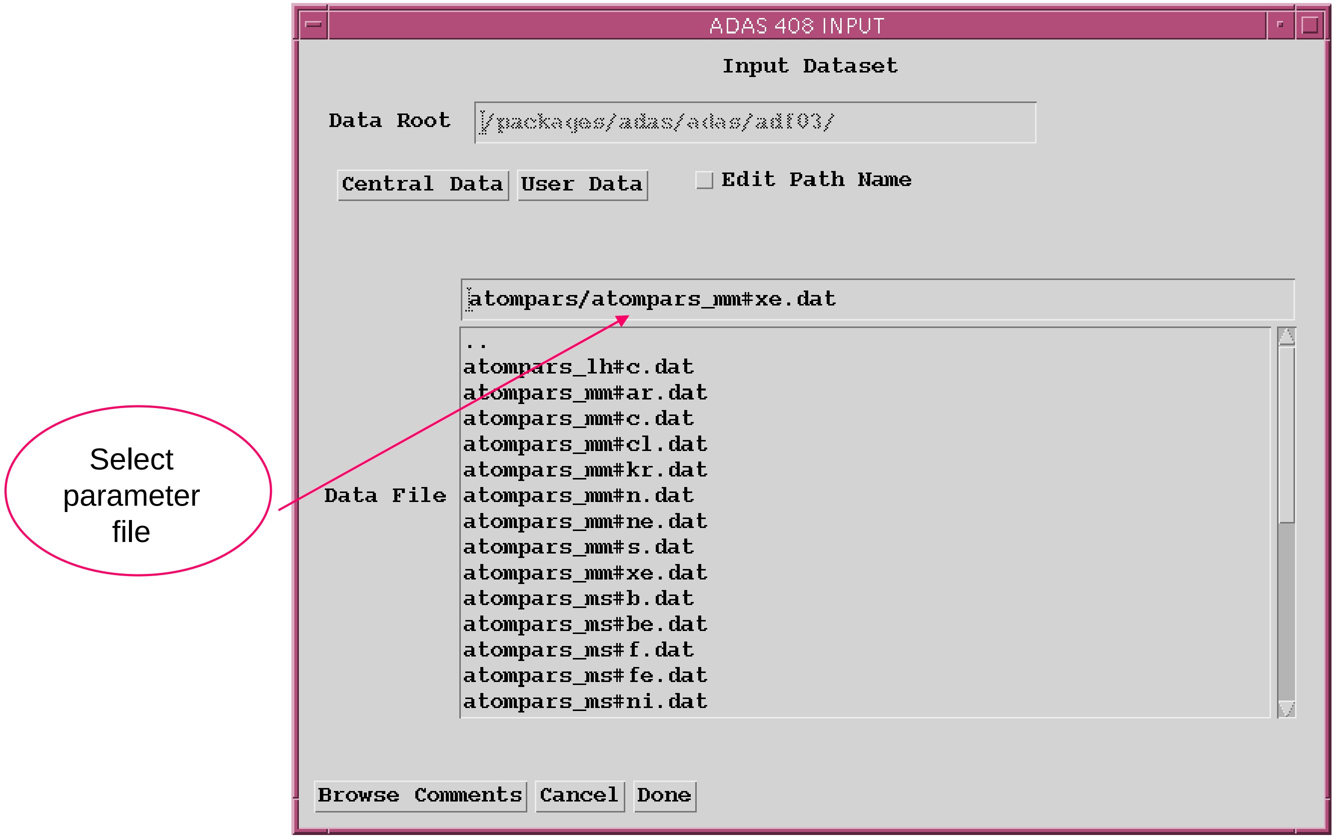
ADAS407 GRAPHICAL OUTPUT

```
TOTAL LINE POWER COEFFICIENT VERSUS TEMPERATURE: USER MANUAL EXAMPLE

ADAS    : ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS407 V1.11 DATE: 17/11/02 TIME: 12:03
FILE    : /packages/adas/adas/adf04/copmm#6/ls#c0.dat                    ELEM: C + 0  MET: 1  FIT: B
KEY     : (FULL LINE - EXACT) (SHORT DASH - INITIAL)(LONG DASH - SIMPLE) (DOT DASH - OPTIMISED)
```

Plot written to print file.

Matching point

ADAS408 Input



Data Root /packages/adas/adas/adf03/

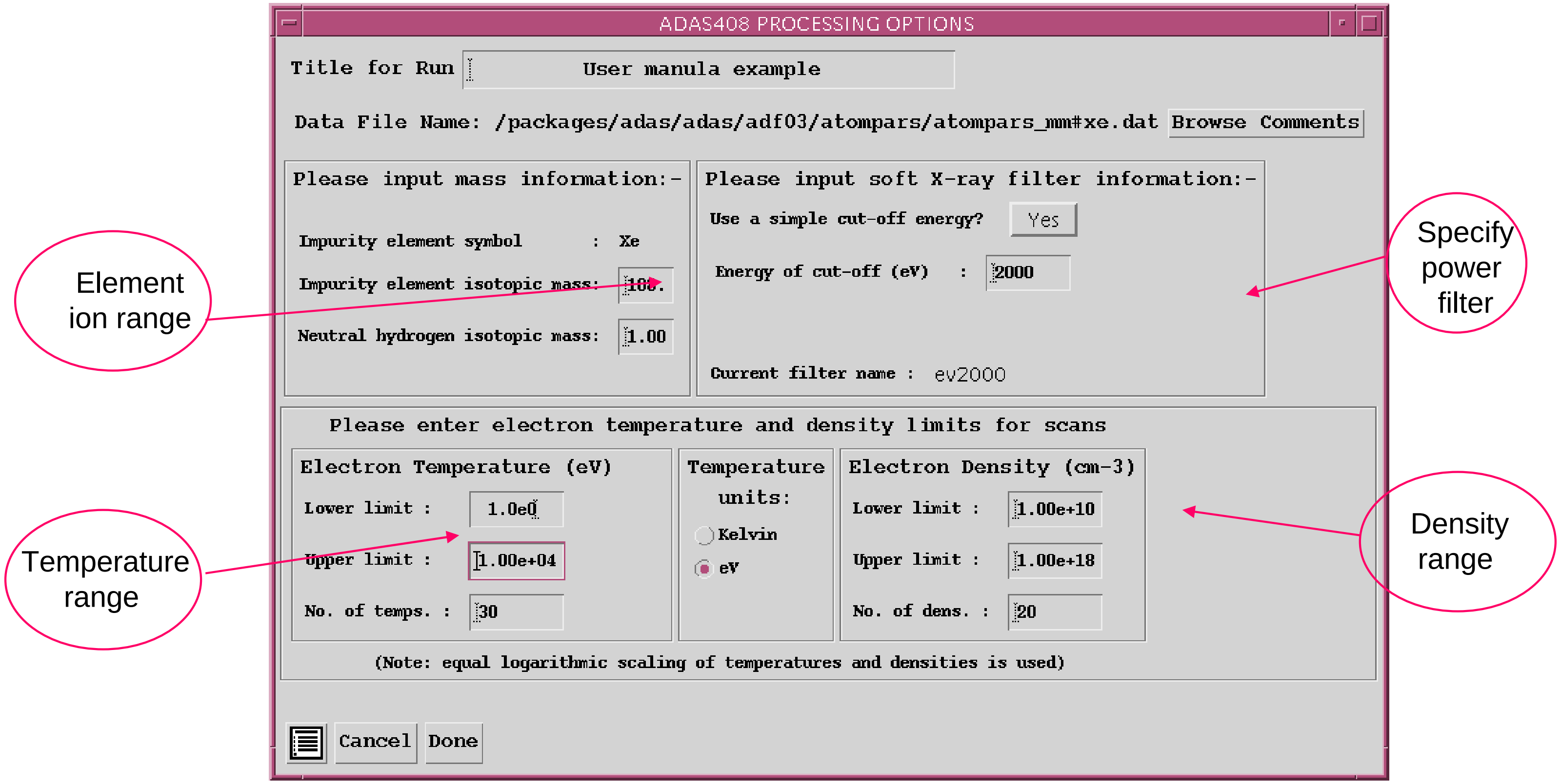
☐ Edit Path Name

Data File atompars/atompars_mm#xe.dat

```
..
atompars_lh#c.dat
atompars_mm#ar.dat
atompars_mm#c.dat
atompars_mm#cl.dat
atompars_mm#kr.dat
atompars_mm#n.dat
atompars_mm#ne.dat
atompars_mm#s.dat
atompars_mm#xe.dat
atompars_ms#b.dat
atompars_ms#be.dat
atompars_ms#f.dat
atompars_ms#fe.dat
atompars_ms#ni.dat
```

Select parameter file

ADAS408 Processing



Title for Run: User manula example

Data File Name: /packages/adas/adas/adf03/atompars/atompars_mm#xe.dat

Please input mass information:-

Impurity element symbol : Xe

Impurity element isotopic mass: 100.

Neutral hydrogen isotopic mass: 1.00

Please input soft X-ray filter information:-

Use a simple cut-off energy? Yes

Energy of cut-off (eV) : 2000

Current filter name : ev2000

Please enter electron temperature and density limits for scans

Electron Temperature (eV)

Lower limit : 1.0e0

Upper limit : 1.00e+04

No. of temps. : 30

Temperature units:

○ Kelvin

● eV

Electron Density (cm-3)

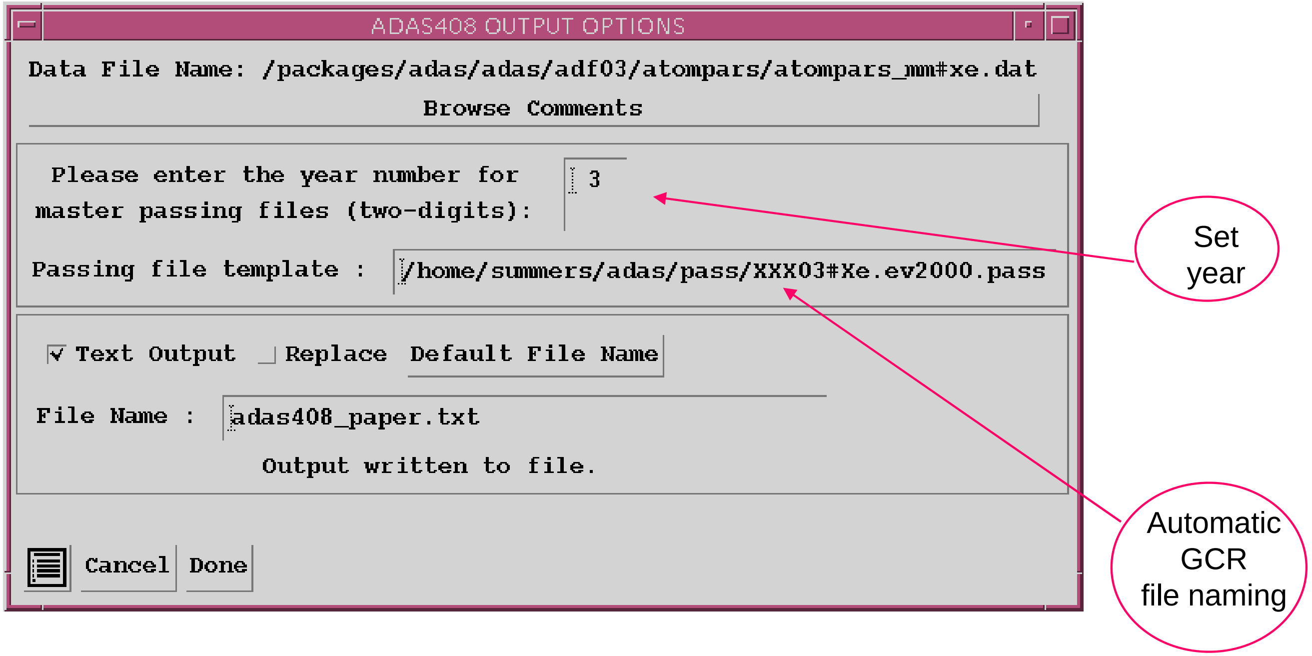
Lower limit : 1.00e+10

Upper limit : 1.00e+18

No. of dens. : 20

(Note: equal logarithmic scaling of temperatures and densities is used)

ADAS408 Output



Data File Name: /packages/adas/adas/adf03/atompars/atompars_mm#xe.dat

Please enter the year number for master passing files (two-digits): 3

Passing file template : /home/summers/adas/pass/XXX03#Xe.ev2000.pass

☑ Text Output ☐ Replace

File Name : adas408_paper.txt

Output written to file.

Set year

Automatic GCR file naming

4a. Charge exchange spectroscopy

- Interrogating state selective charge exchange cross-sections using ADAS301.
- Interrogating CXS effective emission coefficients using ADAS303.
- Calculating and examining effective emission coefficients using ADAS308.

Interrogating charge exchange cross-sections

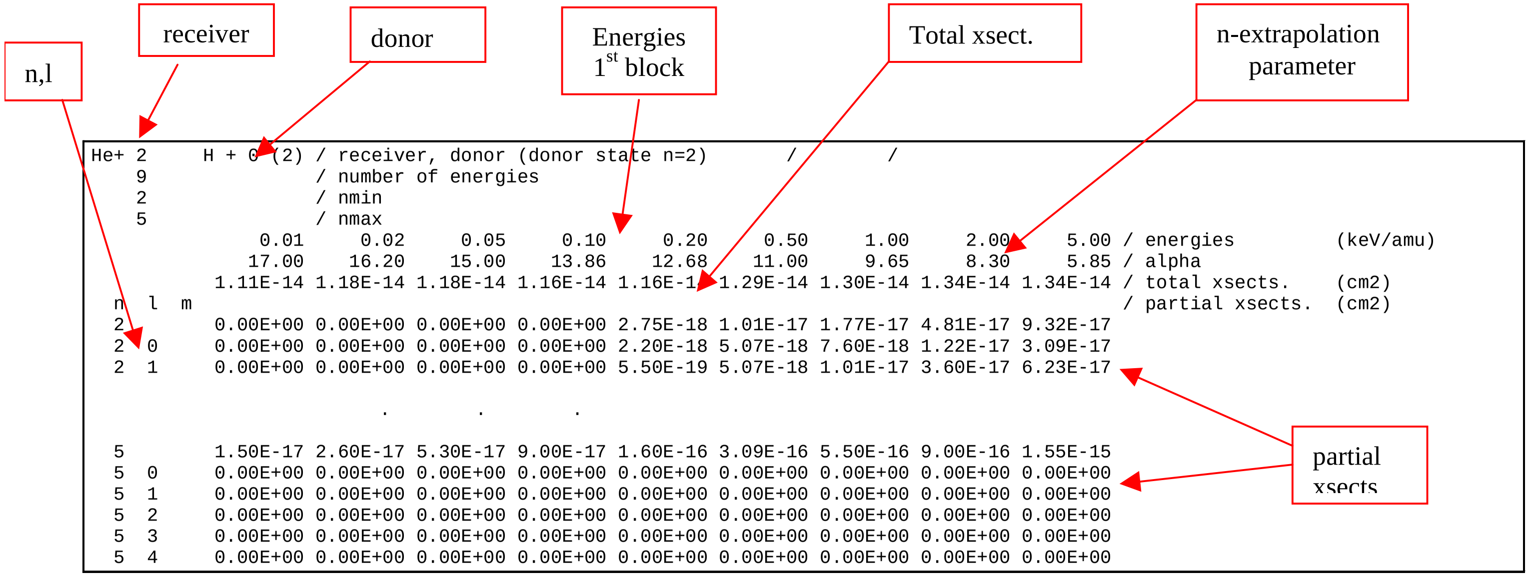
- Datasets of class ADF01 contain state selective charge exchange xsect. (qcx) data as a function of energy.

- These data for bare nucleus light impurity receivers into nl-shells in general.

- The donors may be H, He or Li and can include donation from ground state and excited state. There are separate data sets for each excited donor state.

- Code ADAS301 interrogates ADF01 data sets and displays results at energies of your choice.

ADF01 charge exchange cross-sections



n,l

receiver

donor

Energies 1st block

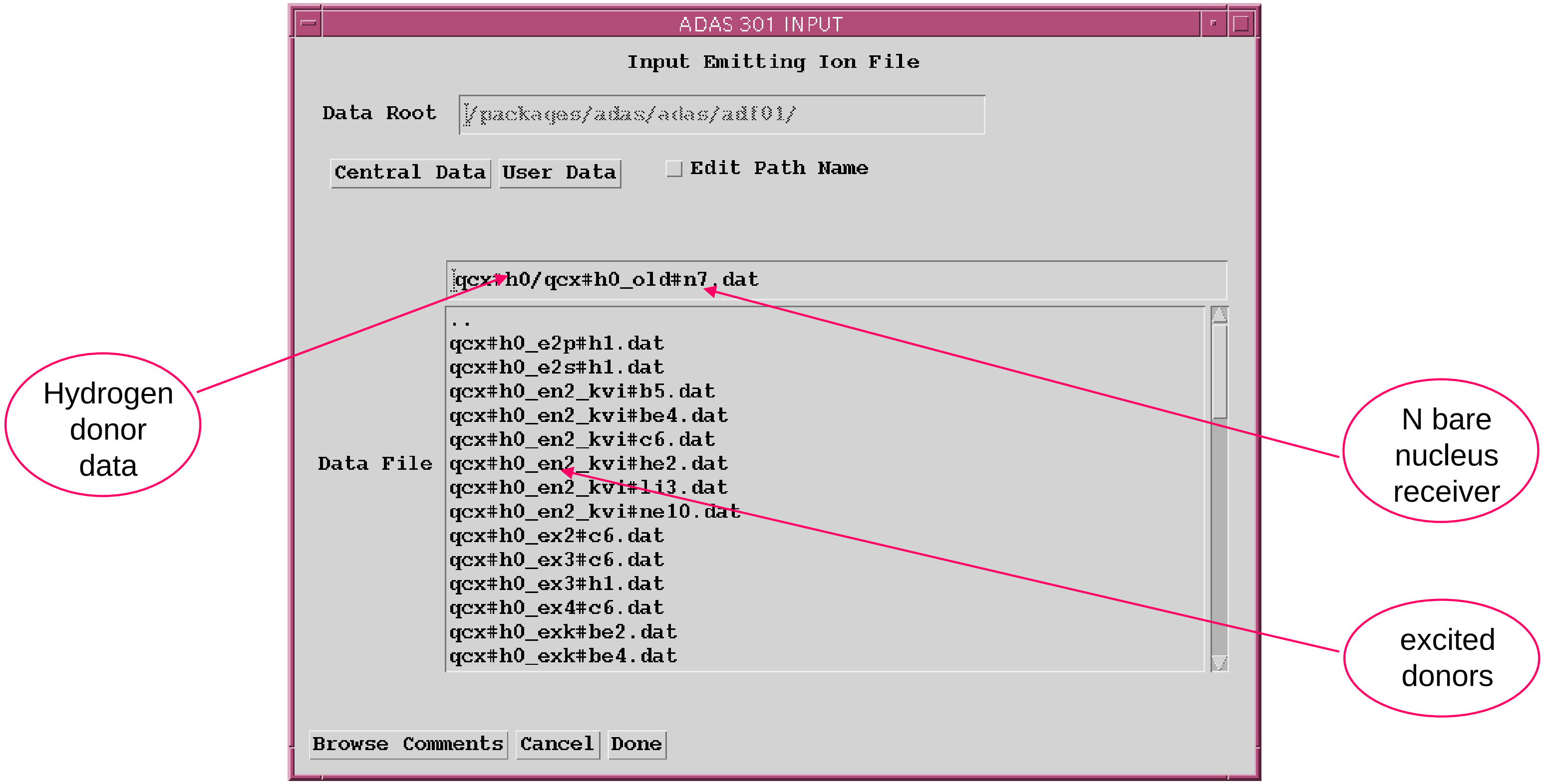
Total xsect.

n-extrapolation parameter

partial xsects

```
He+ 2     H + 0 (2) / receiver, donor (donor state n=2)       /        /
    9               / number of energies
    2               / nmin
    5               / nmax
               0.01      0.02      0.05      0.10      0.20      0.50      1.00      2.00      5.00 / energies          (keV/amu)
              17.00     16.20     15.00     13.86     12.68     11.00      9.65      8.30      5.85 / alpha
           1.11E-14 1.18E-14 1.18E-14 1.16E-14 1.16E-14 1.29E-14 1.30E-14 1.34E-14 1.34E-14 / total xsects.     (cm2)
  n  l  m                                                                                   / partial xsects.  (cm2)
  2        0.00E+00 0.00E+00 0.00E+00 0.00E+00 2.75E-18 1.01E-17 1.77E-17 4.81E-17 9.32E-17
  2  0     0.00E+00 0.00E+00 0.00E+00 0.00E+00 2.20E-18 5.07E-18 7.60E-18 1.22E-17 3.09E-17
  2  1     0.00E+00 0.00E+00 0.00E+00 0.00E+00 5.50E-19 5.07E-18 1.01E-17 3.60E-17 6.23E-17

                            .        .        .

  5        1.50E-17 2.60E-17 5.30E-17 9.00E-17 1.60E-16 3.09E-16 5.50E-16 9.00E-16 1.55E-15
  5  0     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  1     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  2     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  3     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  4     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
```

ADAS301 input



Data Root /packages/adas/adas/adf01/

Data File qcx#h0/qcx#h0_old#n7.dat

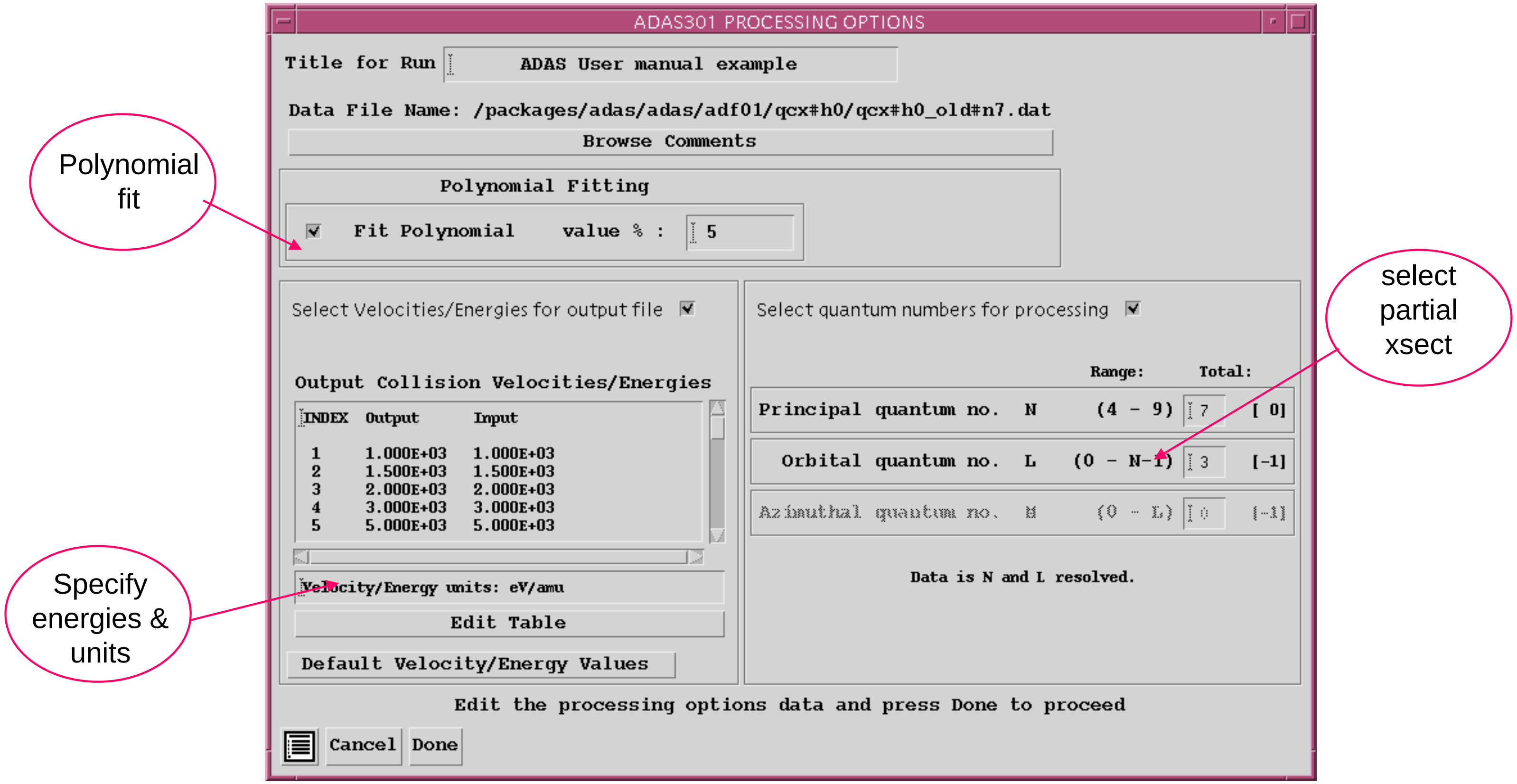
```
..
qcx#h0_e2p#h1.dat
qcx#h0_e2s#h1.dat
qcx#h0_en2_kvi#b5.dat
qcx#h0_en2_kvi#be4.dat
qcx#h0_en2_kvi#c6.dat
qcx#h0_en2_kvi#he2.dat
qcx#h0_en2_kvi#li3.dat
qcx#h0_en2_kvi#ne10.dat
qcx#h0_ex2#c6.dat
qcx#h0_ex3#c6.dat
qcx#h0_ex3#h1.dat
qcx#h0_ex4#c6.dat
qcx#h0_exk#be2.dat
qcx#h0_exk#be4.dat
```

Hydrogen donor data

N bare nucleus receiver

excited donors

ADAS302 Processing



ADAS301 PROCESSING OPTIONS

Title for Run: ADAS User manual example

Data File Name: /packages/adas/adas/adf01/qcx#h0/qcx#h0_old#n7.dat

Polynomial Fitting

☑ Fit Polynomial value % : 5

Select Velocities/Energies for output file ☑

Output Collision Velocities/Energies

INDEX	Output	Input
1	1.000E+03	1.000E+03
2	1.500E+03	1.500E+03
3	2.000E+03	2.000E+03
4	3.000E+03	3.000E+03
5	5.000E+03	5.000E+03

Velocity/Energy units: eV/amu

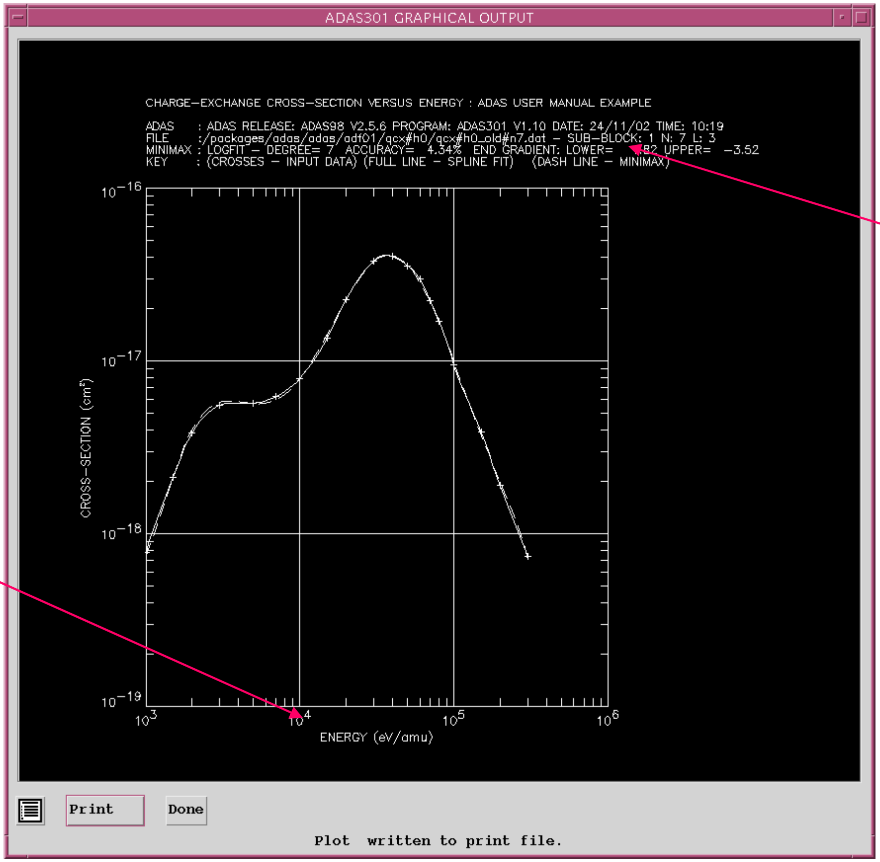
Select quantum numbers for processing ☑

	Range:		Total:
Principal quantum no. N	(4 - 9)	7	[0]
Orbital quantum no. L	(0 - N-1)	3	[-1]
Azimuthal quantum no. M	(0 - L)	0	[-1]

Data is N and L resolved.

Edit the processing options data and press Done to proceed

ADAS301 graph



```
CHARGE-EXCHANGE CROSS-SECTION VERSUS ENERGY : ADAS USER MANUAL EXAMPLE

ADAS    : ADAS RELEASE: ADAS98 V2.5.6 PROGRAM: ADAS301 V1.10 DATE: 24/11/02 TIME: 10:19
FILE    :/packages/adas/adas/adf01/qcx#h0/qcx#h0_old#n7.dat - SUB-BLOCK: 1 N: 7 L: 3
MINIMAX : LOGFIT - DEGREE= 7  ACCURACY=  4.34%  END GRADIENT: LOWER=  [illegible].82 UPPER=  -3.52
KEY     : (CROSSES - INPUT DATA) (FULL LINE - SPLINE FIT)  (DASH LINE - MINIMAX)
```

```
Plot  written to print file.
```

specification of extracted xsect.

graph is a function of energy

Interrogating CXS effective emission coefficients

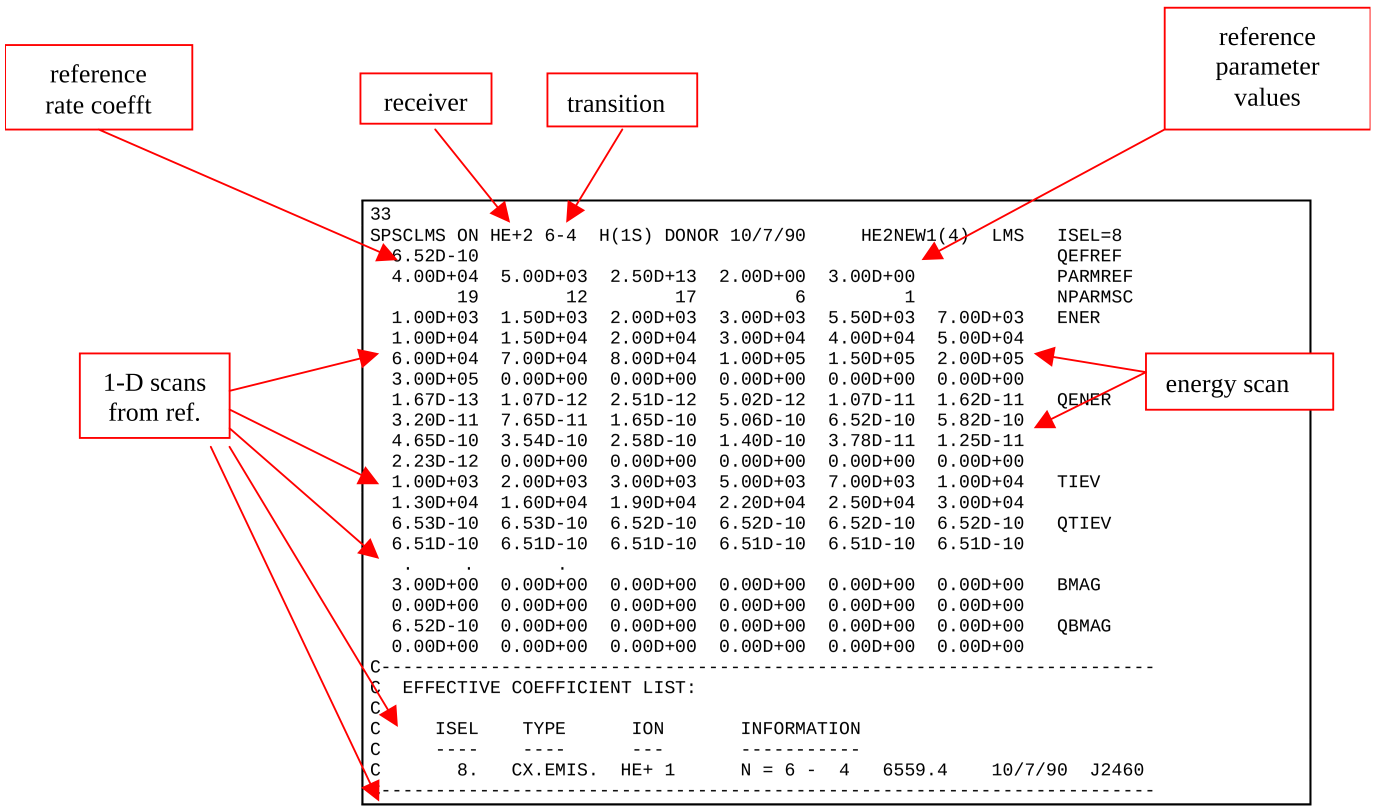
- Datasets of class ADF12 contain CXS effective emission (qef) data as a function of beam and plasma parameters.

- These coefficients include the effect of collisional redistribution of nl-substate populations of the receiver ion in the plasma.

- The individual components of the n->n’ CX transition are not resolvable for bare nucleus receivers so only whole transition arrays are given.

- Code ADAS303 interrogates ADF12 data sets and displays results at beam and plasma conditions of your choice.

ADF12 charge exchange cross-sections



reference rate coefft

receiver

transition

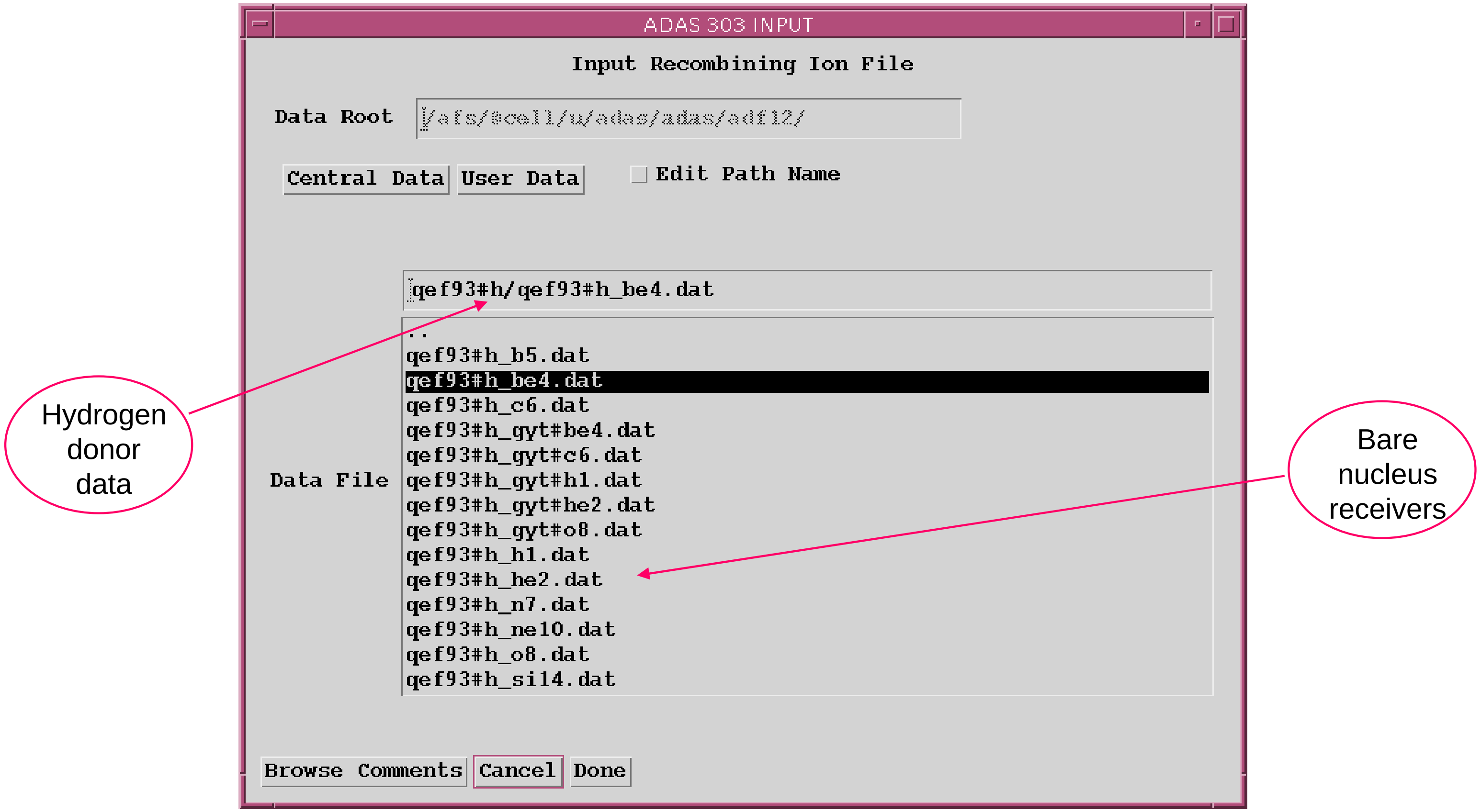
reference parameter values

1-D scans from ref.

energy scan

```
33
SPSCLMS ON HE+2 6-4  H(1S) DONOR 10/7/90     HE2NEW1(4)  LMS    ISEL=8
  6.52D-10                                                      QEFREF
  4.00D+04  5.00D+03  2.50D+13  2.00D+00  3.00D+00              PARMREF
        19        12        17         6         1              NPARMSC
  1.00D+03  1.50D+03  2.00D+03  3.00D+03  5.50D+03  7.00D+03    ENER
  1.00D+04  1.50D+04  2.00D+04  3.00D+04  4.00D+04  5.00D+04
  6.00D+04  7.00D+04  8.00D+04  1.00D+05  1.50D+05  2.00D+05
  3.00D+05  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  1.67D-13  1.07D-12  2.51D-12  5.02D-12  1.07D-11  1.62D-11    QENER
  3.20D-11  7.65D-11  1.65D-10  5.06D-10  6.52D-10  5.82D-10
  4.65D-10  3.54D-10  2.58D-10  1.40D-10  3.78D-11  1.25D-11
  2.23D-12  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  1.00D+03  2.00D+03  3.00D+03  5.00D+03  7.00D+03  1.00D+04    TIEV
  1.30D+04  1.60D+04  1.90D+04  2.20D+04  2.50D+04  3.00D+04
  6.53D-10  6.53D-10  6.52D-10  6.52D-10  6.52D-10  6.52D-10    QTIEV
  6.51D-10  6.51D-10  6.51D-10  6.51D-10  6.51D-10  6.51D-10
    .     .        .
  3.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00    BMAG
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
  6.52D-10  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00    QBMAG
  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
C-----------------------------------------------------------------------
C  EFFECTIVE COEFFICIENT LIST:
C
C     ISEL    TYPE      ION       INFORMATION
C     ----    ----      ---       -----------
C       8.    CX.EMIS.  HE+ 1     N = 6 -  4   6559.4    10/7/90  J2460
 -----------------------------------------------------------------------
```

ADAS303 input



Data Root /afs/@cell/u/adas/adas/adf12/

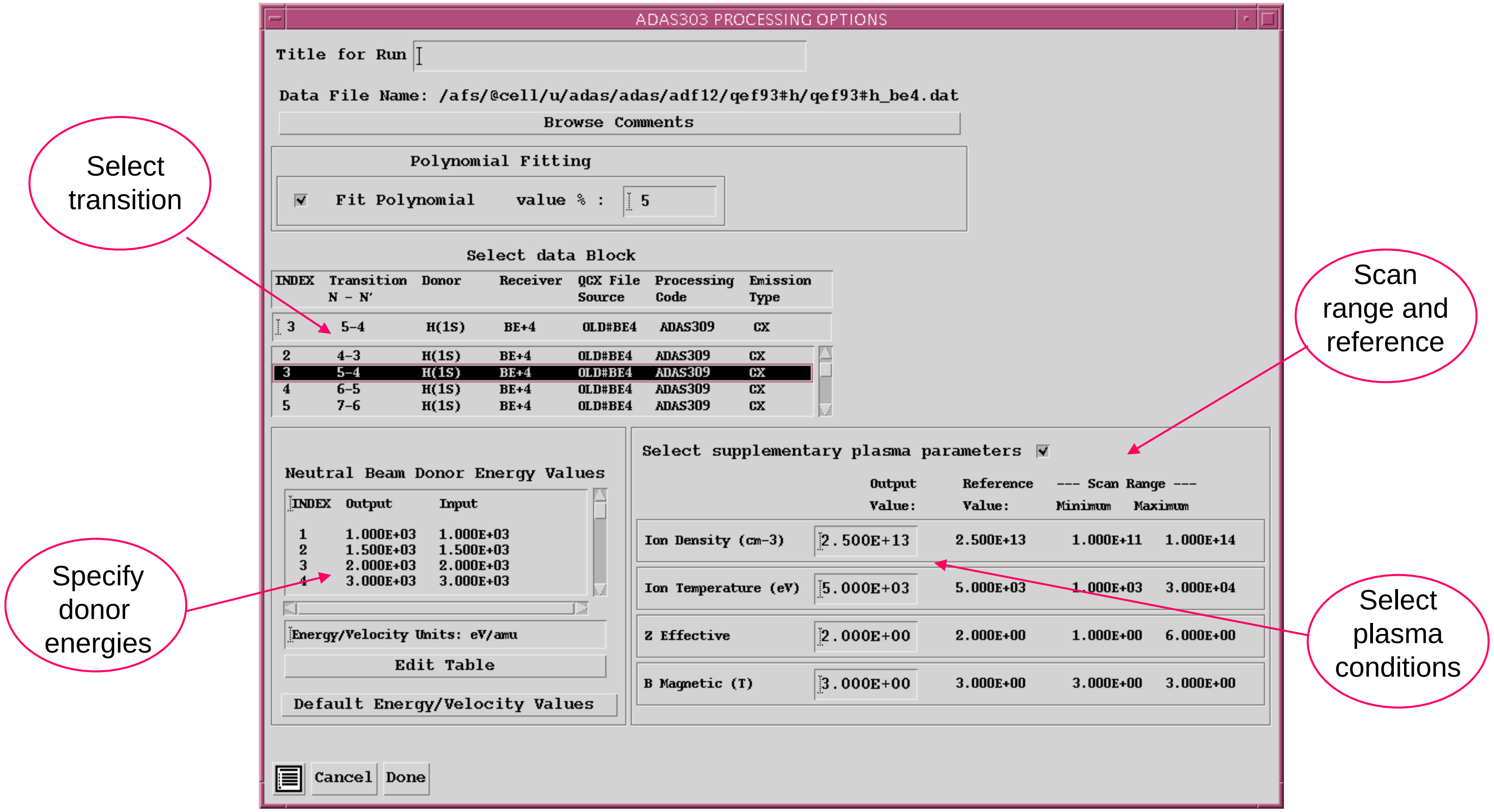
Data File qef93#h/qef93#h_be4.dat

```
..
qef93#h_b5.dat
qef93#h_be4.dat
qef93#h_c6.dat
qef93#h_gyt#be4.dat
qef93#h_gyt#c6.dat
qef93#h_gyt#h1.dat
qef93#h_gyt#he2.dat
qef93#h_gyt#o8.dat
qef93#h_h1.dat
qef93#h_he2.dat
qef93#h_n7.dat
qef93#h_ne10.dat
qef93#h_o8.dat
qef93#h_si14.dat
```

Hydrogen donor data

Bare nucleus receivers

ADAS303 Processing



ADAS303 PROCESSING OPTIONS

Title for Run

Data File Name: /afs/@cell/u/adas/adas/adf12/qef93#h/qef93#h_be4.dat

Polynomial Fitting

☑ Fit Polynomial value % : 5

Select data Block

INDEX	Transition N - N'	Donor	Receiver	QCX File Source	Processing Code	Emission Type
3	5-4	H(1S)	BE+4	OLD#BE4	ADAS309	CX
2	4-3	H(1S)	BE+4	OLD#BE4	ADAS309	CX
3	5-4	H(1S)	BE+4	OLD#BE4	ADAS309	CX
4	6-5	H(1S)	BE+4	OLD#BE4	ADAS309	CX
5	7-6	H(1S)	BE+4	OLD#BE4	ADAS309	CX

Neutral Beam Donor Energy Values

INDEX	Output	Input
1	1.000E+03	1.000E+03
2	1.500E+03	1.500E+03
3	2.000E+03	2.000E+03
4	3.000E+03	3.000E+03

Energy/Velocity Units: eV/amu

Select supplementary plasma parameters ☑

	Output Value:	Reference Value:	--- Scan Range --- Minimum	Maximum
Ion Density (cm-3)	2.500E+13	2.500E+13	1.000E+11	1.000E+14
Ion Temperature (eV)	5.000E+03	5.000E+03	1.000E+03	3.000E+04
Z Effective	2.000E+00	2.000E+00	1.000E+00	6.000E+00
B Magnetic (T)	3.000E+00	3.000E+00	3.000E+00	3.000E+00

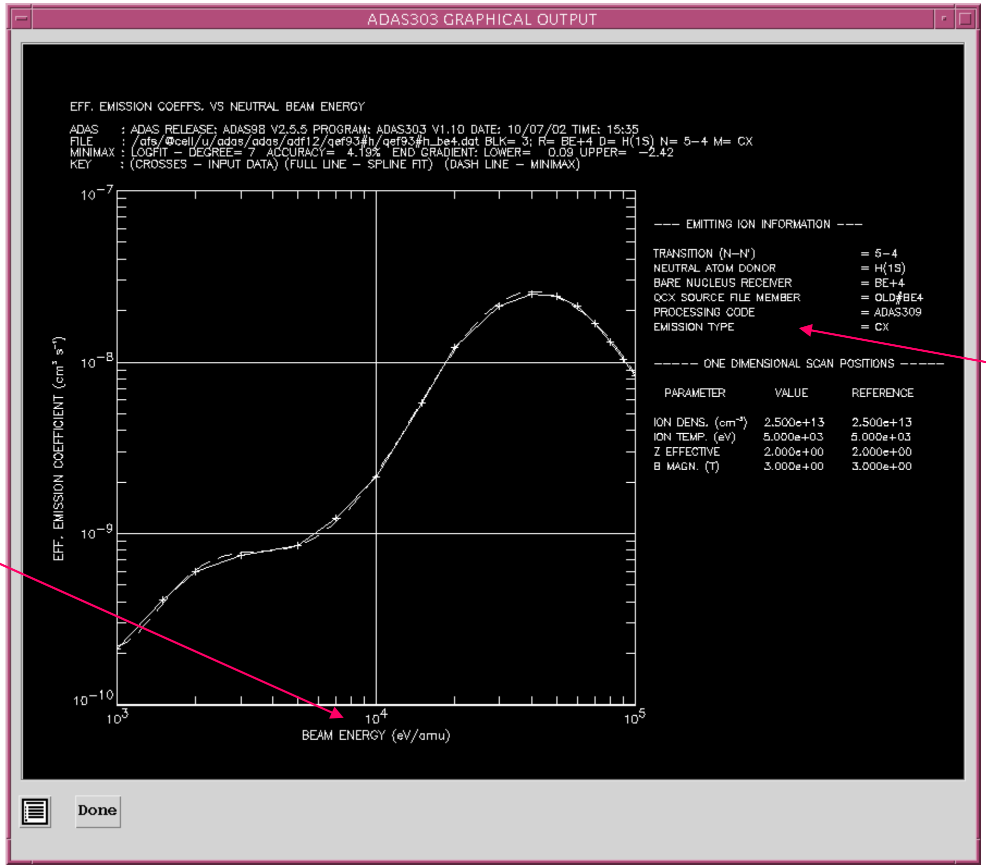
Select transition

Specify donor energies

Scan range and reference

Select plasma conditions

ADAS303 graph



```
EFF. EMISSION COEFFS. VS NEUTRAL BEAM ENERGY

ADAS    : ADAS RELEASE: ADAS98 V2.5.5 PROGRAM: ADAS303 V1.10 DATE: 10/07/02 TIME: 15:35
FILE    : /afs/@cell/u/adas/adas/adf12/qef93#h/qef93#h_be4.dat BLK= 3; R= BE+4 D= H(1S) N= 5-4 M= CX
MINIMAX : LOGFIT - DEGREE= 7  ACCURACY=  4.19%  END GRADIENT: LOWER=   0.09 UPPER=  -2.42
KEY     : (CROSSES - INPUT DATA) (FULL LINE - SPLINE FIT)  (DASH LINE - MINIMAX)

--- EMITTING ION INFORMATION ---

TRANSITION (N-N')              = 5-4
NEUTRAL ATOM DONOR             = H(1S)
BARE NUCLEUS RECEIVER          = BE+4
QCX SOURCE FILE MEMBER         = OLD#BE4
PROCESSING CODE                = ADAS309
EMISSION TYPE                  = CX

----- ONE DIMENSIONAL SCAN POSITIONS -----

  PARAMETER          VALUE        REFERENCE

ION DENS. (cm⁻³)   2.500e+13     2.500e+13
ION TEMP. (eV)     5.000e+03     5.000e+03
Z EFFECTIVE        2.000e+00     2.000e+00
B MAGN. (T)        3.000e+00     3.000e+00
```

graph is a function of beam energy

plasma and beam conditions for graph

Calculating CXS effective emission

- Datasets of class ADF01 state selective charge exchange cross-section data for capture by fully ionised ions.
- Code ADAS308 computes effective emission coefficients, predicts CXS line positions and profiles and deduces the beam plasma emission measure.

Calculating CXS effective emission (contd.)

- The driving reactions are

$$X^{+z_0} + D^0_{beam}(1s) \rightarrow X^{+z_0-1}(nl) + D^+_{beam}$$

- The effective emission coefficient for n-n’ transition is

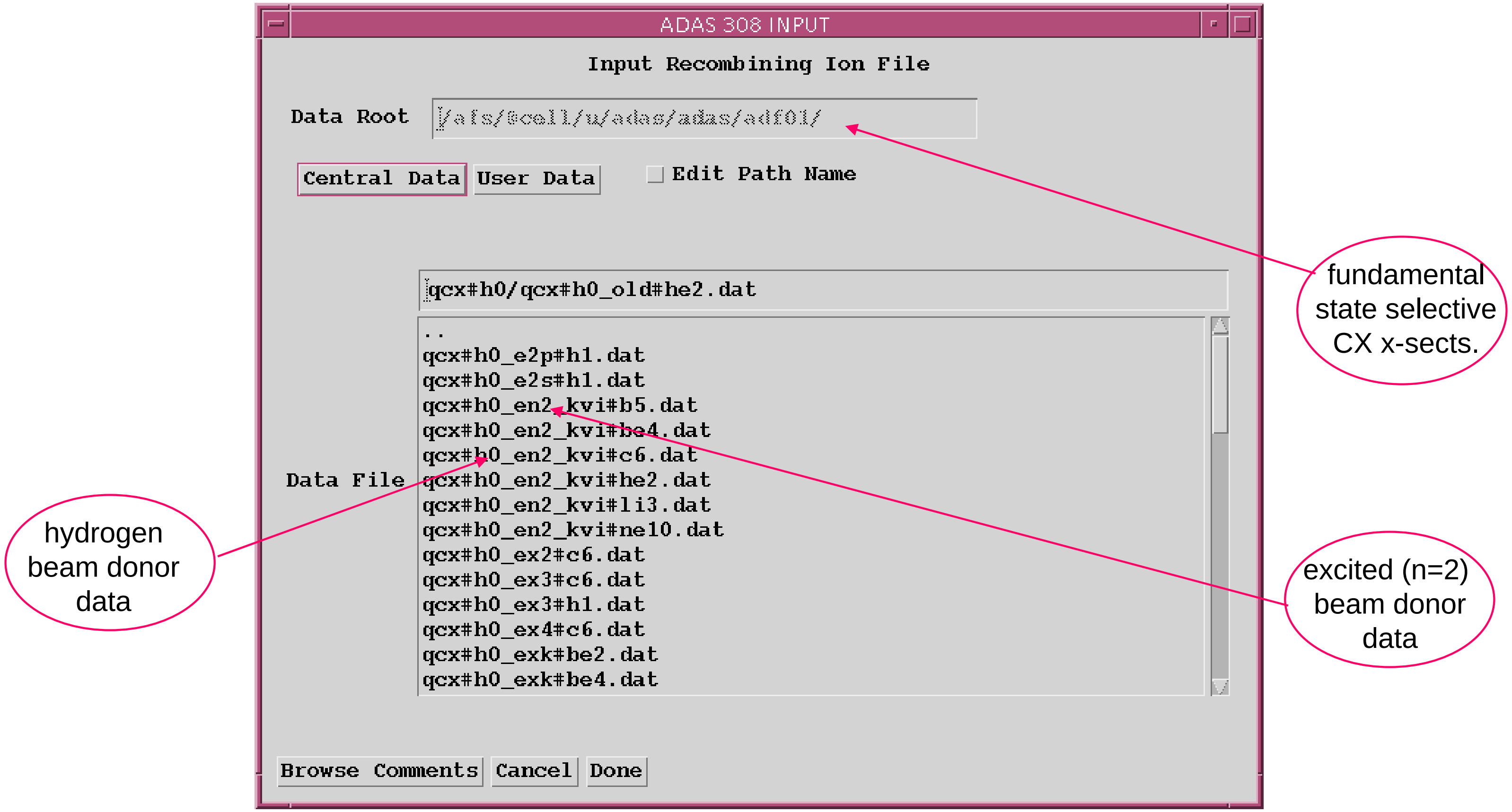
$$q^{(eff)}_{n\rightarrow n'} = \sum_{l,l'} A_{nl\rightarrow n'l'}(N^{(z_0-1)}_{nl} / N_D N^{(z_0)})$$

- Thus a collisional-radiative, resolved-nl population calculation is required to determine the effective emission coefficients.

Calculating CXS effective emission (contd.)

- File selection
  - The fundamental state selective charge exchange x-sect data is format ADF01. These data are resolved into the nl shells of the receiver.
  - Note that there are sub-directories for different donors and separate data sets for ground and excited donor states.
- Processing options
  - *Beam parameter, observed spectrum lines and required emssivity predictions must be entered using Table Editor.*
  - *Then plasma conditions must be entered.*
  - *Finally model for emission measure is chosen.*
- Output options
  - Graphical display of the spectral position, intensity and shape of a designated n-n’ transition is given.
  - Tabulations of predicted intensities of other lines are given together with the estimated emission measure.

ADAS308 Input



Data Root /afs/@cell/u/adas/adas/adf01/

Data File qcx#h0/qcx#h0_old#he2.dat

```
..
qcx#h0_e2p#h1.dat
qcx#h0_e2s#h1.dat
qcx#h0_en2_kvi#b5.dat
qcx#h0_en2_kvi#be4.dat
qcx#h0_en2_kvi#c6.dat
qcx#h0_en2_kvi#he2.dat
qcx#h0_en2_kvi#li3.dat
qcx#h0_en2_kvi#ne10.dat
qcx#h0_ex2#c6.dat
qcx#h0_ex3#c6.dat
qcx#h0_ex3#h1.dat
qcx#h0_ex4#c6.dat
qcx#h0_exk#be2.dat
qcx#h0_exk#be4.dat
```

fundamental state selective CX x-sects.

hydrogen beam donor data

excited (n=2) beam donor data

Calculating CXS effective emission (contd.)

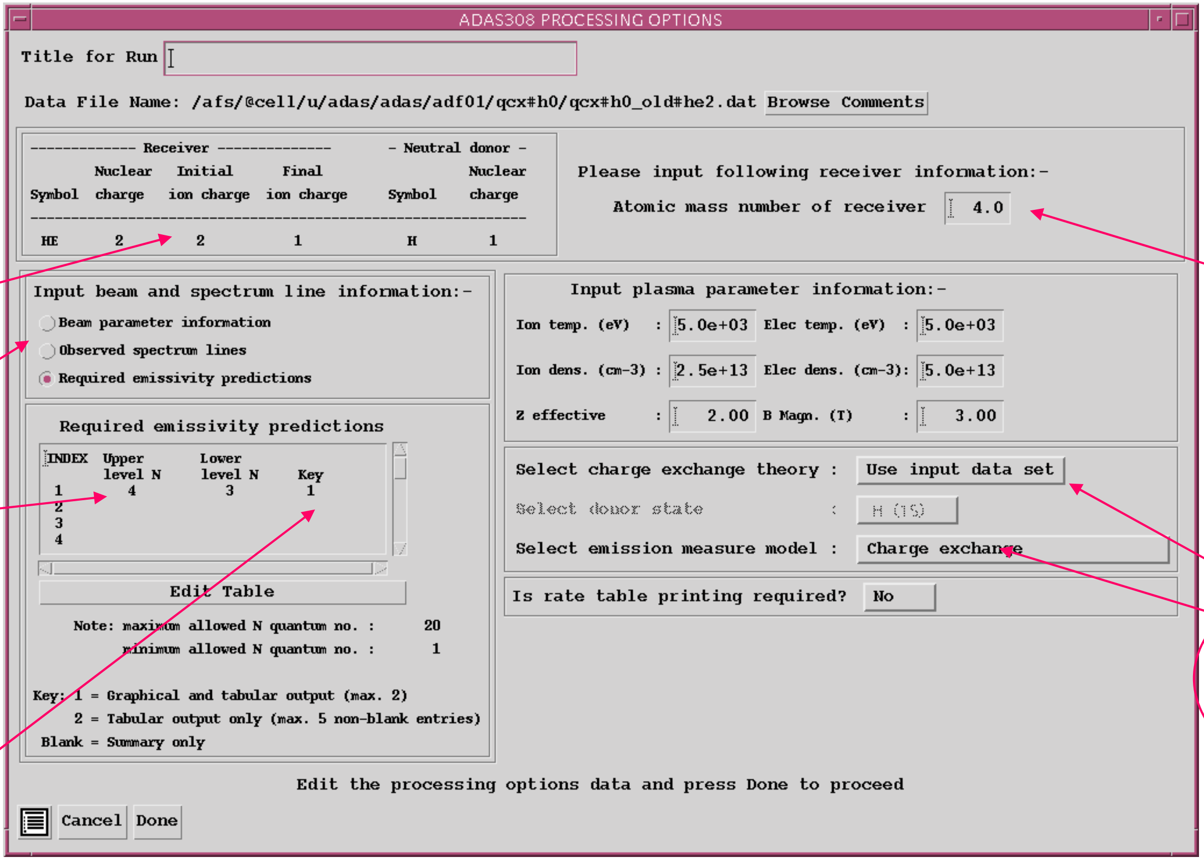
- ADAS308 is designed to do more than solve for the effective emission coefficients, qef.

- The program computes the qef and solves for the emission measure given the line of sight intensity in a charge exchange line as

$$I_{n\to n'}^{(z_0-1)} \approx q_{n\to n'}^{(eff)} \int_s N_D N^{(z_0)} ds$$

- If more than one charge exchange line intensity, with different upper levels, the code can assess the consistency between experimental and theoretical data. ADAS308 casts this onto the consistency of the ADF01 total n-shell capture with observation.
- Most use of ADAS308 has been directed at qef and its components alone.

ADAS308 processing



Title for Run

Data File Name: /afs/@cell/u/adas/adas/adf01/qcx#h0/qcx#h0_old#he2.dat

Receiver				Neutral donor	
Symbol	Nuclear charge	Initial ion charge	Final ion charge	Symbol	Nuclear charge
HE	2	2	1	H	1

Please input following receiver information:-

Atomic mass number of receiver: 4.0

Input beam and spectrum line information:-

○ Beam parameter information
○ Observed spectrum lines
● Required emissivity predictions

Input plasma parameter information:-

Ion temp. (eV) : 5.0e+03 Elec temp. (eV) : 5.0e+03
Ion dens. (cm-3) : 2.5e+13 Elec dens. (cm-3): 5.0e+13
Z effective : 2.00 B Magn. (T) : 3.00

Select charge exchange theory : Use input data set
Select donor state : H (1S)
Select emission measure model : Charge exchange

Is rate table printing required? No

Required emissivity predictions

INDEX	Upper level N	Lower level N	Key
1	4	3	1
2			
3			
4			

Note: maximum allowed N quantum no. : 20
minimum allowed N quantum no. : 1

Key: 1 = Graphical and tabular output (max. 2)
2 = Tabular output only (max. 5 non-blank entries)
Blank = Summary only

Edit the processing options data and press Done to proceed

information from data set

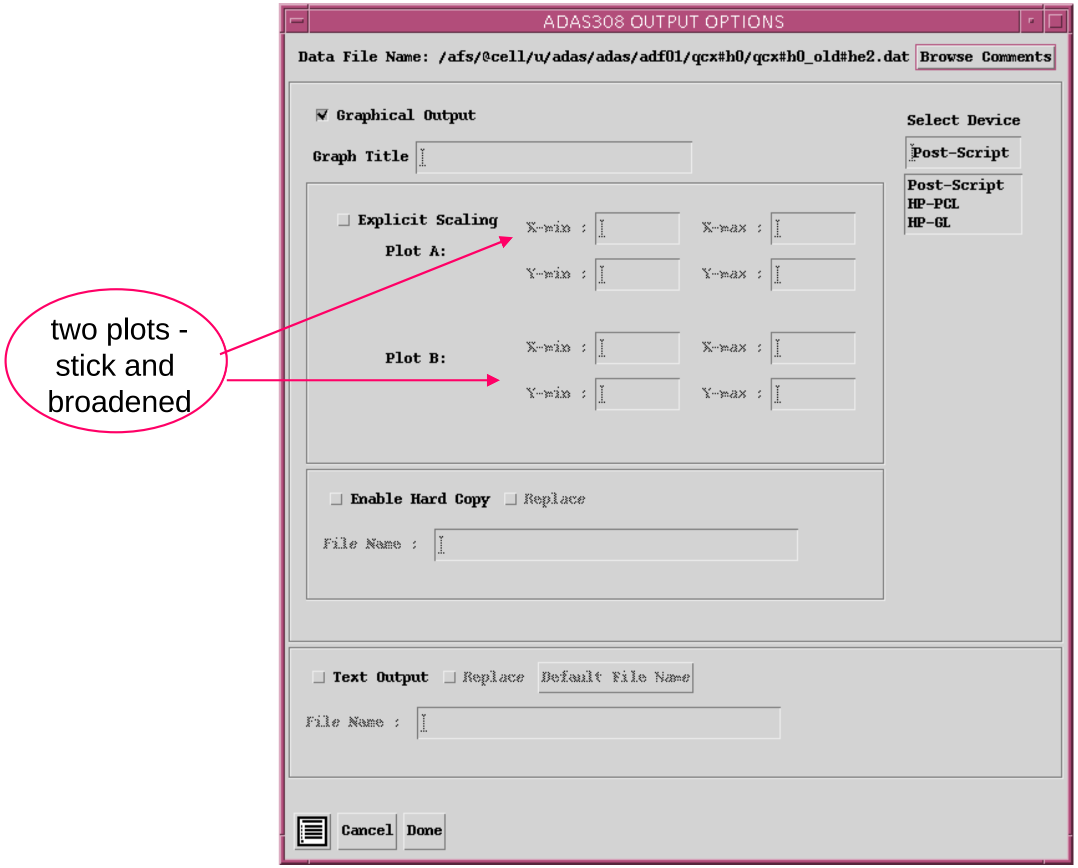
various data required - appropriate is table displayed

key determines tables and graphs

masses required for ion collisions

model choice - usually input data and CX

ADAS308 output



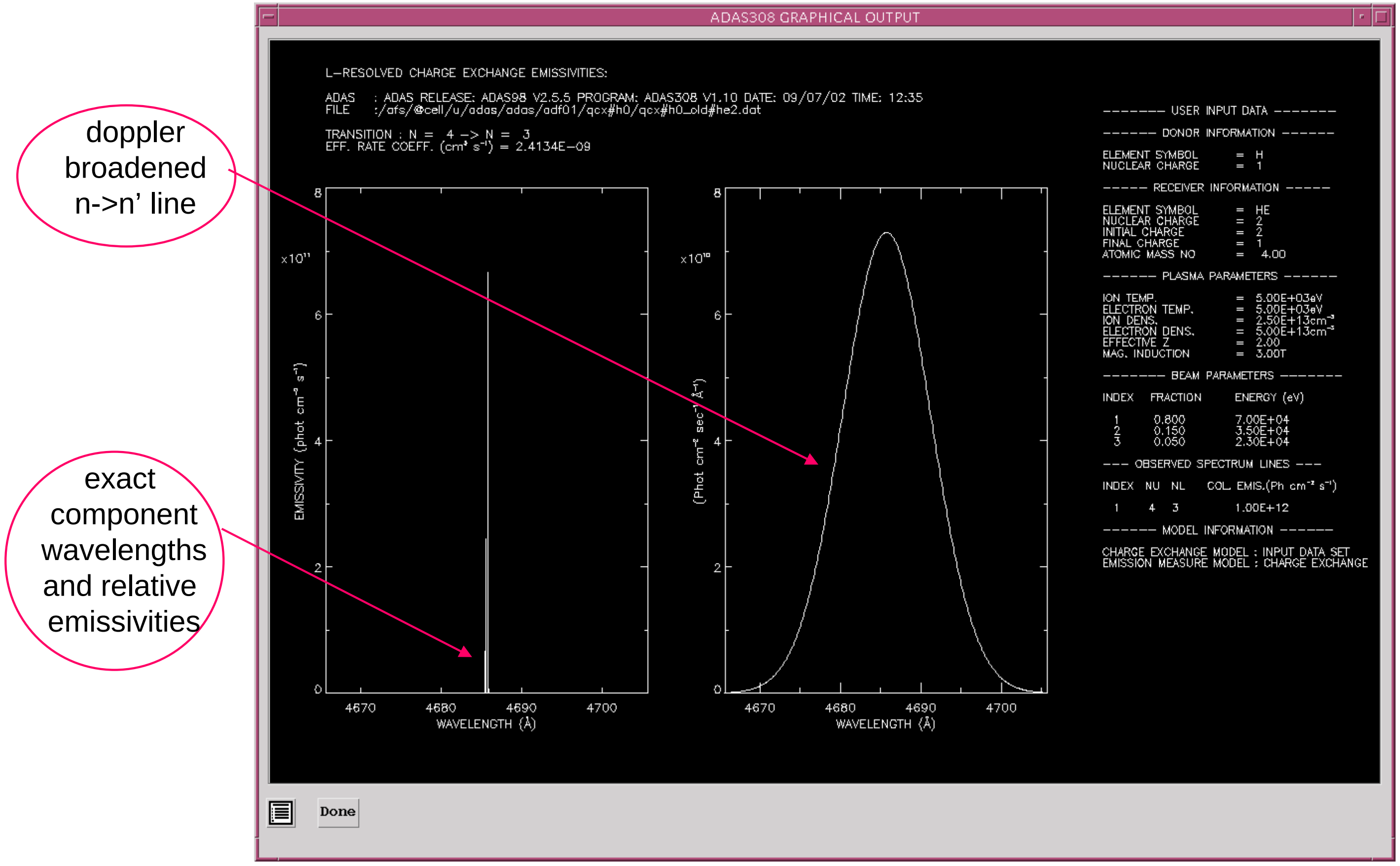
Data File Name: /afs/@cell/u/adas/adas/adf01/qcx#h0/qcx#h0_old#he2.dat

☑ Graphical Output

Select Device: Post-Script

two plots - stick and broadened

ADAS308 graph



```
L-RESOLVED CHARGE EXCHANGE EMISSIVITIES:

ADAS    : ADAS RELEASE: ADAS98 V2.5.5 PROGRAM: ADAS308 V1.10 DATE: 09/07/02 TIME: 12:35
FILE    :/afs/@cell/u/adas/adas/adf01/qcx#h0/qcx#h0_old#he2.dat

TRANSITION : N =  4 -> N =  3
EFF. RATE COEFF. (cm³ s⁻¹) = 2.4134E-09
```

```
-------- USER INPUT DATA --------

------- DONOR INFORMATION -------

ELEMENT SYMBOL       =  H
NUCLEAR CHARGE       =  1

----- RECEIVER INFORMATION -----

ELEMENT SYMBOL       =  HE
NUCLEAR CHARGE       =  2
INITIAL CHARGE       =  2
FINAL CHARGE         =  1
ATOMIC MASS NO       =   4.00

------- PLASMA PARAMETERS -------

ION TEMP.            =  5.00E+03eV
ELECTRON TEMP.       =  5.00E+03eV
ION DENS.            =  2.50E+13cm⁻³
ELECTRON DENS.       =  5.00E+13cm⁻³
EFFECTIVE Z          =  2.00
MAG. INDUCTION       =  3.00T

-------- BEAM PARAMETERS --------

INDEX   FRACTION      ENERGY (eV)

  1      0.800        7.00E+04
  2      0.150        3.50E+04
  3      0.050        2.30E+04

--- OBSERVED SPECTRUM LINES ---

INDEX  NU  NL    COL. EMIS.(Ph cm⁻² s⁻¹)

  1     4   3         1.00E+12

------- MODEL INFORMATION -------

CHARGE EXCHANGE MODEL : INPUT DATA SET
EMISSION MEASURE MODEL : CHARGE EXCHANGE
```

doppler
broadened
n->n’ line

exact
component
wavelengths
and relative
emissivities

Mass production of CX effective emission coeffts.

- ADAS309 is the mass production code for the effective emission coefficients for charge exchange lines.

- The user input is similar to that for ADAS308 but there is no graphical output, nor does it attempt the inversion solution.

- Many transitions can be entered at the one time. An output file of effective emission coefficients is delivered fully formatted to the ADF12 specification.

Extension of the CXS capabilities to heavier species

- Motivated by the need to cope with heavier receiver ions beyond argon, which may be partially ionized.
- There are two new codes ADAS315 and ADAS316. ADAS315 works on a scaleable universal dataset of format ADF49 to produce an ADF01 data set.
- ADAS316 is a bundle-n population model. It requires a driver data set and, for bundle-n in ADAS, these have historically been archived in ADF25. A new sub-directory /a25_p316 has been assigned and a complete redesign of the driver has been carried out.
- Output ADF26 (the bundle-n population solution), ADF12 (charge exchange effective emission coefficients) and ADF40 (feature emissivity coefficients) may be produced.
- For heavy species CXS, because of the very large number of transitions between highly excited states, the ADF40 format becomes more useful that ADF12.

4b. 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

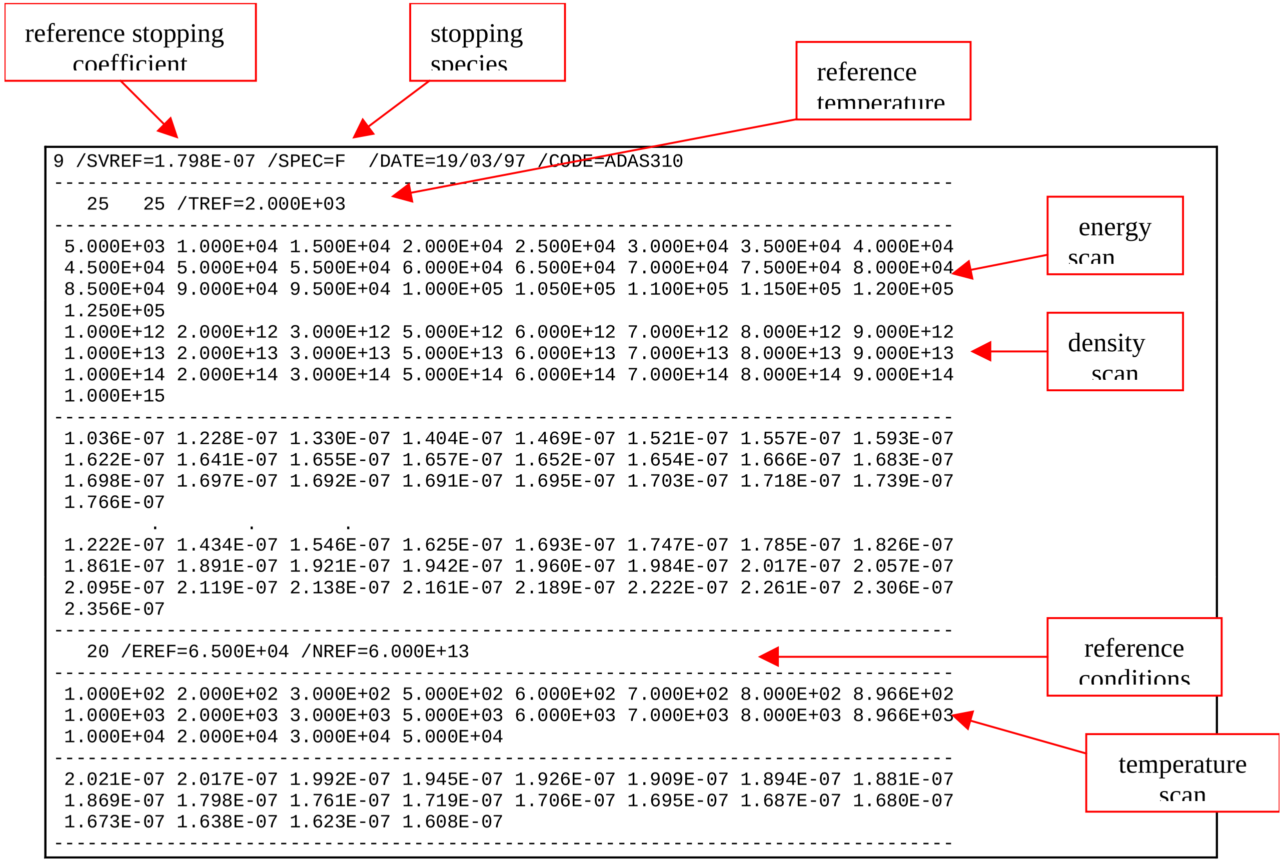
Interrogating effective beam stopping coefficients

- Datasets of class ADF21 contain effective stopping data as a function of beam and plasma parameters for different plasma species.

- Datasets of class ADF22 contain effective beam emission data as a function of beam and plasma parameters for different plasma species.

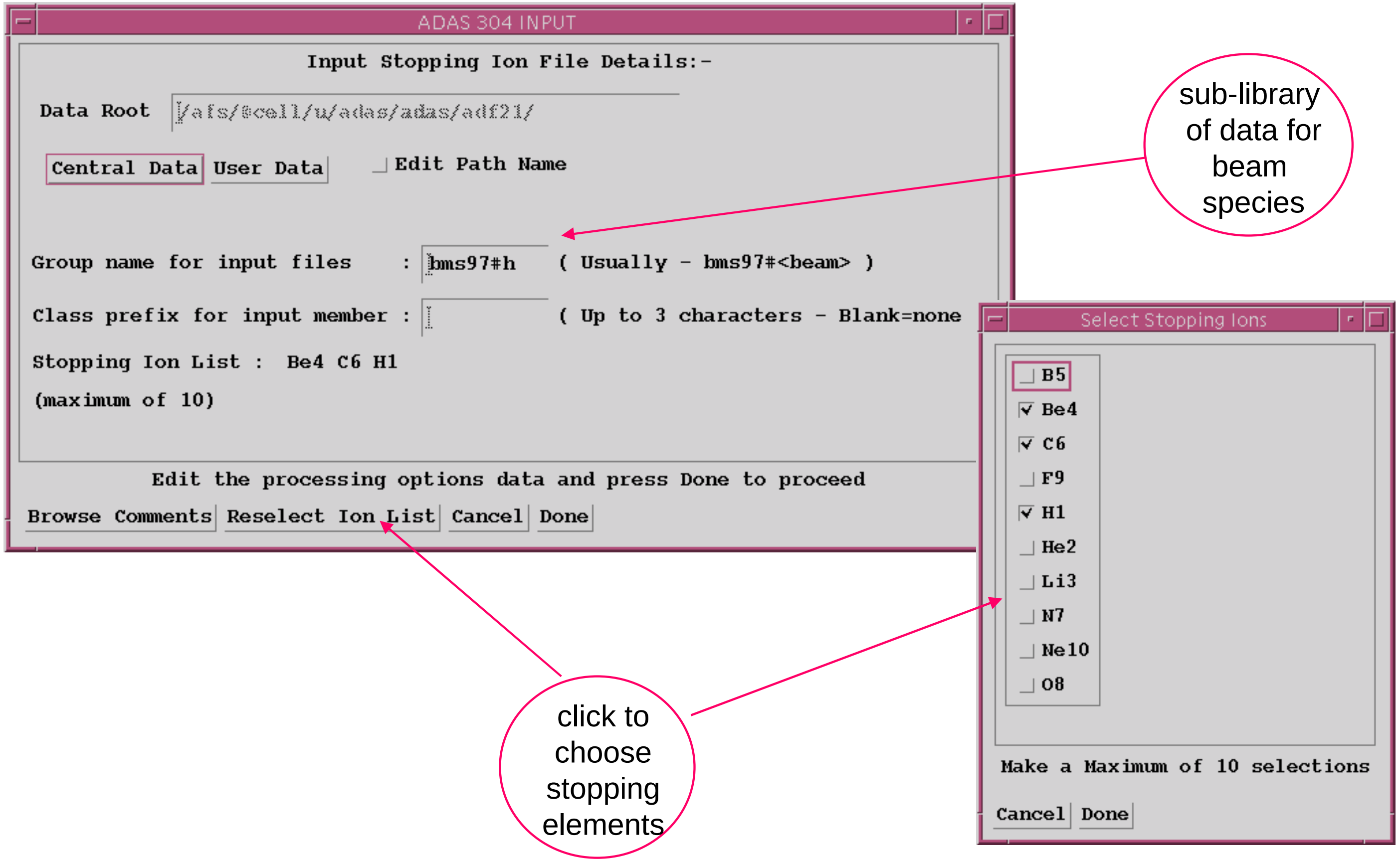
- Code ADAS304 interrogates ADF21 or ADF22 data sets to provide coefficients at beam and plasma conditions of your choice.

ADF21 beam stopping coefficients



```
9 /SVREF=1.798E-07 /SPEC=F  /DATE=19/03/97 /CODE=ADAS310
--------------------------------------------------------------------------------
   25   25 /TREF=2.000E+03
--------------------------------------------------------------------------------
 5.000E+03 1.000E+04 1.500E+04 2.000E+04 2.500E+04 3.000E+04 3.500E+04 4.000E+04
 4.500E+04 5.000E+04 5.500E+04 6.000E+04 6.500E+04 7.000E+04 7.500E+04 8.000E+04
 8.500E+04 9.000E+04 9.500E+04 1.000E+05 1.050E+05 1.100E+05 1.150E+05 1.200E+05
 1.250E+05
 1.000E+12 2.000E+12 3.000E+12 5.000E+12 6.000E+12 7.000E+12 8.000E+12 9.000E+12
 1.000E+13 2.000E+13 3.000E+13 5.000E+13 6.000E+13 7.000E+13 8.000E+13 9.000E+13
 1.000E+14 2.000E+14 3.000E+14 5.000E+14 6.000E+14 7.000E+14 8.000E+14 9.000E+14
 1.000E+15
--------------------------------------------------------------------------------
 1.036E-07 1.228E-07 1.330E-07 1.404E-07 1.469E-07 1.521E-07 1.557E-07 1.593E-07
 1.622E-07 1.641E-07 1.655E-07 1.657E-07 1.652E-07 1.654E-07 1.666E-07 1.683E-07
 1.698E-07 1.697E-07 1.692E-07 1.691E-07 1.695E-07 1.703E-07 1.718E-07 1.739E-07
 1.766E-07
         .        .        .
 1.222E-07 1.434E-07 1.546E-07 1.625E-07 1.693E-07 1.747E-07 1.785E-07 1.826E-07
 1.861E-07 1.891E-07 1.921E-07 1.942E-07 1.960E-07 1.984E-07 2.017E-07 2.057E-07
 2.095E-07 2.119E-07 2.138E-07 2.161E-07 2.189E-07 2.222E-07 2.261E-07 2.306E-07
 2.356E-07
--------------------------------------------------------------------------------
   20 /EREF=6.500E+04 /NREF=6.000E+13
--------------------------------------------------------------------------------
 1.000E+02 2.000E+02 3.000E+02 5.000E+02 6.000E+02 7.000E+02 8.000E+02 8.966E+02
 1.000E+03 2.000E+03 3.000E+03 5.000E+03 6.000E+03 7.000E+03 8.000E+03 8.966E+03
 1.000E+04 2.000E+04 3.000E+04 5.000E+04
--------------------------------------------------------------------------------
 2.021E-07 2.017E-07 1.992E-07 1.945E-07 1.926E-07 1.909E-07 1.894E-07 1.881E-07
 1.869E-07 1.798E-07 1.761E-07 1.719E-07 1.706E-07 1.695E-07 1.687E-07 1.680E-07
 1.673E-07 1.638E-07 1.623E-07 1.608E-07
--------------------------------------------------------------------------------
```

ADAS304 Input



Input Stopping Ion File Details:-

Data Root /afs/@cell/u/adas/adas/adf21/

☐ Edit Path Name

Group name for input files : bms97#h (Usually - bms97#<beam>)

Class prefix for input member : (Up to 3 characters - Blank=none

Stopping Ion List : Be4 C6 H1

(maximum of 10)

Edit the processing options data and press Done to proceed

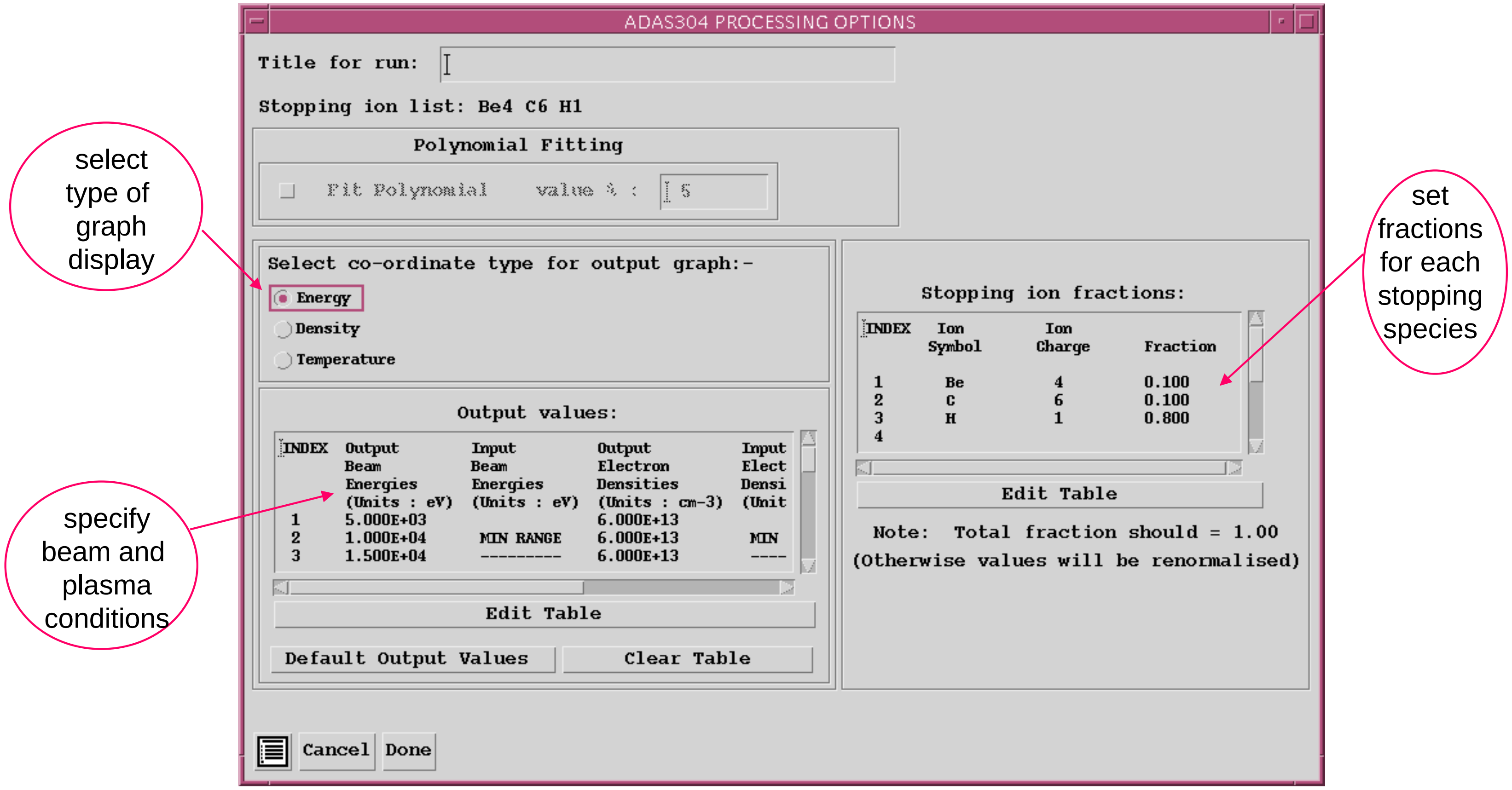
☐ B5
☑ Be4
☑ C6
☐ F9
☑ H1
☐ He2
☐ Li3
☐ N7
☐ Ne10
☐ O8

Make a Maximum of 10 selections

sub-library of data for beam species

click to choose stopping elements

ADAS304 Processing



Title for run:

Stopping ion list: Be4 C6 H1

Polynomial Fitting

☐ Fit Polynomial value % : 5

Select co-ordinate type for output graph:-

● Energy
○ Density
○ Temperature

Output values:

INDEX	Output Beam Energies (Units : eV)	Input Beam Energies (Units : eV)	Output Electron Densities (Units : cm-3)	Input Elect Densi (Unit
1	5.000E+03		6.000E+13	
2	1.000E+04	MIN RANGE	6.000E+13	MIN
3	1.500E+04	---------	6.000E+13	----

Stopping ion fractions:

INDEX	Ion Symbol	Ion Charge	Fraction
1	Be	4	0.100
2	C	6	0.100
3	H	1	0.800
4			

Note: Total fraction should = 1.00
(Otherwise values will be renormalised)

select type of graph display

specify beam and plasma conditions

set fractions for each stopping species

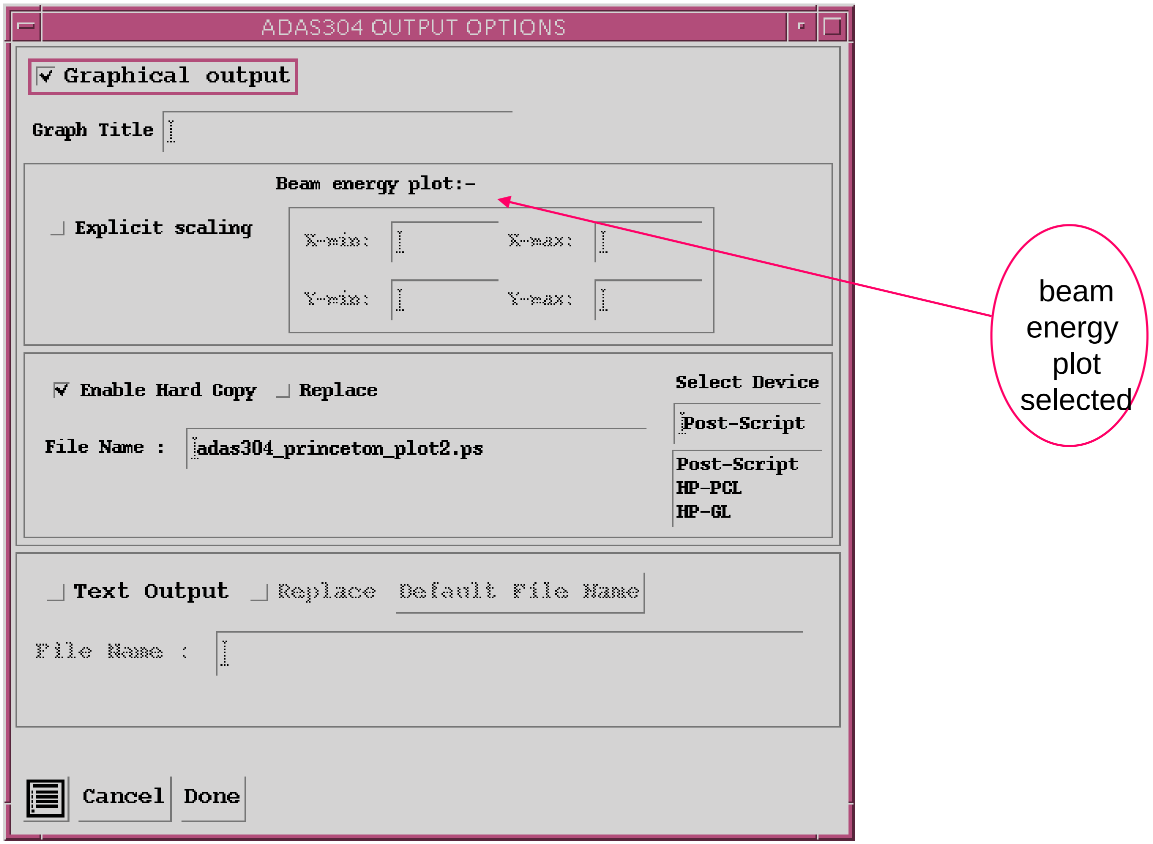
Obtaining effective beam stopping or emission coefficients (contd.)

- The composite stopping for a mixed composition plasma is assembled as

$$N_e S_{CR}^{(A)}(E_B, N_I, T_I) \approx \sum_{i=1}^{I} N_{e,i} [S_{CR}^{(i,e)}(E_B, N_I, T_I) +$$

$$(1/z_{0i}) S_{CR}^{(i,z_0)}(E_B, N_I, T_I)]$$

ADAS304 output



☑ Graphical output

☐ Explicit scaling

☑ Enable Hard Copy ☐ Replace

File Name : adas304_princeton_plot2.ps

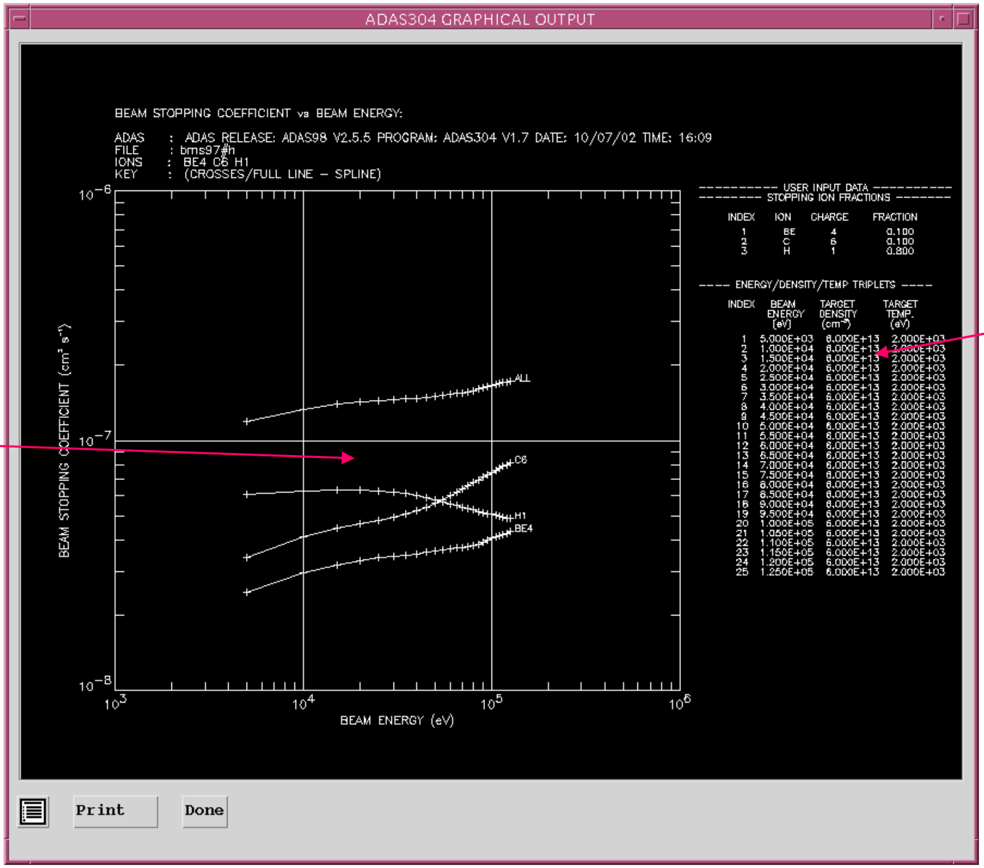
Select Device: Post-Script

☐ Text Output ☐ Replace

File Name :

beam energy plot selected

ADAS304 graph



```
BEAM STOPPING COEFFICIENT vs BEAM ENERGY:

ADAS    :  ADAS RELEASE: ADAS98 V2.5.5 PROGRAM: ADAS304 V1.7 DATE: 10/07/02 TIME: 16:09
FILE    : bms97#h
IONS    :  BE4 C6 H1
KEY     :  (CROSSES/FULL LINE - SPLINE)

----------- USER INPUT DATA -----------
--------- STOPPING ION FRACTIONS ---------

  INDEX    ION    CHARGE    FRACTION

    1       BE      4        0.100
    2       C       6        0.100
    3       H       1        0.800

---- ENERGY/DENSITY/TEMP TRIPLETS ----

  INDEX   BEAM       TARGET      TARGET
         ENERGY     DENSITY      TEMP.
          (eV)      (cm^-3)      (eV)

    1  5.000E+03  6.000E+13  2.000E+03
    2  1.000E+04  6.000E+13  2.000E+03
    3  1.500E+04  6.000E+13  2.000E+03
    4  2.000E+04  6.000E+13  2.000E+03
    5  2.500E+04  6.000E+13  2.000E+03
    6  3.000E+04  6.000E+13  2.000E+03
    7  3.500E+04  6.000E+13  2.000E+03
    8  4.000E+04  6.000E+13  2.000E+03
    9  4.500E+04  6.000E+13  2.000E+03
   10  5.000E+04  6.000E+13  2.000E+03
   11  5.500E+04  6.000E+13  2.000E+03
   12  6.000E+04  6.000E+13  2.000E+03
   13  6.500E+04  6.000E+13  2.000E+03
   14  7.000E+04  6.000E+13  2.000E+03
   15  7.500E+04  6.000E+13  2.000E+03
   16  8.000E+04  6.000E+13  2.000E+03
   17  8.500E+04  6.000E+13  2.000E+03
   18  9.000E+04  6.000E+13  2.000E+03
   19  9.500E+04  6.000E+13  2.000E+03
   20  1.000E+05  6.000E+13  2.000E+03
   21  1.050E+05  6.000E+13  2.000E+03
   22  1.100E+05  6.000E+13  2.000E+03
   23  1.150E+05  6.000E+13  2.000E+03
   24  1.200E+05  6.000E+13  2.000E+03
   25  1.250E+05  6.000E+13  2.000E+03
```

Each contribution to stopping and total

specified conditions

Computing effective beam coefficients

- The first step is the calculation of the full collisional-radiative population structure of the hydrogen beam atoms.
- Code ADAS310 performs these calculations in the bundle-n model.
- It executes these repeatedly for the sets of plasma parameters required to construct tables containing the excited population structure and beam stopping.

Computing effective beam coefficients (contd.)

- The full population structures are archived in ADF26 according to (single) impurity.

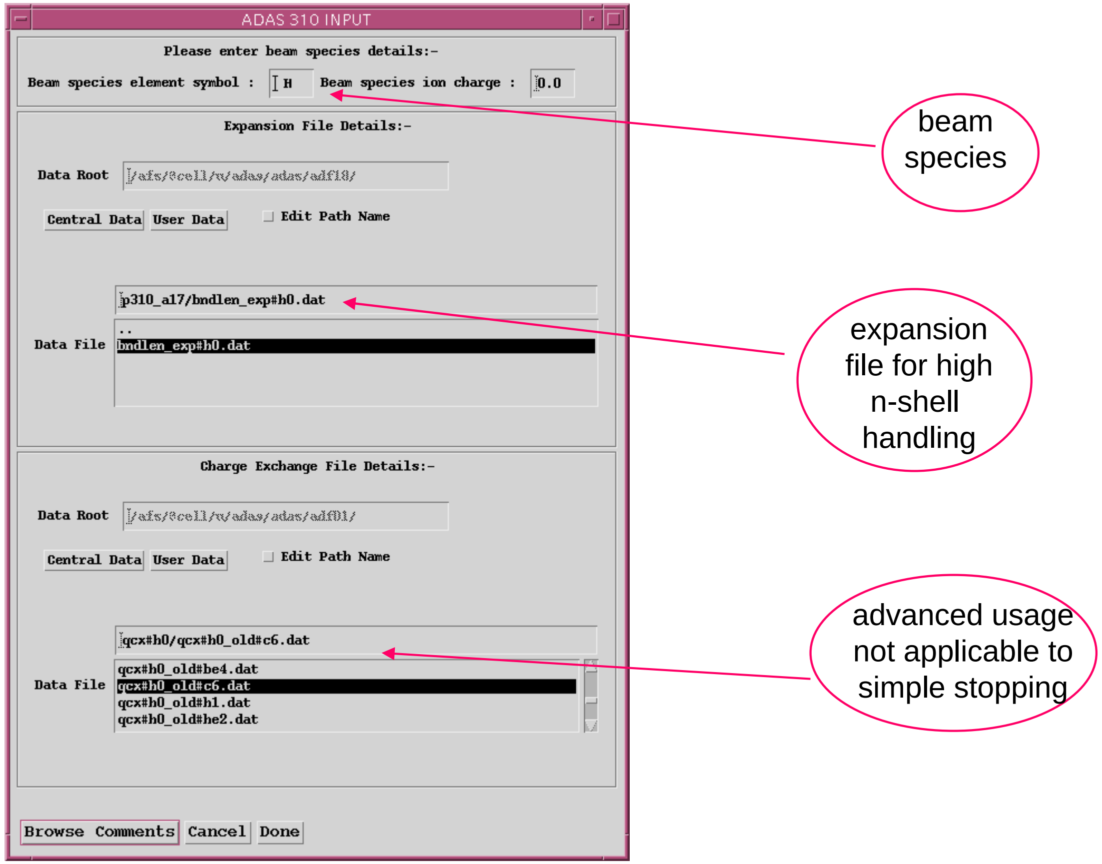
- Code ADAS312 post-processes the ADF25 files to extract the beam stooping and beam emission coefficients of choice.

- The output is structured according to the ADF21 (beam stopping) and ADF22 (beam emission) specifications.

Computing effective beam coefficients (contd.)

- File selection
  - » Two input files may be selected.
  - » The first, called the expansion file, gives the pathway for storing condensed collisional-radiative matrices.
  - » The second, charge exchange file, is not important for the beam case. ADAS310 can compute hydrogen populations in the plasma (including CX) as well as beams

ADAS310 Input



Please enter beam species details:-

Beam species element symbol : H

Beam species ion charge : 0.0

Expansion File Details:-

Data Root /afs/@cell/u/adas/adas/adf18/

p310_a17/bndlen_exp#h0.dat

Data File

..
bndlen_exp#h0.dat

Charge Exchange File Details:-

Data Root /afs/@cell/u/adas/adas/adf01/

qcx#h0/qcx#h0_old#c6.dat

Data File

qcx#h0_old#be4.dat
qcx#h0_old#c6.dat
qcx#h0_old#h1.dat
qcx#h0_old#he2.dat

beam species

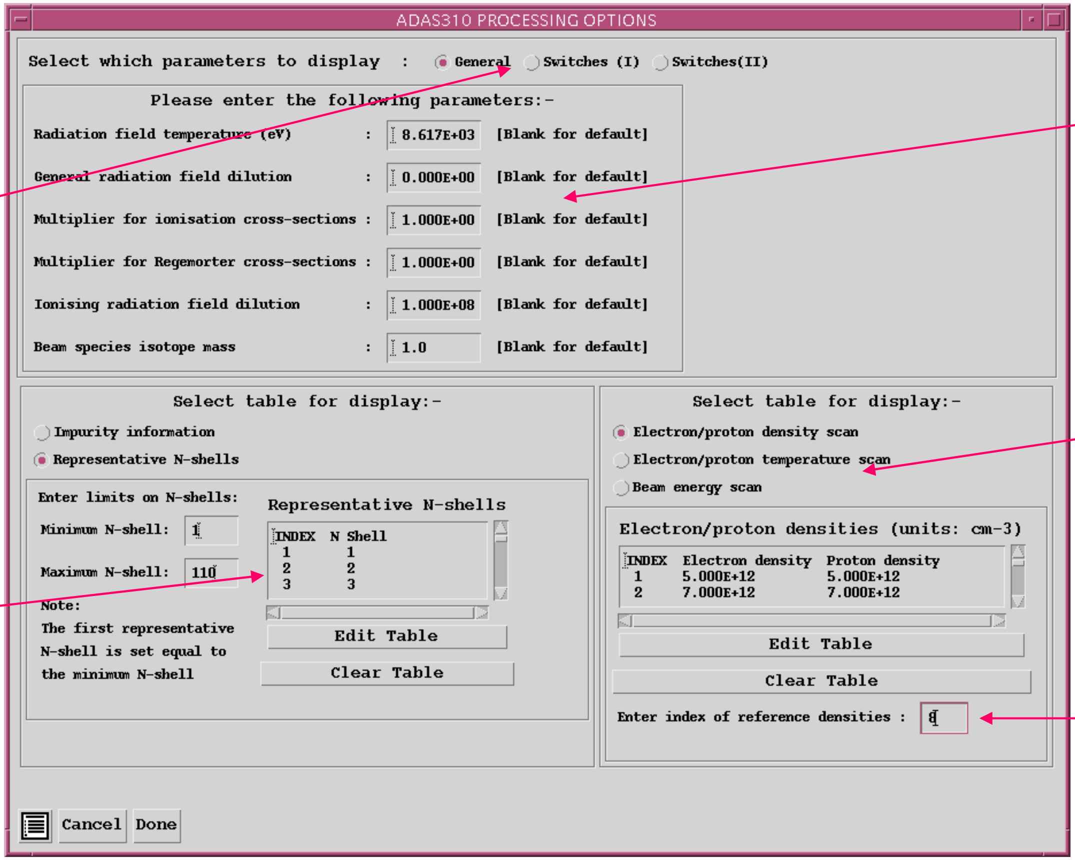
expansion file for high n-shell handling

advanced usage not applicable to simple stopping

Computing effective beam coefficients (contd.)

- Processing options
  - » There are many parameters to specify but most are set with defaults.
  - » The main user data are the impurity specifications and the plasma parameter scans.
  - » ADAS310 can work with mixed impurities but main tabulations are for single impurities which are linearly combined for mixtures at the spectral analysis stage

ADAS310 Processing



Select which parameters to display : ● General ○ Switches (I) ○ Switches(II)

Please enter the following parameters:-

Radiation field temperature (eV)	:	8.617E+03	[Blank for default]
General radiation field dilution	:	0.000E+00	[Blank for default]
Multiplier for ionisation cross-sections	:	1.000E+00	[Blank for default]
Multiplier for Regemorter cross-sections	:	1.000E+00	[Blank for default]
Ionising radiation field dilution	:	1.000E+08	[Blank for default]
Beam species isotope mass	:	1.0	[Blank for default]

Select table for display:-

○ Impurity information

● Representative N-shells

Enter limits on N-shells:

Minimum N-shell: 1

Maximum N-shell: 110

Note:
The first representative
N-shell is set equal to
the minimum N-shell

Representative N-shells

INDEX	N Shell
1	1
2	2
3	3

Select table for display:-

● Electron/proton density scan

○ Electron/proton temperature scan

○ Beam energy scan

Electron/proton densities (units: cm-3)

INDEX	Electron density	Proton density
1	5.000E+12	5.000E+12
2	7.000E+12	7.000E+12

Enter index of reference densities : 1

three sets of switches - defaults are set

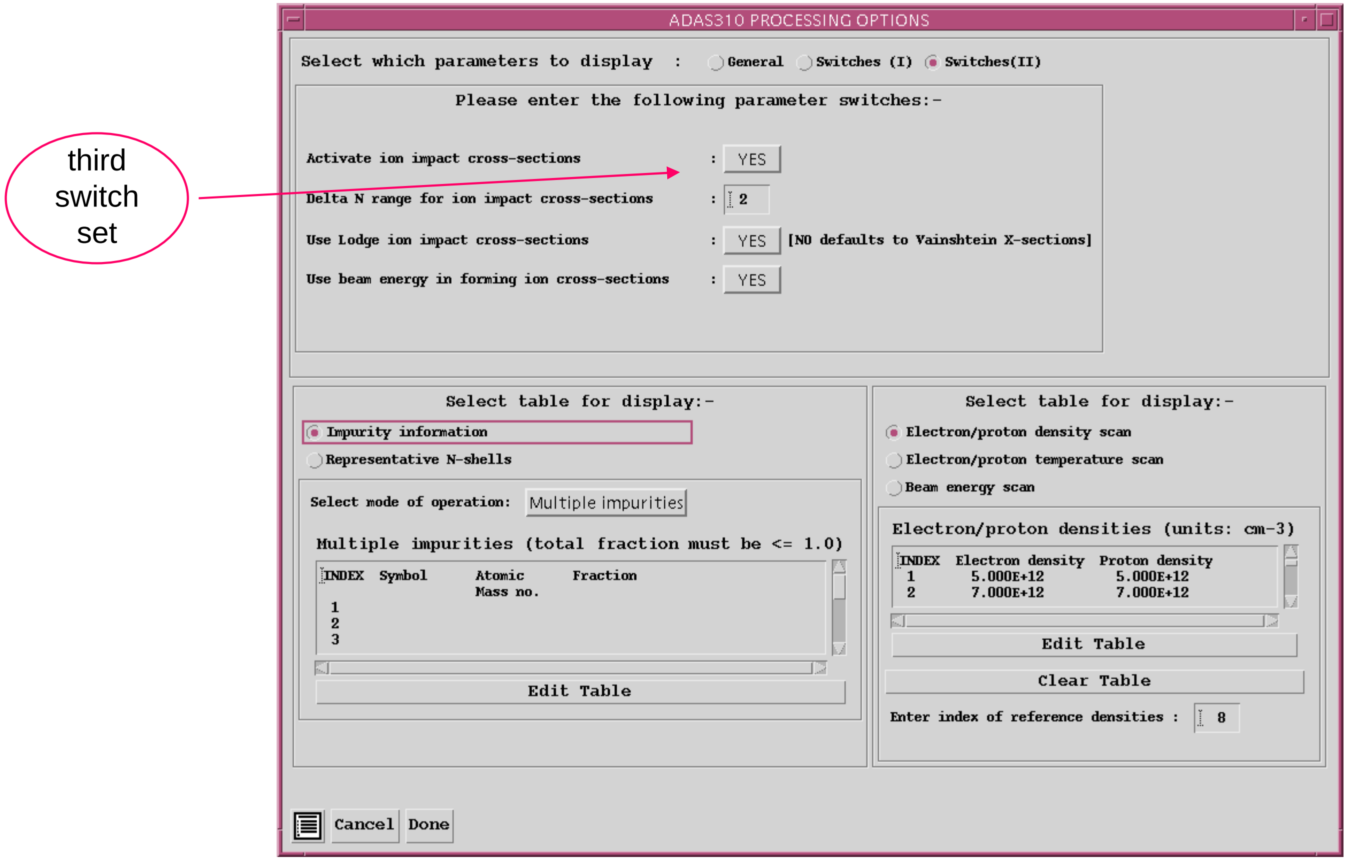
general parameters controlling x-sect. use

specify scans in key parameters

specify details of bundle-n model for hydrogen

note use of reference conditions

ADAS310 Processing (contd.)



ADAS310 PROCESSING OPTIONS

Select which parameters to display : ○ General ○ Switches (I) ● Switches(II)

Please enter the following parameter switches:-

Activate ion impact cross-sections : YES

Delta N range for ion impact cross-sections : 2

Use Lodge ion impact cross-sections : YES [NO defaults to Vainshtein X-sections]

Use beam energy in forming ion cross-sections : YES

Select table for display:-

● Impurity information

○ Representative N-shells

Select mode of operation: Multiple impurities

Multiple impurities (total fraction must be <= 1.0)

INDEX	Symbol	Atomic Mass no.	Fraction
1			
2			
3			

Edit Table

Select table for display:-

● Electron/proton density scan

○ Electron/proton temperature scan

○ Beam energy scan

Electron/proton densities (units: cm-3)

INDEX	Electron density	Proton density
1	5.000E+12	5.000E+12
2	7.000E+12	7.000E+12

Edit Table

Clear Table

Enter index of reference densities : 8

Computing effective beam coefficients (contd.)

- Output options
  - » There is no graphical display from ADAS310.
  - » Several pass files are created
  - » .pass4 is the population structure (ADF26)
  - » Execution time can be ~ 10 mins.

ADAS310 Output

Title for run:

☑ Run Summary Output ☐ Replace

File Name : paper.txt

☐ First Passing File ☐ Replace

File Name :

☐ Second Passing File ☐ Replace

File Name :

☐ Third Passing File ☐ Replace

File Name :

☐ Fourth Passing File ☐ Replace

File Name :

extended set of passing files for post-processing

Beam emission and the Balmer alpha Stark multiplet structure

- The calculation of local Stark/Zeeman emission feature from H (D/T) beams into play as an IDL procedure call *adas305_get_stark.pro* or within FORTRAN by calling the *stark.for* routine in the adas3xx library.

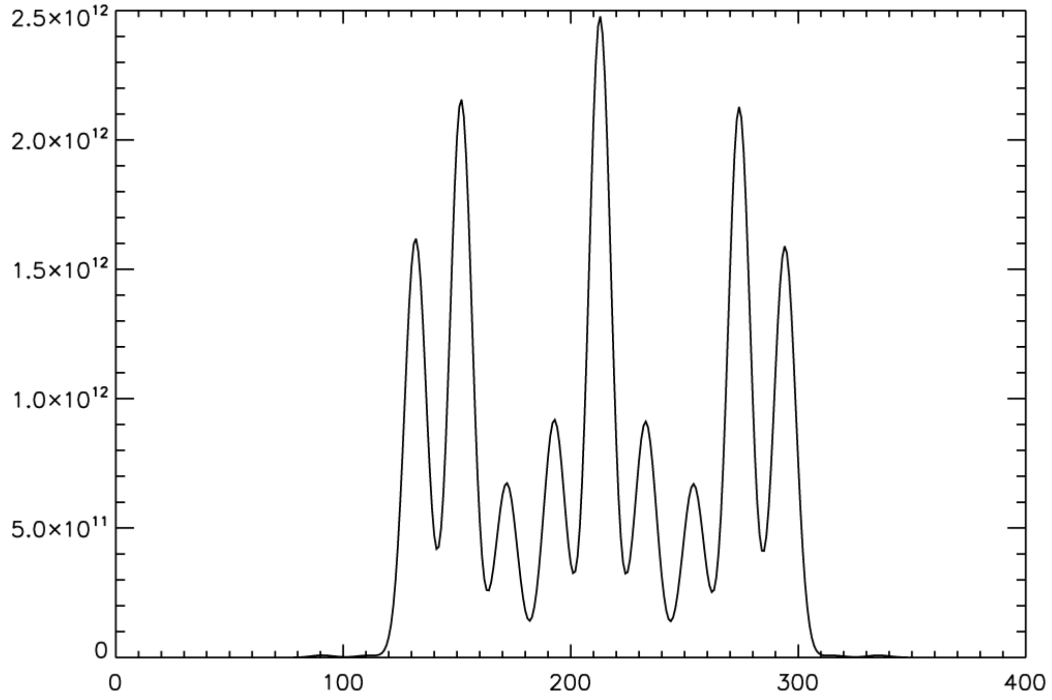
- The beam, plasma, E and B fields and observation orientation must be specified. General geometry specification is defined by direction cosines. The polarisation can be specified by multipliers on the pi and sigma components.

- The feature is returned as either a collection of component wavelengths and emissivities or a Doppler broadened feature over a specified wavelength range (specify minimum and maximum wavelengths and number of pixels).

adas305_get_stark.pro

```
PRO stark_figure

beam   = {mass : 2.0, energy : 40.0e3, te : 10.0, density : 4.27e9}
plasma = {mass : 2.0, te : 4.44e3, density : 2.49e13, zeff : 2.0}
bfield = {value : 3.3915, dc_x : 0.788, dc_y : 0.0053, dc_z : 0.6152}
efield = {value : 0.0000, dc_x : 1.000, dc_y : 0.0000, dc_z : 0.0000}
obs    = {dc_x : 0.8701, dc_y : -0.047, dc_z : 0.4905, sigma : 0.51, pi : 1.0}

adas305_get_stark,beam=beam,plasma=plasma,bfield=bfield,efield=efield, $
obs=obs,n_lower=2,n_upper=3,wave_min=6510,wave_max=6550,npix=400, $
emiss_doppler=emiss_doppler,/doppler

!p.thick=1
!x.thick=1
!y.thick=1
!p.charthick=1
;set_plot, 'PS'
;device, filename=strcompress('fig_stark_cpts.ps',/remove_all)
window,1
plot,emiss_doppler

end
```

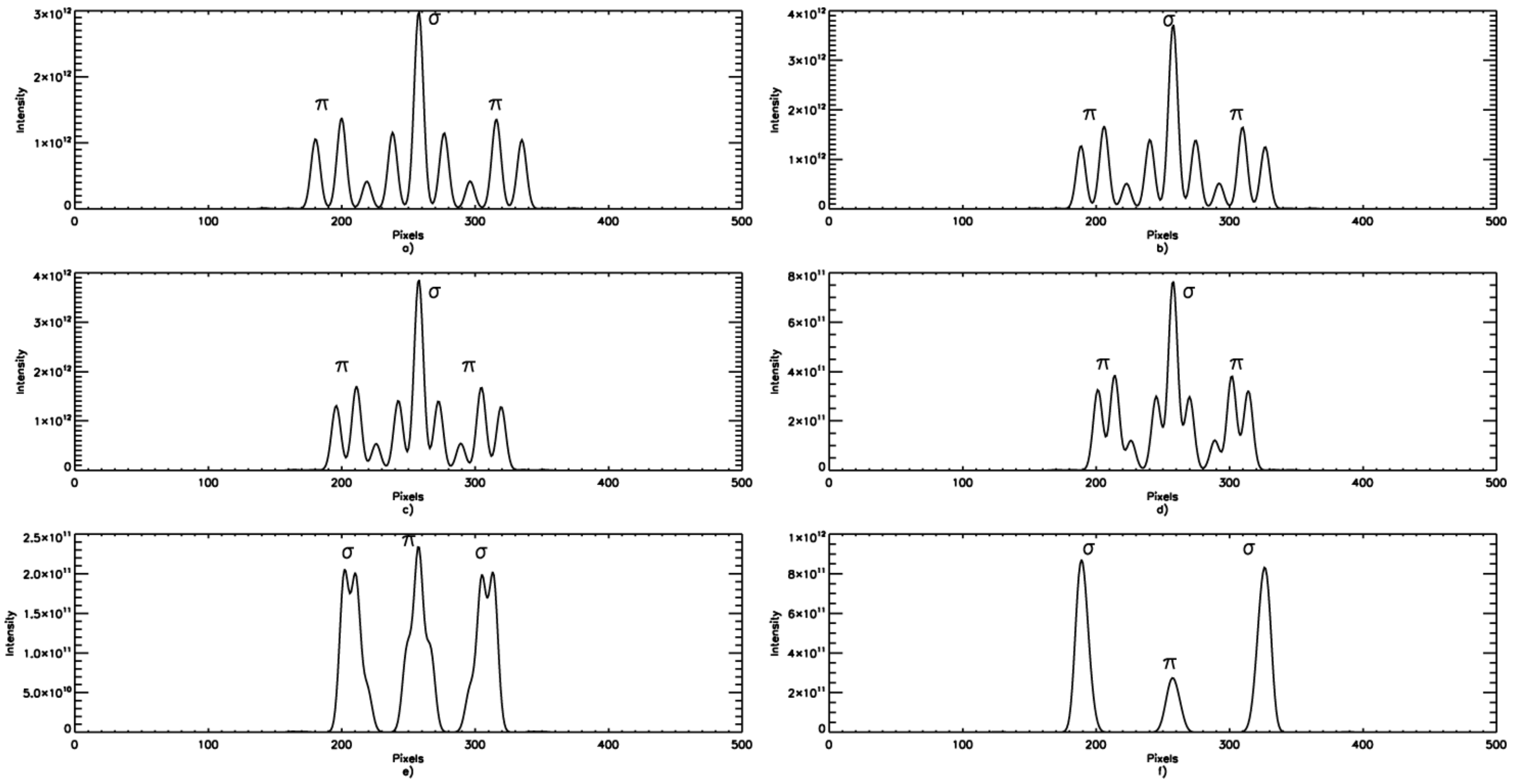
Balmer alpha Stark multiplet



Feature variation

B: 1.4T – 50 T

E: 0.5Mev/amu – 100eV/amu



-

Overview of Atomic Structure and Collision Theory

Nigel Badnell

Department of Physics
University of Strathclyde
Glasgow, UK

– ADAS 2009 –

Atomic Structure Methods

It is deceptively simple to write down the structure problem to be solved

$$\Psi = \sum\!\!\!\!\!\!\!\int_{\nu} a_{\nu}\psi_{\nu} \, . \tag{1}$$

The total wavefunction for the atom Ψ is expanded in terms of a complete set of (antisymmetric) basis states ψ_{ν} (an N-product of one-electron orbitals) with expansion coefficients a_{ν}.

Spherically symmetric problem $\longrightarrow$ (θ, ϕ) problem solved. Use standard angular algebra methods and packages are used, mostly based on Racah algebra but also Condon and Shortley (Slater-states).

Only require to determine radial dependence of wavefunction.

- Hartree/Dirac-Fock: coupled-set of radial equations result from formally varying radial orbitals to give stationary value of an energy functional — self-consistent solution: MCHF (Froese), HFR (Cowan), MCDF (Grant) etc. (Expansion coefficients may also be determined this way, MCHF.)
- Configuration Interaction (CI): radial equations (usually uncoupled) contain variational parameters (e.g. "model potentials") which are varied (numerically) to minimize a computed energy functional: AS/SS, CIV3, HULLAC
- As CI but using a self-consistent model potential: AS, HULLAC, FAC.

All approaches then, usually, construct and diagonalize the Hamiltonian to give the final e-states and e-energies.

Basis expansion is slow to converge in general. A plethora of basis functions are used: spectroscopic, psuedo (Laguerre), B-splines etc.

Pros & Cons: problems with converging HF for excited states. Local vs global minimum, flexible enough variational parameters.

Scattering codes can use only the simplest HF methods, in general: unique, orthogonal...

Hamiltonian

♣ Schrödinger equation based (AS, CIV3, MCHF):

- Non-relativistic: kinetic, nuclear & electrostatic operators.
- Breit-Pauli: as above, plus one-body fine-structure (spin-orbit), and non-fine-structure (Mass-Velocity & Darwin).
  Fine structure mixes terms, non-fine-structure can be added to NR above.
- Breit-Pauli: as above, plus two-body fine-structure (spin-spin, spin-orbit, spin-other-orbit).
- Breit-Pauli: as above, plus two-body non-fine-structure (orbit-orbit, contact-spin-spin, Darwin).

♣ Kappa-averaged Dirac equation based (± small component): radial functions still depend only on nl, not nlj. Then using above Breit-Pauli operators. (HFR one-body only, AS.)

♣ Dirac equation based, large and small component.

- Dirac-Coulomb (HULLAC, FAC)
- $+$ (Generalized) Breit $+$QED (GRASP, Sampson/LANL)

Others: Sapirstein & Johnson, Desclaux, Chen...

Coupling schemes: LS, LSJ, jK, jj (unitary transformations).

What matters more are good quantum numbers...

Atomic Structure Data

Bound-Bound

- Energy levels, ("All")
- E_k and M_k radiative rates ("Most")

Bound-Free

- Autoionization rates, DR (AS, HULLAC, FAC, MCDF(Chen) ...)
- Photoionization cross sections, RR (ditto)

Free-Free

- Infinite and finite energy Plane-wave Born (AS, Cowan)

And More...

- Hyperfine
- Stark-mixing, DR
- ...

Complex (Heavy) Species

- Unresolved Transition Array (UTA) Spectral shape — Bauche-Arnault, Bauche & Klapisch
- Configuration-average (CA) collisions — Cowan driven.

Both neglect configuration interaction.

Atomic Collision Methods

Time-dependent methods solve the full Schrödinger equation — TDCC.

Time-independent methods expand the antisymmetric total wavefunction for the target-plus-colliding particle Ψ in terms of a known complete basis of target states ψ_{ν}.

$$\Psi = \mathcal{A} \sum\!\!\!\!\!\!\!\int_{\nu} \psi_{\nu} \phi \, . \qquad (2)$$

The expansion coefficients ϕ representing the colliding particle (projectile) are then to be freely determined by a variational of the scattering matrix leading to the continuum Hartree/Dirac-Fock equations.

Coupled-channel methods

Resonances arise naturally when the scattering energy of an open-channel coincides with that of a closed-channel.

Traditional close-coupling approximation truncates the expansion to a low-lying set of closely-coupled atomic states — neglects ionization loss.

Pseudo-state expansions attempt to approximate the sum/integral over a wide range of energies and work towards practical numerical convergence — RMPS, CCC.

Complete basis expansions can be used over a limited energy range and volume (particle in a box) — B-spline R-matrix, Intermediate Energy R-matrix.

Distorted-wave methods

DW methods solve (elastic) uncoupled continuum Schrödinger/Dirac equations and treat the (inelastic) coupling as a perturbation — can keep problem small, a series of 2x2 calculations: AS/HULLAC/FAC/LANL & UCL(historic)

Resonances are often neglected from electron-impact excitation, but not recombination — DR. Use of the IPIRDW approximation (Independent Processes Isolated Resonance using DW): AS/HULLAC/FAC

Simple "DW": Coulomb or plane-wave Born for EIE & EII: ATOM or AS/Cowan

Heavy species: can/need we go beyond PWB?

R-matrix

Probably the most successful method/code suite for electron-impact excitation and photoionization (no so much for electron-ionization).

A close-coupling method which is very efficient at mapping-out resonances, compared to CCC, UCL-IMPACT (historic) etc. (But not compared to IPIRDW...)

Need to solve the coupled integro-differential scattering equations at tens, if not hundreds, of thousands of energies and for ~ 100 angular momentum symmetries.

Key Idea

Divide scattering region into two: an inner region that just encompasses the atom/ion (wavefunctions $\lesssim 10^{-3}$, say, outside) and where the scattering potentials are complicated (e.g. short-range); and an outer region where we only have an asymptotic Coulomb potential and, maybe, dipole and quadrupole coupling potentials (with analytic coefficients). Let the dividing boundary radius be r_0.

The inner region is a finite volume and we can expand our (to be determined) continuum wavefunction in terms of a simple orthogonal basis of states $u_i(r)$, say, with a fixed (outer) boundary condition given by the logarithmic derivative:

$$\frac{\mathrm{d}}{\mathrm{d}r}\log(u_i(r))\bigg|_{r=r_0} = \frac{u_i'(r)}{u_i(r)}\bigg|_{r=r_0} = b \tag{3}$$

where b is usually taken to be zero (it must be a constant).

This leads to a set of discrete positive energy solutions k_i^2, say (particle in a box).

The inner region solution at $r = r_0$ for any scattering energy k^2 is completely characterized by the R-matrix:

$$R \equiv \sum_{i=1}^{\infty} \frac{[u_i(r_0)]^2}{k_i^2 - k^2}. \tag{4}$$

The scattering matrix (hence, cross section) is determined by matching the outer region solution to the inner region one at r_0.

For example, for s-wave $(l = 0)$ scattering off a neutral atom

$$K = \frac{-\sin(kr_0) + R(k\cos(kr_0) - b\sin(kr_0))}{\cos(kr_0) + R(k\sin(kr_0) + b\cos(kr_0))}. \tag{5}$$

Here, K is the reactance matrix, which is simply related the the S-matrix.

A more detailed exposition, based on Burke & Robb (1975), is available.

Web Links

http://amdpp.phys.strath.ac.uk/

http://amdpp.phys.strath.ac.uk/tamoc/

http://amdpp.phys.strath.ac.uk/autos/

http://amdpp.phys.strath.ac.uk/UK_APAP/codes.html

R-matrix

Nigel Badnell

Department of Physics
University of Strathclyde
Glasgow, UK

Overview

- R-matrix method
- Parallel codes
- R-matrix with pseudo-states (RMPS)
- Intermediate coupling frame transformation (ICFT) R-matrix
- Dirac R-matrix
- Future thoughts

Motivation

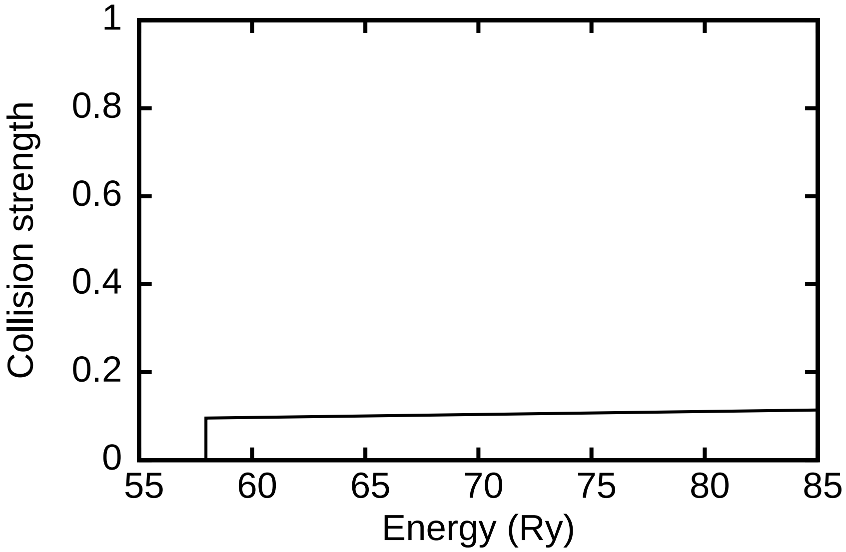
Q. Why atomic collisions?

A. Spectroscopic diagnostic modelling of non-LTE astrophysical and laboratory plasmas.

Simplest model: excited states of an atom/ion are populated by collisional excitation and de-populated by radiative transitions.

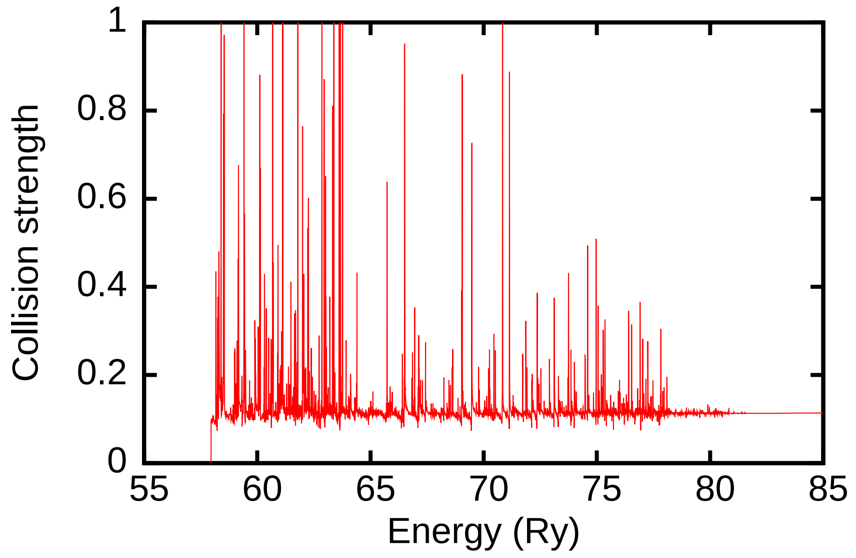
So, need excitation rate coefficients — Maxwellian average of excitation cross sections.

A typical cross section?



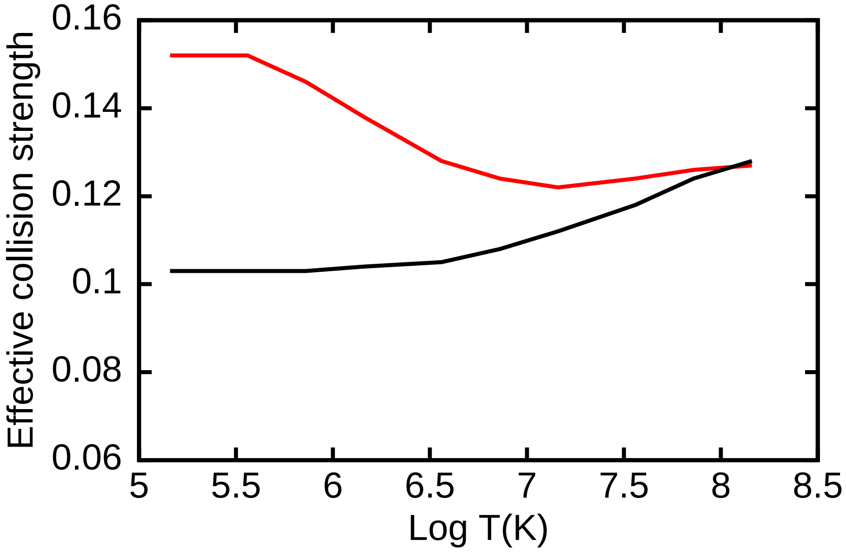
(Collision strength $\Omega = \omega k^2 \sigma / \pi a_0^2$.)

No!



(129CC Dirac–Coulomb R-matrix collision strength for the $3\mathrm{d}^{10}\ {}^1\mathrm{S}_0 - 4\mathrm{d}^1\mathrm{S}_0$ transition in Xe^{26+}.)

The difference!



(Effective (Maxwell-averaged) collision strength $\Upsilon = (kT)^{1/2}\omega q/(2\alpha c a_0^2\sqrt{\pi})$.)

Basic Scattering Theory (in one page)

Write the (anti-symmetric) total wavefunction for the atom-colliding particle system as

$$\Psi = A \sum\!\!\!\!\!\!\int_{\nu} \psi_{\nu} \phi \,, \tag{1}$$

where the ψ_{ν} form a complete set of atomic eigenstates (discrete plus continuous).Then solve for ϕ from

$$H \Psi = E \Psi \,, \tag{2}$$

where H and E are the total Hamiltonian and Energy of the system, respectively. The difference between the large distance asymptotic wavefunction for the colliding particle (ϕ) and that of a plane (or Coulomb) wave leads to the probability of scattering (by a non-Coulomb potential) that has taken place — the S- or scattering matrix, of reactions between initial and final atomic states. A more useful quantity, simply related to the S-matrix, is the cross section, σ.

The Solution

Use of (1) and (2) leads to an infinite set of coupled integro-differential equations (integro because the exchange operator is a non-local). By discretizing the continuum we can form a quadrature for (1) and reduce (2) to a finite-set of close-coupling (CC) equations. Historically, only a few low-lying states of direct interest were included in the CC equations.

In (1) we assumed that we had all atomic eigenstates to any required level of accuracy. In practice, determining a sufficiently accurate atomic structure, while keeping the CC expansion manageable, is a significant issue for any collision calculation.

The wavefunction for the colliding particle (ϕ) is also expanded as an infinite sum of partial waves (angular momentum states). Typically, ≤ 10 angular momentum states couple to a given target state so as to give the same, conserved, total angular momentum for the combined system.

So, given a set of coupled integro-differential equations, how do we best go about solving them, given the complex resonance structure that we must resolve?

The R-matrix Method

The approach of the R-matrix method (Burke & Robb, 1975) to scattering builds upon the idea of dividing-up configuration space into two regions, an inner one where the scattering potential is non-trivial and the scattering wavefunction complicated, and an outer region where the potential is ‘simple’, for example, it vanishes or is Coulombic, and the radial function is represented by its asymptotic form, viz.

$$f_l(r) = f_l^a(r), \tag{3}$$

for $r \geq r_0$, the R-matrix boundary.

For example, a partial plane wave equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} + k^2 \right) f_l^a(r) = 0 \tag{4}$$

with general solution

$$f_l^a(r) = A_l \left[s_l(kr) + K_l c_l(kr) \right] \tag{5}$$

and $K_l = \tan \delta_l$, where δ_l is the phase shift and A_l is a normalization constant.

We denote the two independent real solutions by $s_l(kr)$ and $c_l(kr)$ (the so-called s and c functions). These are related to the spherical Bessel and Neumann functions $j_l(x)$ and $n_l(x)$ via

$$s_l(x) = x j_l(x) \tag{6}$$

and

$$c_l(x) = -x n_l(x). \tag{7}$$

Asymptotically,

$$s_l(x) \underset{x \to \infty}{\sim} \sin\left(x - \frac{l\pi}{2}\right) \tag{8}$$

$$c_l(x) \underset{x \to \infty}{\sim} \cos\left(x - \frac{l\pi}{2}\right). \tag{9}$$

In the inner-region ($r \leq r_0$) we denote the regular solution satisfying $f_l(r = 0) = 0$

by $f_l^b(r)$, i.e.

$$f_l(r) = f_l^b(r) \tag{10}$$

for $r \leq r_0$.

We can determine K_l (and hence σ_l) from $f_l^b(r)$ by matching logarithmic derivatives at the boundary $r = r_0$.

So, define

$$\gamma \equiv \left[\frac{\mathrm{d}f_l^b}{\mathrm{d}r}\frac{1}{f_l^b}\right]_{r=r_0} = \left[\frac{\mathrm{d}f_l^a}{\mathrm{d}r}\frac{1}{f_l^a}\right]_{r=r_0} . \tag{11}$$

Substituting for f_l^a, $f_l^{a\prime}$ from (5) we have

$$K_l = \tan\delta_l = \frac{s_l'(kr_0) - \gamma s_l(kr_0)}{\gamma c_l(kr_0) - c_l'(kr_0)}, \tag{12}$$

where the value of γ is given by the logarithmic derivative of f_l^b. We thus require to determine f_l^b. For $l = 0$, $s_0 = \sin$ and $c_0 = \cos$ and

$$K_0 = \tan\delta_0 = \frac{k\cos(kr_0) - \gamma\sin(kr_0)}{\gamma\cos(kr_0) + k\sin(kr_0)}. \tag{13}$$

Since $f_l^b(r)$ is required only over a finite range, $0 \leq r \leq r_0$, we can approximate it by a suitable linear combination of convenient basis functions $u_i(r)$. Thus,

$$f_l^b(r) = \sum_{i=0}^{\infty} a_i u_i(r). \tag{14}$$

The coefficients a_i are determined by requiring that $f_l^b(r)$ satisfies

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} - V(r) + k^2\right) f_l^b(r) = 0 \tag{15}$$

still, at least to a certain level of accuracy.

Various alternatives are possible. The Wigner–Eisenbud method is one of the most commonly used in atomic physics. We illustrate the case of $l = 0$. Then, we have that

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - V(r)\right) u_i(r) = -k_i^2 u_i(r), \tag{16}$$

for $i = 1, 2, \ldots \infty$, over $0 \le r \le r_0$, subject to the boundary conditions

$$u_i(0) = 0 \tag{17}$$

and

$$\left[\frac{\mathrm{d}u_i}{\mathrm{d}r}\frac{1}{u_i}\right]_{r=r_0} = b, \tag{18}$$

where b is a fixed (which characterizes Wigner–Eisenbud) arbitrary number.

The boundary condition (18) results in a discrete e-value spectrum $\{k_i^2 : i = 1, 2, \ldots \infty\}$.

Note,

$$\int_0^{r_0} u_i u_j \mathrm{d}r = \delta_{ij}, \tag{19}$$

for $i, j = 1, 2, \ldots \infty$, on renormalizing the u_i.

With

$$f_0^b(r) = \sum_{i=1}^{\infty} a_i u_i(r) \tag{20}$$

then

$$a_i = \int_0^{r_0} u_i(r) f_0^b(r) \mathrm{d}r. \tag{21}$$

By multiplying (15) by $u_i(r)$ and (16) by $f_0^b(r)$, subtracting and integrating over r, we have

$$\int_0^{r_0} \mathrm{d}r \left(f_0^b \frac{\mathrm{d}^2 u_i}{\mathrm{d}r^2} - u_i \frac{\mathrm{d}^2 f_0^b}{\mathrm{d}r^2} \right) = (k^2 - k_i^2) \int_0^{r_0} u_i f_0^b \mathrm{d}r. \tag{22}$$

On integrating by parts, we obtain

$$\left[f_0^b \frac{\mathrm{d}u_i}{\mathrm{d}r} - u_i \frac{\mathrm{d}f_0^b}{\mathrm{d}r} \right]_{r=r_0} = (k^2 - k_i^2) a_i, \tag{23}$$

which determines the a_i.

At $r = r_0$,

$$\begin{aligned} f_0^b(r_0) &= \sum_{i=1}^{\infty} a_i u_i(r_0) \qquad (24) \\ &= \sum_{i=1}^{\infty} \frac{u_i(r_0)}{k^2 - k_i^2} \left[f_0^b \frac{\mathrm{d}u_i}{\mathrm{d}r} - u_i \frac{\mathrm{d}f_0^b}{\mathrm{d}r} \right]_{r=r_0} . \qquad (25) \end{aligned}$$

On substituting for the logarithmic derivative γ (11) into (25), and using our boundary condition (18), we have

$$\gamma = b + \frac{1}{R} \qquad (26)$$

where the R-matrix, R, is defined by

$$R \equiv \sum_{i=1}^{\infty} \frac{\left[u_i(r_0)\right]^2}{k_i^2 - k^2}. \qquad (27)$$

Determination of R then enables $K_0 = \tan\delta_0$ to be determined from (via γ)

$$K_0 = \frac{-\sin(kr_0) + R(k\cos(kr_0) - b\sin(kr_0))}{\cos(kr_0) + R(k\sin(kr_0) + b\cos(kr_0))}. \tag{28}$$

Generalization to non-zero angular momentum ($l > 0$) and the Coulomb potential in the external region is straightforward (see Burke & Robb, 1975).

We note that the R-matrix consists of a series of poles along the real k^2 axis. If k^2 is near one of the poles k_i^2, then $R(k^2)$ can be approximated by a single term,

$$R(k^2) \approx \frac{[u_i(r_0)]^2}{k_i^2 - k^2}. \tag{29}$$

Even if the original potential satisfied by $f_l(r)$ is the same one used to determine the $u_i(r)$, there is still an advantage since we need only solve it a small number of times to determine the basis functions but can then determine the scattering cross section at the very large number of energies necessary to resolve resonance structure. Furthermore, if we choose a basis set v_i^0 which is easily evaluated, say

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V_0(r) + k_{0i}^2\right) v_i^0 = 0. \tag{30}$$

Then, if we approximate the first N e-solutions u_i, for $i = 1, 2, \ldots N$, by

$$u_i \approx v_i^{(N)} = \sum_{i'=1}^{N} c_{i'i}^{(N)} v_{i'}^0, \tag{31}$$

we can expand

$$f_0^{b(N)}(r) = \sum_{i=1}^{N} a_i^{(N)} v_i^{(N)}, \tag{32}$$

where $f_0^{b(N)}(r)$ is an approximate solution to the exact solution $f_0^b(r)$ at k^2. Then

$$R^{(N)} = \sum_{i=1}^{N} \frac{\left[v_i^{(N)}(r_0)\right]^2}{k_i^{(N)2} - k^2}, \tag{33}$$

where $k_i^{(N)2} \geq k_i^2$, for $i = 1, 2, \ldots N$ and $k_i^{(N)2}$ and $c_{i'i}^{(N)}$ are determined by diagonalizing

$$L_{ii'}^{(N)} = -\int_0^{r_0} v_i^0 \left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V(r) \right) v_{i'}^0 \mathrm{d}r, \tag{34}$$

for $i, i' = 1, 2, \ldots N$, i.e.

$$\mathbf{c}^{(N)\mathrm{T}} \cdot \mathbf{L}^{(N)} \cdot \mathbf{c}^{(N)} = \left[\mathbf{k}^{(N)}\right]^2 = \mathrm{diag}\left(k_i^{(N)2}\right) . \tag{35}$$

Thus, we only require to converge the sum over N. The rate of convergence can be improved by correcting for the effect of higher poles: $N + 1, \ldots \infty$ — this is the *Buttle correction*:

Solve for $v^0(r)$ at a *non-pole* energy k^2. Then, from (26)

$$R^0 = [\gamma - b]_{r=r_0}^{-1} = v^0(r_0) \left[\frac{\mathrm{d}v^0(r)}{\mathrm{d}r} - bv^0(r) \right]_{r=r_0}^{-1} . \tag{36}$$

The Buttle correction, R^c, is given by

$$R^c = R^0 - \sum_{i=1}^{N} \frac{\left[v_i^0(r_0)\right]^2}{k_{0i}^2 - k^2}. \tag{37}$$

Then, the Buttle-corrected R-matrix is given by

$$R = R^{(N)} + R^c, \tag{38}$$

i.e. the high poles ($> N$) are approximated by the zero order basis.

The power of the R-matrix method lies with the fact that we have replaced solving complex multi-channel coupled integro-differential equations (in the general scattering case) by a small set of uncoupled ordinary differential equations (the potential V_0 can be fairly crude) and a matrix diagonalization (34). This diagonalization has to be carried-out only ONCE to enable the R-matrix to be determined at ALL energies. This is of enormous importance for the low-energy cross sections which are dominated by narrow resonance structures and require a solution at $\sim 10^4$ energies.

The main drawback to the R-matrix method is that it does not scale well to 'high' energies. To determine the R-matrix and, hence, cross section at k^2, say, requires N to be sufficiently large so that the highest few basis energies k_i^2 satisfy $k_i^2 > k^2$. Typically, it is only practical to work with $N = 20 - 50$ as matrix diagonalization is an N_{r}^3 process, where N_{r} is the rank of the matrix. Here $N_{\mathrm{r}} = N \times N_{\mathrm{c}}$ where N_{c} is the number of scattering channels required to describe the problem. In a complex atom the number of channels increases rapidly. The current practical limit utilizing massively parallel machines (e.g. 5000 processors) is a rank of $N_{\mathrm{r}} \approx 150,000$. We also require to carry out this diagonalization ≈ 100 times (so as to converge the partial wave expansion).

However, we only need solve the scattering problem with the R-matrix method up to a few times the ionization energy of the atom so as to establish its high energy behaviour. This is then easily connected to its infinite energy solution, which is identical to that of a (maybe relativistic) plane wave.

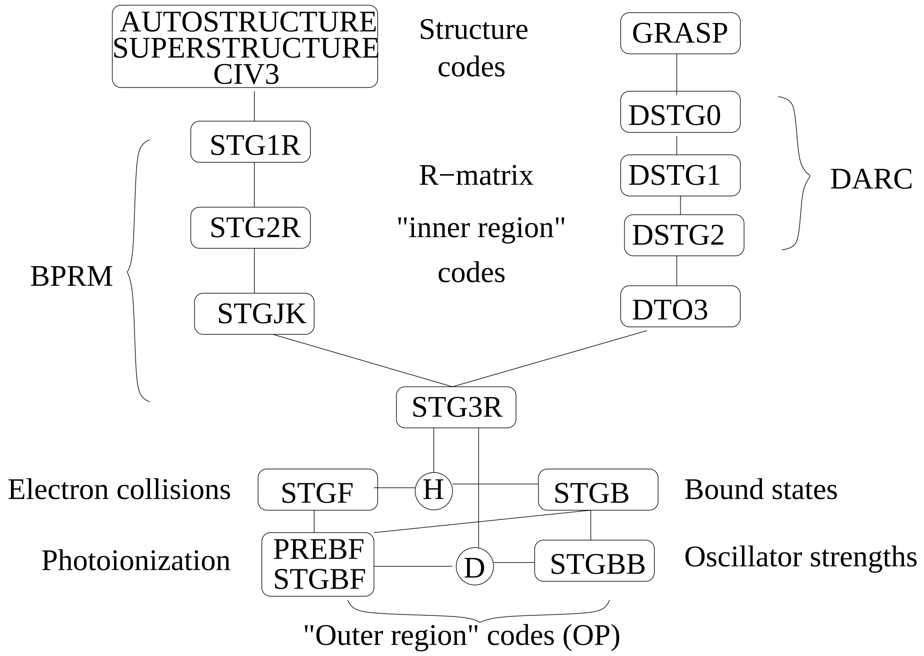
Outer Region Solutions

We have gone into the solution of the collision problem in the inner region in some detail. But, as noted, this must be matched to the outer region solution for us to be able to extract the scattering probability etc. In the outer region we have, maybe, a Coulomb potential plus long-range multipole potentials $(1/r^{\lambda+1}, \lambda \geq 1)$.

Solution in the outer region is computationally non-trivial — the coupled differential equations need to be solved at every energy, maybe several tens of thousands. We initially solve the uncoupled Coulomb (or plane wave) problem and treat the long-range multipole potentials as a perturbation. We can also factor-out much of the strong energy dependence of the scattering matrices, and so interpolate them as a function of energy — multi-channel quantum defect theory. Even so, it is common for the outer region problem to take more computer time than the inner region.

Both regions are amenable to massively parallel calculations — matrix diagonalization via scaLAPACK, while the outer region solution is embarrassingly parallel by energy.

Code Suite Overview



AUTOSTRUCTURE
SUPERSTRUCTURE
CIV3

Structure
codes

GRASP

DSTG0

DSTG1

DSTG2

DARC

STG1R

STG2R

STGJK

BPRM

R−matrix
"inner region"
codes

DTO3

STG3R

Electron collisions

STGF

H

STGB

Bound states

Photoionization

PREBF
STGBF

D

STGBB

Oscillator strengths

"Outer region" codes (OP)

Practical implementation; code suite: `http://amdpp.phys.strath.ac.uk/UK_RmaX`

Parallel Classic R-matrix

- Parallel and serial Classic R-matrix codes are available at the UK RmaX website (userid: UK_RmaX password: H.DAT - only necessary for accessing parallel suite)
  http://amdpp.phys.strath.ac.uk/UK_RmaX/

- Contain many useful features developed over many years.

- Want to use on different parallel architectures: SMP & Beowulf clusters.

- Want to use on many systems: x86 clusters, Itanium Altix SMP, IBM SP, Cray X1E etc. i.e. portability is paramount.

Parallel Strategy

General philosophy: do as little message passing as possible — rather, compute same thing independently on each processor (degrades scaling, but then so does slow MPI). Maintain interchangeability of passing files with serial codes.

- PSTG1R: Distribute generation of bound-continuum and continuum-continuum integrals over a node (whole integrals).
- PSTG2R: Distribute clusters of symmetries over a node.
- PSTG3R, PSTG3NX: Use scaLAPACK (1.7) PDSYEVD to diagonalize a matrix distributed over many processors (NOT a distribution by symmetry — don't have enough memory).
- PSTGB: Distribute clusters of symmetries over a node.
- PSTGF, PSTGICF: Distribute by energy over many processors.

Application: RMPS

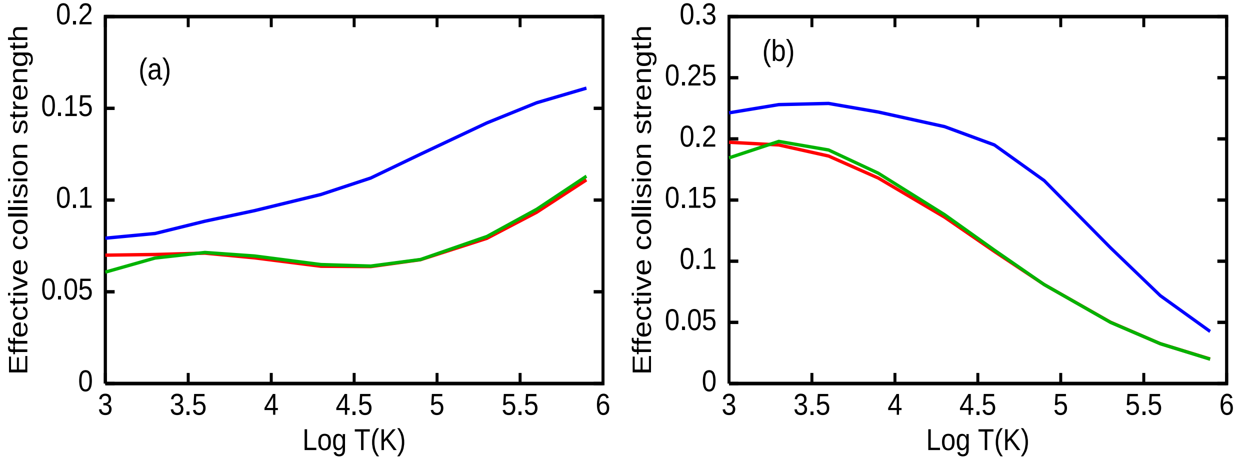
Recall,

$$\Psi = A \sum\!\!\!\!\!\!\int_{\nu} \psi_{\nu} \phi \,. \tag{39}$$

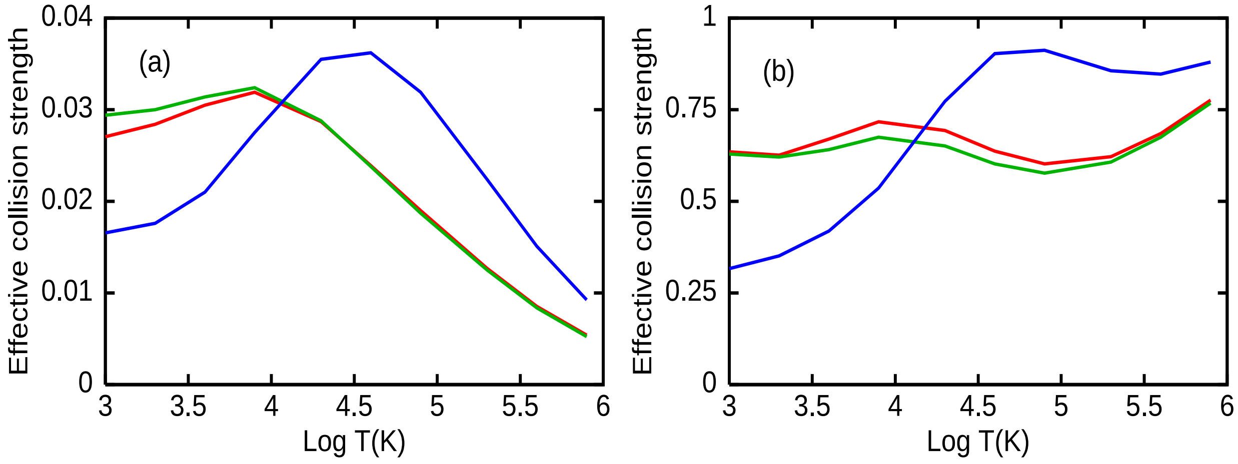
The R-matrix with pseudo-states approach (like CCC) replaces the sum over high Rydberg states and the integration over continuum states by a quadrature over Laguerre states.

The continuum basis plus Laguerre basis is over complete. The original RMPS implementation of Bartschat et al (1996) just Schmidt orthogonalized the two and discarded high-lying basis states. Badnell and Gorczyca (1997) diagonalize the matrix of overlaps to form the reduced linearly independent basis. The Buttle correction is also transformed appropriately, noting that the one-body Hamiltonian is no longer diagonal.

In fusion plasmas, visible-VUV spectroscopy of light neutral atoms and near neutral ions follows from excitation of $n = 3$ and $n = 4$ levels. These are strongly coupled to the continuum. All non-RMPS excitation data is suspect.



B$^+$: Effective collision strengths for excitation, from (a) the 2s^2 ^{1}S ground term and (b) the 2s2p ^{3}P metastable term, to the 2s4s ^{1}S upper term. The blue curves are from the present 20CC R-matrix calculation, the red curves are from the present 114CC RMPS calculation, and the green curves are from the present 134CC RMPS calculation.



B^+: Effective collision strengths for excitation, from (a) the $2s^2\ ^1S$ ground term and (b) the $2s2p\ ^3P$ metastable term, to the $2s4f\ ^3F$ upper term. The blue curves are from the present 20CC R-matrix calculation, the red curves are from the present 114CC RMPS calculation, and the green curves are from the present 134CC RMPS calculation.

RMPS *adf04*

Maxwell-averaged upsilon files exist for:

- H-: H, He$^+$, Li^{2+}, Be^{3+}, B^{4+}, C^{5+}
- He-: He, Li$^+$, Be^{2+}
- Li-: Li, Be$^+$, B^{2+}, C^{3+}
- Be-: Be, B$^+$, C^{2+}
- B-: B

- Neutral Ne, BP, low energy only.

Badnell, Ballance, Griffin, Mitnik in a series of J.Phys.B papers.

MQDT/ICFT

Multi Channel Quantum defect Theory (MQDT):

$$K_{\rm oo} = \mathcal{K}_{\rm oo} - \mathcal{K}_{\rm oc}\left[\mathcal{K}_{\rm cc} - \tan(\pi\nu)\right]^{-1}\mathcal{K}_{\rm co}$$

$$S_{\rm oo} = \mathcal{S}_{\rm oo} - \mathcal{S}_{\rm oc}\left[\mathcal{S}_{\rm cc} - {\rm e}^{-2\pi {\rm i}\nu}\right]^{-1}\mathcal{S}_{\rm co}$$

$$D_{\rm o} = \mathcal{D}_{\rm o} - \mathcal{S}_{\rm oc}\left[\mathcal{S}_{\rm cc} - {\rm e}^{-2\pi {\rm i}\nu}\right]^{-1}\mathcal{D}_{\rm c}$$

- Applies to *all* closed-channels.
- Include long-range coupling potentials by retaining only the finite part of the divergent integrals (Gorczyca et al 1996).
- Intermediate Coupling Frame Transformation R-matrix approach (ICFT) then terms-couples the entire unphysical K- or S-matrix.

ICFT validation

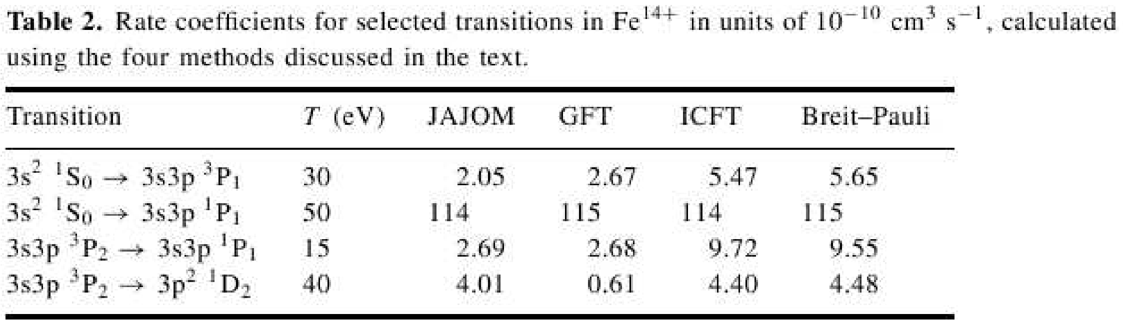


Table 2. Rate coefficients for selected transitions in Fe^{14+} in units of 10^{-10} cm^3 s^{-1}, calculated using the four methods discussed in the text.

Transition	T (eV)	JAJOM	GFT	ICFT	Breit–Pauli
$3s^2\ ^1S_0 \rightarrow 3s3p\ ^3P_1$	30	2.05	2.67	5.47	5.65
$3s^2\ ^1S_0 \rightarrow 3s3p\ ^1P_1$	50	114	115	114	115
$3s3p\ ^3P_2 \rightarrow 3s3p\ ^1P_1$	15	2.69	2.68	9.72	9.55
$3s3p\ ^3P_2 \rightarrow 3p^2\ ^1D_2$	40	4.01	0.61	4.40	4.48

Griffin et al (1998)

- Resonance series converge on levels ICFT, GFT unlike JAJOM.
- Background is correct for ICFT, unlike JAJOM, GFT.

Ni^{4+}

Badnell and Griffin (1999)

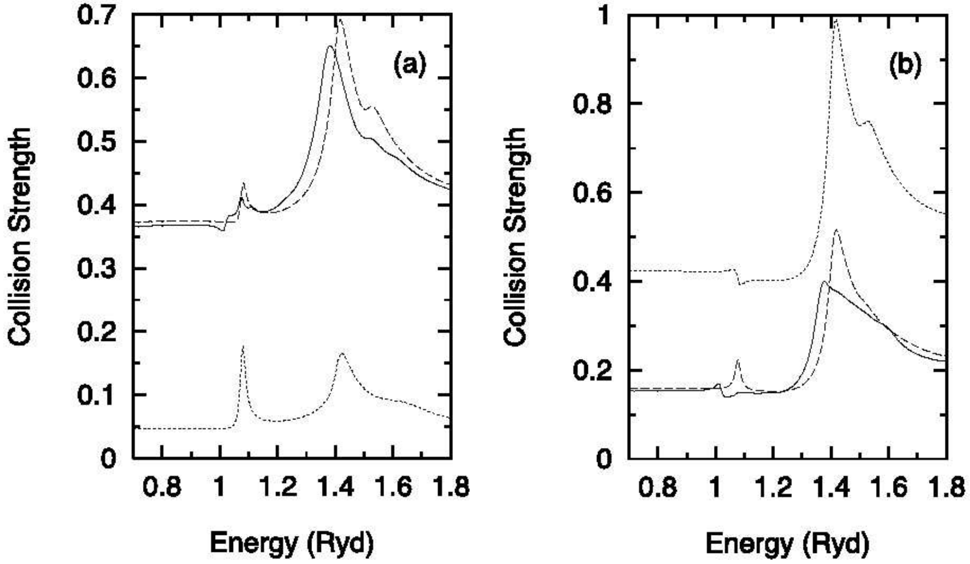


Figure 5. *R*-matrix electron-impact excitation collision strengths for the transitions (*a*) $^5D_4-^3H_4$ and (*b*) $^5D_4-^3F_4$ in Ni^{4+}. Full curve, Breit–Pauli; dashed curve, ICFT; dotted curve, jK-coupling.

- 'Correlation' resonances, which arise in $\mathcal{S}_{\rm oo}$, are well represented.

RM ICFT: along isoelectronic sequences

- Create a baseline database for electron-impact excitation which includes resonant enhancement: all ions of a sequence up to Zn (or Kr).
- Consider shell boundaries: H-, He-, Li- and F-, Ne-, Na-.
- Use (Perl) script to automate R-matrix calculation — requires reliable, robust codes.
- Works on serial or parallel machines.
- Uses AUTOSTRUCTURE (for structure and infinite energy limit points Bethe/Born) and ICFT R-matrix approach.
- End product: $adf04$ file.
- R-matrix analysis package (RAP) has been developed by Mike Witthoeft (Python-based GUI) to validate the large amount of data.

- F-like sequence: see Witthoeft, Whiteford & Badnell J.Phys.B40, 2969 (2007).

- Na-like sequence:

  Outer-Shell: $(nl \rightarrow n'l')$ for $n, n' = 3-6$ — see Liang, Whiteford & Badnell Astron. Astrophys. 500, 1263 (2009)

  Inner-shell: 134CC $(2\mathrm{p}^6 3l, 2\mathrm{p}^5 3l3l'$, ex $3\mathrm{d}^2)$ allowing for Auger and radiation damping of resonances — Liang, Whiteford & Badnell J.Phys.B (At Press)

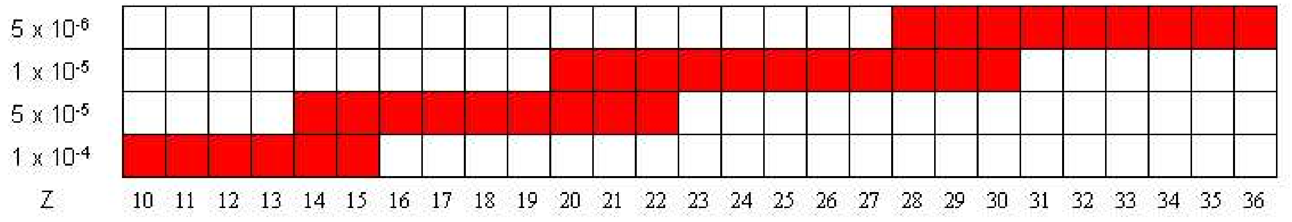
- Ne-like: 209CC $2\mathrm{s}^p 2\mathrm{p}^q nl \, (n = 2-5)$ and $2\mathrm{p}^2 2\mathrm{p}^5 n'l' (n' = 6, 7 \quad l' = 0-2)$ — Liang & Badnell (In progress)

- H-like and He-like sequences in ADAS — Witthoeft & Whiteford, methodology as per previously published for single ions (i.e. allows for radiation damping.)

- Li-like: simpler version of Na-like (TBD)

Example: F-like sequence

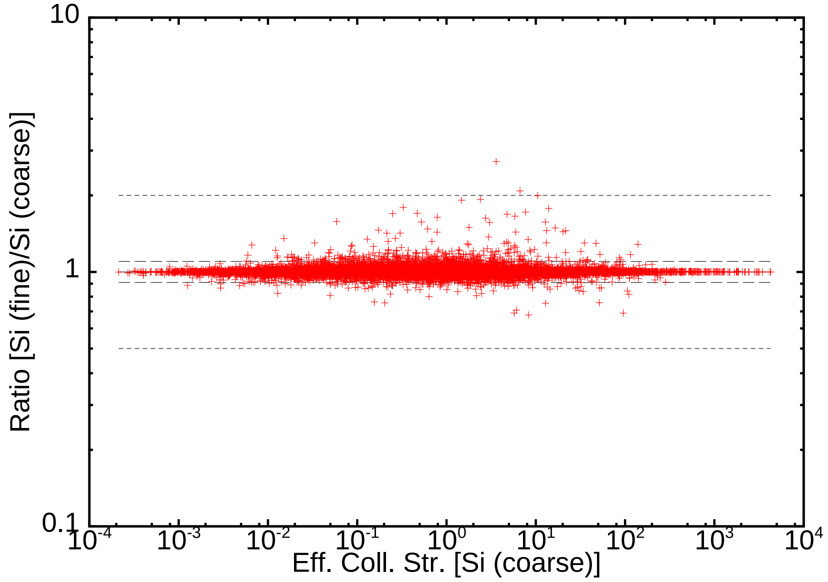
- $2s^2 2p^5$, $2s2p^6$, $2s^2 2p^4 3l$, $2s2p^5 3l$, $2s^2 2p^4 4l$: 87 terms and 195 levels.
- All ions from Ne^{+} to Kr^{27+}.
- Structure automatically optimized for each individual ion.
- Good agreement of gf-values with Fawcett (1984).



5 x 10^{-6}																			🟥	🟥	🟥	🟥	🟥	🟥	🟥	🟥	🟥
1 x 10^{-5}											🟥	🟥	🟥	🟥	🟥	🟥	🟥	🟥	🟥	🟥	🟥						
5 x 10^{-5}					🟥	🟥	🟥	🟥	🟥	🟥	🟥	🟥	🟥														
1 x 10^{-4}	🟥	🟥	🟥	🟥	🟥	🟥																					
Z	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36

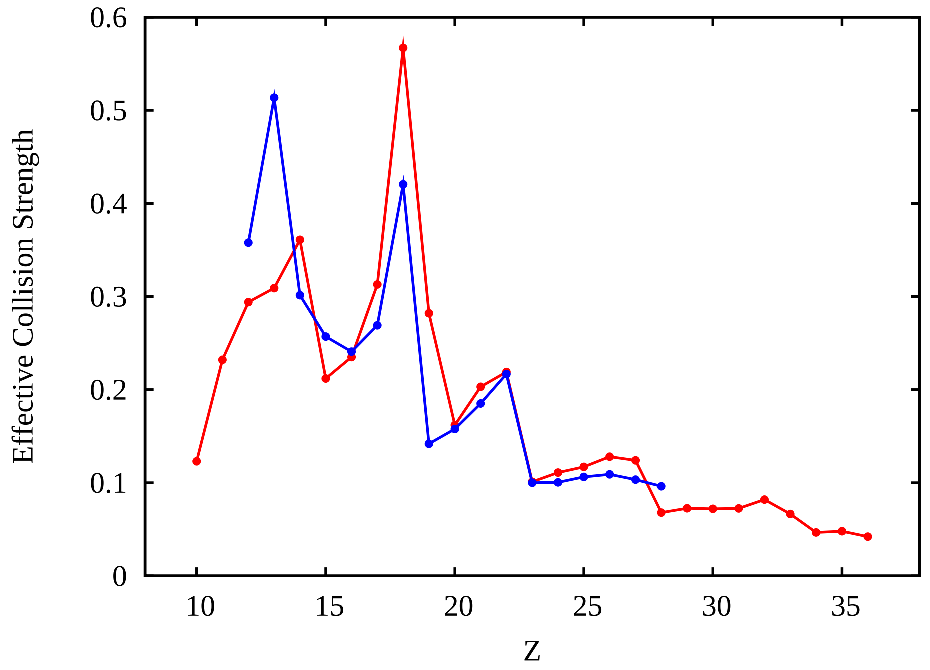
Energy meshes used for each ion - note overlaps as checks.

Energy mesh convergence



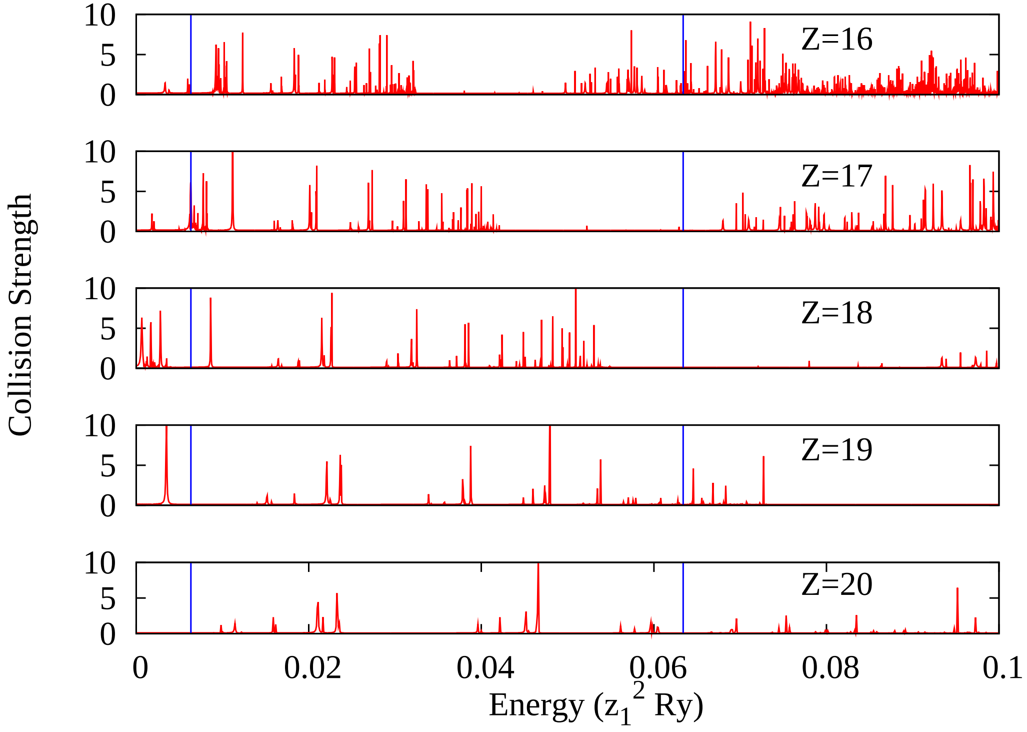
Si^{5+}, at 7.2×10^4K. Only 2.5% of transitions give rise to differences exceeding 10%.

Fine-structure transition

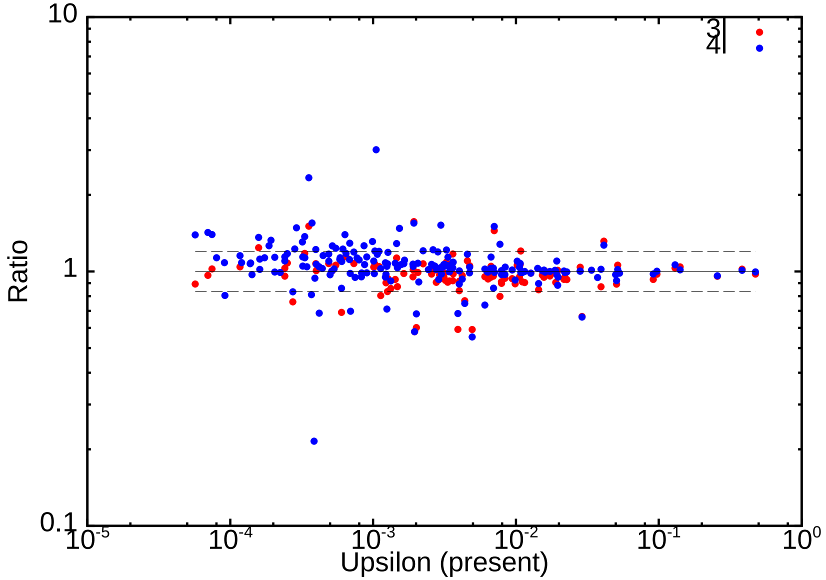


Red curve: ICFT-RM; blue curve: BPRM, Berrington et al (1998). $T = 10^3 z^2 \mathrm{K}$.

The march of the resonances



$\mathbf{Fe}^{17+}$



Comparison, for all transitions from the ground level, with previous results of Witthoeft et al (2006).

Dirac R-matrix for heavy species

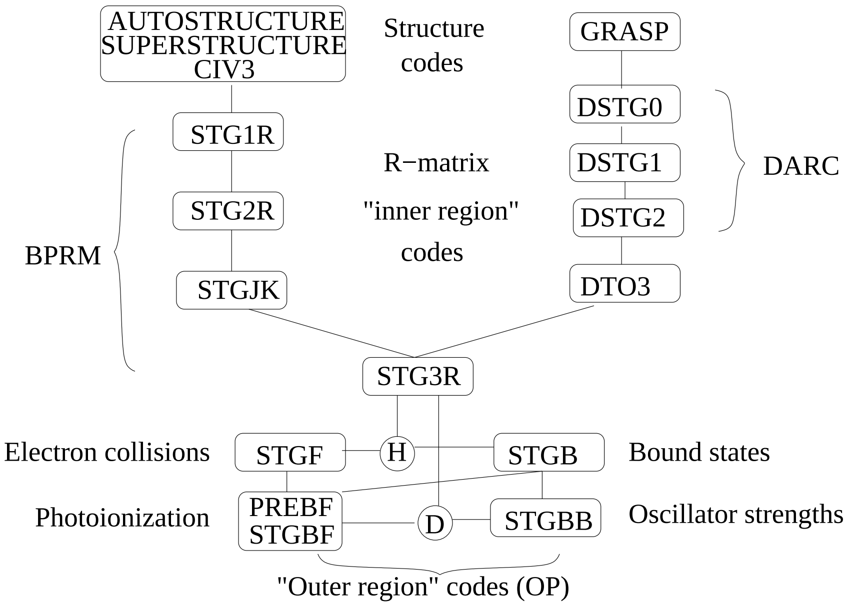
Our preferred approach to electron-impact excitation for ADAS is R-matrix. Autoionizing levels are included implicitly by it rather than explicitly within the GCR modelling.

Main drawback is that R-matrix calculations are computationally demanding (impossible) for complex (i.e. heavy) species.

Semi-relativistic plane-wave Born (SR-PWB) excitation data from Cowan's code (CA and level-resolved) and AUTOSTRUCTURE (level-resolved only) provide complete 'baseline' coverage.

We have incorporated the Dirac R-matrix code within our parallel and radiation damped framework.

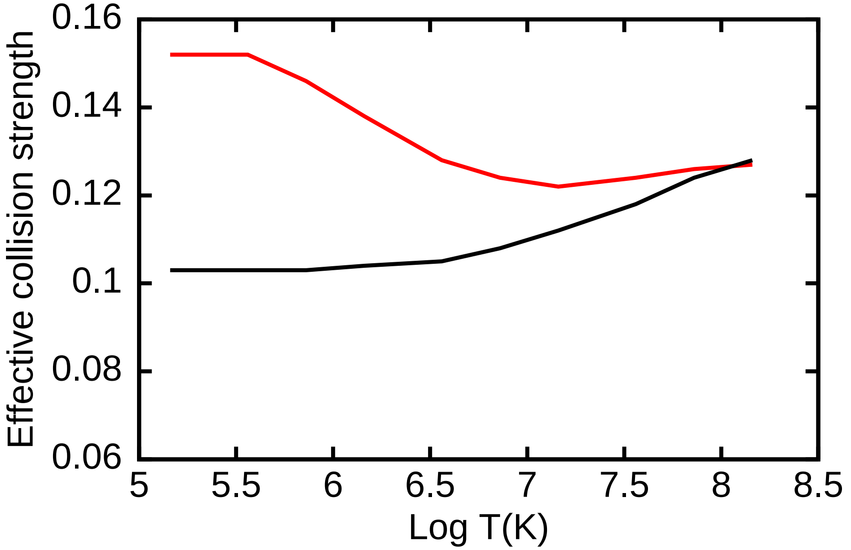
We compare the effect of using R-matrix as opposed to SR-PWB data on the resultant spectral signature of Ni-like Xe^{26+}, as an example, (Badnell et al 2004).



Flow diagram illustrating the interconnectivity between the Breit–Pauli, Dirac–Coulomb and Opacity Project (OP) R-matrix code suites.

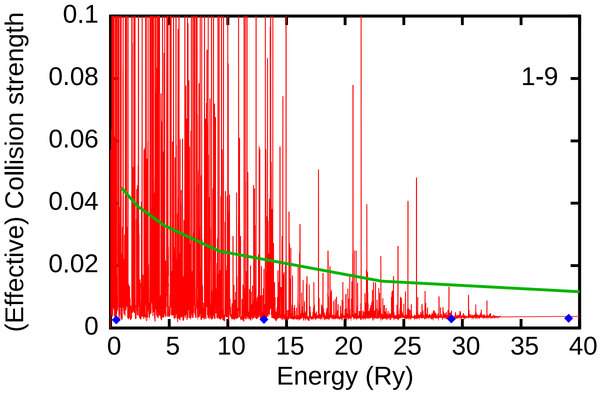
Results of 129CC Dirac-Coulomb R-matrix calculation

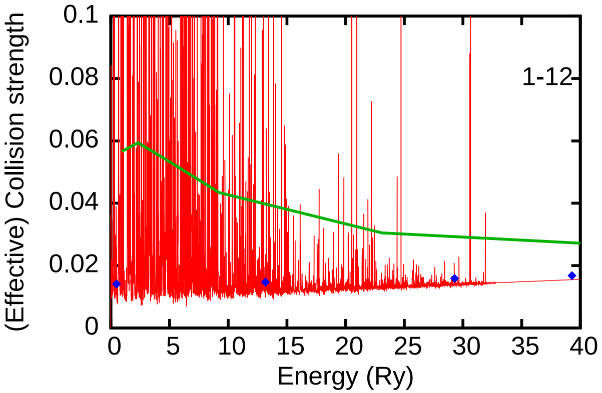
$(3\mathrm{d}^{10}, 3\mathrm{d}^9 nl, n = 4-5, l = 0 \text{ to } n-1.)$

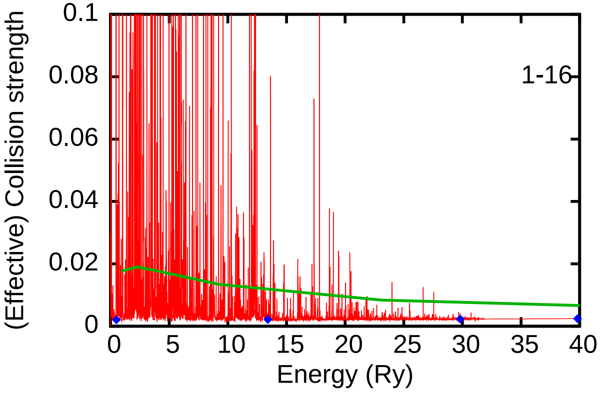


Effective collision strengths for the $3\mathrm{d}^{10}\ {}^1\mathrm{S}_0 - 4\mathrm{d}^1\mathrm{S}_0$ transition in Xe^{26+}:

Red curve, 129CC Dirac–Coulomb R-matrix; black curve, plane-wave Born (baseline data).

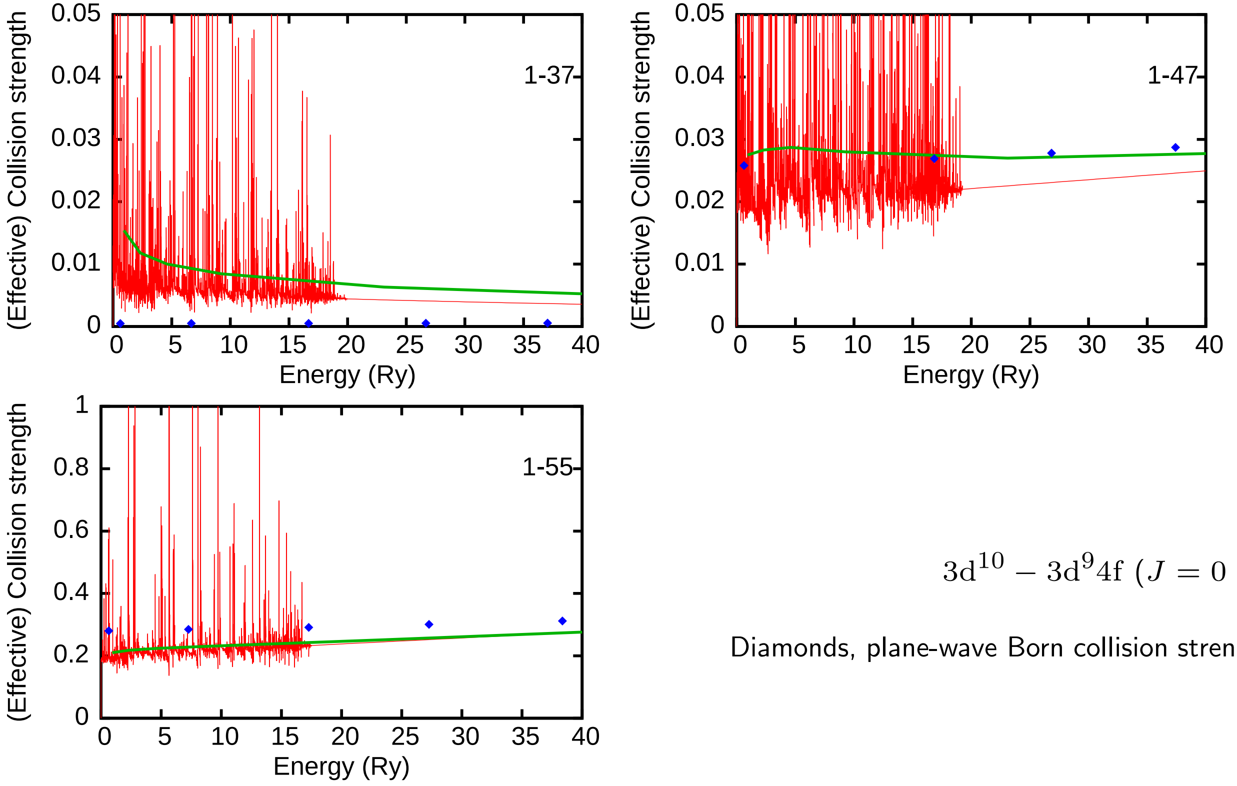






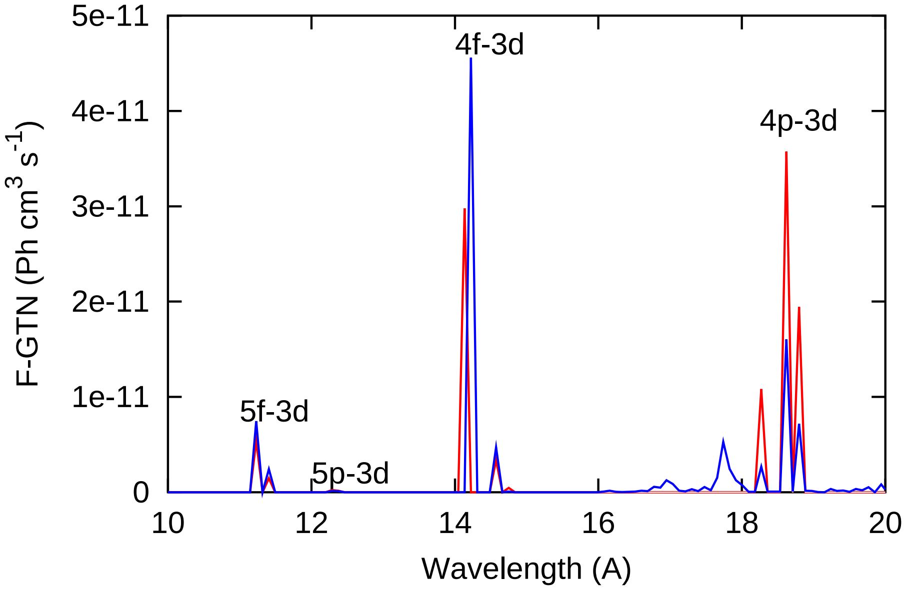
$3\mathrm{d}^{10} - 3\mathrm{d}^9 4\mathrm{p}\ (J = 0 - 1)$

Diamonds, plane-wave Born collision strengths.



$3\mathrm{d}^{10} - 3\mathrm{d}^{9}4\mathrm{f}\ (J = 0 - 1)$

Diamonds, plane-wave Born collision strengths.



$\mathcal{F}\text{-}\mathcal{GTN} = (N^z/N_{\rm tot})|_{\rm eq}\mathcal{F}\text{-}\mathcal{PEC}^z$ for Xe^{q+} at $T_{\rm e} = 550$eV and $N_{\rm e} = 10^{13}$cm^{-3}: red curve, utilizing Dirac–Coulomb R-matrix excitation data; blue curve, utilizing plane-wave Born (baseline) excitation data; both for Xe^{26+} only. (The feature between 16–18 Å arises from other Xe ionization stages.)

Heavy Species - the future

- Stabilize parallel Dirac-Coulomb R-matrix codes —- dipole matrices. (Pretty much done.)

- Port QED/Breit interaction from GRASP to DARC $\Rightarrow$ Dirac-Breit R-matrix.

- Investigate fully-relativistic treatment for the ‘outer region’.

- Dirac RMPS using L-spinors. (Done.)

- ICFTR: ICFT breaks down at $\gtrsim$ Kr $\Rightarrow$ use kappa-averaged relativistic wavefunctions.

Towards ICFTR

ICFT R-matrix method is less computationally demanding than BP/DARC.
⇒ Of interest to extend ICFT via using relativistic orbitals.

The ICR approach (in AUTOSTRUCTURE) averages the orbitals over kappa, neglects the small component (in general) and then carries-out the radial integrals required for the BP structure.

The relativistic analogue of integrals (RI) method takes fully relativistic radial integrals from GRASP and averages over kappa and feeds them back into the BP structure.

Some comparisons:

Energy levels (Ry) in W^{70+}. (From Jonauskas et al JPB v38 L79 (2005), +ICR.)

Index	Level	IC	HFR	DF	RI	ICR
1	2s2 1S0	-14472.2313	-14606.1630	-14661.2007	-14661.2127	-14660.1972
2	2s12p1 3P0	11.8033	9.5122	12.7642	13.3690	12.4027
3	2s12p1 3P1	14.4817	12.5698	15.6393	16.3163	15.4486
4	2p2 3P0	32.9833	29.5304	35.8501	36.6611	35.0358
5	2s12p1 3P2	101.4780	125.3516	123.2548	122.9797	123.2114
6	2s12p1 1P1	107.3621	131.9927	129.7459	129.3913	129.8507
7	2p2 3P1	119.6724	141.7643	142.9160	143.2261	142.6208
8	2p2 1D2	121.6674	143.8498	144.8975	145.2266	144.7094
9	2p2 3P2	210.3791	258.4229	254.3276	253.8651	254.5042
10	2p2 1S0	214.6380	262.8561	258.6676	258.1166	258.9496

Note, I obtain DF ground at -14660.2 with both uniform and Fermi charge nucleus.

Radiative decay of the U^{89+} $\mathrm{1s2s2p}\,{}^4\mathrm{P}_{5/2}$ metastable level.

	$\Delta E(\mathrm{M1})$	$\Delta E(\mathrm{M2})$	$S(\mathrm{M1})$	$S(\mathrm{M2})$
IC	6972.7	7172.1	0.0255	0.00221
ICR	7075.5	7407.2	0.0632	0.00231
DF	7078.0	7409.9	0.0573	0.00236

ICR more elegant — more self-contained ⇒ extend to ICFTR by coding for a BP R-matrix kappa=averaged relativistic continuum basis along the same lines.

Collaborators

Connor Ballance, Dario Mitnik & Don Griffin (Rollins)

Tom Gorczyca (Western Michigan)

Keith Berrington (Sheffield Hallam)

Guiyun Liang, Marin O Mullane, Mike Witthoeft, Allan Whiteford & Hugh Summers (Strathclyde)

Patrick Norrington (QUB)

Overview of Atomic Structure and Collision Theory

Nigel Badnell

Department of Physics
University of Strathclyde
Glasgow, UK

– ADAS 2009 –

Atomic Structure Methods

It is deceptively simple to write down the structure problem to be solved

$$\Psi = \sum\!\!\!\!\!\!\int_{\nu} a_\nu \psi_\nu \,. \tag{1}$$

The total wavefunction for the atom Ψ is expanded in terms of a complete set of (antisymmetric) basis states ψ_ν (an N-product of one-electron orbitals) with expansion coefficients a_ν.

Spherically symmetric problem $\longrightarrow$ (θ, ϕ) problem solved. Use standard angular algebra methods and packages are used, mostly based on Racah algebra but also Condon and Shortley (Slater-states).

Only require to determine radial dependence of wavefunction.

- Hartree/Dirac-Fock: coupled-set of radial equations result from formally varying radial orbitals to give stationary value of an energy functional — self-consistent solution: MCHF (Froese), HFR (Cowan), MCDF (Grant) etc. (Expanion coefficients may also be determined this way, MCHF.)
- Configuration Interaction (CI): radial equations (usually uncoupled) contain variational parameters (e.g. "model potentials") which are varied (numerically) to minimize a computed energy functional: AS/SS, CIV3, HULLAC
- As CI but using a self-consistent model potential: AS, HULLAC, FAC.

All approaches then, usually, construct and diagonalize the Hamiltonian to give the final e-states and e-energies.

Basis expansion is slow to converge in general. A plethora of basis functions are used: spectroscopic, psuedo (Laguerre), B-splines etc.

Pros & Cons: problems with converging HF for excited states. Local vs global minimum, flexible enough variational parameters.

Scattering codes can use only the simplest HF methods, in general: unique, orthogonal...

Hamiltonian

♣ Schrödinger equation based (AS, CIV3, MCHF):

- Non-relativistic: kinetic, nuclear & electrostatic operators.
- Breit-Pauli: as above, plus one-body fine-structure (spin-orbit), and non-fine-structure (Mass-Velocity & Darwin).
  Fine structure mixes terms, non-fine-structure can be added to NR above.
- Breit-Pauli: as above, plus two-body fine-structure (spin-spin, spin-orbit, spin-other-orbit).
- Breit-Pauli: as above, plus two-body non-fine-structure (orbit-orbit, contact-spin-spin, Darwin).

♣ Kappa-averaged Dirac equation based ($\pm$ small component): radial functions still depend only on nl, not nlj. Then using above Breit-Pauli operators. (HFR one-body only, AS.)

♣ Dirac equation based, large and small component.

- Dirac-Coulomb (HULLAC, FAC)
- $+$ (Generalized) Breit $+$QED (GRASP, Sampson/LANL)

Others: Sapirstein & Johnson, Desclaux, Chen...

Coupling schemes: LS, LSJ, jK, jj (unitary transformations).

What matters more are good quantum numbers...

Atomic Structure Data

Bound-Bound

- Energy levels, ("All")
- E_k and M_k radiative rates ("Most")

Bound-Free

- Autoionization rates, DR (AS, HULLAC, FAC, MCDF(Chen) ...)
- Photoionization cross sections, RR (ditto)

Free-Free

- Infinite and finite energy Plane-wave Born (AS, Cowan)

And More...

- Hyperfine
- Stark-mixing, DR
- ...

Complex (Heavy) Species

- Unresolved Transition Array (UTA) Spectral shape — Bauche-Arnault, Bauche & Klapisch
- Configuration-average (CA) collisions — Cowan driven.

Both neglect configuration interaction.

Atomic Collision Methods

Time-dependent methods solve the full Schrödinger equation — TDCC.

Time-independent methods expand the antisymmetric total wavefunction for the target-plus-colliding particle Ψ is expanded in terms of a known complete basis of target states ψ_ν.

$$\Psi = \mathcal{A} \sum\!\!\!\!\!\!\int_{\nu} \psi_\nu \phi \,. \tag{2}$$

The expansion coefficients ϕ representing the colliding particle (projectile) are then to be freely determined by a variational of the scattering matrix leading to the continuum Hartree/Dirac-Fock equations.

Coupled-channel methods

Resonances arise naturally when the scattering energy of an open-channel coincides with that of a closed-channel.

Traditional close-coupling approximation truncates the expansion to a low-lying set of closely-coupled atomic states — neglects ionization loss.

Pseudo-state expansions attempt to approximate the sum/integral over a wide range of energies and work towards practical numerical convergence — RMPS, CCC.

Complete basis expansions can be used over a limited energy range and volume (particle in a box) — B-spline R-matrix, Intermediate Energy R-matrix.

Distorted-wave methods

DW methods solve (elastic) uncoupled continuum Schrödinger/Dirac equations and treat the (inelastic) coupling as a perturbation — can keep problem small, a series of 2x2 calculations: AS/HULLAC/FAC/LANL & UCL(historic)

Resonances are often neglected from electron-impact excitation, but not recombination — DR. Use of the IPIRDW approximation (Independent Processes Isolated Resonance using DW): AS/HULLAC/FAC

Simple "DW": Coulomb or plane-wave Born for EIE & EII: ATOM or AS/Cowan

Heavy species: can/need we go beyond PWB?

R-matrix

Probably the most successful method/code suite for electron-impact excitation and photoionization (no so much for electron-ionization).

A close-coupling method which is very efficient at mapping-out resonances, compared to CCC, UCL-IMPACT (historic) etc. (But not compared to IPIRDW...)

Need to solve the coupled integro-differential scattering equations at tens, if not hundreds, of thousands of energies and for ~ 100 angular momentum symmetries.

Key Idea

Divide scattering region into two: an inner region that just encompasses the atom/ion (wavefunctions $\lesssim 10^{-3}$, say, outside) and where the scattering potentials are complicated (e.g. short-range); and an outer region where we only have an asymptotic Coulomb potential and, maybe, dipole and quadrupole coupling potentials (with analytic coefficients). Let the dividing boundary radius be r_0.

The inner region is a finite volume and we can expand our (to be determined) continuum wavefunction in terms of a simple orthogonal basis of states $u_i(r)$, say, with a fixed (outer) boundary condition. This leads to a set of discrete positive energy solutions k_i^2, say (particle in a box).

The inner region solution at $r = r_0$ for any scattering energy k^2 is completely characterized by the R-matrix:

$$R \equiv \sum_{i=1}^{\infty} \frac{[u_i(r_0)]^2}{k_i^2 - k^2}. \tag{3}$$

The scattering matrix (hence, cross section) is determined by matching the outer region solution to the inner region one at r_0.

For example, for s-wave $(l = 0)$ scattering off a neutral atom

$$K = \frac{-\sin(kr_0) + R(k\cos(kr_0) - b\sin(kr_0))}{\cos(kr_0) + R(k\sin(kr_0) + b\cos(kr_0))}. \tag{4}$$

Here, K is the reactance matrix, which is simply related the the S-matrix.

A more detailed exposition, based on Burke & Robb (1975), is available.

Web Links

http://amdpp.phys.strath.ac.uk/

http://amdpp.phys.strath.ac.uk/tamoc/

http://amdpp.phys.strath.ac.uk/autos/

http://amdpp.phys.strath.ac.uk/UK_APAP/codes.html

This is The End.

Member of the Helmholtz Association

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FORSCHUNGSZENTRUM

Usage of ADAS data in the Monte Carlo codes for particle transport simulations in plasma *(on example of ERO code)*

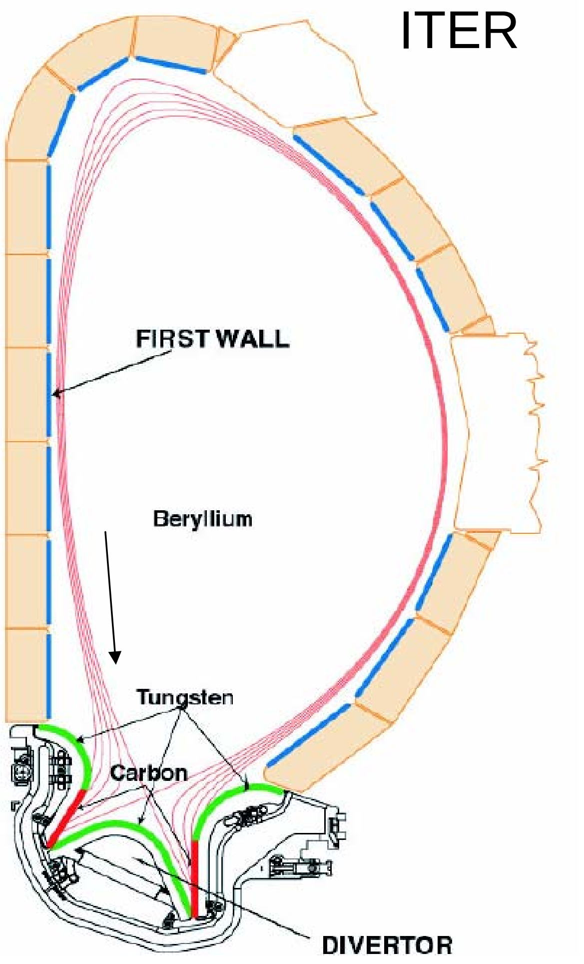
D.Borodin

Institut für Energieforschung – Plasmaphysik, Forschungszentrum Jülich, Germany

Special thanks for contributions from A.Kirschner, D.Reiter, R.Ding and D.Matveev

Motivation: plasma-surface interaction (**PSI**) in fusion devices

ITER – first wall materials



700 m^2 beryllium first wall

- **low Z**
- **oxygen getter**

100 m^2 tungsten baffles, dome

- **high Z**
- **low sputtering**

50 m^2 graphite CFC target plates

- **no melting**

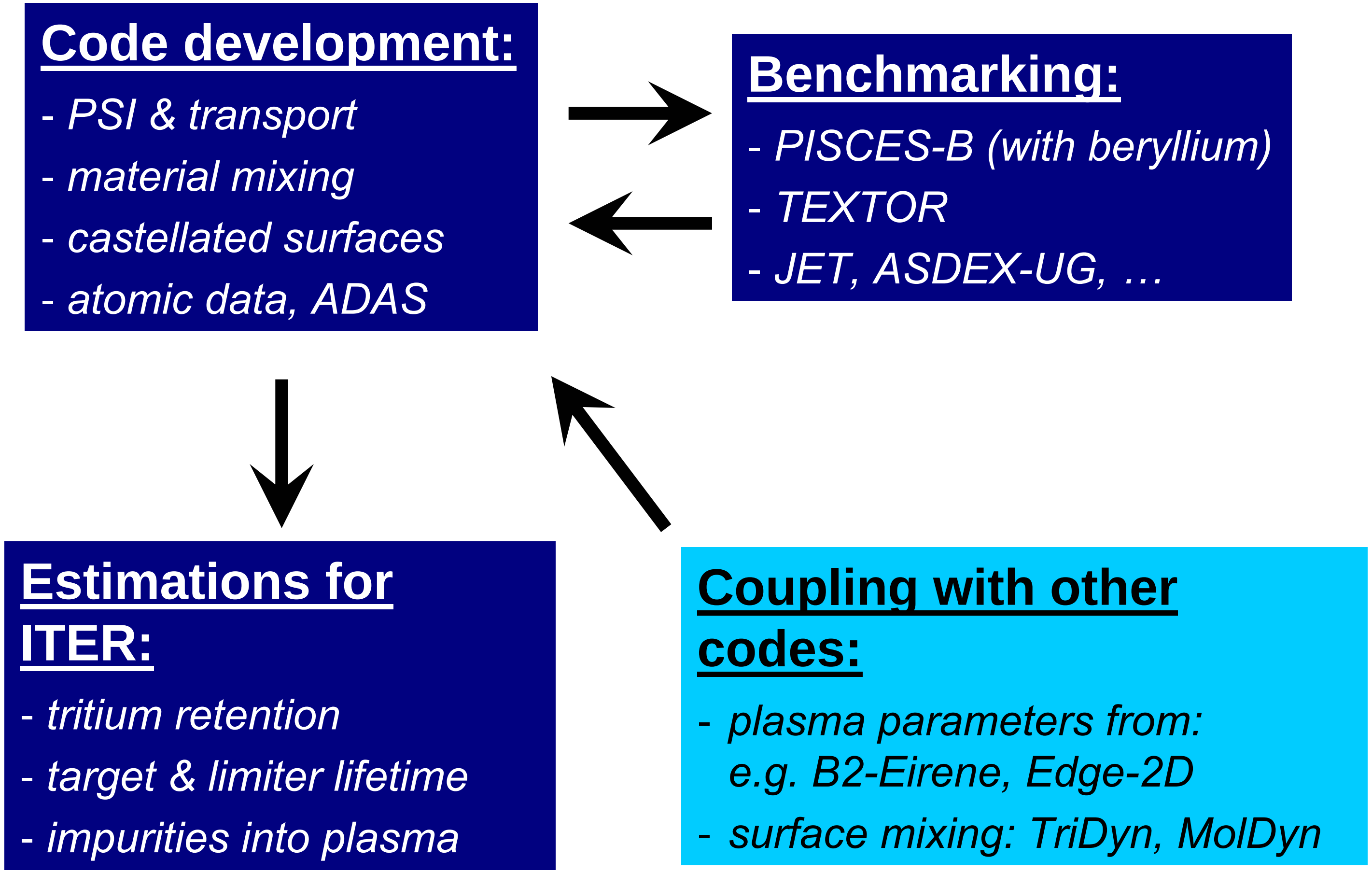
Erosion of wall materials, transport and re-deposition →

- Lifetime & tritium retention

- Material mixing effects

Plasma-surface interaction in divertor can determine the ***ITER availability*** *. . .*

ERO modelling strategy



Code development:

- *PSI & transport*
- *material mixing*
- *castellated surfaces*
- *atomic data, ADAS*

Benchmarking:

- *PISCES-B (with beryllium)*
- *TEXTOR*
- *JET, ASDEX-UG, …*

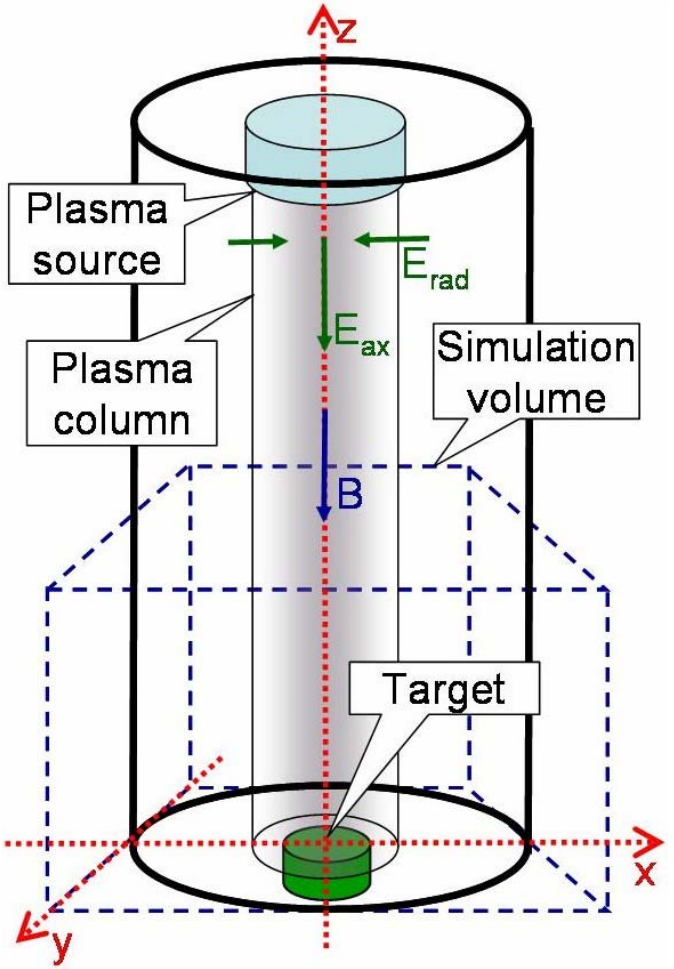
Estimations for ITER:

- *tritium retention*
- *target & limiter lifetime*
- *impurities into plasma*

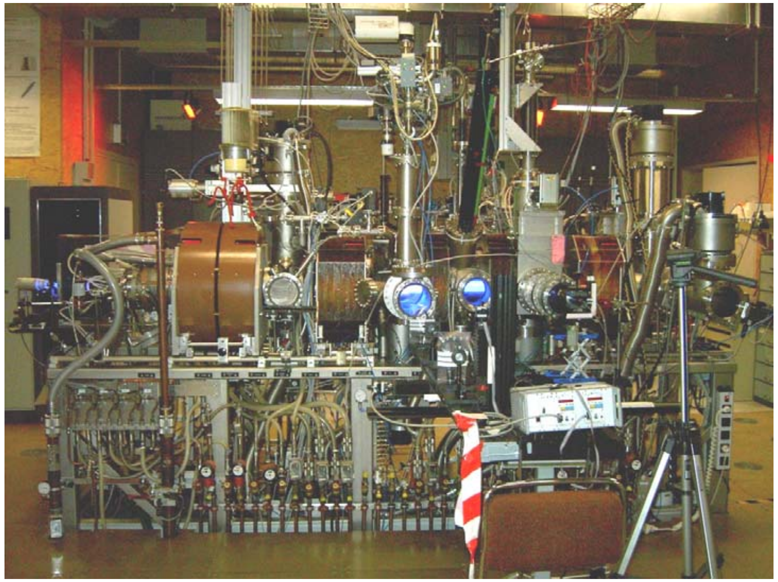
Coupling with other codes:

- *plasma parameters from: e.g. B2-Eirene, Edge-2D*
- *surface mixing: TriDyn, MolDyn*

Linear devices – benchmarking experiments

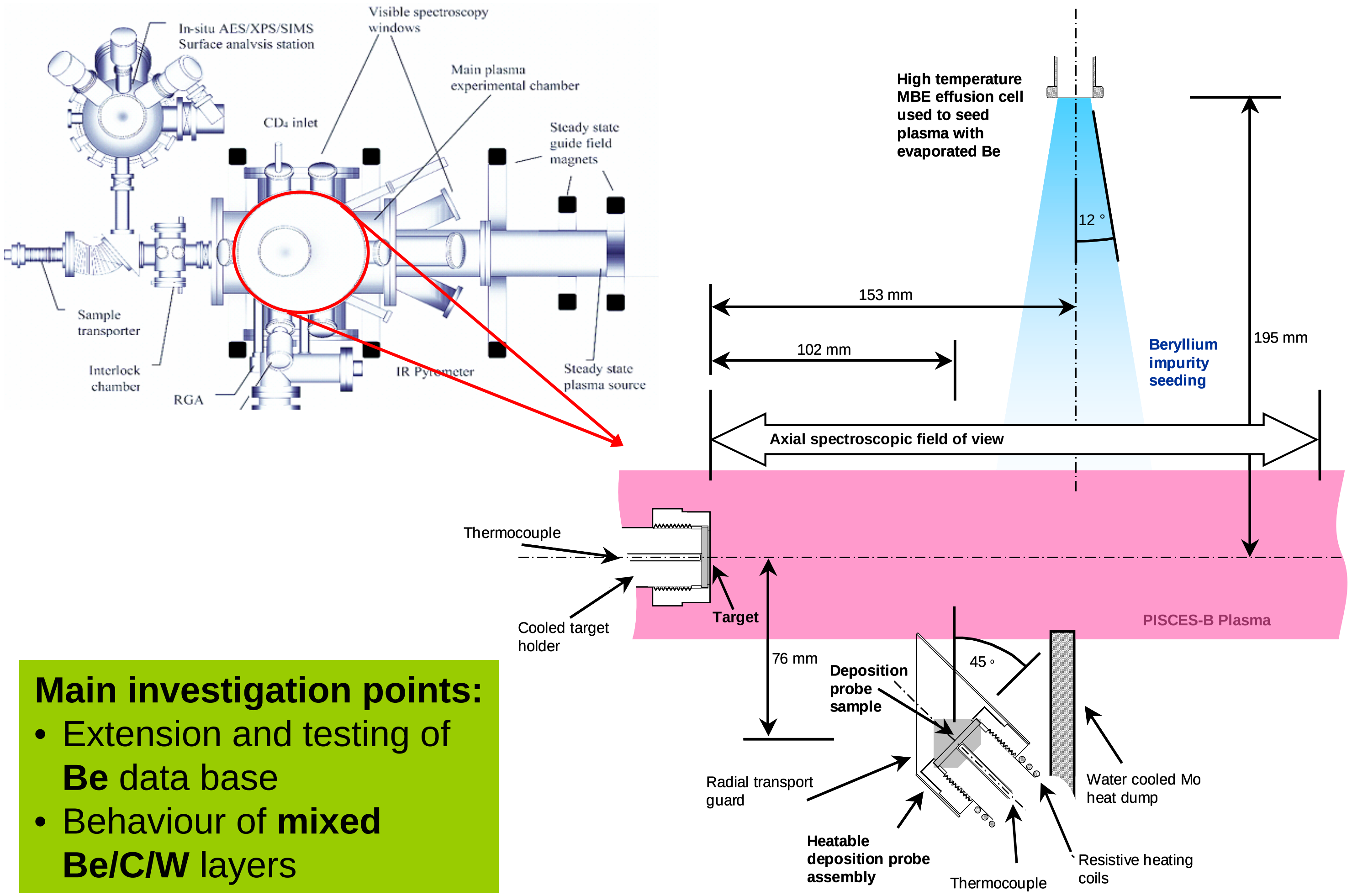


- Less complicated geometry than a tokamak
- Continues operation
- Plasma conditions relevant for ITER divertor



PSI-2 facility (Berlin). Planned to be transferred to FZ Jülich in 2009.

Be experiments at PISCES-B



Main investigation points:
- Extension and testing of **Be** data base
- Behaviour of **mixed Be/C/W** layers

Outline

- **Monte-Carlo (MC) method**
    - Error estimation
    - Random generators
- **Edge plasma and PSI simulations**
    - B2-EIRENE code (SOLPS)
    - ERO code
    - ERO light emission model
    - ERO – PSI modelling (TRIM, TRIDYN, MolDyn)
    - Elastic collisions
    - HYDKIN database
- **ERO – examples of application**
    - Hydrocarbon injection at TEXTOR (D/XB)
    - Test limiters – W and C
    - Be spectroscopy patterns at PISCES-B
    - ITER predictions (divertor plates lifetime, tritium retention)
- **Technical issues (ERO) – paralleliazation, benchmarking**

Monte Carlo basics

MC method – error estimation 1

For numeric calculation of κ-dimensional integral error (“guaranteed error”) can be estimated as

$$\delta \sim dA \cdot N^{-1/\kappa}$$

$$\delta < 0.01dA \Rightarrow N \geq 100^{\kappa}$$

Already by κ=5 really challenging number! . .

Monte-Carlo approach – let’s use mathematical expectation!

$$M(s_i) = \int_G f(P)dP = I(f), \qquad s_i = f(P_i)$$

$$S_N(f) = \frac{1}{N}\sum_{j=1}^{N} s_j \quad \Rightarrow M(S_N) = I(f),\ D(S_N(f)) = \frac{1}{N}D(f)$$

Chebyshev inequality:

$$\delta \sim |S_N(f) - I(f)| \leq \sqrt{D(f)/\eta N} \Leftrightarrow P = 1 - \eta$$

$$\eta = 0.01 \Rightarrow \delta \sim 10\sqrt{D(f)/N}$$

Any pair of s_i independent from each other!

$$\boxed{D(\overline{S_N}) \leq D(S_N) = D(f)}$$

MC method – error estimation 2

More precise estimation is based on central limit theorem:

$$\frac{|S_N(f)-I(f)|}{\sqrt{D(f)/N}} \sim \rho(y)=\frac{1}{2\pi}\int_{-\infty}^{y}\exp\left(-\frac{t^2}{2}\right)dt$$

All s_i are fully independent!

$$|S_N(f)-I(f)| \le \sqrt{D(f)/N} \sim \rho_0(y)=1-\frac{1}{2\pi}\int_{y}^{\infty}\exp\left(-\frac{t^2}{2}\right)dt$$

$$|S_N(f)-I(f)| \le 3\sqrt{D(f)/N} \qquad \mathrm{P}=0.997$$

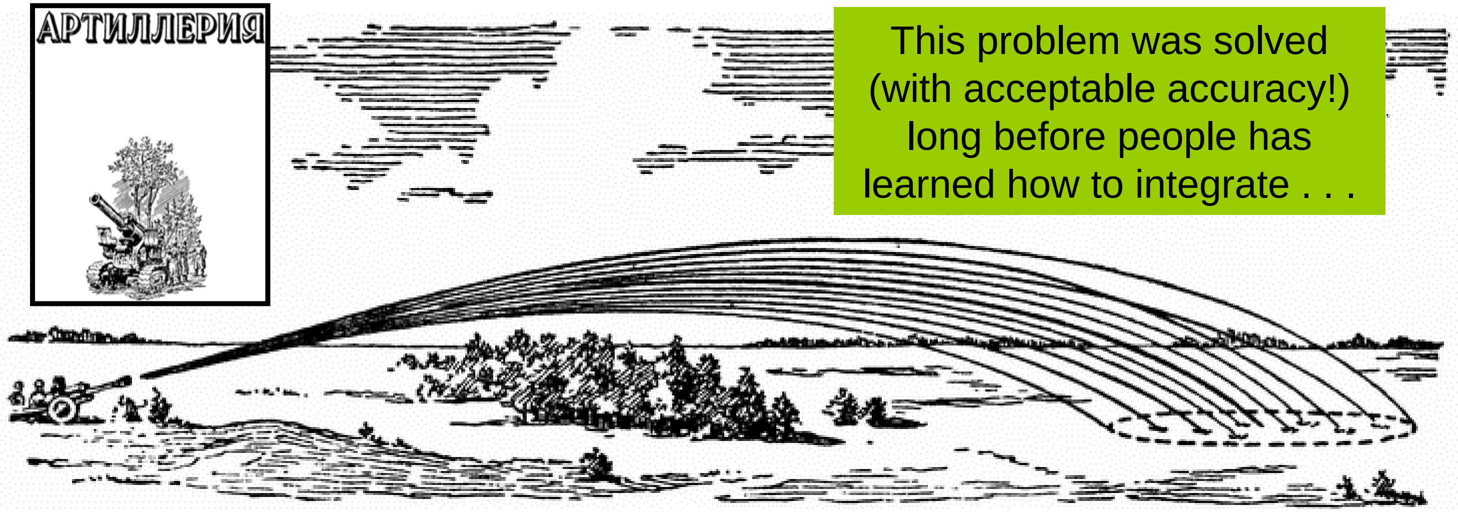
$$|S_N(f)-I(f)| \le 5\sqrt{D(f)/N} \qquad \mathrm{P}=0.99999$$

Some demotivation: *D(f)* should be kept small!..

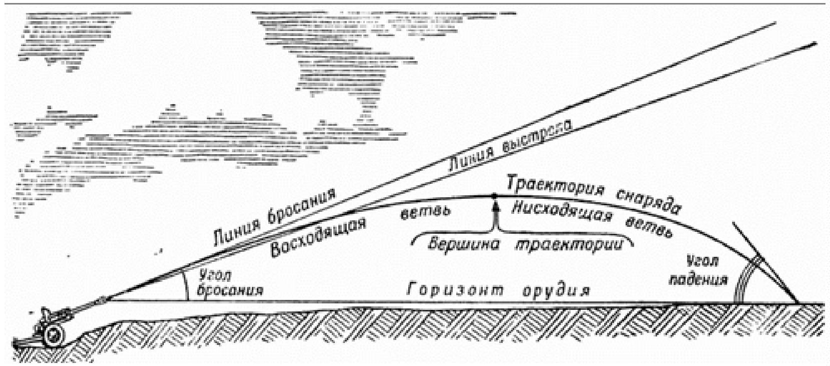
2 main ways to improve performance:

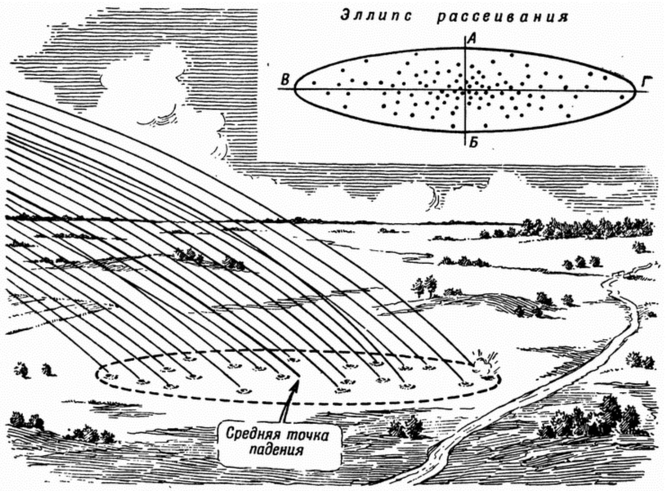
1) Choice of integration points distributed as *g(P)* e.g. such that *f(P)/g(P)=const*.
2) Separate the integration region into sections with various dispersion.

MC method – practical shooting

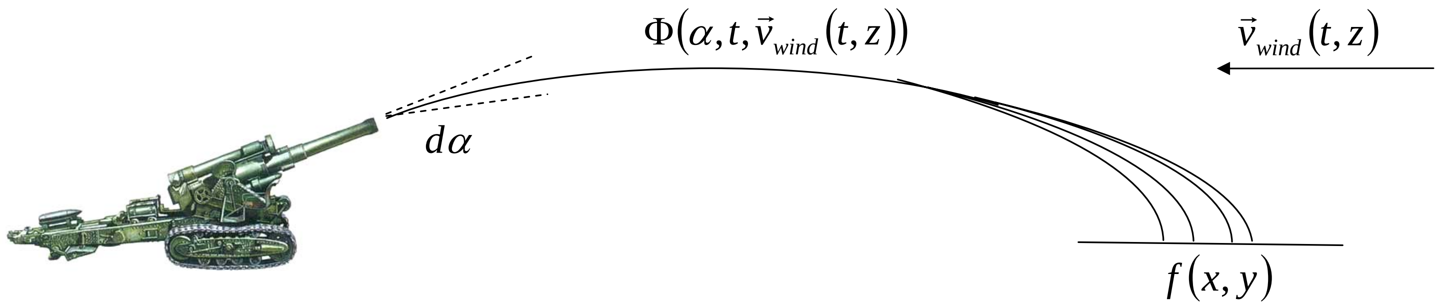


This problem was solved
(with acceptable accuracy!)
long before people has
learned how to integrate . . .





MC method – practical shooting



Determined solution:

$$f(x,y) = \oint \left(\int \Phi(\alpha, t, \vec{v}_{wind}(t,z)) dt \right) \cdot d\alpha$$

α – solid angle!

Monte-Carlo solution:

α – correct distributed arbitrary value

s_i – how many trajectories come to $[x_i \pm dx, y_i \pm dy]$

Typical task – find dispersion.

Determined solution: 2 more integrations by x,y

MC solution: just find dispersion of S_N . . .

Obviously, trajectory of a plasma particle is much more complicated!

MC formulation – elementary processes

Let's assume that on specie can act processes 1, 2, …

$$\frac{dN}{dt} = \langle v\sigma_1 \rangle n_e \cdot N + \langle v\sigma_2 \rangle n_e \cdot N + \ldots$$

$$\beta = n_e \left(\langle v\sigma_1 \rangle + \langle v\sigma_2 \rangle + \ldots \right)$$

$$\int \frac{dN}{N} = \int \beta dt \Rightarrow -\ln N = \beta t + C$$

$$N_{t=0} = 1 \Rightarrow C = 0$$

$$N = \exp(-\beta t)$$

$$P_{\text{change}} \sim \frac{\Delta N}{N} = \Delta N = 1 - \exp(-\beta \Delta t)$$

$$P < .?. > \xi \in [0,1]$$

Monte-Carlo approach: decision is taken based on comparing of probability P with random generated value ξ.

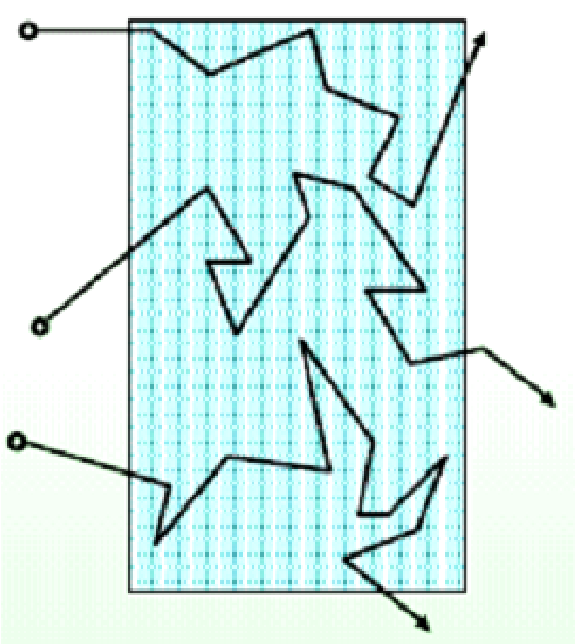
$$P_{\textbf{no}\ \text{change}} \sim \frac{\Delta N}{N} = \Delta N = \exp(-\beta \Delta t)$$

More convenient in this case.

Decision concerning which of processes 1, 2, … has occurred can be taken based on additional random value $\xi_{2.}$

Summary of MC method advantages

- Calculation error does not depend directly on the problem dimensionality
- Usually the mathematical expressions are relatively simple (free from additional integrations)
- Realisation of many physical processes like particle movement is very natural and straightforward. It is easy to control the reasonability of intermediate results.
- Easy to treat complicated 3D geometries.
- MC method is quite time consuming, however very suitable for parallelisation.

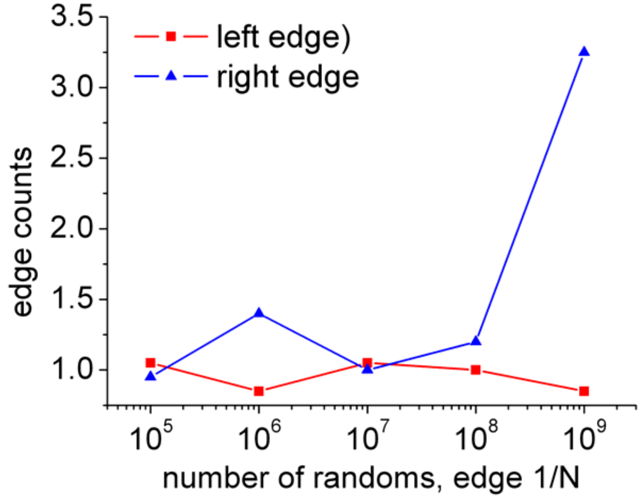


MC – random generator challenges

1) Generated numbers are fully independent!
   - No or at least very long period.
   - Generated numbers are equally distributed along [0,1]
2) Generator does not consume too much CPU time
3) It is possible to reproduce the generation exactly

Example

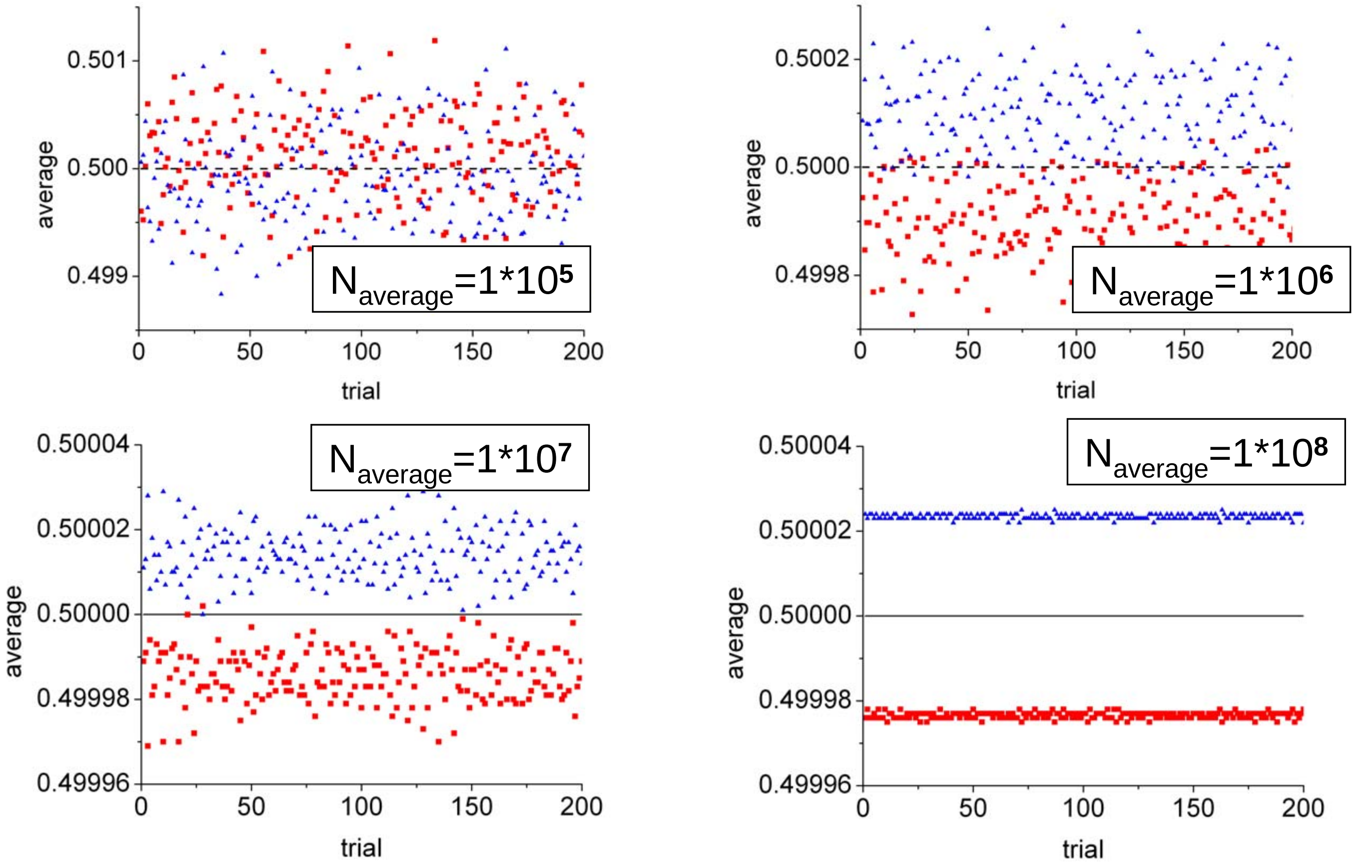
For N uniformly distributed random numbers the average number of hits, <n>, in the ranges (0,ε) and (1-ε,1) should be equal to ε·N. If we select ε=1/N, then <n>=1.



A specific algorithm must be tested together with the random number generator being used regardless of the tests which the generator has passed . . .

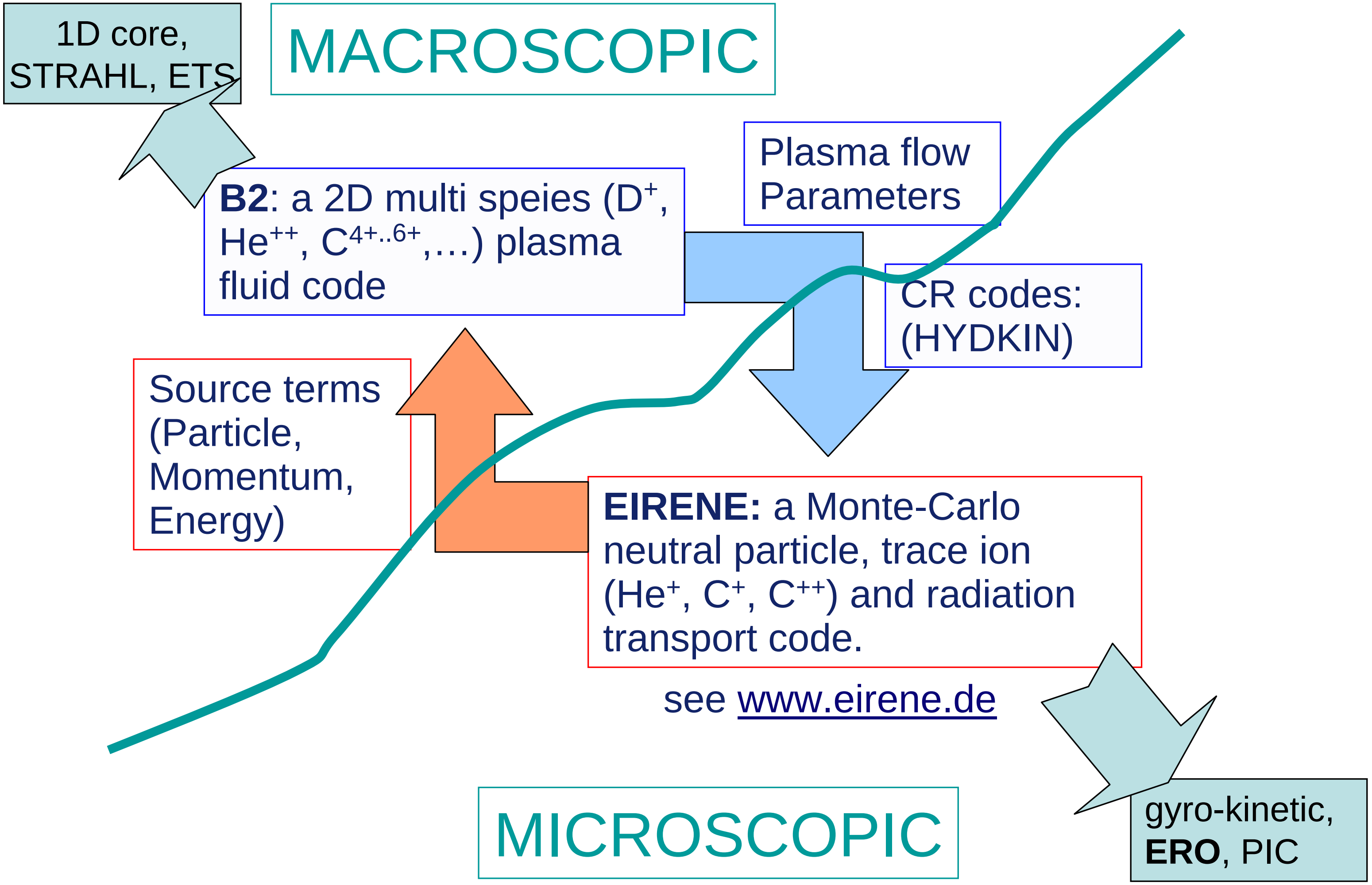
MC – RG negative example

“Not optimal” random generator – combination of 3 recurrent formulas from “Numerical recipes”. Average of **odd (blue)** and **even (red)** numbers.



Plasma simulations,
EIRENE and ERO codes

Codes for fusion plasmas



1D core, STRAHL, ETS

MACROSCOPIC

B2: a 2D multi speies (D^+, He^{++}, $C^{4+..6+}$,…) plasma fluid code

Plasma flow Parameters

CR codes: (HYDKIN)

Source terms (Particle, Momentum, Energy)

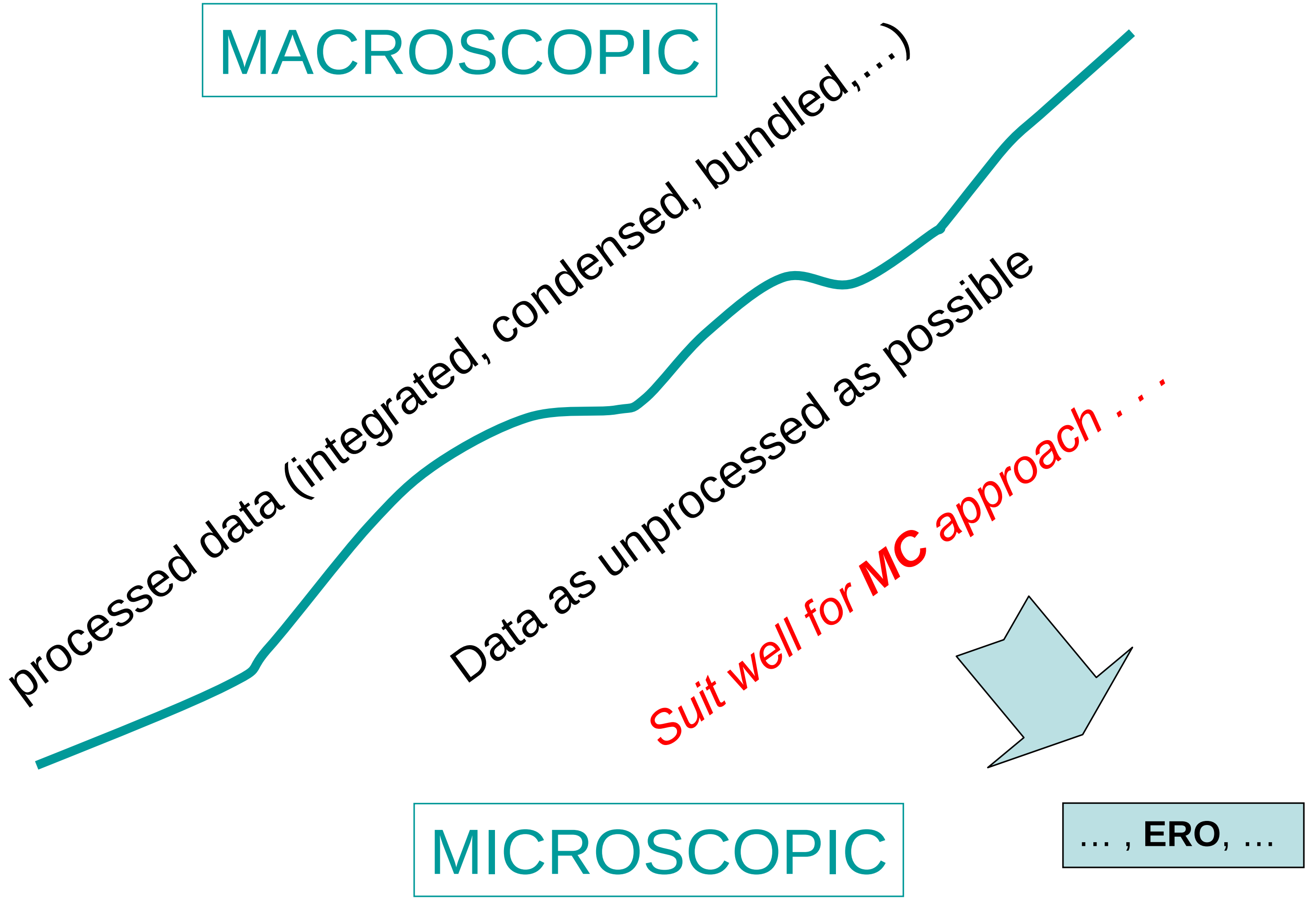
EIRENE: a Monte-Carlo neutral particle, trace ion (He^+, C^+, C^{++}) and radiation transport code.

see www.eirene.de

MICROSCOPIC

gyro-kinetic, **ERO**, PIC

Codes for fusion plasmas



MACROSCOPIC

processed data (integrated, condensed, bundled,…)

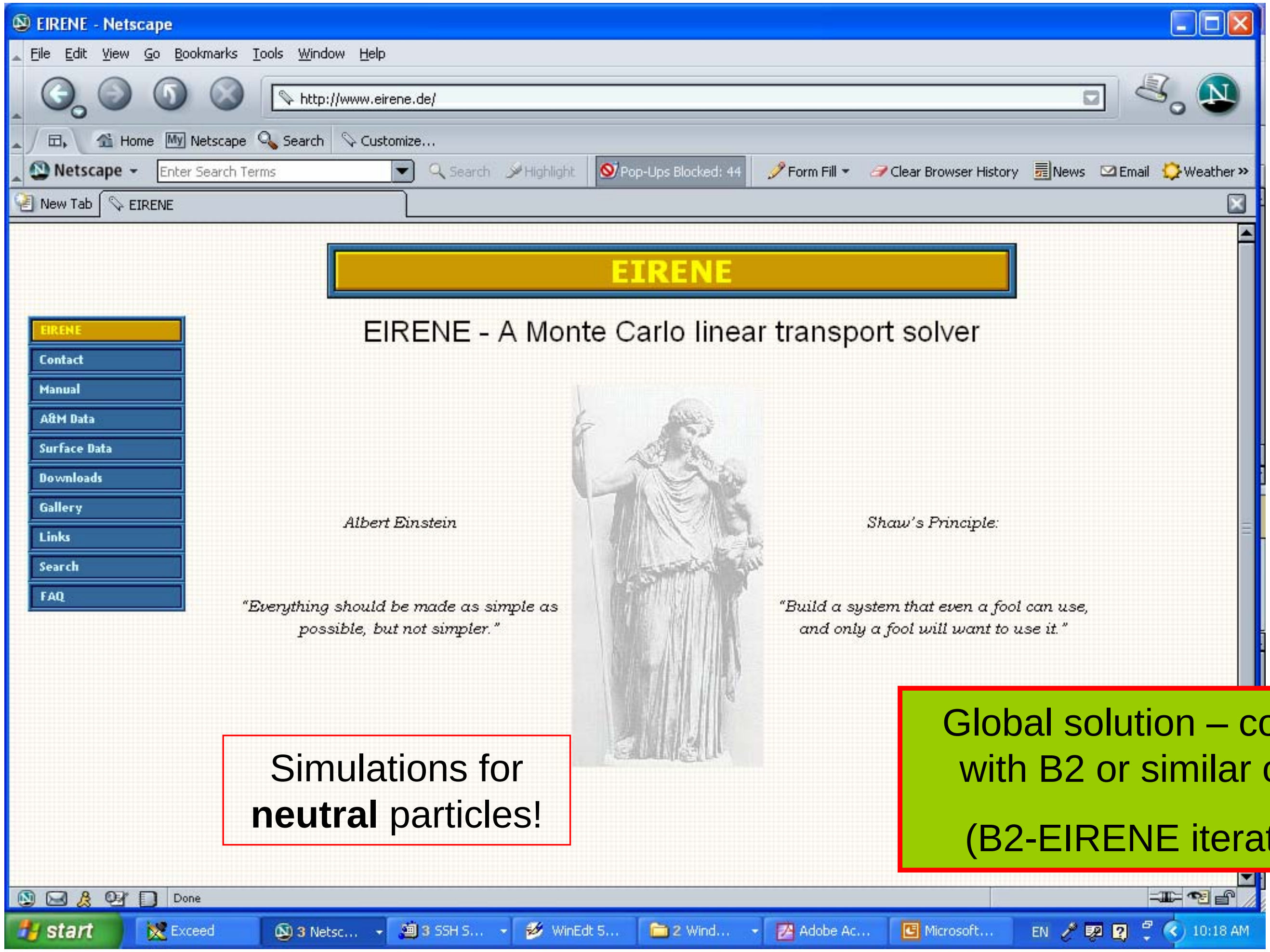
Data as unprocessed as possible

Suit well for **MC** approach . . .

MICROSCOPIC

… , **ERO**, …

EIRENE code



EIRENE

EIRENE - A Monte Carlo linear transport solver

Albert Einstein

"Everything should be made as simple as possible, but not simpler."

Shaw's Principle:

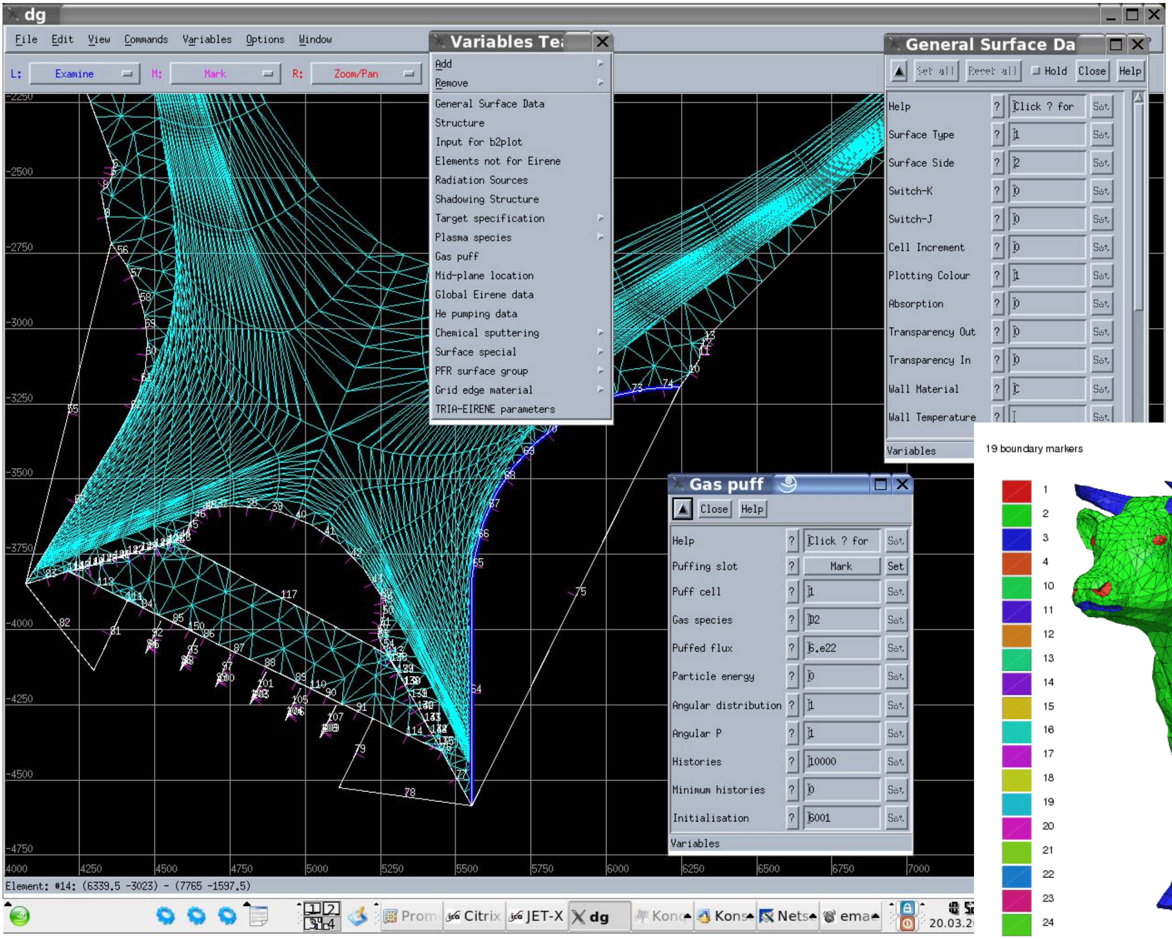
"Build a system that even a fool can use, and only a fool will want to use it."

Simulations for **neutral** particles!

Global solution – coupling with B2 or similar codes

(B2-EIRENE iterations)

EIRENE – mesh generation



Element: #14: (6339.5 -3023) - (7765 -1597.5)

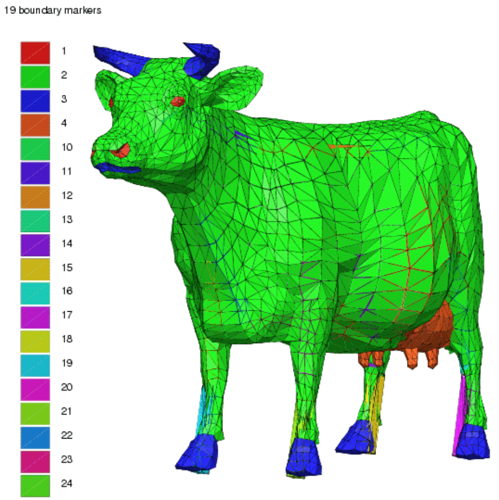
General Surface Da

Help	?	Click ? for
Surface Type	?	1
Surface Side	?	2
Switch-K	?	0
Switch-J	?	0
Cell Increment	?	0
Plotting Colour	?	1
Absorption	?	0
Transparency Out	?	0
Transparency In	?	0
Wall Material	?	C
Wall Temperature	?	

Gas puff

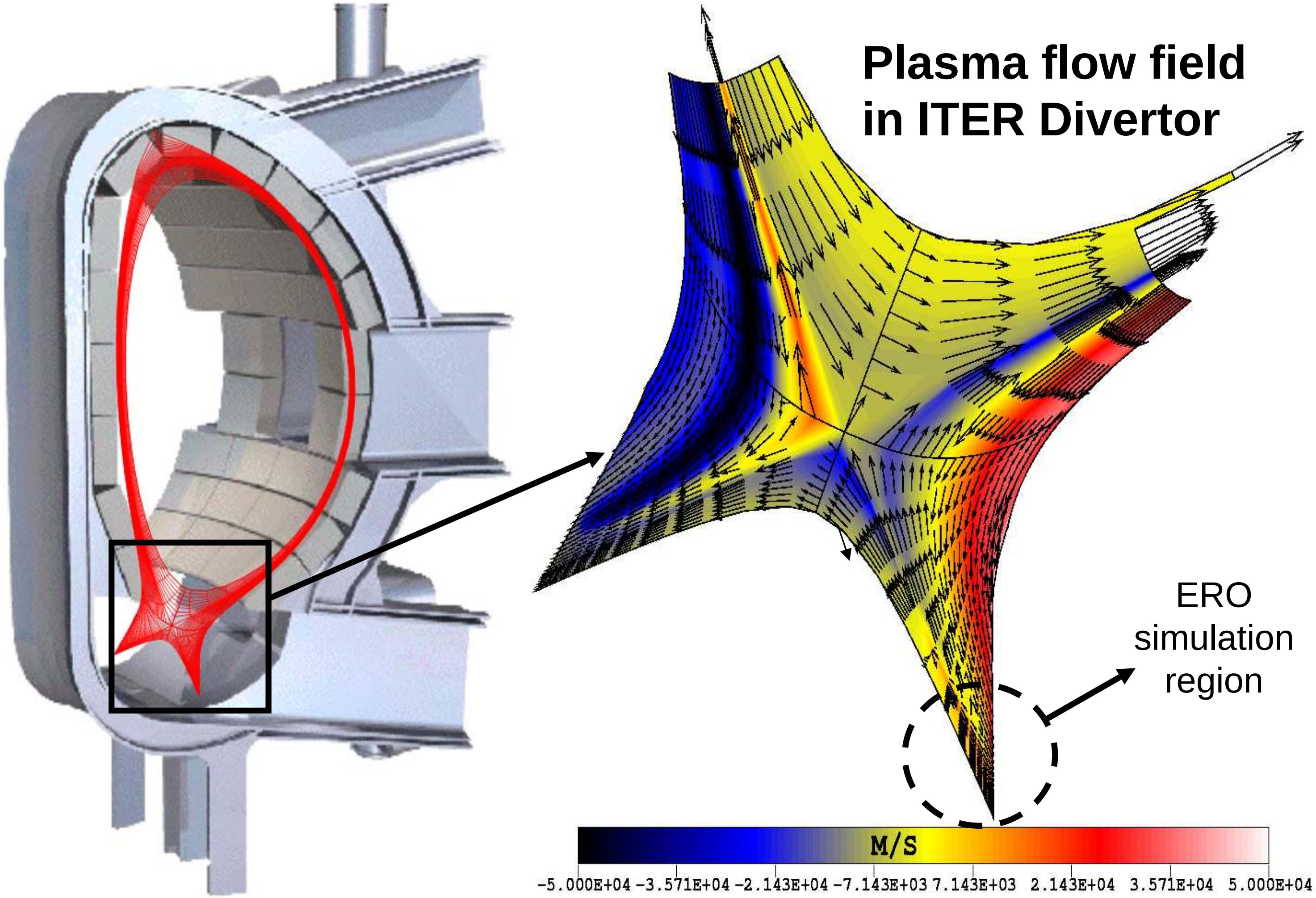
Help	?	Click ? for
Puffing slot	?	Mark
Puff cell	?	1
Gas species	?	D2
Puffed flux	?	6.e22
Particle energy	?	0
Angular distribution	?	1
Angular P	?	1
Histories	?	10000
Minimum histories	?	0
Initialisation	?	6001

Tetrahedral Mesh
Generator and 3D
Delaunay Triangulator



For ITER: 2D GUI, CAD – EIRENE available

EIRENE – simulation region



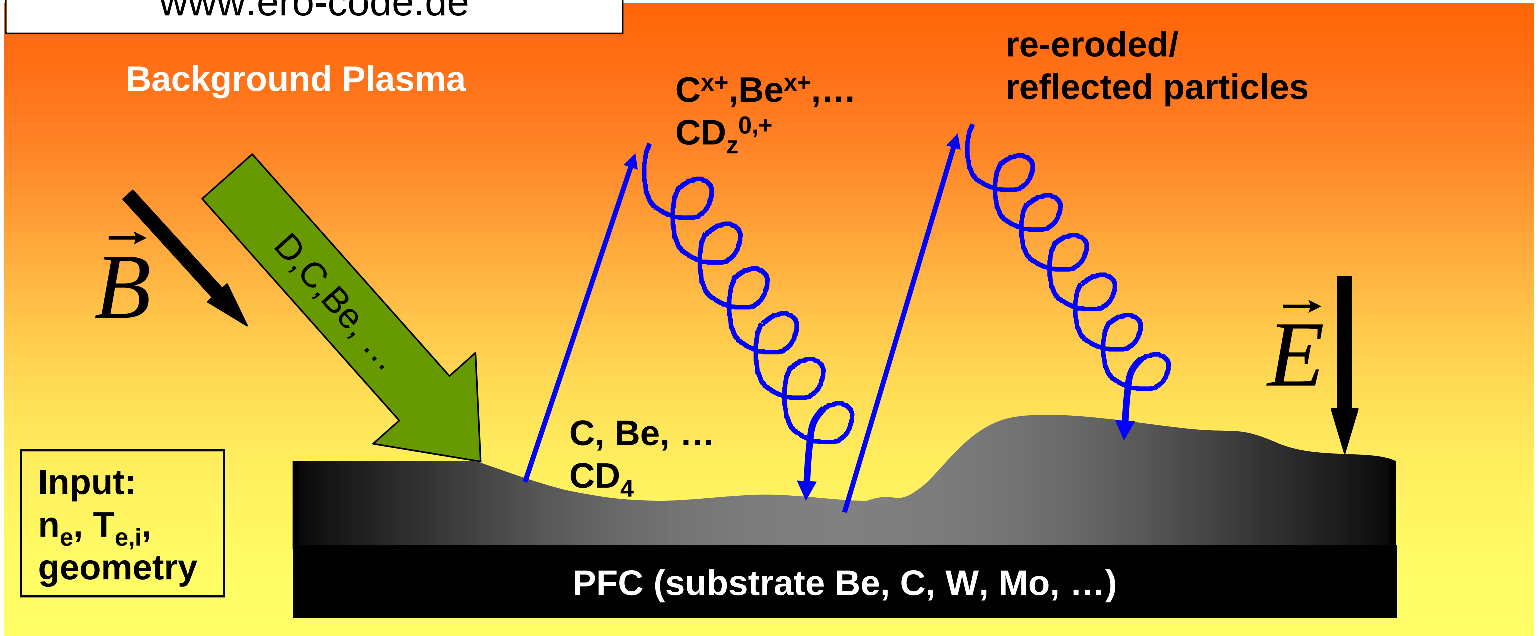
Plasma flow field in ITER Divertor

ERO
simulation
region

ERO code

3D MC impurity transport code ERO

www.ero-code.de



Local transport:

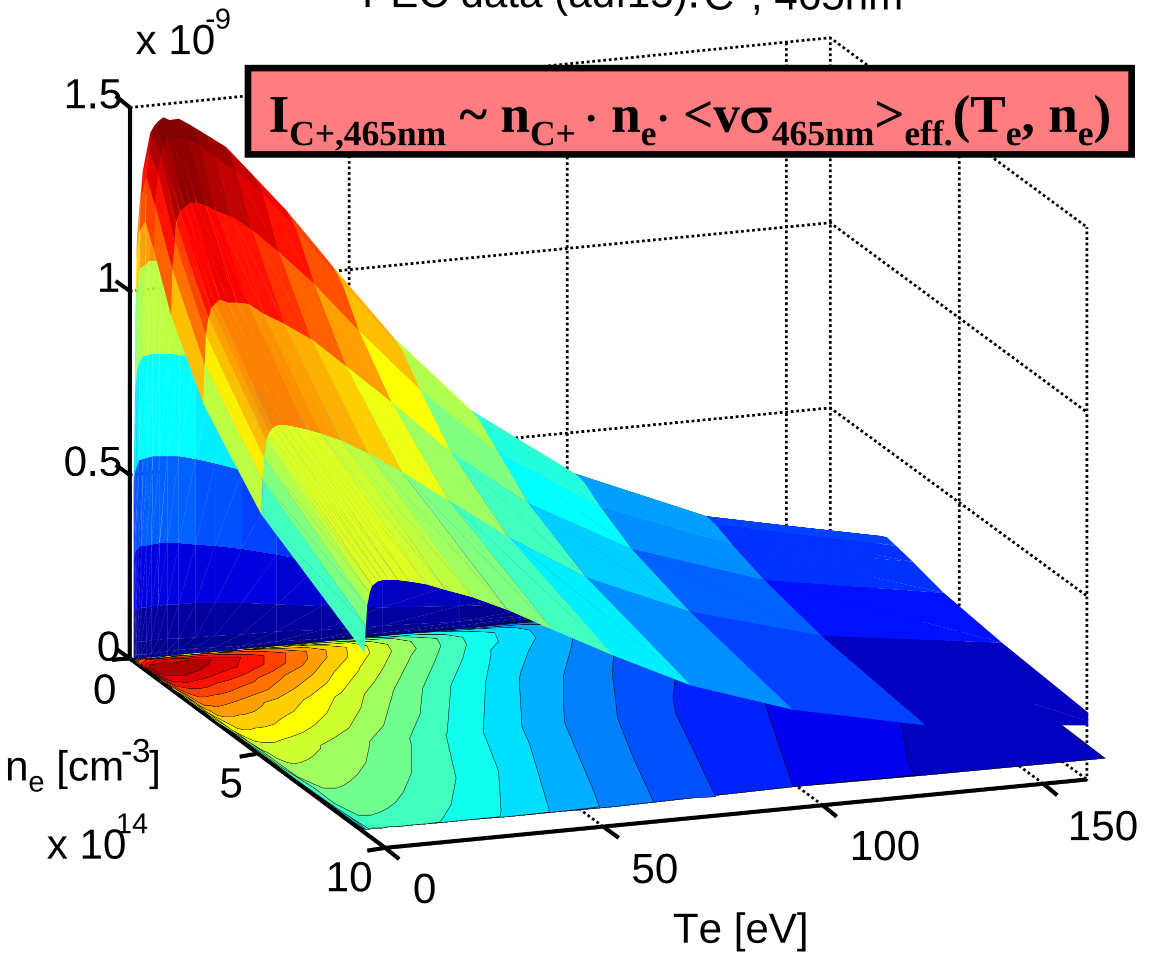
- ✓ ionisation, dissociation
- ✓ friction (Fokker-Planck), thermal force
- ✓ Lorentz force (including ExB component)
- ✓ cross-field diffusion

Plasma-surface interaction:

- ✓ physical sputtering/reflection
- ✓ chemical erosion (CD_4)
- ✓ (re-)erosion and (re-)deposition
- ✓ NEW: coupling with TRIDYN

ERO: calculation of light emission

PEC data (adf15). C^+, 465nm

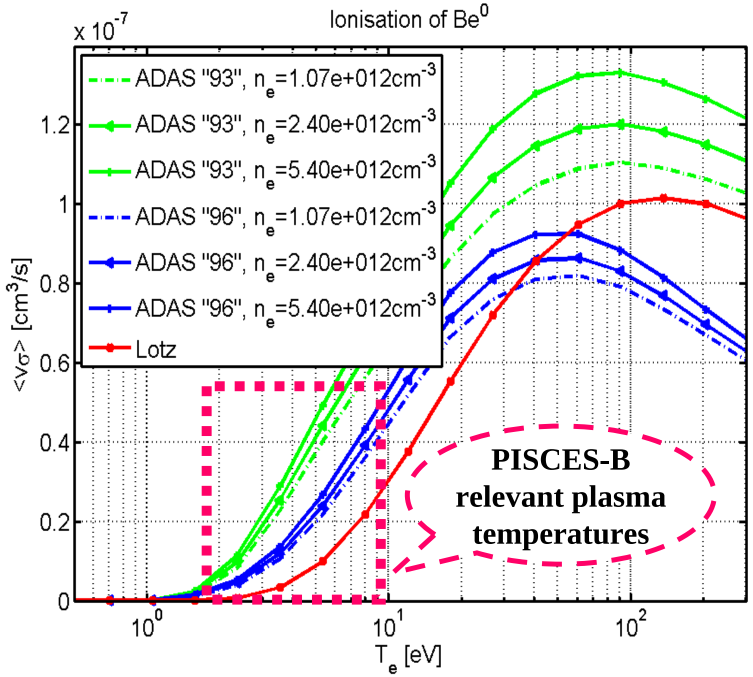


$$I_{C+,465nm} \sim n_{C+} \cdot n_e \cdot \langle v\sigma_{465nm} \rangle_{eff.}(T_e, n_e)$$

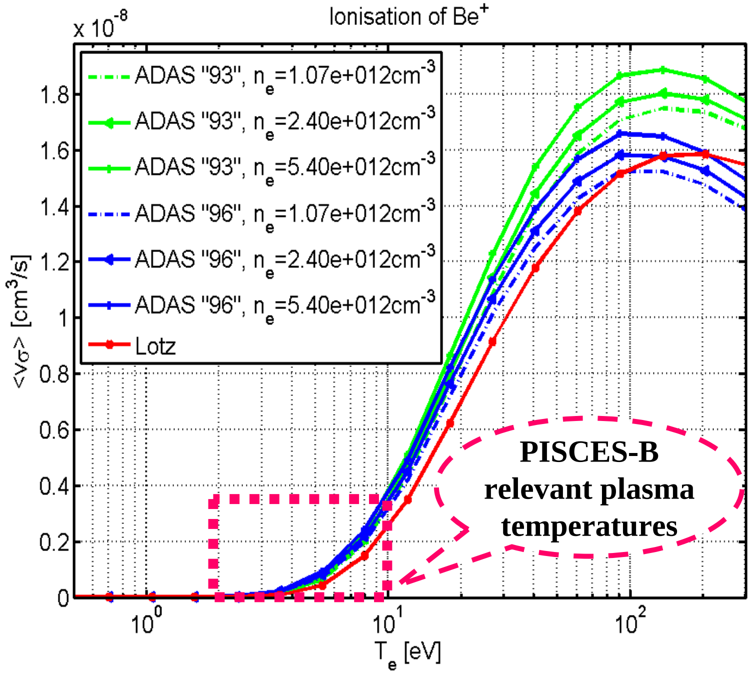
At first, ERO calculates the **3D density** distribution of respective species . . .

This **stationary** approach implies that both excitation and emission acts happen inside the volume cell at hand.

ADAS data: effective ionization of Be



PISCES-B relevant plasma temperatures

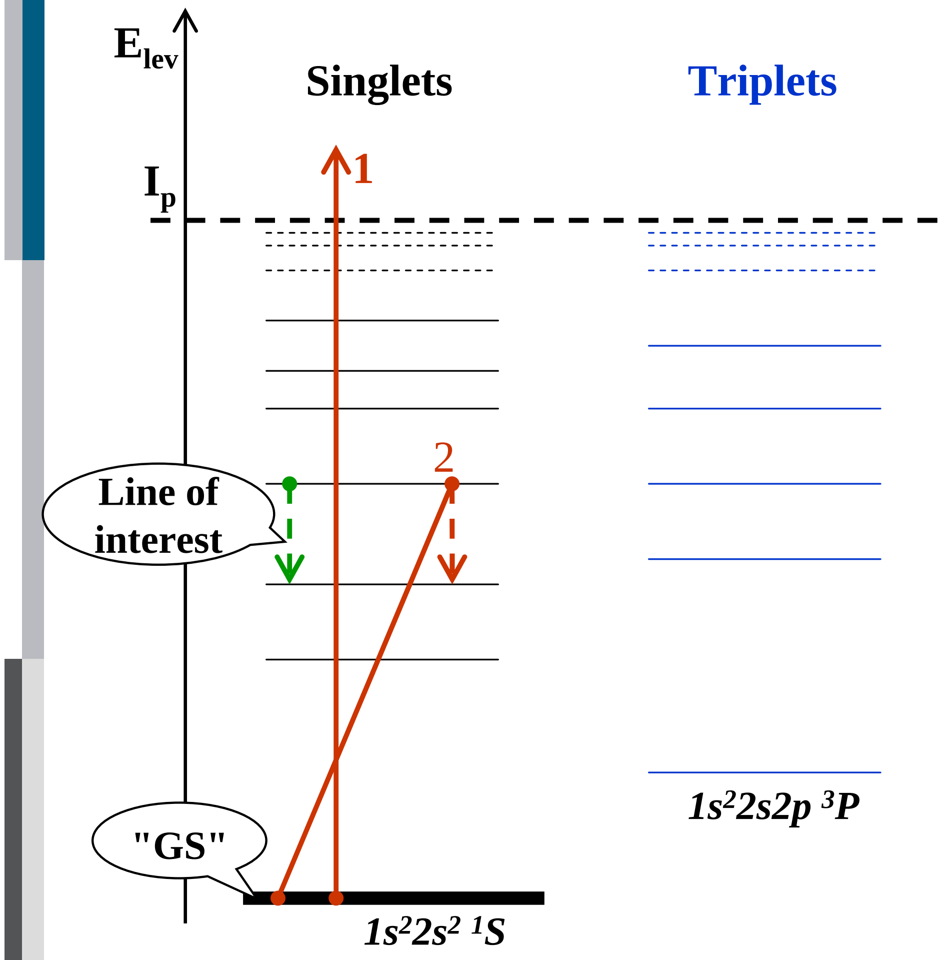


PISCES-B relevant plasma temperatures

ERO database of **atomic data** is continuously updated according to the respective changes in the **ADAS.**

The **density dependence** of **effective rates** was shown to be of importance in a number of cases.

BeI – '2 level' approximation scheme



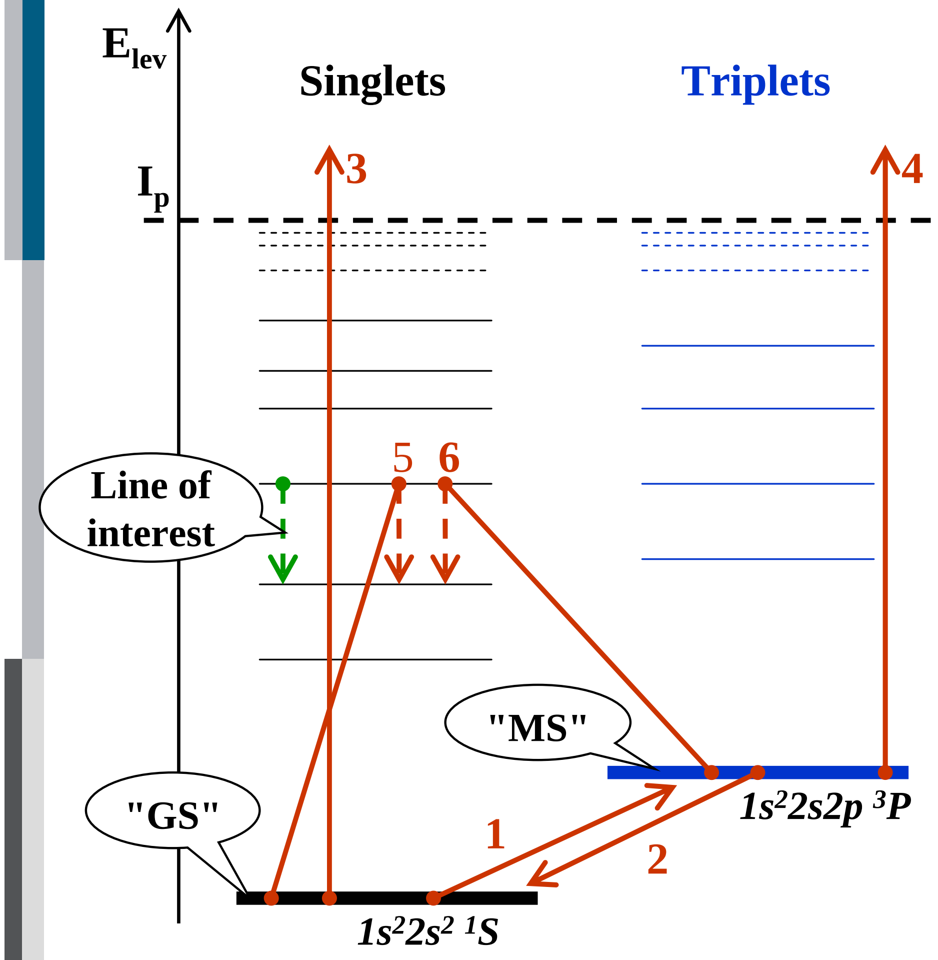
Effective rates:

1) <IzG> - ionization from "GS"
2) <IG> - line intensity, assuming full population of "GS"

One effective PEC (photon efficiency coefficient) for each line + effective ionization

Effective rates represent all possible transitions including cascades, however not the ‘slow’ evolution of level populations.

BeI – 1 MS approximation scheme



Effective rates:

1) <ExGM> - excitation from "GS" to "MS"

2) <ExMG> - deexcitation from "MS" to "GS"

3) <IzG> - ionization from "GS"

4) <IzM> - ionization from "MS"

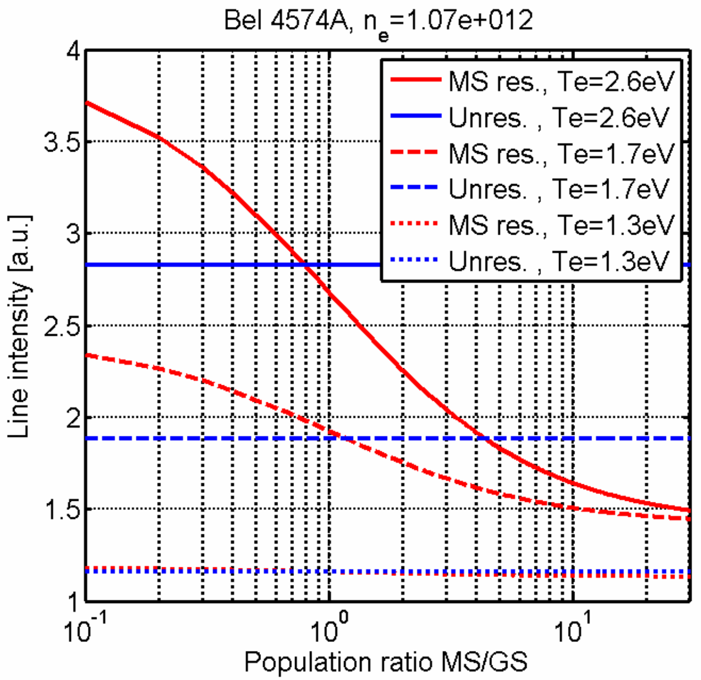
5) <IG> - line intensity, contribution from "GS"

6) <IM> - line intensity, contribution from "MS"

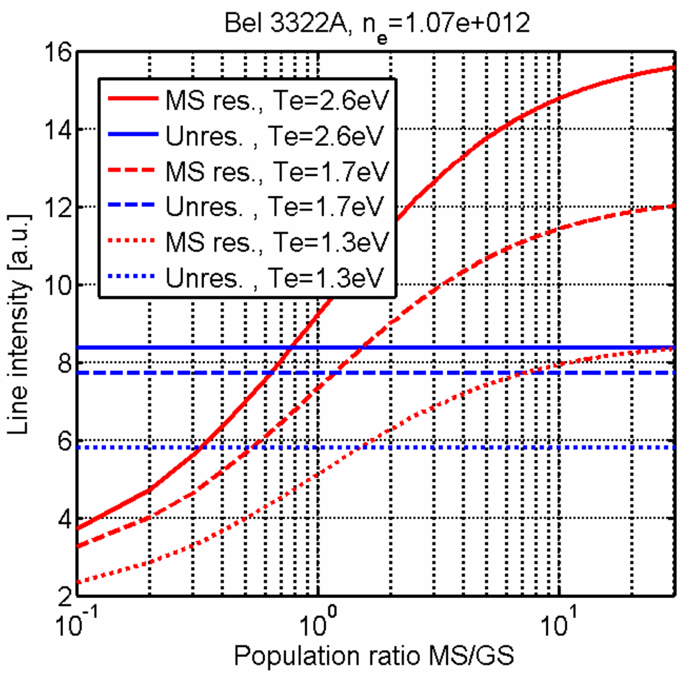
5, 6 are individual for every line of interest!

Line intensities – MS population

Singlet



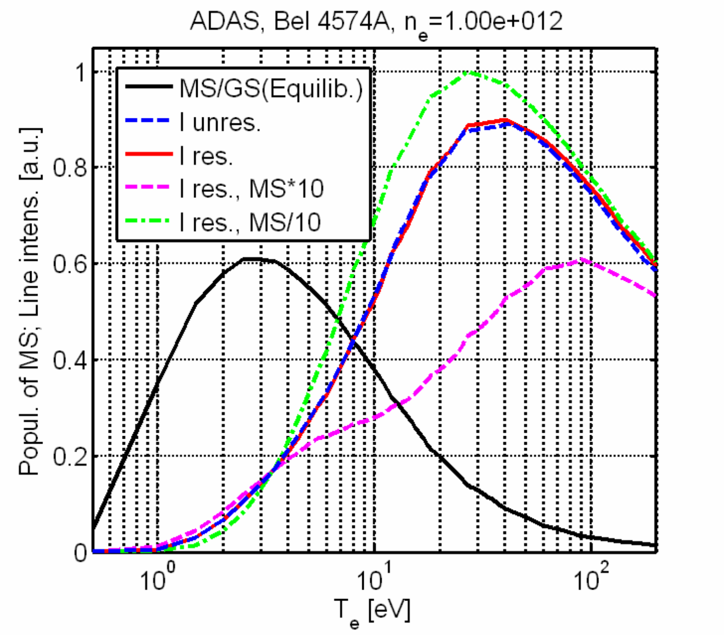
Triplet



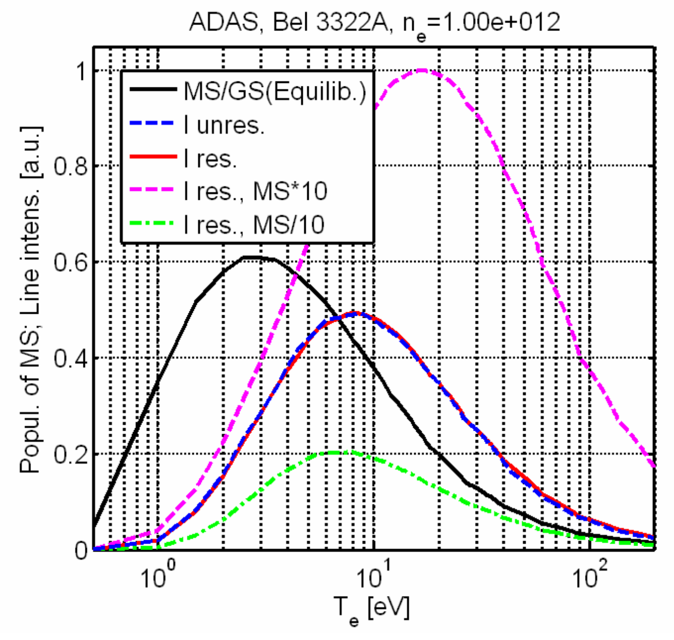
$$I \sim N_{GS} \cdot \underbrace{\langle v\sigma \rangle_{GS}(n_e, T_e)}_{\text{Large for singlets}} \cdot n_e + N_{MS} \cdot \underbrace{\langle v\sigma \rangle_{MS}(n_e, T_e)}_{\text{Large for triplets}} \cdot n_e$$

Line intensities – stationary approach

Singlet



Triplet



$$\begin{cases} \underbrace{0 \equiv}_{\substack{stationary\\approach}} \dfrac{dN_{GS}}{dt} = -\langle ExGM \rangle N_{GS} - \langle IzG \rangle N_{GS} + \langle ExMG \rangle N_{MS} \\ dN_{GS} + N_{MS} = 1 \end{cases} \Rightarrow \quad \frac{N_{MS}}{N_{GS}} = \frac{\langle ExMG \rangle}{\langle ExGM \rangle + \langle IzG \rangle}$$

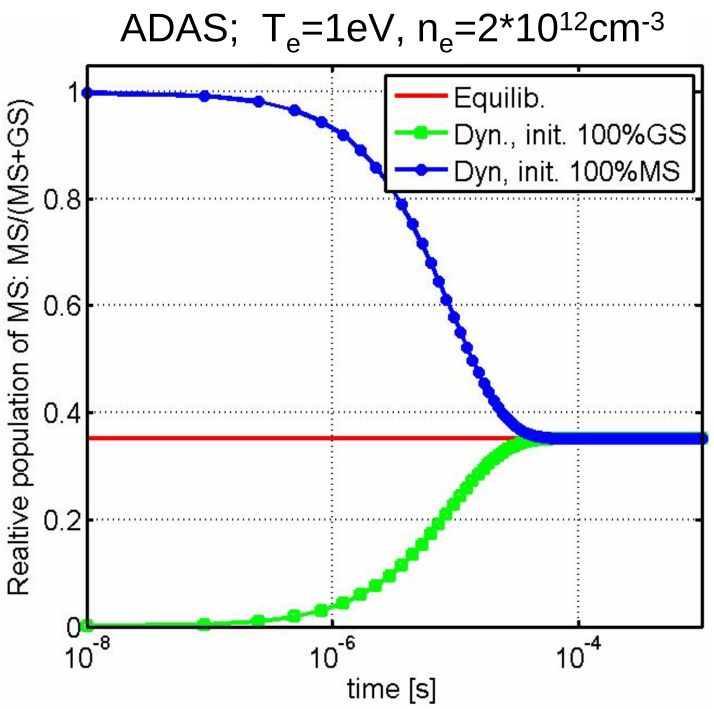
Line intensities – dynamic approach

$$\begin{cases} \dfrac{dN_{GS}}{dt} = -\langle ExGM\rangle N_{GS} - \langle IzG\rangle N_{GS} + \langle ExMG\rangle N_{MS} \\ \dfrac{dN_{MS}}{dt} = -\langle ExMG\rangle N_{MS} - \langle IzM\rangle N_{MS} + \langle ExGM\rangle N_{GS} \end{cases}$$

Analytical solution

$(C_{1i}, C_{2i}, \lambda_p, \lambda_m$ determined by rates) :

$$dN_i(t) = C_{1i}\exp(-\lambda_p t) + C_{2i}\exp(-\lambda_m t)$$



ADAS; T_e=1eV, n_e=2*10^{12}cm^{-3}

Relaxation time between MS and GS is 10^{-5}-10^{-4}s

Higher hydrocarbons

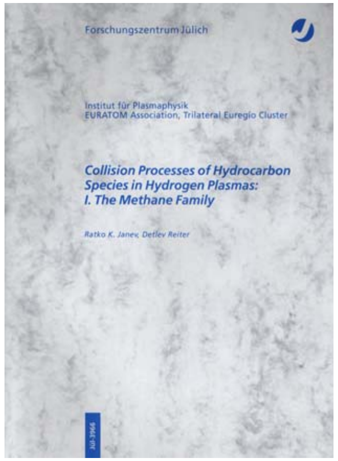
(chemical reaction chains and D/XB for CH)

HYDKIN

Hydride Collision Databases for Technical Plasmas and Fusion Plasmas

Reviewed Database Series 2002-….,
FZ-Jülich (R. Janev, D. Reiter), www.eirene.de www.hydkin.de

Methane (CH_y)


Forschungszentrum Jülich

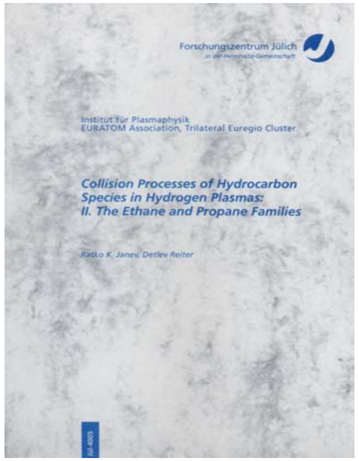
Institut für Plasmaphysik
EURATOM Association, Trilateral Euregio Cluster

Collision Processes of Hydrocarbon Species in Hydrogen Plasmas: I. The Methane Family

Ratko K. Janev, Detlev Reiter

JUEL 3966, Feb 2002
Phys. Plasmas,
Vol 9, 9, (2002) 4071

C_2H_y C_3H_y


Forschungszentrum Jülich
in der Helmholtz-Gemeinschaft

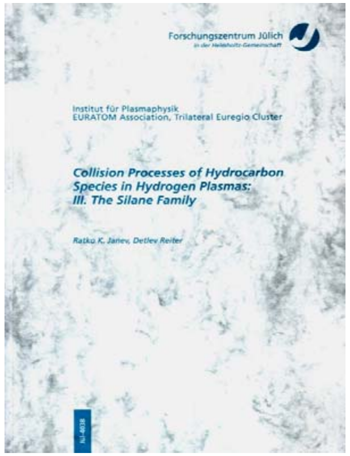
Institut für Plasmaphysik
EURATOM Association, Trilateral Euregio Cluster

Collision Processes of Hydrocarbon Species in Hydrogen Plasmas: II. The Ethane and Propane Families

Ratko K. Janev, Detlev Reiter

JUEL 4005, Oct. 2002
Phys. Plasmas,
Vol 11,2, (2004) 780

Silane (SiH_y)


Forschungszentrum Jülich
in der Helmholtz-Gemeinschaft

Institut für Plasmaphysik
EURATOM Association, Trilateral Euregio Cluster

Collision Processes of Hydrocarbon Species in Hydrogen Plasmas: III. The Silane Family

Ratko K. Janev, Detlev Reiter

JUEL 4038, Mar. 2003
Contr. Plas.Phys,
47, 7, (2003) 401-417

p,H,H^-,H_2,H_2^+,H_3^+


Forschungszentrum Jülich
in der Helmholtz-Gemeinschaft

Institut für Plasmaphysik
EURATOM Association, Trilateral Euregio Cluster

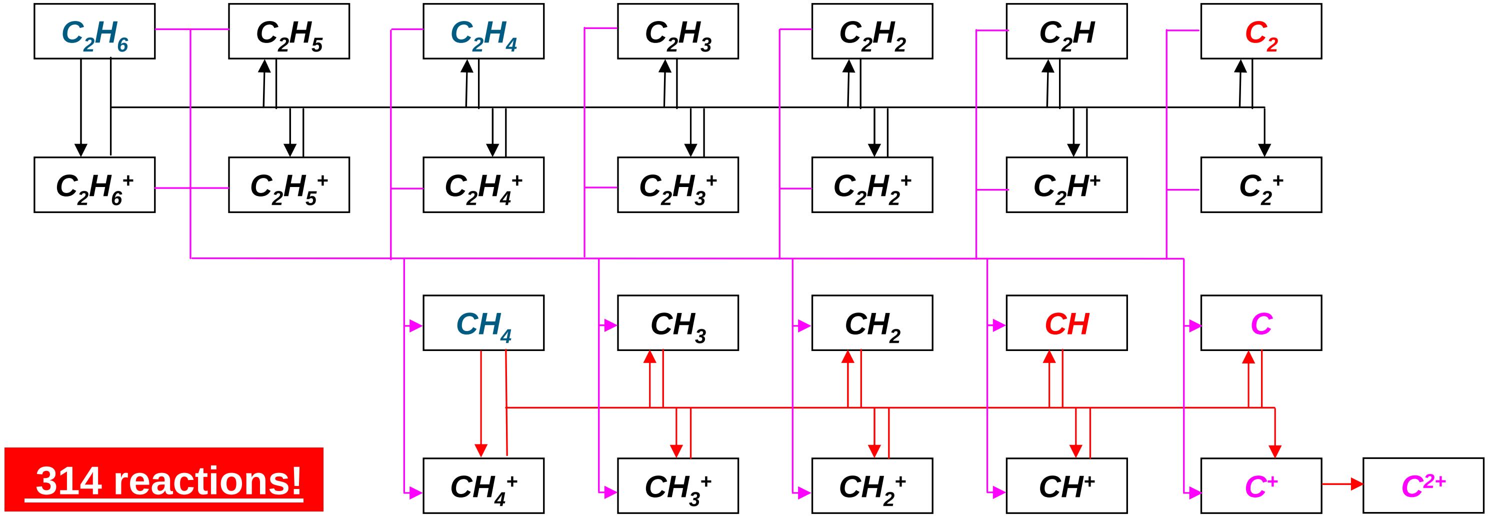
Collision Processes in Low-Temperature Hydrogen Plasmas

Ratko K. Janev, Detlev Reiter, Ulrich Samm

JUEL 4105, Dec. 2003
Encycl. Low. Temp.
Pl. 2007 (in russian)

C-H database in ERO code

Reaction chains of hydrocarbon molecules (Janev / Reiter)



314 reactions!

Emission data

CII, CIII ⇐ **ADAS**

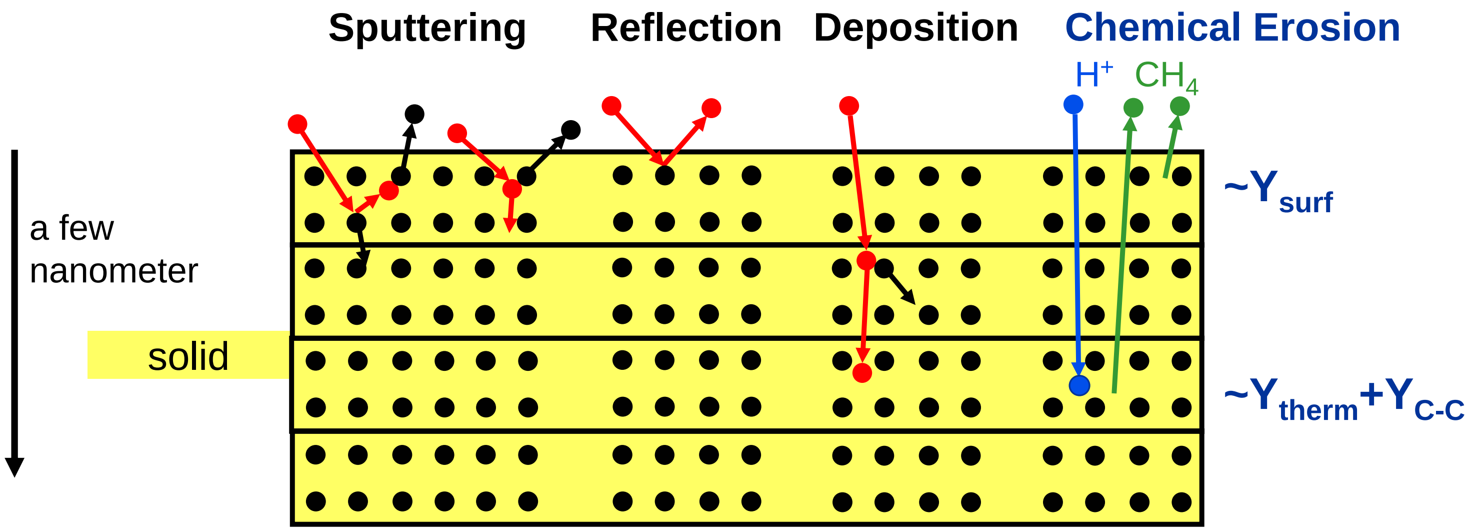
CH A-X, C_2 d-a ⇐ **U. Fantz et al. 2005**

Probably this is not enough . . .

Surface data,
PSI part of ERO

PSI – 1: main processes and TRIM code

Monte-Carlo method: TRIM code (Eckstein et al.)

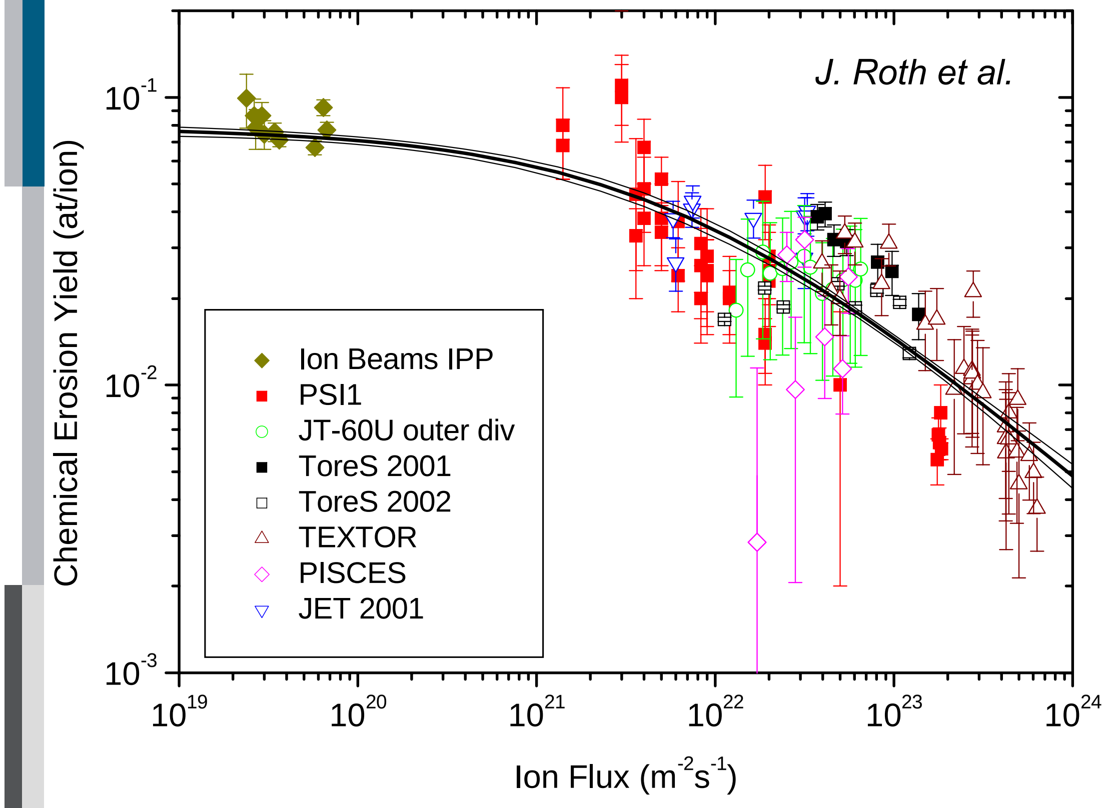


TRIM : TRansport of **I**ons in **M**atter (TriDyn, SDTrimSP)

- using random numbers (e.g. to decide whether collision or not): “Monte-Carlo”
- **binary collisions** between impinging ion and target atoms
  (elastic, screened Coulomb-potential) ⇒ collision cascades
- inelastic electronic energy loss
- **output: reflection coefficients/ physical erosion yields / concentration-depth profiles / layer growth**

PSI – 2: chemical sputtering

Chemical sputtering yield in dependence on impinging flux



Chemical sputtering decreases with increasing flux

Chemical sputtering depends on surface temperature, contance, morphology, . . .

Flux dependence is predicted by model of thermal reaction cycle.

Elastic collisions

Elastic collisions in ERO

Elastic neutral collisions (ENC):

- MC formulation : during time step dt the tracked particle experienses an alastic collition acoording to a random number $\xi, \xi \in [0,1]$:

$$\xi > \exp(-\langle \sigma v \rangle * n_{ntrl} * dt)$$

- The rates $\langle \sigma v \rangle$ are calculated using the routines by A.Pigarov
- The direction of particles is assumed to be opposite to each other and arbitrary in the center of mass system
- For linear devices $n_{ntrl} = n(D_2)$ is often assumed to be uniform in the volume

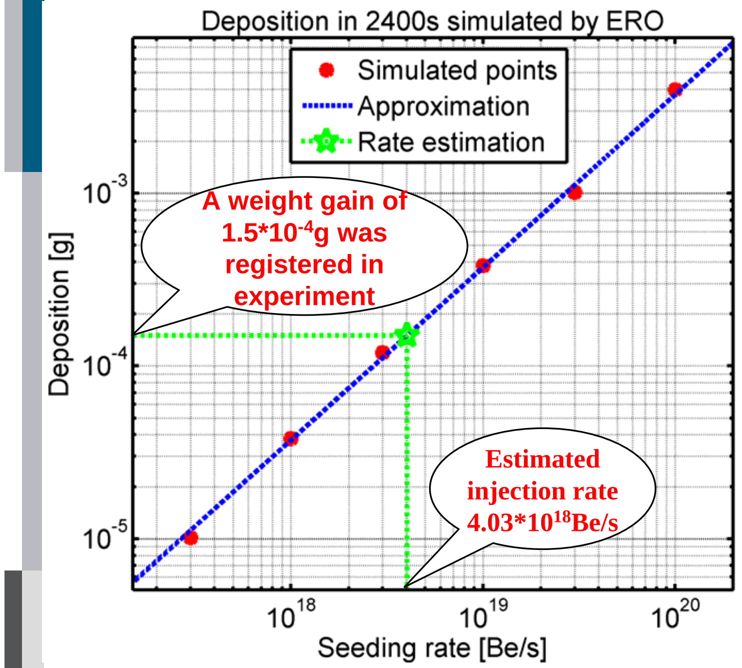
1) In case of injection simulations ENC lead to broadening of the beam

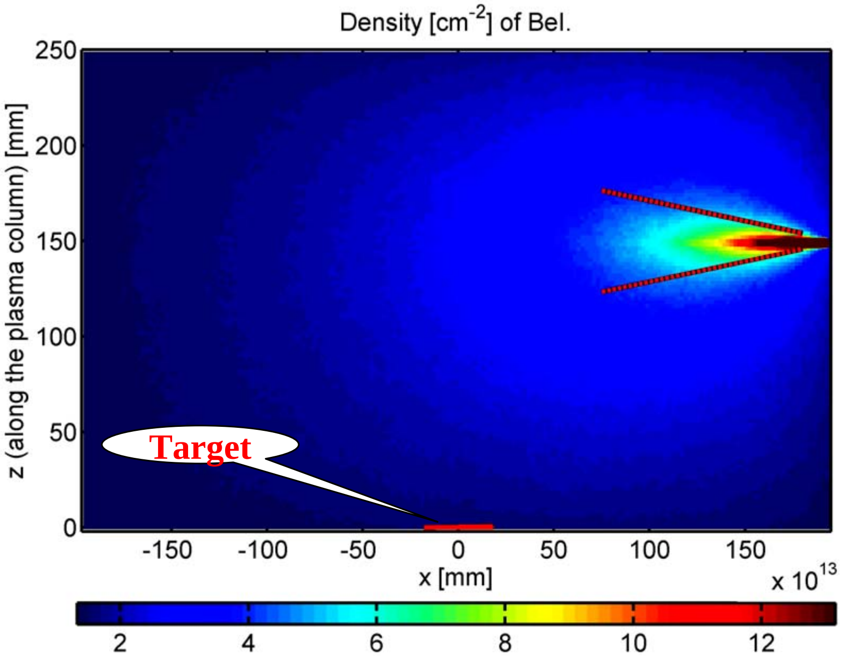
2) ENC lead to an increase of hydrocarbon re-deposition

3) For neutral density B2-EIRENE calculations are necessary . . .

Benchmark of elastic collisions model

Be injection w/o plasma . . .





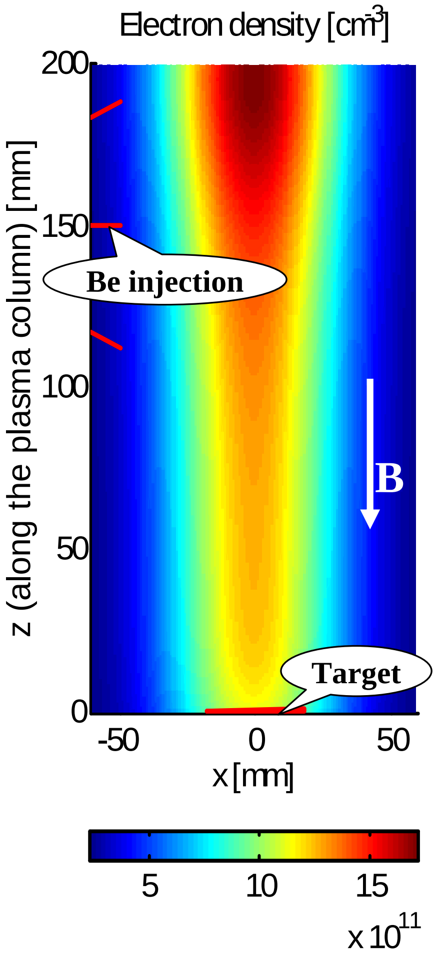
2g of Be is spent in more than 10 hours of oven operation.
This gives a rate of about - **$3.7*10^{18}$Be/s**.

W/o elastic collision with neutrals there would be no Be at target!

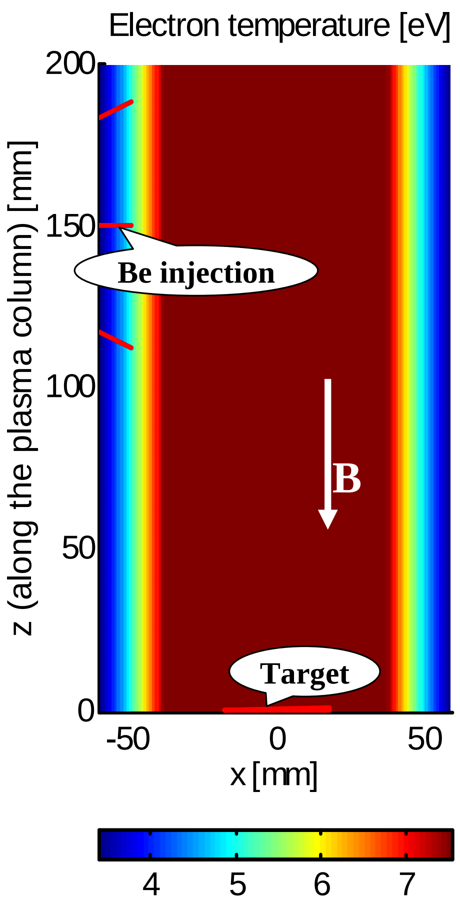
Examples of ERO application

Plasma parameters at PISCES-B

Electron density [cm^{-3}]



Electron temperature [eV]



- Plasma column width is about **5cm**
- Vessel radius is about **20cm** filled with neutral gas
- Be comes into the volume from injection or (and) as a result of Be target erosion

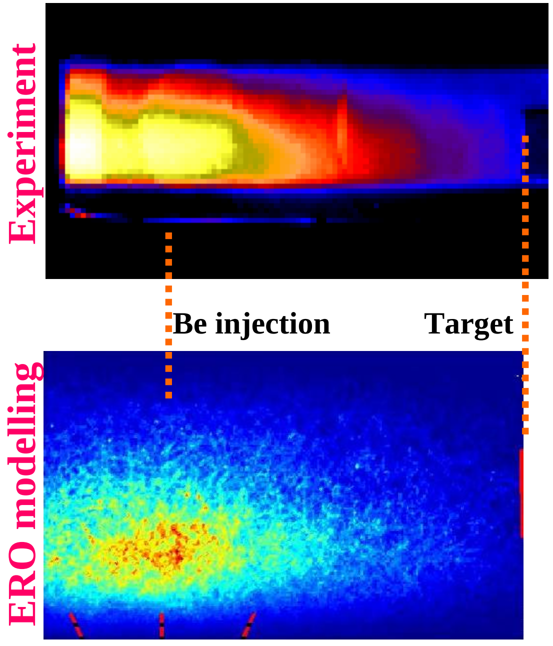
Be spectroscopy at PISCES

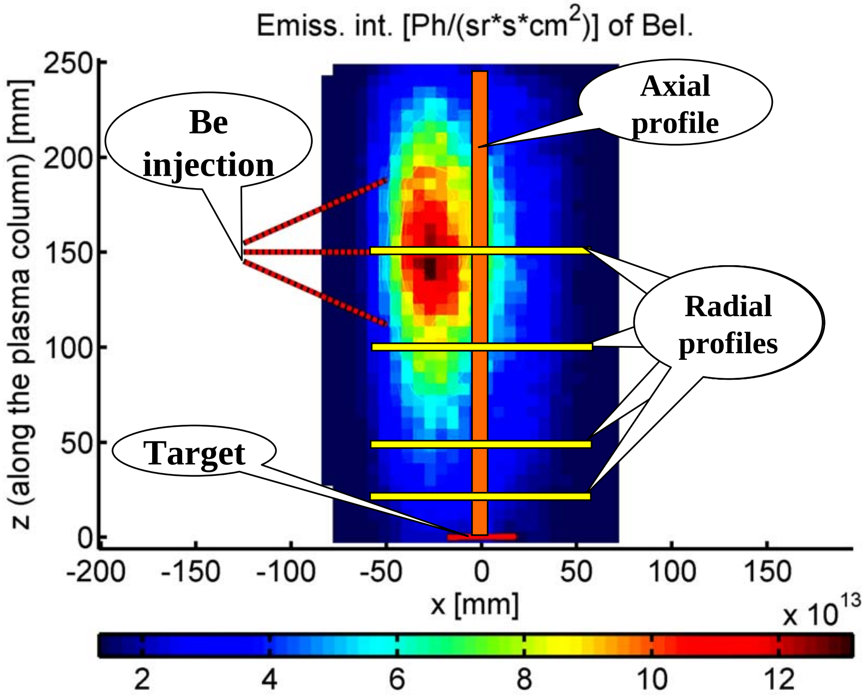
BeI, BeII emission is registered:

by 2D camera

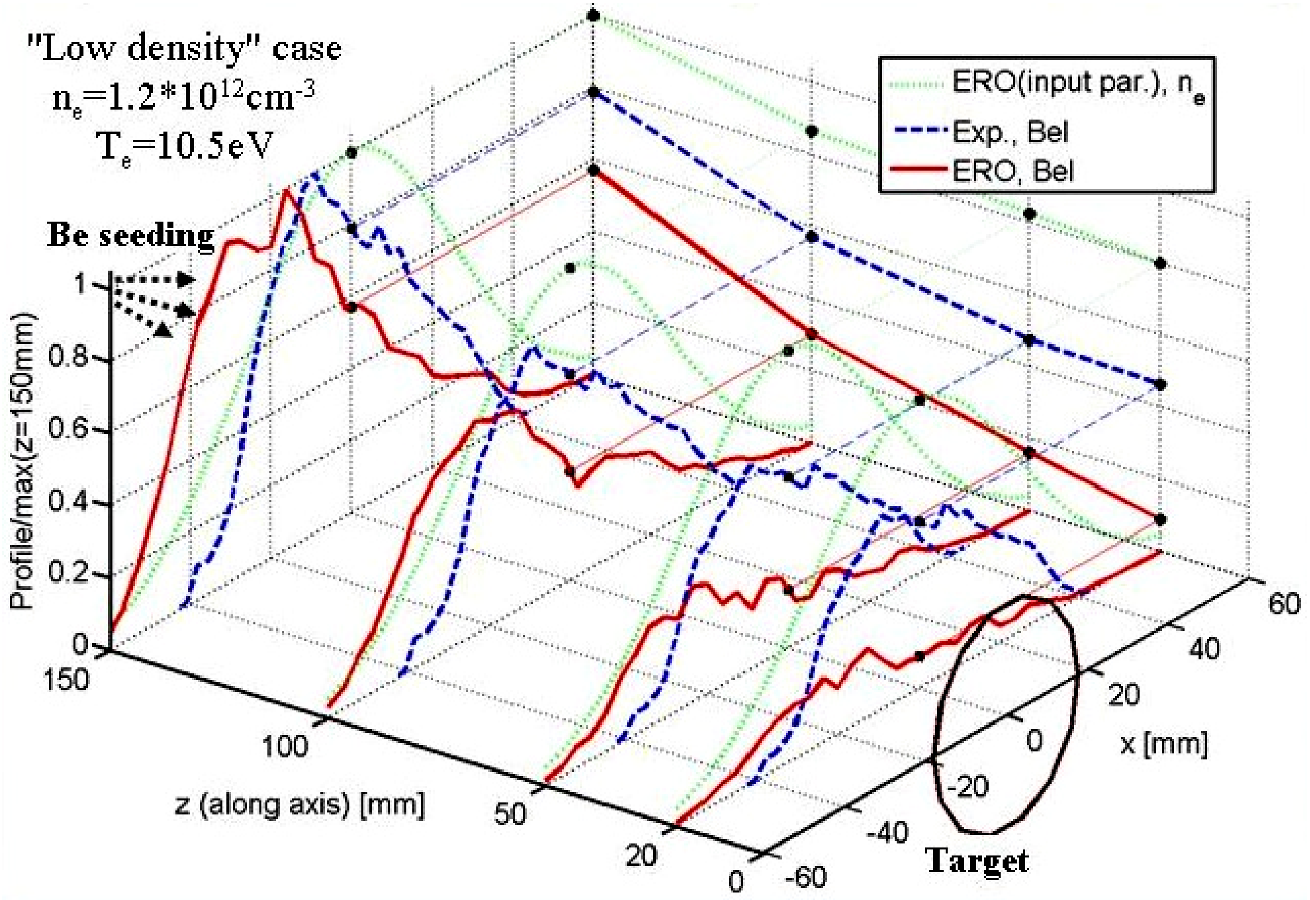
"Low density case"
($1.2*10^{12}cm^{-3}$, T_e=10.5eV)

by spectrometer with a spatial resolution (the radial profile position and direction can be varied)





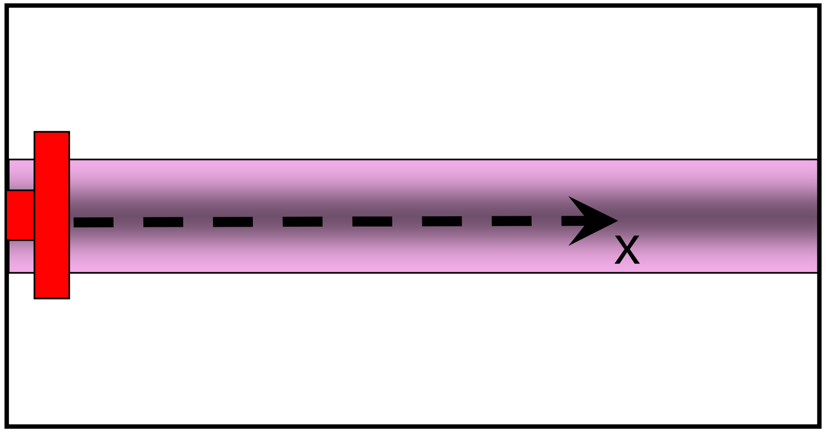
Neutral Be emission 457nm (injection)



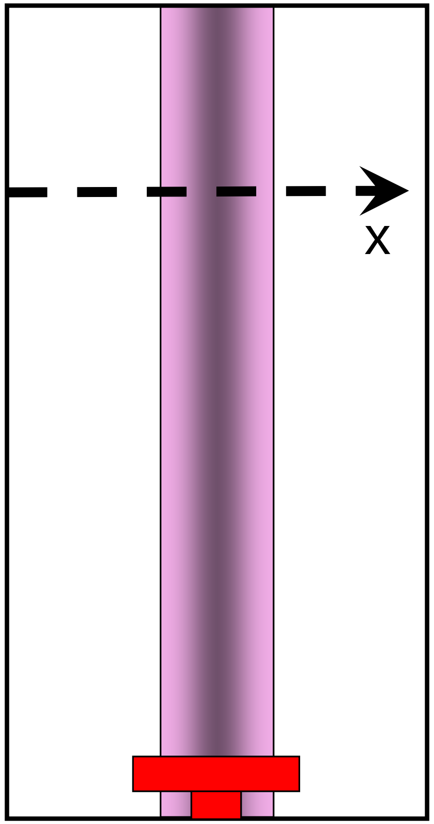
The ERO modelling is in a good agreement with experiment (PSI-2008)

Profiles direction - illustration

Be sputtering from target



Be injection cross plasma

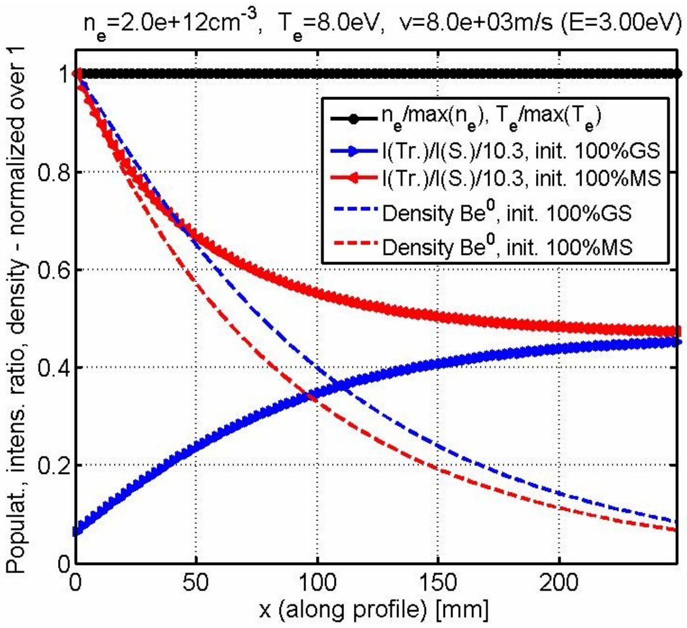


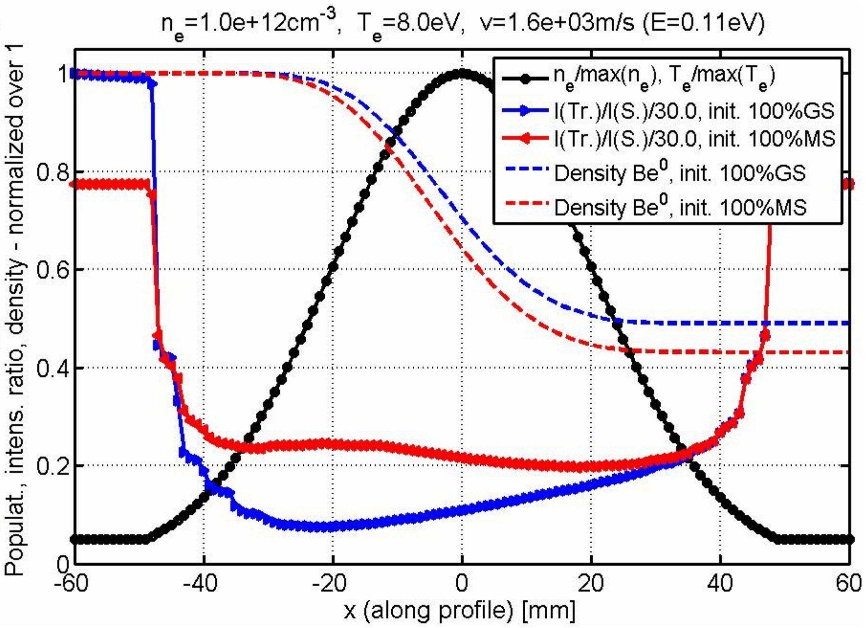
MS implementation into ERO – effect illustration

A narrow monoenergetic beam of Be^0, comming through plasma.

Relevant for sputtering
from Be target . . .

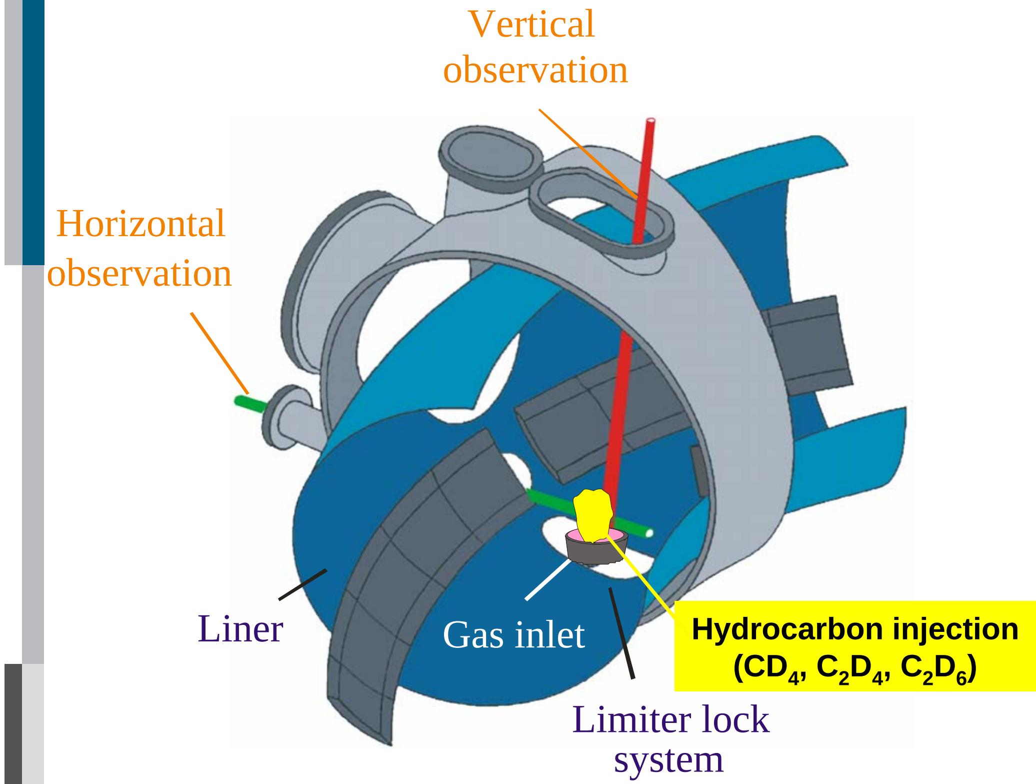
Relevant for seading
from Be oven . . .





Initial MS population and plasma parameters gradient strongly affect:
1) Triplet/singlet line intensity ratio (4573A and 3322A)
2) Be^0 density (MS population affects ionization)

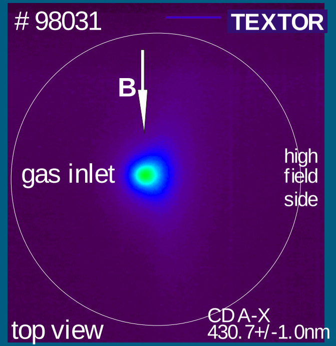
Modelling of experiments with nozzle

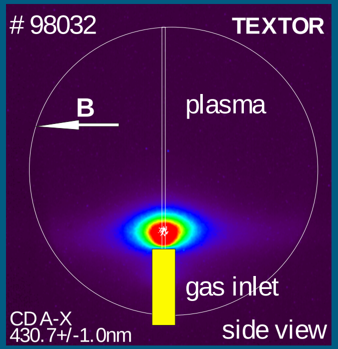


$$\left[\frac{D}{XB}\right]_{A\text{-}X}^{CD_4\rightarrow CD} = \frac{\Gamma_{CD_4}}{\phi_{A\text{-}X}^{CD}}$$

CD light emission

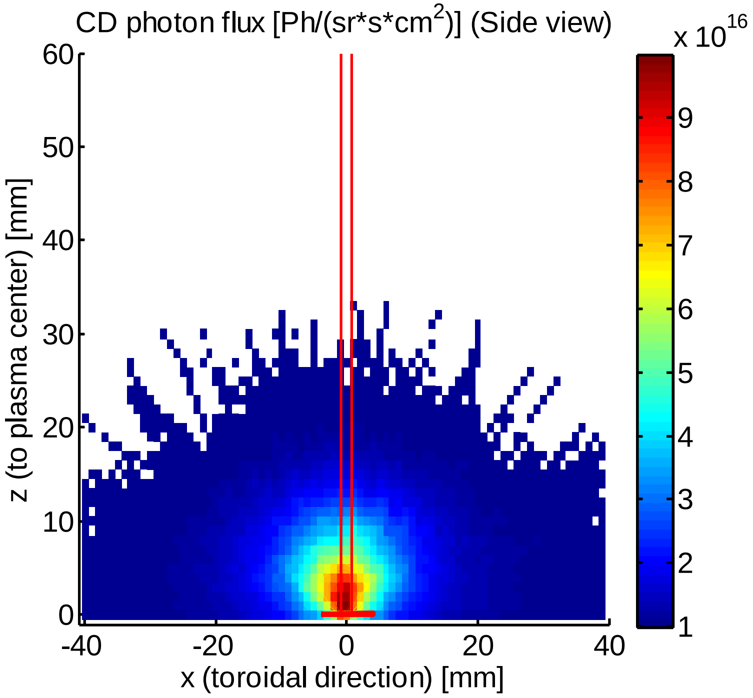
(CD_4 injection)

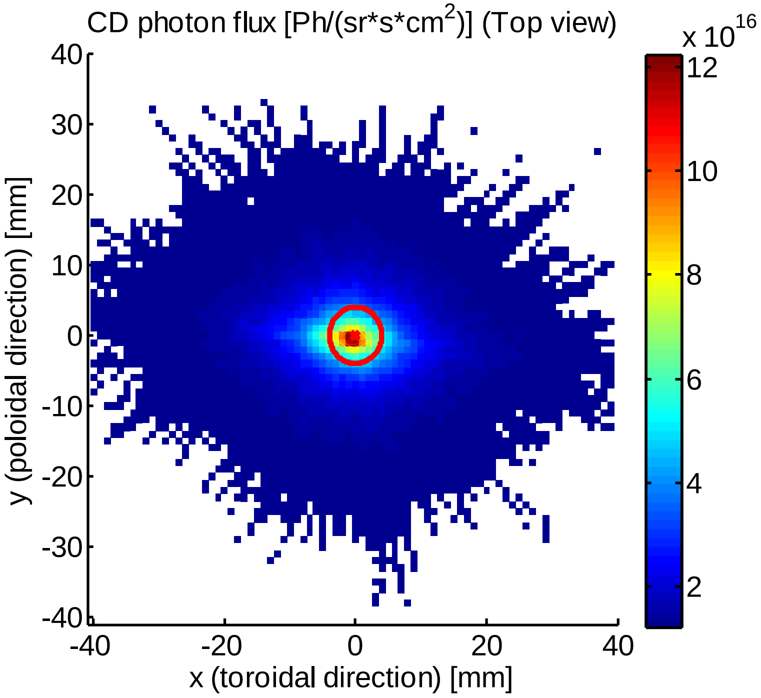




Modelling of experiments with nozzle

Modelled 2D light emission of CD A-X band from CD_4 injection at TEXTOR

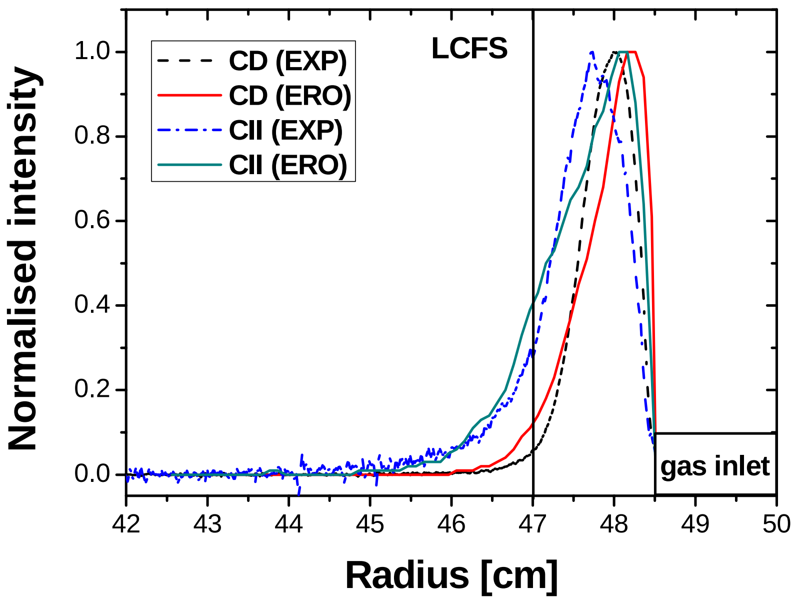




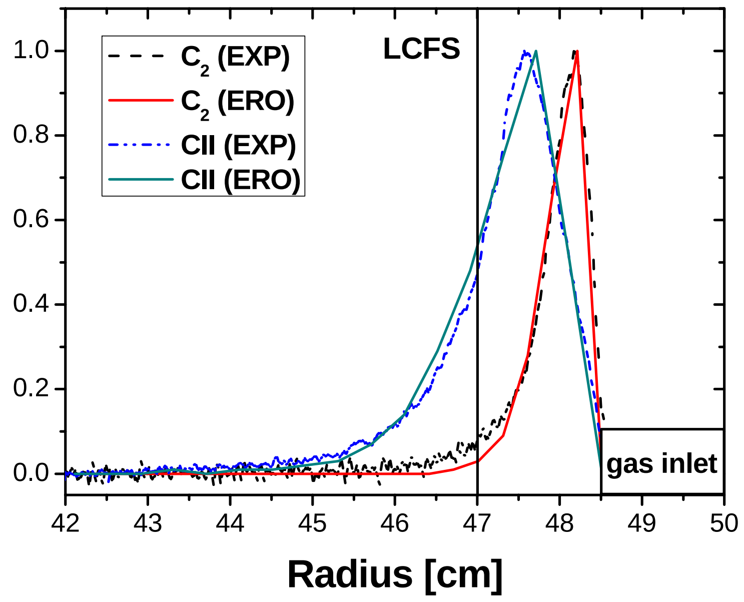
LCFS at 15 mm above inlet tip
T_e (LCFS) = 55 eV

Modelling of experiments with nozzle

Modelling vs. experiment: radial profiles of CD, C_2 and CII emission



CD_4 injection



C_2D_4 injection

Good agreement between modelled and observed penetration depths

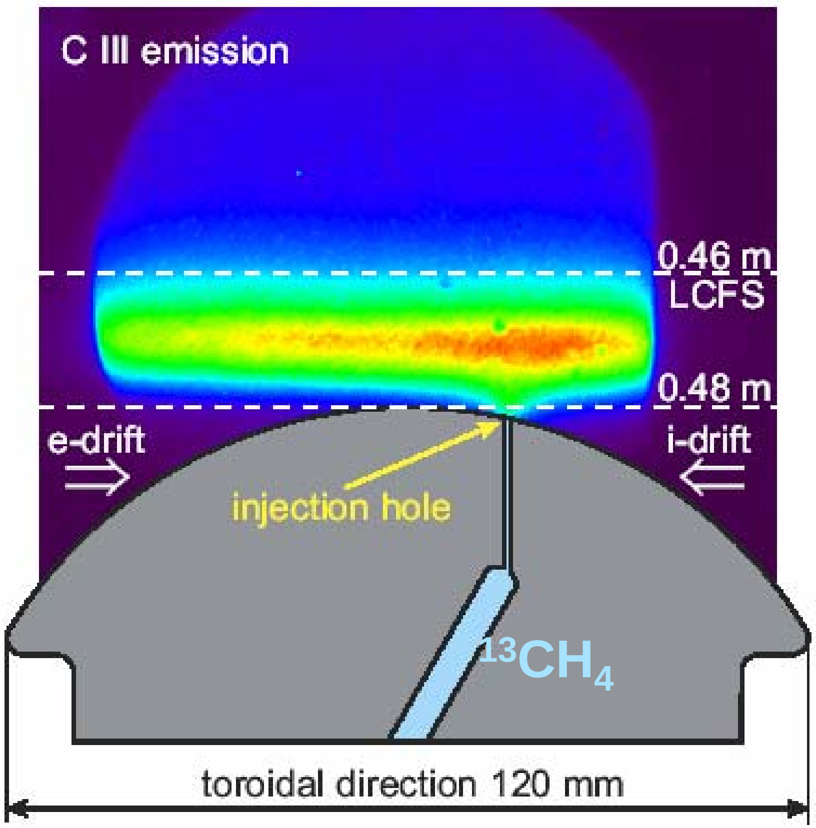
Modelling of experiments with nozzle

Comparison of effective D/XB values for CD A-X and C_2 d-a

Injected species	D/XB (CD A-X band)		D/XB (C_2 d-a band)	
	Experiment	**ERO**	**Experiment**	**ERO**
CD_4	36	65	930	-
C_2D_4	31	80	48	45
C_2D_6	27	76	65	62

Modelling of experiments with spherical limiters

$^{13}CH_4$ injection experiments: deposition and erosion of carbon layers



A. Kreter

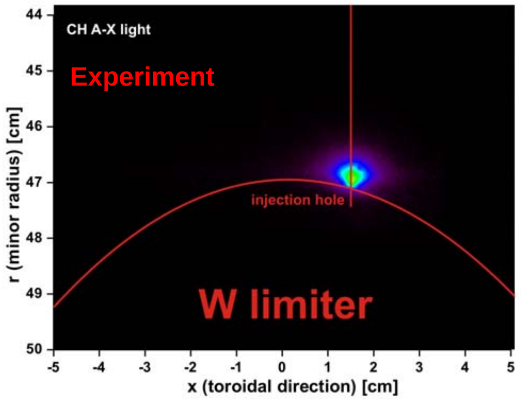
-In-situ observation of light emission above test limiter (dissociation products of CH_4).

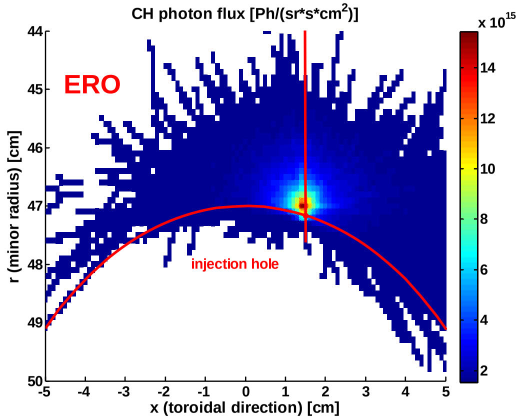
- Post-mortem surface analysis of ^{13}C (and ^{12}C) deposition.

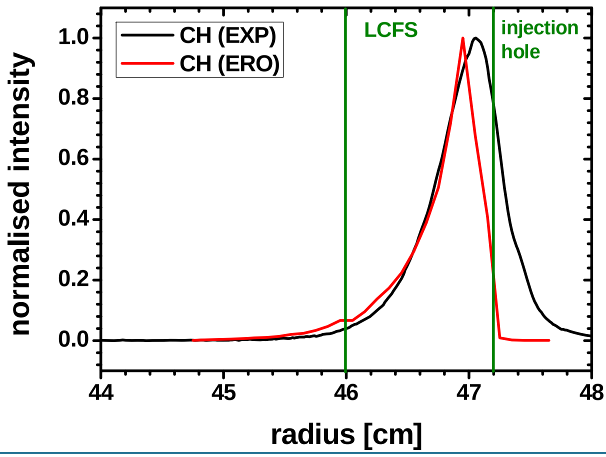
Spherical limiters – spectroscopy patterns

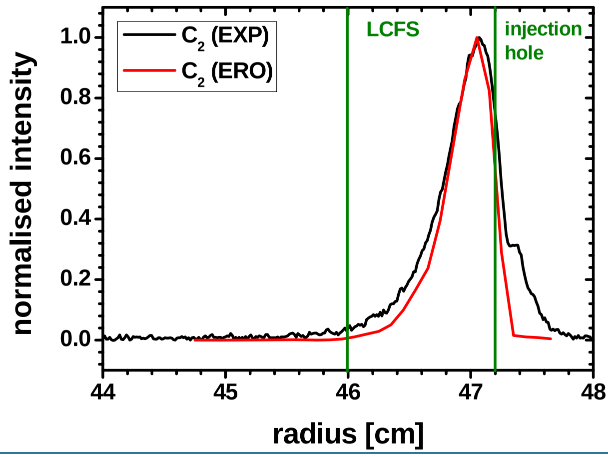
Comparison of light emission: benchmark for n_e, T_e

$^{13}C_2H_4$ injection









Modelling of experiments with spherical limiters

Injection of $^{13}C_2H_4$ and $^{13}CH_4$ through C and W limiters
^{13}C deposition measured by NRA

W

R_{dep}=1.2%

R_{dep}=0.8%

C

R_{dep}=2.1%

R_{dep}=1.7%

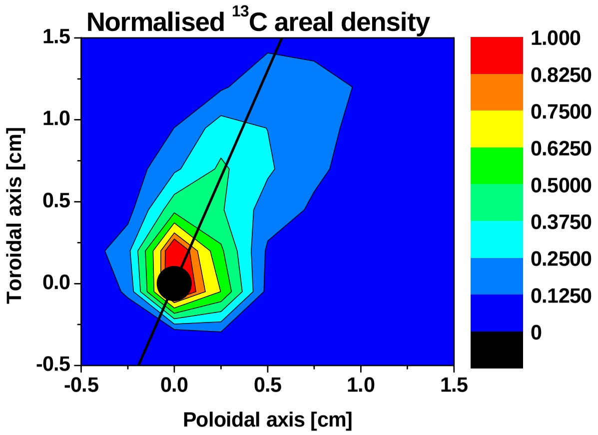
$$\text{Local } ^{13}\text{C deposition efficiency } R_{dep} = \frac{\textit{Locally deposited } ^{13}\text{C}}{\textit{injected } ^{13}\text{C}}$$

R_{dep} is higher for $^{13}C_2H_4$ than for $^{13}CH_4$ and higher on C than on W limiter

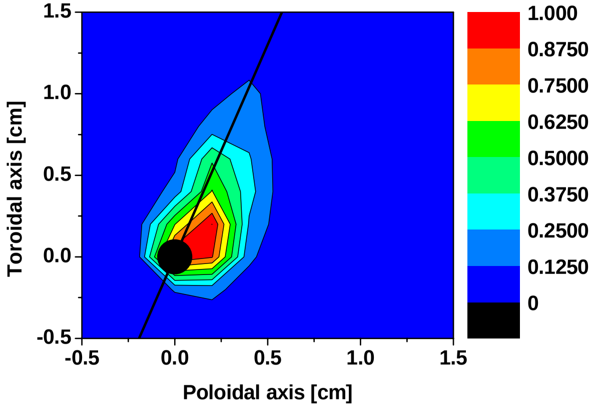
Modelling of experiments with spherical limiters

$^{13}CH_4$ injection through graphite limiter

Experiment

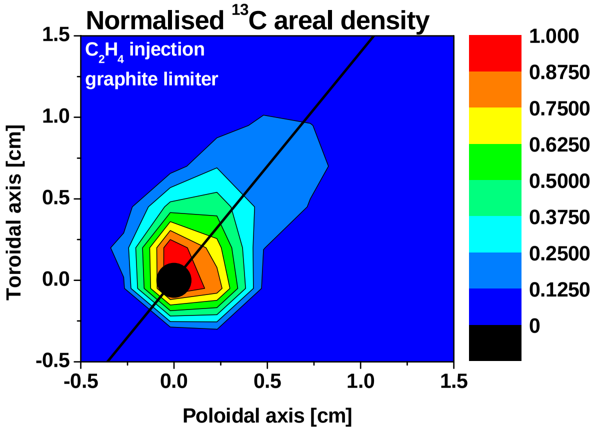

Normalised ^{13}C areal density

Modelling

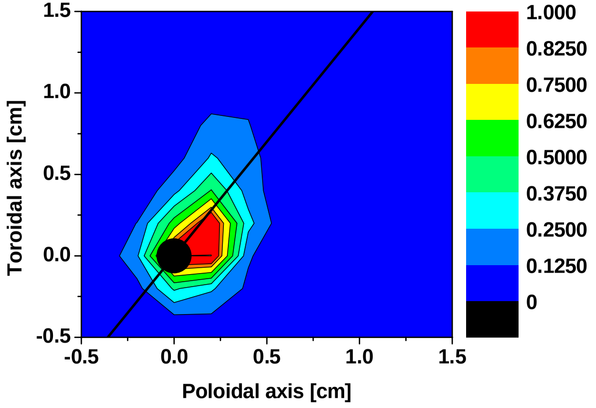


$^{13}C_2H_4$ injection through graphite limiter

Experiment


Normalised ^{13}C areal density

Modelling

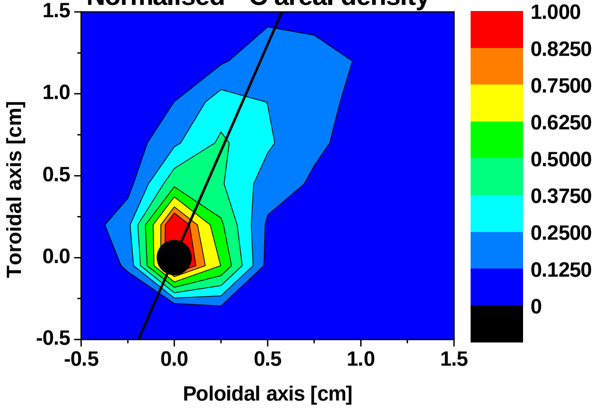


Modelling of experiments with spherical limiters

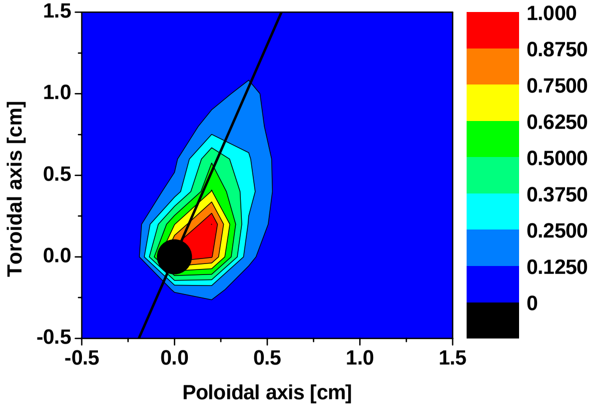
$^{13}CH_4$ injection through graphite limiter

Experiment

Normalised ^{13}C areal density



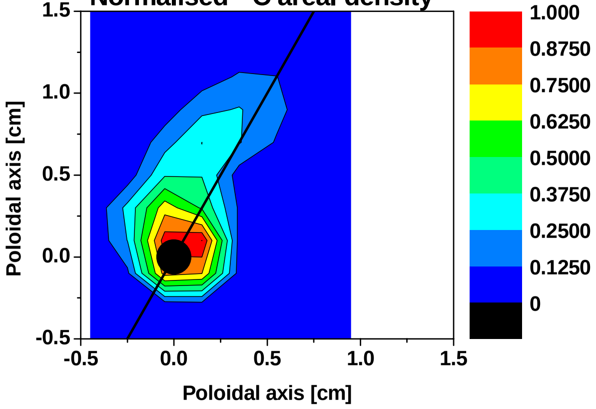
Modelling



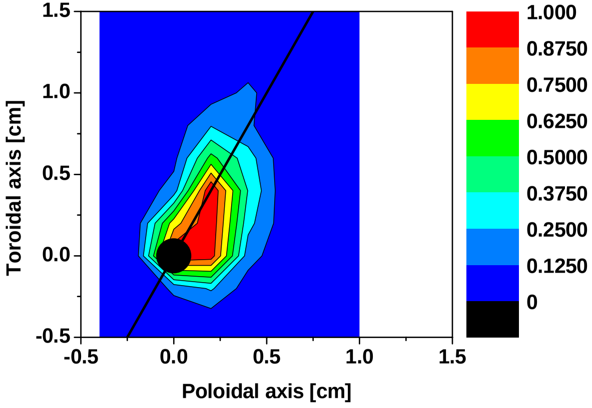
$^{13}CH_4$ injection through tungsten limiter

Experiment

Normalised ^{13}C areal density



Modelling



Spherical limiters – deposition efficiency

$$\text{Local } {}^{13}\text{C deposition efficiency } R_{dep} = \frac{\textit{Locally deposited } {}^{13}C}{\textit{injected } {}^{13}C}$$

Gas	Limiter	R_{dep}	
		Experiment	ERO
$^{13}CH_4$	C	1.7 %	1.9 %
	W	0.8 %	1.1 %
$^{13}C_2H_4$	C	2.1 %	2.3 %
	W	1.2 %	1.3 %

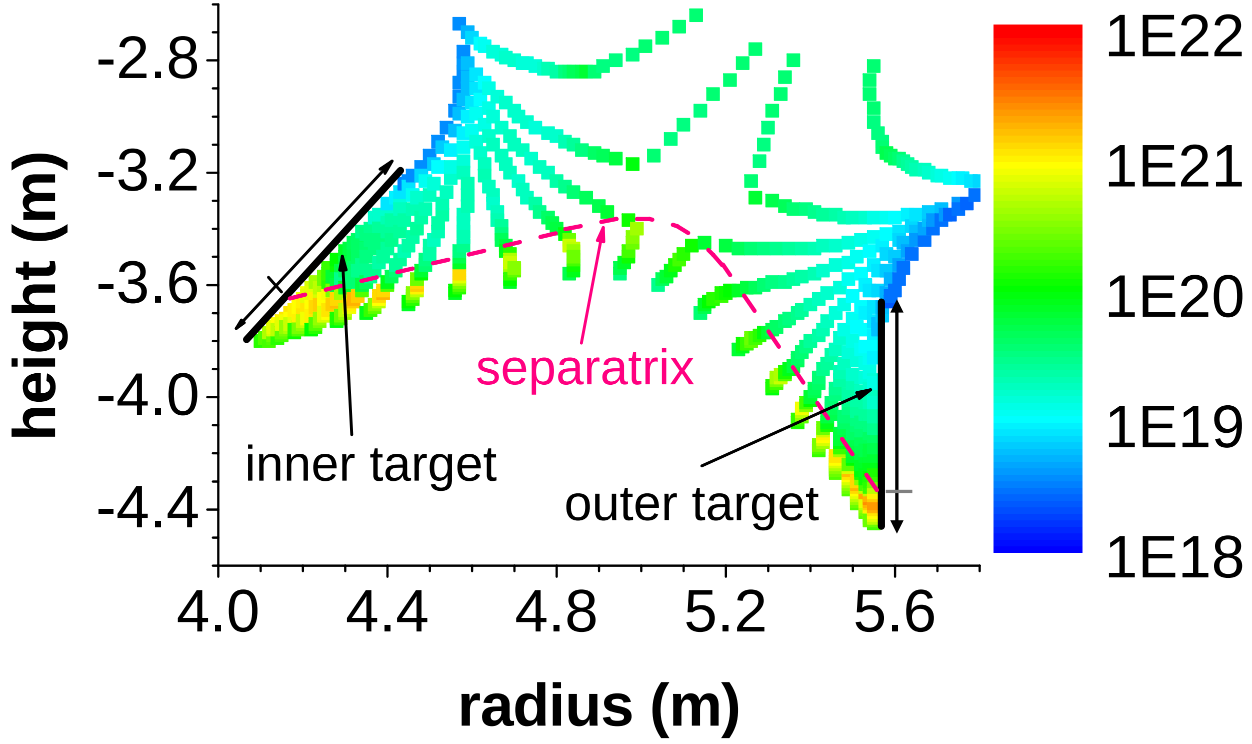
$S_{eff} = 0.15$
$Y_{enh} = 15\%$

- Good agreement between experiment and modelling
- The dependency on substrate material and gases on R_{dep} is reproduced with ERO

ITER availability

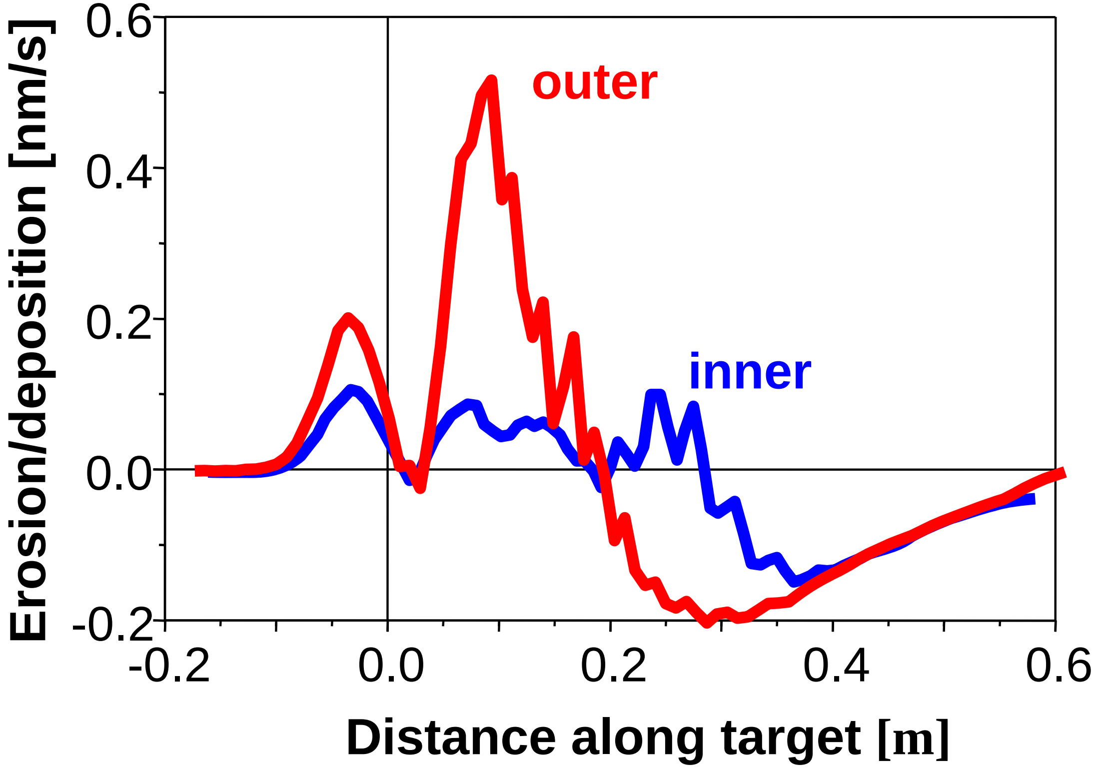
ERO for ITER – plasma parameters

B2-EIRENE simulations



ERO: life time of ITER divertor plates

ERO modelling of target erosion (0.1% of Be)

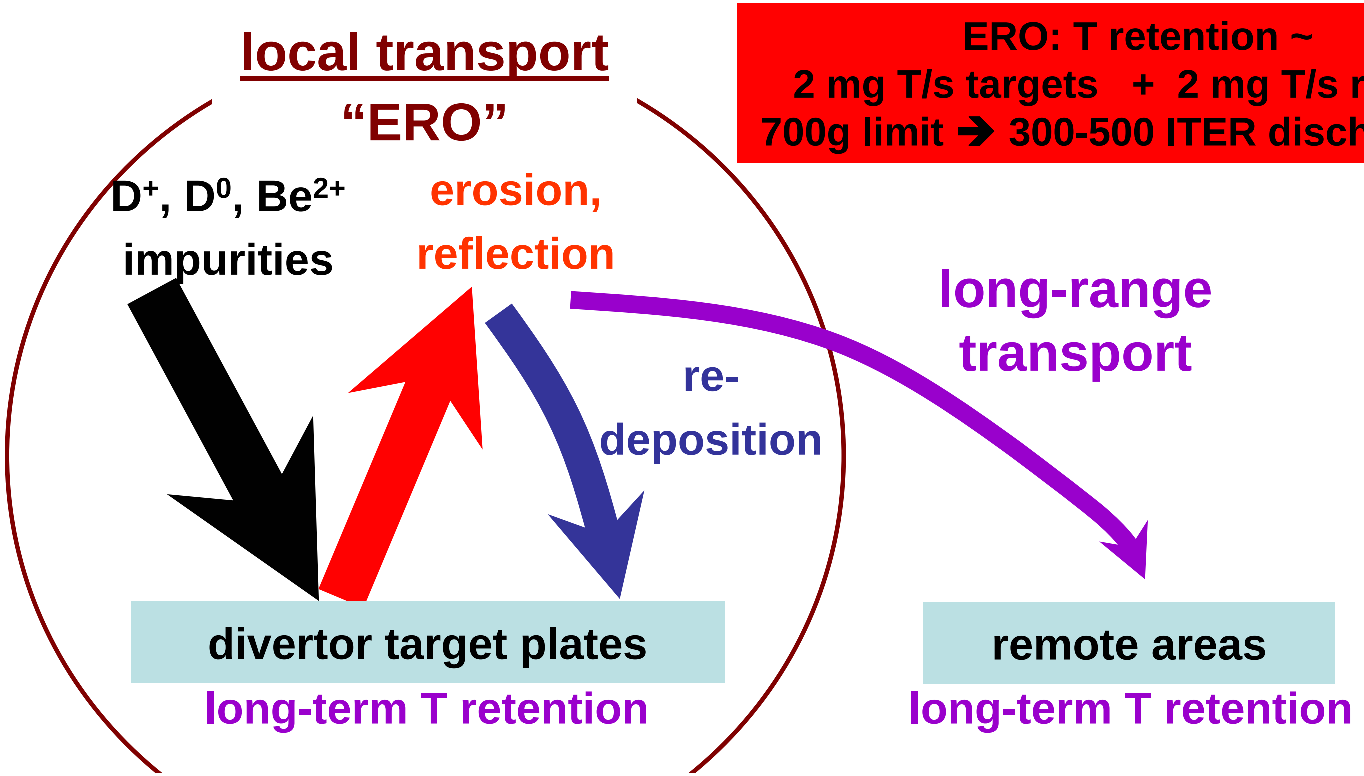


Target plates (0.5 cm) should survive at least 6900 discharges

Sweeping of strike point can increase lifetime

ERO: tritium retention in ITER

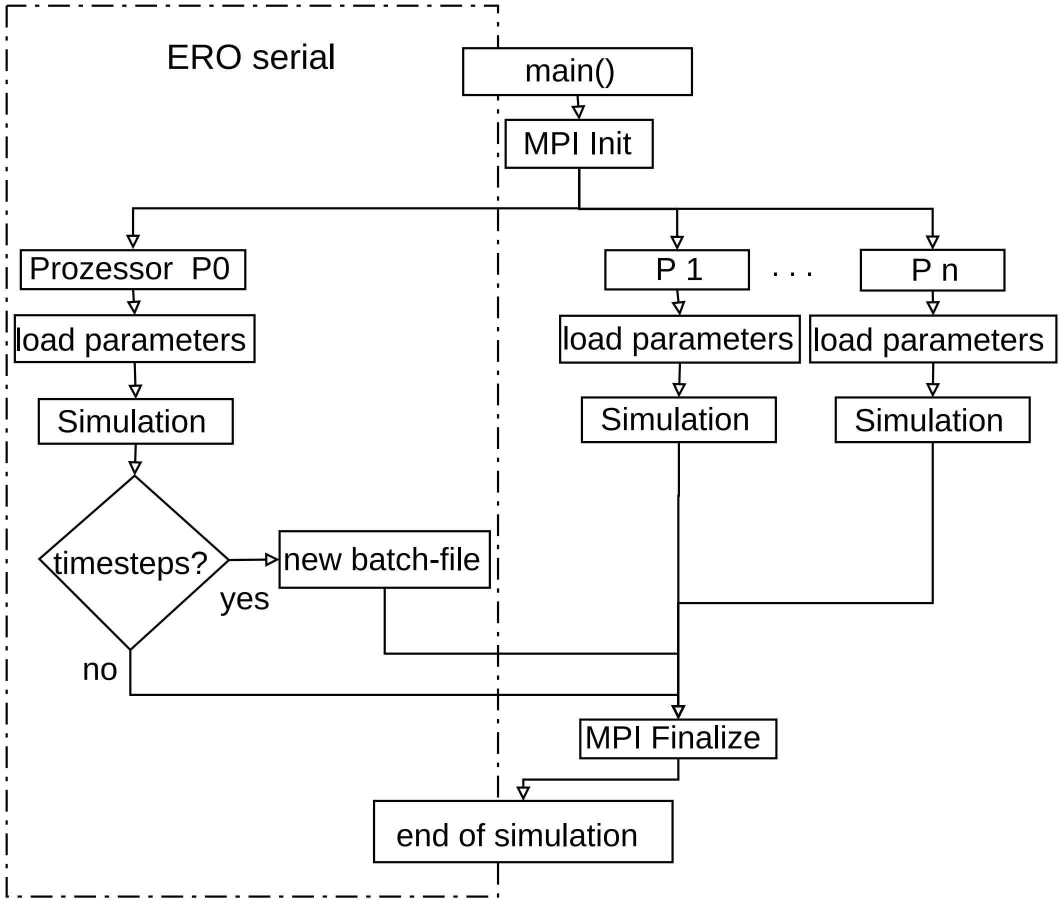
ERO: T retention ~
2 mg T/s targets + 2 mg T/s remote
700g limit ➔ 300-500 ITER discharges?!



ERO:
- local transport near to divertor plates
- background plasma as input (B2 Eirene)
- layer formation (C and Be) ⇒ T retention using T/C, T/Be

Technicalities

Parallelization: parametric (MPI)



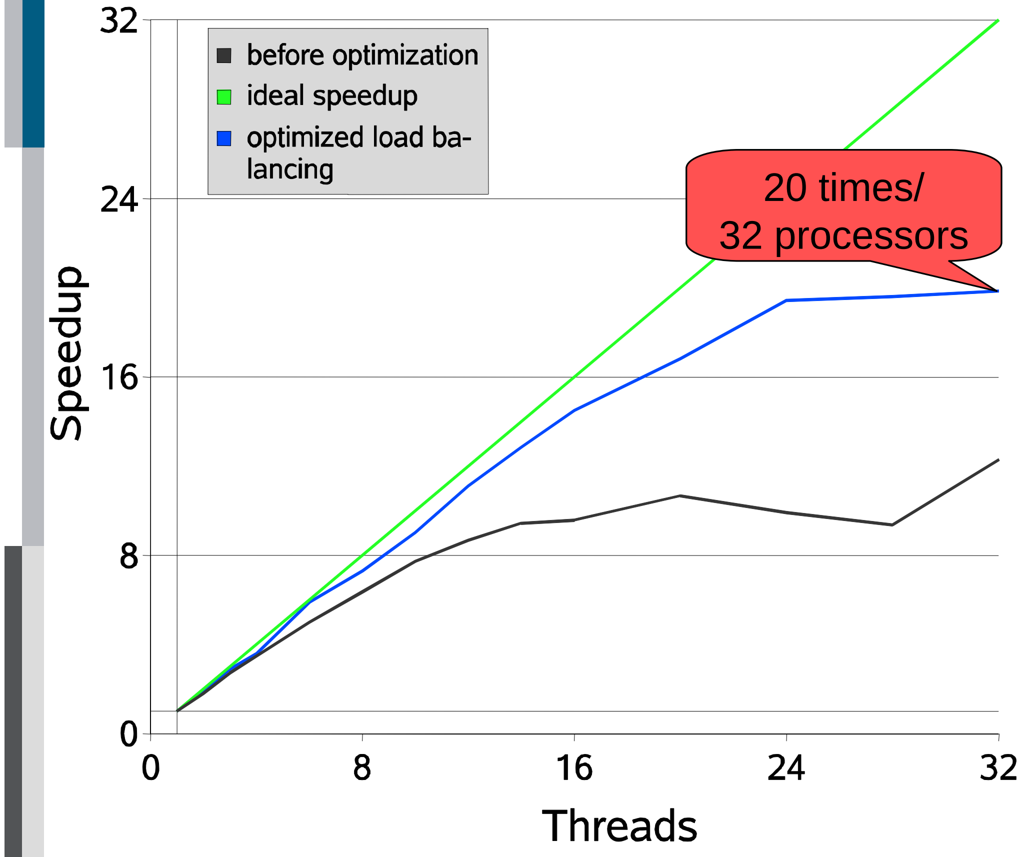
N ERO runs are substituted by 1 run on N processors ***(calculation time remains the same!)***

Each processor gets modified parameter file, working directory, generates all usual ERO output files.

For automatization a special **“starter”** program is developed

Data exchange between processors is minimal – MPI (message passing interface) is optimal

Parallelization: shared memory



Speedup comparison

Processors get portions (“chunks”) of MC test particles for calculation

Particles are not fully independent!

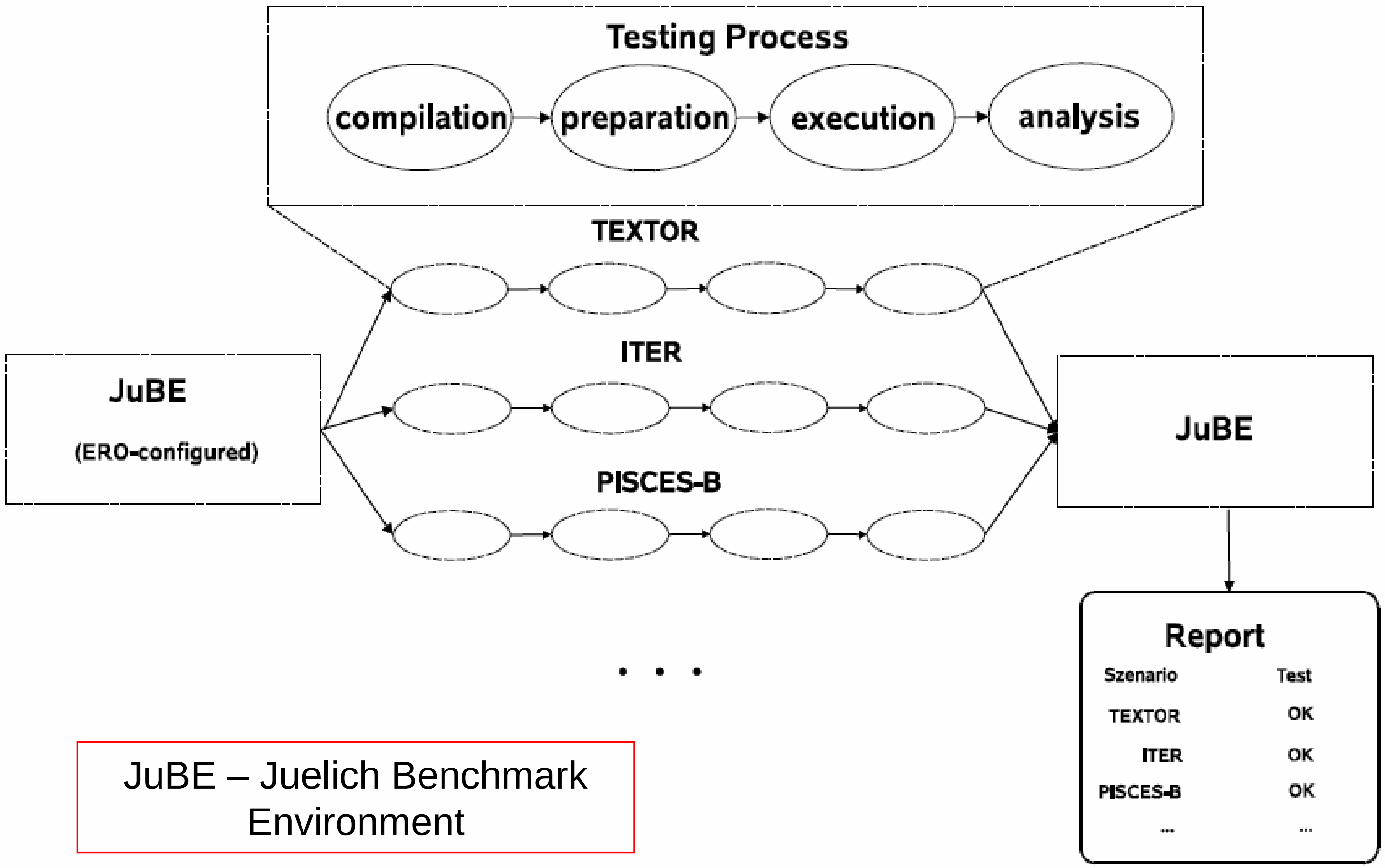
They change the volume and surface meshes (occupying most part of memory used by ERO)

Shared memory (OpenMP) approach is optimal

<u>Optimization:</u>

- Minimization of serial part
- Processor load balancing
- Cashe memory usage

Automatic testing system for ERO



Testing Process

compilation → preparation → execution → analysis

JuBE
(ERO-configured)

TEXTOR

ITER

PISCES-B

• • •

JuBE

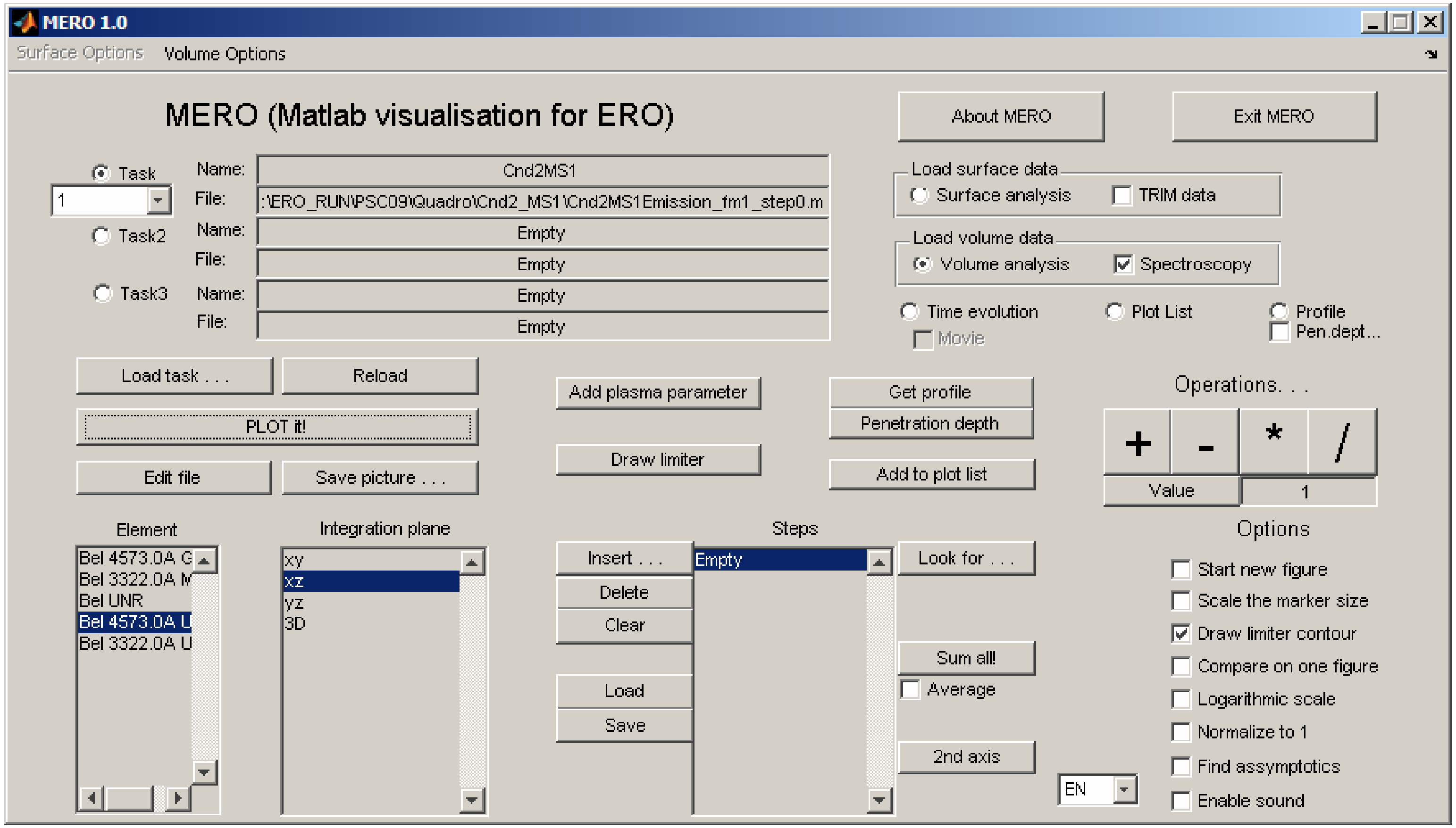
Report

Szenario	Test
TEXTOR	OK
ITER	OK
PISCES-B	OK
...	...

JuBE – Juelich Benchmark Environment

Visualization: MERO

(Matlab visulalization GUI for ERO)



MERO 1.0

MERO (Matlab visualisation for ERO)

● Task: 1
Name: Cnd2MS1
File: :\ERO_RUN\PSC09\Quadro\Cnd2_MS1\Cnd2MS1Emission_fm1_step0.m

○ Task2
Name: Empty
File: Empty

○ Task3
Name: Empty
File: Empty

Load surface data: ○ Surface analysis ☐ TRIM data

Load volume data: ● Volume analysis ☑ Spectroscopy

○ Time evolution ☐ Movie ○ Plot List ○ Profile ☐ Pen.dept...

Element: Bel 4573.0A G, Bel 3322.0A M, Bel UNR, Bel 4573.0A U (selected), Bel 3322.0A U

Integration plane: xy, xz (selected), yz, 3D

Steps: Empty (selected)

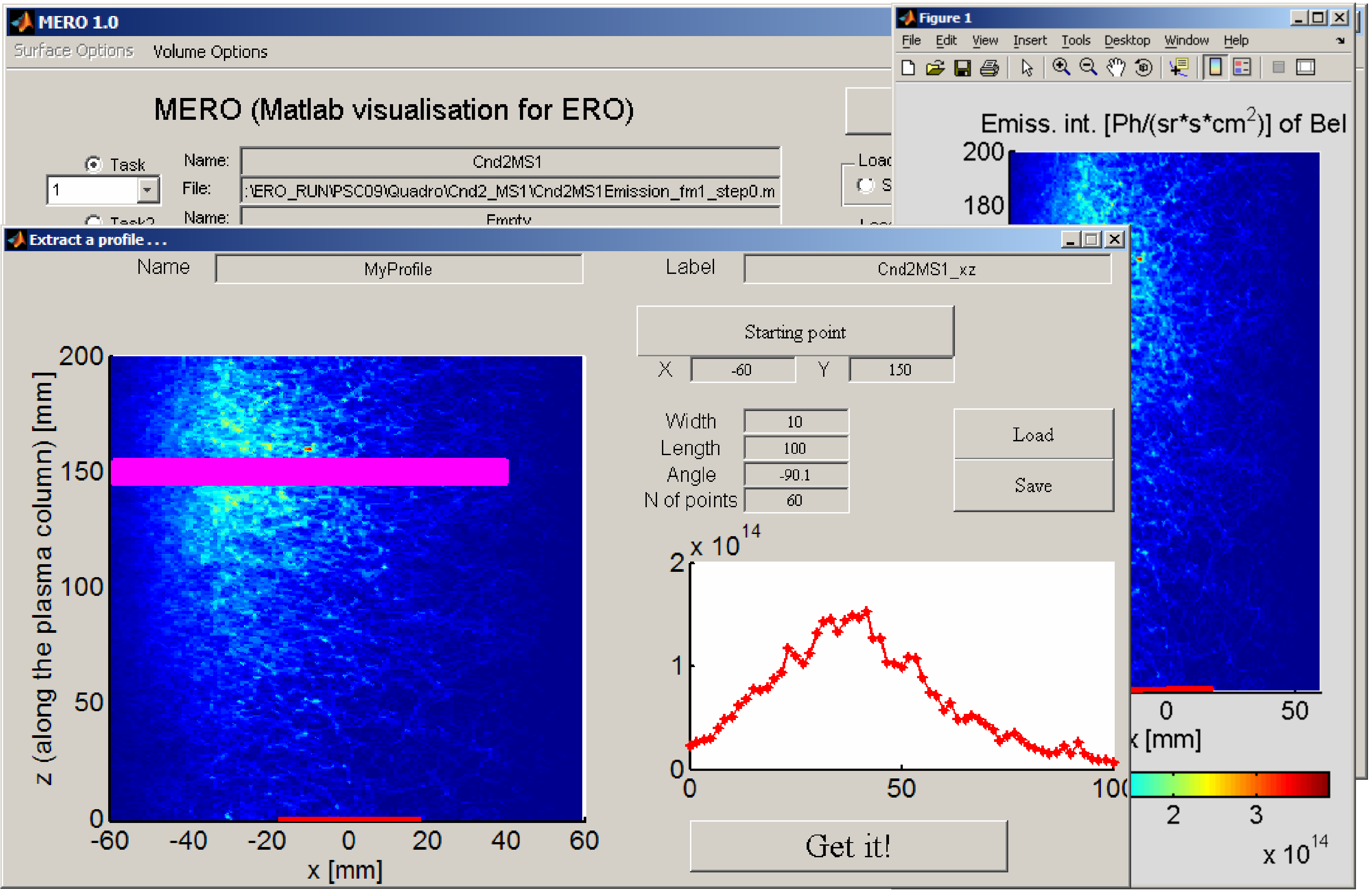
Value: 1

Options:
- ☐ Start new figure
- ☐ Scale the marker size
- ☑ Draw limiter contour
- ☐ Compare on one figure
- ☐ Logarithmic scale
- ☐ Normalize to 1
- ☐ Find assymptotics
- ☐ Enable sound

☐ Average

EN

Visualization: MERO



MERO (Matlab visualisation for ERO)

Name: Cnd2MS1

File: :\ERO_RUN\PSC09\Quadro\Cnd2_MS1\Cnd2MS1Emission_fm1_step0.m

Name: Empty

Name: MyProfile

Label: Cnd2MS1_xz

Starting point X: -60 Y: 150

Width: 10

Length: 100

Angle: -90.1

N of points: 60

In spite of a summary . . .

How important is ADAS for ERO?

1) **Ionization/recombination** processes directly influence the particle **transport** in plasma.

2) For some species (e.g. H) **opacity** is not zero – radiation is an energy **transport channel**.

3) Spectroscopy gives **indispensable information** for model **benchmarking** (both qualitative and quantitative).

End

University of
Strathclyde
Glasgow

Heavy Species in ADAS

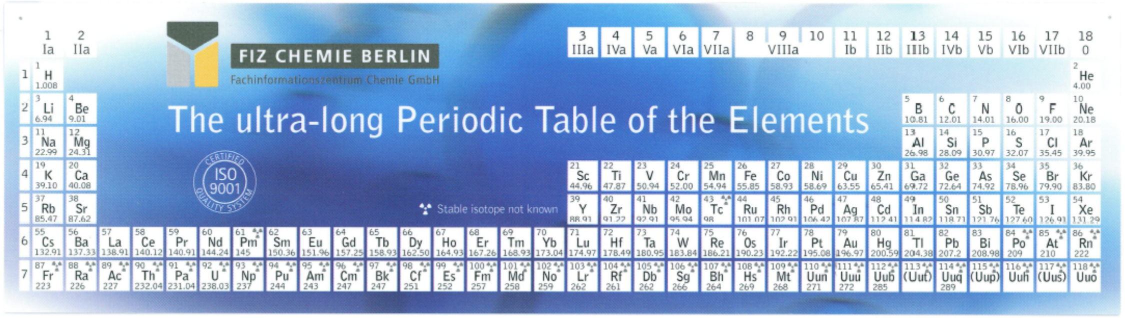
from the viewpoint of one lowly ion

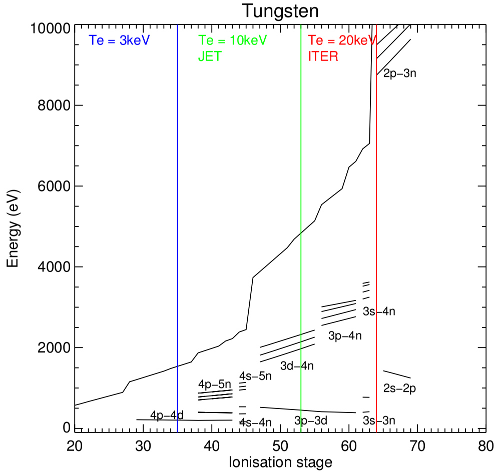
Martin O’Mullane, Adam Foster, Hugh Summers and Allan Whiteford

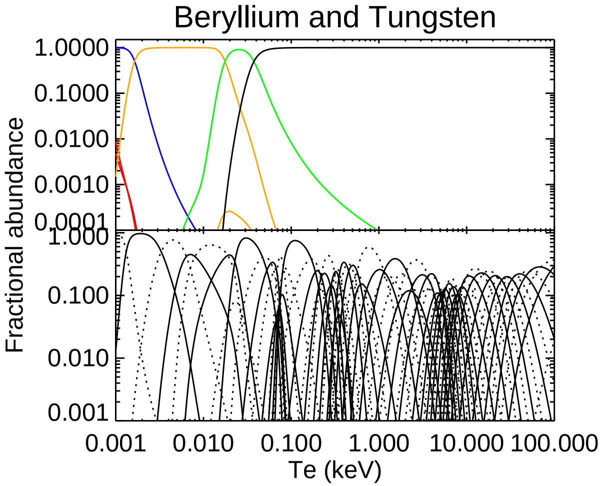
Department of Physics
University of Strathclyde

ADAS-EU Training Course, IPP Garching, 14-Oct-2009

Atomic data requirements







Three aspects of the heavy species question

The data we need

- Source functions — *adf11* acd, scd, ccd
- Power coefficients — *adf11* plt, prb
- Line emission — *adf15* pec
- Spectral feature emission — *adf40* f-pec

How to get it

- Scoping the problem
- Automated generation

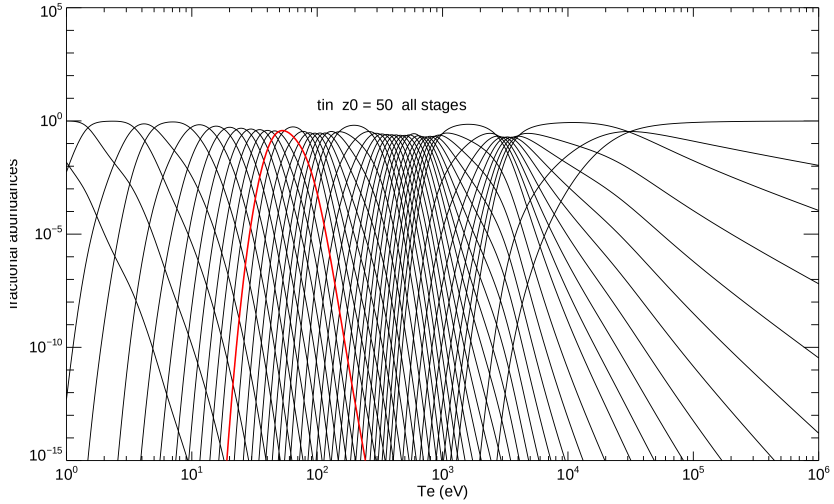
How to use it

- Potentially large datasets
- Partitioning and superstaging.

Let’s choose tin (Z=50)

First questions: Where do its stages radiate? And what if there is no helpful ADAS *adf11* data?

```
preview_natural_partition, z0=50, plot_type=3,   $
                           te_min=1, te_max=1e6, $
                           te_plot=1000,         $
                           frac=frac
oplot, frac.te, frac.ion_all[13,*], color=5, thick=5
```



Now let’s narrow our focus to Sn^{13+}

- What is its ground state configuration?
- What configurations contribute to spectral emission?
- And to radiated power?
- How do we choose which ones to include?

The *adf00* set archives ionisation potential and ground configurations:

```
tin              -50
 0 7.343d+00 1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d10 4f0  5s2  5p2
 1 1.463d+01 1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d10 4f0  5s2  5p1
                          ..
                          ..
12 2.744d+02 1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d2
13 2.995d+02 1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d1
14 3.959d+02 1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6
                              ..
```

What configurations should be considered?

With a ground state of $3d^{10}4s^{2}4p^{6}4d^{1}$ we can

- promote the valence 4d electron to any higher *nl* shell
- allow 4s or 4p electrons to be excited
- or any other electron — from 2p perhaps?
- however where do we stop in Δn or Δl?
- and how many configurations should we consider?

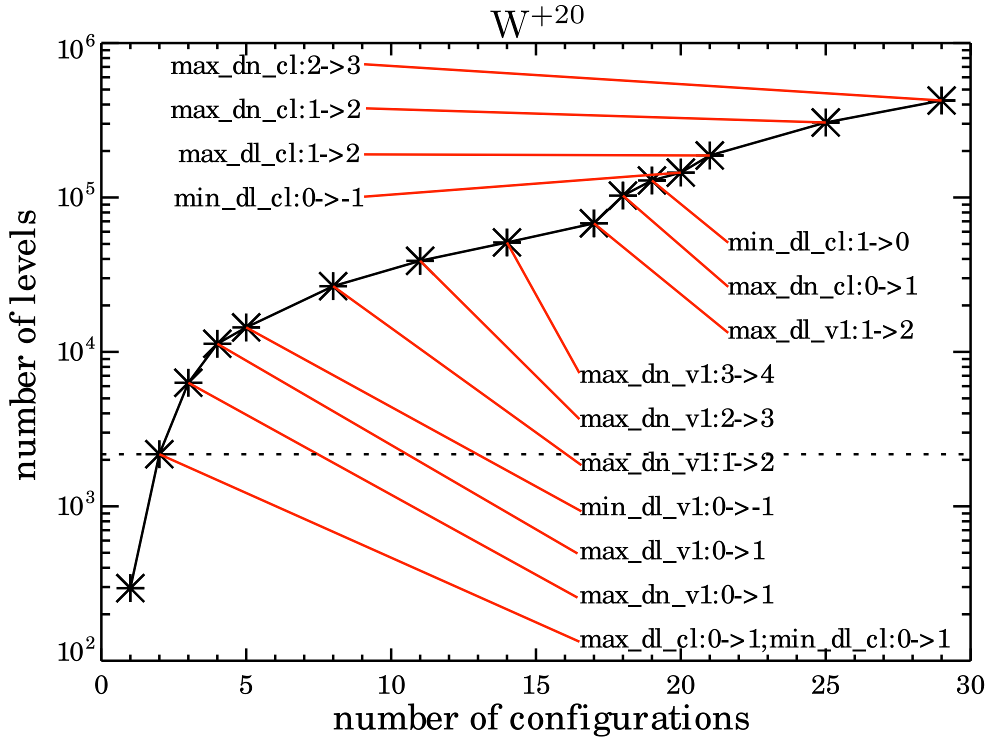
There are 180 distinct ground configurations (for elements up to Radon)

A rule based method is desirable (essential!)

ADAS rules for choosing where to promote electrons

index[]	:	index of ground configuration of each ion of element in *adf54* file
config[]	:	ground configuration for each ion of element
n_el[]	:	number of electrons for each ion of element
no_v_shl[]	:	number of open (valence) shells. Include outer-most shell even if closed.
max_dn_v1[]	:	maximum Δn promotion for first (outer-most) valence shell.
min_dn_v1[]	:	minimum Δn promotion for first (outer-most) valence shell.
		Negative value allows access to inner unoccupied or open shells
max_dl_v1[]	:	maximum delta Δl promotion for first (outer-most) valence shell.
min_dl_v1[]	:	minimum delta Δl promotion for first (outer-most) valence shell.
max_dn_v2[]	:	maximum Δn promotion for second (inner-most) valence shell.
min_dn_v2[]	:	maximum Δn promotion for second (inner-most) valence shell.
max_dl_v2[]	:	maximum delta Δl promotion for second (inner-most) valence shell.
min_dl_v2[]	:	minimum delta Δl promotion for second (inner-most) valence shell.
prom_cl[]	:	promote from inner shell closed shells (1=yes,0=no).
max_n_cl[]	:	maximum inner shell n from which promotions are permitted.
min_n_cl[]	:	minimum inner shell n from which promotions are permitted.
max_l_cl[]	:	maximum inner shell l from which promotions are permitted.
min_l_cl[]	:	minimum inner shell l from which promotions are permitted.
max_dn_cl[]	:	maximum Δn promotion from a permitted inner shell.
min_dn_cl[]	:	minimum Δn promotion from a permitted inner shell.
		Negative values of Δn allow access to inner unoccupied or open shells.
max_dl_cl[]	:	maximum Δl promotion from a permitted inner shell.
min_dl_cl[]	:	minimum Δl promotion from a permitted inner shell.
fill_n_v1[]	:	add all nl configurations of outer valence shell n (1=yes,0=no).
fill_par[]	:	if *n_fill* only add opposite parity to valence shell else add both parities (1=yes, 0=n0).
for_tr_sel[]	:	Cowan option for radiative transitions 1 - first parity, 2 or 3(default).
last_4f[]	:	shift an electron valence shell to unfilled 4f as extra ground.
grd_cmplx[]	:	include configurations of same complex as ground configuation for valence n-shell.

adf54 : rules for automatic data generation



Care needed!! resolved calculations (ic or LS) can overwhelm computers.

Work through Sn^{13+}

- Within ADAS the generation of heavy species data is almost exclusively a non-GUI activity.
- The outputs are standard *adf11, adf15* and *adf40* datasets which can be used and examined with the GUI interactive system.

At the IDL command line:

```
; Let's choose Sn13+

z_nuc = 50
z_ion = 13
tag   = xxesym(z_nuc, /lower) + string(z_ion, format='(i2.2)')

; Use promotion rules from W work

a54file = '/u/adas/adas/adf54/promotion_rules_w_adf54.dat'
```

```
adas8xx_promotion_rules, z0_nuc = z_nuc, z_ion = z_ion, ionpot = ip,  $
                         prom_rules=rules, a54file = file
help, rules, /st

** Structure <9b54e9c>, 25 tags, length=60, data length=60, refs=1:
   CONFIG       STRING '  1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d1'
   INDEX        INT          129
   NO_V_SHL     INT            1
   MAX_DN_V1    INT            3
   MIN_DN_V1    INT            0
   MAX_DL_V1    INT            2
   MIN_DL_V1    INT           -2
   MAX_DN_V2    INT            0
   MIN_DN_V2    INT            0
   MAX_DL_V2    INT            0
   MIN_DL_V2    INT            0
   PROM_CL      INT            1
   MAX_N_CL     INT            4
   MIN_N_CL     INT            4
```

```
MAX_L_CL      INT          1
MIN_L_CL      INT          0
MAX_DN_CL     INT          1
MIN_DN_CL     INT          0
MAX_DL_CL     INT          2
MIN_DL_CL     INT          0
FILL_N_V1     INT          1
FILL_PAR      INT          0
FOR_TR_SEL    INT          3
LAST_4F       INT          0
GRD_CMPLX     INT          0
```

```
adas8xx_promotions, z0_nuc = z_nuc, z_ion = z_ion, ionpot = ip,  $
                    prom_rules        = rules,                   $
                    promotion_results = results

help, results, /st

** Structure <9b530dc>, 11 tags, length=2496, data length=2496, refs=1:
   GRD_CFG         STRING    '4d1  '
   GRD_OCC         INT       Array[36]
   EX_CFG          STRING    Array[25]
   GRD_PAR         INT              0
   EX_PAR          INT       Array[25]
   GRD_ZC_COW      LONG               -14
   EX_ZC_COW       LONG      Array[25]
   OC_STORE        INT       Array[36, 26]
   NO_CONFIGS      LONG      Array[7]
   NO_TERMS        LONG      Array[7]
   NO_LEVELS       LONG      Array[7]
```

```
print, results.grd_occ
       2       2       6       2       6      10       2       6       1       0
       0       0       0       0       0       0       0       0       0       0
       0       0       0       0       0       0       0       0       0       0
       0       0       0       0       0       0
print, results.oc_store[*,1]
       2       2       6       2       6      10       2       6       0       1
       0       0       0       0       0       0       0       0       0       0
       0       0       0       0       0       0       0       0       0       0
       0       0       0       0       0       0
print, results.oc_store[*,2]
       2       2       6       2       6      10       2       6       0       0
       1       0       0       0       0       0       0       0       0       0
       0       0       0       0       0       0       0       0       0       0
       0       0       0       0       0       0
```

```
; Write CA driver files for restricted plasma parameters

files = { adf34_file    : ’adf34_ca_’ + tag + ’.dat’, $
          adf42_ca_file : ’adf42_ca_’ + tag + ’.dat’, $
          adf04_ca_file : ’adf04_ca_’ + tag + ’.dat’, $
          adf40_ca_file : ’adf40_ca_’ + tag + ’.dat’, $
          adf15_ca_file : ’adf15_ca_’ + tag + ’.dat’, $
          adf11_ca_file : ’adf11_ca_’ + tag + ’.dat’}

plasma = {theta         : [  1.0e3, 2.0e3, 5.0e3, 1.0e4, 1.5e4, $
                             2.0e4, 5.0e4, 1.0e5], $
          indx_theta    : indgen(8),
          rho           : [  1.0e8, 1.0e10, 1.0e12, 1.0e14],
          indx_rho      : indgen(4),
          npix          : [  128,   256],
          wvlmin        : [100.0,   1.0],
          wvlmax        : [150.0, 500.0],
          indx_wvl      : indgen(2),
          theta_noscale : 0,
          rho_scale     : 0
```

```
adas8xx_create_drivers, z0_nuc=z_nuc, z_ion=z_ion, ionpot=ip, $
                        promotion_results=results,           $
                        plasma=plasma, files=files
```

The driver file for ADAS801 (Cowan code):

```
2  -5    2   10  1.0    5.d-09    5.d-11-2  0130    1.0 0.65  0.0  0.5
   50  -14   Sn ground z1=13 0   4d1
   50  -14   Sn cfg 01       0   5s1
   50  -14   Sn cfg 02       0   5d1
   50  -14   Sn cfg 03       0   5g1
   50  -14   Sn cfg 04       0   6s1
   50  -14   Sn cfg 05       0   6d1
   50  -14   Sn cfg 06       0   6g1
   50  -14   Sn cfg 07       0   7s1
   50  -14   Sn cfg 08       0   7d1
   50  -14   Sn cfg 09       0   7g1
   50  -32   Sn cfg 10       0   3d10 4s1  4p6  4d2
   50  -32   Sn cfg 11       0   3d10 4s1  4p6  4d1  5s1
```

```
50  -32   Sn cfg 12       0   3d10 4s1  4p6  4d1  5d1
50  -32   Sn cfg 13       0   3d10 4s2  4p5  4d1  4f1
50  -32   Sn cfg 14       0   3d10 4s2  4p5  4d1  5p1
50  -32   Sn cfg 15       0   3d10 4s2  4p5  4d1  5f1
50  -14   Sn cfg 16       1   4f1
50  -14   Sn cfg 17       1   5p1
50  -14   Sn cfg 18       1   5f1
50  -14   Sn cfg 19       1   6p1
50  -14   Sn cfg 20       1   6f1
50  -14   Sn cfg 21       1   7p1
50  -14   Sn cfg 22       1   7f1
50  -32   Sn cfg 23       1   3d10 4s1  4p6  4d1  5p1
50  -32   Sn cfg 24       1   3d10 4s2  4p5  4d2
50  -32   Sn cfg 25       1   3d10 4s2  4p5  4d1  5d1
-1
```

Back to the IDL command line:

```
; Run the CA structure code

adas8xx_create_ca_adf04, z_ion,                                  $
                         z_nuc,                                  $
                         results.oc_store,                       $
                         ionpot           = ip,                  $
                         plasma           = plasma,              $
                         adf04_t3_file    = files.adf04_ca_file
```

adf04 **file for** Sn^{13+}

```
Sn+13        50        14        2415630.6
    1 19                   (0)0(     4.5)          0.0
    2 606527558529         (0)0(   134.5)     604454.8
    3 1B                   (0)0(     0.5)     656865.3
    4 1A                   (0)0(     6.5)     664371.3
    5 1C                   (0)0(     2.5)     810958.4
    6 1D                   (0)0(     4.5)    1048671.2
    7 606517568529         (0)0(    44.5)    1052972.9
    8 60652755851951A      (0)0(   419.0)    1259268.0
    9 1E                   (0)0(     6.5)    1290521.2
   10 1G                   (0)0(     0.5)    1291113.7
   11 1H                   (0)0(     2.5)    1366810.5
   12 1F                   (0)0(     8.5)    1400752.2
   13 60652755851951C      (0)0(   179.5)    1412966.0
   14 1I                   (0)0(     4.5)    1485688.9
   15 1J                   (0)0(     6.5)    1609362.8
   16 1M                   (0)0(     0.5)    1611744.1
   17 60652755851951D      (0)0(   299.5)    1649394.9
   18 1N                   (0)0(     2.5)    1654541.6
   19 1K                   (0)0(     8.5)    1668939.1
   20 60651756851951B      (0)0(    19.5)    1715621.3
   21 1O                   (0)0(     4.5)    1722798.2
   22 1P                   (0)0(     6.5)    1795180.9
   23 1Q                   (0)0(     8.5)    1831229.6
   24 60651756851951C      (0)0(    59.5)    1867168.5
   25 60652755851951E      (0)0(   419.0)    1891442.4
   26 60651756851951D      (0)0(    98.5)    2103915.7
   -1
 14.0    3          1.96+05 3.92+05 9.80+05 1.96+06 2.94+06 3.92+06 9.80+06 1.96+07
    4    1 1.92+11 7.92+00 8.17+00 8.96+00 1.02+01 1.12+01 1.20+01 1.54+01 1.87+01
    3    1 7.69+06 1.99-01 2.02-01 2.09-01 2.17-01 2.23-01 2.27-01 2.39-01 2.47-01
    5    1 1.07+11 3.89-01 4.07-01 4.70-01 5.77-01 6.73-01 7.59-01 1.13+00 1.50+00
    6    1 1.17+07 7.21-01 7.29-01 7.54-01 7.91-01 8.20-01 8.42-01 9.17-01 9.69-01
    9    1 2.22+10 1.34-01 1.35-01 1.35-01 1.37-01 1.39-01 1.41-01 1.59-01 1.83-01
   12    1 1.21+08 5.57-01 5.62-01 5.81-01 6.11-01 6.36-01 6.57-01 7.33-01 7.89-01
   10    1 2.97+06 2.19-02 2.19-02 2.22-02 2.25-02 2.27-02 2.29-02 2.35-02 2.39-02
```

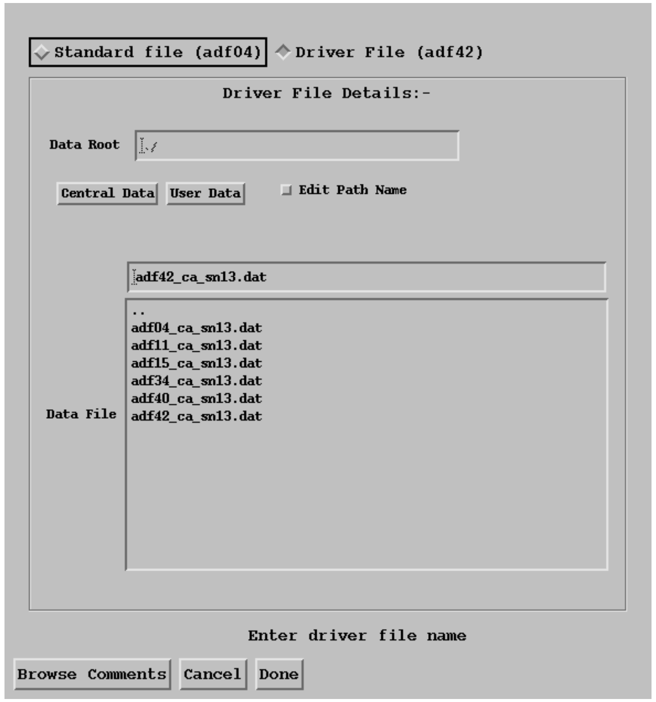
Eissner notation — quick recap

Each occupation/orbital-list pair is separated from the next by 5 (or 6)

```
1s
1

2s  2p
2   3

3s  3p  3d
4   5   6

4s  4p  4d  4f
7   8   9   A

5s  5p  5d  5f  5g
B   C   D   E   F

etc.
```

Generating spectral and power data — ADAS810

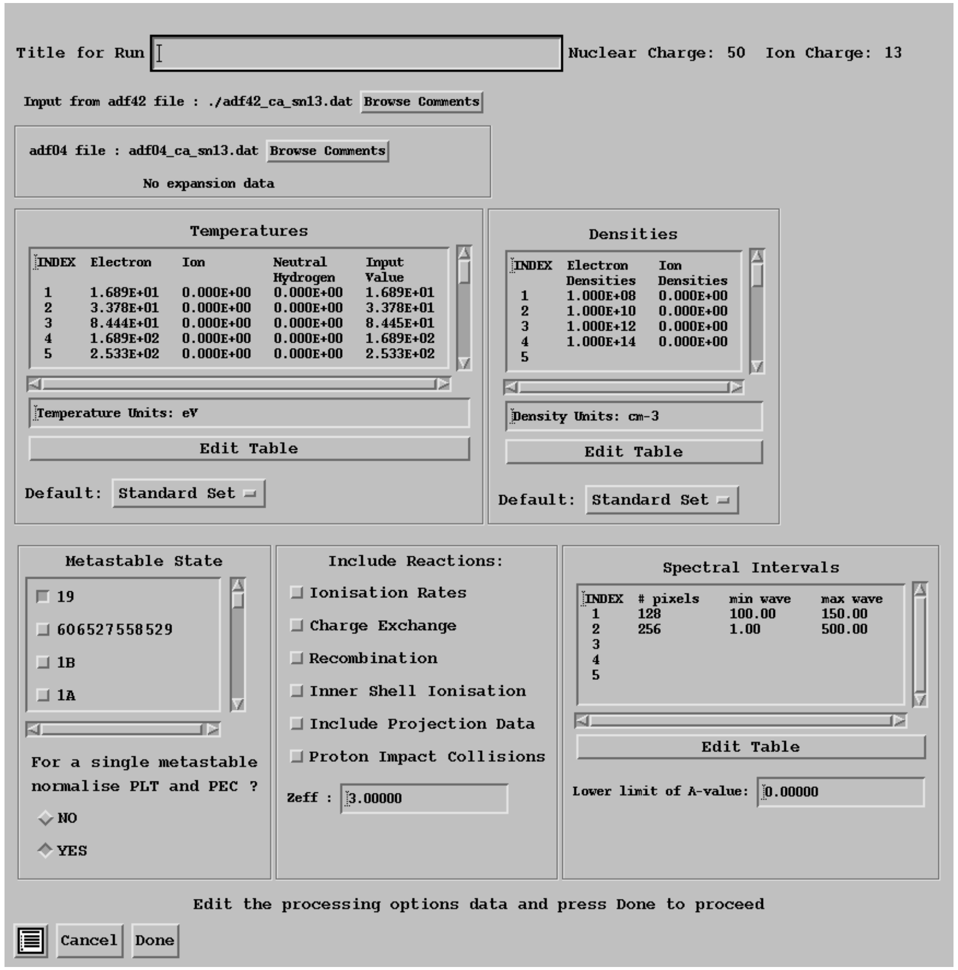
Process the *adf42* file made by `adas8xx_create_drivers` with ADAS810 to generate *adf11*/plt, *adf15* and *adf40* datasets.



Data Root: ./

Data File: adf42_ca_sn13.dat

```
..
adf04_ca_sn13.dat
adf11_ca_sn13.dat
adf15_ca_sn13.dat
adf34_ca_sn13.dat
adf40_ca_sn13.dat
adf42_ca_sn13.dat
```



Title for Run:

Nuclear Charge: 50   Ion Charge: 13

Input from adf42 file : ./adf42_ca_sn13.dat

adf04 file : adf04_ca_sn13.dat

No expansion data

Temperatures

INDEX	Electron	Ion	Neutral Hydrogen	Input Value
1	1.689E+01	0.000E+00	0.000E+00	1.689E+01
2	3.378E+01	0.000E+00	0.000E+00	3.378E+01
3	8.444E+01	0.000E+00	0.000E+00	8.445E+01
4	1.689E+02	0.000E+00	0.000E+00	1.689E+02
5	2.533E+02	0.000E+00	0.000E+00	2.533E+02

Temperature Units: eV

Default: Standard Set

Densities

INDEX	Electron Densities	Ion Densities
1	1.000E+08	0.000E+00
2	1.000E+10	0.000E+00
3	1.000E+12	0.000E+00
4	1.000E+14	0.000E+00
5		

Density Units: cm-3

Default: Standard Set

Metastable State

☑ 19
☐ 606527558529
☐ 1B
☐ 1A

For a single metastable normalise PLT and PEC ?

○ NO
● YES

Include Reactions:

☐ Ionisation Rates
☐ Charge Exchange
☐ Recombination
☐ Inner Shell Ionisation
☐ Include Projection Data
☐ Proton Impact Collisions

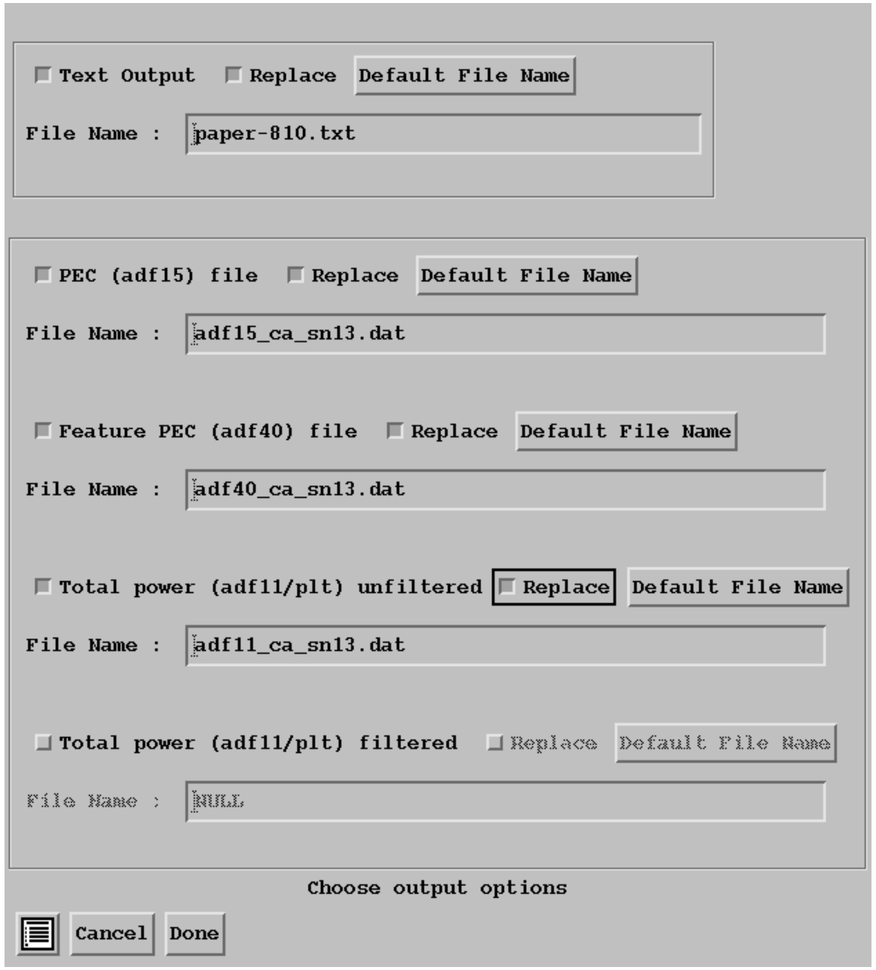
Zeff : 3.00000

Spectral Intervals

INDEX	# pixels	min wave	max wave
1	128	100.00	150.00
2	256	1.00	500.00
3			
4			
5			

Lower limit of A-value: 0.00000

Edit the processing options data and press Done to proceed



☐ Text Output ☐ Replace

File Name : paper-810.txt

☐ PEC (adf15) file ☐ Replace

File Name : adf15_ca_sn13.dat

☐ Feature PEC (adf40) file ☐ Replace

File Name : adf40_ca_sn13.dat

☐ Total power (adf11/plt) unfiltered ☐ Replace

File Name : adf11_ca_sn13.dat

☐ Total power (adf11/plt) filtered ☐ Replace

File Name : NULL

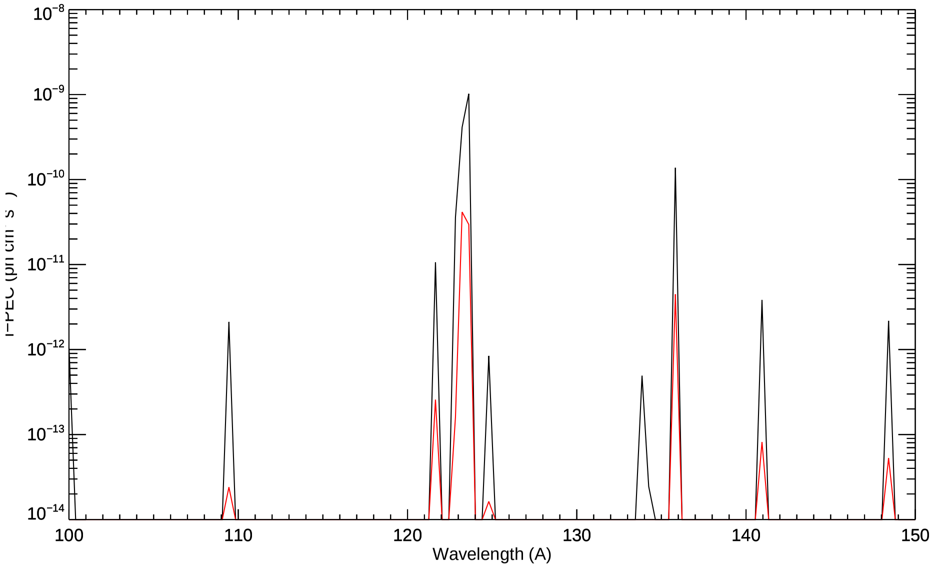
Choose output options

Where lies the emission?

Back to the IDL command line!

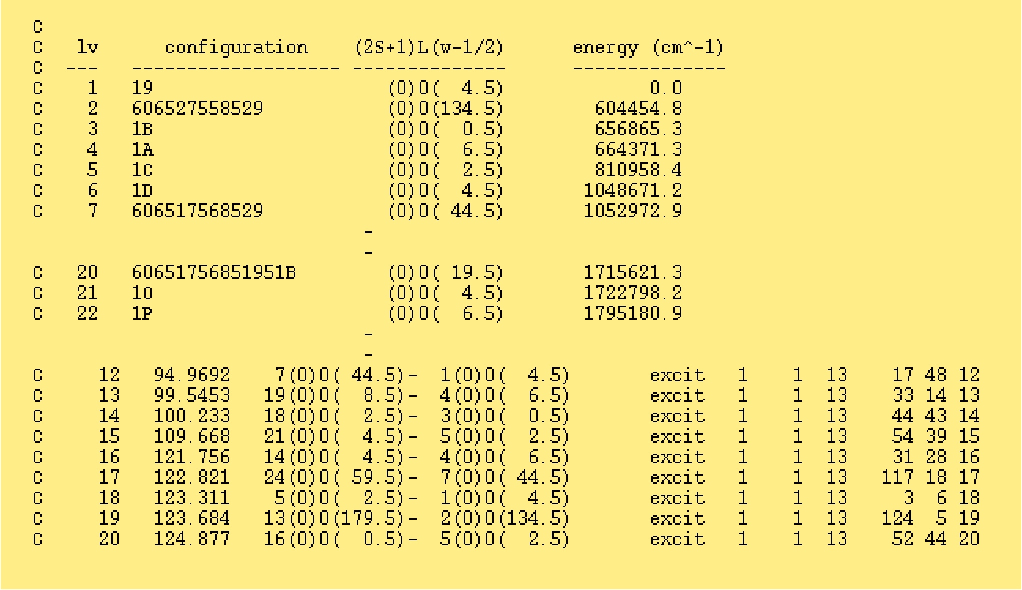
```
read_adf40,file=’adf40_ca_sn13.dat’, fulldata=all

help, all, /st
   ESYM            STRING    ’Sn’
   IZO             LONG                50
   IS              LONG                13
   IS1             LONG                14
   NBLOCK          LONG                 2
   NPIX            LONG      Array[2]
   WAVE_MIN        DOUBLE    Array[2]
   WAVE_MAX        DOUBLE    Array[2]
   NTE             LONG      Array[2]
   TE              DOUBLE    Array[8, 2]
   NDENS           LONG      Array[2]
   DENS            DOUBLE    Array[4, 2]
   FPEC            DOUBLE    Array[256, 8, 4, 2]
   TYPE            STRING    Array[2]
```

```
wave=adas_vector(low=all.wave_min[0], high=all.wave_max[0], $
                 num=all.npix[0], /linear)

plot_io, wave, all.fpec[*, 7, 2, 0] > 1e-14, $
         xtitle='Wavelength (A)', ytitle = 'f-PEC (ph cm!u3!n s!u-1!n)'
oplot, wave, all.fpec[*, 1, 2, 0] > 1e-14, color=5
```



How to identify contributing configurations

It depends of the width of the spectral region of interest



```
C
C   lv      configuration    (2S+1)L(w-1/2)      energy (cm^-1)
C  ---   ------------------- --------------      --------------
C    1   19                      (0)0(  4.5)            0.0
C    2   606527558529            (0)0(134.5)       604454.8
C    3   1B                      (0)0(  0.5)       656865.3
C    4   1A                      (0)0(  6.5)       664371.3
C    5   1C                      (0)0(  2.5)       810958.4
C    6   1D                      (0)0(  4.5)      1048671.2
C    7   606517568529            (0)0( 44.5)      1052972.9
                              -
                              -
C   20   60651756851951B         (0)0( 19.5)      1715621.3
C   21   10                      (0)0(  4.5)      1722798.2
C   22   1P                      (0)0(  6.5)      1795180.9
                              -
                              -
C     12   94.9692    7(0)0( 44.5)-  1(0)0(  4.5)       excit   1    1  13    17 48 12
C     13   99.5453   19(0)0(  8.5)-  4(0)0(  6.5)       excit   1    1  13    33 14 13
C     14   100.233   18(0)0(  2.5)-  3(0)0(  0.5)       excit   1    1  13    44 43 14
C     15   109.668   21(0)0(  4.5)-  5(0)0(  2.5)       excit   1    1  13    54 39 15
C     16   121.756   14(0)0(  4.5)-  4(0)0(  6.5)       excit   1    1  13    31 28 16
C     17   122.821   24(0)0( 59.5)-  7(0)0( 44.5)       excit   1    1  13   117 18 17
C     18   123.311    5(0)0(  2.5)-  1(0)0(  4.5)       excit   1    1  13     3  6 18
C     19   123.684   13(0)0(179.5)-  2(0)0(134.5)       excit   1    1  13   124  5 19
C     20   124.877   16(0)0(  0.5)-  5(0)0(  2.5)       excit   1    1  13    52 44 20
```

- Overplot/look at PEC *adf15* data.
- Refine promotion rules or adf34 driver to home-in
- Note that structure codes are not spectroscopically accurate.

Where next?

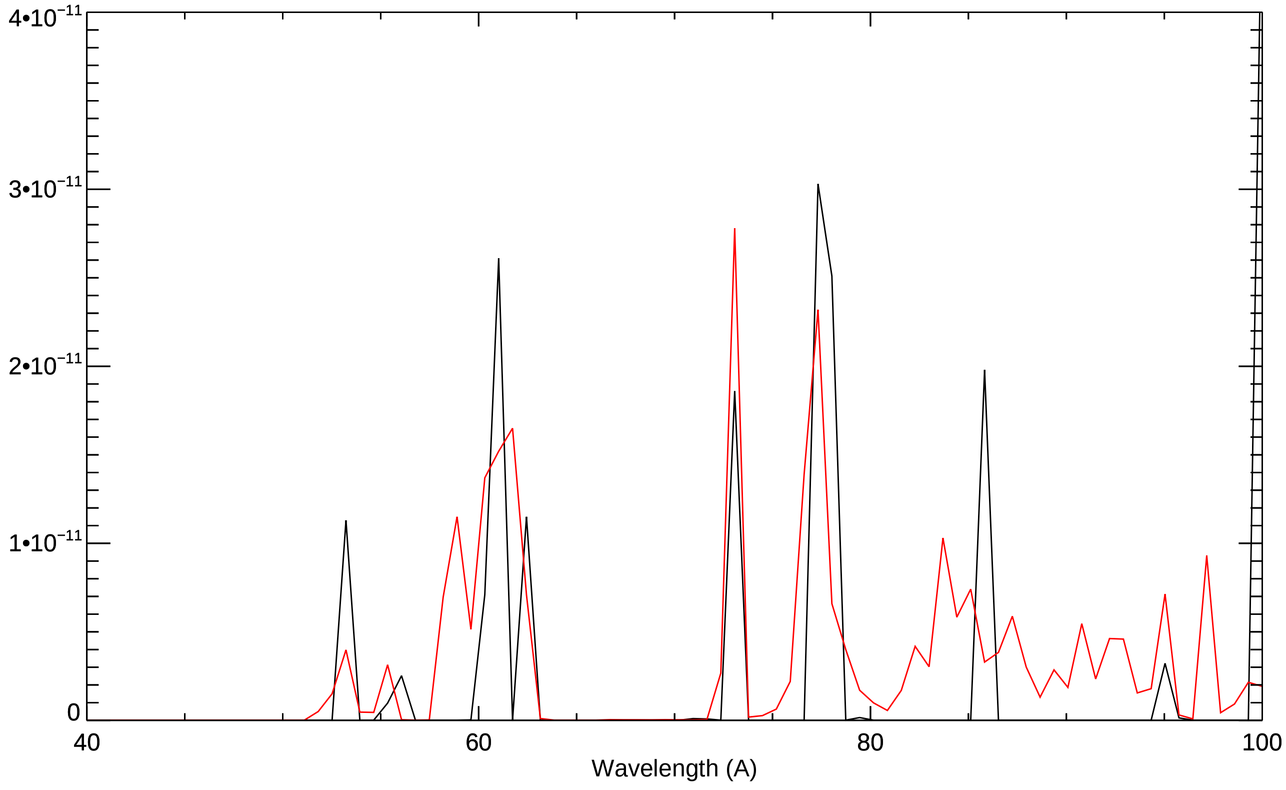
Identify emission region of interest — treat these in intermediate coupling.

For Sn^{13+} :

- 26 configurations, 226 terms, 554 levels

```
read_adf40,file='fpec40#sn_ca#sn13.dat', fulldata=all_ca
read_adf40,file='fpec40#sn_ic#sn13.dat', fulldata=all_ic

wave=adas_vector(low=all_ca.wave_min[1], high=all_ca.wave_max[1], $
                 num=all_ca.npix[1], /linear)

plot, wave, all_ca.fpec[*, 7, 2, 1] > 1e-14,      $
      xtitle = 'Wavelength (A)',                  $
      ytitle = 'f-PEC (ph cm!u3!n s!u-1!n)',      $
      xrange = [40, 100], yrange = [1e-12, 4e-11]

oplot, wave, all_ic.fpec[*, 7, 2, 1] > 1e-14, color=5
```

Configuration average (CA) *vs* intermediate coupling (ic)

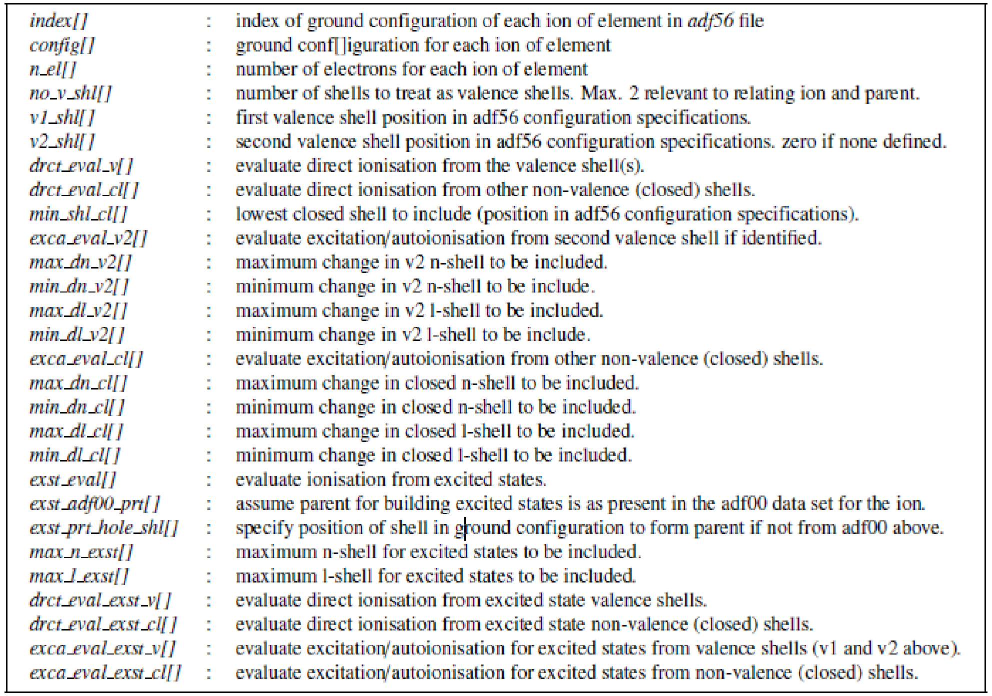


In Reality

- Do not consider each stage by hand — by element is preferable.
- Many scripts available within ADAS to aid this task.
- These impose a directory structure.
- Baseline data identified by the year ‘40’ tag.
- Full instructions in forthcoming ADAS technical report.

Ionisation

Very similar to excitation — driven by *adf56* collection of rules



index[] : index of ground configuration of each ion of element in *adf56* file
config[] : ground conf[]iguration for each ion of element
n_el[] : number of electrons for each ion of element
no_v_shl[] : number of shells to treat as valence shells. Max. 2 relevant to relating ion and parent.
v1_shl[] : first valence shell position in adf56 configuration specifications.
v2_shl[] : second valence shell position in adf56 configuration specifications. zero if none defined.
drct_eval_v[] : evaluate direct ionisation from the valence shell(s).
drct_eval_cl[] : evaluate direct ionisation from other non-valence (closed) shells.
min_shl_cl[] : lowest closed shell to include (position in adf56 configuration specifications).
exca_eval_v2[] : evaluate excitation/autoionisation from second valence shell if identified.
max_dn_v2[] : maximum change in v2 n-shell to be included.
min_dn_v2[] : minimum change in v2 n-shell to be include.
max_dl_v2[] : maximum change in v2 l-shell to be included.
min_dl_v2[] : minimum change in v2 l-shell to be include.
exca_eval_cl[] : evaluate excitation/autoionisation from other non-valence (closed) shells.
max_dn_cl[] : maximum change in closed n-shell to be included.
min_dn_cl[] : minimum change in closed n-shell to be included.
max_dl_cl[] : maximum change in closed l-shell to be included.
min_dl_cl[] : minimum change in closed l-shell to be included.
exst_eval[] : evaluate ionisation from excited states.
exst_adf00_prt[] : assume parent for building excited states is as present in the adf00 data set for the ion.
exst_prt_hole_shl[] : specify position of shell in ground configuration to form parent if not from adf00 above.
max_n_exst[] : maximum n-shell for excited states to be included.
max_l_exst[] : maximum l-shell for excited states to be included.
drct_eval_exst_v[] : evaluate direct ionisation from excited state valence shells.
drct_eval_exst_cl[] : evaluate direct ionisation from excited state non-valence (closed) shells.
exca_eval_exst_v[] : evaluate excitation/autoionisation for excited states from valence shells (v1 and v2 above).
exca_eval_exst_cl[] : evaluate excitation/autoionisation for excited states from non-valence (closed) shells.

adf32 is the driver file for CADW ionisation code from the Auburn group.

Once again to the IDL command line!

```
; Add offline-ADAS IDL library to the path

!path = expand_path('/u/adas/offline_adas/adas8#2/idl') + ':' + !path

; Promotion rules - compiled by Adam Foster (arf)

a56file = '/u/adas/adas/adf56/large_arf09.dat'

; Sn13+ !!

adas8xx_ionis_promotion_rules, z_nuc    = 50,                     $
                               z_ion    = 13,                     $
                               a56file  = a56file,                $
                               adf32    = 'adf32_ca_sn13.dat',    $
                               comments = ['C-------------------', $
                                           'C  I made this!',     $
                                           'C-------------------'  ]
```

```
elem   = Sn
stage  = 13
ip_z   =    3193147.3
ip_z1  =    2415629.2
seq    = rb
--------------------------------------------------------------------------------
Type = Direct /number=3/
#
200-51 1 2  01.   1.   5.0E-08   1.0E-11-2  0130 0 1.00 0.65   71. 0.5       0.70
   50   14  sn+13 ground     4d1                                     4d
   50   15  sn+14 from 4d    3d10 4s2  4p6
   -1
#
200-51 1 2  01.   1.   5.0E-08   1.0E-11-2  0130 0 1.00 0.65   73. 0.5       0.70
   50   14  sn+13 ground     4d1                                     4s
   50   15  sn+14 from 4s    3d10 4s1  4p6  4d1
   -1
#
200-51 1 2  01.   1.   5.0E-08   1.0E-11-2  0130 0 1.00 0.65   72. 0.5       0.70
   50   14  sn+13 ground     4d1                                     4p
   50   15  sn+14 from 4p    3d10 4s2  4p5  4d1
   -1
--------------------------------------------------------------------------------
Type = InDirect /number=2/
#
20 -51 0 2   10  1.0    5.e-08    1.e-11-2   130    1.0 0.65   66.  0.5       0.7
   50   14  sn+13 ground     4d1                                     4s
   50   14  sn+13 via  4d    3d10 4s1  4p6  4d2                      4d
   50   14  sn+13 via  4f    3d10 4s1  4p6  4d1  4f1                 4f
   50   14  sn+13 via  5s    3d10 4s1  4p6  4d1  5s1                 5s
                               -
                               -
   50   14  sn+13 via  7h    3d10 4s1  4p6  4d1  7h1                 7h
   50   14  sn+13 via  7i    3d10 4s1  4p6  4d1  7i1                 7i
   -1
#
20 -51 0 2   10  1.0    5.e-08    1.e-11-2   130    1.0 0.65   66.  0.5       0.7
   50   14  sn+13 ground     4d1                                     4p
   50   14  sn+13 via  4d    3d10 4s2  4p5  4d2                      4d
   50   14  sn+13 via  4f    3d10 4s2  4p5  4d1  4f1                 4f
                               -
                               -
   50   14  sn+13 via  7h    3d10 4s2  4p5  4d1  7h1                 7h
   50   14  sn+13 via  7i    3d10 4s2  4p5  4d1  7i1                 7i
   -1
--------------------------------------------------------------------------------
C-------------------
C  I made this!
C-------------------
```

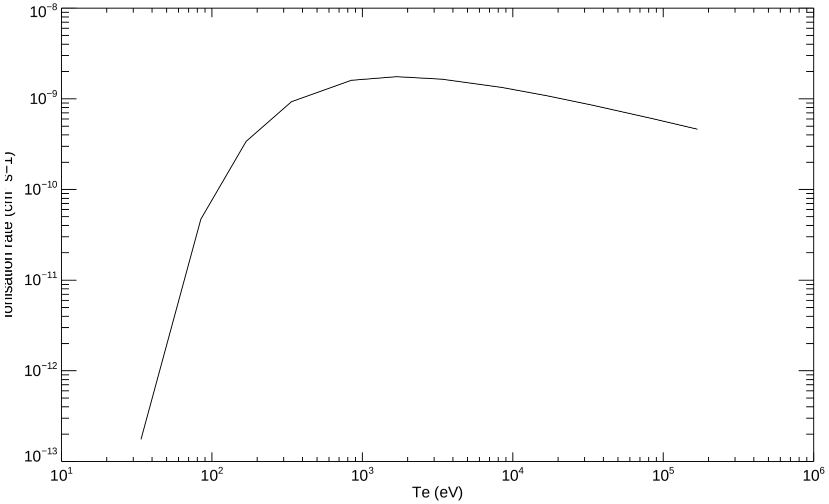
Next to the unix command line

```
 /u/adas/offline_adas/adas8#2/adas8#2.pl adf32_ca_sn13.dat adf23_ca_sn1
```

Return to IDL to inspect the results

```
read_adf23, file='adf23_ca_sn13.dat', fulldata=all, szd_total=szd

help, szd,/st

** Structure <a3e784c>, 7 tags, length=6576, data length=6576, refs=1:
   TE               DOUBLE    Array[12]
   Q_ION            DOUBLE    Array[1, 3, 12]
   IS_Q_ION         LONG      Array[1, 3, 12]
   Q_EXC            DOUBLE    Array[1, 41, 12]
   IS_Q_EXC         LONG      Array[1, 41, 12]
   QTOT             DOUBLE    Array[1, 1, 12]
   IS_QTOT          LONG      Array[1, 1, 12]
```

```
te  = reform(szd.te) / 11605.0
szd = reform(szd.qtot*10.0^szd.is_qtot) > 1.0e-36

plot_oo, te, szd,          $
         xtitle='Te (eV)', $
         ytitle = 'Ionisation rate (cm!u3!n s-1!n)
```



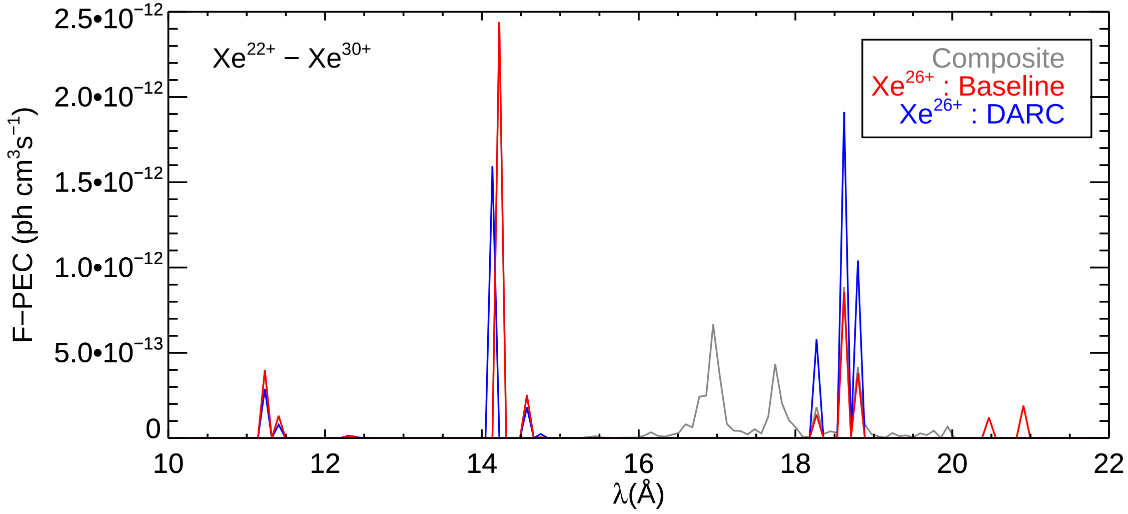
Recombination

- *adf55* rules are imminent.
- However, use ADAS407/ADAS408 for now.

Selectively uplift the quality of baseline

- With increasing atomic number relativistic effects assume a greater importance.
- Compare the baseline Born data to DARC to assess its validity.

Consider Ni-like Xe^{+26} with a $3d^{10}$ ground configuration:



Handling heavy species data

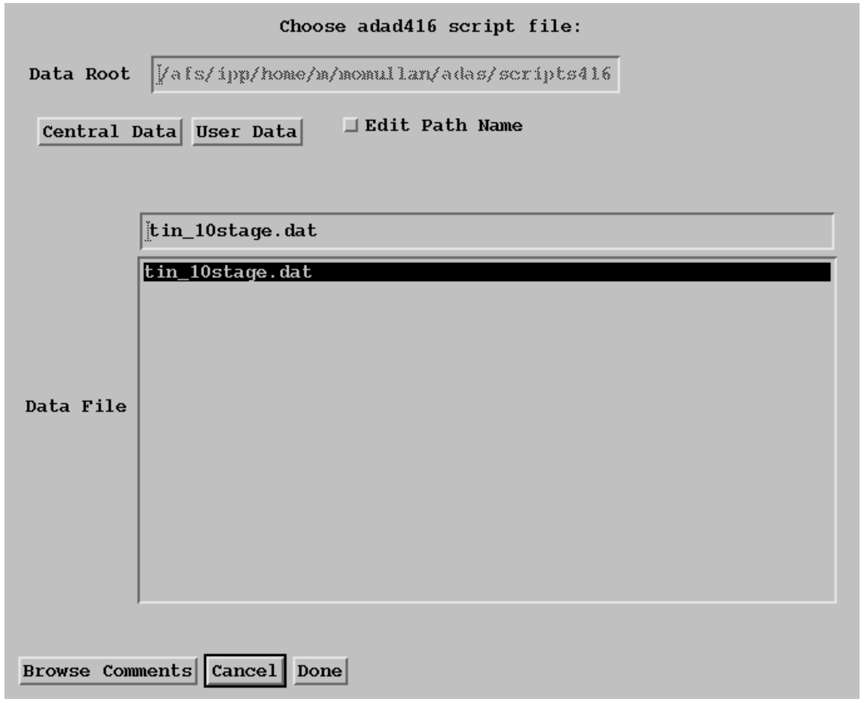
It may not always be necessary to consider all ionisation stages of an element.

Again, for tin, consider the partiton (extract from *scripts416* driver file:

```
//#02/p00/ 00/
      p01/ 01 02 03 04 05 06 07/
      p02/ 08/
      p03/ 09/
      p04/ 10/
      p05/ 11/
      p06/ 12/
      p07/ 13/
      p08/ 14/
      p09/ 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32
      33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49/
      p10/ 50/
```

Generate partitioned *adf11* data

Process with ADAS416 : See `/u/momullan/adas/scripts416/tin_10stage.dat`


Choose adad416 script file:

Data Root: /afs/ipp/home/m/momullan/adas/scripts416

Data File: tin_10stage.dat

Note: *adf11* datasets in `/u/momullan/ADAS-EU_course/`.

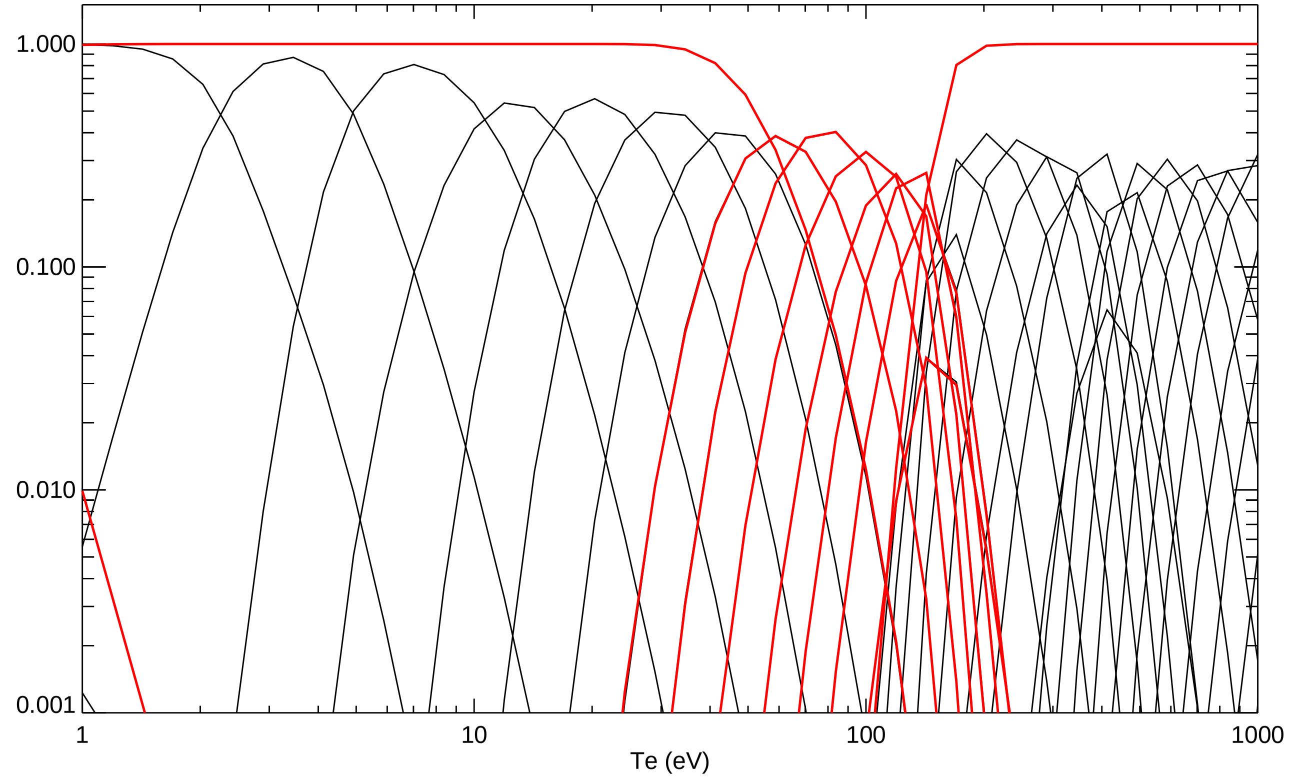
Compare ionisation equilibrium balance

At the IDL command line

```
te = adas_vector(low=1, high=1000, num=40)
dens = fltarr(40) + 1e12

; Explicity name adf11 files

files = {acd : 'acd66_sn#10stage.dat', $
         scd : 'scd66_sn#10stage.dat'  }

run_adas405, uid='adas', elem='sn', year=89, te=te, dens=dens, $
             files=files, frac=frac_par

files = {acd : 'acd89_sn.dat', $
         scd : 'scd89_sn.dat'  }

run_adas405, uid='adas', elem='sn', year=89, te=te, dens=dens, $
             files=files, frac=frac
```

```
xmin = min(te, max=xmax)
ymin = 0.001
ymax = 1.5

plot_oo, [xmin, xmax], [ymin, ymax], /nodata, ystyle=1, $
         xtitle = 'Te (eV)', ytitle = 'Fractional abundance'

for j = 0, n_elements(frac.stage)-1 do begin
   oplot, te, frac.ion[*,j]
endfor

for j = 0, n_elements(frac_par.stage)-1 do begin
   oplot, te, frac_par.ion[*,j], color=5, thick=5
endfor
```

We assume that we have no great interest ouside our chosen ions!



CXSFIT - Charge Exchange Fitting

Allan Whiteford (ADAS)

M G von Hellermann, Thijs Versloot (FOM/Jülich)

L D Horton, C F Maggi, J Schirmer, T Pütterich, R McDermott (IPP-Garching)

K-D Zastrow, T M Biewer⋆, C Giroud and A G Meigs (UKAEA/JET)
⋆ Permanent institution: ORNL

15th September 2009

ADAS-EU Training Course

Contents

- Background.
- KS4FIT.
- CXSFIT.
- Graphical Interface.
- Feature highlights.
- Fit history methodology and automatic processing.
- Benchmarking and testing.

Background

- Fitting charge exchange spectra has always been a complicated process:
  - on the fly wavelength calibration (based on Be line position),
  - the passive signals means a one Gaussian fit is usually not possible,
  - other lines make it difficult to fit the background,
  - using carbon temperatures to aid in the fitting of helium spectra,
  - coupling line positions together based on known wavelengths,
  - now we have tungsten contaminating the spectra,
  - and many many more.

- von Hellermann and co-workers developed advanced techniques to solve all of these issues at JET — resulted in a computer code called KS4FIT.

KS4FIT

- Practical implementation of charge exchange fitting at JET was called KS4FIT:
  - originally written for the IBM but ported to Linux,
  - reads spectra (JPFs) and writes results (PPFs),
  - had a TSO-style interface,
  - now replaced by CXSFIT.

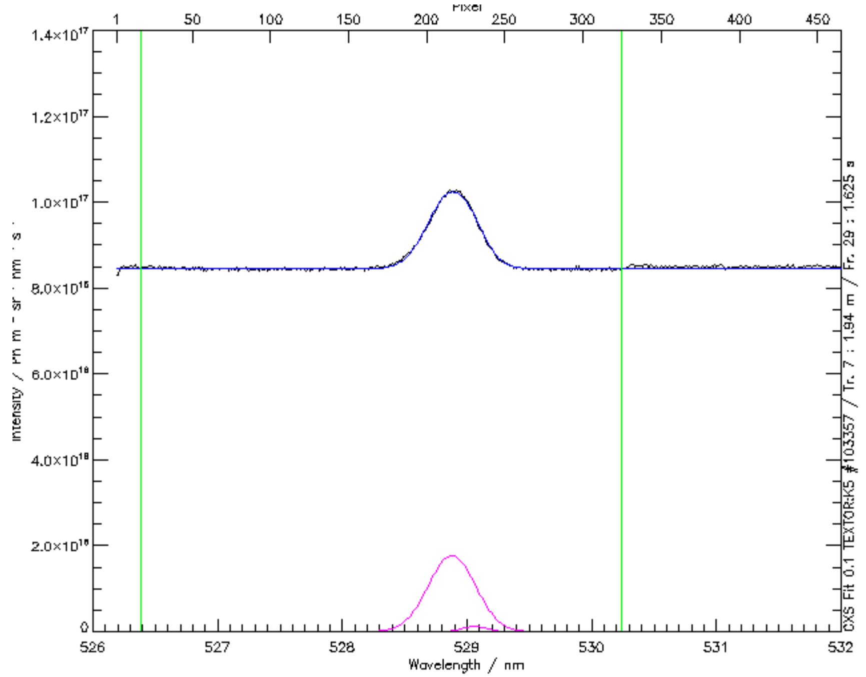
- However, KS4FIT exists outside of JET where it is a different thing:
  - same core fitting algorithm,
  - input and output are completely different,
  - packaged along with InSPECtor (JAVA fitting code).

- It's the latter version of KS4FIT (the pure fitting engine) which CXSFIT uses.

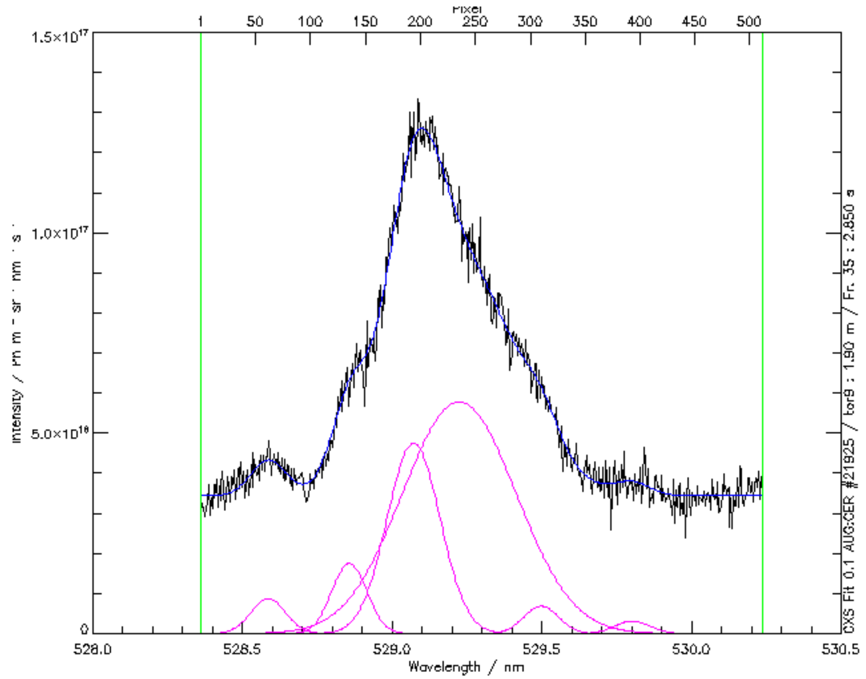
CXSFIT

- CXSFIT is a joint development between ADAS, FOM, Garching, Jülich and UKAEA to provide a universal interface to KS4FIT.
- Graphical user interface written in IDL.
- Contains all of the features present in KS4FIT.
- Provides visualisation of each fit and of the overall results.
- Almost all of the code is machine independent:
  - Machine specific reading/writing routines need to supplied.
  - We really do have an identical code running on AUG, JET and TEXTOR!

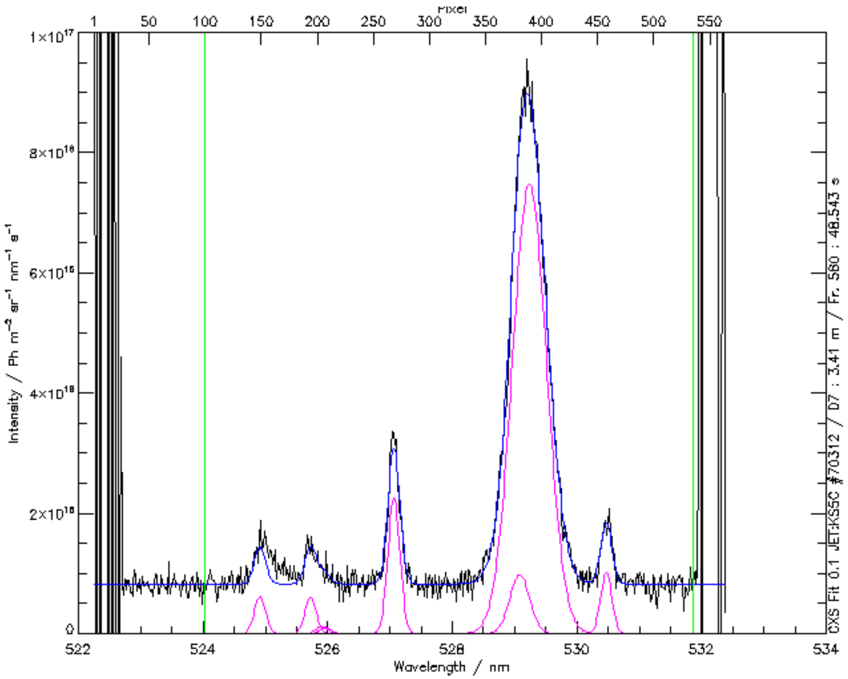
Example spectra — TEXTOR



Example spectra — AUG



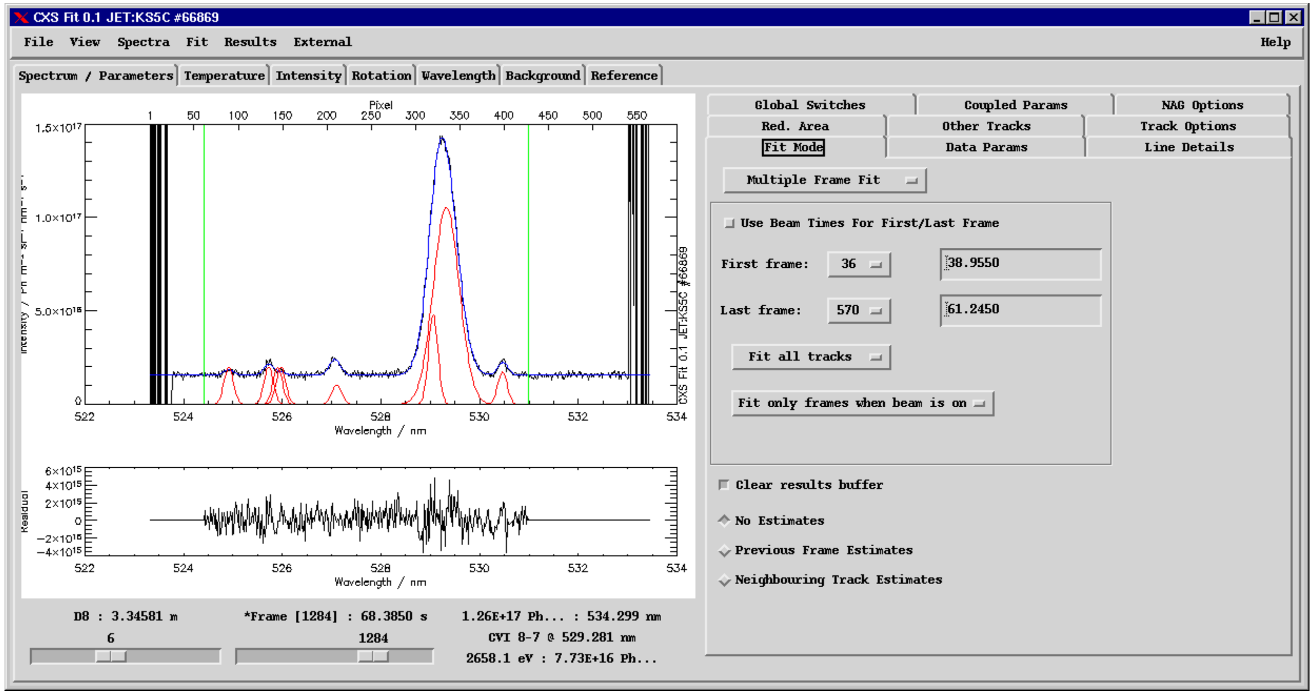
Example spectra — JET



Current usage and deployment

- Used exclusively on all JET core spectroscopy systems (KS5A-E),
  - Reads from JPFs and takes geometry etc. from central location.
  - Writes directly to PPFs.
- Used at AUG on CER and CHR core systems plus CHZ edge system,
  - Reads level-0 shotfiles (spectra) and geometry etc. from central location.
  - Writes directly to level-1 shotfiles compatible with cview.
- Replaced InSPECtor at TEXTOR on all Kameras (1-6).
  - Reads directly from TWU (both spectra and all other information).
  - Writes directly to TEXTOR TPD system.
- First usage at CEA Cadarache last month.

The Graphical Interface



Multiple Frame Fit

☐ Use Beam Times For First/Last Frame

First frame: 36 38.9550

Last frame: 570 61.2450

Fit all tracks

Fit only frames when beam is on

☐ Clear results buffer

◆ No Estimates

◇ Previous Frame Estimates

◇ Neighbouring Track Estimates

D8 : 3.34581 m

6

*Frame [1284] : 68.3850 s

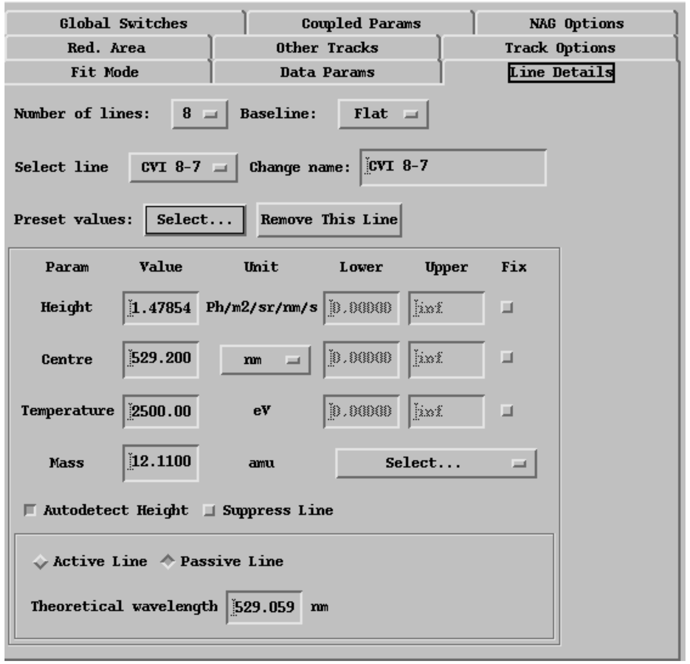
1284

1.26E+17 Ph... : 534.299 nm

CVI 8-7 @ 529.281 nm

2658.1 eV : 7.73E+16 Ph...

Feature Highlights: In-built line database



Number of lines: 8 Baseline: Flat

Select line CVI 8-7 Change name: CVI 8-7

Preset values: Select...

Param	Value	Unit	Lower	Upper	Fix
Height	1.47854	Ph/m2/sr/nm/s	0.00000	inf	☐
Centre	529.200	nm	0.00000	inf	☐
Temperature	2500.00	eV	0.00000	inf	☐
Mass	12.1100	amu	Select...		

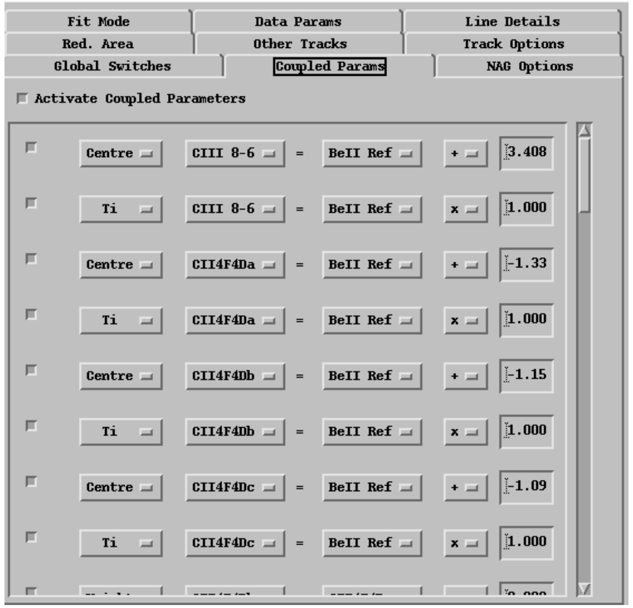
☐ Autodetect Height ☐ Suppress Line

◇ Active Line ◆ Passive Line

Theoretical wavelength 529.059 nm

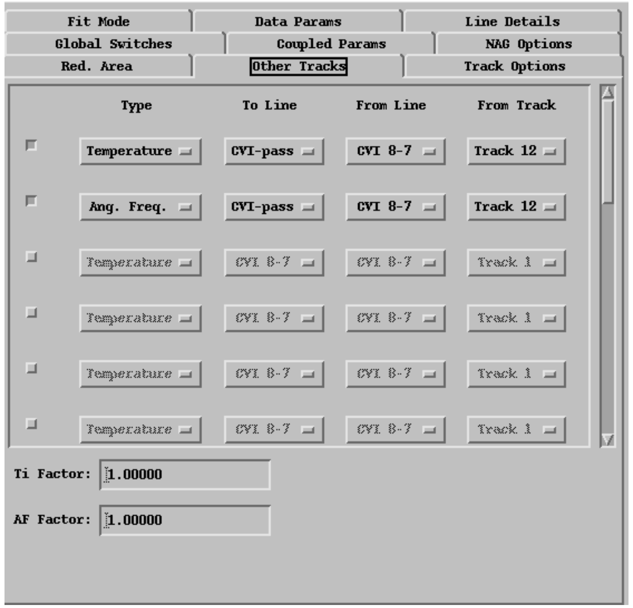
- Very high quality observed wavelengths included in program.
- Gives best quality rotations and on-the-fly calibration.
- If wanted, can be selected automatically based on line position.
- Can be overridden by the user if necessary.

Feature Highlights: Complex coupling



☐ Activate Coupled Parameters

☐ Centre CIII 8-6 = BeII Ref + 3.408
☐ Ti CIII 8-6 = BeII Ref x 1.000
☐ Centre CII4F4Da = BeII Ref + -1.33
☐ Ti CII4F4Da = BeII Ref x 1.000
☐ Centre CII4F4Db = BeII Ref + -1.15
☐ Ti CII4F4Db = BeII Ref x 1.000
☐ Centre CII4F4Dc = BeII Ref + -1.09
☐ Ti CII4F4Dc = BeII Ref x 1.000



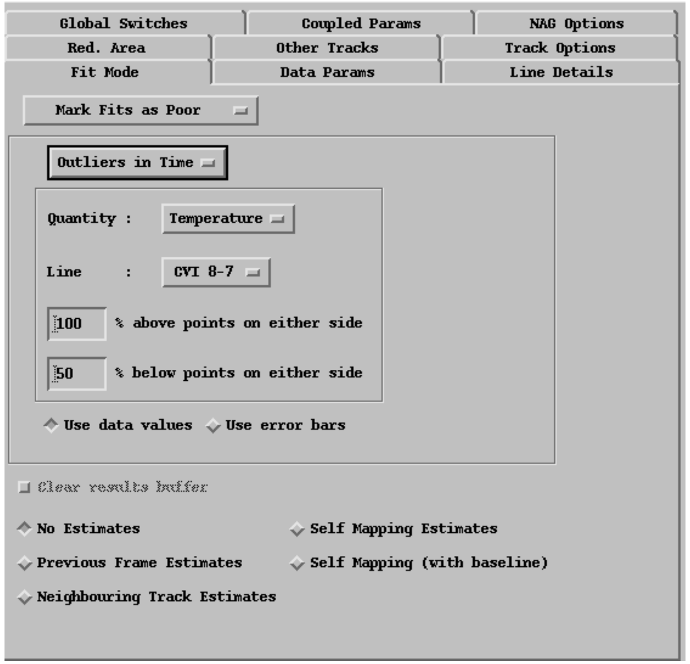
	Type	To Line	From Line	From Track
☐	Temperature	CVI-pass	CVI 8-7	Track 12
☐	Ang. Freq.	CVI-pass	CVI 8-7	Track 12
☐	Temperature	CVI 8-7	CVI 8-7	Track 1
☐	Temperature	CVI 8-7	CVI 8-7	Track 1
☐	Temperature	CVI 8-7	CVI 8-7	Track 1
☐	Temperature	CVI 8-7	CVI 8-7	Track 1

Ti Factor: 1.00000

AF Factor: 1.00000

Can couple inside a spectrum or across tracks.

Highlights: detecting poor data



Mark Fits as Poor

Outliers in Time

Quantity : Temperature

Line : CVI 8-7

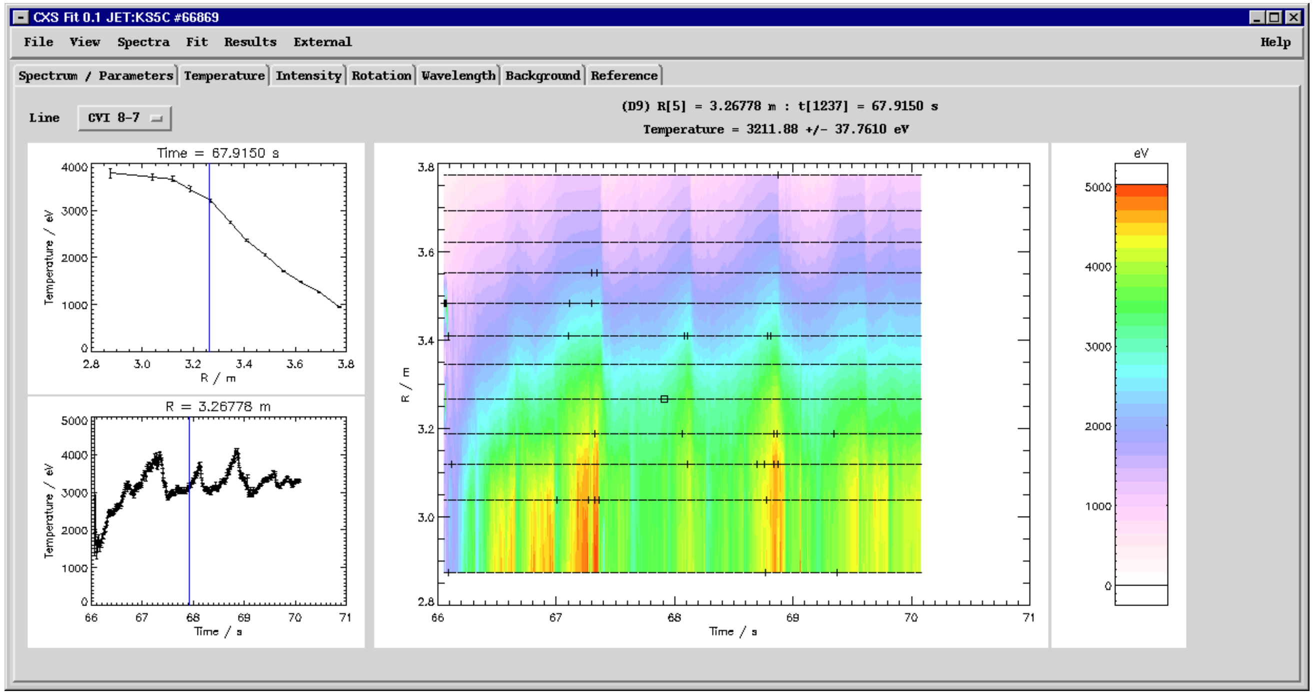
100 % above points on either side

50 % below points on either side

Use data values / Use error bars

- Can do analysis of fit results to check quality/sanity
- Outliers in time or non-physical T_i profiles
- Necessary on systems with high temporal resolution.
- Can be used as part of a more complex analysis.

Preview of results



(D9) R[5] = 3.26778 m : t[1237] = 67.9150 s

Temperature = 3211.88 +/- 37.7610 eV

Repairing spectra

- Even with all the options available, usually a few of the fits don't converge.

- Marked with crosses (poor fits) or stars (failed fits) in the output preview.

- Options exist to refit the failed or poor frames with new fit options:
  - 'standard' current procedure at JET is to use the previous frame estimates,
  - sometimes necessary to do individual fits by hand,
  - conceivable that different temporal regions may need different setup entirely.

- However, this means that to reproduce results or use the same recipe on a different shot there are multiple parameter settings which need to be used.

Fit History

- CXSFIT stores the fit history, i.e.:
  - The list of steps used to produce the current fit in terms of what the fit options were set to each time a fit was initiated.

- Fit histories can be saved as default recipes (also written to default output).

- Very simple history might be:

1. fit all frames with beam on for all times,
2. fit any failed frames using previous frame estimates,
3. fit any remaining failures using neighbouring tracks option.

- Allows the user to load in a spectrum, load a recipe and then “replay” the history. Standard recipes can be developed for particular instruments.

The command line

- CXSFIT can be controlled from the command line for convenience or for batch processing, examples are:

- Load a spectrum at startup:
  - `cxsfit cer:17148`

- Do batch processing using the same recipe:
  - `cxsfit ks5c:66869 ks5c_carbon8-7.fit replay save ks5c_66869.cxf quit`
  - `cxsfit ks5c:66870 ks5c_carbon8-7.fit replay save ks5c_66870.cxf quit`
  - `cxsfit ks5c:66871 ks5c_carbon8-7.fit replay save ks5c_66871.cxf quit`

- Reload a previously saved setup:
  - `cxsfit k5_103357.cxf`

Testing and benchmarking

- Benchmarking between CXSFIT and the TSO KS4FIT has been done at JET. Results were almost identical (expected since the core code is the same).

- Extensive testing has been done on AUG for a number of spectra. Including helium spectra using external estimates.

- Testing at TEXTOR gave very similar results to InSPECtor implementation (expected that the CXSFIT results are better due to the treatment of errors).

- The output of CXSFIT at JET can be processed by the current (IBM-esque) version of CHEAP. Similarly for IDL-CHEAP at AUG and Matlab-CHEAP at TEXTOR.

- Possible CHEAP re-development and rationalisation is an issue.

CXSFIT can be run downstairs, please feel free to have a go. Tutorial sheets are available.

Thank you

-

Introduction to R-matrix calculations

A D Whiteford and N R Badnell

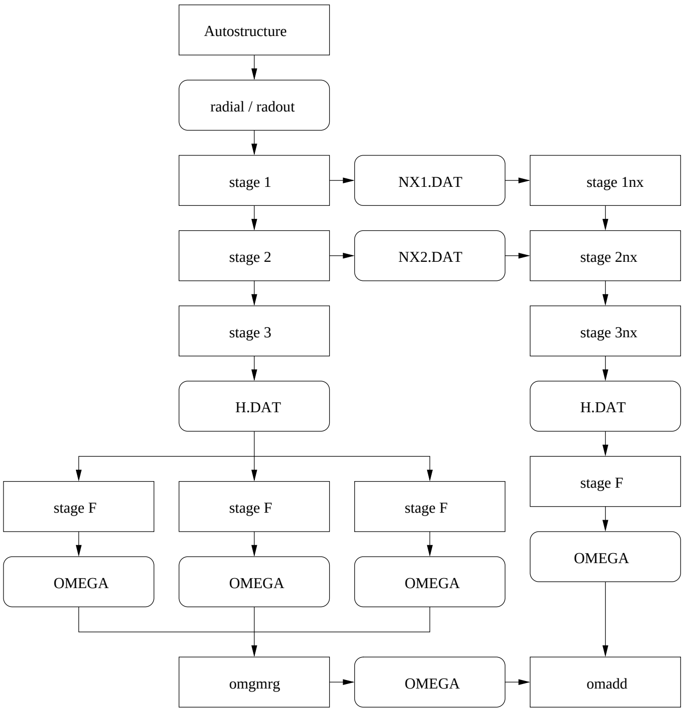
15th October 2009

Contents

1 Introduction

These notes give a rough guide to starting out with R-matrix codes to generate data for Na-like Fe in LS coupling. The examples here should be viewed as a starting point for more advanced R-matrix calculations which could include other physical effects, IC coupling, more levels or different ions.

2 Code layout



.....

3 Structure calculation

The structure is calculated using the code AUTOSTRUCTURE, other structure codes can be used if necessary.

For sodium-like iron, an example input file would look like:

```
A.S.
 &SALGEB RAD='ALL' CUP='IC' MXVORB=3 MXCONF=3 KORB1=1
                           KORB2=3 KUTSO=0 BORN='INF' &END
  3 0  3 1  3 2
   1    0    0
   0    1    0
   0    0    1
 &SMINIM NZION=26 RADOUT='YES' &END
```

`MXVORB` specifys three valance orbitals will be specified, these are 3s, 3p and 3d.

`MXCONF` specifys three configurations will be specified, these are $1s^2 2s^2 2p^6 3s$, $1s^2 2s^2 2p^6 3p$ and $1s^2 2s^2 2p^6 3d$

`RAD="ALL"` implies we also wish the code to calculate all types of radiation, this is not necessary for the resulting R-matrix calculation but for checking an atomic structure it is often useful to compare radiative quantities.

`CUP="IC"` means we wish to perform the calculation in intermediate coupling.

`KORB1=1 KORB2=3` means that we want the first three orbitals to be closed, i.e. all of our confiruations are based on a $1s^2 2s^2 2p^6$ closed core and we only explicitly specify electrons outside of this.

`KUTSO=0` is to turn off the spin orbit interaction, we do this because the R-matrix codes do not include this term so in order to maintain consistency between AUTOSTRUCTURE and R-matrix we turn it off in AUTOSTRUCTURE.

`NZION=26` is specifiying the ion charge, in this case 26 (iron!).

`RADOUT="YES"` causes AUTOSTRUCTURE to produce a file called “radial” which contains radial wavefunctions to be used by the R-matrix codes. This is the only data which AUTOSTRUCTURE passes to R-matrix.

`BORN="INF"` causes AUTOSTRUCTURE to produce infinite energy Born limit points (required later). IC versions end up in a file called `OMGINFIC` and LS versions in a file called `OMGINFLS`.

Here we have included the configurations $1s^2 2s^2 2p^6 3s$, $1s^2 2s^2 2p^6 3p$, $1s^2 2s^2 2p^6 3d$. We specify our three configurations in using occupation numbers, recalling that using the KORB parameters we've already set a $1s^2 2s^2 2p^6$ (21522563) core.

At the end of our structure calculation, it is useful to look at the `olg` file. In particular the energy levels calculated, an extract of the file shows that

```
K          K*CM     2*S+1  L   2J   CF          (EK-E1)/RY
1            0.       2    0    1    1          0.00000000
2       276562.      -2    1    1    2          2.52021562
3       296656.      -2    1    3    2          2.70333129
4       677729.       2    2    3    3          6.17592452
5       681019.       2    2    5    3          6.20590102
```

These are five levels, the first corresponding to configuration (CF) 1 (i.e. $1s^2 2s^2 2p^6 3s$), the second and third to configuration two and the fourth and fifth to configuration five.

NIST quotes the four excited energies as 2.52596, 2.71688, 6.15544 and 6.18198. We can conclude that our structure is reasonable but perhaps some optimisation can be required. For our example, we will continue with this default structure regardless.

4 Inner region exchange calculation

The inner region is run in three stages, interestingly called stage 1, stage 2 and... wait for it... stage 3.

For Na-like iron, an example stage 1 input file would look like:

```
S.S.
 &STG1A &END
 &STG1B MAXLA=2 MAXLT=12 MAXC=20 MAXE=100 &END
```

`MAXLA=2` is the maximum angular momentum of the target.

`MAXLT` is the maximum total angular momentum of the system, typically we make this a factor of 3 or 4 times MAXLA.

`MAXC` is the number of basis orbitals to be used, this limits how high in energy we can scatter.

An example stage 2 input file would look like:

```
S.S.
 &STG2A &END
 &STG2B MAXORB=6 NELC=11 NAST=3 INAST=0 MINLT=0 MAXLT=12
          MINST=1 MAXST=3 &END
 1 0 2 0 2 1 3 0 3 1 3 2
  3
  2 2 6 0 0 0 0 0 0 0
  2 2 6 1 1 1 1 1 1 1
  2 2 6 1 0 0 0 0 0 0  0
  2 2 6 0 1 0 0 0 0 0  0
  2 2 6 0 0 1 0 0 0 0  0
 2 0 0
 2 1 1
 2 2 0
 1
  2 2 6 0 0 0 0 0 0 0
  2 2 6 2 2 2 2 2 2 2
  2 2 6 1 0 0 0 0 0 0  2
```

`MAXORB=6` are the maxium number of orbitals, in this case 6 (1s,2s,2p,3s,3p,3d).

`NELC=11` specifies the number of electrons in the system.

`NAST=3` is the number of atomic states, we are working in LS at the moment and there are 3 terms in the system we are looking at.

`MINLT=0` is the minimum orbital angular momentum we are interested in, this should usually be zero.

`MAXLT=12` is the maximum orbital angular momentum, this should correspond to the MAXLT parameter passed into stage 1.

`MINST=1` and `MAXST=3` are the minimum and maximum spins of the N+1 system. In this case we get singlets and triplets for the intermediate 3 electron system.

We then specify our orbitals in the line which looks like:

```
 1 0 2 0 2 1 3 0 3 1 3 2
```

We give our 6 orbitals as the n of the orbitals followed by the l (e.g. '2 1' ≡ 2p).

Next we specify how many configurations we have and then list them by occupation numbers, note that the fact we have 10 orbitals and 10 configurations is just a conincidence.

```
  3
  2 2 6 0 0 0 0 0 0 0
  2 2 6 1 1 1 1 1 1 1
  2 2 6 1 0 0 0 0 0 0  0
  2 2 6 0 1 0 0 0 0 0  0
  2 2 6 0 0 1 0 0 0 0  0
```

We specify that there are three configurations, on the next line we give the minimum number of electrons which can be in each orbital and on the next the maximum. On the following ten lines we give each configuration. For the moment, ignore the zeros on the end of each line.

Following this we give the 3 allowed terms, we specify multiplicity, orbital angular momentum and parity (0 for even parity and 1 for odd).

After this we list each possible intermediate configurations corresponding to the N+1 electron system:

```
  2 2 6 0 0 0 0 0 0 0
  2 2 6 2 2 2 2 2 2 2
  2 2 6 1 0 0 0 0 0 0  2
```

Again we first specify the minimum number of electrons in each orbital, then the maximum. The line which follows gives a starting configuration and the line on the end the number of promotions from this configuration (so long as we follow the minimum and maximum rules give above it) we allow two promotions. Simple combinatorial analysis will quickly show that these rules generate all intermediate configurations.

The stage 3 input data is somewhat simpler:

```
S.S.
 &STG3A &END
 &STG3B INAST=0 NAST=0 &END
```

At the end of our inner region exchange runs we have an `H.DAT` file. This is the file which is later used by the outer region codes and consists of a series of diagonlised hamiltonians for each symmetry.

5 Outer region exchange runs

The outer region codes are split into two parts, stage f and stage icf. Stage f solves the problem in LS coupling and then stgicf performs a frame transformation and makes use of the term coupling coefficients to resolve the results in an IC picture. We will concentrate here on stage f.

An example input file for stgf would be:

```
&STGF IMESH=1 IQDT=2 PERT='YES' LRGLAM=-12 IPRINT=-1 ELAS='NO'
      IPRKM=4 IBIGE=0 &END
&MESH1 MXE=9000 E0=0.01 EINCR=0.00001 &END
```

`IMESH=1` tells the code how we wish to specify our energy mesh, in this case "1" means we will later specify a starting energy, an energy increment and a number of energies.

`IQDT=2` tells the code to use K-matrices, these are later used by stgicf.

`PERT='YES'` turns on long range coupling potentials, these are usually necessary for accurate results.

`LRGLAM=-12` tells the code to calculate collision strengths up to an L of 12, this can not be higher than the maximum L specified in stage 1 and stage 2. We specify a negative number to suppress top-up since this will be handled with the non-exchange codes.

`IPRINT=-1` controls how much information is printed to the human readable file.

`ELAS='NO'` tells the code we are not interested in elastic transitions.

`IPRKM=4` tells the code to print out K-matrices so that can be used in the following stgicf code.

The energy grid is then specified, in this case we are asking for 9000 points starting at a Z-scaled energy of 0.01 and incrementing 0.00001 Z-scaled rydbergs at a time.

The output of stage f which we are interested in is an `OMEGA` file. This contains the collision strength for each transition as a function of energy.

It is normal to do a number of stage f runs, with a fine mesh to span the resonance region (i.e. up to threshold) and a coarser mesh through the non-resonance region. The input file for the coarser mesh might look like:

```
&STGF IMESH=1 IQDT=2 PERT='YES' LRGLAM=-12 IPRINT=-1 ELAS='NO'
      IPRKM=4 IBIGE=0 &END
&MESH1 MXE=1000 E0=0.1 EINCR=0.001 &END
```

identical to the first file except that the starting energy is where the last file left off and the energy increments is much larger.

6 Inner region non-exchange runs

So far, we have only calculated collision strengths up to a total angular momentum of 12. In order to genereate a complete cross-section we must extend this up to infinity, this is done via the use of the non-exchange codes. They will use a simpler approximation up to another value of L and then apply top-up rules after this.

There are three non-exchange inner region codes, they are all driven by the same input file. A typical one would look like:

```
CONTinuation run
 &STGNX  MINLT=13 MAXLT=60  &END
```

Here we tell it the minimum and maximum values of L it should work for, the rest of the information it can derive from files coming from the exchange codes (NX1.DAT, NX2.DAT and the stage 3 input file).

The three non exchange codes are then run with this input file, producing an `H.DAT` file which can be similarly processed with stage f.

7 Outer region non-exchange runs

These are the same as the exchange codes but a much coarser energy grid can be used since we don't get resonances for the non-exchange calculations.

A typical input files would look like

```
 &STGF IMESH=1 IQDT=2 PERT='YES' LRGLAM=60 IPRINT=-1 ELAS='NO'
       IPRKM=4 IBIGE=0 MINLT=13 &END
 &MESH1 MXE=1090 E0=0.01 EINCR=0.001 &END
```

This will produce an OMEGA file. For partial waves from 13 to 60 calculated explicitly and partial waves of 61 to infinity calculated using 'top-up' rules. We could have turned the top-up off by specifying LRGLAM as a negative value.

8 Merging omega files

By the time you are finished you will have a number of omega files, these will be limited in energy or angular momentum. There are two operations we can perform on two omega files, merge or add.

If we wish to put two omega files together with different energy grids, we merge them using a utility code called OMGMRG.

If we wish to put two omega files together with different angular momenta ranges, we add them using a utility code call OMADD.

We have produced three seperate `OMEGA` files in the examples above, we firstly merge the two exchange runs with OMGMRG and then add the exchange calculations to the non-exchange calculations using OMADD.

9 Results

From our final omega file, we can extract transitions using the `xtrct` program, this will produce an ascii list of collision strength against energy.

Looking at the 3s−3p transition, the different angular momenton contributions are shown in figure 1.

Comparison with the work of Mann is shown in figure 2, the results are showing the correct behaviour at high energy but are perhaps not as close as one would like, the limited inclusion of states and lack of optimisation of the structure could be responsible for the discrepancy.

10 Producing an adf04 file

To do this we use a program called adasex, this works on an OMEGA file and an input file called "adasex.in" which looks like:

```
 &ADASEX NTERM=  3 FIPOT=3946280 IONTRM='1S' IEL='FE' &END
         3s(2S)         0.    1
         3p(2P)    271831.    2
         3d(2D)    649665.    3
NAME: Your name here
DATE: Date here
Free-form comments here
.
```

`NTERM` is the number of levels. We also give the ionisation potential and the term specification of the adjacent ion stage.

Following the namelist we give a temperature grid and then a list of what each level is.

Using this information, an adf04 file can be constructed.

However, we also need to tag on infinite energy limit points, these were generated by autostructure and the file is called `OMGINFLS`, these should be omega merged on to the final `OMEGA` file before ADASEX is run.

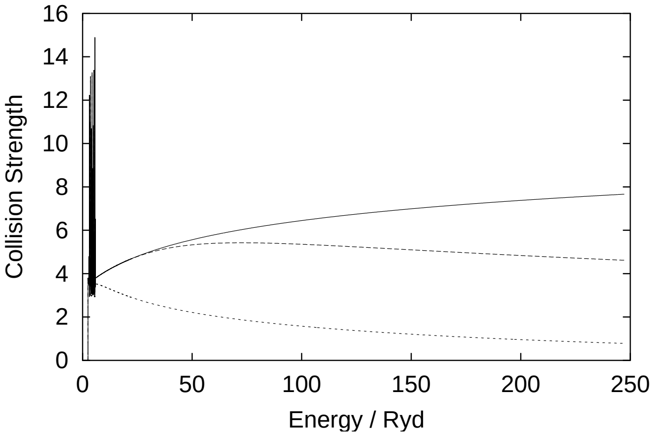


Figure 1: Contribution from different angular momenta regimes, the lower curve shows the inclusion of only the exchange data, the middle curve the inclusion of non-exchange data and the upper curve includes top-up.

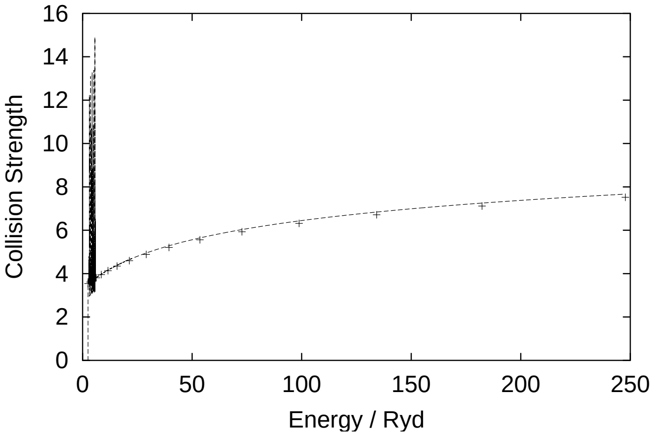


Figure 2: Comparison with the results of Mann

Downloading and compiling *R*-matrix codes

A D Whiteford and N R Badnell

15th October 2009

1 Downloading

For the examples were are running here, you will need to download the following files:

```
http://amdpp.phys.strath.ac.uk/rmatrix/ser/asy/PARAM
http://amdpp.phys.strath.ac.uk/rmatrix/ser/asy/stgf.f

http://amdpp.phys.strath.ac.uk/rmatrix/ser/ipbp/PARAM
http://amdpp.phys.strath.ac.uk/rmatrix/ser/ipbp/stg1r.f
http://amdpp.phys.strath.ac.uk/rmatrix/ser/ipbp/stg2r.f
http://amdpp.phys.strath.ac.uk/rmatrix/ser/ipbp/stg3r.f
http://amdpp.phys.strath.ac.uk/rmatrix/ser/ipbp/stglib.f

http://amdpp.phys.strath.ac.uk/rmatrix/ser/misc/omadd.f
http://amdpp.phys.strath.ac.uk/rmatrix/ser/misc/omgmrg.f
http://amdpp.phys.strath.ac.uk/rmatrix/ser/misc/adasex.f
http://amdpp.phys.strath.ac.uk/rmatrix/ser/misc/xtrct.f

http://amdpp.phys.strath.ac.uk/rmatrix/ser/nxls/PARAM
http://amdpp.phys.strath.ac.uk/rmatrix/ser/nxls/stg1nx.f
http://amdpp.phys.strath.ac.uk/rmatrix/ser/nxls/stg2nx.f
http://amdpp.phys.strath.ac.uk/rmatrix/ser/nxls/stg3nx.f

http://amdpp.phys.strath.ac.uk/autos/ver/asdeck.f
http://amdpp.phys.strath.ac.uk/autos/ver/PARAM
```

To prevent PARAM files from clashing, it's advised that you create different directories for the different codes in the same was as they are on the web.

2 Compling

This will vary from platform to platform, but a rough guide is given here. It is advised that if you don't have one already make a binary directory for yourself via

```
mkdir $\sim$/bin
```

Compile the codes by typing (in whatever directories you created):

```
f90 -O3 -o ~/bin/autos.x asdeck.f

f90 -O3 -o ~/bin/stgf.x stgf.f

f90 -O3 -c -o ~/bin/stglib.o stglib.f
f90 -O3 -o ~/bin/stg1r.x stg1r.f
f90 -O3 -o ~/bin/stg2r.x stg2r.f stglib.o
f90 -O3 -o ~/bin/stg3r.x stg3r.f stglib.o

f90 -O3 -o ~/bin/omadd.x omadd.f
f90 -O3 -o ~/bin/omgmrg.x omgmrg.f
f90 -O3 -o ~/bin/adasex.x adasex.f
f90 -O3 -o ~/bin/xtrct.x xtrct.f

f90 -O3 -o ~/bin/stg1nx.x stg1nx.f
f90 -O3 -o ~/bin/stg2nx.x stg2nx.f
f90 -O3 -o ~/bin/stg3nx.x stg3nx.f
```

Note that as you run the codes, they may need to be redimensioned, these is usually done by changing the appropriate PARAM file, when a code stops it is usually quite helpful about telling you what to change.

Worked example for Na-like Fe

A D Whiteford and N R Badnell

15th October 2009

1 Getting the example input files

Copy the file `allanw/na-fe-example.tar` to your chosen directory.

```
cp ~whitefor/na-fe-example.tar .
```

Untar it.

```
tar -xf na-fe-example.tar
```

You will now have a number of files as explained in the next section.

2 Directory Strucutre

- `str` - Structure run
    - `autos.dat` - Autostrucutre input file
    - `radout` - placeholder for radial wavefunctions
- `ex` - Exchange runs
    - `dstg1` - stg1 input
    - `dstg2` - stg2 input
    - `dstg3` - stg3 input
    - `H.DAT` - placeholder for stg3 output
    - `NX1.DAT` - placeholder for NX data
    - `NX2.DAT` - placeholder for NX data
    - `radial` - symbolic link back to structure run radial wavefunctions
    - `fine/` - sub directory for outer region runs
        - `dstgf` - stgf input [Damping: stgfdamp]
        - `H.DAT` - symbolic link back to stg3 output

  - `coarse/` - as for above

- `nx`- non exchange
  - `dstg3` - copy of stg3 input file
  - `dstgf` - stgf input file
  - `dstgnx` - stg1nx, stg2nx, stg3nx input file
  - `NX1.DAT` - symbolic link back to NX output from exchange run
  - `NX2.DAT` - symbolic link back to NX output from exchange run

- `tot` - merging of all omega files
  - `script` - script to merge all the omega files together
  - `adasexj.in` - input file to generate adf04 file

3 Brief summary

Step	Description	Directory
1	Structure calculation	str
2	Inner region exchange runs	ex
3	Outer region exhcange runs	ex/fine, ex/coarse
4	Inner region non-exchange runs	nx
5	Outer region non-exchange runs	nx
6	Merge omega files	tot
7	Generate adf04 file	tot

4 Running the codes

Starting from the directory na-fe-example, type:

```
cd str
~/bin/autos.x < autos.dat

cd ../ex
~/bin/stg1r.x < dstg1
~/bin/stg2r.x < dstg2
~/bin/stg3r.x < dstg3

cd fine
~/bin/stgf.x < dstgf

cd ../coarse
~/bin/stgf.x < dstgf
```

```
cd ../../nx
~/bin/stg1nx.x < dstgnx
~/bin/stg2nx.x < dstgnx
~/bin/stg3nx.x < dstgnx
~/bin/stgf.x < dstgf

cd ../tot

cp ../ex/fine/OMEGA ./omgmrg1
cp ../ex/coarse/OMEGA ./omgmrg2
~/bin/omgmrg.x

mv omgmrgt omadd1
cp ../nx/OMEGA ./omadd2
~/bin/omadd.x

mv omaddt omgmrg1
cp ../str/OMGINFLS ./omgmrg2
~/bin/omgmrg.x

mv omgmrgt OMEGA
~/bin/adasex.x
```

Be sure that you know what each stage is doing, refer to the notes for further details as to what each program does and what the input files mean.

5 Looking at the results

In your `tot` directory you have two important files, `OMEGA` and `adf04`.

To look at individual collision strengths use the program xtrct.x which you compiled earlier. To look at the level 1 to level 2 collision strength, run xtrct.x then type “1 -2” and press return (note: this is ‘1’ followed by a space, followed by ‘-2’. A file called xout will be produced which is in ascii format and can be interrogated with your favourite graphing package.

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 *mar18-02.pdf.*
    4. Bring up a acrobat viewer for *.pdf* files [*acroread &*] to look at the *mar18-02.pdf* bulletin. ‘Bug fix’ releases and the associated bulletin comes out every four months. New code releases are separate and occur when ready.
    5. Return to the Terminal window, move into the *docs*/ subdirectory *idl-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 *Chap6-03.pdf* and at *appxa-15.pdf*.
    6. Move to the directory */home/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 must not be accessible to the ordinary user.
    7. Now move to the directory */home/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 */Chap1-00.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 */Chap1-00.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.

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 – <u>there may be a lot of electron impact excitation transitions</u>.

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.

7. Example 7

7.1. 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.

8. Example 8

8.1. 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.

8.2. 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 *strathclyde_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.
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.
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 top right box, select *No* for the simple cut-off filter, then 23 for the *Beryllium thickness* and 12 for the *Silicon thickness*. Use integer values. Note that the *Current Filter Name* changes accordingly. This name enters the output power file names.
23. In the lower central box, select *eV* units.
24. In the lower left box for electron temperature, enter *Lower limit* 1.0, *Upper limit* 100.0, *No. of temps* 10.
25. In the lower right box for electron density, enter *Lower limit* 1.00e+10, *Upper limit* 1.00e+15, *No. of dens.* 11.
26. Click *Done* to advance to the Output window.
27. Enter 30 for the two-digit year number. Make sure there are no blanks. The Passing file template changes accordingly. It is editable.
28. Select *Text Output* and *Default File Name* and click *Done*.
29. Note the list of passing files which will be created is shown in an information widget. Click *OK* to accept the list.
30. Click on the *Escape to Menu* button to finish
31. Look at ACD30#C.pass. Note that it is fully formed ADF11 unresolved type file. Note that PLT30#C and PRB30#C appear both with and without the filter '*.ft02312.*'.

3. Example 1

Repeat ADAS405, but this time select the file *strathclyde_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 IDL-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 Qunatum 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.

The tutorial continues with some examples concerned with beam stopping and beam emission.

5. 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.

6. 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.

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The ionisation state of ions in a plasma
Callable ADAS Exercises

Allan Whiteford, Martin O'Mullane and Hugh Summers

9th October 2009

1 Aim

The aim is to familiarise you with callable ADAS for working with the ionisation state of ions in a plasma, mainly in an IDL environment. Please feel free to expand any of the tasks or change them slightly to deal with your favourite ion! The tasks marked with 🥕s should be considered optional and are often more difficult so don't spend too much time on them unless they are of particular interest.

2 Tasks

1. 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 🥕🥕.
2. 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) 🥕🥕🥕.
3. Use `run_adas405` to generate radiated power coefficients and plot them as a function of temperature.
    - Find an interesting density regieme 🥕🥕.
4. Use `read_adf15` to read the PEC for the 977Åline of C3+
    - Compare the power radiated in this line with the total line power for C3+ in coronal equilibrium conditions 🥕🥕🥕.
5. Use `run_adas416` to produce partitioned data using the file `/u/momullan/ADAS-EU_course/partition_example.dat`.
    - Modify the partition and explore how the various ions move in and out of being bundled🥕.

Charge exchange and beam emission spectroscopy
Callable ADAS Exercises

Allan Whiteford, Martin O'Mullane and Hugh Summers

13th October 2009

1 Aim

Presumably you know the aims by now. Harder questions are marked with 🎃s today.

2 Tasks

1. 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🎃🎃🎃.
2. 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🎃🎃.
3. Use `read_adf21` to read beam stopping coefficients for a plasma with 1% carbon content.
    - Integrate a real beam over a sensible profile, find the penetration depth as a function of carbon concentration🎃🎃🎃🎃🎃.
4. Use the AFG (ADAS Feature Generation) system to produce a beam emission feature (`res=afg(/help)`).
    - Have AFG return information about the various parameters to you and print them to screen🎃.
5. Use `run_adas310` to produce beam stopping coefficients.
    - Combine this with `read_adf21` to produce a plot of beam stopping as a function of beam energy without using a central ADAS ADF21 file🎃🎃.
6. Use `read_adf22` to read beam emission (`BME`) coefficients.
    - Integrate this into your (🎃🎃🎃🎃🎃) beam attenuation code to predict absolute beam emission as a function of radius🎃🎃🎃🎃.

CXSFIT Tutorial

Allan Whiteford, Martin O'Mullane and Hugh Summers

15th October 2009

1 Aim

The aim is to run CXSFIT and read AUG data and perform simple fits.

2 Tasks

1. Run CXSFIT by typing `/u/adas/run/cxsfit`
2. Read data for AUG shot 25321🧁.
3. Explore the data by changing the track and frame slider, find a nice CX spectra🧁🧁.
4. Play with the view options, in particular change the colour and contour schemes🧁.
5. Add a single line🧁🧁.
6. Fit the frame🧁🧁.
7. Narrow in the fit range or exclude some data🧁.
8. Refit the frame, is it better🧁🧁?
9. Fit all of the tracks and view the temperature contour plot🧁.
10. Find a fit where the temperature is too high, add parameter bounds and refit this frame — did it work🧁🧁?
11. Try to use multiple Gaussians to describe the passive and active feature🧁🧁🧁.
12. Add some lines to try to fit the other (unrelated) lines🧁🧁🧁🧁.
13. After you've got some good fits, switch to 'refit failed frames mode' and use 'previous frame estimates', do things get better🧁🧁🧁?
14. Try to find someone from AUG to show you how it's really done🧁🧁🧁🧁🧁.
15. Make a PNG of a spectrum as souvenier🧁.

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Appendix D

ADAS-EU external visits

[1] CIEMAT, Madrid, Spain (14-15 Dec. 2009)
[2] University Autonoma, Madrid, Spain (16-23 Dec. 2009)
[3] CEA Cadarache, France (18-22 Jan. 2010)
[4] CEA Cadarache, France (19-21 Jan. 2010)
[5] University Mons-Hainaut, Belgium (28-29 Apr. 2010)
[6] ITER, St Paul-les-Durances, France (7-18 Jun. 2010) - to be included

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ADAS-EU Travel Report

Location: Laboratorio Nacional de Fusion por Confinamiento Magnetico (National Laboratory for Fusion by Magnetic Confinement), Ciemat research centre. Madrid, Spain.
Date: 14-15 December 2009.
ADAS-EU staff: Francisco Guzmán
Persons visited: Francisco Tabares, Bernardo Zurro, Kieran McCarthy, Carlos Hidalgo.
Motivation: Discuss about the role of atomic physics in the work carried in Ciemat and how ADAS can help in a collaborative work.

Items:

1. F. Guzmán was invited to the physics meeting of the laboratory and presented there by F. Tabares who explained the motivation and interests of the visit. Some questions arose about what is ADAS and its role in plasma fusions that were explained by F. Guzmán. F. Tabares said that could be interesting that collaborations could be done with specific experimental Ciemat groups in the frame of ADAS-EU project.
2. A meeting with Bernardo Zurro was made afterwards. Bernardo Zurro exposed his research to study the line ratios of visible lines of CVI and CV ions to get H concentrations by CX recombination obtaining some surprising results as their modelling of the line ratio CV/CVI fails to decay ad the plasma edge and to predict the inner emission peaks [1]. B. Zurro attributes these failures to a some assumption of the model not taken in account as a non-Maxwellian distribution or a possible instrumental failure. His group used a CR model developed by L. Carraro et al. [2] in Padova University and adapted to the system. He wanted to know if something similar could be carried out using ADAS CR models for rate and emission coefficients to obtain the line emission rates. F. Guzmán exposed the capability of ADAS to obtain these results using the series 300 and 400 codes and agreed that could be done in a future collaboration.
3. A third meeting were agreed with C. Hidalgo who explained his diagnostic system. In this Cs^+ is accelerated to 200keV, injected in the plasma and ionized. The resulting Cs^{2+} output intensity is analyzed in function of density, electronic temperature and atomic physics factors [3]. The ratio of Energy between the input and output is used to obtain the plasma electric potential. C. Hidalgo talked about the necessity of having good atomic physics background for Cs. F. Guzmán explained about the current lifting of the data base to include heavy ions but recognized that Cs have been not included yet. C. Hidalgo expressed his hope of have accurate atomic data of this ion in the future. F. Guzmán asked about the possibility of inject other heavy ions that have been or will be included in ADAS such Xe or Kr. C Hidalgo said that could be considered but then the ions should be accelerated to higher energies that are not achievable at the moment.
4. In a talk with K. McCarthy, F. Guzmán was asked to give a tutorial of 1 or 2 days in Ciemat about ADAS, OPEN-ADAS and its use for the necessities of the laboratory. F. Guzmán agreed that this was possible in a future visit to Madrid. A practical demonstration of how to

extract data form OPEN_ADAS web service was done to K. McCarthy by F. Guzmán.

5. A final meeting with F. Tabares was done. In this, different issues where treated. A first issue on an atomic model for obtain the ion temperature profile in the plasma improving the model first published in ref. [4] in collaboration with F. Guzmán. To achieve it, a use of ADAS routines to obtain the HeII to HeI density ratio with a proper CR modeling would allow to calculate ionic temperature in plasma edge from experimental profiles and predict the rotational velocity of the plasma. In this way the He supersonic beam would be a very useful multidiagnostic tool providing several parameters of plasma as electronic density and temperature, ionic temperature and rotational velocity. F. Guzmán agreed to continue working in it in the future in parallel of his other responsibilities.
6. The second part of the meeting with Tabares was around molecules in the frame of the actual task of the visitor that is to create the database and infrastructure and CR codes for H_2 in a molecular amplification of the atomic database. F. Tabares group has a molecular beam where CH_4, CD_4 and C_2H_4 is injected and lines from the fragments of CH and C_2 are detected and its velocity measured making possible to study the possible dissociation path and bound breaking mechanism. F. Tabares talked about the possibility to inject H2,D2 and N2 in a molecular seeding technique where the molecules would be in plasma almost at rest and internal energies and excitation and ionization electronic transitions could be studied from an experimental focus in a plasma environment. That would help to cross check the theoretical data compiled for the ADAS database. That experimental display could serve for the hypothetical lifting of the database to N2 in the future as N is a impurity involved in scavenging and divertor cooling.
7. In a final issue, F. Tabares alluded to transport studies performed in TJ-II in Li and Li+ in the SOL as now TJ-II is coated with Li and N ionization stages time depended population model for the X-ray spectroscopy studies carried out in collaboration with Juelich laboratory in TEXTOR machine. That time dependent model is included into ADAS routines and could be carried out in the future.

F. Guzmán
6/01/2010

REFERENCES

[1] B. Zurro et al. Rev of Sci. Inst. **79**, 10F540 (2008)

[2] L. Carraro et al. Phys. Scr. **55**, 565 (1997)

[3] I.S. Bondarenko et al. Rev of Sci. Inst. **72**, 583 (2001)

[4] F. Guzmán et al. J. Nucl. Mat. **390–391**, 1127 (2009)

ADAS-EU Travel Report

Location: Departamento de Quimica (Chemistry Department). Universidad Autonoma de Madrid,Madrid, Spain.
Date: 16-23 December 2009.
ADAS-EU staff: Francisco Guzmán
Persons visited: Luis Errea, Luis Mendez.
Motivation: Obtain data for atomic collisions to and from excited H in the frame of the collaboration ADAS-EU and UAM.

Items:

1. F. Guzmán was working in the computer of L. Errea group to obtain the previously calculated data for excitation for H(1s) + Ar^{18+}, H(1s) + Li^{3+}, H(1s) + Ne^{10+} and H(1s) + B^{5+} to H(n=2-6) (in the case of B only to n=2) that were calculated previously [1,2] by J. Suarez and himself. These data will expand the atomic database in ADAS.
2. New calculations of CX cross sections B^{5+} + H(n=2-3) were performed in addition to the already existing calculation B^{5+} + H(2s) [3] and comparisons were done with the data in ADAS for H(n=2) donor [4]. A new set of recommended CTMC cross sections data for B^{5+} + H(n=3) collisions has been released after calculations performed by F. Guzmán during the visit. After create the ADAS format files Effective coefficients were calculated using ADAS for fusion plasma relevant parameters. All this work will be submitted to a special number of J. Phys. B dedicated to plasma fusion spectroscopy.
3. It was agreed that all the data from points 1. and 2. will be introduced into ADAS database in the future.

F. Guzmán
6/01/2010

REFERENCES

[1] J. Suarez. Ph.D. Thesis. Universidad Autonoma de Madrid (2005)

[2] L.F. Errea et al. Plasma Phys. Control. Fusion **48**, 1585 (2006)

[3] L.F. Errea et al. J. Phys Conf. Series **58**, 203 (2007)

[4] R. Hoekstra et al. Plasma Phys. Control. Fusion **390-391**, 1127 (2009)

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ADAS-EU Travel Report

Location: CEA, Cadarache, France.
Date: 19-21 January 2010.
ADAS-EU staff: Francisco Guzmán
Persons visited: Remy Guirlet.
Motivation: First Contact visit to discuss possible fields of work and collaborations between the representing ADAS and CEA and ITER staff when the former is based in Cadarache.

Items:

1. F. Guzmán was meeting Remy Guirlet, his contact in Cadarache. R. Guirlet explained about the impurity transport research and about the simulation transport code CRONOS. CRONOS makes use of ITC (Impurity Transport Code). An informal meeting was held after with Thierry Aniel, responsible for the Coupling between ITC and CRONOS. ITC solves coupled time dependant transport equations which depend of the rate coefficients. These rate coefficients came now from Padua but is desired that a review and maintenance would be done from ADAS data. CRONOS uses these results to modelate a self consistent plasma reconstructing the parameters of the plasma. A new genetical algorithm is being implanted to avoid local minima in the iterations of the code.
2. A videoconference meeting was done afterwards. There were present Remy Guirlet, Thierry Aniel, F. Guzman in Cadarache and Frederic Imbeaux and Mireille Schneider at JET at the moment. M. Schneider is in charge of ITER neutral attenuation modeling and F. Imbeaux is responsible for the definition of the atomic data structure in ITM task force. M. Schneider started to ask several questions. First she asked about the stopping coefficients for W in ADAS. F. Guzman answer that there were not available at the moment but they could be generated from the cross section files and in any they could be available soon. The following question was about nuclear reactions in ADAS. F. Guzman answered that ADAS was an atomic data base and was out of its scope to deal with nuclear cross sections. She also expressed the necessity to have beam neutralization coefficients by charge exchange and recombination and cross sections at non thermal conditions. She asked about the existence of stopping coefficients that include contributions from ions and electrons it the same time. F. Guzman answered that he did not know at the moment unless both contributions could be separately added; anyway he had to look for it.
3. In the second part of this meeting F. Imbeaux explained about ITM format specifications. This will be based in the Consistent Physical Objects (CPOs) representing different physical quantities that have a hierarchy in dimensions of dependence and should fulfill several requisites (e.g. be language independent). He suggested that the experience acquired by F. Guzman in ADAS would be of great help to be involved in the filling with data of CPOs from ADAS. F. Guzman agreed with that but expressed his desire to also be involved in a less only-technical work that required a bit of more physical thinking. Was agreed that F. Guzman should go more deep into ITM modeling in a physical way and that could feedback the filling of CPO improving the format of them.
4. A first contact meeting in Atomic Data was held in Cadarache on 20th of January were experimental spectroscopist and theoretical atomic physicist were met with ADAS staff H. Summers and F. Guzman. ADAS data was the central point of the meeting as serves of interface between one and the others. This meeting is explained in detail in H. Summers report.

5. A formal meeting with Alan Becoulet, head of the Plasma Heating and Confinement Unit was held in 21st. There F. Guzman was introduced to A. Becoulet by R. Guirlet. A discussion about future work in CEA followed. A. Becoulet agreed in the possible areas of working that were been considered. New discussions about ITM and other issues were done with R. Guirlet this day. A meeting with J. Garcia working in CRONOS simulation at ITER scenarios was not possible as he was having a period in JET.

F. Guzmán
1/02/2010

ADAS-EU Travel Report

Location: CEA Cadarache, France,
Date: 19-21 January 2010.
ADAS-EU staff: Francisco Guzman, Hugh Summers.
Persons visited: Remy Guirlet, Richard Pitts, Steve Lisgo, Dan Thomas, ~20 participants at the organized mini-workshop meeting.

Items:

(1) The meeting was planned as a first contact between the French Fusion Research Federation and ADAS organized by Remy Guirlet and Yannick Marandet. Participants/presenters represented atomic and molecular calculations at Université du Havre, Laboratory Aimé Coton, Paris, CEA/CELIA Bordeaux and University Aix/Marseille. Local participants, representing CEA Cadarache and ITER, explained required atomic/molecular physics in their fusion plasma/device applications.

(2) An approximate agenda as below was followed:

8.50am. Introduction (R. Guirlet - Y. Marandet)

9.00 am. ADAS presentation (H.P. Summers - ADAS)

9.45am. Molecules in ADAS (F. Guzman - ADAS-EU)

10.45am. ITER context (R. Barnsley, Dan Thomas - ITER IO)

10.45am. Molecular calculations (I. Schneider - Université du Havre)

11.30 am Heavy species calculations (O. Peyrusse - CEA/CELIA Bordeaux)

2.00 pm. Local activity on ITER neutral beam injector (A. Simonin)

2.45 pm Local activity on plasma edge, particles sources and transport (Y. Marandet)

3.30 pm Local activity on impurity transport in the core plasma (R. Guirlet)

Some aspects of the discussions are summarized below.

(3) The ADAS presentation of Hugh Summers focussed on heavy species in ADAS touching on the very complex systems; large-scale, semi-automatic, sized, structure calculations for excitation state and emission; similarly handled and sized ionisation and recombination data calculation for ionisation state; superstage compression.

(4) The ADAS presentation of Francisco Guzman focussed on the steps being taken in ADAS for handling hydrogen molecular data; the new mdf04 format – pre-format and final-format; data sources being accessed and Franck-Condon issues; plans for basic molecular CR model.

(5) An overview of the work at LeHavre was summarized by Ioan Schneider and dealt with collisional (for electron collisions) and quantum chemistry methods (for ion collisions). The multi-channel quantum defect (Jungen) was highlighted and competition between processes addressed. Points of emphasis included H_2^+ dissociation, importance of rotational couplings, vibrational substates and excited (electronic states). Attention was drawn to their own in-house ab initio calculations of potential surfaces.

(6) A more specific talk by Francois Lique of the LeHavre work addressed neutral systems, structure and dynamical studies of the nuclei, x-sect calculations with close-couping, coupled state and IOS sudden approximations mentioned. CN+He has been studied , using MCSCF and MOLPRO for potential surface calculations, with experimental comparisons. $F+H_2$ and O+OH were mentioned – systems picked as of relevance, but not really confirmed by the fusion physicists. Full quantal dynamic calculations (TID) were

described. Request for other systems to be recommended. On quering by Hugh Summers, it seemed that although their work is used by Fantz/Wunderlich there is not really a two-way communication in which feedback and accuracy queries are interchanged. There seems opportunity for a more cohesive, mutually supportive relationship with them on the fundamental molecular data side.

(7) Oliver Peyrusse represented the Bordeaux group and also Jacques Bauch and Madame Bauch from Paris. He focused on NLTE modelling of tungsten in highly ionized plasma coming from the high density laser fusion camp. Described the superconfiguration approach (AVERROES code), together with refinements and split-up to allow for lost couplings. Referred to Bar-Shalom methods for angular and radial separation and non-relativistic (Cowan) structure calculations – but not sophisticated in this respect. Wished to pursue comparison with ADAS CR models and promoted the Ralchenko benchmarking meetings of the laser fusion (Livermore, Los Alamos) group. In discussion, the philosophic differences between low density, time constant ordered collisional-radiative theory and the high density approach were mentioned by Hugh Summers. Hugh Summers also emphasised the difference in use of high efficiency R-matrix methods Vs all states included. The physical role of ion collisions in establishing statistical sub-state populations was explained and it transpired that the source of electrons being principally hydrogen (not the heavy species) had not been taken onboard. How to engage, and the value of engagement with this aspect of the Bordeaux.Aime-Coton group remains unclear at this stage. The high precision heavy species structure work of Wyart (not at the meeting) seems more relevant,

(8) Remy Guirlet gave a broad overview of transport in tokamaks and Tore-Supra in particular, the associated modelling and the spectra diagnostics used to explore it.

(9) Dan Thomas reviewed ITER atomic data needs and queries and used many illustrations of ADAS data calculations supplyingf these needs. Many figures came Robin Barnsley and had been originally from reports to Robin by Martin O'Mullane. He refered to TRIM code data and need for new data (Eckstein 1985). Also mentioned CXS especially at beam energies 100keV (H diagnostic beam), 870keV (H heating beams) 1MeV (D heating beams) from H- sources. Interested in high z impurity radiation rates, tungsten -neutral and low stages- for start-up scenarious. Molecular calculations for tritium inventory – dirty plasmas, Be, C, W walls materials. Mentioned many more diagnostic and interpretative needs. Stressed procurement of diagnostics in 2010-2011 and the role of atomic physics in improving the design specs and capabilities – an influence which is needed in the next 3-5 years. Talk was a bit random and off-the-wall.

(10) A Simonin described the R&D around the ITER NBI systems - principles and modelling. Described D_2 gas target forseen for testing the 1MeV, 17MW D^0 ITER beamline. Note designed for 100-3600 sec operation. He emphasized D chemistry in the negative ion source and refered to the LAPLACE lab., Toulouse. It appears that there quite a lot oc complex codes and lots of plasma chemistry including e, , H_2^+ , H_3^+ , H^- , H^+ and H and linkages to fluid codes and Maxwell equations? Cf W4 modelling? Rather a detailed, self-sufficient kind of talk which did not really open up opportunities for new collaborations or a role for ADAS.

(11) Yannick Marandet (Marseille, CEA) described local activities on plasma edge sources and transport – spectroscopy of source particle movements and applications to Tore Supra. Nice work on D+/D recycling and use of photon efficiencies. Referred to ADAS data but augmented with molecular H_2 contributions. Spatially resolved experimental measurements of sources at different points of the Tore Supra pumped limiter enabled connection with different dissociation sources. Comments on cold divertor issues, $D_2(v>3)$ -> D_2^+ role, molecular assisted recombination, molecular associative recombination – possibly less important than originally thought (cf Fujimoto and Sawada). Discussed chord geometry issues and losses at the wall . Discussed moving on to C. Hugh Summers raised the issue of metastables fluxes in carbon influx. This was an interesting talk by a very competent person and suggests interesting collaboration for us down the line. He had a clear propensity to work with ADAS, using and criticizing contructively.

(12) One to one discussions took place with Steve Lisgo and Richard Pitts over lunch. The expectations and role for ADAS seem large. A working visit to launch ADAS at ITER in the near future would be very welcome.

HPS
27 Jan. 2010

ADAS-EU Travel Report

Location:	Department of Physics and Astrophysics, University of Mons-Hainaut, Mons, Belgium.
Date:	28-29 April 2010.
ADAS-EU staff:	Hugh Summers, Martin O'Mullane, Francisco Guzman (29 Apr).
Persons visited:	Emile Biémont, Patrick Palmeri, Pascal Quinet.

Objectives:

(1) First working visit on the ADAS-EU sub-contract with Mons-Hainaut.

(2) Review plans and progress for the ADAS-EU sub-contract.

(3) Take first steps towards creating a semi-automatic computer code and data transfer interface between Mons-Hainaut spectral data fits and ADAS codes and input datasets.

(4) Compare Mons-Hainaut WI, WII and WIII spectral line reviews with current tokamak observations and line lists.

Items:

(1) Emile and Pascal described the progress of the tungsten studies. A draft paper for J.Phys.B (Special Edition on Spectroscopic Diagnostics of Magnetic Fusion Plasmas) has been prepared summarizing spectral line lists for WI, WII and WIII. For this paper, previously published Mons-Hainaut measurements and lifetime/spectral fits for WII (Eur. Phys. J. D 49, 13 (2008)) and WIII (Physica Scripta 78, 015304 (2008)) were available. The WI spectral line data derived from other sources including Den Hartog and Wyart. Fresh Mons-Hainaut/Lund experiments on WI are some months away. Pascal has meanwhile carried out some Cowan code parametric adjustments and fitting tests on the existing Wyart data. This seems quite successful on the ground state system but less good so far on the alternate spin system. Pascal will continue work on this and is optimistic that he will improve the alternate system fits with an expectation of usable results around August 2010.

(2) Francisco had with him the observed WI lines from Textor at Fz-Juelich and also the earlier calculations and 2008 paper of Beigmann and Vainstein. He was able to cross-identify and a number of WI lines with the Mons-Hainaut review. He will continue this study, including WII and WIII at Fz-Juelich although WII and WIII move us into the VUV region and away from the useful visible emission along directed lines of sight at target surfaces.

(3) ADAS and Mons-Hainaut both use the Cowan atomic structure code, but with somewhat different objectives and options. At Mons-Hainaut, the key issue is choice and optimising of adjustable parameters of the Cowan code – in particular polarisation, finite nuclear dimension and effective interaction parameters. These data are prepared and passed on in the Cowan *rcn2* setup output file *ing.11* for processing in *rcg* for line strengths. This is the endpoint for Mons-Hainaut although they also use *rce* for parameter optimising by fits to experimental line data. ADAS transparently passes *ing.11* through although it is modified slightly. ADAS runs the both the *rcn2* and *rcg* steps twice to produce both line strengths and Born approximation collision strengths Maxwell averaged rates. Martin's ADAS extension code step *ifg* gathers all the necessary output from the Cowan code and executes *ifgpp* to assemble the standard ADAS adf04 dataset type. The latter is the key input file type for population modelling from which SXB, PEC and other derived quantities may be produced automatically by ADAS procedures.

(4) The offline ADAS implementation of Cowan's code (ADAS8#1) was transferred to Patrick's laptop. After some re-dimensioning, choice of Fortran compilers and script adjustments, the code seemed to be working - producing credible output. Sample Mons-Hainaut *ing.11* data sets for WII and WIII were transferred to Martin's ADAS laptop. Some minor reformatting was necessary, but then the ADAS completion steps ran to deliver an *adf04* dataset. It seemed therefore that a connection had been achieved.

(5) The next stage is to coordinate activity and computer processing for systematic, semi-automatic delivery of adf04 datasets from Mons-Hainaut inputs. One suggestion is that there should be transfer to ADAS processing from Mons-Hainaut of two prepared *ing.11* intermediate files (for line strengths and collision strengths). The ADAS8#1 script could be modified to pick up the *ing.11* datasets if present, automatically reformat it appropriately, and then run through the final steps. Agreement of Mons-Hainaut is now required as to whether this is the preferred transfer route. If so Martin will implement the script and code adjustments to ADAS8#1 for both ADAS and Mons-Hainaut to use. Patrick and Pascal will decide on suitable mix of *ing.11* samples and check results for

running and verification by Martin. Patrick will check out correct operation of the modified ADAS8#1 at Mons-Hainaut.

(6) Hugh emphasised the merit of carrying as much as possible of the historic Mons-Hainaut work into the fusion domain via the above processing route. Although tungsten is the immediate focus, related elements such as Re and Ta are of interest, while a whole range of second and third long period elements many be relevant as markers or occasional sources. Influx spectroscopic measurements are most usefully made on the neutral or single ionised stages of such elements. The legacy of work at Mons-Hainaut, systematically converted, can provide a real service to fusion.

(7) There was discussion on whether interpolation was possible between systems explicitly measured at Mons-Hainaut. Emile and Pascal felt that interpolation was feasible between homologous series members and along iso-electronic sequences and pointed out the global scaling work of Wyart. Hugh was particularly interested in interpolation along periods, since it is really neutrals and singly ionised which are of greatest value for influx measurements. Emile was more doubtful about this, but will look further into the matter.

(8) Hugh said that by the end of ADAS-EU, he would like to see a large paper of review character completed - essentially a companion to the light element paper K H Behringer, H P Summers et al. (Plasma Physics & Control. Fusion 31, 2059 (1989)), but for heavy elements. It would be comprehensive and take the generalized collisional radiative viewpoint for SXBs etc. Hugh felt this would be of great value for ITER and would be very well received.

(9) There was general satisfaction with progress so far and agreement on the further steps detailed above. Assignment of on-going tasks from the above are broadly (i) WI fit – Pascal; (ii) Parameter interpolation – Pascal, Emile; (iii) Mons_Hainaut Cowan/ADAS interface – Patrick, Martin; (iv) Fz-Juelich influx line observations – Franscisco; (v) Heavy species review paper design – Hugh.

(10) It was felt that it would be good to hold the next meeting at EFDA-JET in a few months on a date to be decided.

HPS
6 May 2010