jan18-96

ADAS Bulletin

Five new programs are ready. The first pair concern beam stopping and belong to ADAS series 3. ADAS304 is the beam stopping interrogation code operating on beam stopping coefficient compilations (*adf21*). ADAS310 is a population code which allows calculation of effective beam stopping coefficients. Then turning to ADAS series 2, David Brooks has completed his level unbundling code ADAS210 to match the level bundling code ADAS209. The ADAS series 2 menu has been extended accordingly. In preparing ADAS210, David has made some adjustments to ADAS209 so that both routines have a common look. To support ADAS209 and ADAS210, we shall be extending the *adf04* data in the database substantially. In ADAS series 5, two new interrogation routines have been added. These are ADAS502, which interrogates zero-density direct electron impact ionisation rate coefficient data (*adf07*) and ADAS504, which interrogates zero density radiative power loss coefficients (*adf19*).

A number of tiding up and error correction steps have been taken. ADAS207, the line ratio diagnostic program now includes recombination contributions. A new data entry table appears so that the ratio of ionisation stage abundances and of neutral hydrogen to electron density can be entered. Also ADAS401 now permits interrogation of low level line power coefficient data (*adf10*). The escape to menu icon has also been added in several more programs. **Remeber to delete your defaults file for a revised program and let ADAS recreate it if you have problems**.

Alessandro's differential emission measure analysis code has now been decoupled from dependence on the NAG library (not all sites have this package on their workstations). At release 1.6 we shall place it on all sites. It is presently only available at Rutherford-Appleton Laboratory and needs a little extension to increase its flexibility with noisy data before final relase. It is launched from a new ADAS series 6.

1. **ADAS304**

The program interrogates beam stopping coefficient files of type adf21. Data is extracted for stopping by a composite plasma consisting of a mixture of protons (deuterons) and fully ionised impurities. The adf21 data sets are composed of pure species stopping coefficient scans over plasma parameters.

- 1.1. Move to the directory in which you wish any ADAS created files to appear. These include the output text file produced after executing any ADAS program (*paper.txt* is the default) and the graphic file if saved (e.g. *graph.ps* if a postscript file). Initiate ADAS and move to the series 3 menu. Select ADAS304.
- 1.2. The **file selection window** appears first and is illustrated below. Its operation is a little different from usual.
 - 1.2.1. *adf21* is the appropriate format for use by the program ADAS304 (ADAS User Manual, *appxb-21*). 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*.
 - 1.2.2. A root path to the correct data type *adf21* appears automatically a). 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.
 - 1.2.3. At b) a group name for the input files is entered. This is the name of a subdirectory of *adf21* for a particular beam species (usually H or He). The subdirectory contains individual data sets for each impurity contributing to stopping, identified by the element symbol. 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. ADAS304 allows you to select all the impurity files you wish easily. Click the *Reselect Ion List* button. The small pop up selection widget below appears showing available species a). Click the toggle buttons of those you wish to include
 - 1.2.4. Click *Done* to restore the main input widget. Your choices are shown at the Stopping Ion List.

1.2.5. Clicking on the *Browse Comments* button displays any information stored with the selected datafiles. It is important to use this facility to find out what has gone into the dataset and the attribution of the dataset.



1.2.6. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window.



- 1.3. The **processing options window** has the appearance shown below
 - 1.3.1. The Stopping ion list is repeated at a) for information. The *Browse Comments* button is also provided.
 - 1.3.2. 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 at b).
 - 1.3.3. The selection of density, temperature and beam energy sets for data output are made at (e). 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 colums. 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*. *Default Output Values* and *Clear Table* buttons are provided.

- 1.3.4. A choice of which parameter of the input model set to use as the x-coordinate of graphs is given at c). Click on the required button.
- 1.3.5. The mixture of species contibuting 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.
- 1.3.6. 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.



- 1.4. The **Output options window** is shown below. Broadly it follows the pattern of other ADAS interrogation codes.
 - 1.4.1. Graphical output is enabled by clicking on the button at (a). Default scaling of graphs may be over-ridden by appropriate selections at (b). Hard copy may be enabled at (c) and a choice of type of output device made.
 - 1.4.2. As usual a line printer text output file summarising the interrogation may be produced.
 - 1.4.3. Click the *Done* button to show the graph of composite stopping coefficient and the contributuions of the different impurity species. *Cancel* take syou back to the Processing Options window and the *Exit to Menu* icon takes you directly to the ADAS3 series menu.

\square	ADAS304 OUTPUT OPTIONS	
 Graphical Output Graph Title Figure 1 		
Explicit Scaling	Beam energy plot :- X-min : X-max : Y-min : Y-max :	
 Enable Hard Copy File Name : graph.ps 	□ Replace	Select Device Post-script Post-script HP-PCL HP-GL
Text Output R File name : paper.txt Image: Cancel Dor	Default file name	

The program calculates beam stopping coefficients for a neutral hydrogen beam in a plasma of arbitrary composition and conditions of temperature and density. It organises and computes the stopping coefficients as one dimensional scans in the key parameters of neutral beam energy, ion density and ion temperature about a reference condition and outputs them in the format of data type *adf21*. In fact the underlying code is a full bundle-n collisional-radiative model which for the present purpose we are only using to obtain the collisional-radiative ionisation coefficient (the effective stopping coefficient). We have organised the code output so that all the other useful information (beam emission coefficients, thermal emission coefficients, low temperature collisional radiative coefficients etc). is easily accessible. I shall discuss this later in a usernote about off-line subroutines. Because of the comprehensivee nature of this code, there are quite a lot of data to enter. However we have set up default values so as to minimise the problem for those who are not too interested in such details.

- 2.1. Move to the directory in which you wish the ADAS created files to appear. These include the output text file produced after executing any ADAS program (*paper.txt* is the default), and up to four further output data files. There is no graphical output from this program Initiate ADAS310 from the program selection menus in the usual manner.
- 2.2. The **file selection window** appears first as illustrated below.
 - 2.2.1. At a) 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 centra ADAS database at this time.
 - 2.2.2. There are two data files to be selected, the expansion file and the charge exchange file. The procedure is the same in both cases.
 - 2.2.3. 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. 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.

- 2.2.4. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing
- 2.2.5. 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.
- 2.2.6. 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*.
- 2.2.7. The expansion file is selected at b). 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.

\bigtriangledown	ADAS310 INPUT]
	Please enter beam species details :- Beam species element symbol [H] Beam species ion charge [0.0]	
	Expansion File Details Data root //export/home/adas/adas/adf18/	· a)
	Central data User data 🗌 Edit Path Name	
	Dummy Data File: a09-a04 bndlen_exp#h0.dat	b)
	Charge Exchange File Details Data root /export/home/adas/adas/adf01/	
	Central data User data \Box Edit Path Name $axx#b0/axx#b0 a2x#b1 dat $	
	Data File: qcx#h0_e2p#h1.dat qcx#h0_e2s#h1.dat	c)
	Edit the processing options data and press Done to Proceed Browse Comments Cancel Done	

2.2.8. The charge exchange file is selected at c). Again this 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 thje

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.

- 2.2.9. Clicking on the *Browse Comments* button displays any information stored in the selected charge exchange 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.
- 2.2.10. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

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

2.3.1. 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 at b). The default settings are reasonable and they can be ignored as long as only beam stopping is the intent.



- 2.3.2. Switches (I) allow some choices to do with electron collision cross-sections and Switches (II) allow some choices to do with ion collisiion cross-sections. (see the corresponding sub-window inserts below Make sure that Access to low level data is chosen at a) and Use beam energy informing cross-sections at b). It is this latter piece of information that informs the calculation that the neutral hydrogen is in the beam and not in the plasma.
- 2.3.3. The choices at c) above must then be made. Click the *Impurity information* or *Representative N-shell* buttons. The appropriate sub-window is displayed at c).
- 2.3.4. 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.

Please enter the following parameter	switches :-
Delta N range for impact parameter cross-sections	: 2 [max value of 4]
Use Percival-Richards cross-sections	: NO [NO defaults to van Regemorter X-section]
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	: 3 [max value of 3]
Use Lodge ion impact cross-sections	: NO [NO defaults to Vainshtein X-section]
Use beam energy in forming ion cross-sections	: YES
	b

- 2.3.5. The Impurity information sub-window is shown below. There are two modes of operation. Single impurity or Muliple impurites. Click the drop-down list button to make your choice.
- 2.3.6. 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 3.10.16 and 3.10.17 in the ADAS User Manual). The proton and electron density choices to be made next influence this.
- 2.3.7. 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.



2.3.8. At d) the choice of plasma and beam parameters for the scans are 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.

- 2.3.9. Note that a neutral hydrogen density in the beam is requested. This is necessary to allow a mathematical separation of the various influnces on the neutral hydrogen population structure and is not an experimenal beam density. A value of order 10^6 or greater is suitable for the program operation.
- 2.3.10. Clicking the *Done* button causes the output options window to be displayed. Remember that *Cancel* takes you back to the previous window.
- 2.4. The **output options window** is shown below.
 - 2.4.1. It follows the usual pattern except that there is no graphical output.
 - 2.4.2. The Run Summary is given in the output file specified at a). 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.

	ADAS310	OUTPUT OPTIC	DNS]
Title for run :				
Run Summary Output File name :	Append	Replace	Default file name	
First passing file	Append	Replace	Default file name	
File name : data.pass1				
☐ Second passing file File name : data.pass2	Append	Replace	Default file name	
Third passing file	Append	□ Replace	Default file name	
File name : data.pass3				
 Fourth passing file File name : data.pass4 	Append	Replace	Default file name	
	Now			C

- 2.4.3. Four additional passing files may be produced which are placed in your pass directory. The fourth is the assembled stopping coefficients structured according to an *adf21* file. The first passing file 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).
- 2.4.4. Click the *Run Now* button to initiate the calculations. These are run in foreground since they are of fairly modest duration. A thermometer widget illustrated below keeps you informed of the progress of the calculations.



The description of the code is repeated here (cf. bulletin *jul18-95*) since the displays are a little different. This code is not part of JET-ADAS but is only present in the workstation based IDL-ADAS. It is designed to help with the problem of being overwhelmed with data when studying the excited populations and emissivities of complex ions. We seek to simplify by grouping excited populations of similar levels or of levels of minor importance. We call this 'working at different resolution levels' in excited population structure. A specific situation is that in astrophysical studies where intermediate coupling LSJ resolution of populations structure point of view LS resolution is adequate. In fusion, LS resolution is usual for light species. The new code allows controlled 'bundling' of level populations. It does this by operating on a specific ion file (type adf04) of high resolution and generating a new file of the same type but of lower resolution as prescribed by the user. Such an algorithm is also of value with very many level systems where there is a need to focus on the most important levels, for example metastables, and treat other levels more grossly.





3.1.1. 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.

- 3.1.2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
- 3.1.3. 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.
- 3.1.4. 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*.
- 3.1.5. Once a data file is selected, the set of buttons at the bottom of the main window become active.
- 3.1.6. 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.
- 3.1.7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

∇ ADAS209 : PROCESSING OPTIONS Click to edit :-Data File : /disk2/adas/adas/adf04/belike/belike jl1990o.dat ♦ Level Bundling ♦ Parent Bundling V Data File Name : Browse Comments a) /disk2/adas/adas/adf04/belike/belike il19900.dat < Press return after each entry > Browse Comments Ion : 0+4 Nuclear Charge : 8 2s2(1s0) (1)0(0.0) 0.0 1 Specific ion file level list :-(3)1(0.0) 2s2p(3P0) 81942.5 2 Index Configuration Designation Energy(cm-1)2s2p(3P1) (3)1(1.0)82078.6 2 1 2s2(1S0)(1)0(-0.0)0.0 2s2p(3P2) (3)1(2.0) 82385.3 2 2 2s2p(3P0)(3)1(0.0)81942.5 3 2s2p(3P1)(3)1(-1.0)82078.6 Λ 2s2p(3P2)(3)1(-2.0)82385 3 b) \triangleleft Cancel Done

d

 \triangleright

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

e)

3.2.1. At a), two buttons are present to allow bundling of the levels of the selected ion and then bundling of the parents of these levels. The parents are the ground and metastable levels of the next higher ion to which ionisation may take place or from which recombination may take place. For basic studies, you will probably be using adf04 datasets which omit recombination and assume ionisation only to the ground state of the next higher ion. Then the subtleties of parents may be ignored. This parent bundling option is non-trivial only when the advanced adf04 specification is being used. More details are given in the ADAS Manual. Click the appropriate button to fill the left side level display window b) and the right side Bundling window d).

- 3.2.2. The level list displayed in the window at a) is for information only and is a simple transcription of the list from the head of the source *adf04* file.
- 3.2.3. Note that the Data File Name at the left side is the same as the Data file at c) on the right side.
- 3.2.4. In the Level Bundling window, the index number, configuration specification, (2S+1)L(J) quantum numbers and the level energy (cm-1) are given for each level in a separate display window with an editable box to its right d). The editable box is for entering a bundle index number. That is levels which are to be grouped are given the same bundle index number. If no index number is given for a level, then the code treats the level as a distinct bundle. The code reindexes bundles as necessary for consistency. **Remember to press Return after entering each bundle index**.
- 3.2.5. When you have finished the level bundling allocation, click the *Parent Bundling* button at a) to execute parent bundling. Note you may proceed to the next screen directly by clicking the *Done* button after level bundling. The code then puts in the default parent.



- 3.2.6. On clicking the Parent Bundling button the windows at b) and d) are filled with the corresponding parent information. The display is illustrated below. It generally has less than five entries and if the advanced *adf04* format is not in use then only one. The information format is a little different from that of the levels. The first value is the index number, followed by the parent term character string (in brackets) as given on the top line of the *adf04* file. The numerical value of the parent statistical weight follows with finally the parent energy (cm-1) relative to the lowest level of the ion. In the single parent case therefore this is just the ionisation potential.
- 3.2.7. Note that the organisation of all *adf04* datasets at present is such that although energy levels may be at the J-resolved intermediate coupling resolution, the parents are at term resolution. Thus there is usually no need to bundle parents unless there is a wish to focus for example on just the ground parent (lowest ionisation continuum). The latter may be the case if one wishes to bypass the complexities of metastables.

- 3.2.8. Note the icon for *Exit to Menu* at (e). This quits the program and returns you to the ADAS series 2 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen
- 3.3. The **output options window** is of restricted form. It only offers the option of an output file. This part is of the same layout as codes previously described.

	ADAS209 OUTPUT OPTIONS
,	Data File Name : /disk2/adas/adas/adf04/belike/belike_jl19900.dat
a)	Browse Comments
u)/	
	□ File Output □ Replace Default File Name
	File name : /disk2/brooks/adas/pass/bundle.pass
	Cancel Done b)

- 3.3.1. The name of the source data file which has been bundled is repeated at a) for information. The output file is the bundled adf04 file and it is of the correct format for re-entry in the adf04 database. However, if you have used the defaults on parent bundling, it is advisable to check the top line of the file to see that the term allocation of the ground state is what you wish. The comments section at the end of the output adf04 file details the source adf04 file and the bundling imposed.
- 3.3.2. By default the output file is sent to your */pass* file subdirectory as *bundle.pass*. You should ensure that you have created a */pass* sub-directory of you personal */adas* directory to receive such files.
- 3.3.3. There is no graphical output option.

This code is not part of JET-ADAS but is only present in the workstation based IDL-ADAS. It is designed to help with the problem of handling data when studying the excited populations and emissivities of ions at different degrees of fineness. We call this 'working at different resolution levels' in excited population structure. We seek to to change between resolution levels easily. A specific situation is that in astrophysical studies where intermediate coupling LSJ resolution of levels is usual, even for light species, to assist high resolution spectroscopy. From the population structure point of view LS resolution is adequate and so in fusion, LS resolution is usual for light species. We may have data of high quality at LS resolution for some ions which we wish to convert to LSJ resolution for special studies. The new code allows controlled 'unbundling' of level populations. It does this by operating on a specific ion file (type *adf04*) of low resolution and generating a new file of the same type but of higher resolution as prescribed by the user. Such an algorithm is also of value with very many level systems where there is a need to focus on the most important levels perhaps at high resolution while treating other levels more grossly. Such a procedure is of course not a substitute for original high resolution cross-section data. However the procedure tries to maintain precision by using a 'template' file of high resolution (also of type *adf04*) to aid in the 'unbundling' of the low resolution source adf04 file.

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

4.1.1. Selection of the source file to be unbundled is made in the top window. 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.

- 4.1.2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
- 4.1.3. 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.

\bigtriangledown	ADAS210 INPUT		
	Input Dataset		
	Data root //disk2/adas/adas/adf04		
	Central data User data 🗆 Edit Path Name a)		
	/belike/belike_jl1990o.dat		
	b) belike_jl1990o.dat 		
	Browse Comments		
	Select Superstructure file for Template Data root //disk2/adas/adas/adf04 Central data User data □ Edit Path Name d)		
	/copss#be/copss#be_ss#o4j.dat		
	e) Copss#be_ss#o4j.dat Data File:		
	Browse Comments		
	Cancel Done		

- 4.1.4. 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*.
- 4.1.5. Once a data file is selected, the set of buttons at the bottom of the main window become active.
- 4.1.6. 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.

- 4.1.7. Selection of the 'template' file which assists in the unbundling is made in the lower window at d) and e) as for the source file. The information line refers to a 'Superstructure file' as template. It is not obligatory to use an *adf04* file produced from the 'Superstructure' code as a template. However, we have mass producted such files at high resolution and they provide a good starting point. Incidentally such files are held in their own subdirectories of the /*adf04* directory according to isoelectronic sequence. Look for the code letter 'j' at the end of the ion name to tell you that the file is of high (ie. LSJ) resolution. (eg. /.../*adas/adas/adf04/copss#be/copss#be_ss#o4j.dat*
- 4.1.8. Clicking the *Done* button moves you forward to the next screen. Clicking the *Cancel* button takes you back to the previous screen



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

- 4.2.1. At a), two buttons are present to allow unbundling of the levels of the selected ion and then unbundling of the parents of these levels. The parents are the ground and metastable levels of the next higher ion to which ionisation may take place or from which recombination may take place. For basic studies, you will probably be using *adf04* datasets which omit recombination and assume ionisation only to the ground state of the next higher ion. Then the subtleties of parents may be ignored. This parent unbundling option is non-trivial only when the advanced *adf04* specification is being used. More details are given in the ADAS Manual. Click the appropriate button to fill the left side level display window b) and the right side Unbundling window d).
- 4.2.2. The level list displayed in the window at a) is from the source file which is to be unbundled and is for information only. It is a simple transcription of the list from the head of the source *adf04* file.
- 4.2.3. Note that the Data File at the right hand side c) is the template file.
- 4.2.4. In the Level Unbundling window, the index number, configuration specification, (2S+1)L(J) quantum numbers and the level energy (cm-1) are given for each level in a separate display window with an editable box to its right d). The editable box is for entering the index number of the source file level which you wish to associate with the high resolution template file level. Essentially the template levels are bundled first in the procedure for

association with a low resolution source levels. That is template levels which are to be grouped are given the index number of their associated low resolution source file level. Then the low resolution level is unbundled in the proportions of the template file levels forming the group. **Remember to press Return after entering each associated level index**.

- 4.2.5. When you have finished the level allocation, click the *Parent Unbundling* button at a) to execute parent unbundling. Note you may proceed to the next screen directly by clicking the *Done* button after level unbundling. The code then puts in the default parent.
- 4.2.6. On clicking the Parent Unbundling button the window at b) is filled with the parent information from the source file. The window at d) by contrast is filled with level infromation from a template file for the adjacent higher ion of the same sub-directory class as the template file for the level unbundling. Thus if '.../adas/adas/adf04/copss#be/copss#be_ss#o4j.dat' was the level template then '/.../adas/adas/adf04/copss#li/copss#li_ss#o5j.dat' is the parent template. The information format is a little different from that of the levels. The first value is the index number, followed by the parent term character string (in brackets) as given on the top line of the *adf04* file. The numerical value of the parent statistical weight follows with finally the parent energy (cm-1) relative to the lowest level of the ion. In the single parent case therefore this is just the ionisation potential.
- 4.2.7. Note the icon for *Exit to Menu* at (e). This quits the program and returns you to the ADAS series 2 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen
- 4.3. The **output options window** is of restricted form. It only offers the option of an output file. This part is of the same layout as codes previously described.



- 4.3.1. The name of the source data file which has been unbundled is repeated at (a) for information. The output file is the unbundled adf04 file and it is of the correct format for re-entry in the adf04 database. The comments section at the end of the output adf04 file details the source adf04 file and the unbundling imposed.
- 4.3.2. By default the output file is sent to your */pass* file subdirectory as *unbundle.pass*. You should ensure that you have created a */pass* sub-directory of you personal */adas* directory to receive such files.
- 4.3.3. There is no graphical output option.

The program interrogates zero density direct electron impact ionisation rate coefficient (SZD) files of type adf07. The data may be interpolated at electron temperatures of choice. The interpolation may be displayed and a tabulation prepared. A minimax poynomial approximation to the data is also made. Data of type *adf07* is used in ADAS to hold primary collections of stage to stage and resolved metastable to metastable direct ionisation rate coefficients. They constitute the high precision data of this type which is then merged with collisional-radiative calculations to produce the true effective ionisation rate coefficients. ADAS502 is introduced at this stage since we are now moving onto the codes (ADAS204 and ADAS208) which provide these effective coefficients. ADAS208 in effect calls ADAS502 to supplement its internally calculated data with the best we can offer it. The extension and maintenance of the *adf*07 data collection is of importance. At this point only key light species have metastable resolved data in *adf*07. Other species only contain stage to stage values. We are actively improving and building adf07 at this time through Don Griffin's efforts. In fact Don provides a much more complex data type (adf23) for ADAS from which we are extracting only a bit for *adf*07 - more of this later.

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



- 5.1.1. 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. 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.
- 5.1.2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.N B Under the IDL Craphical User Interface which controls the

N. B. Under the IDL Graphical User Interface which controls the window operations, you must remember to press the *return* key on the keyboard for any change to be recorded.

- 5.1.3. 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.
- 5.1.4. 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*.
- 5.1.5. Once a data file is selected, the set of buttons at the bottom of the main window become active.
- 5.1.6. 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.
- 5.1.7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

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

- 5.2.1. An arbitrary title may be given for the case being processed a). 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.
- 5.2.2. The output data extracted from the datafile, in the case of ADAS502, an 'ionisation 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. **Remember to press the** *return* **key on the keyboard to record the value**.
- 5.2.3. Available rate coefficients in the data set are displayed in the coefficient 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 coefficient to select it. The selected rate appears in the selection window c) just above the coefficient list display window.
- 5.2.4. Your settings of electron temperatures (output) are shown in the temperature display window d). The temperature values at which the ionisation rate coefficients are stored in the datafile (input) are also shown for information.
- 5.2.5. The program recovers the output temperatures you used when last executing the program. Pressing the *Default Temperature values* button inserts a default set of temperatures equal to the input temperatures.
- 5.2.6. The Temperature Values are editable. Click on the *Edit Table* button if you wish to change the values.



- 5.3. The **output options window** appearance is shown below
 - 5.3.1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
 - 5.3.2. Graphical display is activated by the *Graphical Output* button a). 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 b) to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.

Browse comments	
Graphical Output	Default Devic
Graph Title Figure 1	Post-script
Explicit Scaling X-min : X-max :	Post-script HP-PCL
Y-min : Y-max :	HP-GL
Enable Hard Copy Replace	
rite traine . graphips	
□ Text Output □ Replace Default file name	
File name : graph.ps	

- 5.3.3. Hard copy is activated by the *Enable Hard Copy* button c). 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.
- 5.3.4. A choice of output graph plotting devices is given in the Device list window d). Clicking on the required device selects it. It appears in the selection window above the Device list window.
- 5.3.5. 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*. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated.
- 5.3.6. The graph is displayed in a following **Graphical Output** window as shown below.

The program interrogates zero density radiative power loss rate coefficient (PZD) files of type *adf19*. The data may be interpolated at electron temperatures of choice. The interpolation may be displayed and a tabulation prepared. A minimax poynomial approximation to the data is also made. The data of type *adf19* is stored by element and includes the total radiated power function and the component radiated power coefficients for each ion. Formally it does not need to be zero-density data, but the data is held as a function of electron temperature only. The *adf19* data collection is by no means exhaustive containing at the moment the tables of Summers and McWhirter and some extra data for light ions. It is easy to extend the *adf19* data using ADAS206. ADAS206 is the radiated power variant of the population code ADAS205 and will be converted to IDL-ADAS soon. Our primary thrust on radiated power in ADAS goes through the much more comprehensive (but more complex) root of isoelectronic and

isonuclear master files (types *adf10* and *adf11*). See *adf19* as a convenient place to hold some quick look data for viewing with ADAS504.



7	ADAS504 INPUT	
	Input Dataset	
	Data root //disk2/adas/adas/adf19/	
	Central data User data 🗆 Edit Path Name	aj
	ionelec/ionelec_pzd#c.dat	
	 ionelec/ionelec_pzd#be.dat ionelec/ionelec_pzd#c.dat	c)
		b)
	Browse Comments Cancel Done	

- 6.1.1. 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. 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.
- 6.1.2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.N. B. Under the IDL Graphical User Interface which controls the

N. B. Under the IDL Graphical User Interface which controls the window operations, you must remember to press the *return* key on the keyboard for any change to be recorded.

- 6.1.3. 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.
- 6.1.4. 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*.
- 6.1.5. Once a data file is selected, the set of buttons at the bottom of the main window become active.
- 6.1.6. 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.
- 6.1.7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

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

6.2.1. An arbitrary title may be given for the case being processed a). 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.



- 6.2.2. The output data extracted from the datafile, in the case of ADAS504, an 'radiated power function', 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. **Remember to press the** *return* **key on the keyboard to record the value**.
- 6.2.3. Available radiative power functions and coefficients in the data set are displayed in the coefficient 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 coefficient to select it. The selected rate appears in the selection window c) just above the coefficient list display window.

- 6.2.4. Your settings of electron temperatures (output) are shown in the temperature display window d). The temperature values at which the ionisation rate coefficients are stored in the datafile (input) are also shown for information.
- 6.2.5. The program recovers the output temperatures you used when last executing the program. Pressing the *Default Temperature values* button inserts a default set of temperatures equal to the input temperatures.
- 6.2.6. 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, appears as shown below:

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

- 6.3.1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
- 6.3.2. Graphical display is activated by the *Graphical Output* button a). 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 b) to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.

Browse comments	
 Graphical Output Graph Title Figure 1 	Default Device Post-script
Explicit Scaling X-min : X-max : Y-min : Y-max :	Post-script HP-PCL HP-GL
Enable Hard Copy Replace File name : graph.ps	
Text Output Replace Default file name File name : graph.ps	
Cancel Done	

- 6.3.3. Hard copy is activated by the *Enable Hard Copy* button c). 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.
- 6.3.4. A choice of output graph plotting devices is given in the Device list windowd). Clicking on the required device selects it. It appears in the selection window above the Device list window.

- 6.3.5. 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*. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated.
- 6.3.6. The graph is displayed in a following **Graphical Output** window as shown below.

You will observe the addition of substantial new data to the ADAS database. These include condensed projection files (adf17), direct resolved radiative recombination coefficients (adf08) and expansion definition data (adf18). Also a new adas data format adf25 has appeared. These are all in preparation for the completion of the advanced parts of ADAS series 2, especially ADAS204 and ADAS208. Also we have done some restructuring and renaming of some sub-directories. This has been mostly to add a date stamp to data collections. Thus the Badnell dielectronic data of type adf09 are now in a sub-directory $/adf09/nrb93 \sim <seq>$ rather than just /Badnell. Also we have added a code such as 'LS' to data set names in a number of ADAS data types such as adf04 so as to distinguish LS-coupled data from intermediate coupling data (code 'j' or 'jj'). The development of the astrophysical side, ADAS210 etc. means that we need to bring over more of such intermediate coupling data and we wish to avoid confusion.

I realise there is a need to direct more clearly as to data available short of going into the comments section of every dataset. I am introducing a */datastatus* sub-directory of */docs* to provide such information. These will again be postscript files. There will be a */general.ps* member giving the overview and then individual ADAS */adfnn.ps* members for each data type as we get round to them. A preliminary */general.ps* will be put in place with the 1.5 data release in a few days.

Meanwhile Lorne Horton at JET has been working very hard with me in preparing for a light element upgrade, from '93' to '96'. We hope to achieve this in the next few weeks now that my heavy teaching committments for the year are over. We are pretty happy with our initial checks and the smooth running of the background support codes. It will mean some further expansion of the database and we do intend to use denser grids. adf10 and adf11 will be the main expansion.

H. P. Summers 20 Feb 1996