ADAS Bulletin

There is one strictly new program in this release. ADAS108 is a cross-section fitting code designed for neutral atoms and molecules. It is similar in general appearance to ADAS101 but with a more sophisticated underlying analysis designed to handle the threshold region of the cross-section. ADAS101 and ADAS102 have been re-examined and now the Burgess options operate correctly. Two programs have been substantially reworked. ADAS503 is the interrogation code for photon emissivity coefficients. Ricky Martin has used ADAS503 as the vehicle for testing our new ideas on versatility in graphical display and pair selection in interrogation of two-parameter data classes. This is a beta version and we would like constructive comments. We plan to rework all the two parameter interrogation programs in this manner over a period of time. ADAS403 is an old code from IBM-ADAS days for handling ADF10 data. It has been extensively reworked by Martin O'Mullane in support of the GCR Project. Then there have been many improvements and adjustments in series 2 and series 4 programs linked to the GCR Project. The codes are now much more robust although there will a final wave of adjustments and refinements linked to the GCR Project in the next release.

There are much new data associated with the GCR Project, that is ADF10, ADF11, ADF13, ADF15 and all the drivers for the elements nitrogen and oxygen. The derived data for the remaining elements of the GCR Project will be in the next release.

1. ADAS101 & ADAS102 These codes have been corrected and the Burgess C-plot analysis method now works. New test data are provided in the central ADAS database in the directories /.../adas/adas/arch101 and /.../adas/adas/arch102 respectively. Use the Old Archive option on the first panel to access these. Note that the first archive is from an 'ADAS' analysis and the second from a 'Burgess' analysis of the same source data. The data can be re-analysed by either method but if the prior analysis was 'ADAS', then a value for the Burgess 'C-parameter' must be entered at the analysis stage. Likewise if the prior analysis was 'Burgess' then optimisation level 1 rather than 2 will be the default. Sample archives are present for type 1, 2 and 3 collision strengths.

2. ADAS108 The program is for entry of electron impact excitation cross-section data for neutral atoms and molecules, examination and comparison with approximate forms, display and conversion to Maxwell averaged rate coefficients for permanent storage in the ADAS database. There is no central ADAS data class associated with input to this program, since new data is entered by hand in the program. However a mechanism is provided for storage and retrieval of the output from the ADAS108 analysis. The output from a case may be stored in an archive file. Such files are present only on the user's own space. Storage is sequential with an index.

Remember to ensure you have a defaults directory allocated. This should have the pathway /..../uid/adas/defaults

where *uid* is your user identifier. The defaults directory records the parameters you set the last time you ran each ADAS code. Move to the directory in which you wish ADAS created output text file (*paper.txt* is the default) and graphic files (e.g. *graph.ps* if a postscript file) to be placed. Initiate ADAS, move to the series 1 menu and click on the button to activate ADAS108.

The **archive selection window** appears first. It is slightly different in operation than the usual file selection window.

1. The recommended root path for user archiving for ADAS108 analysis is .../uid/adas/arch108/

which may be edited in the usual manner.

- 2. Click the appropriate button at a) for opening an old archive file, starting a new archive file or ignoring archiving. In the first case, the usual file display window shows existing archive files from which selection may be made. The selected file is displayed in the selection window. In the second case, the file display window is the same, but the selection window is editable for entry of a new archive file name. **Remember to press the** *return* **key on the keyboard to record an entered value**.
- 3. The capability is given for reworking or re-displaying the results of an earlier analysis stored in an archive file. At b) click on the *Refresh from archive*

button. Then give the *Archive index number*. The selected data will be used as the default data in the subsequent processing and output windows. Archiving is strictly sequential. A new analysis is simply appended at the end of the archive file and the index updated. These is no data replacement or substitution.



- 4. Clicking on the *Browse Index* button displays the index list for the selected archive file. The possibility of browsing the index appears in the subsequent main window also.
- 5. 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

- 6. The button *Browse Index* at a) again allows display of the archive index list.
- 7. Four types of collision cross-section are allowed, namely 1-dipole, 2-nondipole, 3-spin change and 4-other. Enter the *transition type* number at b). For dipole transitions the transition probability is required. Either the line strength (*S*), absorption oscillator strength (*f*) or Einstein A-value (*A*) forms are accepted. Click the appropriate button and enter the value.
- 8. At c) details of the upper and lower levels of the transition are entered. The energies of levels are measured upwards from the lowest level of the ion. Click on the *Select energy form* button to indicate which units are being used for these energies. Note that full statistical weights (including spin parts in the case of terms) are required.
- 9. User input cross-sections, energies and required output temperatures are displayed at d) with the currently selected units shown below. Click the *Edit table* button to 'drop down' the ADAS Table Editor for data input.
- 10. If an archive data set is opened, energy, cross-section and temperature values are filled from this. Otherwise the fields are empty. Pressing the *Default Temperature values* button inserts a default set of temperatures.

	AD	AS108 PROCESSING	OPTIONS	
Data file name :	/home/summers/adas	s/arch108/new_adas108	s_type1.dat	
		Browse Inde	3x	
Nuclear Cha	rge:		Ion Charge:	
Transition T	уре:	Transit	tion Probability:	
•		Form:	♦ s ♦ f	◇ A
	ower Level		Upper I	Level
Index	:]	Index :	
Stat. Wt.	;		Stat. Wt. ;	
Level Ene	rgy :]	Level Energy :	
Select Ene	rgy Form ;	🔷 cm	i-1 🔷 Rydbe	r g s
INDEX	Input Energy	Input X-sect	Output Temp.	Δ
1	1.000E+00	1.000E+00	1.000E+05	
2	2.000E+00	2.000E+00	2.000E+05	
	5.000E+00	5.000E+00	3.000E+05	
	1.000E+01	1.000E+01	4.000E+05	
	2.000E±01 5.000E±01	2.000E+01 5.000E+01	7.000E+03 8.000E+05	
	1.000E+02	1.000E+01	1.000E+05	
8	2.000E+02	2.000E+02	2.000E+06	
				<u>۲</u>
Energy units	X. X-section u	nits : Omega . Temp	erature units : Kelvin .	
		Edit Table		
	De	efault Temperature valu	162	
E Station under			_	

- 11. The ADAS Table Editor window follows the same pattern of operation as described previously. Note however the fairly wide selection of units in which data can be entered. This is to ease the problem of unit conversion for data from the general literature. Click on the buttons for the units with which you wish to work. The program internally converts to the threshold energy parameter *X* and the collision strength *Omega*. If data is returned from archive it will be in these forms. Click the *Done* button if editing is completed satisfactorily.
- 12. 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.

The **output options window** is more complex than in previous programs. It is shown below.

13. There is a choice of method for examination and display of the input data. At a), click either the *ADAS analysis option* which corresponds to the JET analysis or the *Burgess/Summers analysis option*. The sub-window at b) varies depending on this choice. Make the appropriate choices at b), c), d) and e) in the ADAS case or at b'), c') and d') in the Burgess/Summers case.

S . (11 "		1 100 / 1 1		
Data file name : /hoi	ne/summers/adas/arch108/new_a	adas108_type1.dat]
	Browse inde	~		
	Analysis Option			
Burge:	ss/Summers Analysis Option	L		
Optimisation	Level: $\bigcirc 1 \bigcirc 2$	Optimisation Op	tion: \diamond Or	\sim off \checkmark
Bad Point Optio	on: \Diamond on \Diamond o	ff Dipole X-sect. F:	itting : 🔷 Rat	tio 🔷 Difference
Graphical C	Putput			Default Device
Graph Title	Figure 1			Post-script
lst. Defa	ult Graph Scaling	2nd. Default Grap	h Scaling	Post-script
X-min :	X-max :	X-min :	(-max ;	HP-PCL HP-CI
Y-min :	Y-max ;	Y-min : Y	-max :	
Enable Ha	urđ Copy 🗆 Replac	e		(a)
File name :	graph.ps			
Text Output	C Replace D	efault file name		
File name :	graph.ps			
Cance	I Done			
B-value	C-val	ue		
Insert non-dip	ole point at infinity :	\bigcirc Ω_{-value}	:	_
				(IF

14. Two graphs are presented. The first is a scaled comparative graph for assessing the cross-section data and making adjustments if appropriate. The second graph displays the final *Upsilons* at the user's temperatures. Make the required choices of graph scaling and axes choices at f) for the comparative graph and at g) for the *Upsilon* graph.



- 15. The comparative graph is displayed in the Graph Editor window as shown below. The graph displays the scaled input values as daimonds with a spline drawn through these tabular points in the ADAS analysis option case. In the Burgess/Summers analysis option case, the spline is drawn through the special nine knot points which are distinguished as crosses. The points can be modified by using the buttons b) beneath the graph in association with the mouse. In the Burgess/Summers analysis option case, the knot points may only be moved vertically and a special button is present for this case. Also in the Burgess/Summers case, the parameters 'B' and 'C' can be varied to seek an optimum fit. This is done with the sliders at a). Note that the RMS error of the least square fit is displayed and continuously updated at the top of the graph.
- 16. To move a point, click the *move a point* button. Then use the *left* mouse button to pick and drag a point to a new position. The coordinates of the moved point are displayed and continuously updated at the foot of the graph. Note that the x-ordering of points should be maintained although not forced by the editor. Each point has a small active zone around it for picking by the mouse. Terminate point moving operations by pressing the *right* mouse button. To delete a point, click the *delete a point* button. Then click the *left* mouse button with the pointer over the point to be deleted. Terminate point deletion operations by pressing the *right* mouse button. To add a new point in the x-ordered position between two existing points, click the *add X-point*

button. Then click the *left* mouse button with the pointer at the position where the new point is to be inserted. Terminate point insertion operations by pressing the *right* mouse button. For completeness, the capability for adding a point anywhere is given although physically unreasonable. The operation is slightly different. Click the *add anywhere* button. With the *left* mouse button pick a point after which you wish the new point added. Press the *lett* mouse button with the pointer at the insertion point. Multiple insertions may be made by continuing to click the *left* mouse button. Click the *right* mouse button to terminate this particular insertion. Press the *right* mouse button a second time to terminate insertion operations.

- 17. To insert a point by value use sub-window c).
- 18. The buttons at d) provide the usual *Cancel*, *Print* and *Done* options. In addition the *Help* button displays some information on using the graph editing facilities. The original data and graph can be restored by clicking the *Refresh* button. Note that after leaving the graph editor window with the *Done* button, the modified and or additional points replace the original user input data. Note that with the ADAS analysis option, if any points are modified, the program cycles back to the Output Options window for reanalysis. With the Burgess analysis option, movement only of the spline knots does not force reanalysis.
- 19. The Upsilon graph is displayed after graph editing. There is no option to modify this output graph. The graph may be printed, using the *Print* button. If the results of the analysis are acceptable and to be archived, click the *Archive* button.
- **3. ADAS204** A change has been made in the subroutine 'ngffmh'.
- 4. ADAS208 The code has been adjusted to handle 'prb' data consistently. It is now passed through ADAS208 so that ADAS208 delivers a complete set of generalised collisional-radiative files. Also the documentation in the comments section of GCR output files from ADAS208 has been substantially improved. ADAS208 also now allows ionisation rate coefficient data from the levels of the ion under consideration to be present in the adf04 file as 'S-lines'. This means that the tiresome step for fetching better ionisation data via the ADAS208/ADAS502 branch can be avoided. We can include ionisation data from excited levels which are not metastable this way so the program is more versatile. We have been putting the S-lines into new ADF04 files from the GCR Project which are thus complete. Note that the ADAS208/ADAS502 branch can still be used as before but a marker is put on the panel information widget of metastable pairs sought to indicate if the data have already been found in the ADF04 file. You can override the data from the ADF04 file. The data source information is recorded in the comments section of the output files.
- **5. ADAS215** There have been a number of changes to improve the security of extrapolation in temperature of the ADF04 file collisional rate coefficients. In particular a problem with non-dipole, non-spin change data which tend to zero at infinite energy has been trapped. The output 'paper.txt' file records such problems and the corrective action taken. Type 4 collision cross-section data are now accepted.
- 6. ADAS310 A small error in the function subroutine 'gbf' has been discovered and corrected. The error in the bound-free Gaunt factors from this was no more than 0.5% and so is of no general concern.
- **7. ADAS402** The fortran data acquisition routine 'd2data' has been altered in line with changes in the definition of the ADF10 files.
- 8. **ADAS403** The code has been brought to life again but in a different form. It now is a general utility for mapping the primary GCR output from ADAS208 correctly into position in the iso-electronic ADF10 files. This was a tedious hand procedure before. The code functions entirely within IDL and the window structure is a little simpler than usual. There is no output graphical display. Note that we expect to do further work on this code to allow merging of two ADF10 file sets.

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



- 1. At a) identify the directory of the passing files from the ADAS208 run. Note that ADAS208 provides the actual file names within the output directory.
- 2. At b) click to select the particular GCR classes of data which you wish to be inserted/replaced into ADF10 archives.
- 3. Then specify the location of the ADF10 archives by year, prefix and isoelectronic sequence and whether they are to be sought in your user space or in central ADAS. The template file name appears in the text widget which is not editable. It is for information only.
- 4. Clicking the *Done* button moves you forward to the information window. Clicking the *Cancel* button takes you back to the series 4 menu.

The information window appearance is shown below



5. This is a pre-analysis to show if the expected files are present and to allow a check of their content. It checks also if parents and metastables align correctly It is important that the results window be checked to see that operations will

proceed according to plan. There is a separate block for each ADF10 data class. If there are any valid selections, then the code will proceed. You can cancel at the output options stage.

- The output options window has the appearance shown below.
 - 6. If desired select a standard output text file for the summary description of the details of the insertion/replacement at a).
 - 7. At b) specify where the new ADF10 files are to placed. The information required and/or given immediately below depends on the choice of location. If 'passing files' are to be created activate the first button and then give a name for the passing directory in the text widget below at c). There is a button which causes the default directory name to inserted in the text widget.
 - 8. If *Replace Originals* is selected an extra warning is provided as at b') for safety.
 - 9. Finally by activating *New adf10 set* then specification of the file names in the standard manner by year and prefix is offered as at b'') and the template file name is created in the text widget. This is for information only and not editable. An extra button is provided at c'') to warn if the files you have chosen already exist.
 - 10. Click *Done* to run the code, *Cancel* to return to the previous window or else click the *Escape to Menu* button to terminate the program. On clicking Done, an information window summarising the results is presented.



- **9. ADAS404, ADAS405, ADAS406** These codes have been altered to accept the adjustments in ADF10 file structure.
- **10. ADAS501, ADAS503** These are two of our original codes for interrogating and displaying data from ionisation per photon ('sxb' data) of format ADF13 and photon emissivity

coefficient files ('pec' data) of format ADF15. The new facilities are described here for ADAS503. You will recall that although the archived ADF15 data are held as a two dimensional array in electron temperature and electron density for each spectrum line it was only possible to display graphs as a function of electron temperature. Also no choice was given of the temperature units on the graph even though ADAS allows users to choose units on data entry. Finally, ADAS has had no provision for superposing curves on the same graph for comparison purposes. These various items have proved an irritant and the new version of ADAS503 issued as a beta test now is our answer to these criticisms. It is a new 'tour-de force' by Ricky Martin.

The primary operation of ADAS503 is as before and it is possible to simply ignore all the new facilities. However new choices appear on the Processing Options window and on the Graphical Output window which are described here

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

1. At e) some new choices are provided. As well as *Default Te*, *Default Ne* is available. These buttons insert the electron temperature data or electron density data respectively from the input data set as the output values and offers a choice of a fixed electron density or electron temperature respectively to be associated with these.



2. The third button at e) is *Value Selection by display*. It is designed both to provide a display of the actual three-dimensional surface of the density and temperature dependent collisional-radiative emissivity coefficient and to allow selection of temperature/density pairs for the output graphs visually.

The point value selection widget has the appearance shown below

- 3. The emissivity coefficient surface is shown at a). Controls are provided at b) to orientate and alter the appearance of the display. Sliders allow rotation about the X-axis and about the Y-axis so that the whole surface can be examined. The surface styles can be altered by selecting from drop-down menus. The styles include continuous or mesh surfaces and the colour of the surface. Finally the form of the axes, that is logarithmic or linear can be chosen from drop-down menus.
- 4. At b), the two dimensional projection on the Te/Ne plane is displayed. Note that the grid lines are those of the actual data in the source file. The new code provides a sophisticated method for selecting Te/Ne pairs by mouse click which allows the user to track over interesting parts of the surface.
- 5. Move the mouse cursor over the lower Te/Ne grid. A tracking pointer moves over the surface in the upper display. Click the left mouse button to select a Te/Ne pair. A symbol marks the selection on the Te/Ne grid in the lower display and a marker also appears on the surface in the upper display. Continue to select point pairs as required. Note that the position of the cursor in Te/Ne space is shown numerically at c) for precise positioning



- 6. Control buttons at e) allow adjustments to your selection set. Pairs can be added at the beginning or end of the set or inserted between pairs. Also a pair can be deleted. Finally the whole set of pairs can be erased.
- 7. Click *Done* on completion to return to the processing options window. The pairs selected will be present in the editable table. Note that conventional entry or modification of user data with Table Editor remains an option as before.

8. Note that when *Value Selection by display* is activated, the *Fit Polynomial* button is de-activated. It is clearly easy in pair selection over a surface to produce pair orderings which are inappropriate for fitting a polynomial.

The graphical output window has the appearance shown below

- 9. Operation of the output options window is as before but the graphical output window has some extra buttons. *Print* and *Done* are as before at b) with the same action, but *Adjust* and *Retain* buttons are now present at c) and d).
- 10. Click the Adjust button to pop up a new widget for adjusting the graph.
- 11. Click the *Retain* button to keep the graph and allow it to be displayed with other retained graphs. A new window appears called the multiplot window.



The graph adjust widget has the appearance shown below

- 12. Full control is provided at a) to alter the axes styles, the independent variable and the units for the independent variable. These choices are provided by drop-down menus
- 13. At b) the usual manual entry of minima and maxima for the axis scales is supported.
- 14. Click Done to return to the graphical window.

	Graph Adjust Widget				
	Scales :				
a)	Axes: X Log / Y Log				
	X-axis : Temperature				
	X-units : eV				
	Y-units phot. cm-3 s-1				
	xmin xmax				
	ymin ymax				
/					
b)	Done				
	d)				

The multiplot widget has the appearance shown below

- 15. The retained curves appear in the list at a) and b). The current curve is placed at the end of the list and up to seven curves are allowed.
- 16. The editable box in the second column of each row is a numerical selector for the line style used for that curve. This is followed by a brief descriptor for the curve which will also appear on the whole graph when printed. The button in the second last column is activated to display that retained curve and the last button is used to delete a curve from the retained list
- 17. Note that the *Adjust* button is again present . At this point, only the axis maxima and minima can be modified.
- 18. Click *Done* to return to the ordinary graphical window or *Print* to print the multiplot graph.



- **11. ADAS603** The program now includes hydrogenic lines as in the original xPaschen. Also, note that the error preventing fitting with a background only has been corrected.
- **12. ADAS701** The code includes the latest version of *autostructure*.
- **13. READ_ADFXX** A number of new offline IDL procedures have been added to the IDL libraries to allow direct access to ADAS data from IDL. These procedures are equivalent in their delivery to the fortran '##data.for' subroutines. Presently included are *read_adf07*, read_adf11, *read_adf13* and *read_adf15*.
- 14. ADF01 There are new state selective charge exchange cross-sections for capture into the n=16 shell of Ar^{+18}

/.../adas/adas/adf01/qcx#h0/qcx#h0_tmp#ar18.dat

15. ADF02 There are new ion impact data for fully stripped and H-like argon /.../adas/adas/adf02/sia#h/sia#h_j99#h.dat

<u>Note</u> also that we have renamed $sia\#h_j97\#h$ to $sia\#h_j99\#h$ since there has been some more work on these data and the main derived production has been this year. I hope this does not cause confusion.

16. ADF04 There are new data for oxygen and nitrogen ions associated with the GCR Project. Also, data for helium and carbon ions have been extended by inclusion of the electron impact ionisation rate coefficient data in the relevant adf04 files. These are all preferred data and therefore stored in adas#<element> iso-nuclear subdirectories. The new subdirectories are /.../adas/adas/adf04/adas#7/...

/.../adas/adas/adf04/adas#8/...

and the extended ones are

/.../adas/adas/adf04/adas#2/...

/.../adas/adas/adf04/adas#6/...

An intermediate coupling data set for O^{+2} from new calculations by Aggarwal has been prepared

/.../adas/adas/adf04/clike/clike_kma99#o2ic.dat

also there are new data sets in LS-coupling for O^{+5} and C^{+3} from Don Griffin. Note that the latter are R-matrix with pseudo-state calculations and state-of-the-art. They are named as /.../adas/adas/adf04/lilike/lilike/dcg99#c3ls.dat

/.../adas/adas/adf04/lilike/lilike_dcg99#c3is.dat

/.../adas/adas/adf04/lilike/lilike_dcg99#o5ls.dat

An adjustment to the configuration specification in

/.../adas/adas/adf04/helike/helike_kvi97#he0.dat

has been made so that it works correctly when accessed by ADAS311.

17. ADF08 There is a replacement

/.../adas/adas/adf08/rrc98#b/rrc98#b_o3ls.dat

18. ADF10 There are replacements due to the altered format for *prb*, that is

/.../adas/adas/adf10/prb96/...

The previous form has been moved to

/.../adas/adas/adf10/prb96_old/...

for safe keeping. There are updates of all the adf10 classes to include nitrogen and oxygen ions and to update helium and carbon ions.

19. ADF11 There are new resolved and unresolved data for nitrogen and oxygen, new resolved data for helium and carbon and replacement unresolved data for helium and carbon contained in the usual directories

/.../adas/adas/adf11/<class>96r/...

/.../adas/adas/adf11/<class>96/...

- **20. ADF12** There are new charge exchange effective emission coefficients for Ar⁺¹⁷(n=16-15) /.../adas/adas/adf12/qef99#h/qef99#h_ctmc#ar18.dat
- **21. ADF13,ADF15** There are new resolved and unresolved data for nitrogen and oxygen in the iso-electronic sequence directories of the form

/.../adas/adas/adf13/pec96#<seq>/...

/.../adas/adas/adf13/sxb96#<seq>/...

and extension of these directories to include nitrogen-like and oxygen-like. A error in the

helium and carbon ion adf15 data whereby 1.00D+72 appeared instead of zero in underflow positions has been corrected.

22. ADF17 There are new projection files for nitrogen and oxygen ions in the iso-electronic sequence directories of the form

/.../adas/adas/adf17/cbnm96#<seq>/...

and extension of these directories to include nitrogen-like and oxygen-like ions.

23. ADF18 There are new mapping files for nitrogen and oxygen ions in the iso-electronic sequence directories of the form

/.../adas/adas/adf18/a17_p208/... /.../adas/adas/adf18/a09_p204/...

24. ADF21 There are new deuterium beam stopping coefficients for Ar^{+18} and Fe^{+26} as plasma impurity species

 $/.../adas/adas/adf21/bms99\#h/bms99\#h_ar18.dat$

- /.../adas/adas/adf21/bms99#h/bms99#h_fe26.dat
- **25.** ADF22 There are new balmer alpha deuterium beam emission coefficients for Ar^{+18} and Fe^{+26} as plasma impurity species

 $/.../adas/adas/adf22/bme99\#h_ar18.dat$

/.../adas/adas/adf22/bme99#h/bme99#h_fe26.dat

26. ADF26 There are new bundled-n population files for Ar^{+18} and Fe^{+26} as plasma impurity species

These extensions to the data base are documented in the /.../adas/docs/datastatus directory and in the main *idl-adas* manual at /.../adas/docs/idl-manual/appxa-<nn>.pdf. Finally, I do apologise for the delay in this release over the original plan stated in the last bulletin. This arose from the shear volume of work to do with the GCR project and the complexities of testing the elaborate new graphical output capability. We intend to have the next release ready at the end of the year to bring us back onto our usual schedule.

H. P. Summers 18 Oct. 1999