# mar18-95

# **ADAS Bulletin**

Three ADAS series 2 programs are now ready. Together they give a basic capability for looking at electron collision data in the database, excited population modelling and line ratio diagnostic studies. In this bulletin, I wish to give an overview of the user interface to the new programs and draw attention to the rewritten parts of the manual.

Dr. Jalota has now left the project and Dr. Tim Hammond has taken over the program conversion.

We are placing all the ADAS documentation on the world-wide-web as well as on local workstations so that it is more easily available. The ADAS home page is

http://patiala.phys.strath.ac.uk/adas/

## 1. **ADAS201**

This is a conventional interactive interrogation program. Its basic operation is as for ADAS501 and ADAS503 (cf. bulletin *jan18-95*).

1.1. 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.

- 1.2. 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)
- 1.3. Initiate ADAS, move to the series 2 menu and click on the first button to activate ADAS201.
- 1.4. The **file selection window** appears first. Its operation is as described in the bulletin *jan18-95*.
  - 1.4.1. Note that each type of data is stored according to its ADAS data format (*adf* number). *adf04* is the appropriate format for use by the program ADAS201. 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*.
  - 1.4.2. 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. 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. *copsm#16*, where the 16 is the nuclear charge)
  - 1.4.3. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
  - 1.4.4. Once a data file is selected, the set of buttons at the bottom of the main window become active.
  - 1.4.5. 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 has gone into the dataset and the attribution of the dataset. The possibility of browsing the comments appears in the subsequent main window also.
  - 1.4.6. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window
- 1.5. The **processing options window** has the appearance shown below



- 1.5.1. 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.
- 1.5.2. 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. **Remember to press the** *return* key on the keyboard to record the value.

- 1.5.3. 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 c) just above the line list display window.
- 1.5.4. Your settings of electron temperatures (output) are shown in the temperature display window d). The temperature values at which the excitation rate coefficients (in fact 'upsilons') are stored in the datafile (input) are also shown for information.
- 1.5.5. 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
- 1.5.6. 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.
- 1.5.7. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window.
- 1.6. The **output options window** appearance is of the standard form described in bulletin *jan18-95*.

1.6.1. The graph is displayed in a following **Graphical Output** window.

### 2. **ADAS205**

This is the basic excited population structure modelling code. It computes excited populations of an ion in a plasma and relates them to designated metastable populations of the ion. Calculations are performed at arbitrary temperatures and densities. Free electron recombination and charge exchange recombination are handled, **provided such data is in the accessed datafile for the ion**. The coupling to the continuum of the ion is however simplified. A later program ADAS208 treats these more advanced issues.

- 2.1. Initiate ADAS, move to the series 2 menu and click on the fifth button to activate ADAS205.
- 2.2. The **file selection window** appears first. Its operation is as described in the bulletin *jan18-95*. The file selection window and relevant data format (*adf04*) is the same as for ADAS201 above.
- 2.3. The **processing options window** has the appearance shown below
  - 2.3.1. There are three 'pop-up' windows for setting temperatures, densities and for designating metastable levels. For the temperature window a), click on the *Edit Table* button to open up the table editor. The editing operations as as described for ADAS501 but with more columns. 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.
  - 2.3.2. 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.

- 2.3.3. The Metastable State *Selections* button c) pops up a window indexing all the enrgy levels. Activate the buttons opposite levels which you wish treated as metastables. See the ADAS Manual for a detailed explanation of the handling of metastables in the collisional-radiative picture.
- 2.3.4. Various processes, supplementary to the primary electron excitation collisions and bound-bound radiative transitions, are activated as desired by clicking on the appropriate buttons d). 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 autoionising levels in you adf04 dataset but have omitted the details of alternative thresholds etc present in advanced *adf04* files.
- 2.3.5. 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 e).



- 2.4. The **output options window** has the appearance shown below. It follows the same pattern as for ADAS201 but with the added option of creating two output files.
  - 2.4.1. The button *Graph Output* a) is activated to obtain display of graphs. Note the selection of graphic output device d) for hard copy. The *Default Device* is selected by clicking on a device in the lower window and the selection is displayed in the upper window.
  - 2.4.2. The *Contour File* button b) 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 we store such temporary 'passed files' in a *pass* sub-library. You should create this at the first level within the adas database as

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

By default ADAS205 sends the contour file to /..../<uid>/adas/pass/contour.pass

Browse comments	
Graphical Output	Default Device Post-script
Explicit Scaling       X-min :       Y-min :       Y-min :	Post-script HP-PCL HP-GL
Enable Hard Copy     Replace       File name :     graph.ps	
Text Output     Replace     Default file name       File name :     graph.ps	
Contour File     Replace     Default file name       File name :     contour.pass	
METPOP File     Replace     Default file name       File name :     metpop.pass	

2.4.3. The *METPOP File* button b) 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 ADAS series 4 programs. It goes by default into

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

# 3. ADAS207

The program is intended to allow investigation of line ratios of spectrum lines or spectrum line combinations emitted from a single ionisation stage in a plasma. It utilises a data set of excited populations as functions of temperature and density, known as the 'contour passing file' prepared by a prior 'run' of ADAS205.

- 3.1. Initiate ADAS, move to the series 2 menu and click on the seventh button to activate ADAS207.
- 3.2. The **file selection window** appears first. Its operation is as described in the bulletin *jan18-95*. The program requires selection of a data file prepared as output from ADAS205. 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 we store such temporary 'passed files' in a *pass* sub-library. You should create this at the first level within the adas database as

#### /...../<uid>/adas/pass

to which the program looks by default. The window has the appearance shown below

$\bigtriangledown$	ADAS207 INPUT						
Input CONTOUR PASSING FILE							
Data root /home/adas/adas/pass/							
Central data User data 🗆 Edit Path Name							
contour.pass							
	 contour.pass						
Data File							
Browse Comments Cancel Done							

- 3.3. The **processing options window** has the appearance shown below. It displays information from the *contour file* together with information from the *adf04* file used in the prior ADAS205 program run.
  - 3.3.1 Select *Non-equilibrium* or *Equilibrium* conditions by clicking the appropriate case in the list a). 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. The metastables selected in the ADAS205 run are shown in the adjacent window b). 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.

3.3.2. A 'line ratio' in the present context is a ratio of line groups. The current line groups are shown in the list windows. The columns of the each row shows 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.





3.3.4 Each line group is assembled by clicking on the appropriate *Selection* button c) or d). A new window is presented with all available transitions listed. This is shown above. Clicking on the button alongside a transition a) allows it to be selected or de-selected.



$\overline{\nabla}$	7 A	DAS207 OUTPUT OPTIONS				
	Contour Passing File Name : /disl Data File Name : /disk2/adas/adas	k2/adas/adas/pass/contour.pass s/adf04/belike/belike_bkt1988c.	s dat a)			
	В	Browse comments				
	Spectral Line Intensity Ratio rang	e : 0.000D+00 - 6.414D+00				
	□ Graphical Output					
	Diagnostic Contour Plot	of Spectrum Line Ratios in Ter	np/Density Plane			
	□ Spectrum Line Ratios against Temperature for a given Density					
	Spectrum Line Ratios ag	ainst Densitt for a given Temp	erature			
	Default Contour Plot Title	Figure 1				
	Default Contour Scaling					
	Contour Spacing	Contour Values	Contour Interpolation			
	Logarithmic	INDEX	Logarithmic			
	Linear	1 1.00D+00 2	Timer			
	Logarithmic	3	Logarithmic			
d)						
		Edit Table				
			Select Device			
	📋 Enable Hard Copy 🗌	Replace	Post-script			
	File name : graph ps	_	Post-script			
			HP-PCL			
			HP-GL			
r						
	Text Output Replace	Default file name				
	File name : paper.txt					
ſ	Cancel Done					

- 3.4.1. 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 logaithmic and it 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.
- 3.4.2. There are three distinct types of plot of the line ratio allowed b), 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 c) changes according to this choice.

- 3.4.3. For the contour plot case, logarithmic or linear choices of contour are permitted. Click on the required type in the lower list window d). The chosen type appears in the selection window above.
- 3.4.4. 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.
- 4. Until the ADAS program ADAS208 is implemented, you will be dependent on the central *adas* database for derived population data which includes links to different continua of the ion, the high density Saha-Boltzmann equilibrium, three-body recombination etc. Meanwhile we are continuing to put more such data prepared at JET Joint Undertaking into the data base as time permits. We have a substantial capability to put up data for arbitrary ions by processing at JET Joint Undertaking and then file transfer to IDL-ADAS. Please let us know if there are any urgent requests.

H. P. Summers 12 April 1995