Jul18-02   **ADAS Bulletin**

We have not been able to get our large new code release, associated with series 8 and heavy species fully ready yet. However, ADAS811, the work of Martin O'Mullane, is a bit separate so it is added to the present bug fix release. ADAS811 is a general purpose *adf04* file comparison program. It handles most of the rate coefficient data types present in adf04 files including excitation, recombination and ionisation. Also, the excitation data can be displayed as effective collision strengths of as Burgess-Tully scaled values in C-plots. We noted Alessandro Lanzafame's wish for more capability for Burgess plotting in ADAS201 and feel that ADAS811 more than fulfils this. The new manual entry for ADAS811 is appended at the end of the bulletin.

Corrections and additions to codes

C.1 Unintentionally, Allan Whiteford's fix to *run_adas405*.pro did not make it into release 2.5.5. The fix prevents eating up unit numbers when repeat running. It is included now in this release.

C.2 A rogue fortran program *adas406.for* crept into the *idl/adas4xx/adas406* directory where it should not be. It has been removed.

C.3 A syntax error in *cw_adas214_proc.pro* around line 471-472 has been corrected. The *endif* and *endcase* entries are reversed.

C.4 *read_adf04.pro* has been upgraded to provide the extra information on *adf04* files needed by the new *ADAS811* as follow:
  - return ionisation potentials of parents and their statistical weights
  - change *nz* to *iz0* in all structures to preserve the naming
  - carry out some internal renaming by prefixing internal routines with *r04* in accordance with current IDL recommended practice
  - calculate ionisation rates form excited levels and return these in all structures (*r04_add_ecip*) if */ecipcalc* is set. Use *r8necip.pro* for this which call the fortran ECIP calculation.

C.5 There is an increasing need for IDL access to fortran functons. For the more complex routines it is preferable to call the fortran vesion via a wrapper routine. Some of the simpler ones can have direct translations. After discussion, a new directory branch has been introduced, namely,
                        /home/adas/idl_adas/wrapper/
with a similar structure to the fortran branch as:
                        /home/adas/idl_adas/wrapper/adaslib/
                        /home/adas/idl_adas/wrapper/adas4xx/adas401
                                        etc.
The wrapper functions are identified by appending '*_if*' (for interface) to the standard name. For example, *adas2xx/adas208/r8necip_if.for*. Note the following points:
  - the wrapper rouitnes may be in C or fortran
  - each has its own *comp_xxx* script
  - the binaries are made with the *wrapper/adaslib/makeall_wrapper.linux* and other architecture specific files.
  - the IDL calling routine resides in the appropriate sub-directory in the IDL ADAS branch as
                        /home/adas/idl_adas/idl/adas2xx/adas208/r8necip.pro
  - the calling arguments should be the same between fortran and IDL
  - occasionally the IDL version may be altered to make it more IDL-like. For example, single parameter fortran functions may accept vectors. This is introduced in the IDL routine.

   The functions added so far are
                        fortran/adaslib/xxcftr.for
                        fortran/adaslib/xxdtes.for
                        fortran/adas2xx/adas208/r8necip.for

C.6 *ADAS702* has been synchronised with v1.8 of Nigel Badnell's *adasdr.f* off line dielectronic recombination code. This cures some problems for $\Delta n = 0$ DR ins low charge ions when parity split datasets from *AUTOSTRUCTURE* are used.

C.7 There are still some arrays of size 1 issues introduced by IDL 5.5. In *cw_adas208_out.pro*, the *passdir* came back as *strrarr[1]* rather than a string and the inevitable crash occurred when trying to put it into the output structure – which was expecting a string. It was also not possible to de-select the PEC/SXB/GCR output in *ADAS208* and also in getting *ADAS208* to produce PECs. It is unclear if this was an IDL 5.5 problem, but changing the way *cw_adas208_out.pro* dealt with this cured the problem.

C.8 The batch queue system at JET has changed a lot and the new batch.pro reflects these changes. There is no difference for installations outside JET.

C.9 *read_adf24.pro* assumed that *e9spln* used 30 internal knots, but it in fact only had 24. This has been fixed.

C.10 *ADAS409* failed using the '96' *pec* data – due to a dimension change in the arrays used by *e3data*. It is not necessary to tie these dimensions to the global *NTDIM/NDDIM* used in the rest of the program.

C.11 A new IDL utility, *xxeiz0.pro*, converts atomic element symbols into atomic numbers. It is a function version of *i4eiz0.pro*. It was felt to be overkill to use *call_external* to the fortran equivalent in this case.

C.12 There was incorrect labelling of the y-axis in the power plot by ADAS409.

Corrections and updates to data

D.1 More He-like adf09 files and the corresponding adf27/adf28 datasets are included from Manuel Bautista. These include some corrections.

D.2 A new Li^{+2} adf04 file has been completed by Connor Ballance.
    /adf04/hlike/hlike_cpb02#li2ls.dat

D.3 PEC's and SXB's from relatively high n in the h-like low Z elements have been added. These are generated with the off-line *v2bndl* code. Datasets for He and C have been added to the adf13 and adf15 '96' directories with the 'bnd' extension
    /adf13/sxb96#he/sxb96#he_bnd#he1.dat
    /adf15/pec96#he/pec96#he_bnd#he1.dat

D.4 New adf04 files for B^{+2} nd B^{+3} have been prepared by Dimitri Borodin and Nigel Badnell
    /adf04/helike/helike_dvb02#b3.dat
    /adf04/lilike/lilike_dvb02#b2.dat

D.5 The Fe^{25} adf04 file has been updated. This replaces */adf04/hlike/hlike_cpb01\fe25.dat* with the new one.

D.6 A format problem with the adf09 files of James Colgan has been corrected by Allan Whiteford.

D.7 An incorrect ioni charge for carbon in /adf04/copjl#be has been corrected by Allan Whiteford.

D.8 A format problem with some adf08 files has been corrected.

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ADAS811: Compare adf04 files

The program provides extended interrogation of *adf04* files. All types of rate coefficient data in the *adf04* file are handled. Comparison of coefficient data from different adf04 files is supported. The program is a substantial extension and replacement for ADAS201.

Background theory:

The full specification of the adf04 file organisation is given in Appendix A/ADF04. The transition data displayed by ADAS811 includes:

- electron impact excitation - Note that type 1, 2 and 3 transitions are distinguished by the lead character of the transition line data string. The upsilon parameter is tabulated in the adf04 file. The upsilon, excitation rate coefficient and Burgess C-plot scaled upsilon parameter may be displayed (see Chapter 2-02 for details)
- proton impact excitation – P-lines in the adf04 file
- electron impact ionisation – S-lines in the adf04 file.
- free electron recombination – R-lines in the adf04 file.
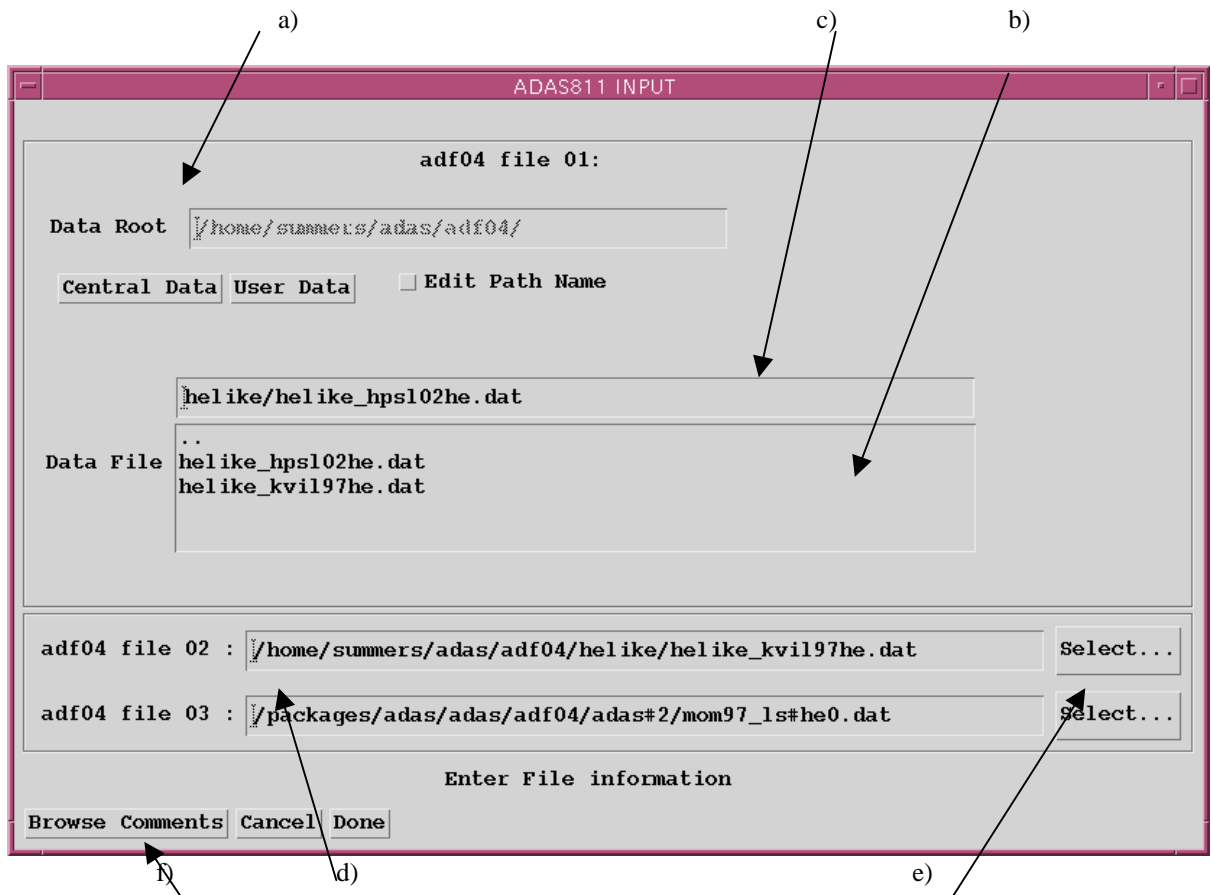- charge exchange recombination – H-lines in the adf04 file.

Program steps:

The code is implemented entirely in the IDL language. Access to the *adf04* file data is by the procedure *read_adf04.pro*. Note that such procedures are FORTRAN wrappers with parameter checking and control mediated through a C language interface.
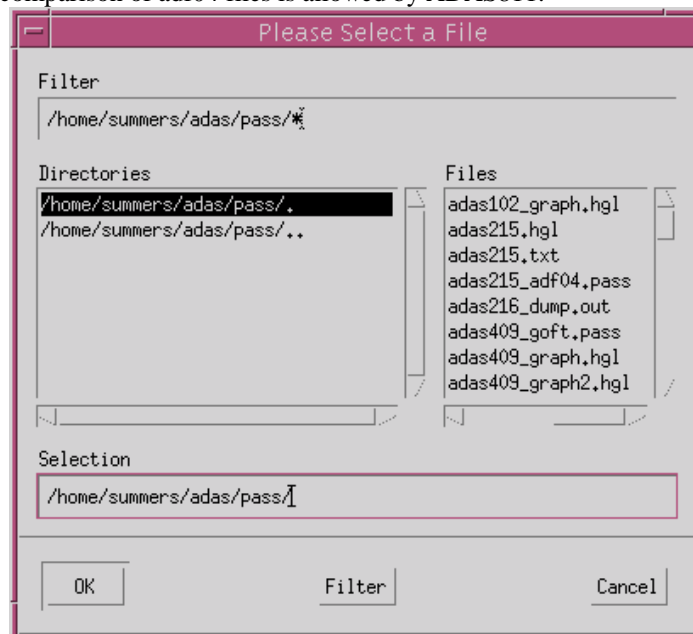
Interactive parameter comments:

The program interrogates archived ADAS datasets of format *adf04* and initiates an interactive dialogue with the user in two parts, namely, input file selection and display/comparison of selected data. There is only graphical output.

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

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

a)

c)

b)

ADAS811 INPUT

adf04 file 01:

Data Root   /home/summers/adas/adf04/

Central Data   User Data   ☐ Edit Path Name

helike/helike_hpsl02he.dat

Data File   ..
helike_hpsl02he.dat
helike_kvil97he.dat

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

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

Enter File information

Browse Comments   Cancel   Done

f)   d)   e)

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

Please Select a File

Filter

/home/summers/adas/pass/*

Directories   Files

/home/summers/adas/pass/.   adas102_graph.hgl
/home/summers/adas/pass/..   adas215.hgl
                                     adas215.txt
                                     adas215_adf04.pass
                                     adas216_dump.out
                                     adas409_goft.pass
                                     adas409_graph.hgl
                                     adas409_graph2.hgl

Selection

/home/summers/adas/pass/

OK   Filter   Cancel

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

1. The selected adf04 files are shown at the top of the screen at a). If there is more than one file, click the appropriate button for the primary file you wish to scan through. If there is more than one adf04 file, the program will seek to match transitions between them. The matching does depend on standard configuration labelling and formatting in the adf04 files. The graphical display plots the coefficients from each transition from the primary file but plots the same coefficient from the other files only if it is unambigously matched.

2. Five types of rate coefficient can be displayed, namely electron impact excitation, positive ion excitation, recombination, ionisation and charge exchange. Make the appropriate selection at b). A number of different forms for display of the selected coefficient may be permitted. The choices are displayed at c) and are selected by button click.

a)   b)
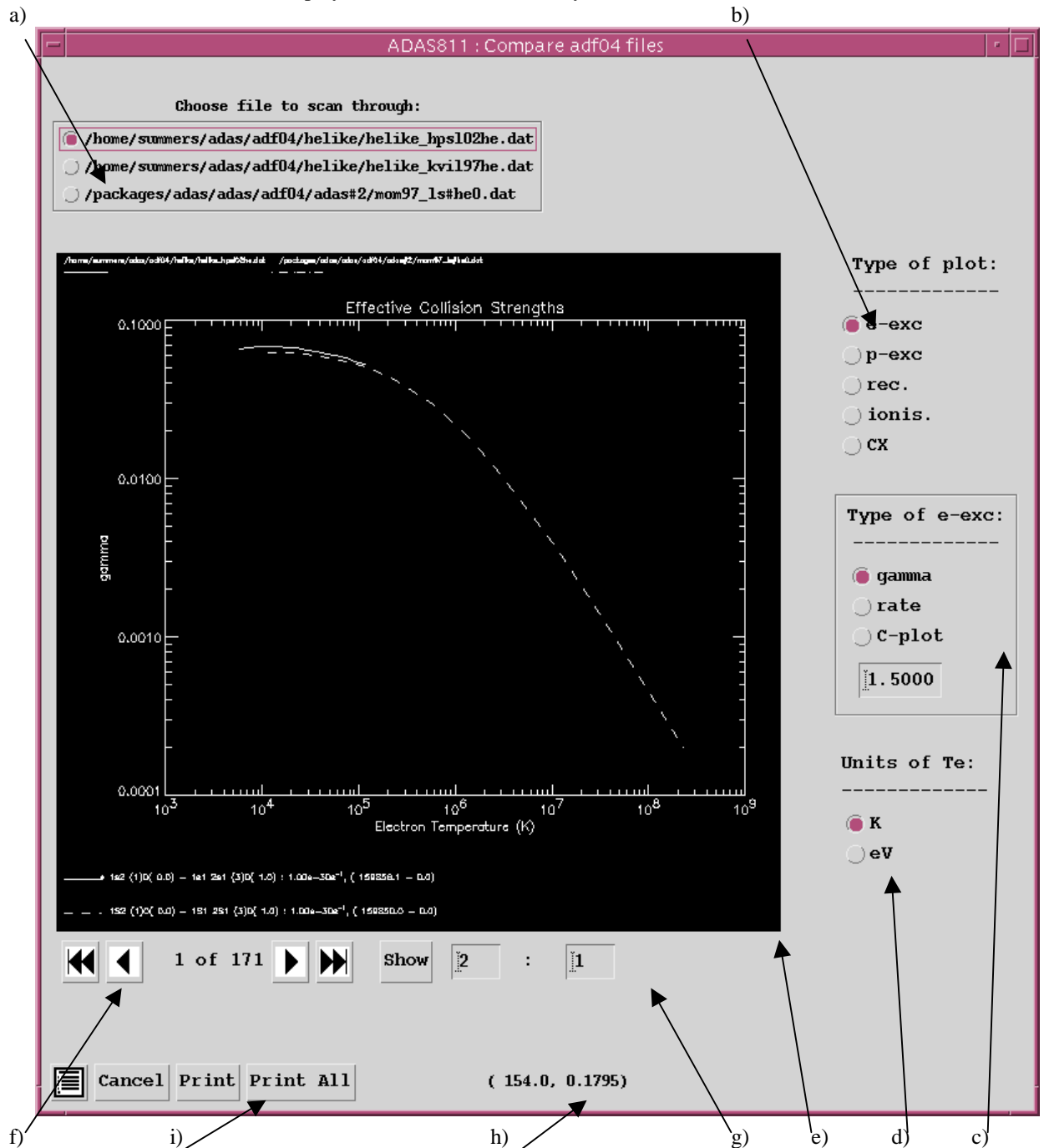
3. Coefficients are plotted as a function of temperature. The units, K or eV, may be chosen at d).
4. The plots are displayed at e). The legend of the graph plot line appearances is at the top of the graph and the identification of the particular transition given at the bottom.
5. Tape recorder type controls are given at f) to move between transitions, or the indices of the transiiton may be typed in explicitly at g).
6. Note that the cursor position in graph axis coordinates is given at h).
7. The button controls at i) allow printing of the current graph , *Print*, or of all the graphs, *Print All*. . The *Escape to Menu* icon is also available for a quick exit to the main ADAS menu. The *Cancel* button returns the user to the input file selection screen.

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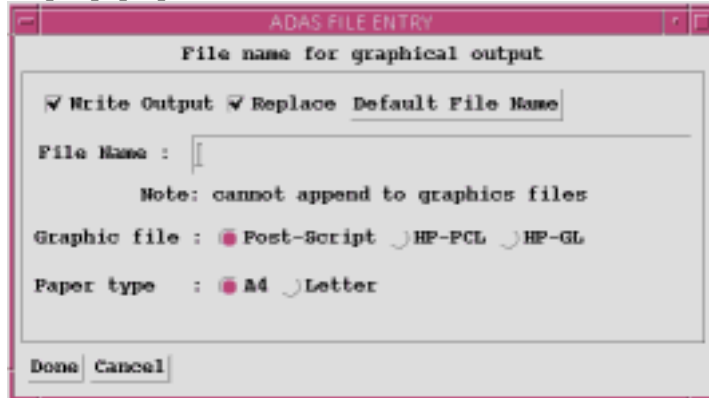
Illustration:

A typical output graph from the program is illustrated for an electron impact excitation transition in figure 9.2.
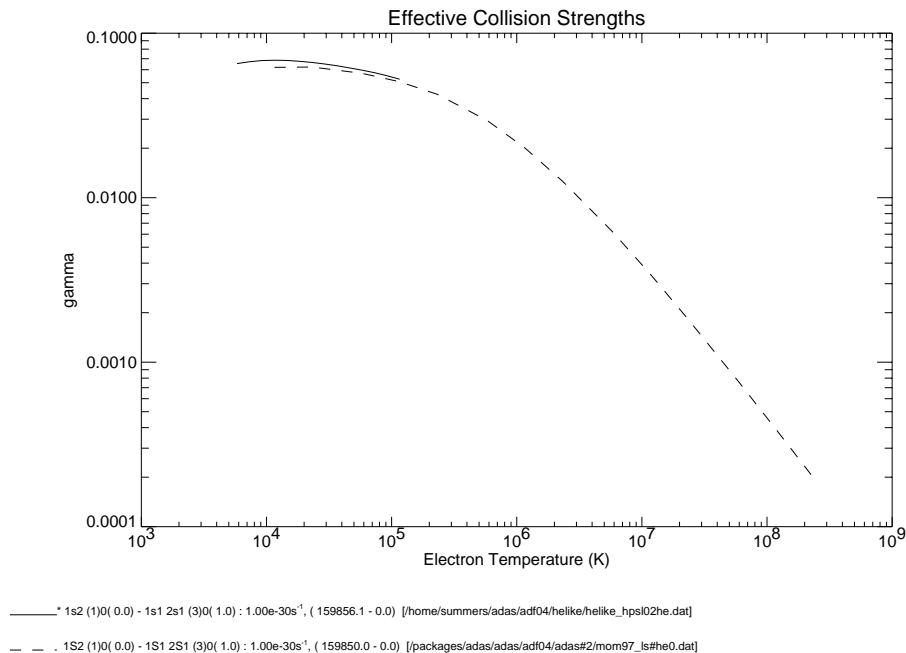
Figure 9.2

Figure 9.2 shows the Upsilon (effective collision strength) parameter versus electron temperature (K) for the He^0 transition $1s^2\ {}^1S_0 - 1s2s\ {}^3S_1$ The comparison is of the 2002 revised preferred data with the older 1997 preferred data. See the comments on the data sets for more details.