ADAS809: Non-Maxwellian modelling - change adf04 file type

The program converts an ADF04 – type 1 file to a standard ADF04 – type 3 file. That is an ADF04 file with collision strength data is converted to an ADF04 file with Maxwell averaged collision strengths.

Background theory:

The tabulation of the electron impact excitation and ionisation data in an ADF04 – type 1 file is of collision strength Ω versus threshold parameter X. $X = \varepsilon_i / \Delta E_{ij}$ where ΔE_{ij} is the energy of the transition $i \rightarrow j$ and ε_i is the incident electron energy with the target in the lower energy state i. At the finest energy resolution, collision strengths display detailed resonance structure. It is assumed that the tabulated collisions strengths in the ADF04 – type 1 file are smoothly varying, that is they have been subject to some averaging over resonant structure. It is evident that if the 'width' of the averaging interval above is $\Delta E_{res-avge}$, then the generation of Maxwell averaged collision strengths at temperature T_e is meaningful only if $kT_e >> \Delta E_{res-avge}$. The numerical quadrature procedure takes account of dipole, non-dipole and spin change forms for excitation. The behaviours for transition $i \rightarrow j$ are as

$$dipole: \qquad \Omega_{ij} \approx F_3 S_{ij} \log(X + F_2)$$
$$non-dipole: \quad \Omega_{ij} \approx F_3 + F_2 / X \qquad\qquad 9.9.1$$
$$spin\ change: \quad \Omega_{ij} \approx F_3 / (X + F_2)^2$$

where F_2 and F_3 are constants. In the dipole case, asymptotically $F_3 = \frac{4}{3}$. S_{ij} is the *line strength* for the transition. For ionisation, the dipole form with $F_3 S_{ij}$ replaced by the single constant F_3' is appropriate. For electron impact excitation of ions, the collision strength tends to a finite value at threshold. In contrast, for neutral atom excitation and ionisation, the collision strength tends to zero at theshold, with the threshold behaviour $\Omega \sim a X^{\alpha}$. Usually $\alpha = 1/2$ for neutral atom excitation and $\alpha \sim 1$ for ionisation of both atoms and ions.

For the tabulation $\{(X_k , \Omega_k) : k = 1,...,n \}$, the quadrature

$$Y_{ij} = \int_0^\infty \Omega_{ij}(\varepsilon_j) \exp(-\varepsilon_j / kT_e) d(\varepsilon_j / kT_e) \qquad\qquad 9.9.2$$

is expressed as

$$Y_{ij} = (\Delta E_{ij} / kT_e) exp(\Delta E_{ij} / kT_e)$$
$$\int_1^\infty \Omega_{ij}(X) exp[- X(\Delta E_{ij} / kT_e))] dX \qquad\qquad 9.9.2$$

and the integral divided into the ranges $\int_1^{X_1}$, $\int_{X_1}^{X_n}$ and $\int_{X_n}^\infty$. The asymptotic behaviours extrapolating from the first and last two tabular points are used in the evaluation of the first and last integrals respectively. The second integral is evaluated piece-wise in each tabular interval with the integrand locally fitted to a quadratic in either a linear scale (ie. $\Omega = c_1 + c_2 X + c_3 X^2$) or logarithmic scale picture (ie. $\ln\Omega = c_1 + c_2 \ln X + c_3 \ln X^2$).

Quadrature precision is checked from the exact integrals of the approximate forms, namely,

$$dipole: \qquad \mathrm{Y}_{ij} \approx F_3 S_{ij} \, [ln(1 + F_2) + EEI((1 + F_2)\Delta E_{ij} / kT_e)]$$

$$non - dipole : \mathrm{Y}_{ij} \approx F_3 + F_2(\Delta E_{ij} / kT_e)EEI(\Delta E_{ij} / kT_e) \qquad \qquad 9.$$

$$spin \ change : \mathrm{Y}_{ij} \approx \frac{F_3(\Delta E_{ij} / kT_e)}{1 + F_2} EE2((1 + F_2)\Delta E_{ij} / kT_e)$$

9.3

where $EEI(x) = \exp(x)E_1(x)$ and $EE2(x) = \exp(x)E_2(x)$ with E_1 and E_2 the first and second exponential integrals. A further verification on the quadratures is from the exact integrals for $\Omega = $ constant, $\Omega = X - 1$ and $\Omega = (X - 1)^2$ which are exact for the quadratic fit, linear scale option.

The program has a capability for comparison and display. In addition to the input ADF04 – type 1 file for conversion, it can accept a second ADF04 – type 3 file. The temperature set for output is copied from the latter reference file. Additionally, the collision data for a selected single transition may be graphed along with the corresponding data from the reference file if it exists. The usual display and output routing facilities are provided.

Program steps:

These are summarised in figure 8.9.

Figure 8.9
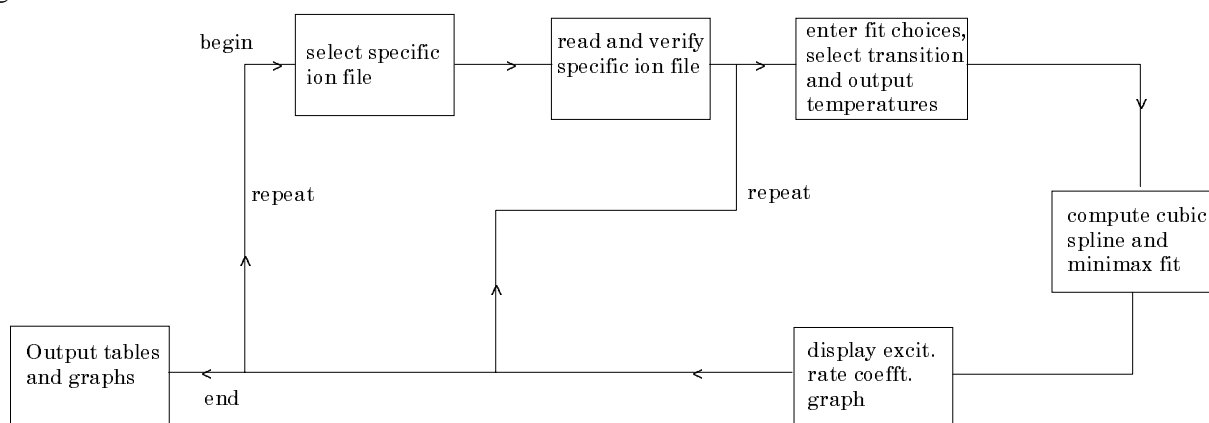
Interactive parameter comments:

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 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, move to the series 2 menu and click on the first button to activate ADAS201.
The **file selection window** has the appearance shown below

1. Selection of two adf04 files is permitted. The first selected in the upper sub-window is of *adf04 – type1* and is mandatory. The second optional file, selected in the lower sub-window is of adf04-type3. It provides a temperature grid for the conversion. Selection of the *adf04* files follows the standard ADAS.

2. Data root shows the full pathway to the appropriate *adf04* data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier

replacing the first *adas,* to use this facility. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.

3. Available sub-directories are shown in the large file display window. Scroll bars appear if the number of entries exceed the file display window size. Click on a name to select it. The selected name appears in the smaller selection window above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat.*
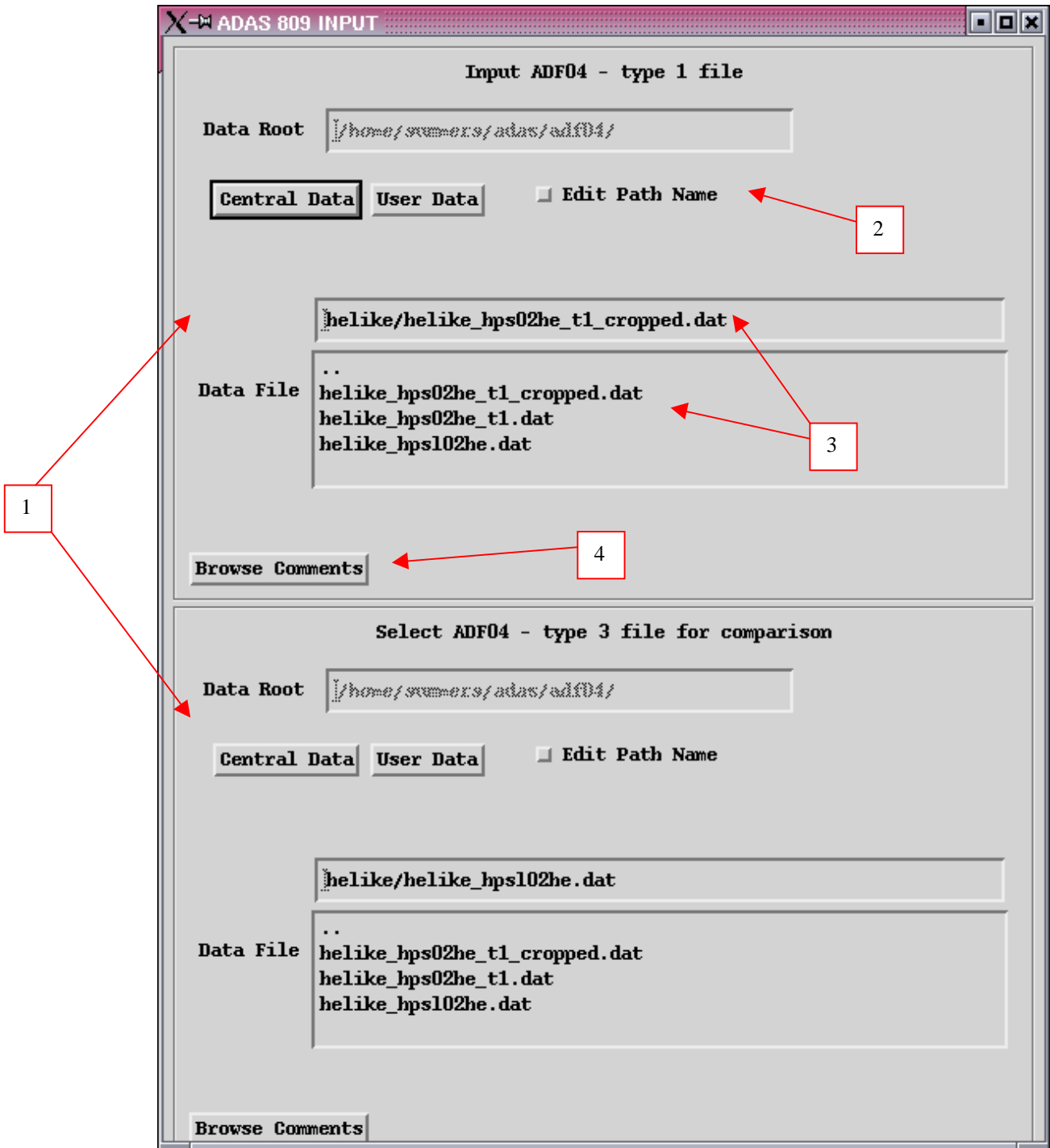

4. Once the *adf04* files are selected, the set of buttons at the bottom of the main window become active. Clicking on the *Browse Comments* button displays the comment line information stored with the *adf04* datafile. It

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.

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

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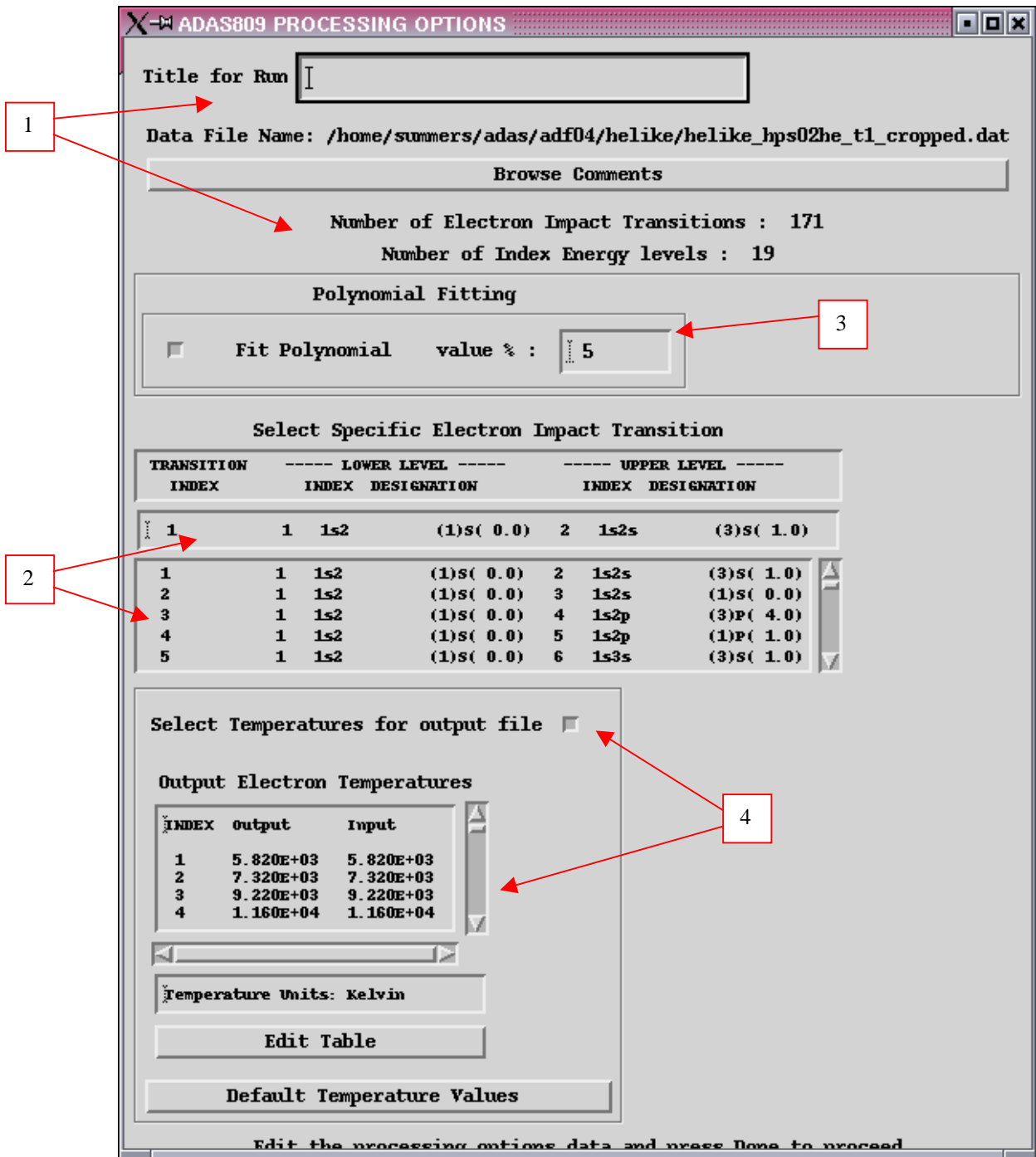

2. Transitions for which electron impact excitation data are available in the data set are displayed in the line list display window. This is a scrollable window using the scroll bar to the right of the window. Click anywhere on

the row for a line to select it. The selected transition appears in the selection window just above the line list display window. This single transition will displayed.

3. The output rate coefficient for the selected transition may be fitted with a polynomial. This is as a function of temperature. Clicking the *Fit Polynomial* button activates this. The accuracy of the fitting required may be specified in the editable box. The value in the box is editable only if the *Fit Polynomial* button is active.

4. To obtain an output *adf04-type3* file output temperatures must be selected. If a comparative *adf04-type3* file was selected, the Input temperatures are taken from that file. Otherwise temperatures from the Defaults file are used. Pressing the *Default Temperature values* button inserts a default set of temperatures equal to the input temperatures

5. 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.

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

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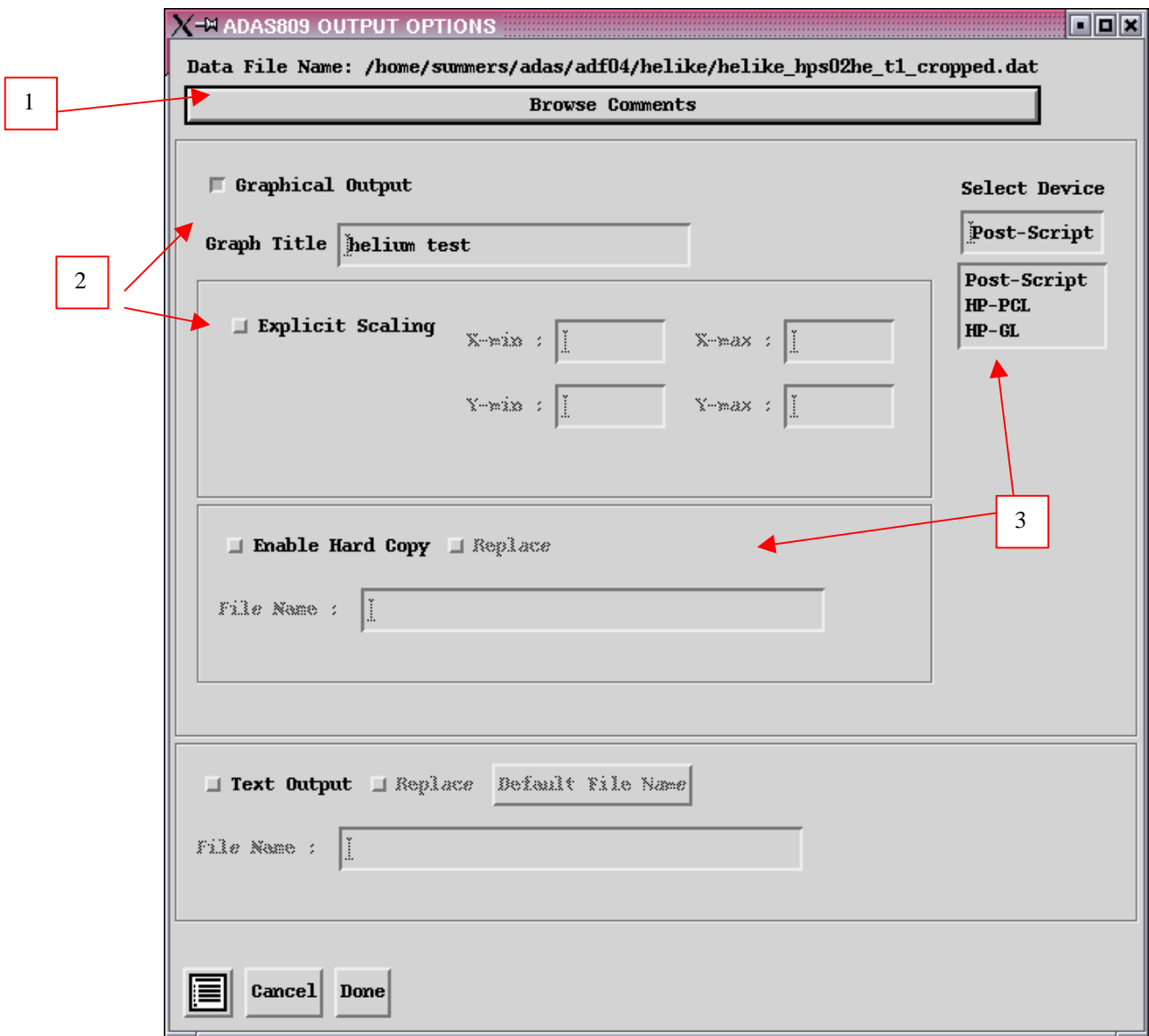
2. Graphical display is activated by the *Graphical Output* button. This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph. By default, graph scaling is adjusted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

3. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. If the output graphic file already exits and the *Replace* button has not been activated, a 'pop-up' window issues a warning. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.

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

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