

ADAS810: Generate envelope feature photon emissivity coefficient

The program calculates envelope feature emissivities of type ADF40 for an ion of a complex element. The program is a foreground, interactive, version of the mass production, paralised background code ADAS810_offline. The interactive version is designed for small sample testing and test result production prior to large scale execution. It can use the same driver data file type (ADF42) as the offline version, but allows the user to modify some driver parameters. ADAS810 includes the full population, emissivity and radiated power calculation functionality of ADAS208.

Background theory:

An envelope feature photon emissivity coefficient, denoted by \mathcal{F}_{PEC} , is defined on a wavelength interval and is a composite feature arising from very many lines from a single ionisation stage. The \mathcal{F}_{PEC} is suitable as a descriptor in wavelength intervals and at spectral resolutions where the individual component lines are unresolved or only partly resolved. This situation occurs with very complex heavy element ions for which it becomes helpful and economical to handle the envelope feature rather than the individual line emissivity coefficients (\mathcal{PEC} s). Following Chap 3.8, the emissivity of an individual line is specified as

$$\varepsilon_{j \rightarrow k} = A_{j \rightarrow k} \left(\sum_{\sigma=1}^M \mathcal{F}_{j\sigma}^{(exc)} N_e N_{\sigma} + \sum_{v'=1}^{M+1} \mathcal{F}_{jv'}^{(rec)} N_e N_{v'} \right). \quad 9.10.1$$

This allows specification of the *excitation* photon emissivity coefficient

$$\mathcal{PEC}_{\sigma, j \rightarrow k}^{(exc)} = A_{j \rightarrow k} \mathcal{F}_{j\sigma}^{(exc)} \quad 9.10.2$$

and the *recombination* photon emissivity coefficient

$$\mathcal{PEC}_{v', j \rightarrow k}^{(rec)} = A_{j \rightarrow k} \mathcal{F}_{jv'}^{(rec)}. \quad 9.10.3$$

There are similar coefficients, namely, the *charge exchange* photon emissivity coefficient and the *ionisation* photon emissivity coefficient, which are of less relevance here. Each of these coefficients is associated with a particular metastable σ or v' of the X^{+z} , or X^{+z+1} ions respectively.

Consider a spectral interval, $[\lambda_0, \lambda_1]$, subdivided into N_{pix} intervals as $\{\Delta\lambda_i^{[0,1]} \equiv [\lambda_0 + i(\lambda_1 - \lambda_0)/N_{pix}, \lambda_0 + (i+1)(\lambda_1 - \lambda_0)/N_{pix}] : i = 0, \dots, N_{pix} - 1\}$ Also suppose that the $j \rightarrow k$ spectrum line has a normalised emission profile $\varphi_{j \rightarrow k}(\lambda)$. In general, such a profile is a convolution of Doppler and instrumental functions. Then the envelope feature photon emissivity coefficient vector is defined as

$$\mathcal{F}_{\text{PEC}_{\sigma, i}^{(exc)}/[0,1]} = \sum_{\substack{j,k \\ \lambda_{j \rightarrow k} \in [0,1]}} \mathcal{PEC}_{\sigma, j \rightarrow k}^{(exc)} \int_{\lambda_i}^{\lambda_{i+1}} \varphi_{j \rightarrow k}(\lambda) d\lambda \quad 9.10.4$$

$\lambda_{j \rightarrow k}$ is the natural wavelength of the $j \rightarrow k$ spectrum line. The default broadening assumed is Doppler with a Maxwellian distribution for the emitting ion at temperature, T_{ion} , equal to the electron temperature, T_e , used in the collisional–radiative modelling of the \mathcal{PEC} s. This constitutes a minimum broadening. The integral in equation 9.10.4 is then expressible in terms of error functions as

$$\mathcal{F}_{\text{PEC}_{\sigma, i}^{(exc)}/[0,1]} = \sum_{\substack{j,k \\ \lambda_{j \rightarrow k} \in \Delta\lambda_i^{[0,1]}}} \mathcal{PEC}_{\sigma, j \rightarrow k}^{(exc)} \frac{1}{2} \{ \text{erfc}((\lambda_i - \lambda_{j \rightarrow k})/\sigma) - \text{erfc}((\lambda_{i+1} - \lambda_{j \rightarrow k})/\sigma) \} \quad 9.10.5$$

where $\sigma = \lambda_{j \rightarrow k} \alpha \left(\frac{kT_{ion}}{I_H} \cdot \frac{m_p}{m_X} \cdot \frac{m_e}{m_p} \right)^{1/2}$ and m_X is the emitting ion mass.

In actual spectral analysis involving complex heavy species, individual strong spectrum lines may be distinguishable from the envelope. It is therefore appropriate to archive a restricted number of the strongest individual PEC s and these can be identified and ordered as processing for the \mathcal{F}_PEC s takes place. Again, while passing through the complete set of radiative transitions for assignment to excitation $\mathcal{F}_PEC^{(exc)}$ s, the line radiative power coefficient for the ion, $P_{LT}^{(z)}$, can be totalled. This total line power coefficient (archived in the data class ADF11, subcategory PII), which is the part driven by excitation for the ground or metastable levels of the ion, is a more precise estimate than computed by the code ADAS408 and so is a preferred substitute for that data. For application to actual measurements of total radiation emission, it is normally necessary to calculate $P_{LT}^{(z)}$ as modified by appropriate soft x-ray and /or bolometer filter transmission functions. Such modification can not be done retrospectively on the unfiltered $P_{LT}^{(z)}$. In contrast, the $\mathcal{F}_PEC^{(exc)}$ is suited to further processing which can include imposition of spectrometer instrument functions as well as filtering and integration over extended wavelength regions. Such additional operations on \mathcal{F}_PEC s are treated as separate from ADAS810 will be handled by a new code for. Note that preparation of filters is provided by the codes ADAS414 and ADAS415. It is also assumed that this is the route for preparation of higher precision filtered $P_{LT}^{(z)}$ s and requires the initial creation of appropriate \mathcal{F}_PEC s via the present ADAS810 code.

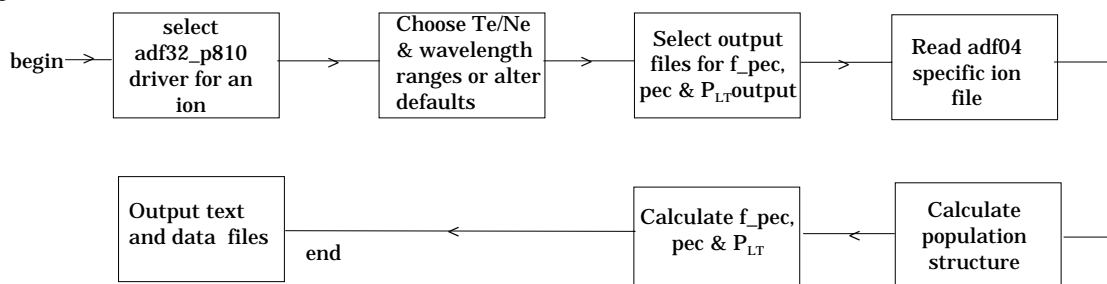
In like manner, $PEC^{(rec)}$ s can be produced, provided the input data (ADF04) supports this. Note that for ease and consistency in modelling, the same spectral intervals apply to both the $\mathcal{F}_PEC^{(exc)}$ s and the $PEC^{(rec)}$ s and to each of the metastable drivers – if more than one. Also, the selection of the strong individual PEC s is determined from the whole ground excitation driven set and the selected set is then used for all other metastable drivers and for recombination. The rank ordering of individual PEC s is from the maximum of each PEC viewed as a tabular function of T_e and N_e .

Note finally that \mathcal{F}_PEC s are tabulated as a function of selected wavelength range, wavelength interval bin, T_e and N_e with $T_i = T_e$.

Program steps:

These are summarised in figure 9.10.

Figure 9.10



It is noted again that the code is designed to allow single ion testing of \mathcal{F}_PEC production. The primary intent is nonetheless mass production and so the interactive code ADAS810 makes use of the driver data sets and file naming conventions of the mass production codes. As ADAS810 is in essence a variant of the population code ADAS208, instead of direct selection of an ADF42 driver file, the data set selected on the INPUT screen may be an ADF04 file.

As noted above, the driver files for this application are of format ADF42. The planned organisation in central ADAS will be according to pathways `./.../adas/adf42/iso_nucl/<element>/`. The primary parameter settings for operation of ADAS810 are contained in the driver, which may be copied to the equivalent user area and edited directly to modify operation. The driver structure is shown in the illustration below.

Note the various file pathways which include the input ADF04 file and then the output PII , PEC and \mathcal{F}_PEC files. In interactive operation, ADAS810 allows re-specification of some parameters such as wavelength intervals, temperatures etc. (on the processing screen and of output file routing (on

the output screen)) over-riding the adf42 driver file. All other parameters are predetermined or set in the driver file. Note the use of namelists where possible in the driver file structure

```

&FILES
  dsn04 = '/home/adas/adas/adf04/adas#6/mom97_ls#c2.dat',
  dsn18 = 'NULL',
  dsn35 = 'NULL',
  dsn15 = 'test_adf15_pec.dat',
  dsn40 = 'test_adf40_fpec.dat',
  dsn11 = 'test_adf11_plt.dat',
  dsn11f = 'test_adf11_plt_filter.dat'
&END

&ION
  element = 'C',
  z0      = 6,
  z1      = 2,
  ip      = 386241.0
&END

&META
  lnorm   = .TRUE.,
  nmet    = 1,
  imetr(1) = 1
&END

&PROCESS
  liosel = .FALSE.,
  lhsel  = .FALSE.,
  lrsel  = .FALSE.,
  lisel  = .FALSE.,
  lnsl   = .FALSE.,
  lpsele = .FALSE.,
  zeff   = 0.0
&END

&OUTPUT
  lmetr  = .FALSE.,
  ltsc1  = .FALSE.,
  ldsc1  = .FALSE.,
  lbrdi  = .FALSE.,
  numte  = 5,
  numtion = 0,
  numth  = 0,
  numdens = 5,
  numdion = 0,
  numwv1 = 3
&END

1.800e+04 4.500e+04 9.000e+04 1.800e+05 4.500e+05

1.000E+11 1.000E+12 1.000E+13 1.000E+14 1.000E+15

64 1.500e+00 3.00e+00
32 1.000e+01 1.00e+02
32 4.500e+02 8.00e+02

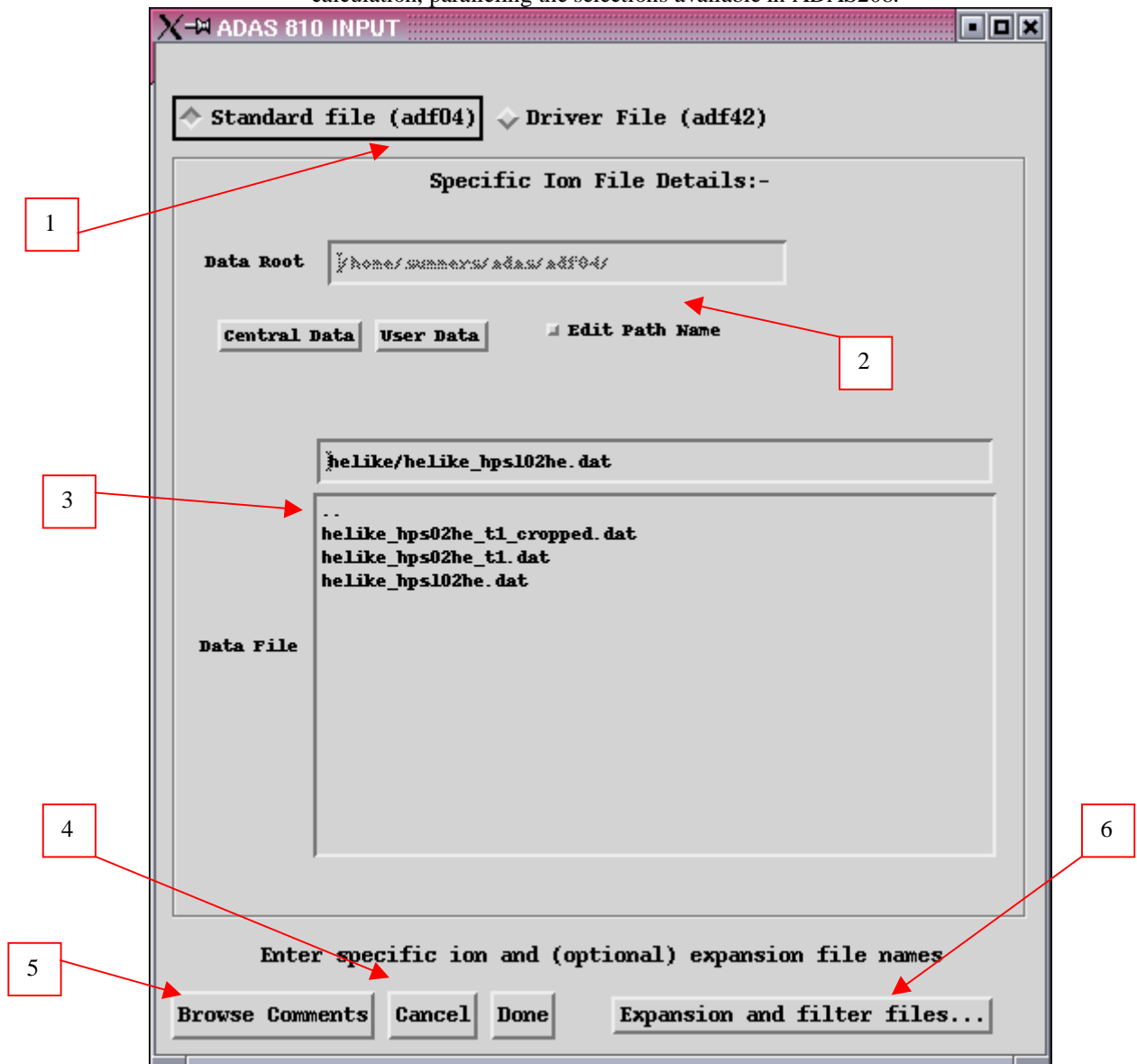
```

Interactive parameter comments:

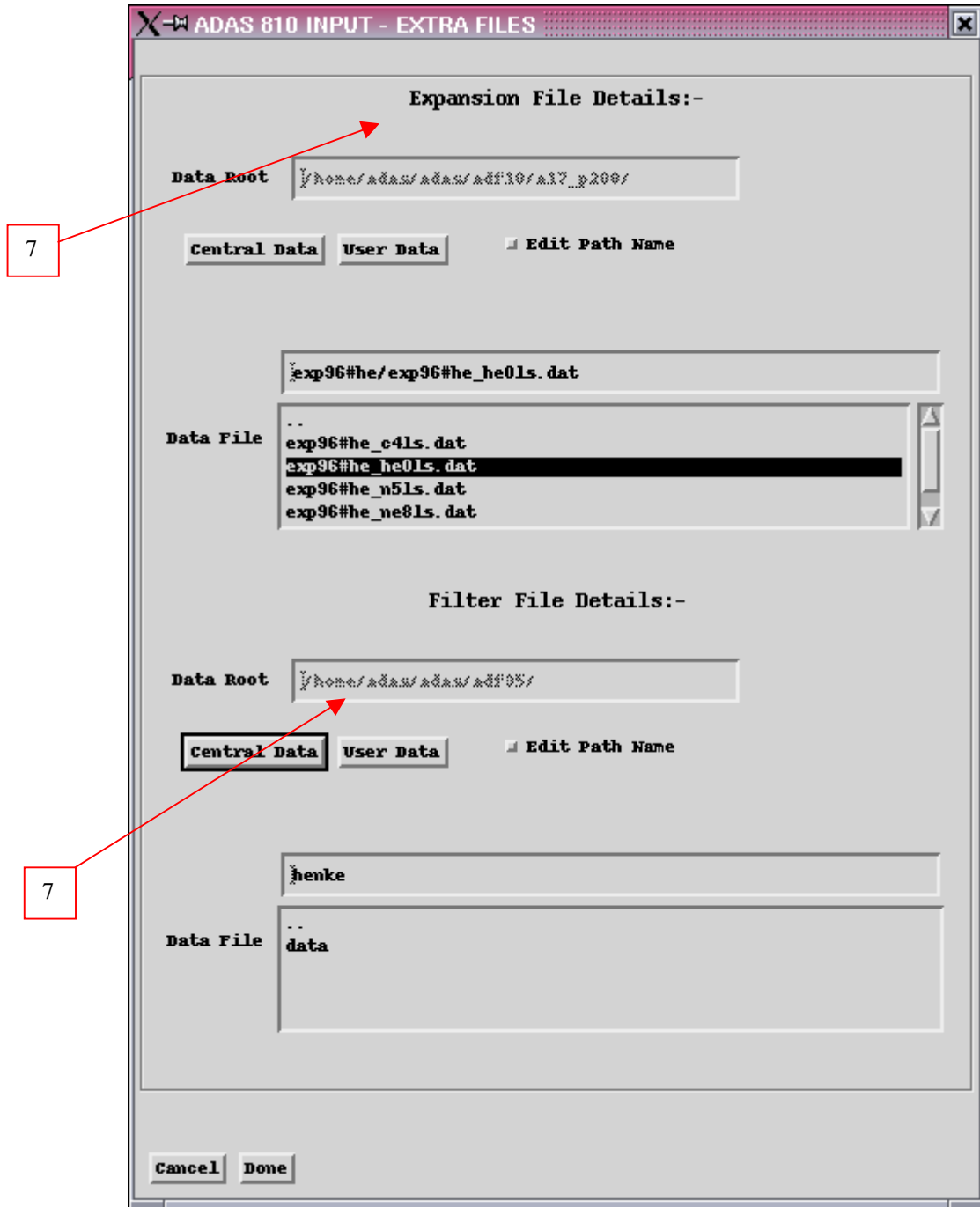
The **file selection window** is as shown below

1. A primary file, either an adf04 for the ion whose spectral line and envelope emissivities are required, or a driver file of format adf42 is required. The driver file route maintains compatibility of operation of the interactive ADAS810 with the automatic offline mass production codes. Data from the driver file fills the editable fields in on the following Processing window. With an ADF04 file selected, these fields must be edited in.

2. Note that each type of data is stored according to its ADAS data format (*adf* number). Your personal data should be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*.
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 the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
4. Once a data file is selected, the set of buttons at the bottom of the main window become active.
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. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window.
6. An extra button, *Expansion and filter files*, is present. Click it to pop-up a supplementary file selection window shown below. These supplementary files may be included, if available, to extend the population and emissivity calculation, paralleling the selections available in ADAS208.



7. On the upper sub-window, an expansion file may be selected. This is the same expansion file as used by ADAS208 and is drawn from the cross-referencing file subclass *adf18/a17_p208*.
8. On the lower sub-window, a filter file of format *adf35* may be selected. ADAS810 provides total radiative power and filtered power as well as the line and envelope emisivities.



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

1. An arbitrary title may be given for the case being processed.
2. For information the full pathways to the datasets being processed are also shown. The button *Browse comments* again allows display of the information field section at the foot of the selected dataset, if it exists.
3. The main inputs follow that those of ADAS208. Your settings of electron temperature, ion temperature and neutral hydrogen temperature are shown in

the temperature display window. The temperature values at which the excitation rate coefficients (in fact 'upsilons') are stored in the selected adf04 (input) are also shown for information. The program obtains the output from the adf42 driver file if available. A similar pattern is shown in the Density sub-window although there is no 'Input' from the adf04 file.

4. Selection of *Default* temperatures is somewhat different from the usual ADAS pattern. A drop-down menu allows choice from a number of favoured sets, such as the GCR Standard set. Personal preferred sets are allowed. These should be stored in your `./.../<uid>/adas/defaults/` directory as `adas810_te.dat` (for temperature defaults) and `adas810_dens.dat` (for density defaults). Samples are illustrated below.

```

2
-----
Low Te set
11
ev
1.0
2.0
3.0
5.0
7.0
10.0
20.0
30.0
50.0
70.0
100.0
-----
Another set
4
K
500.0
1000.0
4000.0
8000.0

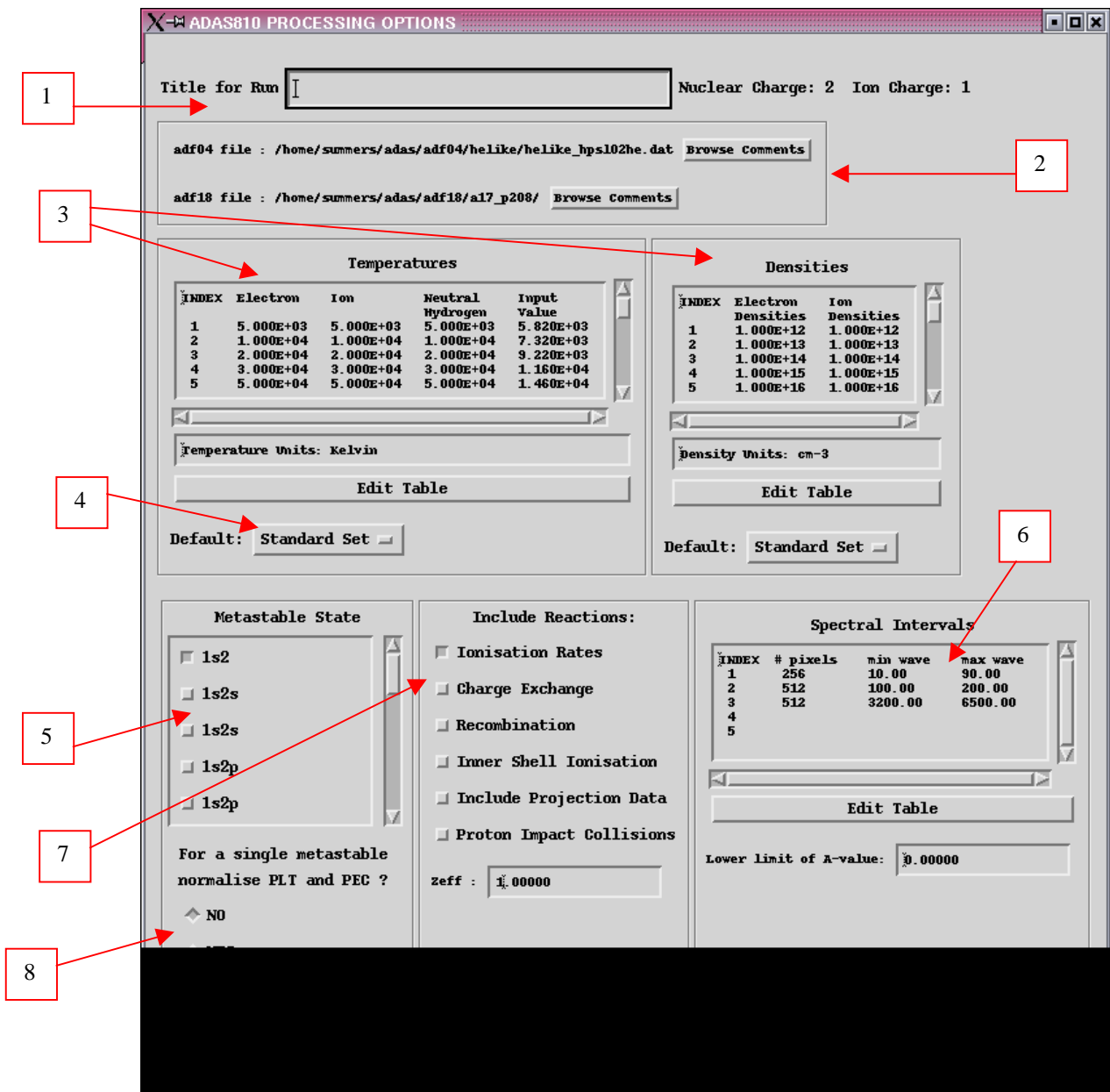
```

```

2
-----
Low Ne set
4
cm-3
1.0e11
2.0e11
3.0e11
4.0e11
-----
Another set
4
cm-3
1.0e12
2.0e12
3.0e12
4.0e12

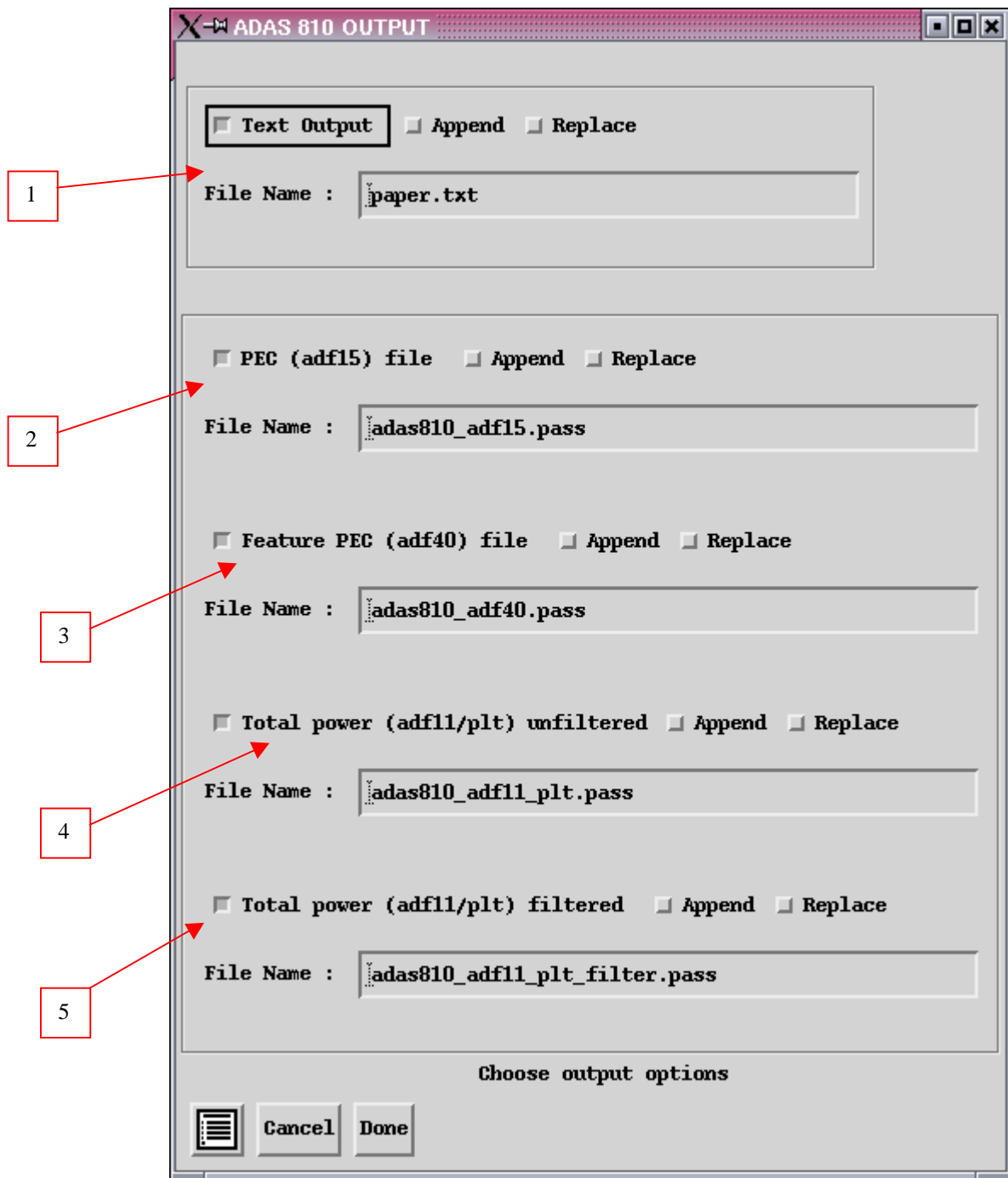
```

5. Selection of metastables is done from a scrollable button list rather than a pop-up.
6. Wavelength ranges and associated pixels are specified in an editable table.
7. The set of control parameters for the calculation follows ADAS208.
8. The Normalisation option should be chosen when there is only a single metastable..



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

1. 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. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated.
2. The *PEC* (*adf15*) file comprises the set of individual line emissivity coefficients.



3. The *Feature PEC (adf40)* file comprises the envelope feature data for each selected wavelength interval and each metastable, tabulated in pixel space as a function of temperature and density .
4. The *Total power (adf11/plt) unfiltered* file comprises the total radiated power in the spectral intervals.
5. The *Total power (adf11/plt) filtered* file comprises the radiated power in the spectral intervals as transmitted by the filter specified in the input filter file – if selected.

Notes: