Beam stopping and beam emission spectroscopy

For a neutral beam species A being stopped by fully stripped impurity species and electrons in the plasma, the stopping coefficient is the effective loss rate coefficient of electrons from A. This corresponds closely to the effective ionisation rate coefficient or *collisional-radiative* ionisation coefficient from the ground state of A, where charge transfer losses as well as direct ionisation losses are included. It is usual to write the coefficient in terms of the plasma electron density N_e so that the loss rate is $N_e S_{CR}^{(A)}$.

One can apply almost the same modelling approach to hydrogen (or helium) atoms in a thermal plasma or to hydrogen atoms in a beam. The practical distinction is made by the assignment of a translational velocity for beam atoms. This velocity is incorporated in the integrals of beam particle / plasma particle cross-sections over the Maxwellian distributions in the thermal plasma. For hydrogen forming part of the thermal plasma, the translational velocity is set to zero. In the latter circumstance, ion impact collision rates are very small compared with electron impact rates. Also recombination (both free-electron capture and charge exchange capture) become significant processes. For the hydrogen atoms in a fast beam, recombination is not relevant and although formally present is ignored in the results. However the translational velocity can make ion impact collisions more important than electron collisions.

For hydrogen or hydrogenic ions in a plasma, the largest collision cross-sections are those for which n=n' and l=l'± 1. For these cases the transition energy is nearly zero and the cross-sections are so large for electron and ion densities of relevance for fusion that it is very good approximation to assume relative statistical population for the l-states. Thus for hydrogenic systems only populations of complete n-shells need be evaluated, the *bundle-n* approximation. The equilibrium populations of the n-shells, N_n, are the solution of the statistical balance equations

$$\begin{aligned}
&\sum_{n'>n}[A_{n'\to n} + u(\nu)B_{n'\to n} + N_e q^{(e)}_{n'\to n} + N_e q^{(p)}_{n'\to n}]N_{n'} \\
&+\sum_{n''<n}[u(\nu)B_{n''\to n} + N_e q^{(e)}_{n''\to n} + N_e q^{(p)}_{n''\to n}]N_{n''} \\
&+N_e N_+ \alpha_n^{(r)} + N_e^2 N_+ \alpha_n^{(3)} + N_e N_+ \int u(\nu)B_{\kappa\to n}d\kappa \\
&= \{\sum_{n'>n}[u(\nu)B_{n\to n'} + N_e q^{(e)}_{n\to n'} + N_e q^{(p)}_{n\to n'}] \\
&+ \sum_{n''<n}[A_{n\to n''} + u(\nu)B_{n\to n''} + N_e q^{(e)}_{n\to n''} + N_e q^{(p)}_{n\to n''}] \\
&+\int u(\nu)B_{n\to\kappa}d\kappa + N_e q^{(e)}_{n\to\varepsilon} + N_e q^{(p)}_{n\to\varepsilon}\}N_n
\end{aligned}$$

N_n is the population of the state $X_n^{+z_0-1}$ and N_+ of the parent ion X^{+z_0}. N_e is the free electron density and N_p the free proton density. A and B are the usual Einstein coefficients, $q^{(e)}$ and $q^{(p)}$ denotes collisional rates due to electrons and protons, $\alpha_n^{(r)}$ and $\alpha_n^{(\tau)}$ denote radiative and three-body recombination and $u(\nu)$ is the energy density of the radiation field. There is one such equation for each value of n from 1 to ∞. The equations may be extended by including reactions for other impurity ions additional to the protons. The radiation field presence in the equations is not of direct relevance to hydrogen population modelling in a fusion plasma, but it can be exploited in a purely technical manner to separate the influence of different driving populations in the collisional-radiative sense.

Population results and preparing tabulations

ADAS 310 is the primary code for evaluating beam stopping and emission coefficients for hydrogen beams. It is too slow in execution for a direct link to inter-pulse experiment analysis and so it is used to prepare tabulations of effective beam stopping and beam emission coefficients for subsequent look-up. The effective coefficients are most sensitive to the beam particle energy and the plasma ion density

and less sensitive to plasma ion temperature and Z-effective. Suitable tabulations can therefore be built on a reference set of plasma and beam conditions, a two-dimensional array of coefficients as functions of beam energy and plasma density at the reference conditions of the other parameters and then one-dimensional vectors of the coefficients as functions of each minor parameter at the reference condition of all the other parameters. ADAS310 accepts as input the definition of these scans, establishes an extended list of cases required to achieve these scans and then executes repeated population calculations at each set of plasma conditions in the list. ADAS310 can compute the populations for any mixture of light impurities (hydrogen to neon) in the plasma. It is impractical to deal with all possible mixtures of impurities. It is our usual practice to execute ADAS310 in turn for each light impurity from hydrogen to neon treated as a pure species. The mixed species effective coefficients are constructed from these pure impurity solutions by the theoretical data acquisition routines. The main population output is very complete and in principle contains all information on possible emitted spectrum lines up to very high n-shells together with both ionisation and recombination collisional-radiative coefficients. It is archived as ADAS data format ADF26. ADAS310 can also produce directly the final tabulations of beam stopping coefficient according to ADAS data format ADF21, however this is normally done using the post-processor program ADAS312.

ADAS304 is the interrogation code on the beam stopping coefficient data base ADF21. It also works with the beam emission coefficient data base, which is of identical organisation to the stopping coefficients, and is assigned to ADF22.

In creation of compact interpolable datasets of type ADF21 and ADF22, some simplifications are made. The stopping coefficient data sets for each impurity species are calculated as though that species alone is present in the plasma. For species X^{+z_0}, of nuclear charge z_0, of number density $N^{(z_0)}$, the electron density used in the stopping calculation is $N_e = z_0 N^{(z_0)}$ consistent with charge neutrality. Let the stopping coefficient for the impurity species X^{+z_0} be $S_{CR}^{(\mathrm{A},X)}$ then the loss rate is

$$N_e S_{CR}^{(\mathrm{A},X)}(E_B, N^{(z_0)}, T^{(z_0)}) = N_e S_{CR}^{(\mathrm{A},e)}(E_B, N^{(z_0)}, T^{(z_0)}) + N^{(z_0)} S_{CR}^{(\mathrm{A},z_0)}(E_B, N^{(z_0)}, T^{(z_0)})$$

distinguishing parts driven by excitation from the ground state of A by electron collisions and by X^{+z_0} ions respectively. The coefficient is

$$S_{CR}^{(\mathrm{A},X)}(E_B, N^{(z_0)}, T^{(z_0)}) = S_{CR}^{(\mathrm{A},e)}(E_B, N^{(z_0)}, T^{(z_0)}) + (1/z_0) S_{CR}^{(\mathrm{A},z_0)}(E_B, N^{(z_0)}, T^{(z_0)})$$

The density dependence of the collisional-radiative coefficient is written in terms of the impurity ion density $N^{(z_0)}$ since ion collisions primarily determine the collisional redistribution..

Consider a set of species $\{X_i^{+z_{0i}} : i = 1,..,I\}$ with fractions $\{f_i : i = 1,..,I\}$, in the plasma causing a composite stopping. The loss rate may be written approximately as

$$\begin{aligned} N_e S_{CR}^{(\mathrm{A})}(E_B, N_I, T_I) &\approx N_e S_{CR}^{(\mathrm{A},e)}(E_B, N_I, T_I) + \sum_{i=1}^{I} N_i^{(z_{0i})} S_{CR}^{(\mathrm{A},z_{0i})}(E_B, N_I, T_I) \\ &= \sum_{i=1}^{I} N_{e,i} [S_{CR}^{(\mathrm{A}e)}(E_B, N_I, T_I) + (1/z_{0i}) S_{CR}^{(\mathrm{A},z_{0i})}(E_B, N_I, T_I)] \end{aligned}$$

where

$$N_e = \sum_{i=1}^{I} N_{e,i} = \sum_{i=1}^{I} z_{0i} N^{(z_{0i})} = N_I (\sum_{i=1}^{I} z_{0i} f_i)$$

defines the proportions of the electron density contributed by each impurity species. From an ion collisional redistribution point of view, in a composite plasma the $\sum_{k=1}^{I} z_{0k}^2 N_k^{(Z_{0k})}$ z-weighted density

sum is meaningful so the equivalent density of the single impurity $X_i^{+z_{0i}}$ to correspond to the summed impurity ion density for this purpose is

$$N_i^{(z_{0i}),equiv} = N_I(\sum_{k=1}^{I} z_{0k}^2 f_k)/z_{0i}^2$$

and the equivalent electron density is

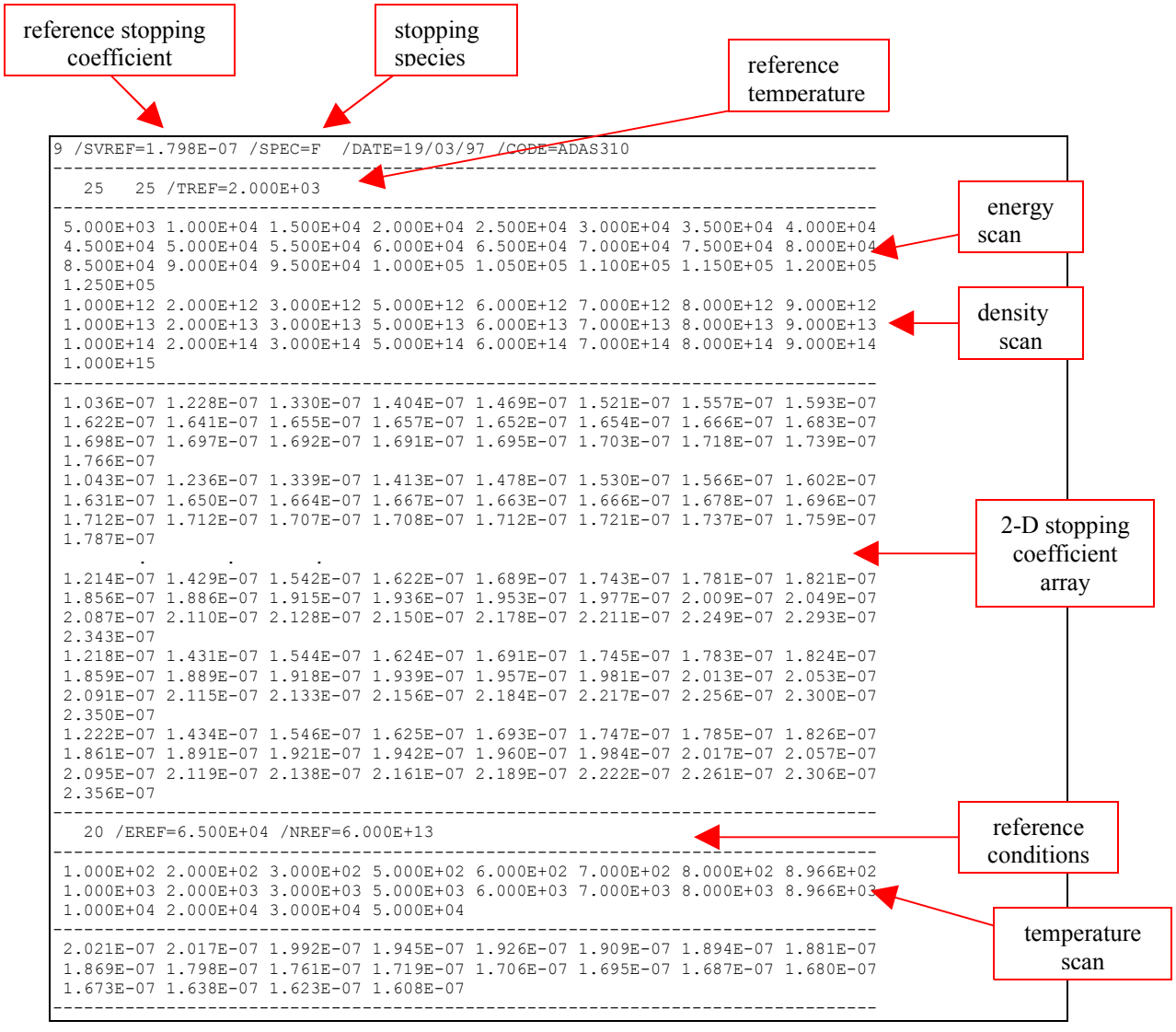
$$N_{ei}^{(z_{0i}),equiv} = \left(\frac{N_e}{\sum_{k=1}^{I} z_{0k} f_k}\right)(\sum_{k=1}^{I} z_{0k}^2 f_k)/z_{0i}$$

ADAS310 evaluates the stopping & emission coefficients as a function of electron density. The approximate composite stopping coefficient is assembled from the pure species coefficients as

$$S_{CR}^{(A)}(E_B, N_e, T_I) \approx \sum_{i=1}^{I}[z_{0i} f_i S_{CR}^{(A,X_i)}(E_B, N_{ei}^{(z_{0i}),equiv}, T_I)]/(\sum_{k=1}^{I} z_{0k} f_k)$$

The prescription outlined is equally applicable for the storage and handling of beam emission coefficients.

ADF21

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 2.350E-07
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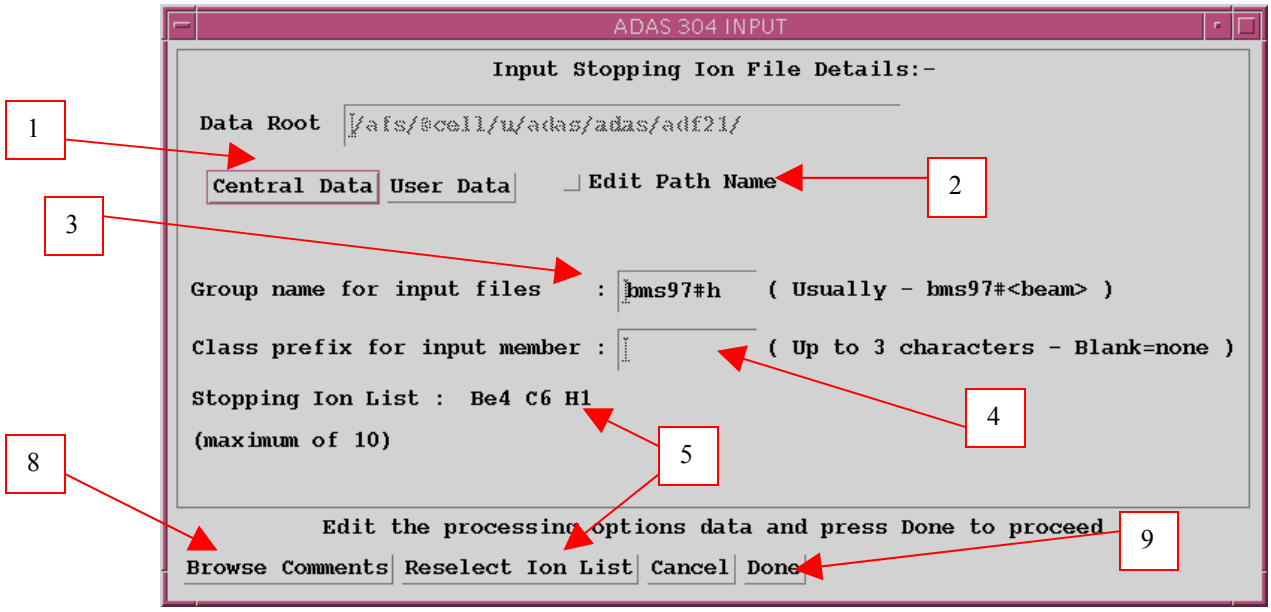
ADAS304

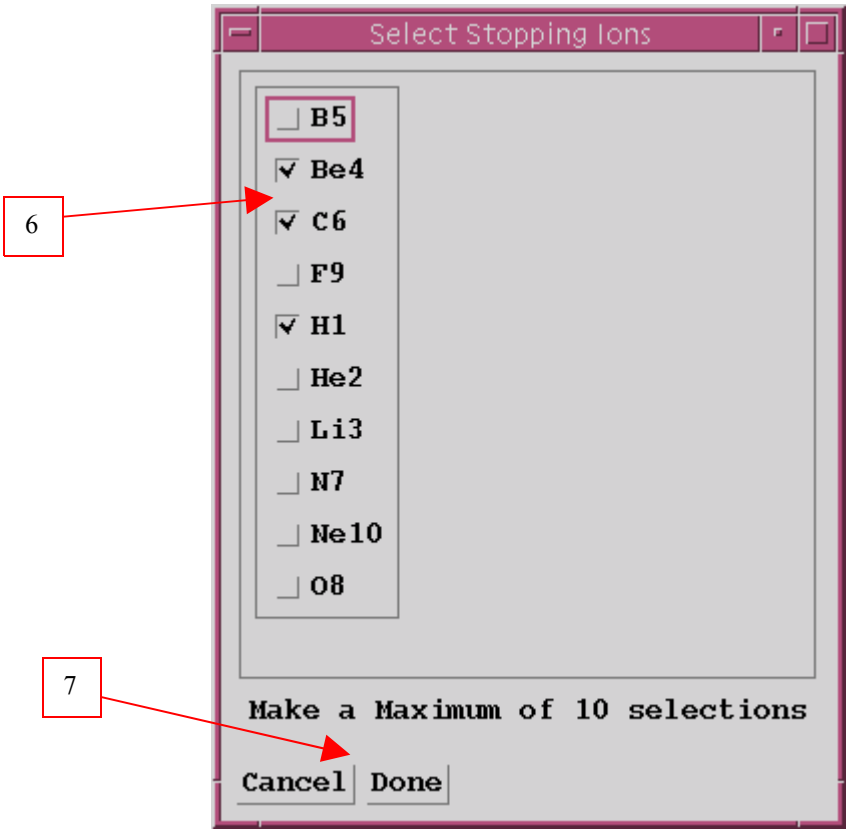
The code interrogates beam stopping or beam emission coefficient files of type ADF21 or ADF22. Data is extracted for stopping by a composite plasma consisting of a mixture of protons (deuterons) and fully ionised impurities. The data is interpolated using cubic splines at selected beam energy, target density and target temperature triplets. Minimax polynomial fits are made to the interpolated data. The total stopping and partial stopping by each species are given. The beam emission coefficients are handled in a similar manner. The interpolated data are displayed and a tabulation prepared. The tabular and graphical output may be printed and includes the polynomial approximations.

The **file selection window** is shown below. Its operation is a little different from usual.

1. ADF21 is the appropriate format for use by the program ADAS304 (ADAS User Manual, *appxb-21*). A root path to the correct data type ADF21 appears automatically. 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*.



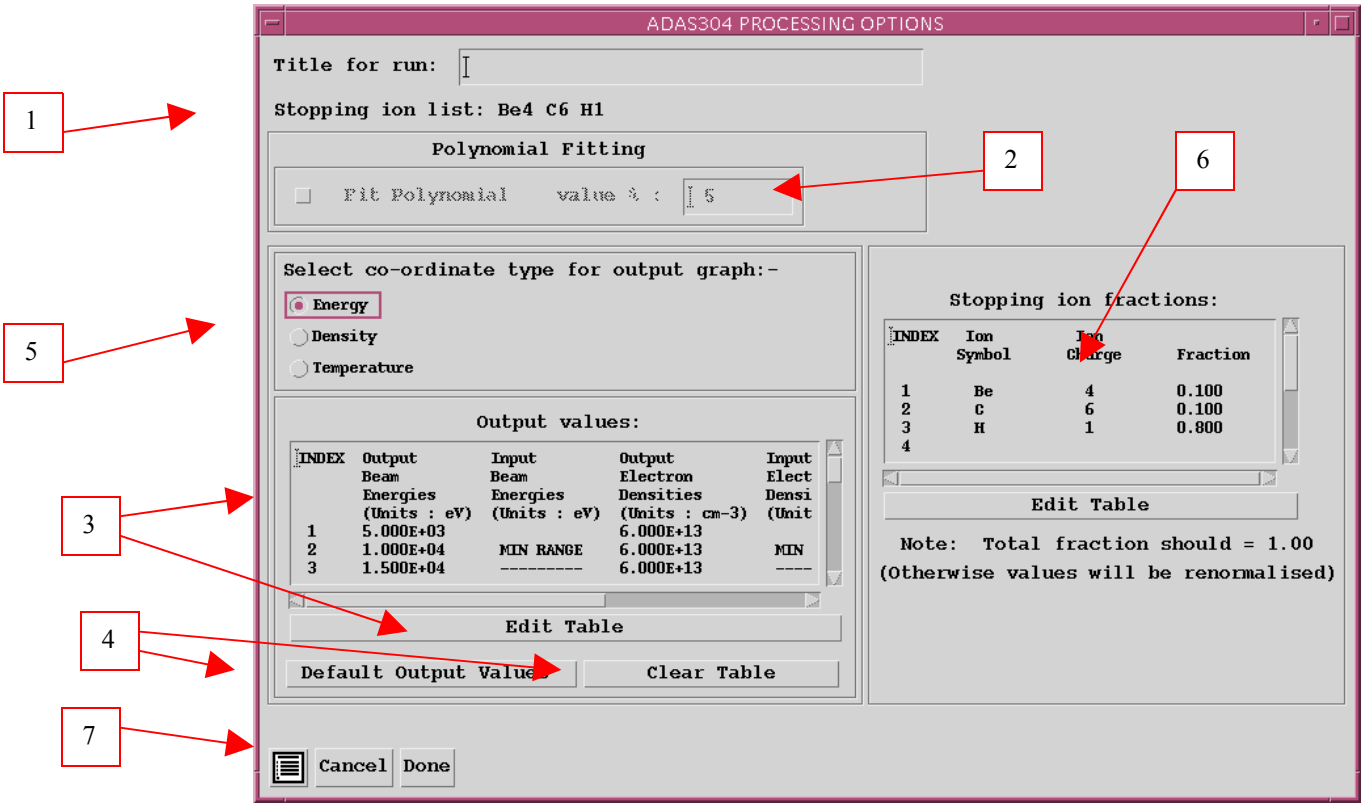
2. Buttons are present to set the data root to that of the *Central data* or to your personal *User data* (provided it is in ADAS organisation. Alternatively the 'data root' may be edit explicitly.



3. A group name for the input files is entered. This is the name of a sub-directory of ADF21 for a particular beam species (usually H or He). The sub-directory contains individual data sets for each impurity contributing to stopping , identified by the element symbol.
4. To increase flexibility in naming a three letter class prefix may be added to the data set name. The primary data in central ADAS has no prefix and so a typical data set name would be */../adas/adas/adf21/bms#h/bms#h_be.dat*.
5. ADAS304 allows you to select all the impurity files you wish easily. Click the *Reselect Ion List* button.
6. The small pop up selection widget appears showing available species. Click the toggle buttons of those you wish to include
7. Click *Done* to restore the main input widget. Your choices are shown at the Stopping Ion List.
8. Clicking on the *Browse Comments* button displays any information stored with the selected data-files. It is important to use this facility to find out what has gone into the data-set and the attribution of the data-set.
9. 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

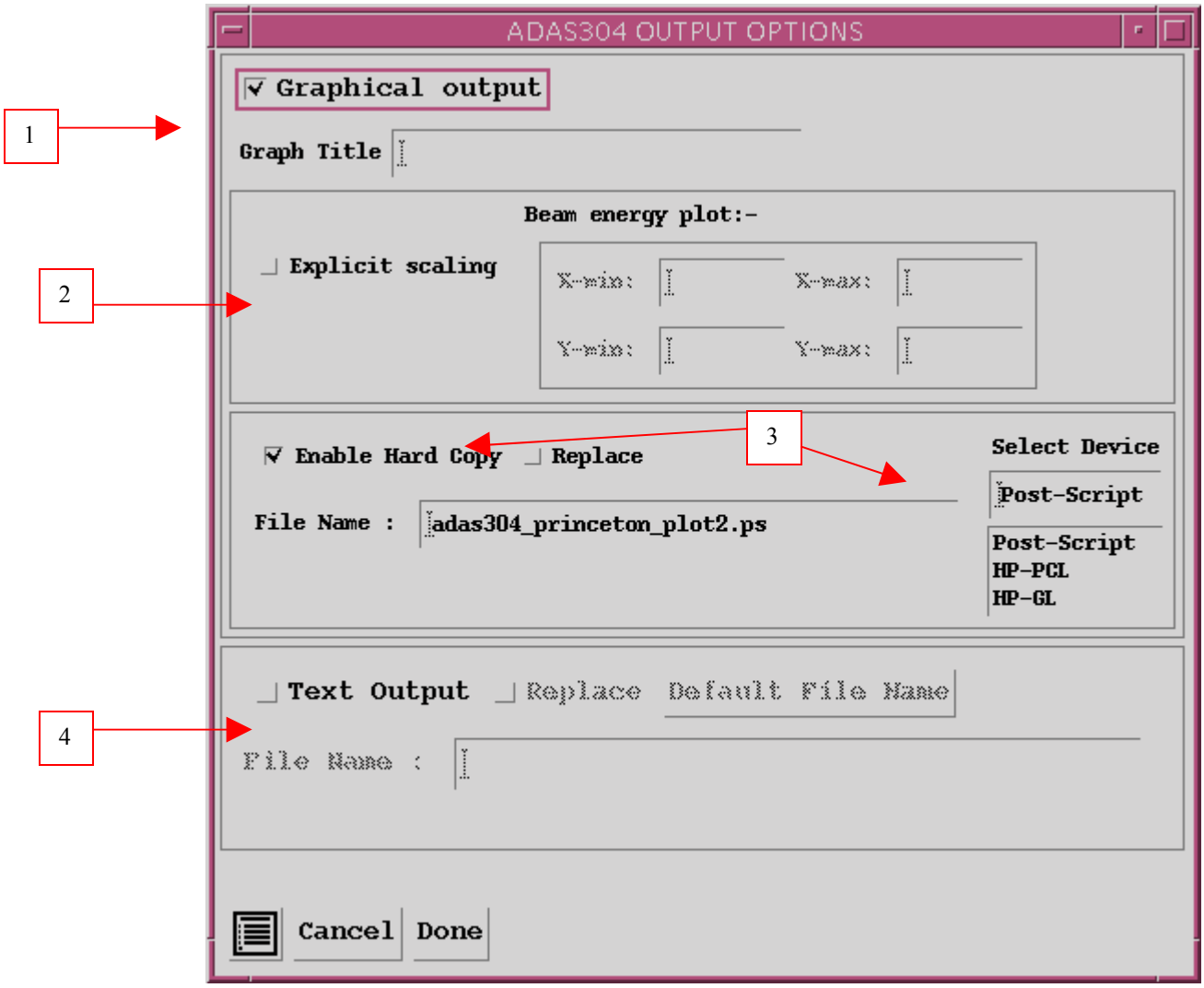
1. The Stopping ion list is repeated for information. The *Browse Comments* button is also provided.



2. The extracted data for a selected ion is interpolated by a cubic spline at user selected plasma parameters for graphical display and tabular output. Additionally a polynomial approximation may obtained by making the appropriate selections.
3. The selection of beam energy, density and temperature sets for data output must be made. The source values are held as one-dimensional scans relative to reference values for each impurity separately. The minimum and maximum for each impurity is shown in the Input columns. The table may be edited by clicking on the *Edit Table* button.
4. *Default Output Values* and *Clear Table* buttons are provided.
5. A choice of which parameter of the input model set to use as the x co-ordinate of graphs is given. Click on the required button.
6. The mixture of species contributing to the stopping is assembled at d). This again is an editable table. Click *Edit Table* to pop up the ADAS Table Editor. The required fractions may then be entered. Normalisation to unity takes place.
7. The *Exit to Menu* icon is present in ADAS304. Clicking the *Done* button causes the output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

The **Output options window** is shown below.

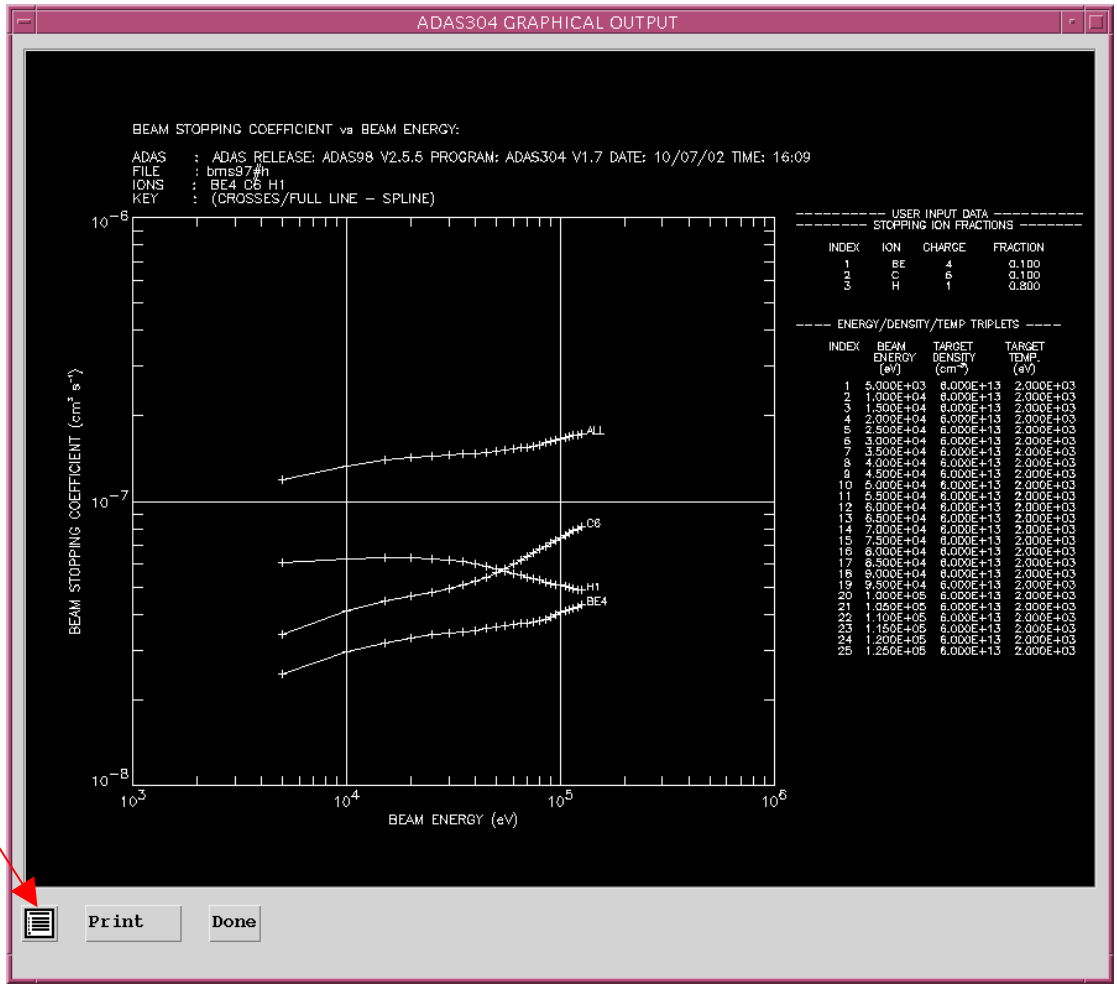
1. Graphical display is activated by the *Graphical Output* button. This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph.
2. By default, graph scaling is adjusted 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. 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*.

The **Graphical output window** is shown below

1. Printing of the currently displayed graph is activated by the *Print* button.



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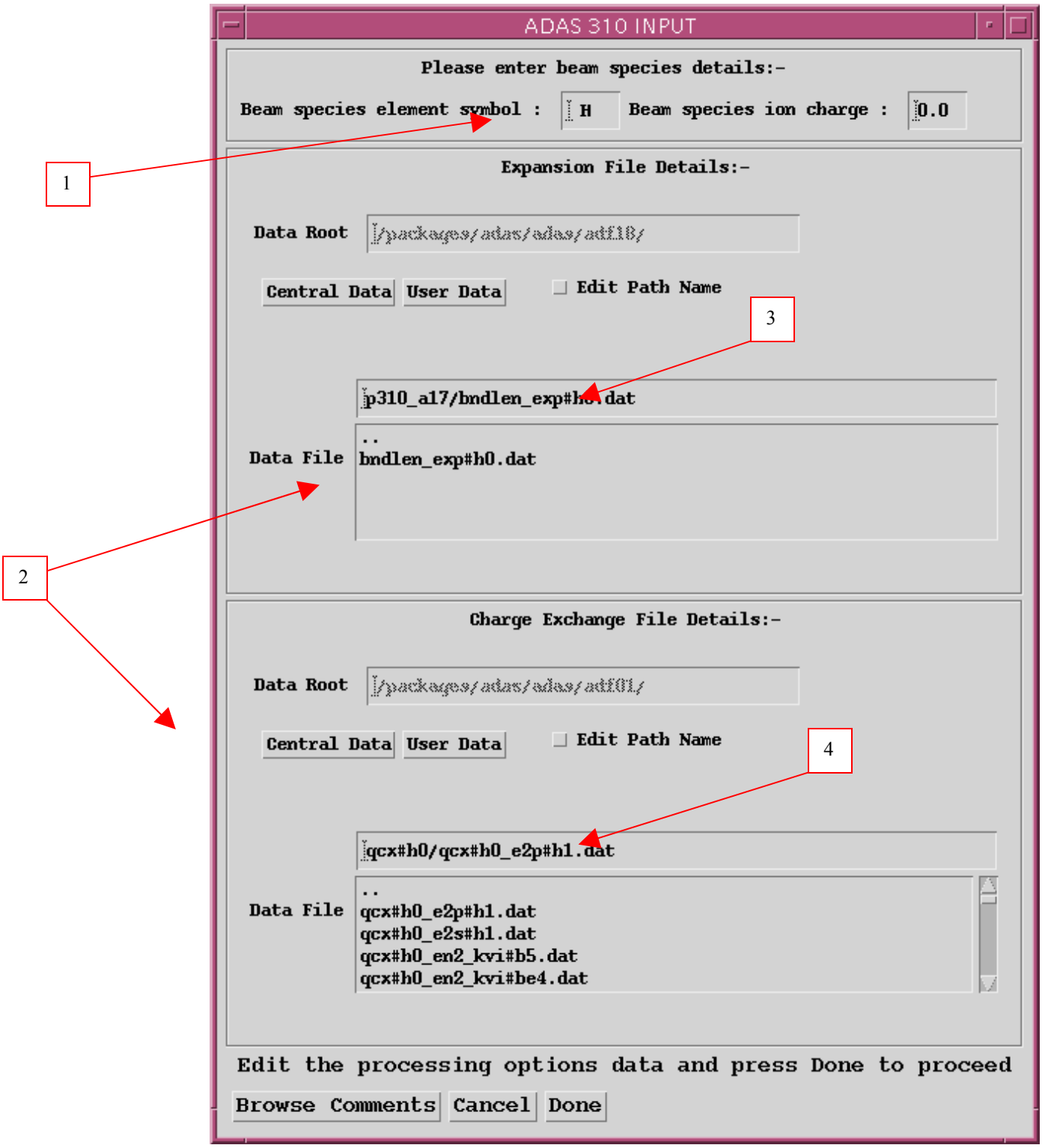
ADAS310

The code calculates the excited population structure, effective ionisation and recombination coefficients of hydrogen atoms or hydrogenic ions in an impure plasma. A very many n-shell bundle-n approximation is used. The hydrogen atoms may be part of the thermal plasma or may be in a beam. The latter case is the only one of relevance for this manual, however the full flexibility of the program has been retained.

The **file selection window** appears first as illustrated below.

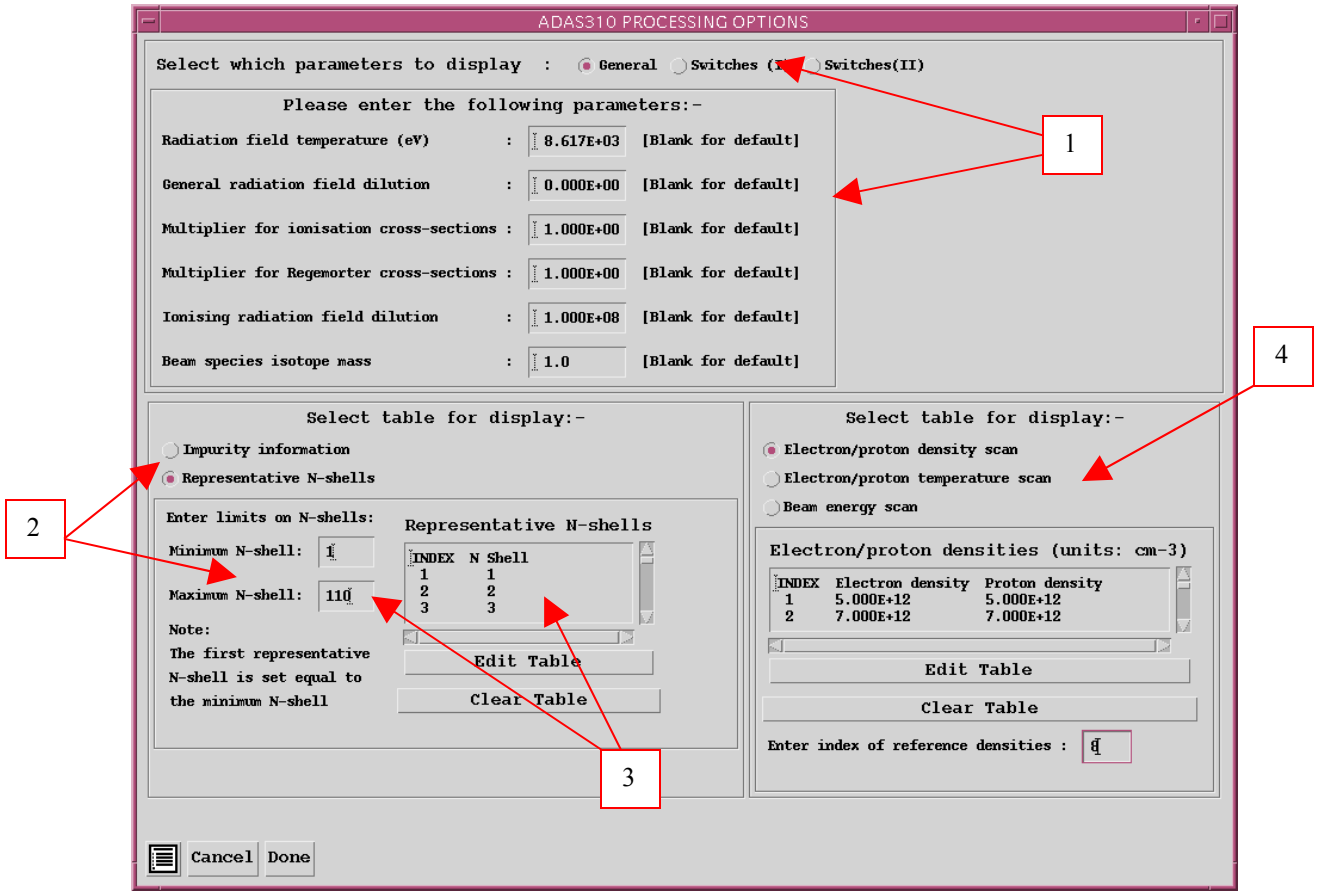
1. Enter the beam species (H for hydrogen and its isotopes) and the atomic charge of the beam species. Only data for neutral beam species is present in the central ADAS database at this time.
2. There are two data files to be selected, the expansion file and the charge exchange file. The procedure is the same in both cases.
3. A special ADAS data type *adf18* is used for such 'expansion' and 'cross-referencing' files. They fall into various categories, kept in sub-directories, according to where they map from and to. Thus the sub-directory *a09_a04* contains data sets mapping from the *adf09* data type into the *adf04* data type. We shall deal with the purposes of these in the discussion of advanced population modelling in the next release. For the moment note that *bndlen_exp#h0.dat* is the one needed here and it sits alone as shown in the illustration. Always select it.
4. The charge exchange file is not of importance for neutral beam stopping. The charge exchange data set is required when hydrogen nuclei can act as electron receivers from other species. You will see no effect of your selection here on the beam stopping coefficient but the selection is kept in for the future. Once a charge exchange data file is selected, the set of buttons at the bottom of the main window become active.



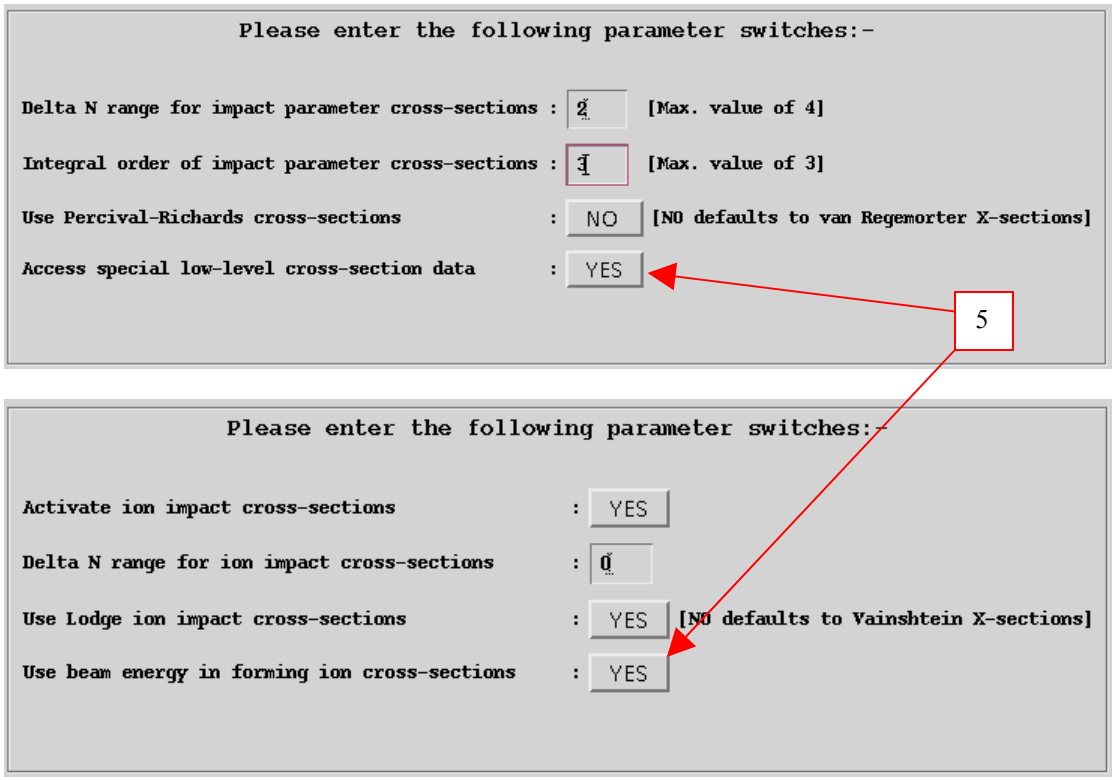
The **processing options window** has the appearance shown below

1. The various control parameters of the collisional-radiative population calculation are organised into three groups selected in turn by the buttons *General*, *Switches (I)* and *Switches (II)*. These cause the appropriate set of parameters to be displayed in the sub-window immediately below the switches. The default settings for these are reasonable and they can be ignored as long as only beam stopping is the intent. *Switches (I)* allow some

choices to do with electron collision cross-sections and *Switches (II)* allow some choices to do with ion collision cross-sections.

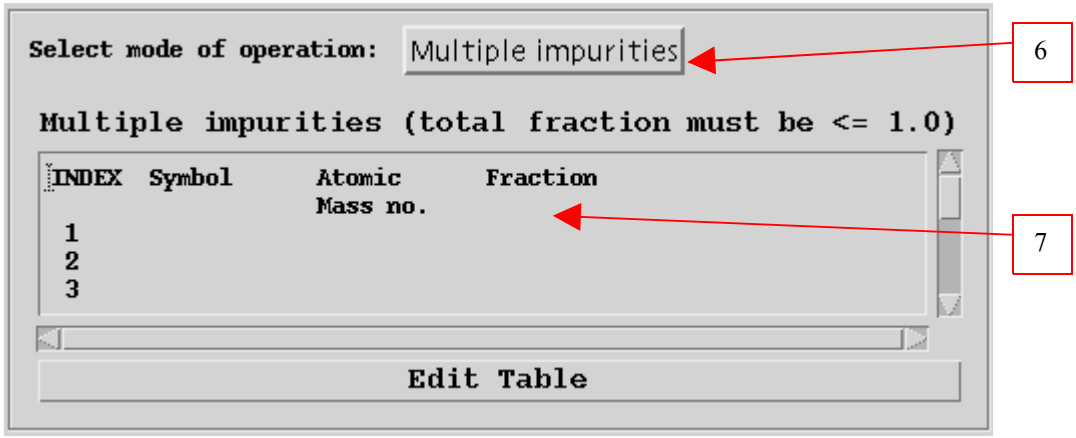


2. Impurity and representative N-shell information is required. Click the *Representative N-shell* buttons to display the appropriate sub-
3. The representative N-shells requires specification of the lowest N-shell, Highest N-shell and a set of sensibly spaced 'representative' N-shells spanning the range. Make sure the lowest is 1 for hydrogen. Make the highest around 110 and use about 20 representative levels. Use all levels up to N=10 and then start to space more widely.
1. A choice of plasma and beam parameters for the scans must be made Click on the appropriate button to work on each scan in turn. Note that you edit in a set of values and then choose one to be the reference value of that parameter. The table may be edited by clicking on the *Edit Table* button.. The ADAS Table Editor window is then presented with the same set of editing operations available as are described in bulletin *nov18-94*. Values should be monotonic increasing. It has proved helpful to add a *Clear Table* button to remove all entries in the output field. When specifying *the Beam energy scan*, note that a neutral hydrogen density in the beam is requested. This is necessary to allow a mathematical separation of the various influences on the neutral hydrogen population structure and is not an experimental beam density. A value of order 10^6 or greater is suitable for the program operation.
4. Details of the switches I and II sub-windows are shown. Make sure that *Access to low level data* is chosen and *Use beam energy informing cross-sections*. It is this latter piece of information that informs the calculation that the neutral hydrogen is in the beam and not in the plasma.
5. In the impurity information sub-window, there are two modes of operation. Single impurity or Multiple impurities. Click the drop-down list button to make your choice.



6. The multiple impurity choice enables us to investigate the influence of an impurity mixture on the stopping with greater precision. Edit in the fractions you wish in the usual manner. Note that the impurity density acts non-linearly in the stopping coefficient and so the linear superposition implied by the use of ADAS304 is imprecise. It is however very fast which is necessary in large scale experimental data analysis.

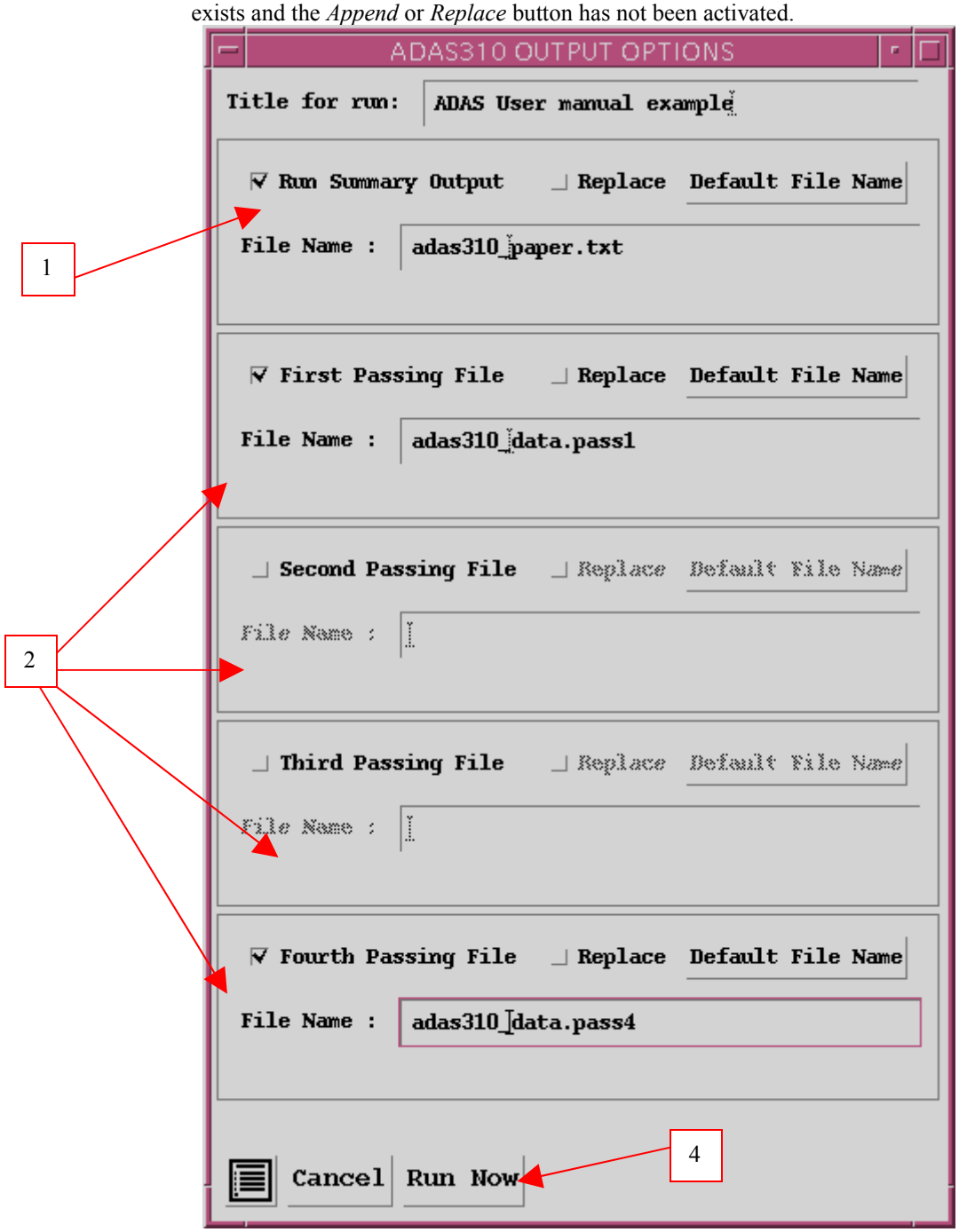
The single impurity case has only one impurity nucleus in addition to protons present in the plasma. The single impurity case is used to build up such data sets in *adf21*. Note how the impurity and protons fit together (equations 4.10.16 and 4.10.17 in the ADAS User Manual). The proton and electron density choices to be made next influence this.



The **output options window** is shown below. It follows the usual pattern except that there is no graphical output.

1. The *Run Summary Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Run Summary Output* is on. If the file already exits a choice to *Replace* or *Append* may be made. 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 *Append* or *Replace* button has not been activated.



2. Four additional passing files may be produced which are placed in your pass directory. The first passing file is of ADAS data format ADF26 and contains line printer formatted pages of data, one page for each individual population structure case run. The data held on these sheets is very comprehensive. By appropriate choice of the parameters mentioned in the processing section above and choice of input files, hydrogen in all its possible conditions in a fusion plasma can be obtained (beam and non-beam).
3. Click the *Run Now* button to initiate the calculations. These are run in fore-ground since they are of fairly modest duration. A thermometer widget keeps you informed of the progress of the calculations.