ADAS304: Effective beam emission spectroscopy stopping data - graph and fit coefficient

The program 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.

Background theory:

For a neutral beam species $\mathscr{A}$ being stopped by fully stripped impurity species and electrons in the plasma, the stopping coefficient is the effective loss rate coefficient of electrons from $\mathscr{A}$. This corresponds closely to the effective ionisation rate coefficient or *collisional-radiative* ionisation coefficient from the ground state of $\mathscr{A}$, 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 $N_e S_{CR}^{(\mathsf{A})}$.

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 $S_{CR}^{(\mathscr{A},X)}$ then the loss rate is

$$N_e S_{CR}^{(\mathscr{A},X)}(E_B, N^{(z_0)}, T^{(z_0)}) = N_e S_{CR}^{(\mathscr{A},e)}(E_B, N^{(z_0)}, T^{(z_0)}) + N^{(z_0)} S_{CR}^{(\mathscr{A},z_0)}(E_B, N^{(z_0)}, T^{(z_0)}) \qquad 4.4.1$$

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

$$S_{CR}^{(\mathscr{A},X)}(E_B, N^{(z_0)}, T^{(z_0)}) = S_{CR}^{(\mathscr{A},e)}(E_B, N^{(z_0)}, T^{(z_0)}) + (1/z_0) S_{CR}^{(\mathscr{A},z_0)}(E_B, N^{(z_0)}, T^{(z_0)}) \qquad 4.4.2$$

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

$$\begin{aligned} N_e S_{CR}^{(\mathscr{A})}(E_B, N_I, T_I) &\approx N_e S_{CR}^{(\mathscr{A},e)}(E_B, N_I, T_I) + \sum_{i=1}^{I} N_i^{(z_{0i})} S_{CR}^{(\mathscr{A},z_{0i})}(E_B, N_I, T_I) \\ &= \sum_{i=1}^{I} N_{e,i} [S_{CR}^{(\mathsf{A},e)}(E_B, N_I, T_I) + (1/z_{0i}) S_{CR}^{(\mathsf{A},z_{0i})}(E_B, N_I, T_I)] \end{aligned} \qquad 4.4.3$$

where

$$N_e = \sum_{i=1}^{I} N_{e,i} = \sum_{i=1}^{I} z_{0i} N^{(z_{0i})} = N_I (\sum_{i=1}^{I} z_{0i} f_i) \qquad 4.4.4$$

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

$$N_i^{(z_{0i}),equiv} = N_I (\sum_{k=1}^{I} z_{0k}^2 f_k) / z_{0i}^2 \qquad 4.4.5$$

and the equivalent electron density is

$$N_{ei}^{(z_{0i}),equiv} = (\frac{N_e}{\sum_{k=1}^{I} z_{0k} f_k})(\sum_{k=1}^{I} z_{0k}^2 f_k) / z_{0i} \qquad 4.4.6$$

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

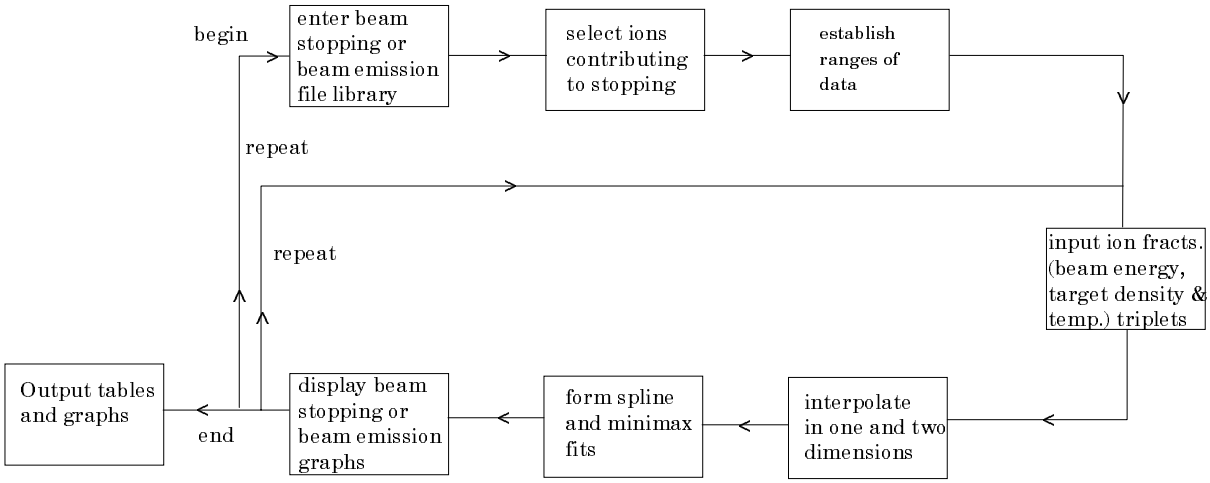
$$S_{CR}^{(\mathscr{A})}(E_B, N_e, T_I) \approx \sum_{i=1}^{I} [z_{0i} f_i S_{CR}^{(\mathscr{A}, X_i)}(E_B, N_{ei}^{(z_{0i}),equiv}, T_I)] / (\sum_{k=1}^{I} z_{0k} f_k) \qquad 4.4.7$$

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

Program steps:

These are summarised in the figure below.

Figure 4.4

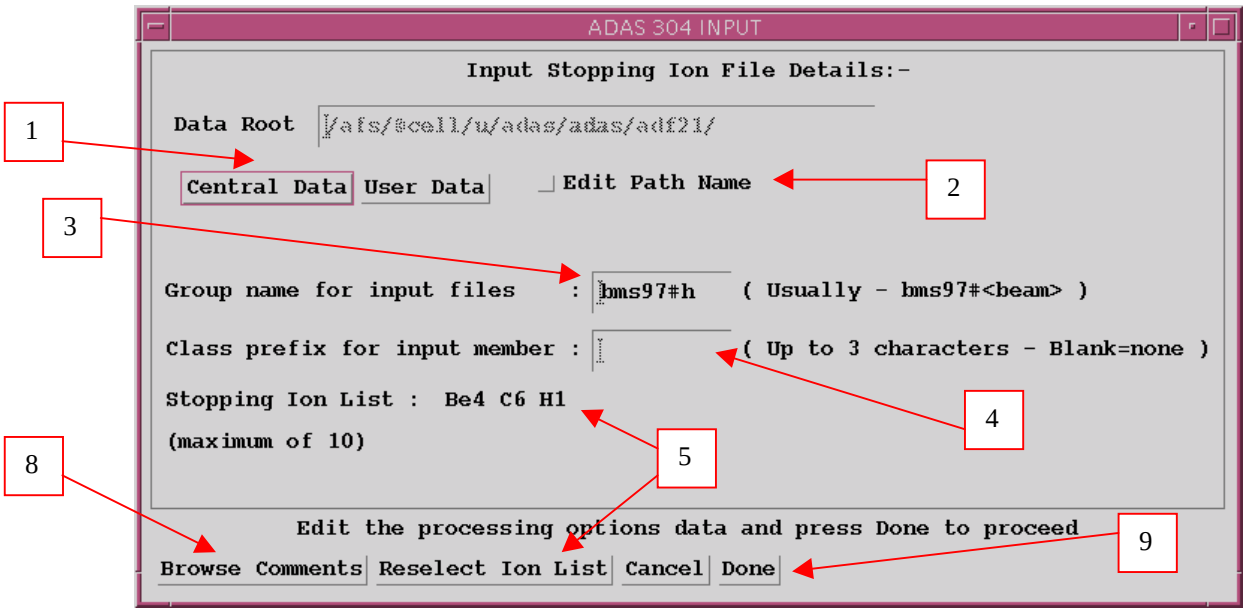


Interactive parameter comments:

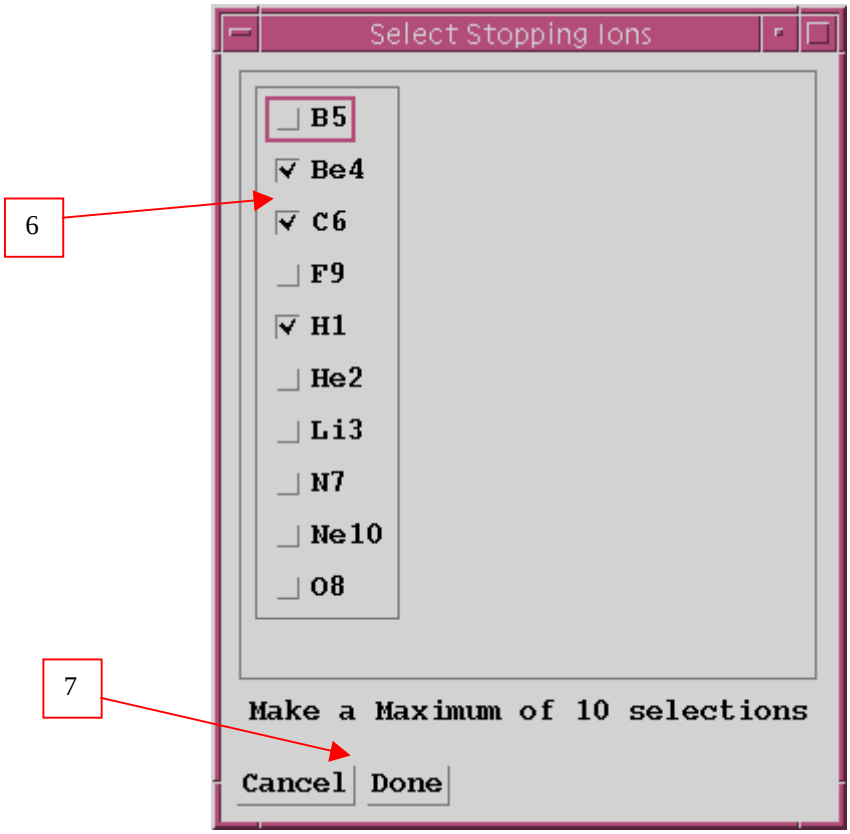
Move to the directory in which you wish any ADAS created files to appear. These include the output text file produced after executing any ADAS program (*paper.txt* is the default) and the graphic file if saved (e.g. *graph.ps* if a postscript file). Initiate ADAS and move to the series 3 menu. Select ADAS304.

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.



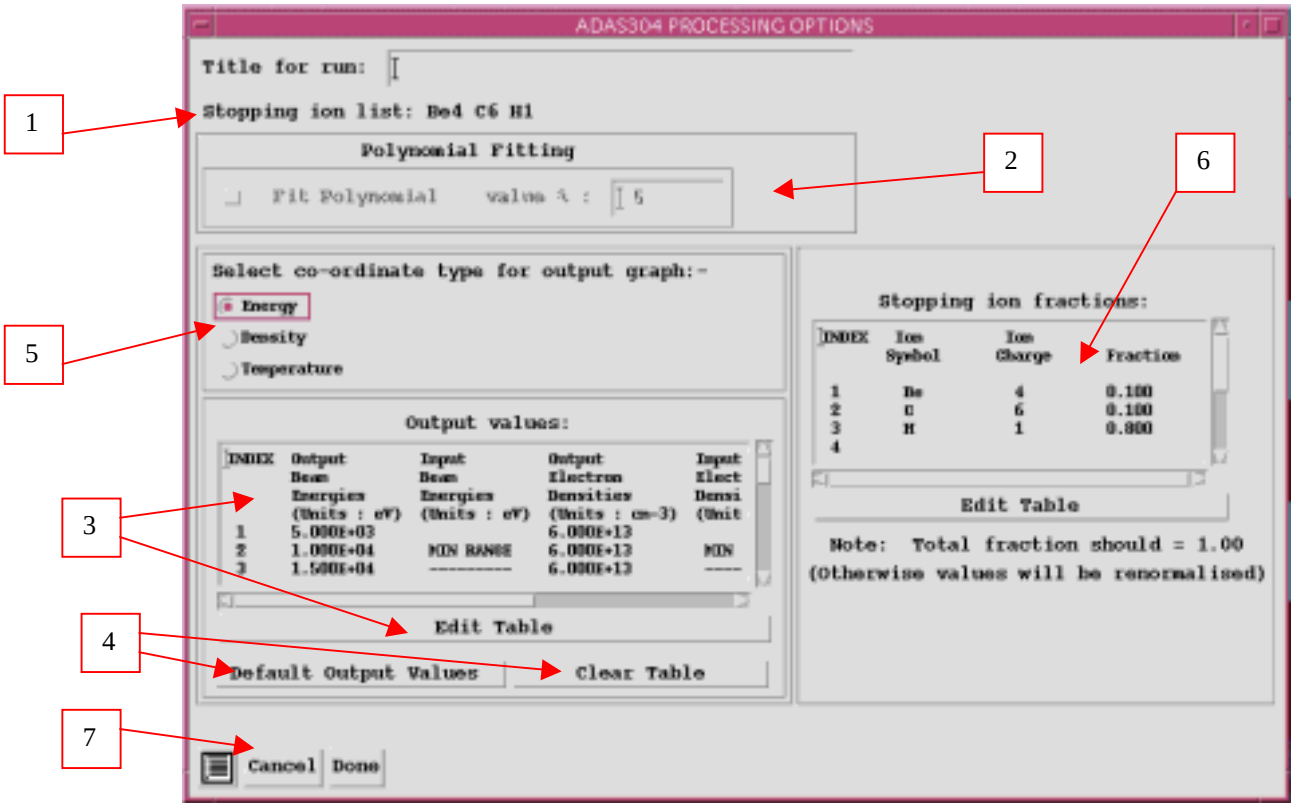
3. A group name for the input files is entered. This is the name of a sub-directory of ADF21 for a particular beam species (usually H or He).

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.

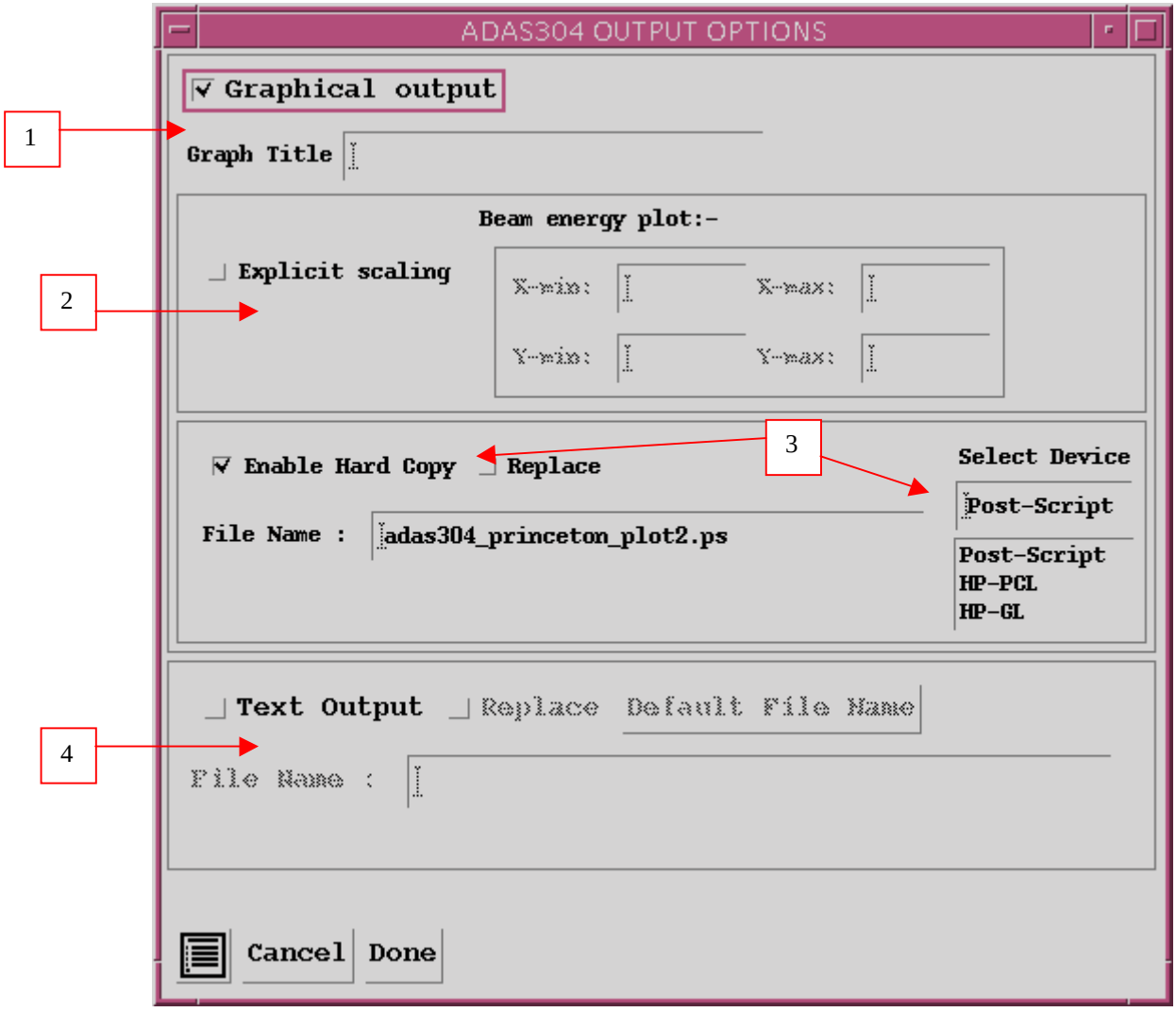


2. The extracted data for a selected ion is interpolated by a cubic spline at user selected plasma parameters for graphical display and tabular output. Additionally a polynomial approximation may obtained by making the appropriate selections.
3. The selection of beam energy, density and temperature sets 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.

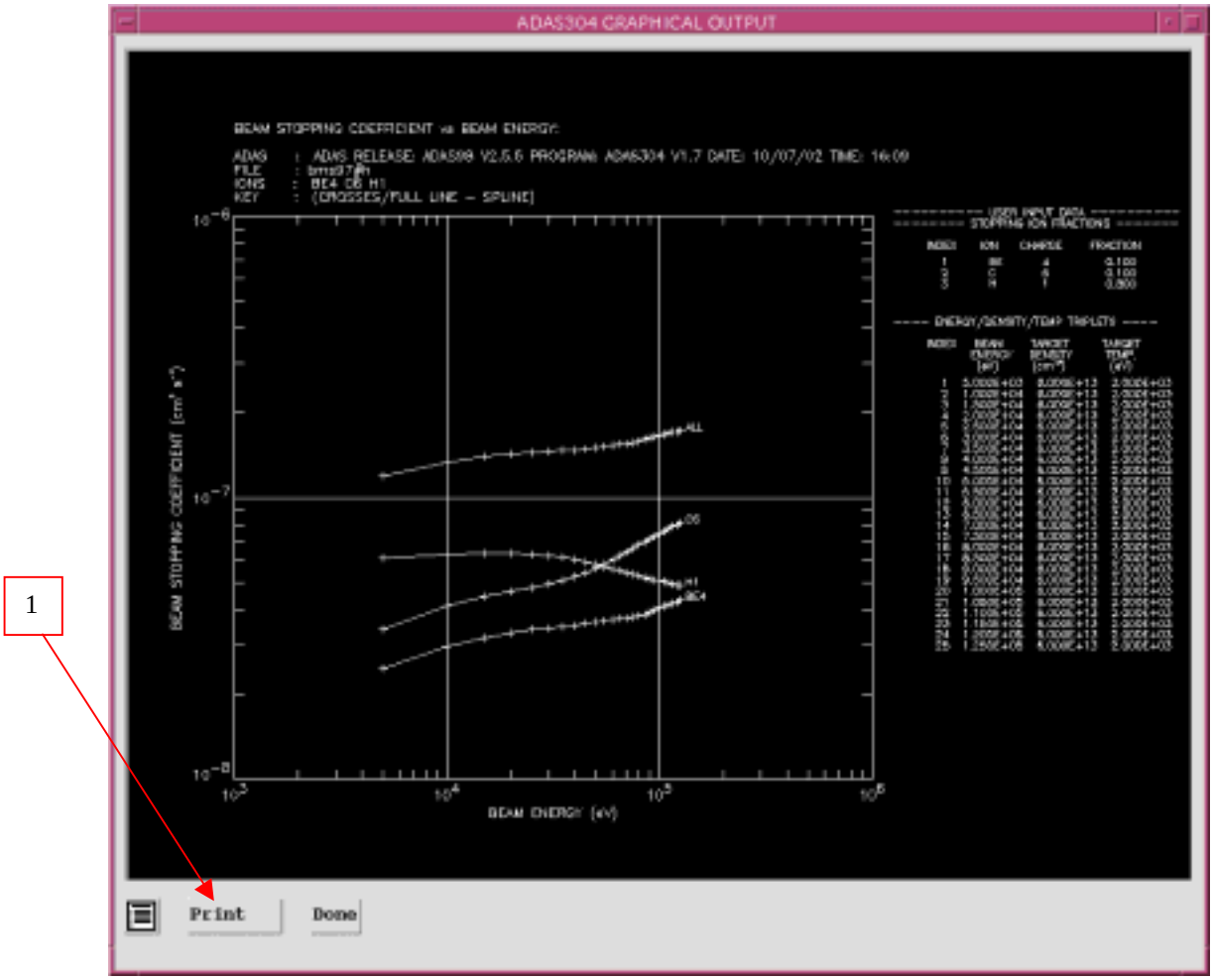


Illustration:

The output from the programme for hydrogen beam stopping in a composite plasma of H^+, He^{+2} and B^{+5} is illustrated in figure 4.4a. The total stopping rate coefficient is given as well as the individual species contributions to the stopping. The solid lines are spline fits and the dotted lines give the minimax polynomial fits. The tabulated output is shown in table 4.4a.

Figure 4.4a

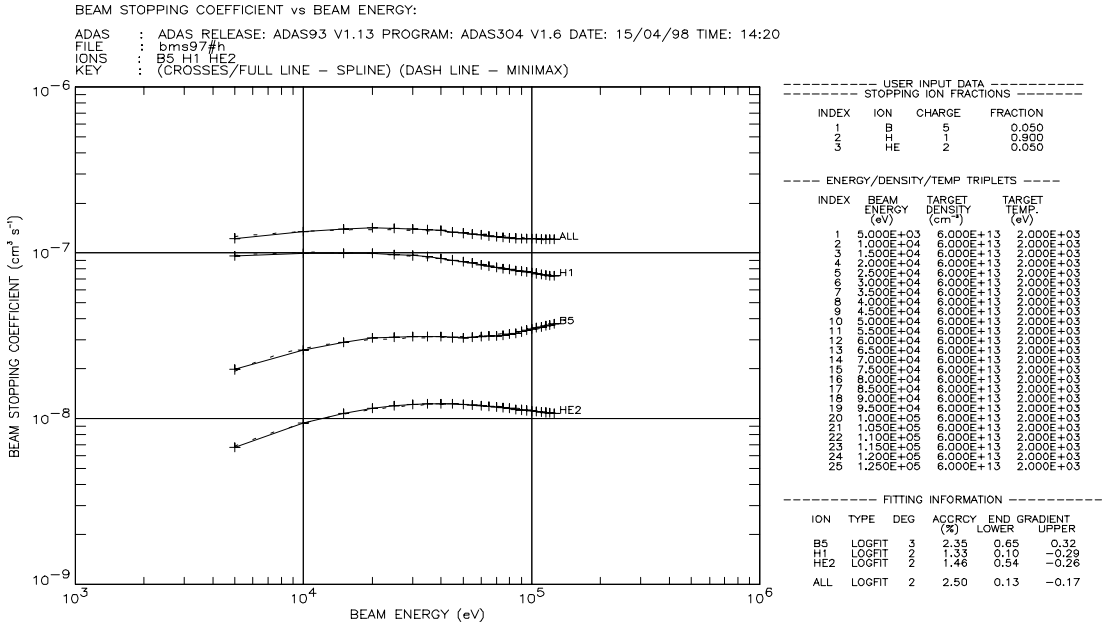


Table 4.4a

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ADAS RELEASE: ADAS93 V1.13 PROGRAM: ADAS304 V1.6 DATE: 15/04/98 TIME: 14:32
****** TABULAR OUTPUT FROM BEAM STOPPING COEFFICIENT INTERROGATION PROGRAM: ADAS304 - DATE: 15/04/98 *****
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BEAM STOPPING COEFFICIENTS AS A FUNCTION OF BEAM ENERGY AND TARGET DENSITY AND TEMPERATURE
-------------------------------------------------------------------------------------------
                     DATA GENERATED USING PROGRAM: ADAS304
                     -------------------------------------
 INPUT DATA SET:  bms97#h
       MEMBERS: B5 H1 HE2
                              ------------------------
 --------------------------- STOPPING ION FRACTIONS ---------------------------
                              ------------------------
 ION  CHARGE  FRACTION
 ----------------------
   B      5      0.050
   H      1      0.900
   HE     2      0.050
                         ----------------------------------
 ---------------------- TOTAL BEAM STOPPING COEFFICIENTS ----------------------
                         ----------------------------------
   BEAM    TARGET   TARGET  BEAM STOPPING
  ENERGY   DENSITY   TEMP.   COEFFICIENT
   (EV)    (CM-3)    (EV)     (CM3 S-1)
 ---------------------------------------
 5.00D+03 6.00D+13 2.00D+03   1.22D-07
 1.00D+04 6.00D+13 2.00D+03   1.35D-07
 1.50D+04 6.00D+13 2.00D+03   1.39D-07
 2.00D+04 6.00D+13 2.00D+03   1.41D-07
 2.50D+04 6.00D+13 2.00D+03   1.41D-07
-------------------------------------------------------------------------------------------
 NOTE: * => BEAM STOPPING COEFFICIENT EXTRAPOLATED FOR ENERGY/DENSITY/TEMPERATURE TRIPLET.
 -------------------------------------------------------------------------------------------
                      -----------------------------------------
 ------------------ INDIVIDUAL ION BEAM STOPPING COEFFICIENTS ------------------
                      -----------------------------------------
   BEAM    TARGET   TARGET  ---- BEAM STOPPING COEFFICIENT (CM3 S-1) ----------------------
  ENERGY   DENSITY   TEMP.      B5        H1        HE2
   (EV)    (CM-3)    (EV)    (0.05)    (0.90)    (0.05)
-------------------------------------------------------------------------------------------
 5.00D+03 6.00D+13 2.00D+03  1.98D-08  9.59D-08  6.76D-09
 1.00D+04 6.00D+13 2.00D+03  2.60D-08  9.92D-08  9.39D-09
 1.50D+04 6.00D+13 2.00D+03  2.90D-08  9.97D-08  1.08D-08
 2.00D+04 6.00D+13 2.00D+03  3.07D-08  9.92D-08  1.15D-08
 2.50D+04 6.00D+13 2.00D+03  3.11D-08  9.79D-08  1.19D-08
-------------------------------------------------------------------------------------------
 NOTE: 1) * => BEAM STOPPING COEFFICIENT EXTRAPOLATED FOR ENERGY/DENSITY/TEMPERATURE TRIPLET.
       2) ION FRACTIONS GIVEN IN BRACKETS BELOW ION SYMBOLS.
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The output from the programme for hydrogen beam emission coefficients for a composite plasma of H^+, He^{+2} and B^{+5} is illustrated in figure 4.4b and the tabulated output in table 4.4b.

Figure 4.4b

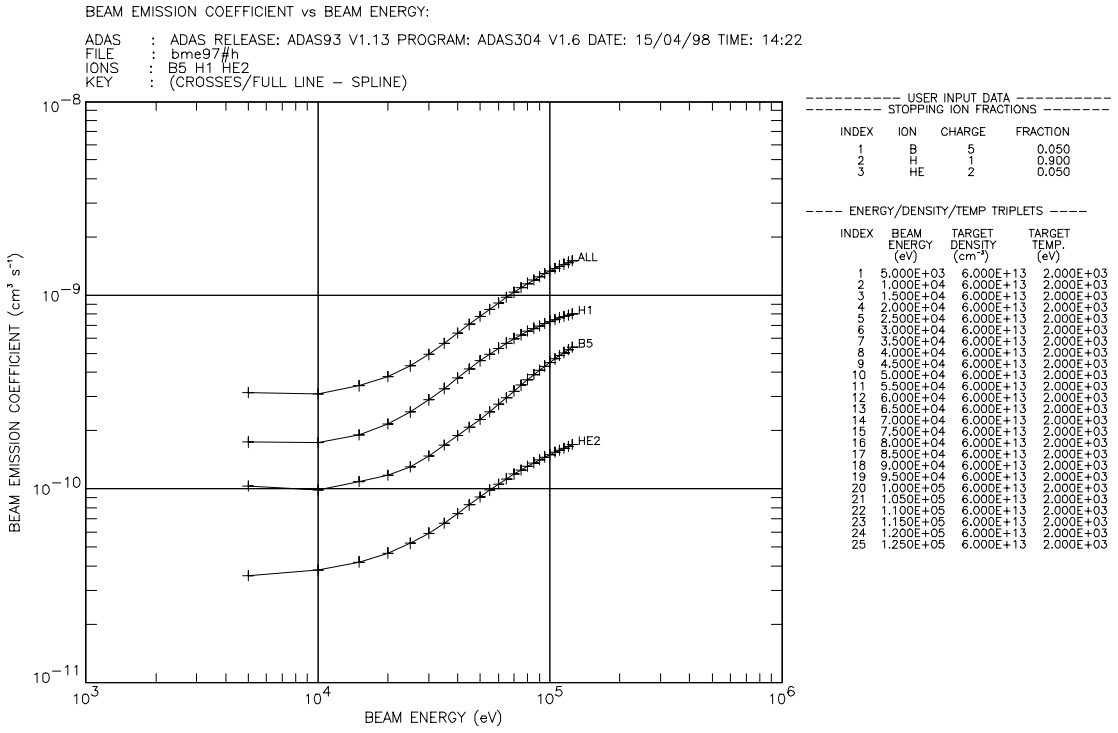

Table 4.4b

ADAS RELEASE: ADAS93 V1.13 PROGRAM: ADAS304 V1.6 DATE: 15/04/98 TIME: 14:34
***** TABULAR OUTPUT FROM BEAM EMISSION COEFFICIENT INTERROGATION PROGRAM: ADAS304 - DATE: 15/04/98 *****

BEAM EMISSION COEFFICIENTS AS A FUNCTION OF BEAM ENERGY AND TARGET DENSITY AND TEMPERATURE

DATA GENERATED USING PROGRAM: ADAS304

INPUT DATA SET: bme97#h
MEMBERS: B5 H1 HE2

STOPPING ION FRACTIONS

ION	CHARGE	FRACTION
B	5	0.050
H	1	0.900
HE	2	0.050

TOTAL BEAM EMISSION COEFFICIENTS

BEAM ENERGY (EV)	TARGET DENSITY (CM-3)	TARGET TEMP. (EV)	BEAM EMISSION COEFFICIENT (CM3 S-1)
5.00D+03	6.00D+13	2.00D+03	3.13D-10
1.00D+04	6.00D+13	2.00D+03	3.10D-10
1.50D+04	6.00D+13	2.00D+03	3.41D-10
2.00D+04	6.00D+13	2.00D+03	3.81D-10
2.50D+04	6.00D+13	2.00D+03	4.32D-10

NOTE: * => BEAM EMISSION COEFFICIENT EXTRAPOLATED FOR ENERGY/DENSITY/TEMPERATURE TRIPLET.

```
              ----------------------------------------
 ------------------ INDIVIDUAL ION BEAM EMISSION COEFFICIENTS ------------------
                   ----------------------------------------

   BEAM    TARGET   TARGET  --------BEAM EMISSION COEFFICIENT (CM3 S-1) ------------------
  ENERGY   DENSITY   TEMP.       B5        H1        HE2
    (EV)    (CM-3)    (EV)    (0.05)    (0.90)    (0.05)
 ------------------------------------------------------------------------------------------
 5.00D+03 6.00D+13 2.00D+03  1.03D-10  1.74D-10  3.56D-11
 1.00D+04 6.00D+13 2.00D+03  9.86D-11  1.73D-10  3.80D-11
 1.50D+04 6.00D+13 2.00D+03  1.09D-10  1.90D-10  4.19D-11
 2.00D+04 6.00D+13 2.00D+03  1.18D-10  2.16D-10  4.66D-11
 2.50D+04 6.00D+13 2.00D+03  1.30D-10  2.50D-10  5.24D-11
------------------------------------------------------------------------------------------
 NOTE: 1) * => BEAM EMISSION COEFFICIENT EXTRAPOLATED FOR ENERGY/DENSITY/TEMPERATURE TRIPLET.
       2) ION FRACTIONS GIVEN IN BRACKETS BELOW ION SYMBOLS.
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Notes: