ADAS313 Post-process population data for helium beam stopping and emission

The tabulated population structure and cross coupling coefficients calculated by ADAS311 are stored as a function of plasma parameters in the ADAS data format of *adf26*. The rapid assembly of coupling or emission coefficients for experimental analysis warrants the need for fast look-up tables. ADAS313 is used to construct such tables by extracting cross coupling or beam emission data from the *adf26* files. The extracted data is tabulated and stored in a convenient format of type *adf21* or *adf22*. Such data types consists of two dimensional arrays of coefficients in density and beam energy and then one dimensional scans in temperature.

Background theory:

The interactive code provides the facility to study the behaviour of the effective cross coupling and emission coefficients as a function of electron density and neutral beam energy. The production of fast look-up tables of type *adf21* or *adf22* is also another feature of ADAS313. The construction of convenient look up tables to enable the fast assembly of cross coupling or emission coefficients is important for daily experimental analysis were the *ab intio* calculation of these quantities would be impractical. Particularly since the solution of the following set of coupled equations is required to model the beam attenuation,

$$v_b \frac{dN_{1^1S}}{dx} = n_e S_{1^1S} N_{1^1S} - n_e S_{2^1S \to 1^1S} N_{2^1S} - n_e S_{2^3S \to 1^1S} N_{2^3S}$$

$$v_b \frac{dN_{2^1S}}{dx} = -n_e S_{1^1S \to 2^1S} N_{1^1S} + n_e S_{2^1S} N_{2^1S} - n_e S_{2^3S \to 2^1S} N_{2^3S} \qquad 4.13.1$$

$$v_b \frac{dN_{2^3S}}{dx} = -n_e S_{1^1S \to 2^3S} N_{1^1S} - n_e S_{2^1S \to 2^3S} N_{2^1S} + n_e S_{2^3S} N_{2^3S}$$

where N_{2S+1} is the population of the level specified by the quantum numbers n, S and L. The quantity v_b is the beam velocity and dx is along the path taken by the beam. n_e is the electron density and the collisional-radiative cross coupling coefficients are represented by the symbol $S_{\rho\sigma}$, where the subscripts specify the initial and the final non-equilibrium level.

Program steps:

These are summarised in the figure below.

Figure 4.13
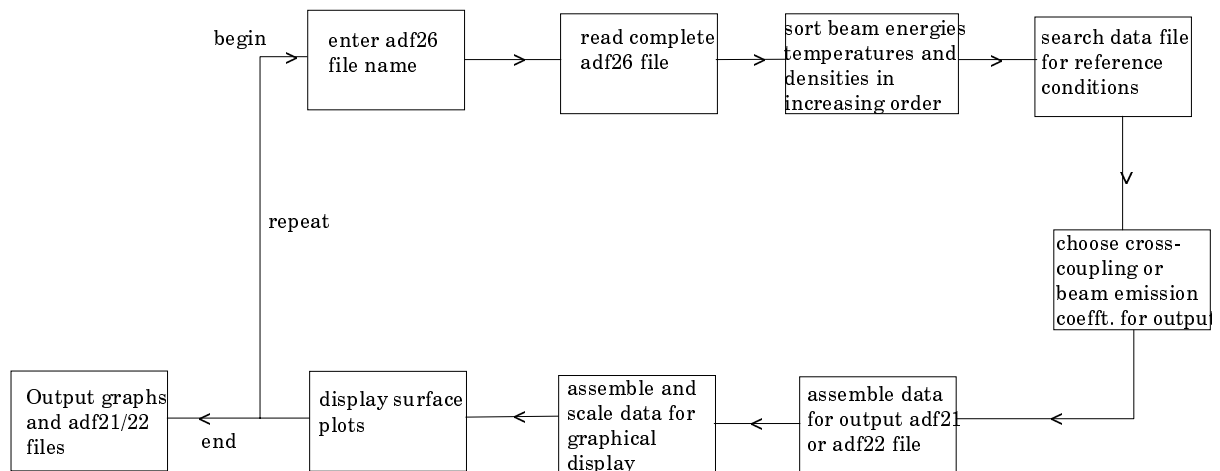
Interactive parameter comments:

The program which makes use of data from archived ADAS data-sets initiates an interactive dialogue with the user in three parts, namely, input data file selection, entry of user data and disposition of output.

Move to the directory in which you wish the ADAS created files to appear. These include the output text file produced after executing any ADAS program (*paper.txt* is the default), and either an *adf21* or *adf22* type file. The program can also produce surface plots of the derived data which can be written to appropriate graphics files. Initiate ADAS313 from the program selection menus in the usual manner.

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

1.   Data root a) shows the full pathway to the appropriate data sub directories. 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.

2.   The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
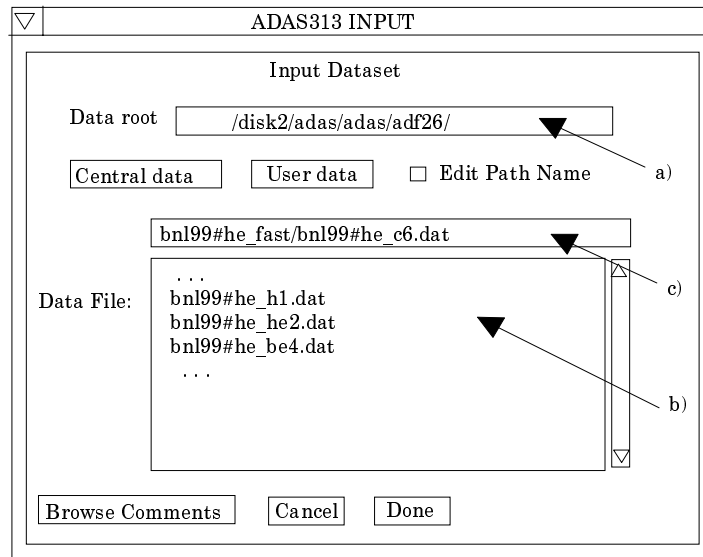
3.   Available sub-directories are shown in the large file display window b). Scroll bars appear if the number of entries exceed the file display window size.

4.   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 data-files are presented for selection. Data-files all have the termination *.dat*.

5.   Once a data file is selected, the set of buttons at the bottom of the main window become active.

6.   Clicking on the *Browse Comments* button displays any information stored with the selected data-file. It is important to use this facility to find out what is broadly available in the data-set. The possibility of browsing the comments appears in the subsequent main window also.

7.   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.

8.   An arbitrary title may be given for the case being processed. For information the full pathway to the data-set being analysed is also shown at a). The button *Browse*

comments again allows display of the information field section at the foot of the selected data-set, if it exists.

9. At b) some additional information on the beam donor species and the impurity in the plasma which is the receiver in charge exchange reactions. These data are extracted from the data set name. Note that a bundle-nlSL population data set of type *adf26* being analysed is for a single plasma impurity.

```
┌─────────────────────────────────────────────────────────────────────────────┐
│ ▽                        ADAS313 : PROCESSING OPTIONS                          │
│                                                                               │
│   Title for Run        demonstration                                          │
│                                                                               │
│   Data File Name :    /disk2/adas/adas/adf26/bnl99#he_fast/bnl99#he_c6.dat    │
│                                                                               │
│                    Browse Comments                                            │
│                                                                               │
│   --------------------Receiver------------------------   ------Neutral donor ------    │
│            Nuclear      Initial       Final                        Nuclear     │
│   Symbol   charge     ion charge   ion charge    Symbol            charge      │
│   ------------------------------------------------------------------------    │
│      C        6            6            5          He                 2         │
│                                                                               │
│      ◇   Generate beam stopping file      ◇   Generate beam emission file      │
│                                                                               │
│            Input plasma parameter information :-                               │
│                                                                               │
│   Temperature range (eV)  :   1.000E+02 - 5.000E+04    Ref. temp. (eV) :  2.000E+03  │
│                                                                               │
│   Beam energy range (eV/amu)  5.000E+03 - 1.250E+05   Ref. ener. (eV/amu)  6.500E+04 │
│                                                                               │
│   Density range (cm-3)  :    1.000E+12 - 1.000E+15    Ref. dens. (cm-3)  6.000E+13  │
│                                                                               │
│   Select coupling coefficient        Select quantum numbers & reference metastables │
│                                                                               │
│              Lower    Upper              Lower   Upper        ◇  1s2(1)S        │
│              index    index              level   level       ◇  1s2s(1)S       │
│   Range (1-3)  2        3       N(1-4)     2       4          ◇  1s2s(3)S       │
│                                 L(0-3)     0       1            Singlet         │
│                                                                               │
│   [≡]   Cancel    Done                                                         │
└─────────────────────────────────────────────────────────────────────────────┘
```

a) b) c) d) e) f)

10. The code scans the very extensive tabulations in the data set and extracts selected data from them according to the type of output file required by the user. The choices available at this time are cross coupling coefficients and beam emission coefficients. Select the output you wish to be generated at c). The *adf26* data sets in fact contain a large variety of other population information which may be provided at a later stage. With *Generate beam stopping file* selected, additional information must be entered in at e). Similarly when the *Generate beam emission file* button is activated, additional information must be entered in at f).

11. Additional information on the plasma temperature, beam energy and plasma density ranges used in the creation of the adf26 data set is given at d) together with the reference conditions used. Note that the adf26 data set contains two-dimensional arrays of beam energy and ion density data and a one dimensional array in ion temperature from a reference condition.

12. The sub-window at e) becomes active if generation of beam emission data is requested. The choices available are the indices corresponding to the initial and final non-equilibrium levels of interest. The non-equilibrium levels include the ground state

and the two metastable levels i.e. He(2 ^{1}S) and He(2 ^{3}S). The index 1 corresponds to the ground state, while the indices 2 and 3 respectively correspond to the He(2 ^{1}S) and the He(2 ^{3}S). There are nine cross coupling coefficients in total.

13. The sub-window at f) becomes active if generation of beam emission file is requested. There are a variety of choices available. The most obvious concerns the specification of the upper and lower level of the radiative transition of interest. The range of principal and angular quantum numbers has been restricted to 1-4 and 0-3 respectively. The adf26 data set contains results for much higher quantum shells also, so we can extended the available range in the future is desired. The multiplicity of the spin system is also selected. Finally, since the quasi-static exited population is calculated relative to each non-equilibrium level we also have to specify which level, we refer to the level as the reference metastable.

14. At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 3 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

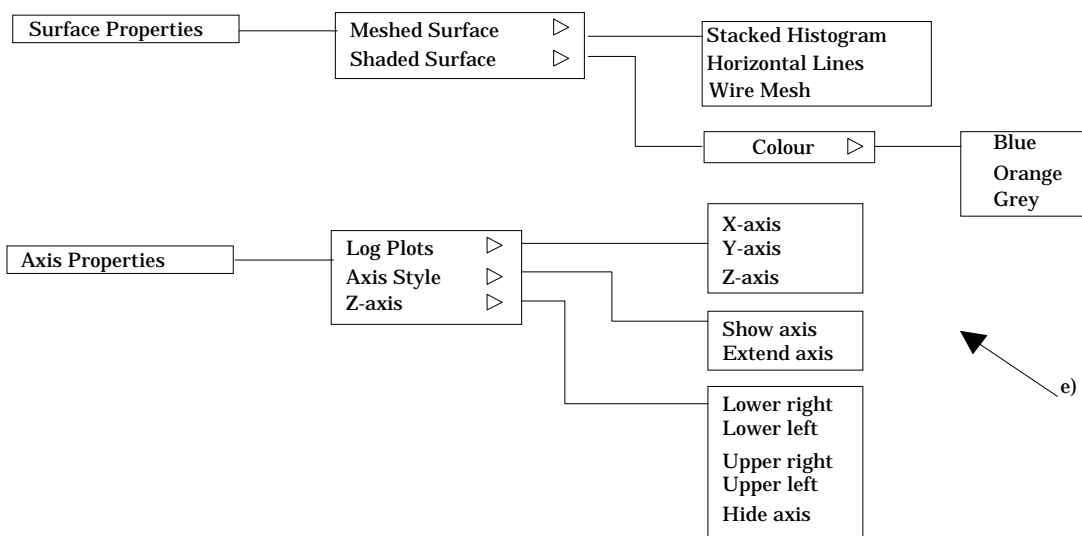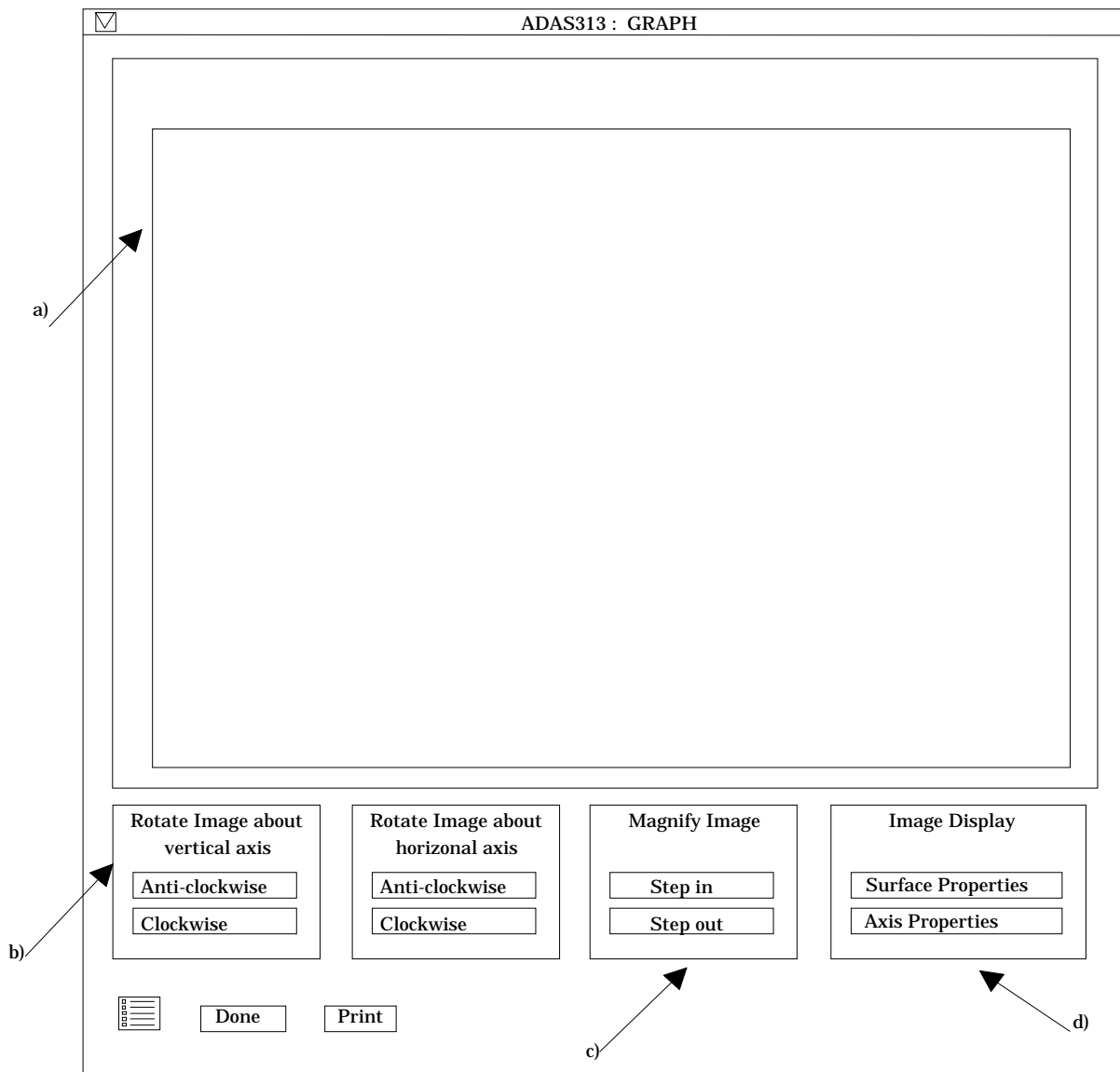The **output options window** appearance is shown below

15. As in the previous window, the full pathway to the file being analysed is shown for information at a). Also the *Browse comments* button is available.

16. Graphical display is activated by the *Graphical Output* button a). 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.

17. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button at b) to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable. In this case, a three-dimensional surface plot is presented with x-axis: beam energy, y-axis: density, z-axis: selected coefficient.

18.   The surface plot is produced at a selected plasma ion temperature. Make this choice at c).

19.   Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. If the output graphic file already exists and the *Replace* button has not been activated, a 'pop-up' window issues a warning.

20.   A choice of output graph plotting devices is given in the Device list window at d). Clicking on the required device selects it. It appears in the selection window above the Device list window.

21.   At e) output of the *Passing File* of results is enabled. This is of *adf21* or *adf22* format according to earlier choices.. The *passing* is written on exiting ADAS313 and is placed by default in your */pass* directory as *ADAS313.pass*. It is fully structured for reassignment into your personal ADAS data base of the appropriate data format.

The **graphical output window** appearance is shown below

22.   This is a new style of graphical output widget to ADAS. A three-dimensional surface plot is given at a). There is much more control over it than in our usual graph displays.

23.   At b), there are the controls for the orientation of the figure. By clicking repeatedly on a button, the figure may be rotated clockwise or anti-clockwise is small steps. You may rotate about a vertical or horizontal axis.

24.   At c), there are two buttons to zoom in or out on the figure.

25.   At d), the controls on the appearance of the figure are available. Note the nesting of menu buttons in more than one layer. The choices are laid out at e) below the main figure. Thus one may choose a meshed surface or shaded surface, the colour of the shaded surface may be selected and so on. You may feel we have gone to overkill here.

26.   Then there are choices on the axes, whether they are linear or logarithmic, whether they are to be displayed or not etc. There is an additional point. At b) when the figure is rotated the position of the axis of rotation matters.   For rotations about a vertical axis, the figure Z-axis is used and it may be moved to any corner of the projected area on the X/Z plane.

27.   Finally note that when the figure is printed, it is the figure as displayed in the graphic output window which you get.

28.   At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 3 menu. Remember that *Done* takes you back to the previous screen. The *Print* button appears if graphical hard-copy is selected on the output options window.

a)

Rotate Image about vertical axis

| Anti-clockwise |
| Clockwise |

Rotate Image about horizonal axis

| Anti-clockwise |
| Clockwise |

Magnify Image

| Step in |
| Step out |

Image Display

| Surface Properties |
| Axis Properties |

b)

c)

d)

| Done | | Print |

| Surface Properties | ——— | Meshed Surface ▷
Shaded Surface ▷ |

| Stacked Histogram
Horizontal Lines
Wire Mesh |

| Colour ▷ | ——— | Blue
Orange
Grey |

| Axis Properties | ——— | Log Plots ▷
Axis Style ▷
Z-axis ▷ |

| X-axis
Y-axis
Z-axis |

| Show axis
Extend axis |

e)

| Lower right
Lower left

Upper right
Upper left

Hide axis |

Illustration:

The graphical output from the programme is shown in figure 4.13a for the behaviour of the coupling coefficient describing the total loss rate form the ground state for a pure hydrogen

target plasma. The behaviour of the beam emission coefficient for the transition He(3^1P) $\rightarrow$ He($3\ ^1$S) for a pure hydrogen target plasma is shown in figure 4.13b.

The tabulated output for the effective stopping and emission coefficients are respectively shown in tables 4.13a and 4.13b.

Figure 4.13a.

CROSS COUPLING COEFFICIENT SURFACE PLOT :
ADAS RELEASE: ADAS93 V1.13 PROGRAM: ADAS313 V1.0 DATE : 08/03/99 TIME :10:59
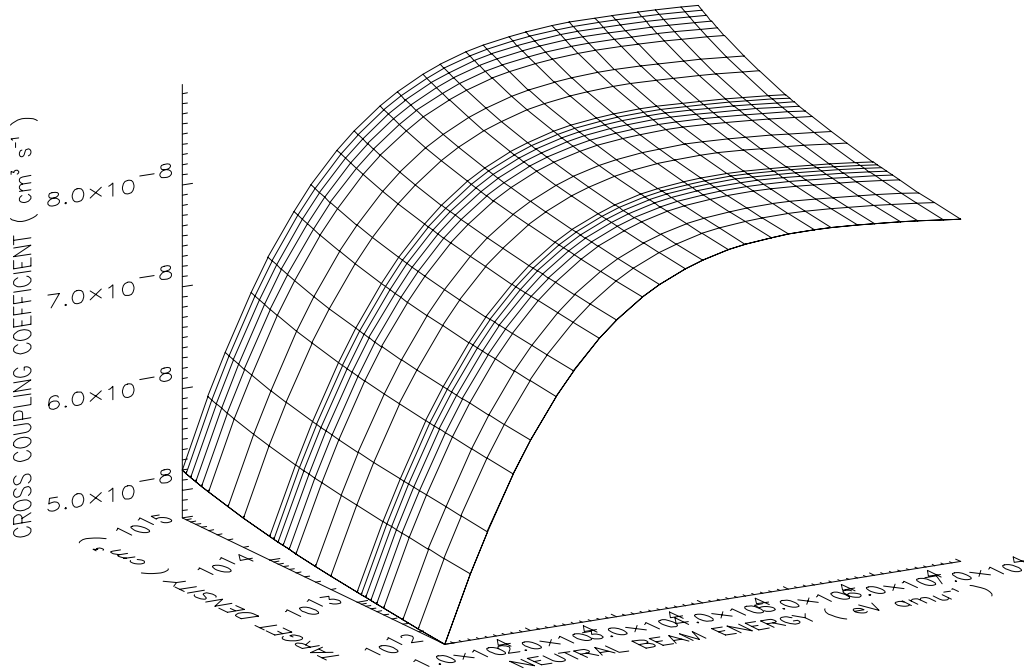FILE : /packages/adas/adas/adf26/bnl99#he_fast/bnl99#he_h1.dat

Table 4.13b.

```
    1 /GCRC1=7.566E-08 /SPEC=H   /DATE=08/03/99 /CODE=ADAS313
-------------------------------------------------------------------------------
   25    25 /TREF=2.000E+03
-------------------------------------------------------------------------------
 1.000E+04 1.300E+04 1.500E+04 1.800E+04 2.000E+04 2.300E+04 2.500E+04 2.800E+04
 3.000E+04 3.300E+04 3.500E+04 3.800E+04 4.000E+04 4.300E+04 4.500E+04 4.800E+04
 5.000E+04 5.300E+04 5.500E+04 5.800E+04 6.000E+04 6.300E+04 6.500E+04 6.800E+04
 7.000E+04
 1.000E+12 2.000E+12 3.000E+12 5.000E+12 6.000E+12 7.000E+12 8.000E+12 9.000E+12
 1.000E+13 2.000E+13 3.000E+13 5.000E+13 6.000E+13 7.000E+13 8.000E+13 9.000E+13
 1.000E+14 2.000E+14 3.000E+14 5.000E+14 6.000E+14 7.000E+14 8.000E+14 9.000E+14
 1.000E+15
-------------------------------------------------------------------------------
 4.432E-08 5.042E-08 5.407E-08 5.901E-08 6.187E-08 6.552E-08 6.762E-08 7.023E-08
 7.165E-08 7.339E-08 7.431E-08 7.536E-08 7.589E-08 7.648E-08 7.673E-08 7.694E-08
 7.702E-08 7.705E-08 7.699E-08 7.683E-08 7.670E-08 7.649E-08 7.633E-08 7.606E-08
 7.586E-08
 4.458E-08 5.069E-08 5.435E-08 5.929E-08 6.215E-08 6.581E-08 6.791E-08 7.053E-08
 7.196E-08 7.370E-08 7.462E-08 7.568E-08 7.621E-08 7.681E-08 7.706E-08 7.727E-08
 7.735E-08 7.738E-08 7.733E-08 7.717E-08 7.704E-08 7.683E-08 7.668E-08 7.641E-08
 7.621E-08
 4.474E-08 5.085E-08 5.452E-08 5.947E-08 6.233E-08 6.600E-08 6.810E-08 7.073E-08
 7.215E-08 7.390E-08 7.483E-08 7.588E-08 7.642E-08 7.702E-08 7.727E-08 7.749E-08
 7.757E-08 7.760E-08 7.755E-08 7.739E-08 7.726E-08 7.706E-08 7.690E-08 7.664E-08
 7.644E-08
 4.494E-08 5.107E-08 5.474E-08 5.970E-08 6.257E-08 6.624E-08 6.835E-08 7.098E-08
 7.241E-08 7.417E-08 7.510E-08 7.616E-08 7.670E-08 7.730E-08 7.756E-08 7.778E-08
 7.786E-08 7.790E-08 7.785E-08 7.770E-08 7.757E-08 7.737E-08 7.722E-08 7.695E-08
 7.675E-08
 4.502E-08 5.115E-08 5.482E-08 5.978E-08 6.266E-08 6.633E-08 6.844E-08 7.107E-08
 7.251E-08 7.426E-08 7.520E-08 7.626E-08 7.680E-08 7.741E-08 7.767E-08 7.789E-08
 7.798E-08 7.801E-08 7.797E-08 7.782E-08 7.769E-08 7.749E-08 7.734E-08 7.707E-08
 7.688E-08
        .            .          .
 4.843E-08 5.482E-08 5.863E-08 6.376E-08 6.673E-08 7.056E-08 7.276E-08 7.554E-08
```

```
      7.708E-08 7.898E-08 8.001E-08 8.123E-08 8.188E-08 8.263E-08 8.300E-08 8.337E-08
      8.355E-08 8.374E-08 8.379E-08 8.378E-08 8.374E-08 8.368E-08 8.361E-08 8.348E-08
      8.336E-08
      4.858E-08 5.498E-08 5.879E-08 6.392E-08 6.690E-08 7.073E-08 7.294E-08 7.573E-08
      7.726E-08 7.918E-08 8.021E-08 8.144E-08 8.209E-08 8.285E-08 8.322E-08 8.360E-08
      8.379E-08 8.398E-08 8.404E-08 8.403E-08 8.400E-08 8.394E-08 8.388E-08 8.375E-08
      8.364E-08
      4.872E-08 5.512E-08 5.893E-08 6.407E-08 6.706E-08 7.089E-08 7.310E-08 7.589E-08
      7.744E-08 7.935E-08 8.040E-08 8.163E-08 8.228E-08 8.305E-08 8.342E-08 8.381E-08
      8.400E-08 8.420E-08 8.426E-08 8.426E-08 8.424E-08 8.418E-08 8.413E-08 8.400E-08
      8.390E-08
      ----------------------------------------------------------------------------
         20 /EREF=3.300E+04 /NREF=5.000E+13
      ----------------------------------------------------------------------------
      1.000E+02 2.000E+02 3.000E+02 5.000E+02 6.000E+02 7.000E+02 8.000E+02 8.966E+02
      1.000E+03 2.000E+03 3.000E+03 5.000E+03 6.000E+03 7.000E+03 8.000E+03 8.966E+03
      1.000E+04 2.000E+04 3.000E+04 5.000E+04
      ----------------------------------------------------------------------------
      8.073E-08 8.498E-08 8.548E-08 8.436E-08 8.358E-08 8.281E-08 8.206E-08 8.136E-08
      8.068E-08 7.566E-08 7.248E-08 6.843E-08 6.703E-08 6.589E-08 6.497E-08 6.421E-08
      6.357E-08 6.011E-08 5.877E-08 5.722E-08
      ----------------------------------------------------------------------------
      C
      C
      C      ADAS FILE TYPE :   ADF21
      C      SOURCE FILE    :   /packages/adas/adas/adf26/bnl99#he_fast/bnl99#he_h1.dat
      C
      C      USER ID        :   anderson
      C
      ----------------------------------------------------------------------------
```

Figure 4.13b.

BEAM EMISSION COEFFICIENT SURFACE PLOT :
ADAS RELEASE: ADAS93 V1.13 PROGRAM: ADAS313 V1.0 DATE : 08/03/99 TIME :11:01
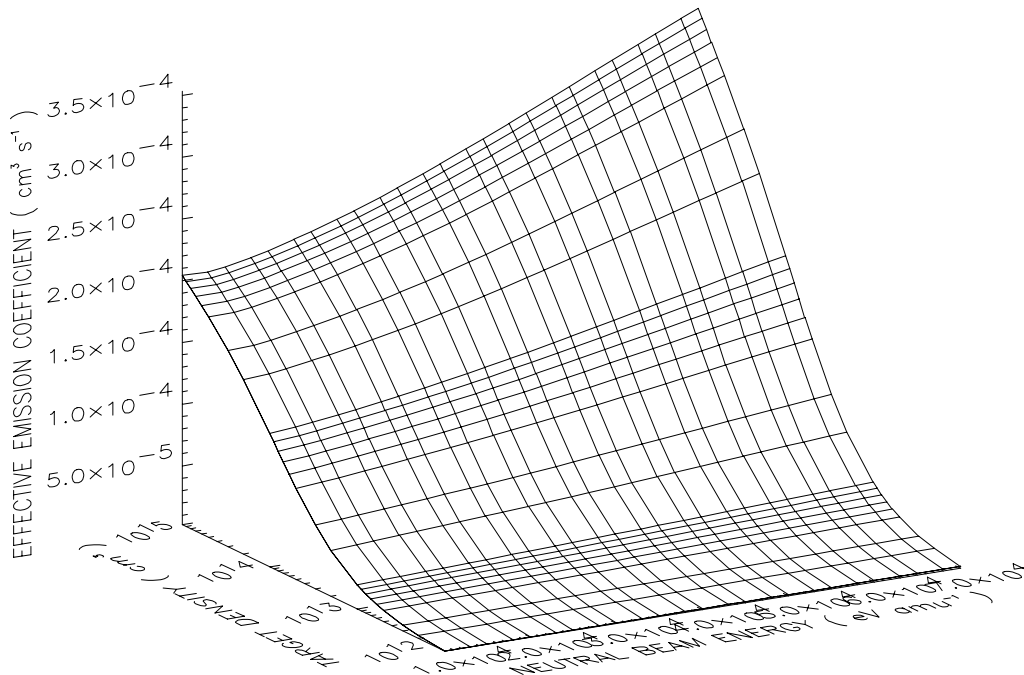FILE : /packages/adas/adas/adf26/bnl99#he_fast/bnl99#he_h1.dat

Table 4.13b.

```
        1 /ECMT1=4.637E-13 /SPEC=H  /DATE=08/03/99 /CODE=ADAS313
      ----------------------------------------------------------------------------
         25   25 /TREF=2.000E+03
      ----------------------------------------------------------------------------
      1.000E+04 1.300E+04 1.500E+04 1.800E+04 2.000E+04 2.300E+04 2.500E+04 2.800E+04
      3.000E+04 3.300E+04 3.500E+04 3.800E+04 4.000E+04 4.300E+04 4.500E+04 4.800E+04
      5.000E+04 5.300E+04 5.500E+04 5.800E+04 6.000E+04 6.300E+04 6.500E+04 6.800E+04
      7.000E+04
      1.000E+12 2.000E+12 3.000E+12 5.000E+12 6.000E+12 7.000E+12 8.000E+12 9.000E+12
      1.000E+13 2.000E+13 3.000E+13 5.000E+13 6.000E+13 7.000E+13 8.000E+13 9.000E+13
      1.000E+14 2.000E+14 3.000E+14 5.000E+14 6.000E+14 7.000E+14 8.000E+14 9.000E+14
      1.000E+15
      ----------------------------------------------------------------------------
```

```
 5.955E-13 6.161E-13 6.294E-13 6.486E-13 6.609E-13 6.792E-13 6.913E-13 7.096E-13
 7.222E-13 7.417E-13 7.552E-13 7.761E-13 7.905E-13 8.126E-13 8.276E-13 8.506E-13
 8.662E-13 8.896E-13 9.052E-13 9.286E-13 9.441E-13 9.672E-13 9.823E-13 1.005E-12
 1.019E-12
 5.912E-13 6.121E-13 6.257E-13 6.454E-13 6.581E-13 6.768E-13 6.892E-13 7.079E-13
 7.208E-13 7.406E-13 7.542E-13 7.753E-13 7.897E-13 8.119E-13 8.270E-13 8.500E-13
 8.655E-13 8.888E-13 9.044E-13 9.276E-13 9.430E-13 9.659E-13 9.810E-13 1.003E-12
 1.018E-12
         .           .
 6.115E-14 6.107E-14 6.166E-14 6.291E-14 6.392E-14 6.561E-14 6.683E-14 6.878E-14
 7.018E-14 7.239E-14 7.394E-14 7.636E-14 7.803E-14 8.063E-14 8.240E-14 8.511E-14
 8.694E-14 8.973E-14 9.158E-14 9.437E-14 9.623E-14 9.902E-14 1.009E-13 1.036E-13
 1.054E-13
 5.541E-14 5.529E-14 5.581E-14 5.693E-14 5.785E-14 5.939E-14 6.051E-14 6.229E-14
 6.357E-14 6.558E-14 6.700E-14 6.921E-14 7.074E-14 7.311E-14 7.473E-14 7.720E-14
 7.887E-14 8.141E-14 8.311E-14 8.565E-14 8.735E-14 8.990E-14 9.158E-14 9.408E-14
 9.572E-14
 5.070E-14 5.054E-14 5.101E-14 5.203E-14 5.288E-14 5.429E-14 5.532E-14 5.696E-14
 5.814E-14 6.000E-14 6.130E-14 6.334E-14 6.475E-14 6.693E-14 6.842E-14 7.070E-14
 7.224E-14 7.458E-14 7.614E-14 7.848E-14 8.005E-14 8.239E-14 8.394E-14 8.624E-14
 8.775E-14
--------------------------------------------------------------------------------
   20 /EREF=3.300E+04 /NREF=5.000E+13
--------------------------------------------------------------------------------
 1.000E+02 2.000E+02 3.000E+02 5.000E+02 6.000E+02 7.000E+02 8.000E+02 8.966E+02
 1.000E+03 2.000E+03 3.000E+03 5.000E+03 6.000E+03 7.000E+03 8.000E+03 8.966E+03
 1.000E+04 2.000E+04 3.000E+04 5.000E+04
--------------------------------------------------------------------------------
 3.988E-13 4.727E-13 4.947E-13 5.036E-13 5.028E-13 5.008E-13 4.982E-13 4.952E-13
 4.920E-13 4.637E-13 4.454E-13 4.256E-13 4.203E-13 4.169E-13 4.149E-13 4.140E-13
 4.138E-13 4.299E-13 4.572E-13 5.049E-13
--------------------------------------------------------------------------------
C
C
C     SOURCE FILE   :  /packages/adas/adas/adf26/bnl99#he_fast/bnl99#he_h1.dat
C     ADAS FILE TYPE :   ADF22
C
C     REF. METASTABLE: 1s2(1)S
C     TRANSITION    :  1s3p(1)P-1s3s(1)S
C     A-VALUE       :  2.530E+05
C
C     USER ID       :   anderson
C
--------------------------------------------------------------------------------
```

Notes: