

# ADAS507: GCF - graph and fit generalised contribution functions

The program interrogates GCF files of type ADF16. The coefficient is extracted for a selected radiative transition of an ion. The data may be interpolated using cubic splines at selected electron temperature. A minimax polynomial approximation is made to the interpolated data. The interpolated data are displayed and a tabulation prepared. The tabular and graphical output may be printed and includes the polynomial approximation.

## Background theory:

The GCF function is designed to provide a flexible extension to the  $G(T_e)$  functions described in ADAS506.

The emissivity in a transition  $j \rightarrow k$  of an ion may be written (see equation 3.8.7) as

$$\begin{aligned} \varepsilon_{j \rightarrow k} = A_{j \rightarrow k} & \left( \sum_{\sigma=1}^{M_z} \mathcal{F}_{j\sigma}^{(exc)} N_e N_{\sigma} + \sum_{v'=1}^{M_{z+1}} \mathcal{F}_{jv'}^{(rec)} N_e N_{v'}^+ + \right. \\ & \left. \sum_{\mu'=1}^{M_{z-1}} \mathcal{F}_{j\mu'}^{(ion)} N_e N_{\mu'}^- \right) \end{aligned} \quad 6.7.1$$

where  $N_{\sigma}$  denotes the population density of the specified ion in the metastable state  $\sigma$ ,  $N_{v'}^+$  denotes the population density of ions in the metastable state  $v'$  of the adjacent higher ionisation stage and  $N_{\mu'}^-$  denotes the population density of ions in the metastable state  $\mu'$  of the adjacent lower ionisation stage. The  $\mathcal{F}_{j\sigma}^{(exc)}$ ,  $\mathcal{F}_{jv'}^{(rec)}$ , and  $\mathcal{F}_{j\mu'}^{(ion)}$  are the effective contributions to the population of the upper excited level  $j$  of the transition from excitation from the metastables, from free electron capture, and from ionisation respectively. Charge exchange is omitted. All these coefficients depend on density as well as temperature.  $N_e$  is the electron density.

A time-dependent ionisation or spatially non-equilibrium ionisation model for a particular plasma allows determination of the metastable population densities as a function of space or time (see ADAS406).

$$N_{\sigma}(x) \equiv N_{\sigma}^{(z)}(x) = \frac{N_{\sigma}^{(z)}(x)}{N_{tot}(x)} N_{tot}(x) \quad 6.7.2$$

$x$  is the appropriate spatial (temporal) coordinate. Thus the ratio  $N_{\sigma}^{(z)} / N_{tot}$  is not necessarily in equilibrium at the local temperature and density. The ionisation equilibrium case may be incorporated in this description but with the spatial (temporal) coordinate  $x$  merely an index of temperature/density pairs.

Define  $G_{j \rightarrow k}(x)$  by

$$\begin{aligned} G_{j \rightarrow k}(x) &= A_{j \rightarrow k} \sum_{\sigma=1}^{M_z} \mathcal{F}_{j\sigma}^{(exc)} \frac{N_{\sigma}^{(z)}}{N_{tot}} + A_{j \rightarrow k} \sum_{v'=1}^{M_{z+1}} \mathcal{F}_{jv'}^{(rec)} \frac{N_{v'}^{(z+1)}}{N_{tot}} + \\ & A_{j \rightarrow k} \sum_{\mu'=1}^{M_{z-1}} \mathcal{F}_{j\mu'}^{(ion)} \frac{N_{\mu'}^{(z-1)}}{N_{tot}} \\ &= \mathcal{GCF}_{j \rightarrow k}^{(exc)}(x) + \mathcal{GCF}_{j \rightarrow k}^{(rec)}(x) + \mathcal{GCF}_{j \rightarrow k}^{(ion)}(x) \end{aligned} \quad 6.7.3$$

The  $\mathcal{GCF}_{j \rightarrow k}(x)$  constitute the extension of contribution functions suitable for arbitrary dynamic plasmas. In practise, such functions are usually required for a modest number of spectrum lines of special diagnostic importance and are grouped for application to each particular plasma scenario. The data type ADF16 is specified as indexed lists for such purposes. Codes such as ADAS405 and ADAS406 prepare generalised contribution function data to the ADF16 specification directly as prescribed by their *scripts*.

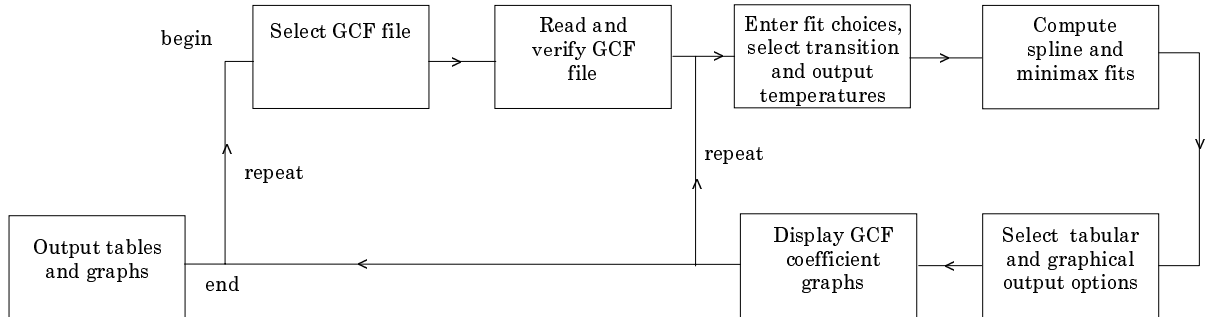
The GCF functions are stored at a set of plasma model triplets, that is of spatial (temporal) coordinate, electron temperature and density in archived files of type ADF16. The code interpolates in this one-dimensional model by cubic splines to provide results at an arbitrary

interpolated model triplet. The data interpolation uses the temperature coordinate as the independent variable, the spatial (temporal) and density values also being interpolated. The interpolated GCF functions are approximated by a minimax polynomial and a graph produced. A tabulation of the the interpolated spline data and the minimax approximation is prepared.

## Program steps:

These are summarised in figure 6.7.

Figure 6.7



## Interactive parameter comments:

Programs of this series (ADAS5) which make use of data from archived ADAS datasets initiate an interactive dialogue with the user in three parts, namely, input file selection, entry of user data and disposition of output.

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

1. Data root a) shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Note that each type of data is stored according to its ADAS data format (*adf* number). 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 datafiles are presented for selection. Datafiles 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 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.
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

a) Title for run

b) Data file name

c) Select data block table

d) Temperature & Density Values table

**ADAS507 PROCESSING OPTIONS**

Title for run

Data file name :

**Polynomial Fitting**

Fit Polynomial value % :

**Select data block**

Index	Wavelength	Ion Stage	Processing Code	Metastable Index
3	3321.1A	be+0	ADAS405	1
1	2349.3A	be+0	ADAS405	1
2	1661.5A	be+0	ADAS405	1
3	3321.1A	be+0	ADAS405	1
4	2651.4A	be+0	ADAS405	1
5	2495.4A	be+0	ADAS405	1

**Temperature & Density Values**

Index	Output	Temperature Input	Density Input	Reference Input
1	1.000E+00	1.000E+00	1.000E+12	1.000E+00
2	2.000E+00	2.000E+00	1.000E+12	2.000E+00
3	5.000E+00	5.000E+00	1.000E+12	3.000E+00
4	1.000E+01	1.000E+01	1.000E+12	4.000E+00
5	2.000E+01	2.000E+01	1.000E+12	5.000E+00
6	5.000E+01	5.000E+01	1.000E+12	6.000E+00
7	1.000E+02	1.000E+02	1.000E+12	7.000E+00
8	2.000E+02	2.000E+02	1.000E+12	8.000E+00

Temperature units : eV      Density units : cm-3

8. An arbitrary title may be given for the case being processed a). 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.

9. The output data extracted from the datafile, in the case of ADAS507, an 'generalised contribution function', may be fitted with a polynomial. This is as a function of temperature. Clicking the *Fit polynomial* button b) 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. **Remember to press the return key on the keyboard to record the value.**
10. Spectrum lines for which functions 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 line appears in the selection window c) just above the line list display window.
11. Your settings of electron temperature are shown in the temperature/density display window d). The temperature and density values at which the functions are stored in the datafile (inputs) are also shown for information.
12. The program recovers the output temperature/density pairs you used when last executing the program. Pressing the *Default Temperature values* button inserts a default set of temperatures equal to the input temperatures
13. 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, appears as shown below:

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

14. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
15. 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. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button b) to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.

ADAS507 OUTPUT OPTIONS

Data file name : /packages/adas/adas/adf16/gcf93#be/gcf93#be\_be0.dat

Browse comments

Graphical Output

Graph Title : demonstration

Default Device : HP-GL

Explicit Scaling

X-min : [ ] X-max : [ ]

Y-min : [ ] Y-max : [ ]

Post-script : HP-PCL, HP-GL

Enable Hard Copy  Replace

File name : adas5-07.hgl

Text Output  Replace

Default file name

File name : adas5-07.txt

Cancel Done

16. Hard copy is activated by the *Enable Hard Copy* button c). 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.

17. A choice of output graph plotting devices is given in the Device list window d). Clicking on the required device selects it. It appears in the selection window above the Device list window.
18. 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.
19. The graph is displayed in a following **Graphical Output** window.

## Illustration:

Figure 6.7a

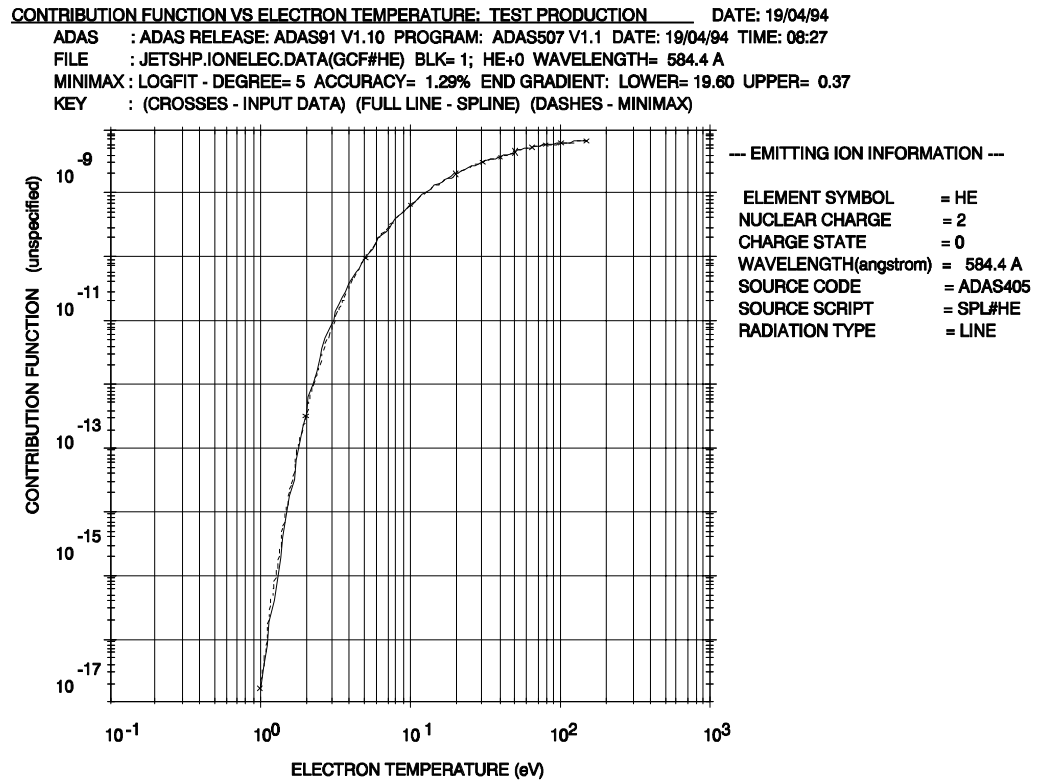


Table 6.7a

```

ADAS RELEASE: ADAS91 V1.10 PROGRAM: ADAS507 V1.1 DATE: 19/04/94 TIME: 08:27
** TABULAR OUTPUT FROM GENERALISED CONTRIBUTION FUNCTION INTERROGATION PROGRAM: ADAS507 - DATE: 19/04/94 ***

----- TEST PRODUCTION 19/04/94 -----
GENERALISED CONTRIBUTION FUNCTION AS A FUNCTION OF ELECTRON TEMPERATURE
-----
DATA GENERATED USING PROGRAM: ADAS507
-----

FILE: JETSHPIONELEC.DATA(GCF#HE) - DATA-BLOCK: 1

EMITTING ION INFORMATION:
-----
ELEMENT NAME           = HELIUM
ELEMENT SYMBOL         = HE
NUCLEAR CHARGE        (Z0) = 2
CHARGE STATE          (Z)  = 0
WAVELENGTH (angstrom) = 584.4 A
SOURCE CODE           = ADAS405
SOURCE SCRIPT         = SPL#HE
RADIATION TYPE        = LINE

----- ELECTRON TEMPERATURE -----
Kelvin      eV      K/Z1**2      CONTR. FUNC.  DENSITY      T PARM.
unspecified unspecified cm-3      unspecified
1.161D+04   1.000D+00   1.161D+04   1.660D-17    1.000D+11    1.000D+00
1.741D+04   1.500D+00   1.741D+04   8.224D-15    1.503D+11    1.554D+00
2.321D+04   2.000D+00   2.321D+04   3.160D-13    2.000D+11    2.000D+00
2.901D+04   2.500D+00   2.901D+04   2.587D-12    2.488D+11    2.298D+00
5.803D+04   5.000D+00   5.803D+04   9.550D-11    5.000D+11    3.000D+00
8.124D+04   7.000D+00   8.124D+04   2.722D-10    7.172D+11    3.453D+00
1.161D+05   1.000D+01   1.161D+05   6.540D-10    1.000D+12    4.000D+00
1.741D+05   1.500D+01   1.741D+05   1.359D-09    1.364D+12    4.545D+00
2.321D+05   2.000D+01   2.321D+05   2.010D-09    2.000D+12    5.000D+00

```

```
3.482D+05 3.000D+01 3.482D+05 3.100D-09 5.000D+12 6.000D+00
2.321D+06 * 2.000D+02 2.321D+06 7.131D-09 8.862D+14 1.254D+01
```

```
-----
NOTE: * => CONTRIBUTION FUNCTIONS EXTRAPOLATED FOR ELECTRON TEMPERATURE VALUE
-----
```

```
MINIMAX POLYNOMIAL FIT - TAYLOR COEFFICIENTS:
```

```
-----
- LOG10(CONTRIB. FUNC. <unspecif>) VERSUS LOG10(ELECTRON TEMPERATURE<eV>) -
-----
```

```
A( 1) = -1.677430890D+01      A( 2) =  1.959942229D+01
A( 3) = -2.168046216D+01      A( 4) =  1.347406444D+01
A( 5) = -4.372675335D+00      A( 6) =  5.703404655D-01
```

```
LOGFIT - DEGREE= 5 ACCURACY= 1.29% END GRADIENT: LOWER= 19.60 UPPER= 0.37
-----
```

## Notes: