ADAS505: QTX - graph and fit thermal charge exchange coefficients

The program interrogates thermal charge transfer rate coefficient (QTX) files of type ADF14. The coefficient is extracted for total or selective capture by a thermal ion from a thermal donor. The data may be interpolated using cubic splines at selected donor/receiver temperature pairs. 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:

In the situation of electron-ion collisions, the assumption that electron speeds are fast compared with ion speeds can usually be made. Since the electron distribution function is also usually Maxwellian, rate coefficients are the preferred form in ADAS for storage of electron collision data. For ion-ion and ion-atom collisions, by contrast, target and projectile speeds are comparable and collision cross-sections are the preferred means of storage (see ADAS3 series codes). Then, various relevant integrals over target and projectile velocity distribution functions may be made for particular experimental cases. The situation when both target and projectile have thermal velocity distribution functions is however common. With independent temperatures assigned to the two distributions, reasonable description of, for example tokamak divertor processes, without the complexity of handling explicit non-thermal distribution functions may be made.

For particles of masses m_1 and m_2 with speeds v_1 and v_2, since the collision cross-section depends only on the relative velocity of the collision partners, it is convenient to orientate the direction of the first particle along the z-axis and measure the direction of the second particle relative to this. Since $v_{rel} = \sqrt{v_1^2 + v_2^2 - 2v_1 v_2 \cos\theta_{12}}$, the integral over the angle θ_{12} is performed first as

$$q_{rel}(v_1, v_2) = \int_0^\pi |v_{rel}| Q(|v_{rel}|) \sin\theta_{12} d\theta_{12}$$

$$= \frac{1}{v_1 v_2} \int_{|v_1 - v_2|}^{v_1 + v_2} |v_{rel}|^2 Q(|v_{rel}|) dv_{rel}$$

6.5.1.

followed by the integral over the speed of the second particle v_2 as

$$q(v_1, T_2) = 2\pi \left(\frac{m_2}{2\pi k T_2} \right)^{3/2} \int_0^\infty v_2^2 e^{-\frac{1}{2}m_2 v_2^2 / kT_2} q_{rel}(v_1, v_2) dv_2$$

6.5.2

where T_2 is the thermal temperature of the second particle. This integral is relevant to beam plasma reactions and is used extensively in the ADAS3 series codes.

The final double Maxwell averaged rate coefficient is

$$q(T_1, T_2) = 4\pi \left(\frac{m_1}{2\pi k T_1} \right)^{3/2} \int_0^\infty v_1^2 e^{-\frac{1}{2}m_1 v_1^2 / kT_1} q(v_1, T_2) dv_1$$

6.5.3

where T_1 is the thermal temperature of the first particle.

Two dimensional arrays of the coefficients $q(T_1, T_2)$ are available together with the equal temperature vector (that is, $T_1 = T_2$) in QTX files of type ADF14. QTX data are extracted from these files and interpolated by cubic splines in donor and receiver temperature to provide results at an arbitrary set of donor/receiver temperature pairs. The interpolated data are approximated by a minimax polynomial and a graph produced. A tabulation of the the interpolated spline data and the minimax approximation is prepared.
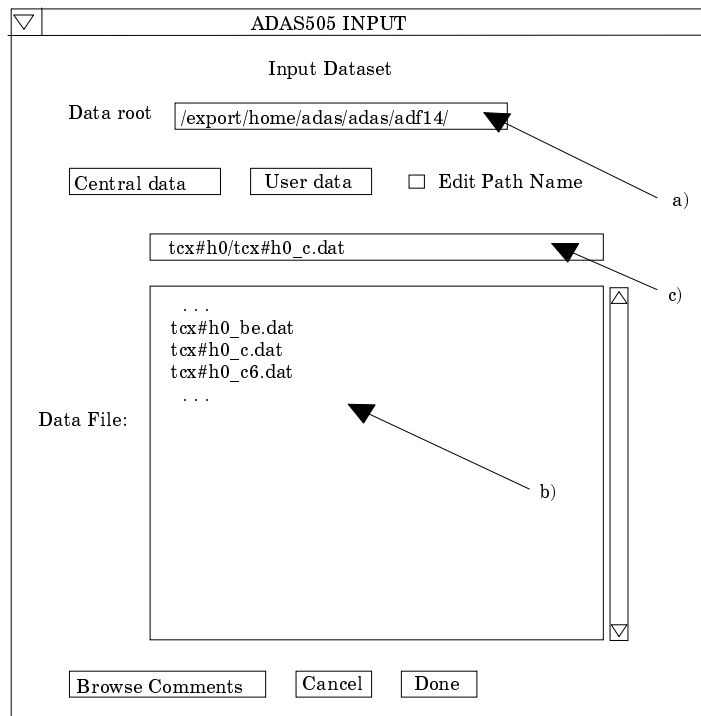
Program steps:

These are summarised in figure 6.5.

Figure 6.5
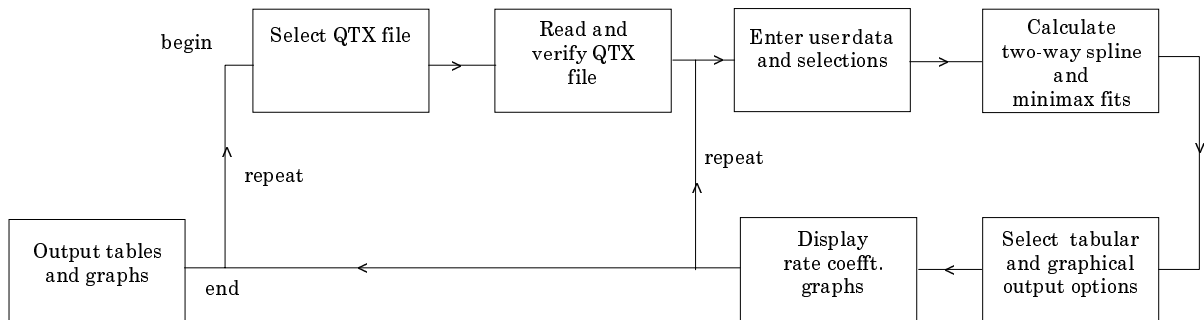
Interactive parameter comments:

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. 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. 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*.

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 is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.

6. 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

ADAS505 PROCESSING OPTIONS

Title for Run   cxs-manu demonstration   a)
Data File Name : /export/home/adas/adas/adf14/tcx#h0/tcx#h0_c.dat

Browse Comments

Polynomial Fitting

◇   Fit Polynomial   Value % :   5

f)

Select Data Block

INDEX Reciever Donor   Final State
       Identity Identity Spec.

1   C+1 (1)   H+0 (1)   TOTAL

1   C+1 (1)   H+0 (1)   TOTAL
2   C+2 (1)   H+0 (1)   TOTAL
3   C+3 (1)   H+0 (1)   TOTAL

b)

Plot and fit as function of

◇   receiver temperature

◇   donor temperature

d)

Receiver and Donor Temperature Values

           Receiver   Donor

INDEX Output   Input   Output   Input
  1   4.80e+01 4.80E+01 1.00E+01 1.00E+00
  2   8.40E+01 8.40E+01 1.00E+01 1.00E+01   . . .

c)

Temperature Units : eV

Edit Table

Default Temperature Values

Select Isotopic A.M.   Receiver   Donor

Atomic Mass   12.00   1.00
Isotopic Atomic Mass   12.00   1.00

e)

Edit the processing options data and press Done to continue

Cancel   Done

7. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being analysed is also shown. The button *Browse comments* a) again allows display of the information field section at the foot of the selected dataset, if it exists.

8. The output data extracted from the datafile, in the case of ADAS505, a double Maxwell averaged charge transfer rate coefficient , may be fitted with a polynomial. This is as a function of temperature. Clicking the *Fit polynomial* button f) 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

9. Available rate coefficients in the data set are displayed in the coefficient list display window at b). This is a scrollable window using the scroll bar to the right of the window. Click anywhere on the row for a coefficient to select it. The selected rate appears in the selection window just above the coefficient list display window.

10. Your settings of temperatures (output) for donor and receiver are shown in the temperature display window c). The donor and receiver temperature values at which the rate coefficients are stored in the datafile (input) are also shown for information.

11. The program recovers the output temperatures you used when last executing the program. 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.

12. Pressing the *Default Temperature values* button inserts a default set of temperatures. This depends on the switch settings at d). For plot as a function of receiver temperature, the source receiver temperatures are used and a pop-up window allows choice of a single donor temperature from the source set. Conversely, for plot as a function of donor temperature, the source donor temperatures are used and the pop-up allows choice of a single receiver temperature.

13. At e) choice of donor and receiver atomic mass numbers is available. For information, the isotope mass numbers in the source dataset are given. Note that these masses are simply used to locate the effective donor and receiver temperatures in the source dataset.

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 5 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

The **output options window** is shown below. It is of standard form with the same layout as codes previously described.

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 b). 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 to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.

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

18. 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.

19. 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.

20. The graph is displayed in a following Graphical Output window.

Illustration:

Figure 6.5a shows the total thermally averaged charge exchange capture coefficient for $C^{+4}(3s\ ^2S)$ from H(1s) from the review by Maggi. The solid line connects the spline fit points obtained in the main interpolation and the dashed curve is the minimax fit. The code provides a set of data lines for supplementation of an ADF04 file illustrated in table 6.5a. The normal text summary is shown in table 6.5b.

Figure 6.5a
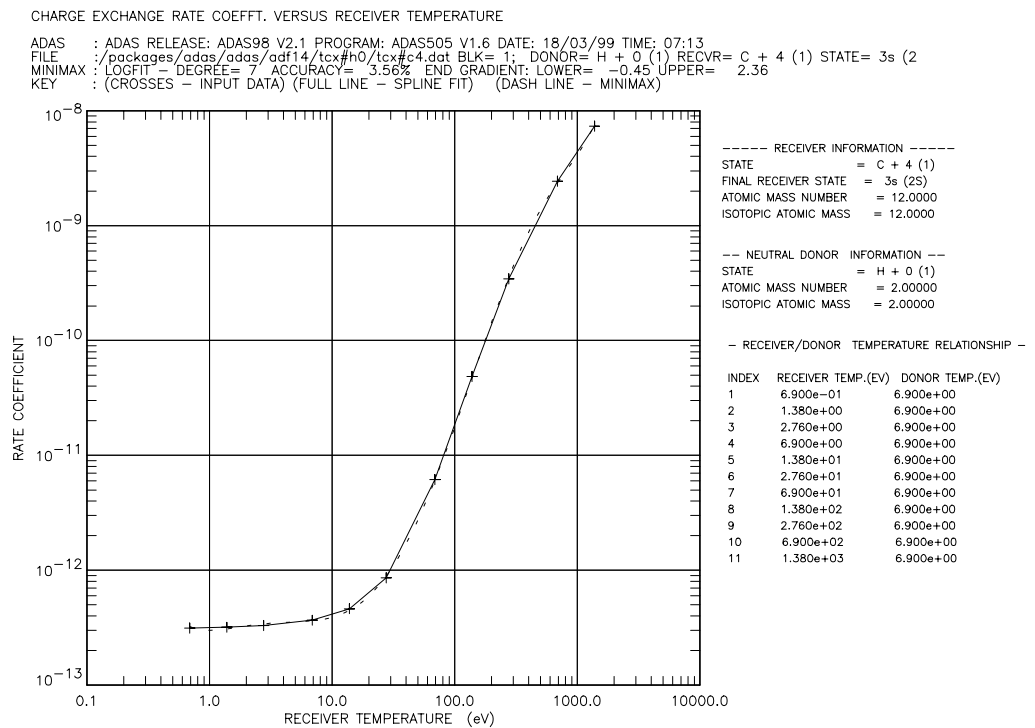
Table 6.5a

```
CX H line for input to ADF04 dataset
Line 1 : Receiver Temperature
Line 2 : CX rate for T receiver / T donor pairs
Line 3 : CX rate for T donor set equal to T receiver


            6.90-01 1.38+00 2.76+00 6.90+00 1.38+01 2.76+01 6.90+01 1.38+02 2.76+02 6.90+02 1.38+03
H  ?  +?    3.13-13 3.19-13 3.30-13 3.67-13 4.63-13 8.60-13 6.15-12 4.85-11 3.43-10 2.44-09 7.35-09
H  ?  +?    1.00-13 1.42-13 2.00-13 3.67-13 3.40-12 6.46-11 1.02-09 3.98-09 1.11-08 3.02-08 5.13-08
```

Table 6.5b

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ADAS RELEASE: ADAS98 V2.1 PROGRAM: ADAS505 V1.6 DATE: 18/03/99 TIME: 07:13


***.TABULAR OUTPUT FROM CHARGE EXCHANGE RATE-COEFFICIENT INTERROGATION PROGRAM: ADAS505 - DATE: 18/03/99 **


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  CHARGE EXCHANGE RATE-COEFFICIENTS AS A FUNCTION OF RECEIVER/DONOR TEMPERATURE
  ----------------------------------------------------------------------------
                    DATA GENERATED USING PROGRAM: ADAS505
                    -------------------------------------
 FILE : /packages/adas/adas/adf14/tcx#h0/tcx#c4.dat  - DATA-BLOCK:  1

                            RECEIVER        NEUTRAL DONOR
                            --------        -------------
                            C + 4 (1)       H + 0 (1)
 ELEMENT NAME             = CARBON          HYDROGEN
 ELEMENT SYMBOL           = c               h
 NUCLEAR CHARGE      (Z0) =      6               1
 RECOMBINING ION CHARGE (Z1) =  4               -
 RECOMBINED ION CHARGE  (Z) =   3               -
 FINAL STATE SPECIFICATION  = 3s (2S)           -
 ATOMIC MASS NUMBER      =   12.00           2.00
 ISOTOPIC ATOMIC MASS NUMBER =  12.00        2.00


--- RECEIVER TEMPERATURE ---   - NEUTRAL DONOR TEMPERATURE -   RATE COEFFICIENT
     kelvin        eV             kelvin        eV              cm**3/sec
    8.008D+03  6.900D-01        8.008D+04  6.900D+00           3.130D-13
    1.602D+04  1.380D+00        8.008D+04  6.900D+00           3.190D-13
    3.203D+04  2.760D+00        8.008D+04  6.900D+00           3.300D-13
    8.008D+04  6.900D+00        8.008D+04  6.900D+00           3.670D-13
    1.602D+05  1.380D+01        8.008D+04  6.900D+00           4.631D-13
    3.203D+05  2.760D+01        8.008D+04  6.900D+00           8.600D-13
    8.008D+05  6.900D+01        8.008D+04  6.900D+00           6.151D-12
    1.602D+06  1.380D+02        8.008D+04  6.900D+00           4.854D-11
    3.203D+06  2.760D+02        8.008D+04  6.900D+00           3.430D-10
    8.008D+06  6.900D+02        8.008D+04  6.900D+00           2.440D-09
    1.602D+07 * 1.380D+03       8.008D+04  6.900D+00           7.351D-09
-----------------------------------------------------------------------------
NOTE: * => RATE-COEFFICIENT EXTRAPOLATED FOR THIS TEMPERATURE VALUE
-----------------------------------------------------------------------------


MINIMAX POLYNOMIAL FIT TO RECEIVER TEMPERATURES - TAYLOR COEFFICIENTS:
 -----------------------------------------------------------------------------
 - LOG10(RATE-COEFFICIENT<cm**3/sec>) versus LOG10(RECEIVER TEMPERATURE<eV>) -
 -----------------------------------------------------------------------------
           A( 1) = -1.252233238D+01        A( 2) = -1.443747602D-02
           A( 3) =  8.824693154D-01        A( 4) = -1.722730073D+00
           A( 5) =  1.003429345D+00        A( 6) =  1.085655124D-01
           A( 7) = -1.725557123D-01        A( 8) =  2.784024322D-02

LOGFIT - DEGREE= 7 ACCURACY=  3.56%  END GRADIENT: LOWER=  -0.45 UPPER=   2.36
-----------------------------------------------------------------------------
```

Notes: