

ADAS509: SCX - graph and fit charge exchange cross-sections

This code interrogates state selective charge exchange cross-sections ('scx') files of type *adf24*. The cross-section is extracted for capture by a receiver ion from a neutral donor. The data is interpolated at selected donor/receiver energies. The usual minimax polynomial fit, graph and tabular outputs are available. Additionally Maxwell averaged rate coefficients (over donor and receiver temperature ranges) may be obtained and a 'tcx' file of type *adf14* output.

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 $v_{rel} = \sqrt{v_1^2 + v_2^2 - 2v_1v_2 \cos \theta_{12}}$, the integral over the angle θ_{12} is performed first as

$$\begin{aligned} q_{rel}(v_1, v_2) &= \int_0^\pi |v_{rel}| Q(|v_{rel}|) \sin \theta_{12} d\theta_{12} \\ &= \frac{1}{v_1 v_2} \int_{|v_1 - v_2|}^{v_1 + v_2} |v_{rel}|^2 Q(|v_{rel}|) dv_{rel} \end{aligned} \quad 6.9.1$$

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

$$q(v_1, T_2) = 2\pi \left(\frac{m_2}{2\pi k T_2} \right)^{3/2} \int_0^\infty v_2^2 e^{-\frac{1}{2} m_2 v_2^2 / k T_2} q_{rel}(v_1, v_2) dv_2 \quad 6.9.2$$

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

$$q(T_1, T_2) = 4\pi \left(\frac{m_1}{2\pi k T_1} \right)^{3/2} \int_0^\infty v_1^2 e^{-\frac{1}{2} m_1 v_1^2 / k T_1} q(v_1, T_2) dv_1 \quad 6.9.3$$

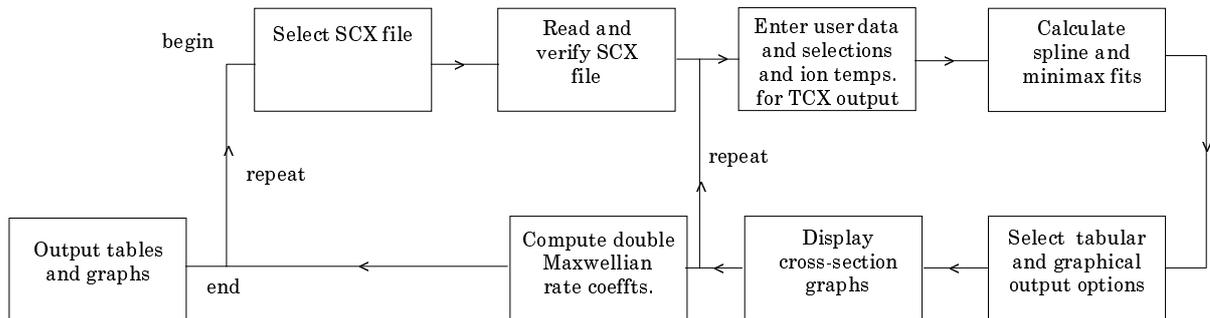
where T_1 is the thermal temperature of the first particle.

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 6.9.

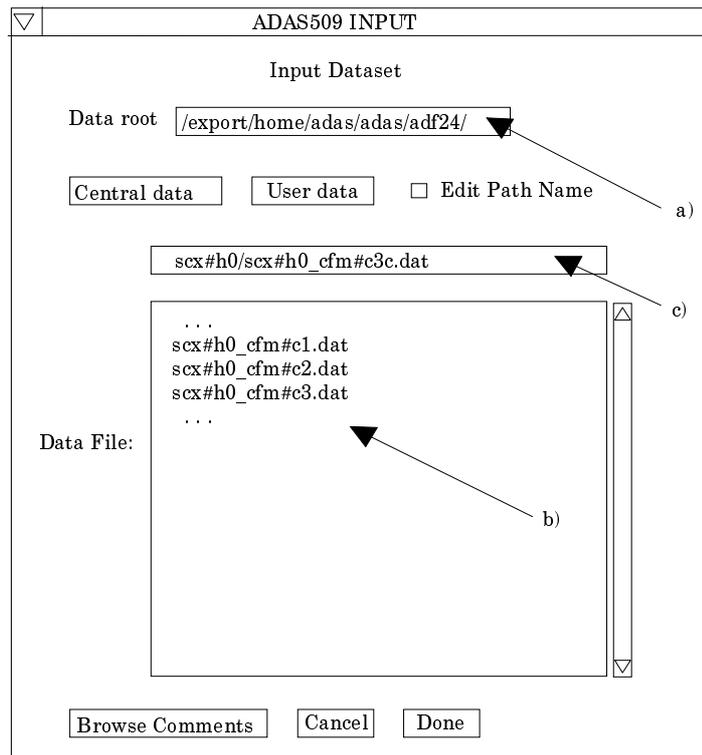
Figure 6.9



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.
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

8. 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.

ADAS509 PROCESSING OPTIONS

Title for Run

Data File Name : /export/home/adas/adas/adf24/scx#h0/scx#h0_cfm#c3.dat

Polynomial Fitting

Fit Polynomial Value % :

Select Data Block

INDEX	Donor Ion	Receiver Ion	Final State	Type
1	H+0 (1)	C+3 (1)	Tot. Singl.	1
1	H+0 (1)	C+3 (1)	Total	1
2	H+0 (1)	C+3 (1)	Tot. Singl.	1
3	H+0 (1)	C+3 (1)	Tot. Tripl.	1

Please enter the reactant mass numbers Donor : Receiver :

Select Energies for Output File

Output Collision Energies

INDEX	Output	Input
1	3.50E-03	3.50E-03
2	...	

Energy Units : eV/amu

Select Temperatures for TCX File

Output Temperatures

INDEX	Output	Input
1	1.16e+04	1.16E+04
2	...	

Energy Units : eV Don.

Edit the processing options data and press Done to continue

9. The output data extracted from the datafile, in the case of ADAS509, a state selective charge transfer cross-section, may be fitted with a polynomial. This is as a function of energy. Clicking the *Fit polynomial* button g) 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

10. Available cross-sections in the data set are displayed in the cross-section 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 cross-section to select it. The selected cross-section appears in the selection window just above the cross-section list display window.
11. For production of rate coefficients, the donor and receiver isotopic mass numbers are required. Enter these at c)
12. To obtain an output text file of the interpolated cross-section at chosen energies click the button at d). Your settings of collision energy (output) are shown in the energy display window c). The energy values at which the cross-sections are stored in the datafile (input) are also shown for information.
13. The program recovers the output energies you used when last executing the program. Pressing the *Default Energy Values* button inserts a default set of energies equal to the input energies.
14. The Energy Values are editable. Click on the *Edit Table* button if you wish to change the values.
15. Note that you can work in a choice of energy units, namely eV/amu, atomic velocity units or cm s^{-1} .
16. To obtain an output 'tex' file Maxwell averaged charge exchange rate click the button at e). Your settings of temperature (output) are shown in the temperature display window. The energy values at which the cross-sections are stored in the datafile (input) are also shown for information.
17. The program recovers the output temperatures you used when last executing the program. Pressing the *Default Temperatures Values* button f) inserts a default set of temperatures equal to the input energies.
18. The Temperature Values are editable. Click on the *Edit Table* button if you wish to change the values.
19. Note that you can work in a choice of temperature units. ADAS509 creates a two-dimensional array of thermal charge exchange rate coefficients from the selected cross-section. The same set of temperatures is used for both donor and receiver.
20. 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** appearance is shown below

21. 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.
22. 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.
23. 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.
24. 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.

ADAS509 OUTPUT OPTIONS

Data File Name : /export/home/adas/adas/adf24/scx#h0/scx#h0_cfm#c3.dat

Browse Comments

Graphical Output

Graph Title : cxs-manu demonstration

Select Device

Post script

Post script

HP-PCL

HP-GL

Explicit scaling

X-min : X-max :

Y-min : Y-max :

Enable Hard Copy Replace

File Name : graph.ps

Text Output Replace Default File Name

File Name : paper.txt

TCX Coeff. File Replace Default File Name

File Name : tcxout.pass

NB. Only when you exit ADAS 509 will TCX output be sent to this file

Cancel Done

25. At d) 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.
26. At e) output of the 'tcx' file may be enabled. The *Default file name* and *Replace* options are set up at the first pass through this window. Note that the actual output is deferred. This is to allow processing of further cross-sections so that a complete 'tcx' file for applications may be built up in one session. The TCX file is written on exiting ADAS509 and is placed by default in your */pass* directory
27. The graph is displayed in a following Graphical Output window.
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 5 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

Illustration:

Figure 6.9a total charge transfer cross-section for C^{+3} from H(1s) from the review by Maggi. Table 6.9a provides the text summary of the interrogation. Table 6b shows the thermally averaged rate coefficient file of type ADF14. The file is fully structured for use by ADAS505.

Figure 6.9a

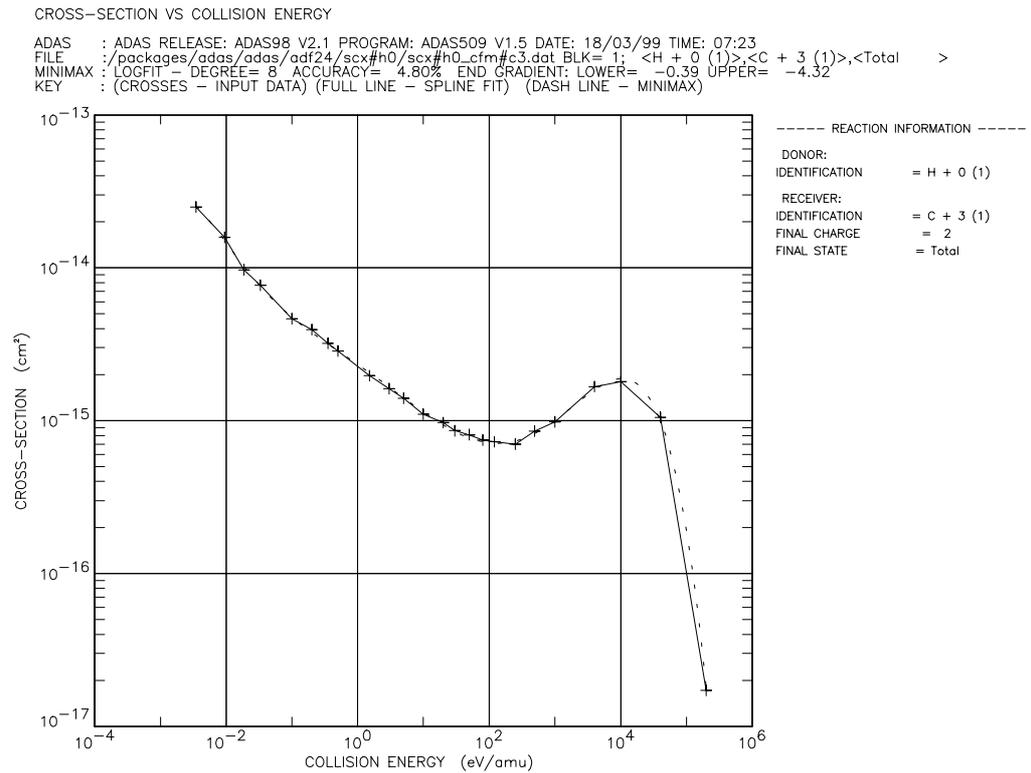


Table 6.9a

ADAS RELEASE: ADAS98 V2.1 PROGRAM: ADAS509 V1.5 DATE: 18/03/99 TIME: 07:23

**** TABULAR OUTPUT FROM CHARGE EXCHANGE CROSS-SECTION INTERROGATION PROGRAM: ADAS509 - DATE: 18/03/99 ****

CHARGE EXCHANGE COLLISION CROSS-SECTIONS AS A FUNCTION OF COLLISION ENERGY

DATA GENERATED USING PROGRAM: ADAS509

/packages/adas/adas/adf24/scx#h0/sc - DATA-BLOCK: 1

REACTION INFORMATION:

ELEMENT SYMBOL = C
 NUCLEAR CHARGE (Z0) = 6

DONOR:
 IDENTIFICATION = H + 0 (1)

RECEIVER:
 IDENTIFICATION = C + 3 (1)
 FINAL CHARGE (Z) = 2
 FINAL STATE = Total

--- COLLISION ENERGIES/VELOCITIES ---			COLLISION CROSS-SECTION
AT. UNITS.	CM S-1	EV/AMU	CM**2
3.757D-04	8.219D+04	3.501D-03	2.490D-14
6.163D-04	1.348D+05	9.420D-03	1.580D-14
8.683D-04	1.900D+05	1.870D-02	9.700D-15
1.157D-03	2.531D+05	3.320D-02	7.700D-15
2.008D-03	4.393D+05	1.000D-01	4.640D-15
2.840D-03	6.213D+05	2.000D-01	3.950D-15
3.762D-03	8.230D+05	3.510D-01	3.210D-15
4.490D-03	9.823D+05	5.000D-01	2.850D-15
7.777D-03	1.701D+06	1.500D+00	1.970D-15
1.100D-02	2.406D+06	3.001D+00	1.620D-15
1.420D-02	3.107D+06	5.001D+00	1.400D-15
2.008D-02	4.393D+06	1.000D+01	1.100D-15
2.840D-02	6.213D+06	2.000D+01	9.699D-16
3.478D-02	7.609D+06	3.000D+01	8.600D-16

```

4.486D-02  9.814D+06  4.991D+01  8.090D-16
5.672D-02  1.241D+07  7.979D+01  7.470D-16
6.956D-02  1.522D+07  1.200D+02  7.270D-16
1.004D-01  2.196D+07  2.500D+02  7.030D-16
1.406D-01  3.076D+07  4.903D+02  8.541D-16
2.008D-01  4.393D+07  1.000D+03  9.820D-16
4.016D-01  8.786D+07  4.000D+03  1.670D-15
6.350D-01  1.389D+08  1.000D+04  1.800D-15
1.270D+00  2.778D+08  4.000D+04  1.050D-15
2.840D+00 * 6.213D+08 * 2.000D+05  1.719D-17
-----
NOTE: * => CX CROSS-SECTION EXTRAPOLATED FOR COLLISION ENERGY VALUE
-----

MINIMAX POLYNOMIAL FIT - TAYLOR COEFFICIENTS:
-----
- LOG10(CX CROSS-SECTION <CM**2>) VERSUS LOG10(COLLISION ENERGY <EV/AMU>) -
-----
A( 1) = -1.463171806D+01      A( 2) = -2.998103315D-01
A( 3) = -2.023791879D-02      A( 4) = -1.122748620D-02
A( 5) =  1.963704877D-02      A( 6) =  2.891296687D-04
A( 7) = -1.380328465D-03      A( 8) =  2.081053698D-04
A( 9) = -1.419031099D-05
LOGFIT - DEGREE= 8  ACCURACY=  4.80%  END GRADIENT: LOWER=  -0.39  UPPER=  -4.32
-----

```

Table 6.9b

```

1
H + 0 (1)/C + 3 (1) 24 24/AMD= 2.0/AMR= 12.0/FST=Total /ISEL= 1
7.00D-03 1.88D-02 3.74D-02 6.64D-02 2.00D-01 4.00D-01 7.02D-01 1.00D+00
3.00D+00 6.00D+00 1.00D+01 2.00D+01 4.00D+01 6.00D+01 9.98D+01 1.60D+02
2.40D+02 5.00D+02 9.80D+02 2.00D+03 8.00D+03 2.00D+04 8.00D+04 4.00D+05
*EQUAL** 7.00D-03 1.88D-02 3.74D-02 6.64D-02 2.00D-01 4.00D-01 7.02D-01
1.00D+00 3.00D+00 6.00D+00 1.00D+01 2.00D+01 4.00D+01 6.00D+01 9.98D+01
1.60D+02 2.40D+02 5.00D+02 9.80D+02 2.00D+03 8.00D+03 2.00D+04 8.00D+04
4.00D+05
1.90D-09 1.90D-09 1.96D-09 1.96D-09 2.03D-09 2.22D-09 2.51D-09 2.72D-09
2.86D-09 3.52D-09 4.02D-09 4.49D-09 5.23D-09 6.47D-09 7.27D-09 8.75D-09
1.06D-08 1.32D-08 2.07D-08 3.42D-08 6.08D-08 1.66D-07 2.47D-07 2.02D-07
6.31D-08
1.97D-09 1.94D-09 1.97D-09 1.97D-09 2.02D-09 2.23D-09 2.51D-09 2.72D-09
2.86D-09 3.52D-09 4.02D-09 4.49D-09 5.23D-09 6.47D-09 7.27D-09 8.75D-09
1.06D-08 1.32D-08 2.07D-08 3.42D-08 6.08D-08 1.66D-07 2.47D-07 2.02D-07
6.31D-08
1.84D-07 2.16D-07 2.16D-07 2.16D-07 2.16D-07 2.16D-07 2.16D-07 2.16D-07
2.16D-07 2.16D-07 2.17D-07 2.17D-07 2.17D-07 2.17D-07 2.17D-07 2.17D-07
2.18D-07 2.18D-07 2.20D-07 2.23D-07 2.29D-07 2.53D-07 2.64D-07 1.84D-07
5.16D-08
4.06D-08 2.24D-07 2.24D-07 2.24D-07 2.24D-07 2.24D-07 2.24D-07 2.24D-07
2.24D-07 2.24D-07 2.24D-07 2.24D-07 2.24D-07 2.24D-07 2.23D-07
2.23D-07 2.23D-07 2.22D-07 2.21D-07 2.19D-07 2.09D-07 1.93D-07 1.32D-07
4.06D-08
-----
C THERMAL CHARGE EXCHANGE RATE COEFFICIENT SOURCE LIST
C
C ISEL DONOR RECEIVER FINAL STATE SOURCE
C -----
C 1 H + 0 (1) C + 3 (1) Total /packages/adas/adas/adf24/scx#h0/scx#h0_cfm#c3.dat
C
C
C Processing code: ADAS509
C Producer:
C Date: 18/03/99
C
C
-----

```

Notes: