## ADAS405: Equilibrium ionisation - process metastable populations and emission functions

The program calculates the fractional abundances of resolved metastable or unresolved stage populations of the ions of an element in equilibrium in a thermal plasma. It also evaluates the radiated power function and line emission contribution functions $\left(G\left(T_{e}\right)\right)$. The evaluation of emission functions (and ratios of emission functions between lines os possibly different ions of the same element) is controlled by a 'script file'. This specifies the composition of the lines required.

## Background theory:

## The unresolved case:

Consider the evolution of populations of ions of an element in a plasma. For an element $X$ of nuclear charge $z_{0}$, the populations of the ionisation stages are denoted by

$$
N^{(z)}: z=0, \ldots, z_{0}
$$

The time dependence of the ionisation stage populations is given by the equations

$$
\begin{align*}
d / d t N^{(z)}= & N_{e} S_{C D}^{(z-1 \rightarrow z)} N^{(z-1)} \\
& -\left(N_{e} S_{C D}^{(z \rightarrow z+1)}+N_{e} \alpha_{C D}^{(z \rightarrow z-1)}+N_{H} C_{C D, \rho \rightarrow \rho^{\prime}}^{(z \rightarrow z-1)}\right) N^{(z)} \\
& +N_{e} \alpha_{C D}^{(z+1 \rightarrow z)} N^{(z+1)}+N_{H} C_{C D}^{(z+1 \rightarrow z)} N^{(z+1)}
\end{align*}
$$

This is called an unresolved or stage to stage picture. The coefficients are the (ordinary) collisional radiative coefficients. In equilibrium ionisation balance, the time derivatives are set to zero and the stage populations are the solutions of the matrix equation
$N_{e}\left[\begin{array}{cccc}-S_{C D}^{(0 \rightarrow 1)} & \alpha_{C D}^{(1 \rightarrow 0)}+\left(N_{H} / N_{e}\right) C_{C D}^{(1 \rightarrow 0)} & 0 & 0 \\ S_{C D}^{(0 \rightarrow 1)} & -\left(S_{C D}^{(1 \rightarrow 2)}+\alpha_{C D}^{(1 \rightarrow 0)}+\left(N_{H} / N_{e}\right) C_{C D}^{(1 \rightarrow 0)}\right) & \alpha_{C D}^{(1 \rightarrow 0)} & 0 \\ 0 & S_{C D}^{(1 \rightarrow 2)} & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot\end{array}\right]\left[\begin{array}{c}N^{(0)} \\ N^{(1)} \\ N^{(2)} \\ \cdot\end{array}\right]=0$
subject to the normalisation

$$
N_{t o t}=\sum_{z=0}^{z_{0}} N^{(z)}
$$

where $N_{\text {tot }}$ is the number density of ions of element $X$ in any ionisation stage. The equilibrium fractional abundances $N^{(z)} / N_{\text {tot }}$ at a set of temperatures and densities are sought. The code accesses standard isonuclear master file data of type ADF11 to obtain the coefficients of equations 5.5.3. In practical solution of the equations, note must be taken of the very small fractions which can obtain for ionisation stages distant from the dominant ionisation stage at a given temperature and density. Therefore the progressive elimination algorithm for the triagonal matrix equations is performed towards the dominant ionisation stage from both the neutral and fully ionised stages to avoid overflows rather than the usual 'single pass'.
From the equilibrium stage population solution, the total radiated power function $P_{t o t}$, is calculated as

$$
\begin{align*}
P_{t o t} & =\sum_{z=0}^{z_{0}} P^{(z)}\left(N^{(z)} / N_{t o t}\right) \\
& =\sum_{z=0}^{z_{0}}\left[P_{L T}^{(z)}+P_{R B}^{(z)}+\left(N_{H} / N_{e}\right) P_{R C}^{(z)}\right]\left(N^{(z)} / N_{t o t}\right)
\end{align*}
$$

with separate radiated power coefficient $\left(P^{(z)}\right)$ contributions arising from low level line power, recombination-bremsstrahlung-cascade power and charge exchange recombination power. Also contribution functions to line emission known as $G\left(T_{e}\right)$ functions may be evaluated for arbitrary lines as

$$
\begin{align*}
G_{i \rightarrow j}^{(z)}= & {\left[\varepsilon_{i \rightarrow j}^{e x c} N^{(z)}+\varepsilon_{i \rightarrow j}^{r e c} N^{(z+1)}\right.} \\
& \left.+\left(N_{H} / N_{e}\right) \varepsilon_{i \rightarrow j}^{C X} N^{(z+1)}\right] / N_{t o t}
\end{align*}
$$

The $\varepsilon_{i \rightarrow j}$ are called photon emissivity coefficients (c.f. $\mathscr{P} \mathscr{C} \mathscr{C}$ coefficients in the metastable resolved case - see the descriptions of ADAS503 and ADAS208 in the last chapter) They occur in independent parts $\varepsilon_{i \rightarrow j}^{e x c}, \varepsilon_{i \rightarrow j}^{\text {rec }}$ and $\varepsilon_{i \rightarrow j}^{C X}$, distinguished by the driving process.

## The resolved case:

Properly, although the populations of excited states may be neglected compared with those of metastable and ground states of ions, it is not correct to combine the ground and metastable populations into a single stage population in the time dependent equations. This is because ground and metastable populations may have comparable populations and evolve on similar timescales. The ground and metastable populations

$$
N_{\rho}^{(z)}: z=0, \ldots, z_{0} ; \rho=1, \ldots, M_{z}
$$

where $M_{z}$ is the number of metastable states (including the ground state) of ionisation stage $z$, should be treated separately The time dependence of the metastable populations is then given by the equations

$$
\begin{aligned}
d / d t N_{\rho}^{(z)} & =N_{e} \sum_{\rho^{\prime}=1}^{M_{z-1}} S_{C D, \rho^{\prime} \rightarrow \rho}^{(z-1 \rightarrow z)} N_{\rho^{\prime}}^{(z-1)} \\
& -\left(N_{e} \sum_{\rho^{\prime \prime}=1}^{M_{z+1}} S_{C D, \rho \rightarrow \rho^{\prime \prime}}^{(z \rightarrow z+1)}+N_{e} \sum_{\rho^{\prime}=1}^{M_{z-1}} \alpha_{C D, \rho \rightarrow \rho^{\prime}}^{(z \rightarrow z-1)}+N_{H} \sum_{\rho^{\prime}=1}^{M_{z-1}} C_{C D, \rho \rightarrow \rho^{\prime}}^{(z \rightarrow z-1)}\right. \\
& \left.+N_{e} \sum_{\sigma=1}^{M} Q_{C D, \rho \rightarrow \sigma}^{(z \rightarrow z)}+N_{e} \sum_{\rho^{\prime}=1}^{M_{z}} X_{C D, \rho \rightarrow \sigma}^{(z \rightarrow z)}\right) N_{\rho}^{(z)} \\
& +N_{e} \sum_{\rho^{\prime \prime}=1}^{M_{z+1}} \alpha_{C D, \rho^{\prime \prime} \rightarrow \rho}^{(z+1 \rightarrow z)} N_{\rho^{\prime}}^{(z+1)}+N_{H} \sum_{\rho^{\prime \prime}=1}^{M_{z+1}} C_{C D, \rho^{\prime \prime} \rightarrow \rho}^{(z+1 \rightarrow z)} N_{\rho^{\prime \prime}}^{(z+1)} \\
& +N_{e} \sum_{\sigma=1}^{M_{z}} Q_{C D, \sigma \rightarrow \rho}^{(z \rightarrow z)} N_{\sigma}^{(z)}+N_{e} \sum_{\sigma=1}^{M_{z}} X_{C D, \sigma \rightarrow \rho}^{(z \rightarrow z)} N_{\sigma}^{(z)}
\end{aligned}
$$

5.5.8
where there is such an equation for each $z$ and $\rho$. This is called a resolved or generalised picture. The coefficients are the generalised collisional radiative coefficients. In equilibrium ionisation balance, the time derivatives are set to zero and the metastable populations are the solutions of the partitioned matrix equations

$$
N_{e}\left[\begin{array}{cccc}
-\mathbf{S}_{C D}^{(0)} & \mathbf{a}_{C D}^{(1 \rightarrow 0)}+\left(N_{H} / N_{e}\right) \mathbf{C}_{C D}^{(1 \rightarrow 0)} & 0 & 0 \\
\mathbf{S}_{C D}^{(0 \rightarrow 1)} & -\left(\mathbf{S}_{C D}^{(1)}+\mathbf{Q}_{C D}^{(1 \rightarrow 1)}+\mathbf{X}_{C D}^{(1 \rightarrow 1)}+\mathbf{a}_{C D}^{(1)}+\left(N_{H} / N_{e}\right) \mathbf{C}_{C D}^{(1)}\right) & \mathbf{a}_{C D}^{(2 \rightarrow 1)}+\left(N_{H} / N_{e}\right) \mathbf{C}_{C D}^{(2 \rightarrow 1)} & 0 \\
0 & \mathbf{S}_{C D}^{(1 \rightarrow 2)} & \cdot & \cdot \\
0 & 0 & \cdot & \cdot
\end{array}\right]\left[\begin{array}{l}
\mathbf{N}^{(0)} \\
\mathbf{N}^{(1)} \\
\mathbf{N}^{(2)} \\
\cdot
\end{array}\right]=0
$$

which must be interpreted for the metastable resolved case. Each element of the matrix in eqns. 5.5.9 is now itself a matrix extending over the metastable sets of the ionisation stage involved. Thus

$$
\mathbf{S}_{C D}^{(0 \rightarrow 1)}=\left[\begin{array}{cccc}
. & \cdot & \cdot & \cdot \\
. & S_{C D, \rho-1 \rightarrow \sigma-1}^{(0 \rightarrow 1)} & S_{C D, \rho-1 \rightarrow \sigma}^{(0 \rightarrow 1)} & \cdot \\
. & S_{C D, \rho \rightarrow \sigma-1}^{(0 \rightarrow \rightarrow 1)} & S_{C D, \rho \rightarrow \sigma}^{(0 \rightarrow 1)} & \cdot \\
. & \cdot & \cdot & \cdot
\end{array}\right]
$$

and

$$
\mathbf{S}_{C D}^{(0)}=\left[\begin{array}{cccc}
\cdot & \cdot & \cdot & \cdot \\
\cdot & \sum_{\sigma=1}^{M_{1}} S_{C D, \rho-1 \rightarrow \sigma}^{(0 \rightarrow 1)} & 0 & \cdot \\
\cdot & 0 & \sum_{\sigma=1}^{M_{1}} S_{C D, \rho \rightarrow \sigma}^{(0 \rightarrow 1)} & \cdot \\
\cdot & \cdot & \cdot & \cdot
\end{array}\right]
$$

where the index $\rho: 1, \ldots, M_{0}$ spans the metastables of stage 0 and $\sigma: 1, \ldots, M_{1}$ spans the metastables of stage 1. Also

$$
\mathbf{Q}_{C D}^{(1 \rightarrow 1)}=\left[\begin{array}{cccc}
. & \cdot & \cdot & \cdot \\
\cdot & -\sum_{\rho^{\prime}=1 ; \rho^{\prime} \neq \rho-1}^{M_{1}} Q_{C D, \rho^{\prime} \rightarrow \sigma-1}^{(1 \rightarrow 1)} & Q_{C D, \rho-1 \rightarrow \sigma}^{(1 \rightarrow 1)} & \cdot \\
. & Q_{C D, \rho \rightarrow \sigma-1}^{(1 \rightarrow 1)} & -\sum_{\rho^{\prime}=1 ; \rho^{\prime} \neq \rho}^{M_{1}} Q_{C D, \rho^{\prime} \rightarrow \sigma}^{(1 \rightarrow 1)} & \cdot \\
& & \cdot & \cdot
\end{array}\right]
$$

Similar definitions apply for the $\mathbf{a}_{C D}^{(1 \rightarrow 0)}, \mathbf{X}_{C D}^{(1 \rightarrow 1)}$ etc. Also the population vector is

$$
\mathbf{N}^{(0)}=\left[\begin{array}{c}
N_{1}^{(0)} \\
\cdot \\
\cdot \\
N_{M_{0}}^{(0)}
\end{array}\right]
$$

and the normalisation

$$
N_{t o t}=\sum_{z=0}^{z_{0}} \sum_{\rho=1}^{M_{z}} N_{\rho}^{(z)}
$$

The equilibrium fractional abundances $N_{\rho}^{(z)} / N_{\text {tot }}$ at a set of temperatures and densities are sought. The code accesses partial isonuclear master file data of type ADF11 to obtain the coefficients of the equations 5.5.9. Practical solution in the resolved case is achieved by an equivalent method to the unresolved case but with matrix operations replacing the scalar operations.
From the population solution, the total radiated power function is calculated as

$$
P_{\text {tot }}=\sum_{z=0}^{z_{0}} \sum_{\rho=1}^{M_{z}}\left[P_{L T, \rho}^{(z)}+P_{R B, \rho}^{(z)}+\left(N_{H} / N_{e}\right) P_{R C, \rho}^{(z)}\right]\left(N_{\rho}^{(z)} / N_{t o t}\right)
$$

with contributions arising from low level line power, recombination-bremsstrahlungcascade power and charge exchange recombination power. Also contribution functions to line emission known as $\mathrm{G}\left(\mathrm{T}_{\mathrm{e}}\right)$ functions may be evaluated for arbitrary lines as

$$
\begin{align*}
G_{i \rightarrow j}^{(z)}= & {\left[\sum_{\rho=1}^{M_{i}} \mathscr{P} \mathscr{E} \mathscr{C}_{\rho, i \rightarrow j}^{(e x c)} N_{\rho}^{(z)}+\sum_{v^{\prime}=1}^{M_{z+1}} \mathscr{P} \mathscr{E} \mathscr{C}_{v^{\prime}, i \rightarrow j}^{(r e c)} N_{\rho^{\prime}}^{(z+1)}\right.} \\
& \left.+\left(N_{H} / N_{e}\right) \sum_{v^{\prime}=1}^{M_{z+1}} \mathscr{P} \mathscr{E} \mathscr{C} \mathscr{V}_{v^{\prime}, i \rightarrow j}^{(C X)} N_{\rho^{\prime}}^{(z+1)}\right] / N_{\text {tot }}
\end{align*}
$$

(c.f. the description of ADAS208 in the last chpater of this manual). In practice, there may be very many choices of $G\left(T_{e}\right)$ functions of interest.

## Program steps:

These are summarised in figure 5.5.
Figure 5.5


## Interactive parameter comments:

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

The file selection window appears first as illustrated below

1. Two types of data file are identified in the file selection, namely, the isonuclear master files required for the ionisation balance and power calculations and the script file. The top part of the file selection window is concerned with identifying the master file data required and the lower part with identifying the script file.
2. Click on the Select button to drop down a selection list of master file data classes. Activate the buttons at the data classes required for your analysis. It is obligatory to select the ' $a c d$ ' and ' $s c d$ ' electron impact effective recombination and ionisation data classes since otherwise an ionisation balance cannot proceed. However the other data classes selected are at the user's choice. This enables investigative studies of the importance of different contributions for example to radiated power.
3. Effective radiated power coefficients ('prb', 'plt' and 'prc') are often made available both as the whole emitted power and as the power which would pass through certain filters (such as $\mathrm{Be} / \mathrm{Si}$ windows). The filter is specified either simply as an energy cut-off (eg. ev2000) or as filter specification (eg. ft1235). These codes appear as an extension in the relevant master file names. Specify the filter choice.
4. Some flexibility for subdivision within a data year is provided by allowing a two character 'member prefix' (eg. 'pj') which may be present in the final part of a file name (eg. ‘/../acd93r/acd93r_pj\#c.dat').
5. Select the directory branch, that is the central ADAS or user data area.
6. Select the year of data. In general the two digit year number is used to provide the main groupings of data. Thus ' 89 ' is the standard, unresolved, JET base line data of low precision but fairly complete. ' 93 ' is metastable resolved data, but available only for light elements of primary importance to fusion. Note that a default year must be specified. Often the complete set of
data classes for a particular year and type are not available and the capability of filling in from a default (perhaps less accurate but more complete) year is allowed.
7. Specify the element.

8. Specify the type of master file. The distinctions between standard and partial master file types and resolved and unresolved types must be clarified. Standard data is stage to stage and has a specific layout. Partial data distinguishes metastables and has a different layout.
9. Within the partial data layout specify the partial type. .It is possible simply to have each stage represented only by its ground state and therefore to be similar to standard data. However the layout is the partial one. We call such data partial but unresolved. The usual partial data with metastables present is called resolved. This distinction and added flexibility are helpful in iso-nuclear master file preparation and archiving.
10. Clicking the Display data set availability button at causes display of a file availability summary window as illustrated below. It is important to use this facility since it shows which master files classes sought by the user were not available, where default data files were substituted etc.

11. A script file selection may be made. The structure of script file is shown below. We have found it convenient to group script files in a personal ADAS database under a subdirectory classification /scripts $405 /$. Also, it is possible to bypass contribution function calculation and display by selecting the ' $N U L L$ ' script. You may find it helpful to copy the ' $N U L L$ ' script from the central ADAS database to your own space. Note that scripts apply to particular cases. Thus the references to emissivity coefficient data in a script applying to metastable resolved will not in general work for unresolved data, indeed will probably crash. We have not built much protection against faulty references into script files at the moment. More protection may be added if this proves a stumbling point for users. You may find it helpful to fetch the test_c script from central ADAS for first trials.

A script file is illustrated below. Details of the species, number of (composite) lines and line ratios to be obtained are at the head of the file (SPECIES, NLINE, NRATIO). Note that you must follow the positional layout exactly. Emissivity coefficient data are obtained from 'pec' files of ADAS format ADF15. The number of such files to be searched in the ADAS database are specified at NFILE and the full Unix paths to the files themselves in following lines at PHOTON EMISSIVITY FILE NAMES. The subsequent table identifies the index number of the pecs in these files required to build the particular line emission function. The lines are indexed at ILINE, the number of component parts of each line is at NCOMP, the charge of the ion to which the component attaches is at IZION and the components simply indexed at ICOMP. The metastable of the ion to which the component is attached is specified by its ranked index number at IMET (the ground state is 1). INDPH gives the selection index of the component pec in the ADF15 file identified at IFILE from the list given earlier. Note the letter qualification on the INDPH index to distinguish electron collision driven pecs and charge exchange driven pecs. The composite lines may be ratioed as specified by IRATIO, an index number of the ratio; ILINE, the upper composite line of the ratio; JLINE, the lower composite line of the ratio. All other text is for information. Note that a 'c------' line is used to separate comments which follow it. Each comment line begins with ' $c$ ' and we conventionally put in a 'c-----' terminator line for the comments section.


The processing options window has the appearance shown below

1. The script file selected by the user is identified. The Browse Comments button displays the comments field at the foot of the script file.
2. Information is presented of the element and master files classes selected in the previous file selection option step.
3. Enter isotope mass numbers for the selected element and background neutral hydrogen in the plasma. This information is only used if charge exchange recombination master file data has been selected.
4. The spectrum lines set up in the script file are shown in the display window. This operates in the same manner as dataset display and selection windows in the input option window of a code such as ADAS205 (see chapter 2). Click on a line to select it. The selected line is shown in the selection window above the display window. Only one line is treated at a time for graphical display. However all lines and line ratios in the script file are computed and tabulated in the output text file.
5. Select temperature and density pairs for data output. The table may be edited by clicking on the Edit Table button.. The ADAS Table Editor window is then presented with the same set of editing operations available as are described in the introductory chapter. Electron temperatures should be monotonic increasing. It has proved helpful to add a Clear Table button to remove all entries in the temperature and density output fields.
6. 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. It follows the usual pattern except that there is a choice of graphs to display. Thus the fractional abundances, power functions and contribution functions are all of potential interest. Click on the appropriate button. Generally, we find that on the first one or two occasions we wish to see the fractional abundances and powers but then have a more sustained interested in the contribution function shapes and their location in temperature. All the graphs are provided as a function of electron temperature.
2. The sub-window presented depends on the graph choice above. The default scaling may be over-ridden and explicit values for the graph limits entered.
3. Graphical output may enabled in the window together with hard copy device and output file name. This follows the pattern of other ADAS programs. Likewise text output selection is standard.
4. The 'GCF Passing File' is the name used for the output dataset of calculated contribution functions. It is organised according to an ADAS data format ADF16. The widget is active only if a non NULL script file has been selected on input Specify an output file name. Note that $\mathrm{G}(\mathrm{Te})$ functions of type ADF20 (gft) are organised differently and have a slightly different definition from the output here of generalised contribution functions of type ADF16 ( $g c f$ ). The expected practice is that ADAS405 will be used either recursively or in distinct runs to examine contribution functions and then decide which to put into the $g c f$ file.
5. The Replace and Default file name buttons have their usual meanings.

## ADAS405 OUTPUT OPTIONS

Script file: /afs/@cell/u/adas/adas/scripts405/NULL Browse Comments
$\checkmark$ Graphical output
Graph Title
(- Fractional abundance plot
Power function plot
Contribution function plot

$\checkmark$ Text output $\quad$ Replace Default File Name
File Name : paper.txt


5

The Graphical output window is shown below

1. The graph has at its foot a Done button, and possibly Next and Previous buttons if there is a sequence of graphs to be displayed. A Print and Print all button is also present if the Enable Hard Copy button on the previous window was activated.
2. Press the Next button to show the next graph in a sequence and the Previous button to show the previous graph.
3. Press the Print button to make a hard copy of the currently displayed picture. Print all makes a hard copy of all the pictures.
4. Pressing the Done button restores the previous Output Options window.


## Illustration:

The output from the program is illustrated for carbon in the resolved case. Figure 5.5a shows the equilibrium metastable fractional abundances for the first seven metastables as a function of temperature at a fixed density. The balance is at the electron density $10^{+13} \mathrm{~cm}^{-3}$. Figure 5.5 b shows shows the total equilibrium radiated power function (TOT) for carbon, the separation into recombination + bremsstrahlung power function (PRB) and total line power function (PLT) and the line power function contributions from the last seven metastables states evaluated using the generalised collisional radiative coefficients. Seven curves only are displayed on each graph
Figure 5.5 c shows the equilibrium generalised contribution function for the CI 1561A resonance line. As can be seen from the script file, contributions from each of the four $\mathrm{C}^{+0}$ metastables are included. The contribution function omits the $\mathrm{N}(\mathrm{C}) / \mathrm{N}(\mathrm{H})$ and $\mathrm{N}(\mathrm{H}) / \mathrm{Ne}$ factors usually included in the solar coronal $\mathrm{G}(\mathrm{Te})$ function definition.

Figure 5.5a


Figure 5.5b


Figure 5.5c


Table 5.5a shows the tabular output from the carbon equilibrium ionisation balance. The option to calculate a ratio of contribution functions for two lines is tabulated but is not available graphically. FILTER applies only to radiated power. Isoelectronic master files which include the effect of an energy filter are of two qualities, namely, precisely estimated for a window of specified thicknesses of beryllium and quartz (FT) and secondly a simple sharp energy cut-off (EV). FILTER gives the master file name subfield of the form EV<nnnn> or FT<ll><mm> by which they identified.
Table 5.5a

```
ADAS RELEASE: ADAS98 V2.0 PROGRAM: ADAS405 V1.9 DATE: 28/07/98 TIME: 15:55
************* TABULAR OUTPUT FROM EQUILIBRIUM IONISATION AND EMISSION PROGRAM: ADAS405 - DATE: 28/07/98
***************
------_-----_---------
ELEMENT NAME : CARBON
RESOLUTION : PARTIAL
MASTER FILE SELECTION:
SELECTED YEAR : 93
DEFAULT YEAR : 9
\begin{tabular}{crcc} 
CLASS & TYPE & SELECT & FILTER \\
----- & --- & ------- & ---- \\
ACD & P & S & \\
SCD & P & S & \\
CCD & P & & \\
PRB & P & S & \\
PRC & P & & \\
QCD & P & S & \\
XCD & P & S & \\
PLT & P & S & \\
KEY: & & &
\end{tabular}
SELECT: S=SELECTED, D=DEFAULT, blank= not available
TYPE : P=PARTIAL, S=STANDARD
FILTER: FT=FILTER THICKNESS SPECIFICATION, EV=ENERGY CUT-OFF, blank=no filter
SCRIPT FILE: u/hps/adas/scripts405/test_resolved_c
PHOTON EMISSIVITY COEFFICIENT FILES:
```






## Notes:

