ADAS408: Iso-nuclear master data - prepare from iso-nuclear parameter sets

The program uses parametric forms for zero density recombination, ionisation and radiated power loss coefficients to prepare standard (unresolved, stage to stage) iso-nuclear master files for a particular element. The iso-nuclear master files may be prepared over arbitrary ranges of electron temperature and electron density

Background theory:

The practice in the past in fusion research has been to adopt a substantially simpler and more approximate approach to acquiring the atomic data for plasma models than that which forms the basis of the Atomic Data and Analysis Structure. This is the parametric approximate form approach. It assumes that

1. Simple parametric forms for atomic processes, which apply to any ion of any element, are available.
2. The low density coronal limit may be assumed in all circumstances.
3. Each ionisation stage of an element may be represented by its ground state alone.
4. Each ion may be assumed to experience two effective electron collisional excitations which can be used to represent adequately radiant power losses and dielectronic recombination.

These assumptions and approximations can not be sustained in modern fusion device studies. However the earlier procedures do have the merit of providing atomic data for modelling codes for virtually any element desired (unlike the selective nature of more refined data) as long as too searching questions are not asked. For this reason such data is still widely used. It is necessary that such data can still be generated for comparative purposes and low quality data fill-in. The Atomic Data and Analysis Structure is based on absolute numerical data and interpolation rather than parametric databases, since thereby no data constraint or precision limit is intrinsic to the structure and best available data of whatever type may be used. The ADAS408 code creates data sets of standard iso-nuclear master file organisation from the old parametric forms. The access subroutines to the iso-nuclear master files provided with ADAS allow a seamless switch to the Atomic Data and Analysis Structure with older calculations and assumptions still reproducible.

The following classes of data of standard type are generated:- the collisional-dielectronic recombination coefficient (ACD),the collisional-dielectronic ionisation coefficient (SCD), the collisional-radiative charge exchange recombination coefficient (CCD), the collisional-dielectronic recombination / cascade / bremsstrahlung radiated power coefficient (PRB), the collisional-radiative charge exchange recombination / cascade power coefficient (PRC), the collisional-radiative excitation total line power coefficient (PLT) and the collisional-radiative excitation specific line power coefficient (PLS). However, the data does not constitute true collisional-radiative coefficients. For the various classes, the most prevalent assumptions forced by the parametric forms are summarised below.

Mnemonic	Class simplification	Forms
ACD	zero density radiative + representative dielectronic parent transitions with a finite density cut-off	S
SCD	zero density ground state ionis. coefft.	S
CCD	total zero density coefft.	S
PRB	zero density recom./brems. + two dielectronic transition contributions with simplified energy loss per recombination	S
PRC	zero density with simplified energy loss per recombination.	S
PLT	effective excitations in coronal approximation.	S
PLS	single resonance line in coronal approximation	S

The parametric approximate forms for the above coefficient classes used historically are called here the (A) forms. From the considerations of section 2 of this manual

and provided more accurate numerical data is available, some improvement both of the parametric forms and of the actual values of parameters used may be made. The improved parametric forms, called here the (B) forms are those which provide the basis for comparative assessment of new data is the ADAS series 1 codes. Both (A) and (B) parametric forms are allowed by the ADA407 code. They are as follow:

ACD: the coefficient is composed of a sum of radiative and dielectronic recombination parts

$$\alpha^{(z+1 \to z)}(T_e, N_e) = \alpha_r(T_e, N_e) + \alpha_d(T_e, N_e) \qquad 5.8.1$$

(A) Hydrogenic formulae are used for radiative recombination with Gaunt factors unity. The ground principal quantum shell is adjusted with an effective principal number ν_0 and lowest shell occupancy factor $phfrac$. The Burgess zero density general formula is used for dielectronic recombination including two parent transitions only.

$$\alpha_r = \alpha^H(n_0) + \sum_{n \geq n_0 + 1}^{n_G} \alpha^H(n_0)$$

$$= [2.6^{-14}] z_1 (z_1^2 I_H / kT_e)^{1/2} \{$$

$$\frac{2 \, phfrac}{n_0} (z_1^2 I_H / kT_e n_0^2) EEI(z_1^2 I_H / kT_e n_0^2) \qquad 5.8.2$$

$$+ \sum_{n \geq n_0 + 1}^{n_G} \frac{2}{n} (z_1^2 I_H / kT_e n^2) EEI(z_1^2 I_H / kT_e n^2) \} \quad cm^3 s^{-1}$$

where $z_1 = z + 1$, n_0 is the principal quantum number of the valence shell of the ion of the recombined ion, $phfrac$ is the statistical weight fraction of the valence shell unoccupied before recombination and $EEi(x) = e^x E_1(x)$ with E_1 the first exponential integral. The principal quantum shell sum is terminated at

$$n_G = 126.0 \{ z_1^{12} (kT_e / I_H)(cm^{-6} / N_e^2) \}^{1/17} \qquad 5.8.3$$

The dielectronic recombination part is given by

$$\alpha_d = [4.78^{-11}] (z_1^{1/2} (z_1 + 1)^{5/2} / (z_1^2 + 13.4)^{1/2})$$

$$(I_H / kT_e)^{3/2} D(T_e, N_e) \sum_{j=1}^{2} f_j A(y_j) e^{-\overline{\Delta E_j} / kT_e} \quad cm^3 s^{-1} \qquad 5.8.4$$

where the sum is over at most two parent transitions with oscillator strengths f_j and effective transition energies $\overline{\Delta E_j} = \Delta E_j / a$ with ΔE_j the transition energy and $a = 1.0 + 0.015 \{ z_1^3 / (z_1 + 1)^2 \}$. The factor A and finite density reduction D depend on whether the parent transition is of '$\Delta n = 0$' type

$$D = n_t / (200 + n_t)$$

$$A(y) = y^{1/2} / (1 + 0.105 y + 0.015 y^2) \qquad 5.8.5$$

or of '$\Delta n = 1$' (excluding 1s initial parent states) type

$$D = 0.0015 [(z_1 + 1) n_t]^2 / (1 + 0.0015 [(z_1 + 1) n_t]^2)$$

$$A(y) = y^{1/2} / (2 + 0.41 y + 0.06 y^2) \qquad 5.8.6$$

with

$$n_t = [5.57^{17} (cm^{-3} / N_e) z_1^6 (kT_e / I_H)^{1/2}]^{1/7} \text{ and } y_j = (\Delta E_j / I_H) / (z_1 + 1).$$

(B) The hydrogenic expression for radiative recombination to the lowest principal quantum shell uses the effective principal quantum number ν_0 for the shell and is improved by factors *scale* and *edisp* obtained from improved sources. The density dependent n-shell cut-off is not applied. The dielectronic coefficient is based on the Burgess zero density general formula as for the $\Delta n = 0$ case above, adjusted

to fit improved data with factors $scale_1, edisp_1, scale_2, edisp_2$. An extended set of parent transitions but combined into at most two groups.

$$\alpha_r = scale(z_1^2 I_H / kT_e v_0^2)^{edisp} \alpha^H(v_0) + \sum_{n \geq n_0 + 1} \alpha^H(n_n) \qquad 5.8.7$$

$$\alpha_d = scale_1 \exp(-edisp_1 / akT_e) D(T_e, N_e) \sum_{i_1 \in grp_1} \alpha^{GF}(g \to i_1)$$

$$+ scale_2 \exp(-edisp_2 / akT_e) D(T_e, N_e) \sum_{i_2 \in grp_2} \alpha^{GF}(g \to i_2) \qquad 5.8.8$$

SCD: The coefficient is a zero density coefficient from the ground state of the ion obtained as a sum over contributing shells. It may include direct ionisation (*shd*) or excitation auto-ionisation (*excit*)

$$S^{(z \to z+1)}(T_e) = S_{shd}^{approx}(T_e) + S_{excit}^{approx}(T_e) \qquad 5.8.9$$

(A) The expressions of Lotz are used for direct ionisation. Only two shells are allowed and there is no excitation auto-ionisation part.

$$S_{shd}^{approx}(T_e) = \sum_{i=1,2} S^{LOTZ}(z, \chi_i, \zeta_i, T_e) \qquad 5.8.10$$

where

$$S_{shd}^{Lotz} = 1.42^{-6}(I_H / kT_e)^{3/2} a \zeta [E_1(\chi / kT_e) / (\chi / kT_e)$$
$$- be^c E_1(\chi / kT_e + c) / (\chi / kT_e + c)] \quad cm^3 s^{-1} \qquad 5.8.11$$

The a, b, c are constants given for each shell, ζ is the number of equivalent electrons in the shell and χ is the ionisation energy of the shell.

(B) The expressions of Burgess & Chidichimo are used together with a contribution from excitation / auto-ionisation.

$$S_{shd}^{approx}(T_e) = \sum_I c_I \sum_{i \in I} S^{BCHID}(z, \chi_i, \zeta_i, T_e) \qquad 5.8.12$$

where

$$S^{BCHID} = 2.1715^{-8} c \zeta (I_H / \chi)^{3/2} (\chi / kT_e)^{1/2}$$
$$E_1(\chi / kT_e) w \quad cm^3 s^{-1} \qquad 5.8.13$$

with

$$w = \{\ln(1.0 + kT_e / \chi)\}^{\beta/(1.0 + kT_e/\chi)}$$
$$\beta = 0.25[\{(100z + 91)/(4z + 3)\}^{1/2} - 5] \qquad 5.8.14$$

and

$$S_{excit}^{approx}(T_e) = \sum_R c_R \sum_{r \in R} 1.45 \, WT_r \, (I_H / \Delta E_r)(I_H / \varepsilon) \pi a_0^2 \qquad 5.8.15$$

CCD: Only charge transfer from neutral hydrogen in its ground state is included. The total charge exchange cross-section is used at a mean hydrogen collision speed to obtain the rate coefficient.

(A) A constant cross-section for total charge transfer is used except for the ions of carbon, nitrogen and oxygen

$$\alpha_{CX}^{(z+1 \to z)}(T_i) = 3.07^{-9}((kT_i / I_H)(m_H / m_i))^{1/2} z_1^{1.07} \quad cm^3 s^{-1} \qquad 5.8.16$$

(B) There is no separate expression

$$\alpha_{CX}^{(z+1 \to z)}(T_i) = 3.07^{-9}((kT_i / I_H)(m_H / m_i))^{1/2} z_1^{1.07} \quad cm^3 s^{-1} \qquad 5.8.17$$

PRB: The power coefficient is a zero density coefficient obtained as a sum of radiative recombination, dielectronic recombination and bremsstrahlung parts

(A) A radiative recombination is assumed to release energy equal to ground state ionisation energy of the recombined ion. Dielectronic recombination energy loss

is summed over the two parent transitions and each is assumed to release an energy equal to the parent transition energy together with the ionisation energy of the ground state of the recombined ion. Bremsstrahlung is taken to be hydrogenic with free-free Gaunt factor set to unity.

$$P_{RB}^{(z+1\to z)} = 1.6^{-19}\{\alpha_r^{(z+1\to z)}\,\chi + \sum_{j=1}^{2}[\alpha_d^{(z+1\to z)}(\Delta E_j + \chi)])\}$$

$$+5.68^{-32}z_1^2(kT_e/I_H)\quad Wcm^3$$

.5.8.18

(B) A radiative recombination is assumed to release energy equal to ground state ionisation energy of the recombined ion. Dielectronic recombination energy loss is summed over the two parent transitions and each is assumed to release an energy equal to the parent transition energy together with the ionisation energy of the ground state of the recombined ion. Bremsstrahlung is taken to be hydrogenic with free-free Gaunt factor set to unity.

$$P_{RB}^{(z+1\to z)} = 1.6^{-19}\{\alpha_r^{(z+1\to z)}\,\chi + \sum_{j=1}^{2}[\alpha_d^{(z+1\to z)}(\Delta E_j + \chi)])\}$$

$$+5.68^{-32}z_1^2(kT_e/I_H)\quad Wcm^3$$

5.8.19

PRC: The coefficient is a zero density coefficient based on the total charge exchange recombination coefficient

(A) A recombination is assumed to release an amount of energy equal to the ionisation energy of the ground state of the recombined ion..

$$P_{RC}^{(z+1\to z)}(T_e) = 1.60^{-19}\chi\,\alpha_{CX}^{(z+1\to z)}(T_e)\quad Wcm^3$$

5.8.20

(B) There is no separate expression

$$P_{RC}^{(z+1\to z)}(T_e) = 1.60^{-19}\chi\,\alpha_{CX}^{(z+1\to z)}(T_e)\quad Wcm^3$$

5.8.21

PLT: The coefficient is a zero density coefficient obtained by assuming a coronal picture and represented by effective collisional excitations from the ground state of the ion.

(A) A $\overline{g}$ dipole approximation is assumed, specified by an oscillator strength and a constant effective Gaunt factor

$$P_{LT}^{(z)}(T_e) = \sum_{j=1}^{2}\Delta E_j q_{g\to j}^{(e)}(T_e)$$

5.8.22

where

$$\Delta E_j q_{g\to j}^{(e)} = 2.18^{-18}(\Delta E_j/I_H)4.28^{-6}(I_H/kT_e)^{1/2}$$

$$(I_H/\Delta E_j)f_j\overline{g}_j e^{-\Delta E_j/kT_e}\quad Wcm^3$$

5.8.23

(B) Similar expressions are used but with the $\overline{g}$ replaced with the $P(\Delta E/kT_e)$ of Van Regemorter. The expressions are based on two effective transitions with mean transition energies and oscillator strengths. Multipliers c_j are chosen to optimise the fit to best available data at one temperature

$$P_{LT}^{(z)}(T_e) = \sum_{j=1}^{2}c_j\overline{\Delta E}_j\overline{q}_{g\to j}^{(e)}(T_e)$$

5.8.24

where

$$\overline{\Delta E}_j\overline{q}_{g\to j}^{(e)} = 2.18^{-18}(\overline{\Delta E}_j/I_H)4.28^{-6}(I_H/kT_e)^{1/2}$$

$$(I_H/\overline{\Delta E}_j)\overline{f}_j P(\overline{\Delta E}_j/kT)e^{-\overline{\Delta E}_j/kT_e}\quad Wcm^3$$

5.8.25

PLS: The coefficient is a zero density coefficient for the power in a resonance line excited from the ground state of the ion.

(A) A $\overline{g}$ dipole approximation is assumed, specified by an oscillator strength and a constant effective Gaunt factor

$$P_{LS}^{(z)}(T_e) = \Delta E \, q^{(e)}(T_e) \qquad\qquad 5.8.26$$

where

$$\Delta E \, q^{(e)} = 2.18^{-18}(\Delta E / I_H) 4.28^{-6}(I_H / kT_e)^{1/2}$$
$$(I_H / \Delta E) f \overline{g} e^{-\Delta E / kT_e} \quad Wcm^3 \qquad\qquad 5.8.27$$

(B) A similar expression is used but with the $\overline{g}$ replaced with the $P(\Delta E / kT_e)$ of Van Regemorter. The expression is based on an effective dipole excitation with the transition energy and oscillator strength specified. A multiplier c is chosen to optimise the fit to best available data at one temperature

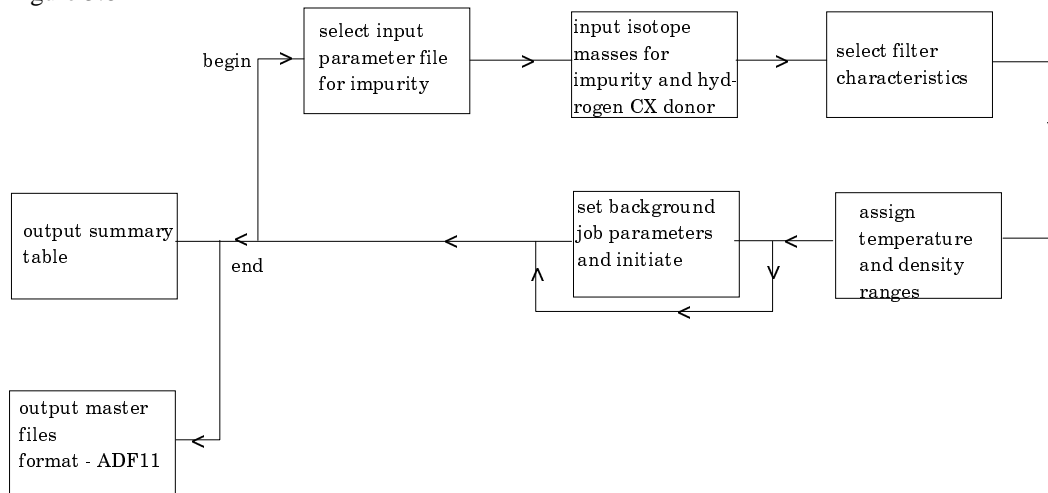$$P_{LS}^{(z)}(T_e) = c \, \Delta E \, q^{(e)}(T_e) \qquad\qquad 5.8.28$$

where

$$\Delta E \, q^{(e)} = 2.18^{-18}(\Delta E / I_H) 4.28^{-6}(I_H / kT_e)^{1/2}$$
$$(I_H / \Delta E) f \, P(\Delta E / kT) e^{-\overline{\Delta E}_j / kT_e} \quad Wcm^3 \qquad\qquad 5.8.29$$

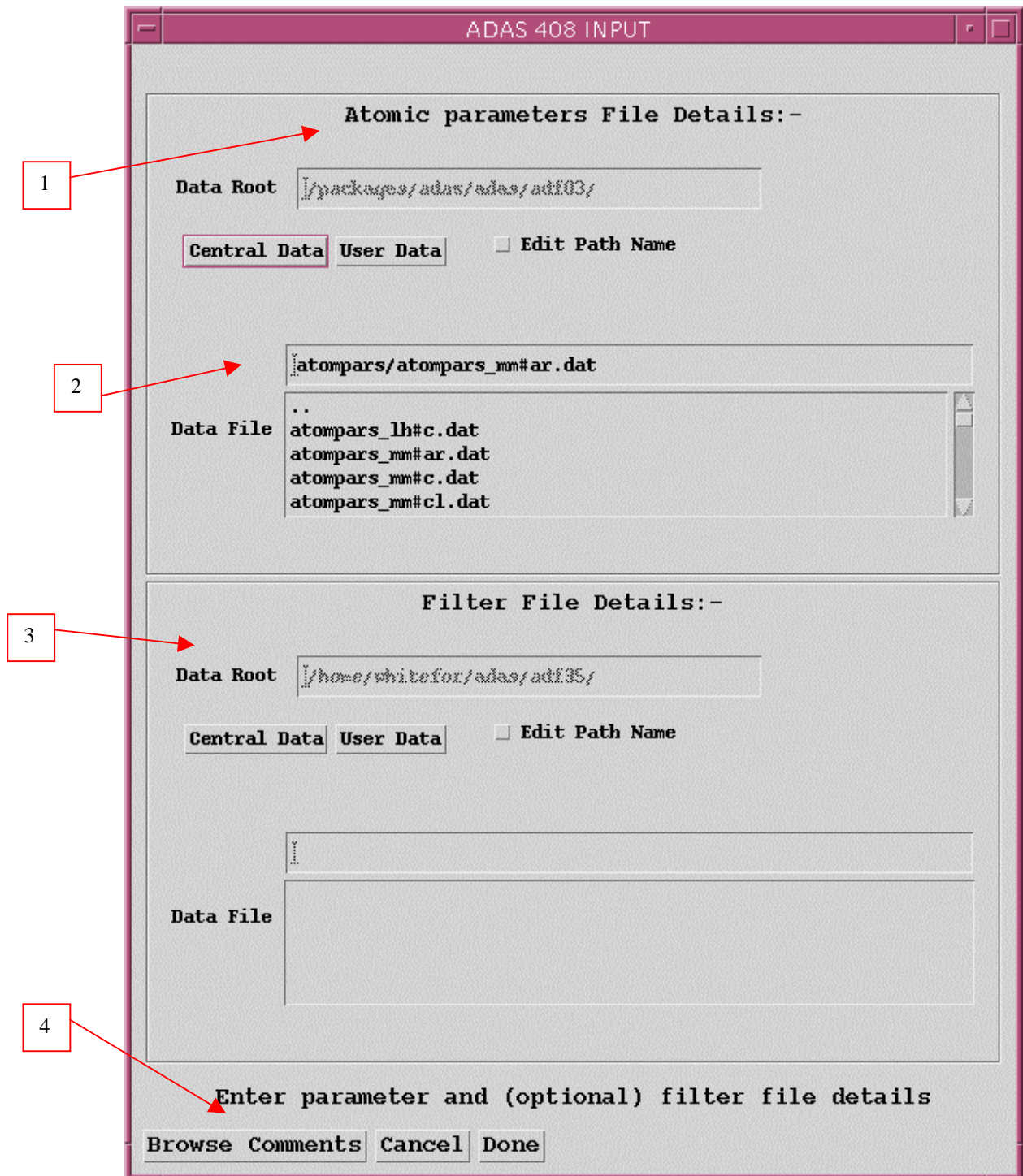## Program steps:

These are summarised in figure 5.8.

Figure 5.8

Interactive parameter comments:

The program uses parametric forms for zero density recombination, ionisation and radiated power loss coefficients, type *adf03*, to prepare standard (unresolved, stage to stage) iso-nuclear master files for a particular element of type *adf11*. The iso-nuclear master files may be prepared over arbitrary ranges of electron temperature and electron density.

The **file selection window** is shown below:

ADAS 408 INPUT

Atomic parameters File Details:-

1

Data Root /packages/adas/adas/adf03/

[Central Data] [User Data] ☐ **Edit Path Name**

2

atompars/atompars_mm#ar.dat

Data File
..
atompars_lh#c.dat
atompars_mm#ar.dat
atompars_mm#c.dat
atompars_mm#cl.dat

Filter File Details:-

3

Data Root /home/whitefor/adas/adf35/

[Central Data] [User Data] ☐ **Edit Path Name**

Data File

4

Enter parameter and (optional) filter file details

[Browse Comments] [Cancel] [Done]

1. Data root 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. The appropriate ADAS data format for input to this program is *adf03* ('atompars files'). 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. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.

2. Available sub-directories are shown in the large file display window. Click on a name to select it. The selected name appears in the smaller selection window 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*.

3. A second file may be selected which specifies a spectral filtration to be applied to the radiated power. Filter files are archived in format *adf35* and can be prepared and interrogated using the codes ADAS414 and ADAS415 respectively.

4. Once the data file is selected, the set of buttons at the bottom of the main window become active. Clicking on the *Browse Comments* button displays any information stored with the selected data-set. 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
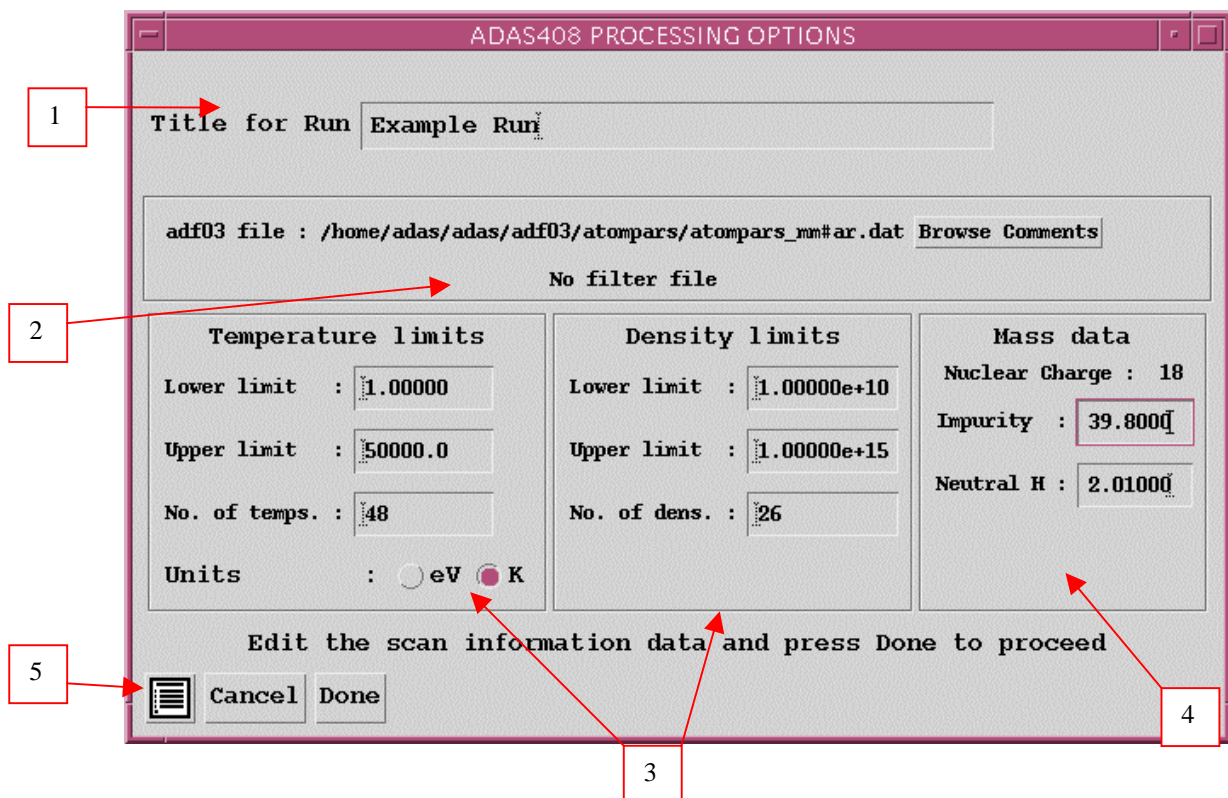
1. At the top of the window, an arbitrary title may be given for the case being processed.

2. The name of the data file under analysis and any filter file being used are shown. The button *Browse Comments* allows display of the information field section at the foot of the named atompars file, if it exists.

3. The lower sub-windows allow the plasma electron temperature and electron density for production of the output *adf11* standard master files to be specified. Select on the required temperature units. This choice determines to the units used in the adjacent temperature range selection window. Specify lower temperature limit, upper temperature limit and number of temperatures in the editable boxes. ADAS408 then creates the temperature grid equally spaced in the logarithm. Note that the output files in fact contain the temperatures in eV (see the ADAS User Manual, appxb-11). Similarly specify the electron density limits and number of grid points.

4. Enter the mass number for the actual isotope of the element required. For information the element chemical symbol is displayed. Also, the mass number of hydrogen isotope constituting the primary plasma species is required.

5. The *Exit to Menu* icon is present in ADAS408. 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 of restricted form. It only offers the option of an output files. There is no output graph.

1. The *adf11* iso-nuclear master file output comprises several. The template shows the file naming structure
2. Collections of *adf11* files are held by year number and element. Enter a two digit year number for the output. Note that any two digits are acceptable and 'fictitious' years can be used for special collections if so desired. The element name is inserted automatically from the atompars input file.
3. The filter name field of the template is only sensitised if a filter file has been selected on input. The convention in the past was that in the simple cut-off case, the filter name had the prefix 'ev' followed by the numerical value of the cut-off energy in eV. In the true filter case (which was restricted to beryllium/silicon, the filter name had the prefix 'ft' followed by the first two

significant figures of the beryllium and silicon thicknesses. The much greater flexibility of the full Henke filter implementation is not encompassed by the old convention. Filter names are at your own choice although central ADAS will continue to have *adf11* data following the old naming. Note also that the output files can be placed in a directory of your choice rather than entering the pass directory.

4. Click on the buttons for the output adf11 file classes you wish. The filtered power classes are only sensitized if a filter file has been selected.

5. The standard line printer text output file summarising the options selected for ADAS408 is available. The *Replace* and *Default File Name* buttons are present for the text output file as usual.

6. The *Exit to Menu* icon is present in ADAS408. Clicking the *Done* button causes the output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

Illustration:

There is no graphical display from this code.

Table 5.8a

```
*****************    RUN SUMMARY FOR PROGRAM GENERATING STANDARD   ******************
 ****************   ISONUCLEAR MASTER FILES FROM PARAMETRIC FORMS   ******************
 **************************** ADAS408 - DATE: 19.08.03 ****************************


 INPUT PARAMETER FILE      : /home/adas/adas/adf03/atompars/atompars_mm#ar.dat



 Output files:

  /home/mog/pass/acd89_ar.pass
  /home/mog/pass/scd89_ar.pass
  /home/mog/pass/ccd89_ar.pass
  /home/mog/pass/prb89_ar.fil_jet.pass
  /home/mog/pass/plt89_ar.fil_jet.pass
  /home/mog/pass/pls89_ar.pass
  /home/mog/pass/prc89_ar.fil_jet.pass
  /home/mog/pass/prb89_ar.pass
  /home/mog/pass/plt89_ar.pass
  /home/mog/pass/prc89_ar.pass

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 IMPURITY INFORMATION:
  ---------------------
   ELEMENT SYMBOL          =      ar
   NUCLEAR CHARGE          =      18
   LOWEST ION CHARGE       =       0
   HIGHEST ION CHARGE      =      17
   ATOMIC MASS NUMBER      =   40.00


 NEUTRAL DONOR INFORMATION:
  -------------------------
   ELEMENT SYMBOL          =       H
   NUCLEAR CHARGE          =       1
   ATOMIC MASS NUMBER      =    2.01


 FILTER INFORMATION:
  -------------------
```

```
   Filter from : /home/adas/adas/adf35/jet_filter.dat


  ELECTRON TEMPERATURE/DENSITY INFORMATION:
  -----------------------------------------

                          TEMPERATURE (EV)      DENSITY (CM-3)
                          ----------------      --------------
  NUMBER OF VALUES      =        48                  26
  MINIMUM VALUE         =     1.0000D+00          1.0000D+10
  MAXIMUM VALUE         =     5.0000D+04          1.0000D+15

  (NOTE: EQUAL INTERVALS IN THE LOGARITHM ARE SET)
```

Notes: