6. Ionisation and emission, part II

- Calculating effective ionisation, recombination, power and emissivity data of high quality requires much attention to detail and data sources
  - » The generalised collisional-radiative approach is required.
  - » Density effects must be included at root.
  - » Best data sources must be accessed and tailored for their usage.

Building the specific ion file

- The basic ADF04 specific ion file contains energy level, A-value and electron impact rate coefft. data for an ion.
- It must be supplemented with recombination, ionisation and charge exchange data from best sources for the complete solution.

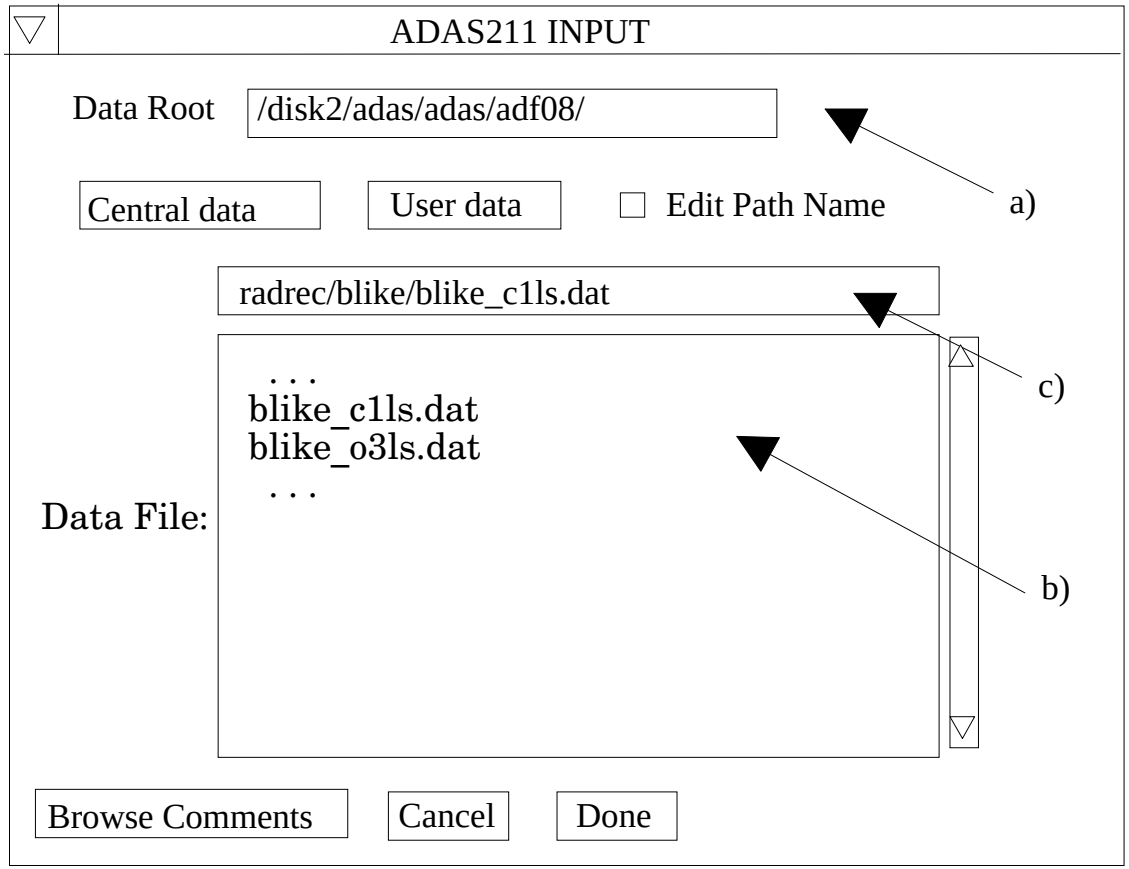
Building the specific ion file (contd.)

- Such extra data is added as electron collision data but with a code in the first column.
  - » ADAS211 prepares state selective radiative recombination data (‘R-lines’).
  - » ADAS212 prepares state selective dielectronic recombination data (‘R-lines’).
  - » ADAS213 prepares state selective electron impact ionisation data (‘S-lines’).

ADF08 template file

```
SEQ='BE'     NUCCHG= 6

   PARENT TERM INDEXING            BWNP=    520178.4  NPRNTI= 1
   --------------------
   INDP    CODE                 S L   WI        WNP
   ----    ----                 - -   --  ----------
     1     1S2 2S1             (2)0( 0.5)        0.0

   LS RESOLVED TERM INDEXING       BWNR=    386214.0    NTRM=  6
   -------------------------
   INDX    CODE                 S L   WJ        WNR
   ----    ----                 - -   --  ----------
     1     2S2                 (1)0( 0.0)        0.0  {1}2.000
     2     2S1 2P1             (3)1( 4.0)    52419.4  {1}1.000
     3     2S1 2P1             (1)1( 1.0)   102352.0  {1}1.000
     4     2P2                 (3)1( 4.0)   137477.7  {X}
     5     2P2                 (1)2( 2.0)   145876.1  {X}
     6     2P2                 (1)0( 0.0)   182519.9  {X}



   INDX TE=  9.00D+03  1.80D+04  4.50D+04  9.00D+04  1.80D+05  4.50D+05  9.00D+05  1.80
```

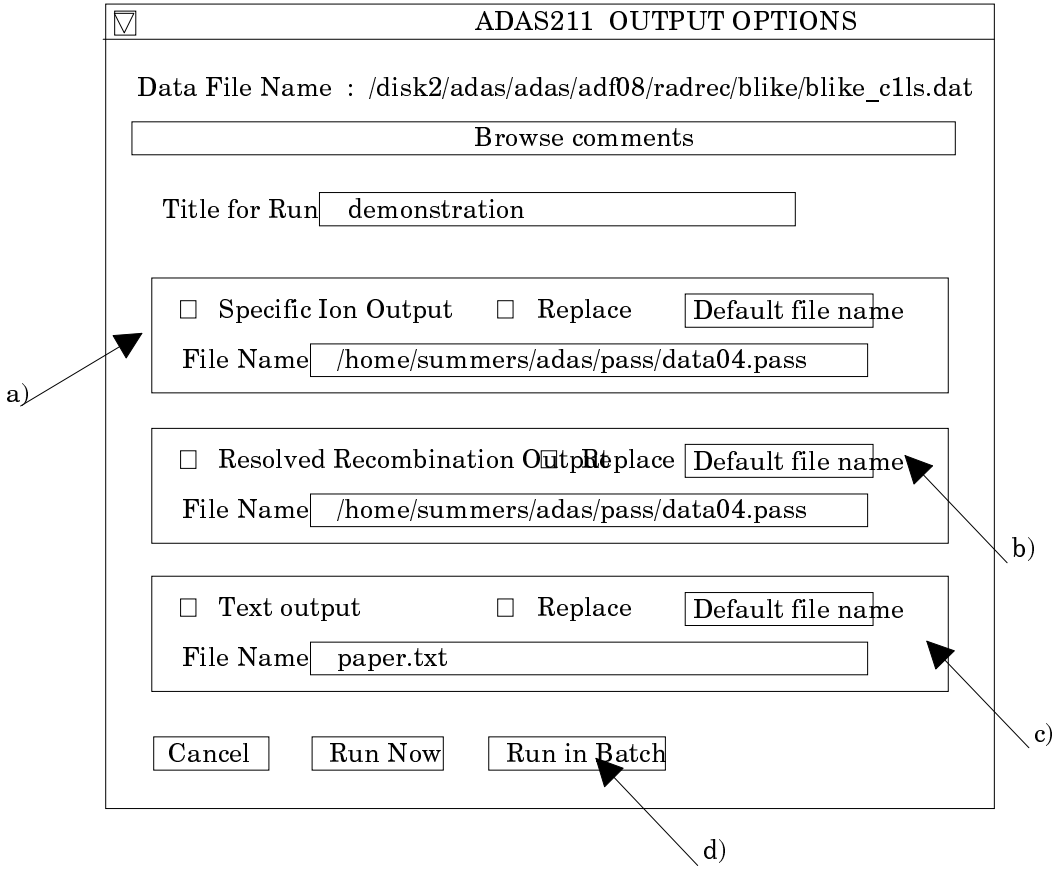
ADAS211 Input



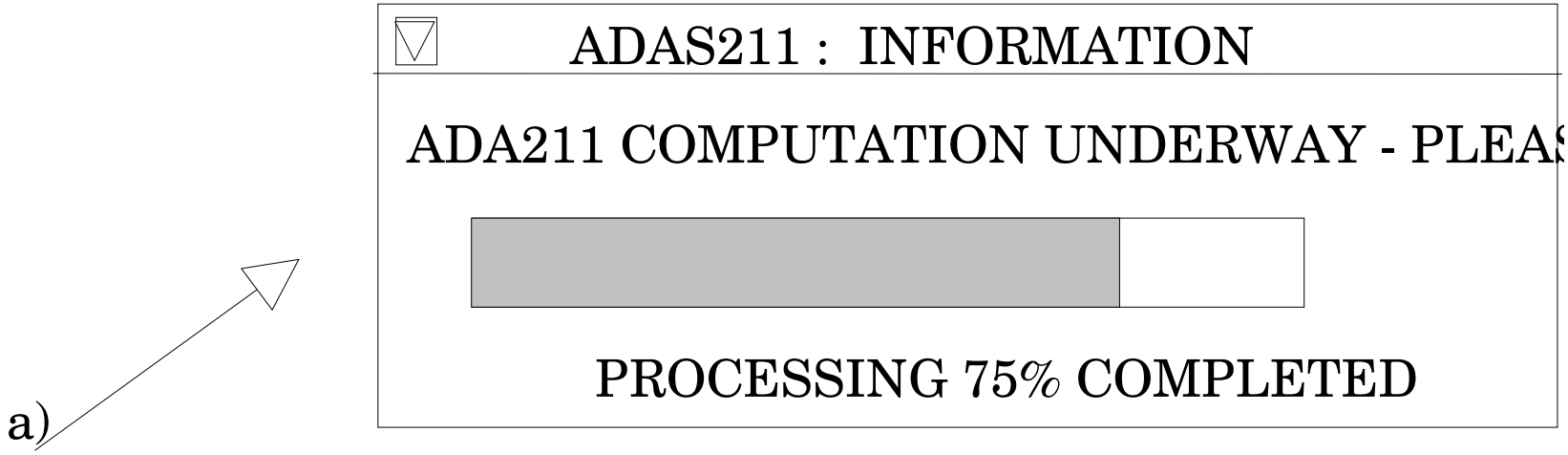
Adding radiative recombination to the specific ion file (contd.)

- There is no graphical output from ADAS211.
- Calculations may be quite long so a foreground or batch execution choice is given.
- In foreground a thermometer widget keeps you informed of progress

ADAS211 Output



ADAS211 Output (contd.)



ADAS211 Output (ADF08)

```
SEQ='BE'     NUCCHG= 6

   PARENT TERM INDEXING            BWNP=    520178.4  NPRNTI= 1
   --------------------
   INDP    CODE                 S L   WI        WNP
   ----    ----                 - -   --  ----------
     1     1S2 2S1             (2)0( 0.5)        0.0

   LS RESOLVED TERM INDEXING       BWNR=    386214.0    NTRM=  6
   -------------------------
   INDX    CODE                 S L   WJ        WNR
   ----    ----                 - -   --  ----------
     1     2S2                 (1)0( 0.0)        0.0  {1}2.000
     2     2S1 2P1             (3)1( 4.0)    52419.4  {1}1.000
     3     2S1 2P1             (1)1( 1.0)   102352.0  {1}1.000
     4     2P2                 (3)1( 4.0)   137477.7  {X}
     5     2P2                 (1)2( 2.0)   145876.1  {X}
     6     2P2                 (1)0( 0.0)   182519.9  {X}



 ---------------------------------
 PRTI= 1  TRMPRT= (2S)  SPNPRT= 2

   INDX TE=  9.00D+03  1.80D+04  4.50D+04  9.00D+04  1.80D+05  4.50D+05  9.00D+05  1.80
     1       1.47D-13  1.05D-13  6.79D-14  4.97D-14  3.69D-14  2.50D-14  1.81D-14  1.24
     2       1.10D-12  7.67D-13  4.68D-13  3.14D-13  2.02D-13  1.04D-13  5.75D-14  2.94
     3       2.61D-13  1.82D-13  1.10D-13  7.31D-14  4.65D-14  2.32D-14  1.26D-14  6.29
```

ADAS211 Output (R-lines)

```
R  1  +1        1.47-13 1.05-13 6.79-14 4.97-14 3.69-14 2.50-14 1.81-14 1.24-14
R  2  +1        1.10-12 7.67-13 4.68-13 3.14-13 2.02-13 1.04-13 5.75-14 2.94-14
R  3  +1        2.61-13 1.82-13 1.10-13 7.31-14 4.65-14 2.32-14 1.26-14 6.29-15
C-------------------------------------------------------------------------------
C
C   RADIATIVE RECOMBINATION DATA ADDED
C
C   PROCESSED BY ADAS211 ON :
C   /u/hps/adas/adf08/rrc96#li/rrc96#li_c3ls.dat
C
C                                          14/04/98
C
C-------------------------------------------------------------------------------
```

Building the specific ion file (contd.)

- State selective charge exchange recombination data from neutral hydrogen must also be added.
  - » ADAS509 prepares state selective CX cross-sections (ADF24) into thermally averaged rate coefficients (ADF14)
  - » ADAS505 interrogates thermal charge exchange rate coefficients and prepares (‘H-lines’) for the ADF04 file.

Calculating the generalised collisional-radiative coeffts.

- There are two stages in the calculation
  - » ADAS204 computes the metastable resolved, bundle-nS very many n-shell population structure and its influence on low levels via projection matrices (ADF17).
  - » ADAS208 computes the low level population structure using the projection matrices (ADF17) and the high quality ADF04 file.
  - » ADA208 outputs PEC (ADF15), SXB (ADF13) and GCR (ADF10) coefficients

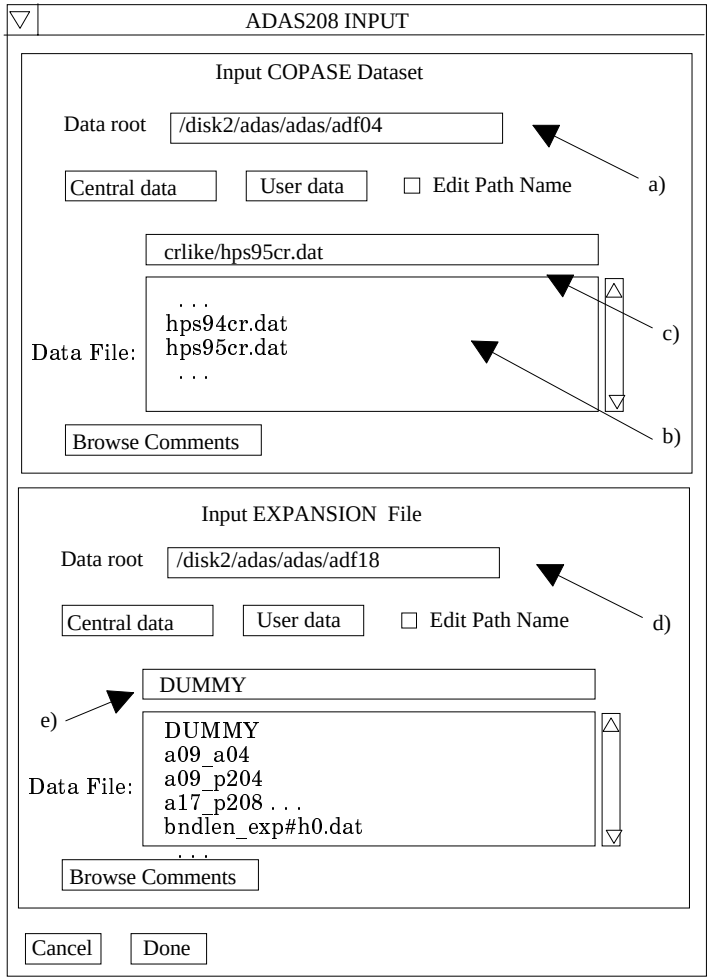
Calculating populations, GCR, PEC and SXB coeffts.

- Start ADAS208 as follows
  - » *Start ADAS*
  - » *Move to ADAS series 2*
  - » *Click button for ADAS208*
- ADAS208 has the standard sequential three screen structure, namely *file selection*, *processing options* & *output options* screens

Calculating populations, GCR, PEC and SXB coeffts.

- File selection
  - » *Two input files may be selected.*
  - » *The first is the fully featured ADF04 specific ion file.*
  - » *The second is an expansion file (ADF18/a17_p208) which tells where the projection matrices are and how they are to be expanded over the low levels.*
  - » *Enter DUMMY for the second file to by-pass high n-shell projection.*

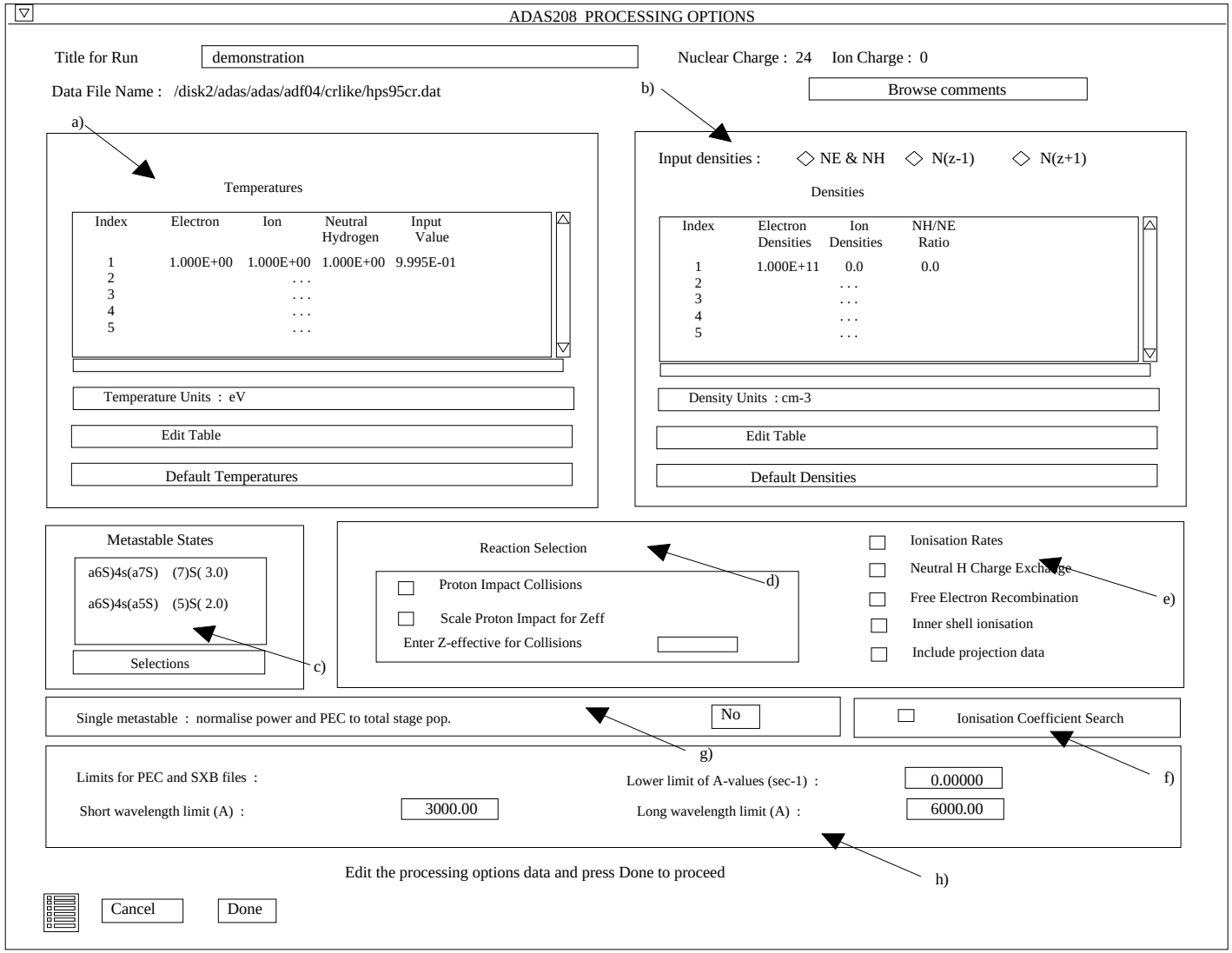
ADAS208 Input



Calculating populations, GCR, PEC and SXB coeffts.

- Processing options
  - » *First the choice of temperatures and densities must be entered.*
  - » *Designation of metastables must be made.*
  - » *Switches control the inclusion and exclusion of specific processes*
  - » *Emissivity output may be large and can be limited by wavelength range appropriately for a particular spectrometer.*

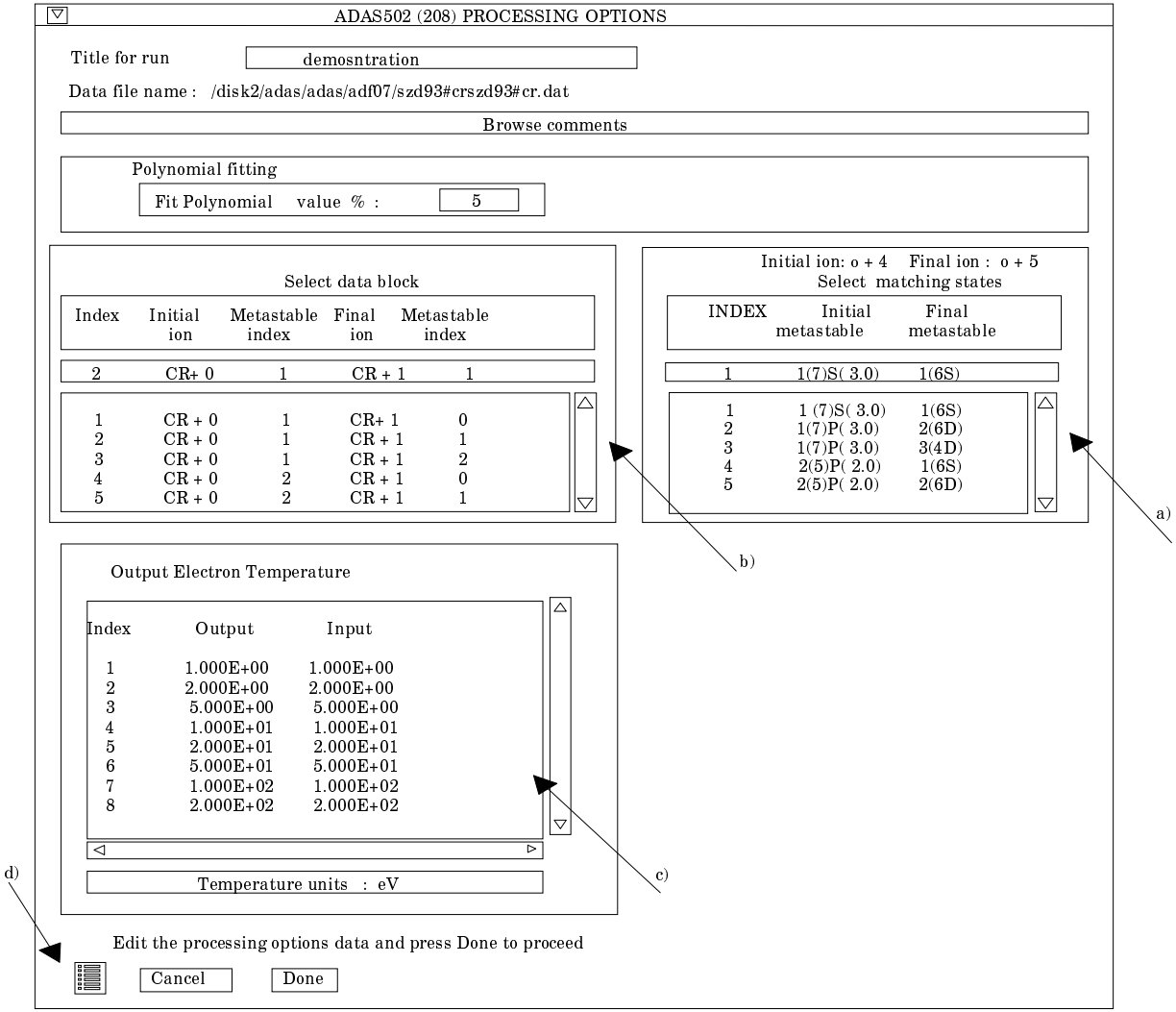
ADAS208 Processing



Calculating populations, GCR, PEC and SXB coeffts.

- Best available direct ionisation coefficients from the metastables are sought to improve the precision.
  - » Click *Ionisation Coefficient Search*
  - » *Find the correct ionisation data file*
  - » *Match demand from ADAS208 from the ionisation data source according to initial and final metastable.*

ADAS502(208) Processing



Calculating populations, GCR, PEC and SXB coeffts.

- The program solves for excited level populations in terms of the metastables. That is for the F's and F$^+$'s where

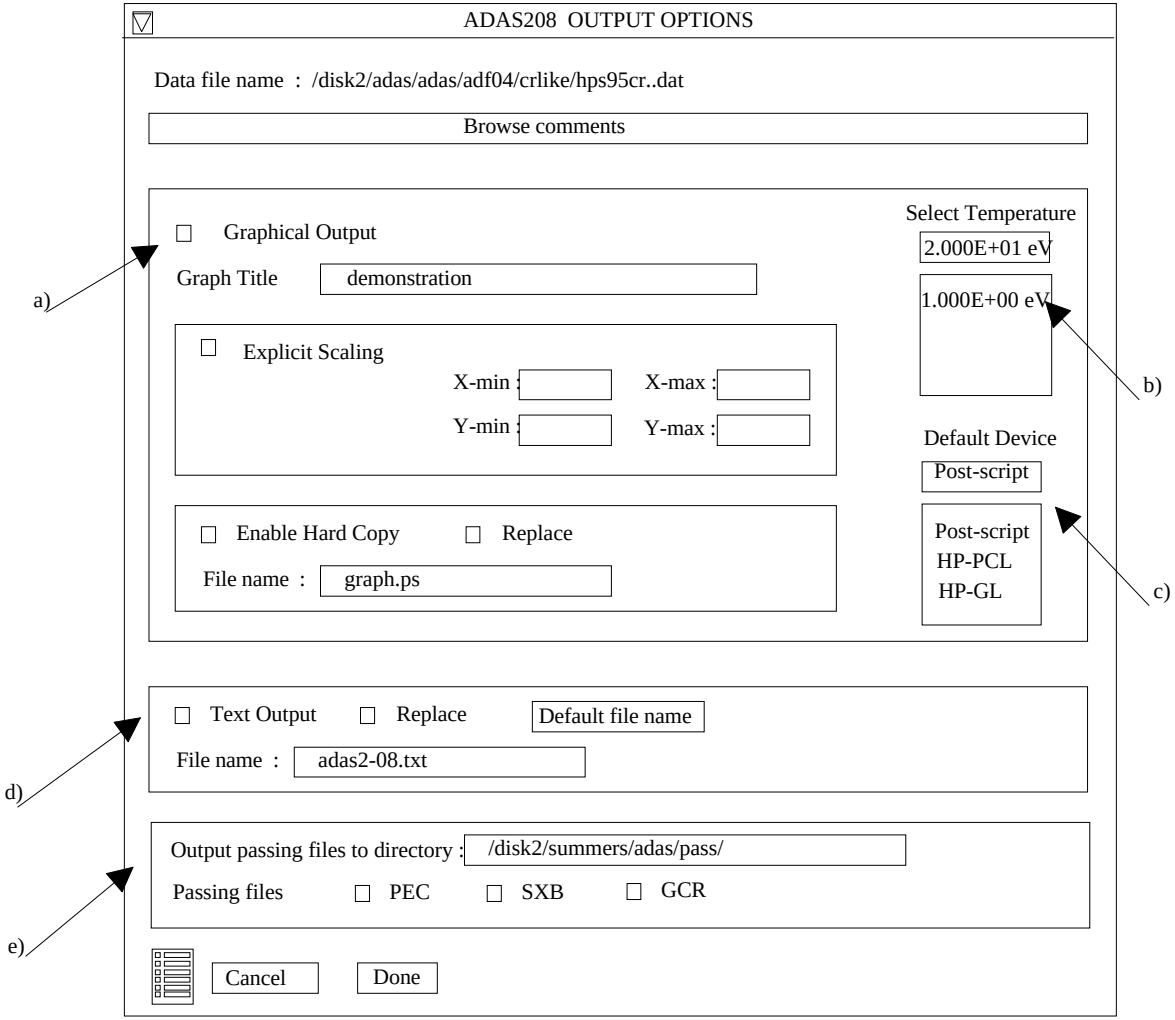
$$N_i = N_e \sum_{\rho=1}^{M} F_{i\rho}(T_e, N_e) N_\rho + N_e \sum_{\sigma=1}^{M^+} F_\sigma^+(T_e, N_e) N_\sigma^+$$

- The code then computes collisional radiative coefficients, photon emissivities and ionisations per photon.

Calculating populations, GCR, PEC and SXB coeffts.

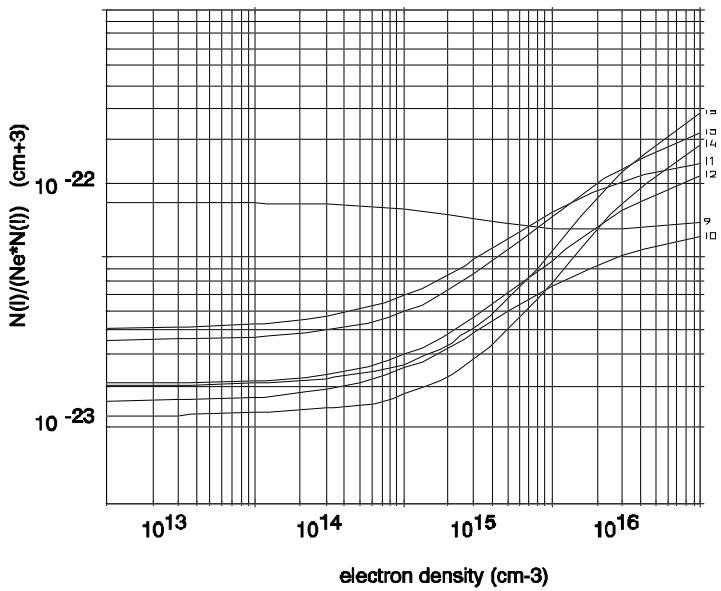
- Output options
  - » *Graphical display of the F's as a function of density is allowed*
  - » *PEC, SXB and GCR output files are produced as required ready for addition to the ADAS database.*

ADAS208 Output



ADAS208 graph

POPULATION DEPENDENCE ON METASTABLES : O+5 ELECTRON TEMP. = 2.00E+01 (EV)
ADAS RELEASE : ADAS91 V1.01 PROGRAM: ADAS205 V1.0 DATE: 26/05/93 TIME: 16:15
GRAPH TITLE : POPULATION GRAPH
INPUT FILE : /JETSHP.COPSM#LI.DATA(SM#O5)



O+5 POPULATIONS

------ LEVEL ASSIGNMENTS ------

INDEX	DESIGNATION	
1	2s1	(2)S(0.5)
2	2p1	(2)P(0.5)
3	2p1	(2)P(1.5)
4	3s1	(2)S(0.5)
5	3p1	(2)P(0.5)
6	3p1	(2)P(1.5)
7	3d1	(2)D(1.5)
8	3d1	(2)D(2.5)
9	4s1	(2)S(0.5)
10	4p1	(2)P(0.5)
11	4p1	(2)P(1.5)
12	4d1	(2)D(1.5)
13	4d1	(2)D(2.5)
14	4f1	(2)F(2.5)
15	4f1	(2)F(3.5)
16	5s1	(2)S(0.5)
17	5p1	(2)P(0.5)
18	5p1	(2)P(1.5)
19	5d1	(2)D(1.5)
20	5d1	(2)D(2.5)
21	5f1	(2)F(2.5)
22	5f1	(2)F(3.5)
23	5g1	(2)G(3.5)
24	5g1	(2)G(4.5)