The ionisation state of ions in a plasma

- Effective ionisation and recombination
  - » Data sets of class ADF11
  - » Interrogating ADF11 using ADAS402.
- Equilibrium ionisation balance
  - » Using adas405 to examine the temperature and density dependent equilibrium ionisation balance

Effective ionisation and recombination

- Collisional-radiative modelling
  - » Full modelling for the populations of an ion also gives the collisional-radiative ionisation and recombination coefficients.
  - » In basic CR modelling, the coeffts. give stage to stage connections. In GCR modelling, the coeffts. give connections between metastables within and across ionisation stages.
  - » The data format ADF11 is assigned to Maxwell averaged, Te and Ne dependent CR and GCR coeffts.

Collisional-radiative theory

Then the quasi-equilibrium statistical balance is

$$\frac{d}{dt} N_1 = \sum_{j \neq 1} C_{1j} N_j + C_{11} N_1 + N_e N_+ r_1$$

$$0 = \sum_{j \neq 1} C_{ij} N_j + C_{i1} N_1 + N_e N_+ r_i \quad , \quad i = 2,..$$

In matrix form these become

$$\begin{bmatrix} \frac{d}{dt} N_1 \\ 0 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{1j} \\ C_{i1} & C_{ij} \end{bmatrix} \begin{bmatrix} N_1 \\ N_j \end{bmatrix} + N_e N_+ \begin{bmatrix} r_1 \\ r_i \end{bmatrix}$$

The populations of the excited levels in quasi-equilibrium, N_j^{eq} are given by

$$N_j^{eq} = -N_e N_+ \sum_{i \neq 1} C_{ji}^{-1} r_i - \sum_{i \neq 1} C_{ji}^{-1} C_{i1} N_1$$

Collisional-radiative theory (contd.)

Collisional-dielectronic ionisation coefficient

$$S_{CD} = C_{11} - \sum_{j\neq 1}\sum_{i\neq 1} C_{1j}C_{ji}^{-1}C_{i1}$$

and collisional-dielectronic recombination coefficient

$$\alpha_{CD} = r_1 - \sum_{j\neq 1}\sum_{i\neq 1} C_{1j}C_{ji}^{-1}r_i$$

$$d/dt\, N_1 = -N_e S_{CD} N_1 + N_e \alpha_{CD} N_+$$

Collisional-radiative theory (generalised)

The ionisation coefficients

$$S_{CD,\sigma\to\upsilon} = (\mathsf{S}_{\upsilon\sigma} - \sum_{j=1}^{O} \mathsf{S}_{\upsilon j} \sum_{i=1}^{O} \mathsf{C}_{ji}^{-1} \mathsf{C}_{i\sigma})$$

the free electron recombination coefficients

$$\alpha_{CD,\upsilon'\to\rho} = (\mathsf{R}_{\rho\upsilon'} + \sum_{j=1}^{O} \mathsf{C}_{\rho j} \sum_{i=1}^{O} \mathsf{C}_{ji}^{-1} \mathsf{R}_{i\upsilon'})$$

the charge exchange recombination coefficients

$$C_{CD,\upsilon'\to\rho} = (\mathsf{Q}_{\rho\upsilon'} + \sum_{j=1}^{O} \mathsf{C}_{\rho j} \sum_{i=1}^{O} \mathsf{C}_{ji}^{-1} \mathsf{Q}_{i\upsilon'})$$

the metastable cross-coupling coefficients

$$X_{CD,\sigma\to\rho} = (\mathsf{C}_{\rho\sigma} - \sum_{j=1}^{O} \mathsf{C}_{\rho j} \sum_{i=1}^{O} \mathsf{C}_{ji}^{-1} \mathsf{C}_{i\sigma}) / N_e$$

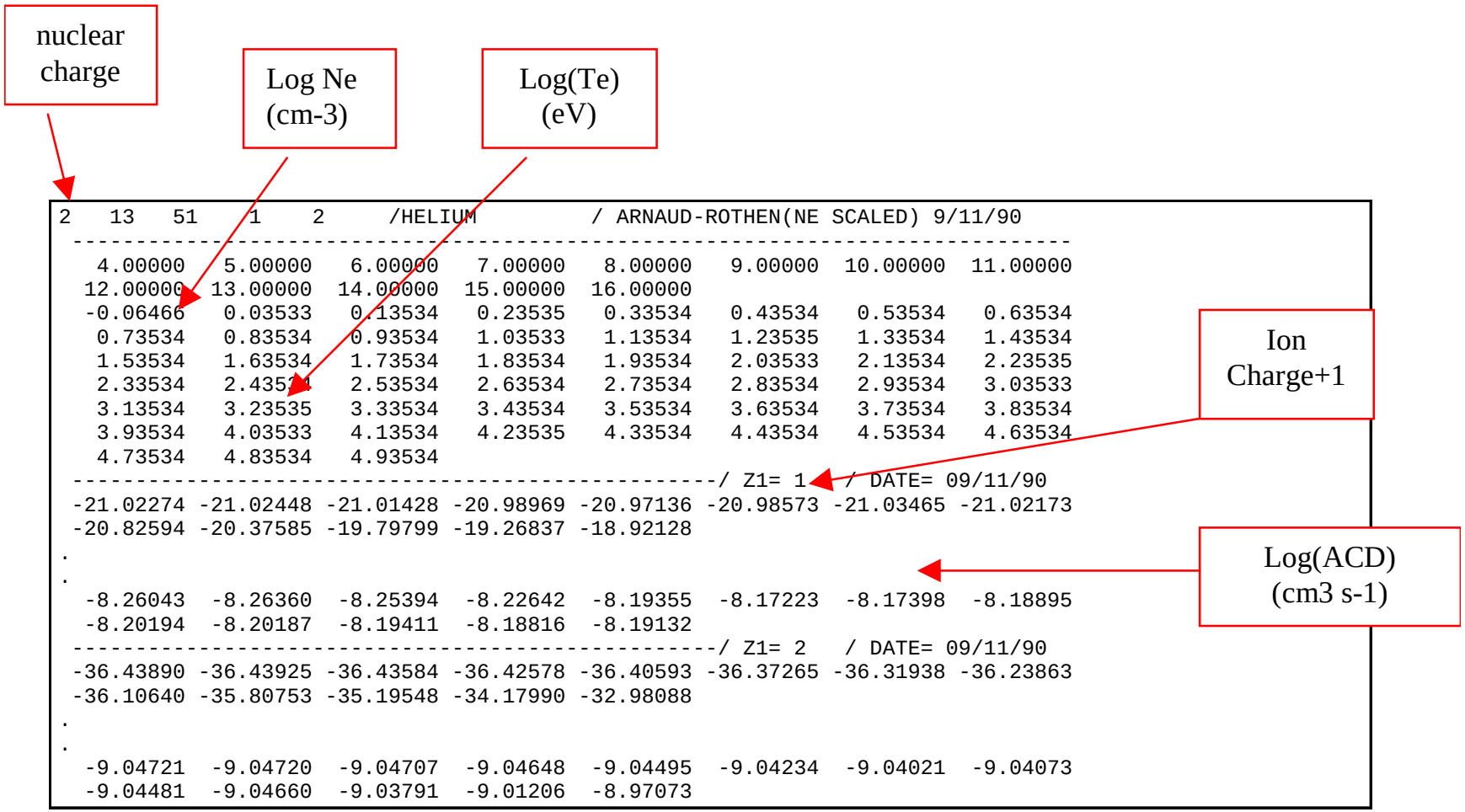
and the parent metastable cross-coupling coefficients

$$Q_{CD,\upsilon'\to\upsilon} = \sum_{j=1}^{O} \mathsf{S}_{\upsilon j} \sum_{i=1}^{O} \mathsf{C}_{ji}^{-1} \mathsf{R}_{i\upsilon'}{}_{e}$$

ADF11 iso-nuclear master file classes

Mnemonic	Class	Data prefix
ACD	Coll.-diel. recom. coefft.	R & U (or none)
SCD	Coll.-diel. ionis. coefft.	R & U (or none)
CCD	Coll.-rad. charge exch. coefft.	R & U (or none)
PRB	Coll.-diel. recom./brems. power coefft.	R & U (or none)
PRC	Coll.-rad. charge exch. recom. power coefft.	R & U (or none)
QCD	Coll.-rad. metastable cross coupling coefft.	R
XCD	Coll.-diel. parent meta. cross-coupling coefft.	R
PLT	Coll.-rad. excit. line power coefft.	R & U (or none)
PLS	Coll.-rad. specific line excit. power coefft.	R & U (or none)

ADF11 iso-nuclear master file layout (standard- unresolved)




```
2   13   51    1    2     /HELIUM          / ARNAUD-ROTHEN(NE SCALED) 9/11/90
 ------------------------------------------------------------------------------
   4.00000   5.00000   6.00000   7.00000   8.00000   9.00000  10.00000  11.00000
  12.00000  13.00000  14.00000  15.00000  16.00000
  -0.06466   0.03533   0.13534   0.23535   0.33534   0.43534   0.53534   0.63534
   0.73534   0.83534   0.93534   1.03533   1.13534   1.23535   1.33534   1.43534
   1.53534   1.63534   1.73534   1.83534   1.93534   2.03533   2.13534   2.23535
   2.33534   2.43534   2.53534   2.63534   2.73534   2.83534   2.93534   3.03533
   3.13534   3.23535   3.33534   3.43534   3.53534   3.63534   3.73534   3.83534
   3.93534   4.03533   4.13534   4.23535   4.33534   4.43534   4.53534   4.63534
   4.73534   4.83534   4.93534
 -------------------------------------------------/ Z1= 1   / DATE= 09/11/90
 -21.02274 -21.02448 -21.01428 -20.98969 -20.97136 -20.98573 -21.03465 -21.02173
 -20.82594 -20.37585 -19.79799 -19.26837 -18.92128
.
.
  -8.26043  -8.26360  -8.25394  -8.22642  -8.19355  -8.17223  -8.17398  -8.18895
  -8.20194  -8.20187  -8.19411  -8.18816  -8.19132
 -------------------------------------------------/ Z1= 2   / DATE= 09/11/90
 -36.43890 -36.43925 -36.43584 -36.42578 -36.40593 -36.37265 -36.31938 -36.23863
 -36.10640 -35.80753 -35.19548 -34.17990 -32.98088
.
.
  -9.04721  -9.04720  -9.04707  -9.04648  -9.04495  -9.04234  -9.04021  -9.04073
  -9.04481  -9.04660  -9.03791  -9.01206  -8.97073
```

ADF11 iso-nuclear master file layout (partial- resolved)

```
      4   26   35    1    4     /BERYLLIUM          /DICKSON ET AL 1992
-------------------------------------------------------------------------------
    2    1    2    1    1
-------------------------------------------------------------------------------
  10.00000  10.20003  10.40002  10.59999  10.80003  11.00000  11.20003  11.40002
  11.59999  11.80003  12.00000  12.20003  12.40002  12.59999  12.80003  13.00000
  13.20003  13.40002  13.59999  13.80003  14.00000  14.20003  14.40002  14.59999
  14.80003  15.00000
   0.00015   0.10016   0.20015   0.30015   0.40015   0.50015   0.60015   0.70015
   0.80015   0.90015   1.00015   1.10016   1.20015   1.30015   1.40015   1.50015
   1.60015   1.70015   1.80015   1.90015   2.00015   2.20015   2.40015   2.60015
   2.80015   3.00015   3.20015   3.40015   3.60015   3.80015   4.00015   4.20015
   4.40015   4.60015   4.70015
----------------------/ IPRT= 1   / IGRD= 1   /--------/ Z1= 1    / DATE= 16/11/93
 -11.57681 -11.55926 -11.53861 -11.51437 -11.48604 -11.45315 -11.41518 -11.37166
 -11.32210 -11.26598 -11.20285 -11.13244 -11.05561 -10.97341 -10.88689 -10.79719
 -10.70532 -10.61241 -10.51952 -10.42769 -10.33806 -10.25165 -10.16957 -10.09290
 -10.02268  -9.96003
.
.
  -7.20840  -7.21561  -7.22233  -7.22831  -7.23329  -7.23700  -7.23918  -7.23957
  -7.23791  -7.23394  -7.22740  -7.21811  -7.20627  -7.19216  -7.17605  -7.15822
  -7.13895  -7.11852  -7.09722  -7.07531  -7.05308  -7.03080  -7.00876  -6.98724
  -6.96650  -6.94684
  -6.85348  -6.85100
.
.
.
.
--------------------/ IPRT= 1   / IGRD= 1   /--------/ Z1= 4    / DATE= 16/11/93
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 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000
 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000 -74.00000
 -74.00000 -74.00000
```

Connection vector

Metastable

Parent metastable

ADF11 (contd.)

- ADF11 year numbers
  - » baseline CR data are assigned the ‘89’ year number. They are stage to stage data and available for very many elements.
  - » GCR data on the restricted Te/Ne grid are assigned the ‘93’ year number. They are LS-coupled, metastable resolved data for selected light elements.
  - » GCR data on the extended Te/Ne grid are assigned the ‘96’ year number. They are LS-coupled, metastable resolved data for selected light elements. CR data ‘condensed’ from the GCR data is also provided.
  - » Other approximations, eg. Arnaud/Rothenflug. are available but sub-categories are generally incomplete.

appxa-11.pdf

ADF11: iso-nuclear master files

Isonuclear master file data. Formatting conventions and variable storage are given below.

Utilising subroutines :

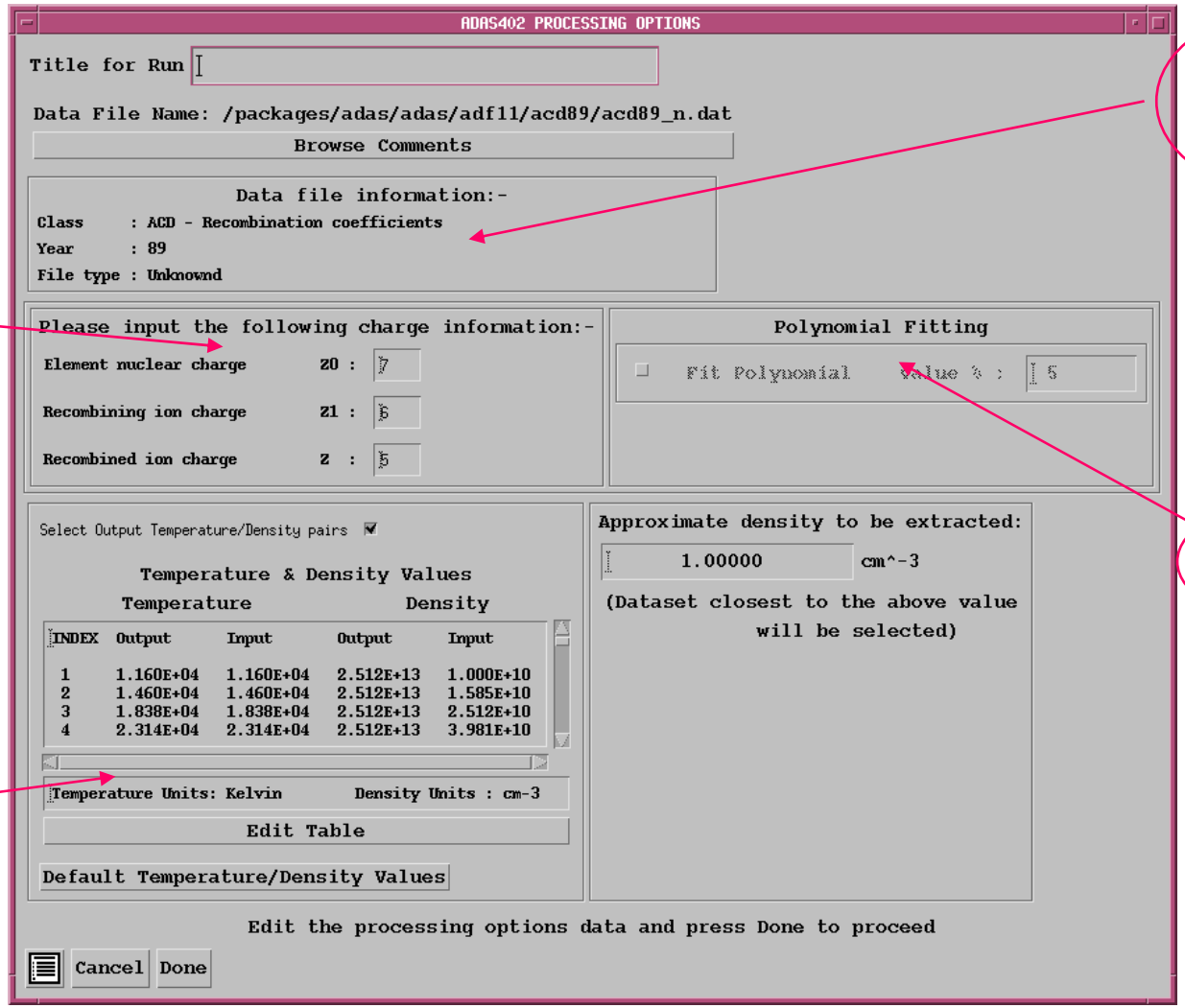
ADAS405 ADAS406

Formatted files to ADF11 specification :

Database Status Date = March 17, 2003 Data type = isonuclear master files Data root = /.../adas/adas/adf11/

Element	*Cluster*	*Dataset*	*Comments*	*Resolution*	*Quality*
Hydrogen	acd, scd, ccd, prb, prc, plt, pls	/<class>89/<class>89h.dat	JET base line	unresolved	low
Hydrogen	acd, scd, qcd, xcd, prb, plt	/<class>93e/<class>93e_h.dat	ADAS208, c-r	resolved	high
Hydrogen	acd, scd, ccd, prb, plt, prc	/<class>96/<class>96_h.dat	ADAS208, c-r	unresolved	high
Helium	acd, scd	/<class>74/<class>74_he.dat	Summers, c-r	unresolved	medium
Helium	acd, scd	/<class>85/<class>85_he.dat	Amund & Rotherflug *HPS c-r	unresolved	medium
Helium	acd, scd,ccd,prb,prc,plt,pls	/<class>89/<class>89_he.dat	JET base line	unresolved	low
Helium	acd, scd,qcd,xcd,prb,plt	/<class>93e/<class>93e_he.dat	ADAS208, c-r	resolved	high
Helium	acd, scd, ccd, prb, plt, prc	/<class>96/<class>96_he.dat	ADAS208, c-r	unresolved	high
Helium	acd, scd, ccd, qcd, xcd, prb, plt, prc	/<class>96/<class>96_he.dat	ADAS208, c-r	resolved	high
Lithium	acd, scd,ccd,prb,prc,plt,pls	/<class>89/<class>89_li.dat	JET base line	unresolved	low
Lithium	acd, scd, ccd, prb, plt, prc	/<class>96/<class>96_li.dat	ADAS208, c-r	unresolved	high
Lithium	acd, scd, ccd, qcd, xcd, prb, plt, prc	/<class>96/<class>96_li.dat	ADAS208, c-r	resolved	high
Beryllium	acd, scd,ccd,prb,prc,plt,pls	/<class>89/<class>89_be.dat	JET base line	unresolved	low
Beryllium	acd, scd,qcd,xcd,prb,plt	/<class>93e/<class>93e_be.dat	ADAS208, c-r	resolved	high

ADAS402 Processing



Data class selected

ion required

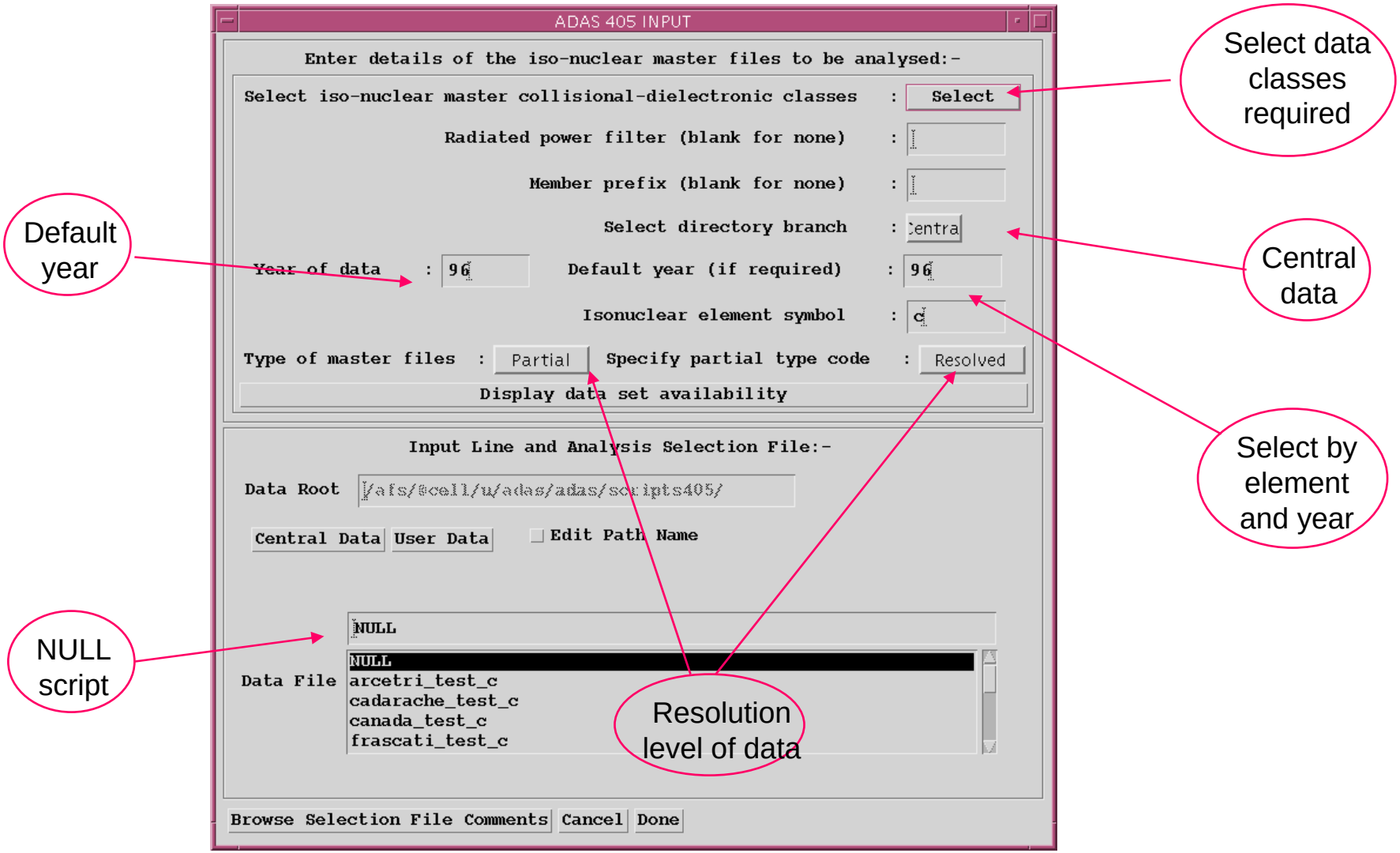
Polynomial fit

Specify Te/Ne pair values

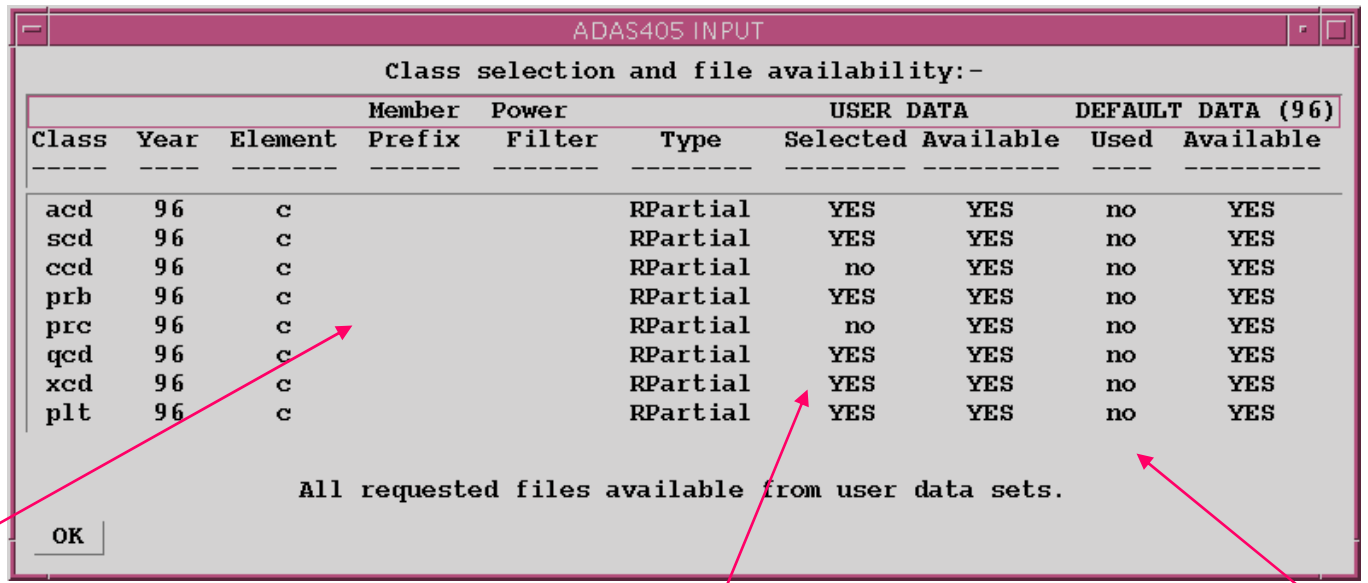
Equilibrium ionisation balance

- The ionisation balance is often a weakness in the theoretical input.
- Code ADAS405 is provided for examining and contrasting ionisation balances as a function of Te and Ne.
- It has also capability for examining radiated power and the ingredients of G(Te(h),Ne(h)) functions

ADAS405 Input



Availability of ADF11 data

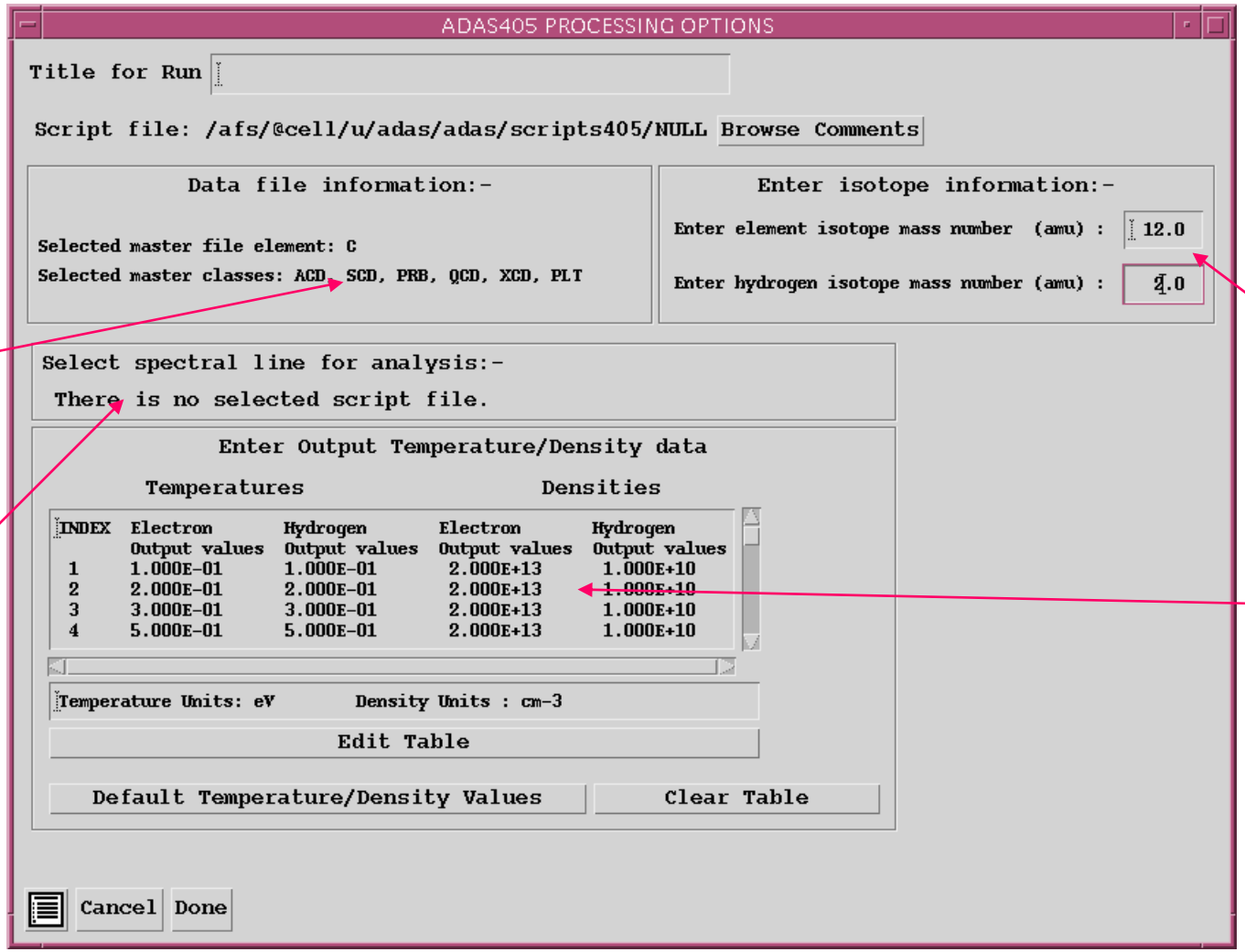


Data set information

Data obtained from primary year

Data obtained from default year

ADAS405 processing



ADF11 classes selected

No script file present- no lines for selection

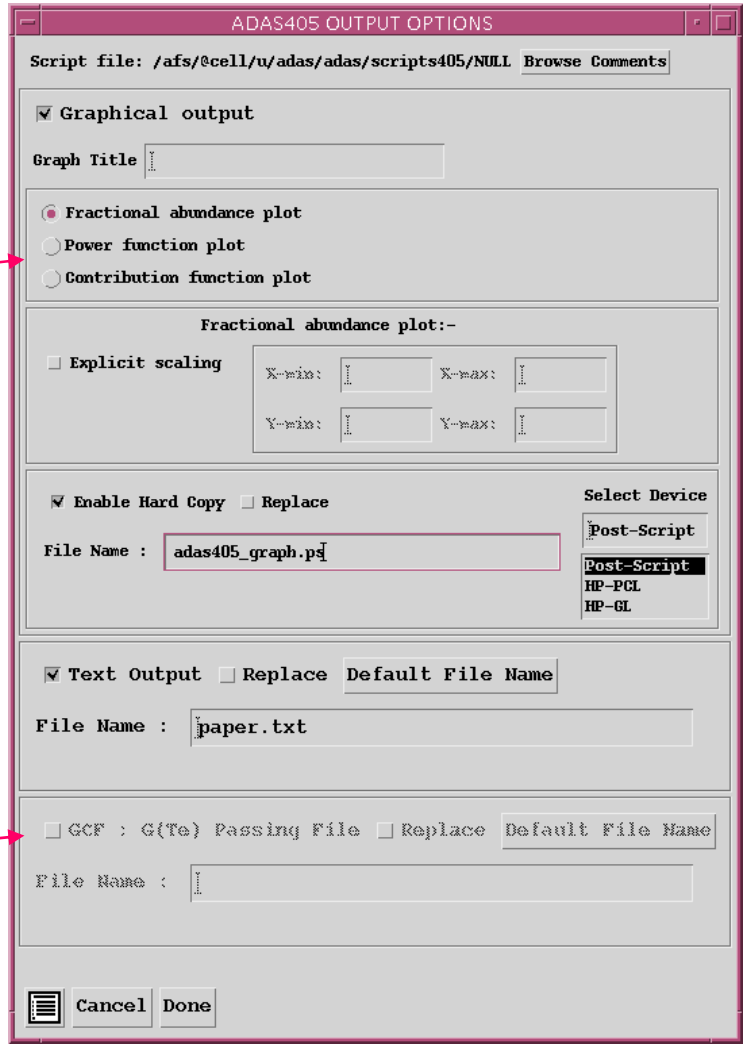
Set element parameters

Select Te and Ne pairs

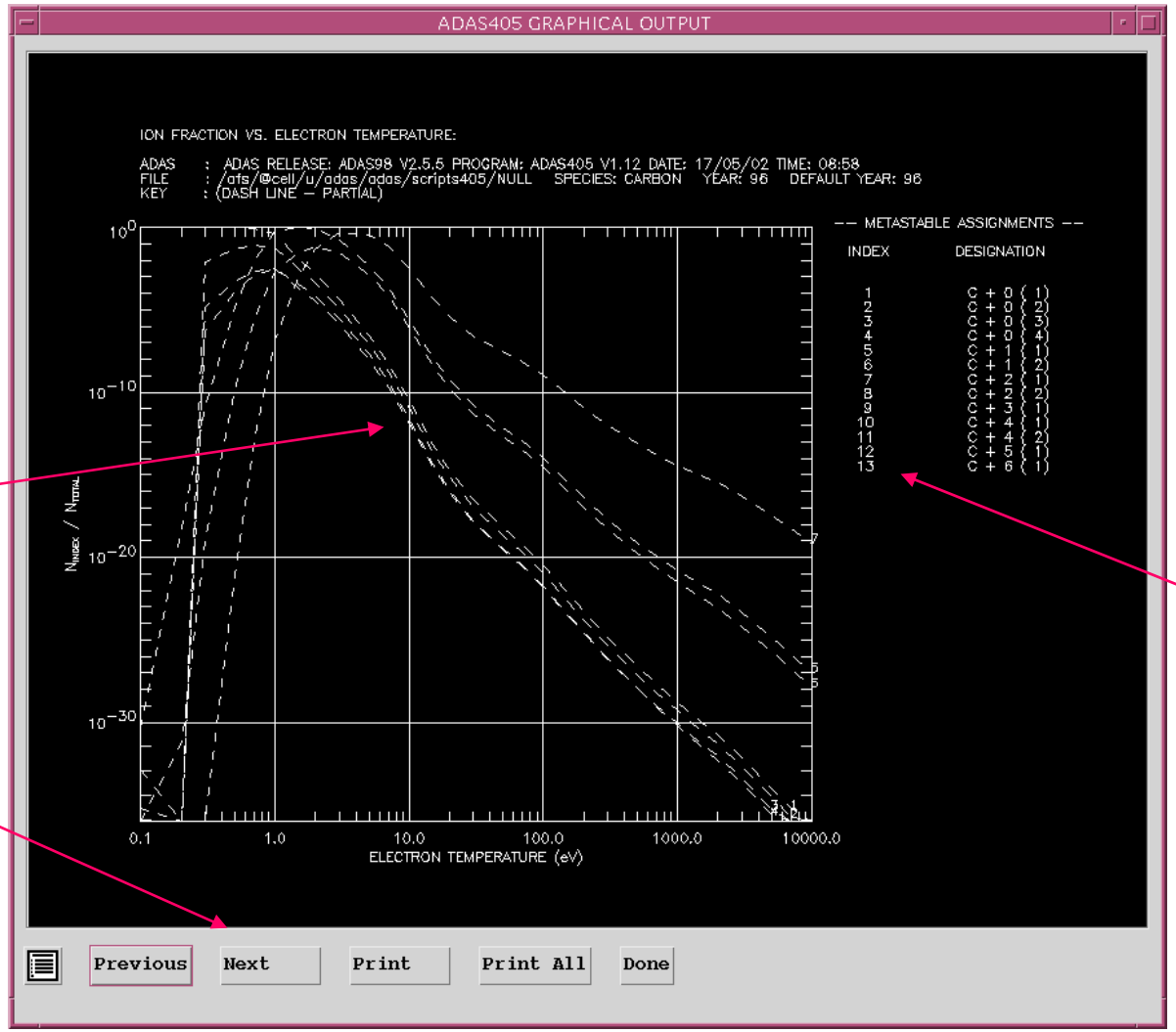
ADAS405 Output

Choice of graphs

No GCF output since no script



ADAS405 fractional abundance graph

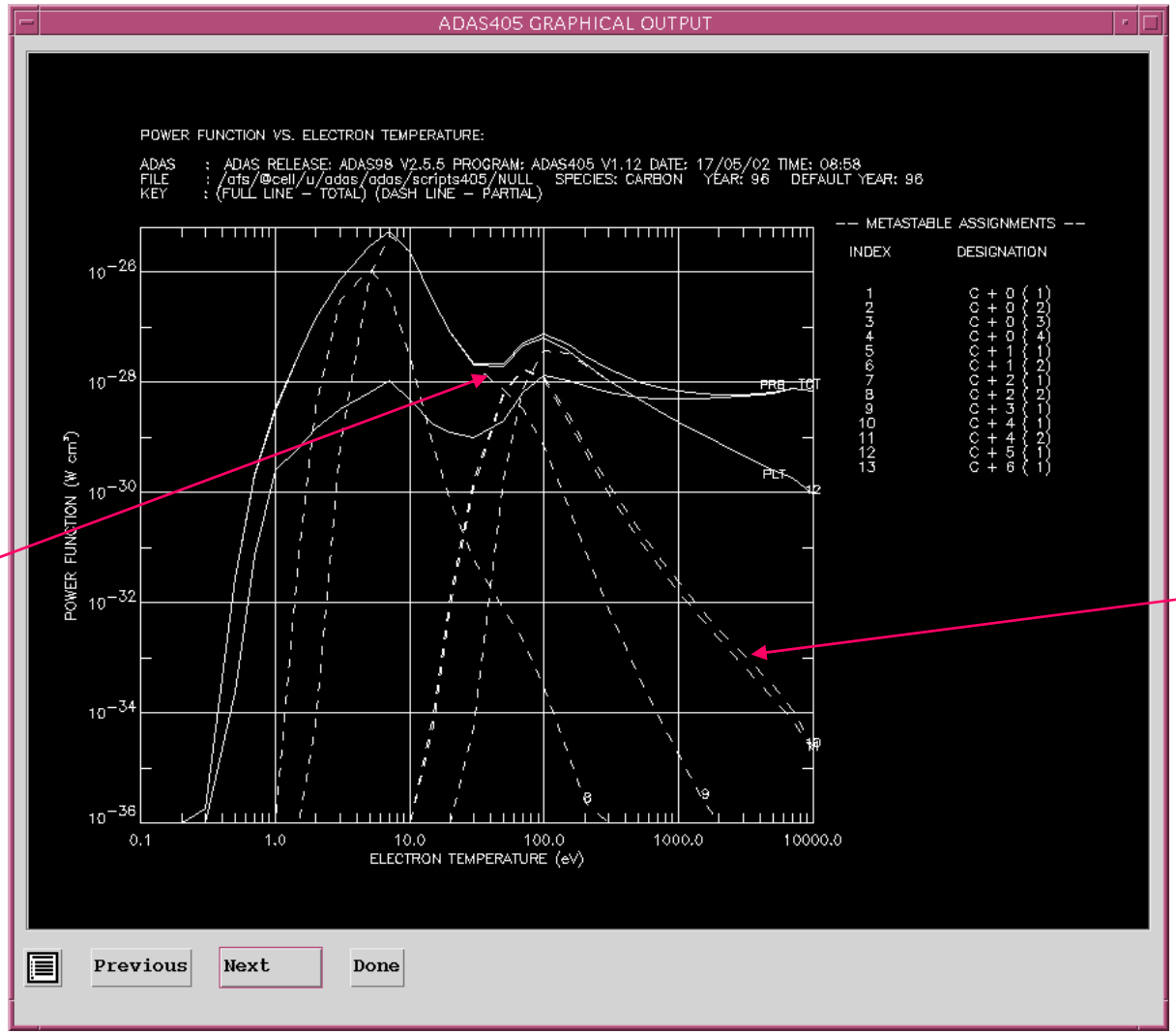


Fractional abundances - seven curves / screen

Index - note metastable resolved case

Page through graphs

ADAS405 power graph



Total power and components

Metastable contributions to total