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EURATOM/UKAEA Fusion

FISPACT-99: User manual

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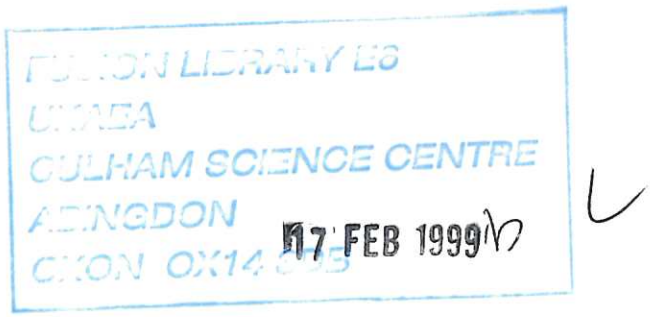

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EASY Documentation Series **UKAEA FUS 407**

FISPACT-99: User manual

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charged particles are in 1 MeV bins covering the energy range 0-24 MeV.

EAF_XN-99

EAF_XN describes the cross sections of p, d, h, t and α particles on 745 targets. Seven reactions types are considered: (p,n), (d,n), (h,n), (t,n), (α,n), (d,2n) and (t,2n). This is the third of the KfK libraries. Most of the data are calculated by a theoretical model code due to the lack of experimental data. The data are given at 1 MeV intervals over the energy range 0-24 MeV.

EAF_ABS-99

EAF_ABS-99 contains the photon mass energy attenuation coefficient (μ/ρ) for all the elements $Z = 1$ - 100 in increasing Z order. The attenuation coefficient (μ) and energy absorption coefficient (μ_{en}/ρ) for air are also listed. All data are stored in the same 24-group energy structure as described in Appendix 10.

Appendix 7 - Bremsstrahlung corrections

The contribution of high energy β particle bremsstrahlung to the total γ dose rate can be significant in cases where the γ emission is small. FISPACT uses a similar approach to Jarvis [29] who considers γ emission from a monoenergetic electron.

The energy distribution of γ rays emitted by a monoenergetic electron in a matrix of charge Z is given by equation A7.1,

$$dN = aZ\frac{E_0 - E}{E}dE \quad \text{.....(A7.1)}$$

where

dN = number of γ rays with energy E (keV)
E_0 = energy of electron (keV)
a = $2.76\ 10^{-6}$

Consider a group structure where $\varepsilon(n)$ is the upper limit of the n-th energy group in units of E_k = 0.1 MeV. Only energies greater than 100 keV are used, so that only 19 of the 24 energy groups are required. Integrating equation A7.1 over the n-th group,

$$N(n) = aZ\int_{\varepsilon(n-1)E_k}^{\varepsilon(n)E_k}\frac{E_0 - E}{E}dE = aZE_k t_n(\alpha) \quad \text{.....(A7.2)}$$

where

α = E_0 / E_k
$t_n(\alpha) = \alpha \ln(\varepsilon(n)/\varepsilon(n-1)) - \varepsilon(n) + \varepsilon(n-1)$
$\varepsilon(0) \equiv 1$

Equation A7.2 shows that the γ spectrum $N(n)$ depends on the matrix through Z and the nuclide through α.

If equation A7.2 is used to calculate the correction due to β particles with low energies then the discrete nature of the group structure can cause problems. Integrating over the first group gives a term $\int_1^2 \frac{\alpha - e}{e}de$ (in units of 0.1 MeV), and as α is reduced this integral becomes zero. This occurs when

$\alpha = 1/\ln 2 \approx 1.45$. It is assumed in FISPACT that such low energy bremsstrahlung corrections can be ignored and thus if the energy of the β particle is less than 0.145 MeV then the correction is set to zero.

The above discussion is valid only for monoenergetic electrons, but it is assumed that the same expressions are valid for the emission of β particles which have a continuous energy distribution if the mean β energy is used for E_0.

The value of Z used in equation A7.2 is calculated from equation A7.3,

$$Z = \sum_j Z_j n_j \quad \text{(A7.3)}$$

where

Z_j = atomic number of the j th element

n_j = atomic fraction of the j th element (number of atoms of j / total number of atoms)

Only a subset of all the nuclides in the decay library need to be considered for bremsstrahlung production. The nuclides shown in Table A7.1 may make a contribution to the γ dose rate because of bremsstrahlung emission from energetic β particles. The bremsstrahlung correction can be estimated by including nuclides from the mass range of interest using the code word **BREM**.

The following criteria applied to the EAF_DEC-99 decay library give the nuclides shown in the Table.

- The nuclide is radioactive with a half-life ≥ 0.1 years or in the case of a short-lived nuclide, the half-life of the parent ≥ 0.1 years.
- The nuclide has an average β-energy > average γ-energy.
- The nuclide has an average β-energy > 0.145 MeV.

Column 1 in the Table specifies the nuclide giving the bremsstrahlung correction, column 2 the half-life of the nuclide or the parent, column 3 the decay parent and column 4 the percentage branching ratio of the nuclide from the parent.

Table A7.1. Possible bremsstrahlung nuclides.

Nuclide	Half-life (y)	Parent	Branching ratio (%)
^{10}Be	1.60 10^{6}		
^{32}P	330.0	^{32}Si	100.0
^{36}Cl	3.02 10^{5}		
^{39}Ar	269.0		
^{40}K	1.28 10^{9}		
^{42}Ar	33.00		
^{42}K	33.00	^{42}Ar	100.0
^{85}Kr	10.73		
^{89}Sr	0.14		
^{90}Sr	28.87		
^{90}Y	28.87	^{90}Sr	100.0
^{91}Y	0.16		
^{95m}Nb	0.18	^{95}Zr	1.1
^{106}Rh	1.01	^{106}Ru	100.0
^{108}Ag	418.0	^{108m}Ag	8.7
^{110}Ag	0.68	^{110m}Ag	1.3
^{113m}Cd	13.7		
^{115m}Cd	0.12		
^{114}In	0.14	^{114m}In	96.5
^{115}In	4.41 10^{14}		
^{115m}In	0.12	^{115m}Cd	7.0 10^{-3}
^{123}Sn	0.35		
^{127}Te	0.30	^{127m}Te	97.6
^{137}Cs	30.17		
^{144}Pr	0.78	^{144}Ce	98.5
^{148}Pm	0.11	^{148m}Pm	5.0
^{177}Lu	0.44	^{177m}Lu	22.6
^{186}Re	2.00 10^{5}	^{186m}Re	100.0
^{188}Re	0.19	^{188}W	100.0
^{194}Ir	5.99	^{194}Os	100.0
^{206}Hg	22.3	^{210}Pb	1.9 10^{-6}
^{204}Tl	3.79		
^{206}Tl	3.00 10^{6}	^{210m}Bi	100.0
^{210}Bi	22.3	^{210}Pb	100.0
^{223}Fr	21.77	^{227}Ac	1.4
^{237}U	14.4	^{241}Pu	2.4 10^{-3}
^{240}U	8.00 10^{7}	^{244}Pu	99.9
^{231}Th	7.04 10^{8}	^{235}U	100.0
^{236}Np	1.52 10^{5}		
^{239}Np	7.36 10^{3}	^{243}Am	100.0
^{243}Pu	1.60 10^{7}	^{247}Cm	100.0
^{242}Am	141.0	^{242m}Am	99.6

Appendix 8 - Pathways

FISPACT calculates the inventory of nuclides after irradiation with no reference to the actual paths that are followed in the production of the various nuclides. The code can be used to carry out a sensitivity calculation to determine by how much the amount of a nuclide will vary if a particular cross section or half-life is varied. However, although very valuable for identifying important reactions and in the calculation of errors, this method requires a great deal of computer time and the results are not always easy to understand.

To overcome these problems the method of pathway analysis has been implemented in FISPACT. This technique enables the percentage of the final nuclide produced by a particular pathway to be calculated. Although the concept of 'pathway' is intuitive it requires careful definition. In this context a pathway refers to a series of nuclides all of which are distinct, joined in a linear fashion by links which either represent reactions or decays. There are no additional entry points on the pathway and all the depletion modes for each nuclide can be assumed to go to a sink and play no further part in the pathway. Note that because of the way that the first five nuclides in the decay library (the 'gas' nuclides) are labelled it is possible for these nuclides to be repeated in a pathway. This inconsistency is of little practical importance, but is noted as an area for improvement in a future version of FISPACT.

An example of a pathway is the production of ^{59}Ni from ^{59}Co:

^{59}Co(n,γ) ^{60m}Co(IT) ^{60}Co(β^-)^{60}Ni(n,2n) ^{59}Ni.

This is the most important pathway (in the first wall of the EEF fusion device) contributing (see reference 5) 54% of all the ^{59}Ni formed from ^{59}Co. This pathway contains 4 links consisting of 2 reactions and 2 decays. A diagram of this pathway is shown in Figure A8.1.

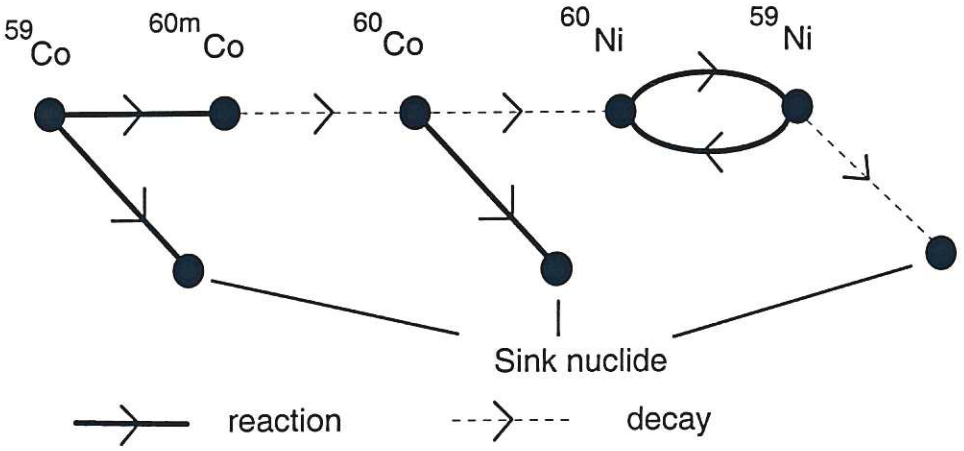

Figure A8.1. Diagram of a pathway from ^{59}Co to ^{59}Ni.

Several points in this definition require further discussion. The pathway is linear because any side paths either in or out can be considered as part of some other linear pathway. Also shown are the reactions or decays to a sink nuclide, this is a fictitious nuclide which is not followed by FISPACT, the reaction to it is actually the sum of all physical reactions on the target which do not lead to the next nuclide on the pathway. In the case of a radionuclide on the pathway connected to the next nuclide by a reaction, then a decay is shown to the sink nuclide.

The nuclides are all distinct as written down, although this conceals an important improvement in the calculation of pathways since version 3.0. As can be seen in Figure A8.1, a reaction arrow is shown between ^{59}Ni and ^{60}Ni, this means that the 'backward' reaction ^{59}Ni(n,γ) ^{60}Ni is included with the other 'forward' reactions in the calculation. This 'loop', involving (n,γ) and (n,2n) reactions allows the effects of burn-up of the parent in high fluxes to be included correctly. Note that in the first step of the pathway there is no loop as the half-life of ^{60m}Co is too short to have reaction data in the cross section library. Physically the inclusion of these loops means that in addition to the standard pathway all the others of the form shown below are also considered.

^{59}Co(n,γ)^{60m}Co(IT)^{60}Co(β$^-$)^{60}Ni(n,2n)^{59}Ni(n,γ)^{60}Ni(n,2n)^{59}Ni

$^{59}Co(n,\gamma)^{60m}Co(IT)^{60}Co(\beta^-)^{60}Ni(n,2n)^{59}Ni(n,\gamma)^{60}Ni(n,2n)^{59}Ni$
$(n,\gamma)^{60}Ni(n,2n)^{59}Ni$

It is important to note that these parallel pathways ***MUST*** not be asked for explicitly, the code will include them automatically whenever they are required.

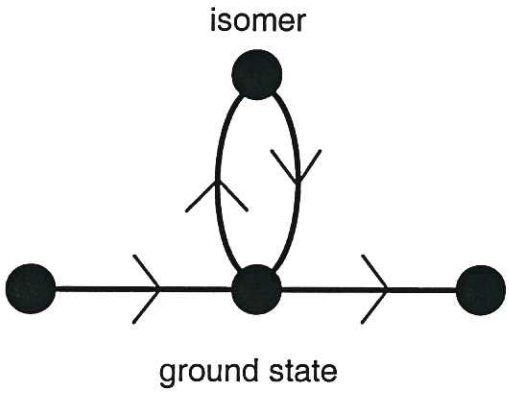

Figure A8.2. Detail of a diagram for a pathway containing an isomer loop.

There is a further type of loop, the inclusion of which is at the discretion of the user. If one of the nuclides on the pathway has an isomeric state of short half-life which decays back to the nuclide via an isomeric transition (IT), then a loop of the form X(n,n')X*(IT)X could also be included in the pathway replacing the X alone. An example of this is shown in Figure A8.2. The user is able to decide which isomers should be considered by means of the **LOOPS** code word, and this is often essential for the correct calculation of the pathway contribution if short-lived isomers of any of the nuclides in the pathway exist.

Since version 3.1 a change has been made during the routine calculation of pathways at the end of each time interval. By default the **LOOPS** code word is used with the time parameter set to the larger of 1 second or (time interval / 1000). For pathway calculations made using **PATHS** or **ROUTES** it is still necessary to switch on this feature with **LOOPS**, by default it is not used.

Since version 3.0 the output of 'generic' pathways has been possible. This was introduced because if many of the nuclides

on the path have isomeric states then a large number of separate pathways are identified all with the same basic structure and only differing by the presence of $X^{m}(IT)X^{g}$ links. Thus the two following pathways have the same generic pathway.

$^{190}Os(n,\gamma)^{191m}Os(IT)^{191}Os\ (\beta^-)^{191}Ir(n,\gamma)^{192}Ir$

$^{190}Os(n,\gamma)^{191}Os(\beta^-)^{191}Ir(n,\gamma)^{192m}Ir(IT)^{192}Ir$

$^{190}Os(n,\gamma)^{191}Os(\beta^-)^{191}Ir(n,\gamma)^{192}Ir$ [Generic]

By default the generic pathways are listed, but their output can be switched off by using the **GENERIC** code word.

FISPACT calculates the amount of the final daughter formed by a particular pathway in exactly the same way as for a full inventory, except that the number of nuclides is very much smaller. Only the nuclides in the pathway and a fictitious nuclide which acts as the sink for all the depletion modes of the nuclides (and any isomers specified by the **LOOPS** code word) are considered. The fictitious nuclide is ^{49}Fe which is assumed stable with zero reaction cross section. This nuclide is used in other calculations (impurities in an unreactive iron matrix) so it is convenient to also use it for this purpose.

When using the pathway option either routinely or in special runs it ***MUST*** be remembered that only a single irradiation step should be considered. If it is necessary to consider many irradiations (say for pulsed operation) then two possible solutions should be considered.

- Carry out pulsed calculations for the detailed inventory calculations, but in a separate run use an average flux over the total irradiation time to calculate pathways.
- Model the irradiation history so that the large majority of the fluence is in the initial irradiation step. Pathways will be calculated for this interval and the contribution of the final few pulses will be ignored.

In most cases the second option will be most useful as uncertainty estimates can also be given based on these approximate pathways.

Appendix 9 - Uncertainties

EAF3 was the first activation library to contain uncertainty information. Details of this uncertainty file for EAF3.1 are given in Reference 18. The file has been substantially improved for EAF-99 and some details of these changes are given below. The use of the uncertainty file and half-life uncertainties by FISPACT to calculate uncertainty estimates of the radiological quantities (*e.g.* activity) is then explained.

EAF_UN-99

Since version 4.1 both capture and fission cross sections have 3 rather than 2 uncertainty values in the file. The energy regions are defined in Table A9.1.

Table A9.1. Definition of uncertainty energy regions.

Low energy region	Medium energy region	High energy region
$1.0\ 10^{-5}$ eV - E_V	E_V - E_H	E_H - 20 MeV
E_V - End of $1/v$ behaviour of the cross section.	E_H - End of resolved resonance region of the cross section.	

The systematic values of the error factor used for capture and fission reactions are given in Table A9.2.

Table A9.2. Systematic values of error factor (f) used for capture and fission reactions.

Reaction	Low energy region	Medium energy region	High energy region
Capture	10	2	2.0
Fission	5	2	2.0

In EAF-99 the general principle that has been followed is that wherever experimental data are available these are used to estimate the error factors (f) for threshold reactions. The remainder of the error estimates are based on systematics.

FISPACT uncertainty estimation

FISPACT can use the sensitivity coefficients defined in Appendix 5 to calculate uncertainties in the number of atoms of a particular nuclide due to an uncertainty in a cross section. While practicable for particular cases the computer time involved in using this method for routine estimation of uncertainties of total radiological quantities would be too large. An alternative approach followed in FISPACT involves a simplified procedure which nevertheless gives an estimate adequate both for the quality of the cross section uncertainty data and for fusion applications.

The main steps in the simplified procedure are:

1. At the end of each time interval FISPACT lists the 20 most important nuclides for each of the five radiological quantities (activity, heating, γ dose rate, potential ingestion hazard and potential inhalation hazard) and the percentage contribution that each makes.
2. For each of these dominant nuclides the pathways and fractional contributions are calculated.
3. The uncertainty for each pathway is calculated using the 'sum of squares' of the errors of each reaction.
4. The errors for all parallel pathways contributing to a particular dominant nuclide are calculated.
5. The errors for each dominant nuclide contributing to a radiological quantity are calculated.

In order to describe each step mathematically several terms need to be defined. When deriving systematics of 14.5 MeV cross sections it was noted [30] that the quantities $\log(\sigma_{expt} / \sigma_{calc})$ were approximately normally distributed and that the best representation of error limits on σ_{calc} were $\sigma_{calc} f$ and σ_{calc} / f where f is termed the 'error factor'. The 'error' (ε) of a quantity is defined as the 'maximum estimate' - 'best value', thus $\varepsilon = \sigma f - \sigma$. The 'relative' or 'fractional error' (Δ) is the 'error' /

'best value', thus $\Delta = \varepsilon / \sigma$, and $f = 1 + \Delta$. If a cross section was 'known to 20%' then $\Delta = 0.2, f = 1.2$ and $\varepsilon = 0.2\ \sigma$.

The value of one of the radiological quantities at a particular time (Q) is given by equation A9.1.

$$Q = \sum_i q_i \quad \text{(A9.1)}$$

where q_i is the value of the quantity for nuclide i and the sum is over all dominant nuclides.

The fractional contribution (c_i) of each dominant nuclide is given by equation A9.2.

$$c_i = q_i / Q \quad \text{(A9.2)}$$

The error on the quantity Q (ΔQ) is given by equation A9.3.

$$(\Delta Q)^2 = \sum_i (\Delta q_i)^2 \quad \text{(A9.3)}$$

The radiological quantities are linearly dependant on the number of atoms present as shown by equation A9.4.

$$q_i = \alpha N_i \quad \text{(A9.4)}$$

where N_i is the number of atoms of nuclide i.

The error on the quantity q_i (Δq_i) is given by equation A9.5.

$$\Delta q_i = \left(\frac{\Delta N_i}{N_i} \right) q_i \quad \text{(A9.5)}$$

The dominant nuclide i can be produced by a set of parallel pathways, the total number of atoms of i is given by equation A9.6.

$$N_i = \sum_j N_{ij} \quad \text{(A9.6)}$$

where N_{ij} is the number of atoms of i formed by pathway j and the sum is over all pathways.

The fractional contribution (d_{ij}) of each pathway to i is given by equation A9.7.

$$d_{ij} = N_{ij} / N_i \quad \text{(A9.7)}$$

The error on the number of atoms N_i (ΔN_i) is given by equation A9.8.

$$(\Delta N_i)^2 = \sum_j (\Delta N_{ij})^2 \quad \text{(A9.8)}$$

Each pathway is a series of reactions (and decays) and the total number of atoms formed is the product of the individual cross sections as shown by equation A9.9.

$$N_{ij} = \beta \prod_k \sigma_k \quad \text{(A9.9)}$$

The error on the number of atoms formed by a particular pathway (ΔN_{ij}) is given by equation A9.10.

$$\left(\frac{\Delta N_{ij}}{N_{ij}}\right)^2 = \sum_k \left(\frac{\Delta \sigma_k}{\sigma_k}\right)^2 \quad \text{(A9.10)}$$

Using A9.5 to rewrite A9.3 gives equation A9.11.

$$(\Delta Q)^2 = \sum_i \left(\frac{\Delta N_i}{N_i}\right)^2 q_i^2 \quad \text{(A9.11)}$$

Using A9.8 to rewrite A9.11 gives equation A9.12.

$$(\Delta Q)^2 = \sum_i \frac{q_i^2}{N_i^2} \sum_j (\Delta N_{ij})^2 \quad \text{(A9.12)}$$

Using A9.10 to rewrite A9.12 gives equation A9.13.

$$(\Delta Q)^2 = \sum_i \frac{q_i^2}{N_i^2} \sum_j N_{ij}^2 \sum_k \left(\frac{\Delta \sigma_k}{\sigma_k}\right)^2 \quad \text{(A9.13)}$$

Using A9.2 to rewrite A9.13 gives equation A9.14.

$$(\Delta Q)^2 = \sum_i c_i^2 Q^2 \sum_j \left(\frac{N_{ij}}{N_i}\right)^2 \sum_k \left(\frac{\Delta \sigma_k}{\sigma_k}\right)^2 \quad \text{(A9.14)}$$

Using A9.7 to rewrite A9.14 gives equation A9.15.

$$\left(\frac{\Delta Q}{Q}\right)^2 = \sum_i c_i^2 \sum_j d_{ij}^2 \sum_k \left(\frac{\Delta \sigma_k}{\sigma_k}\right)^2 \quad \text{(A9.15)}$$

Equation 9.15 shows how the error of a radiological quantity depends on the individual cross section errors. This formula is correct in cases where there are no fission reactions on

actinides, but requires modification if actinides are included in the input materials.

In the derivation above it has been assumed that all errors are completely uncorrelated; however this assumption is no longer valid if fission is included. A particular fission product which is also a dominant nuclide can be produced by pathways that either include a fission reaction or do not. In the latter case the formalism derived above is correct, but if the pathway includes fission then it must be extended. If fission occurs then this can involve one of several actinide nuclides. This occurs because the input actinide is transmuted, by say, capture reactions and many fissionable actinides are therefore present. All pathways from a particular actinide to the dominant nuclide contain the same fission cross section and thus errors in these pathways are completely correlated. This means that the errors are added linearly rather than by the sum of squares procedure.

The set of pathways must therefore be partitioned into subsets labelled by the actinide from which it is produced. This is shown by equation A9.16

$$\{P_{ij}\} = \{P_{ij}\}_0 + \sum_m \{P_{ij}\}_m \quad \text{.....(A9.16)}$$

where

P_{ij} indicates the j th pathway forming nuclide i

the index 0 indicates pathways with no fission and the index m indicates that the fission was on actinide m.

To each of these subsets there corresponds a subset of j values (S_m) such that choosing a subset of j values defines a subset of pathways. Equation A9.8 can then be rewritten as equation A9.17

$$(\Delta N_i)^2 = \sum_{j \in S_0} (\Delta N_{ij})^2 + \sum_m \left(\sum_{j \in S_m} \Delta N_{ij} \right)^2 \quad \text{.....(A9.17)}$$

If A9.17 is used in the derivation then the final equation (A9.15) is modified as shown in equation A9.18.

$$\left(\frac{\Delta Q}{Q}\right)^2 = \sum_i c_i^2 \sum_{j \in S_0} d_{ij}^2 \sum_k \left(\frac{\Delta \sigma_k}{\sigma_k}\right)^2 + \sum_i c_i^2 \sum_m \left(\sum_{j \in S_m} d_{ij} \sqrt{\sum_k \left(\frac{\Delta \sigma_k}{\sigma_k}\right)^2} \right)^2$$

.....(A9.18)

The above derivation is correct so long as only cross section uncertainties are considered. In FISPACT-97 the facility to consider half-life uncertainties was included. The derivation therefore needs to be extended, to do this requires additional justification of the whole of the pathway methodology, this is included in the current Appendix for completeness. Note that this extends the original theoretical development given in Appendix 1 of reference 31.

Pathways containing 2 reactions only

Consider the 2-link pathway (both reactions) shown in Figure A9.1, where it is assumed that the final nuclide neither reacts nor decays. This constraint is removed in the treatment of a later section. Note that it is assumed that there is no cross section for a parent nuclide to be reformed from its daughter - this is true in the low burn-up limit.

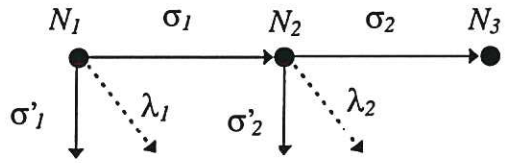

Figure A9.1. A 2-link pathway, consisting of reactions only.

The symbols used in Figure 1 are defined below, the label *i* can be used for nuclides 1, 2 or 3:

N_i Number of atoms of nuclide

λ_i Decay constant (s^{-1})

σ_i Cross section of a pathway reaction (cm^2)

σ'_i Sum of all cross sections of a target excluding the pathway reaction (cm^2)

The differential equation satisfied by nuclide 1 is given in equation A9.19.

$$\frac{dN_1}{dt} = -\lambda_1 N_1 - (\sigma_1 + \sigma_1')\phi N_1 = -\Lambda_1 N_1 \quad \text{(A9.19)}$$

The solution is given in equation A9.20.

$$N_1(t) = N_{10} e^{-\Lambda_1 t} \quad \text{(A9.20)}$$

The differential equation satisfied by nuclide 2 is given in equation A9.21.

$$\frac{dN_2}{dt} = -\lambda_2 N_2 - (\sigma_2 + \sigma_2')\phi N_2 + \sigma_1 \phi N_1 = -\Lambda_2 N_2 + \sigma_1 \phi N_{10} e^{-\Lambda_1 t} \quad \text{(A9.21)}$$

Using a standard integrating factor, the solution is given in equation A9.22.

$$N_2(t) = e^{-\Lambda_2 t} \int \sigma_1 \phi N_{10} e^{-\Lambda_1 t} e^{\Lambda_2 t} dt \quad \text{(A9.22)}$$

Evaluating the integral in equation A9.22, assuming that $N_2(0) = 0$, yields equation A9.23.

$$N_2(t) = \frac{\sigma_1 \phi N_{10}}{(\Lambda_1 - \Lambda_2)} \left[e^{-\Lambda_2 t} - e^{-\Lambda_1 t} \right] \quad \text{(A9.23)}$$

The differential equation satisfied by nuclide 3 is given in equation A9.24.

$$\frac{dN_3}{dt} = \sigma_2 \phi N_2 \quad \text{(A9.24)}$$

The solution obtained by integrating equation A9.23 is given in equation A9.25.

$$N_3(t) = \frac{\sigma_1 \sigma_2 \phi^2 N_{10}}{(\Lambda_1 - \Lambda_2)} \left[(1 - e^{-\Lambda_2 t})/\Lambda_2 - (1 - e^{-\Lambda_1 t})/\Lambda_1 \right] \quad \text{(A9.25)}$$

We can consider two limiting cases of equation A9.25 termed 'long-lived' and 'short-lived'. Consider typical values for the quantities ϕ, $(\sigma + \sigma')$ and the irradiation time T: 10^{15} $cm^{-2}s^{-1}$, 10^{-25} cm^2 and 10^8 s. When a nuclide has a half-life of 1 s then $\lambda = 0.693$, $\lambda >> \phi(\sigma + \sigma')$ and $\lambda >> T^{-1}$. When a nuclide has a half-life of 1000 y then $\lambda = 2.196\ 10^{-11}$, $\lambda << \phi(\sigma + \sigma')$ and $\phi(\sigma + \sigma') << T^{-1}$.

If both nuclides 1 and 2 are long-lived then $\Lambda_i t << 1$ and the exponential can be expanded, keeping terms up to $O(t^2)$. This limit is given in equation A9.26.

$$N_3(t) \xrightarrow{L} \sigma_1\sigma_2\phi^2 N_{10} t^2/2 \quad \text{..... (A9.26)}$$

If both nuclides 1 and 2 are short-lived then $\Lambda_i t >> 1$ and the exponential can be set to zero. This limit is given in equation A9.27.

$$N_3(t) \xrightarrow{S} \sigma_1\sigma_2\phi^2 N_{10}/\lambda_1\lambda_2 \quad \text{..... (A9.27)}$$

Equations A9.26 and A9.27 suggest that in these two limits the number of atoms of the final nuclide in the pathway is obtained by multiplying the starting number of atoms by a factor for each link. If the nuclide is long-lived then the factor is $\sigma\phi t$, while if the nuclide is short-lived then the factor is $\sigma\phi/\lambda$. In addition, in the case of long-lived nuclides there is a multiplicative constant factor.

Pathways containing arbitrary number of reactions

In general there can be an arbitrary number of links; if there are $(n+1)$ links then equation A9.28 expresses how the number of atoms N_{n+1} is related to the number of atoms N_n.

$$\frac{dN_{n+1}}{dt} = -\Lambda_{n+1}N_{n+1} + \sigma_n\phi N_n \quad \text{..... (A9.28)}$$

This is valid for all $n \geq 1$. A solution can be found using the method of Laplace transforms. The Laplace transform of $N_{n+1}(t)$ is $\hat{N}_{n+1}(p)$, which is defined in equation A9.29.

$$\hat{N}_{n+1}(p) = \int_0^\infty e^{-pt} N_{n+1}(t)dt = L(N_{n+1}(t)) \quad \text{..... (A9.29)}$$

Using the standard result for the Laplace transform of a differential given by equation A9.30, it is possible to transform equation A9.28 as shown in equation A9.31.

$$L\left(\frac{dN_{n+1}}{dt}\right) = pL(N_{n+1}) - N_{n+1}(0) \quad \text{..... (A9.30)}$$

$$p\hat{N}_{n+1} = -\Lambda_{n+1}\hat{N}_{n+1} + \sigma_n\phi\hat{N}_n$$

$$\Rightarrow \hat{N}_{n+1}(p) = \frac{\sigma_n\phi}{p+\Lambda_{n+1}}\hat{N}_n(p) \quad \text{..... (A9.31)}$$

Equation A9.31 can be applied repeatedly until $n = 1$, yielding equation A9.32.

$$\hat{N}_{n+1}(p) = \frac{\phi^n \prod_{i=1}^{n} \sigma_i}{\prod_{i=2}^{n+1} (p + \Lambda_i)} \hat{N}_1(p) \quad \text{(A9.32)}$$

The solution for N_1 is given in equation A9.20, the Laplace transform of this is given in equation A9.33.

$$\hat{N}_1(p) = \frac{N_{10}}{(p + \Lambda_1)} \quad \text{(A9.33)}$$

Combining equations A9.32 and A9.33 yields equation A9.34, the final expression for the transform.

$$\hat{N}_{n+1}(p) = \frac{\phi^n N_{10} \prod_{i=1}^{n} \sigma_i}{\prod_{i=1}^{n+1} (p + \Lambda_i)} \quad \text{(A9.34)}$$

In order to obtain the expression for $N_{n+1}(t)$ it is necessary to use the inverse Laplace transform which is given in equation A9.35, where the variable p has been written as z to emphasise that the integral is defined in the complex plane.

$$N_{n+1}(t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \hat{N}_{n+1}(z) e^{zt} dz \quad \text{(A9.35)}$$

The value of c can be set to zero, since all poles in the transform are for Real(z) < 0 (this corresponds to all decay constants and cross sections being positive). Given the form of the transform shown in equation A9.34, it can be seen that completing the path of integration by a semicircle at infinity in the negative half-plane will contribute nothing to the integral and it is therefore possible to replace it with a contour enclosing all the poles of the transform. The value of the contour integral is given by $2\pi i$ times the sum of the residues at the poles. Equation A9.34 shows that all the poles are simple, and for the pole at $-\Lambda_j$ the residue is given by equation A9.36. The prime on the product sign in all equations in this section indicates that the term with $i = j$ is excluded.

$$R(-\Lambda_j) = \frac{\phi^n N_{10} \prod_{i=1}^{n} \sigma_i \cdot e^{-\Lambda_j t}}{\prod_{i=1}^{n+1}{}' (\Lambda_i - \Lambda_j)} \quad \text{..... (A9.36)}$$

There are n+1 simple poles and the sum of the residues is given in equation A9.37.

$$\sum R = \phi^n N_{10} \prod_{i=1}^{n} \sigma_i \cdot \sum_{j=1}^{n+1} \left(e^{-\Lambda_j t} \Big/ \prod_{i=1}^{n+1}{}' (\Lambda_i - \Lambda_j) \right) \quad \text{..... (A9.37)}$$

Combining equations A9.34, A9.35 and A9.37 and introducing the factor $(-1)^n$ since the factor in the product in the denominator has the labels i and j interchanged, yields equation A9.38, the final form of the solution of equation A9.28.

$$N_{n+1}(t) = (-1)^n N_{10} \phi^n \prod_{i=1}^{n} \sigma_i \cdot \sum_{j=1}^{n+1} \left(e^{-\Lambda_j t} \Big/ \prod_{i=1}^{n+1}{}' (\Lambda_j - \Lambda_i) \right) \quad \text{(A9.38)}$$

Corresponding to equation A9.25 for the final nuclide in the 2-link case, the number of atoms of the final nuclide in the n+1 link case is given by equation A9.39.

$$N_{n+2}(t) = (-1)^{n+1} N_{10} \phi^{n+1} \prod_{i=1}^{n+1} \sigma_i \cdot \sum_{j=1}^{n+1} \left((e^{-\Lambda_j t} - 1) / \Lambda_j \prod_{i=1}^{n+1}{}' (\Lambda_j - \Lambda_i) \right)$$

..... (A9.39)

An identity can be derived by using equation A9.38 and solving equation A9.28 by direct integration. The solution of equation A9.28 using a standard integrating factor is given in equation A9.40.

$$N_{n+1} = e^{-\Lambda_{n+1} t} \int \sigma_n \phi N_n e^{\Lambda_{n+1} t} dt \quad \text{..... (A9.40)}$$

Using equation A9.38 and rearranging yields equation A9.41.

$$N_{n+1}(t) = (-1)^{n-1} N_{10} \phi^n \prod_{i=1}^{n} \sigma_i \cdot e^{-\Lambda_{n+1} t} \sum_{j=1}^{n} \left(\int e^{-(\Lambda_j - \Lambda_{n+1}) t} dt \Big/ \prod_{i=1}^{n}{}' (\Lambda_j - \Lambda_i) \right)$$

..... (A9.41)

Performing the integrals and using the relationship in equation A9.42 yields equation A9.43.

$$\prod_{i=1}^{n+1}{}' (\Lambda_j - \Lambda_i) = (\Lambda_j - \Lambda_{n+1}) \prod_{i=1}^{n}{}' (\Lambda_j - \Lambda_i) \quad \text{..... (A9.42)}$$

$$N_{n+1}(t) = (-1)^n N_{10} \phi^n \prod_{i=1}^{n} \sigma_i \cdot \left[\sum_{j=1}^{n} (e^{-\Lambda_j t} \Big/ \prod_{i=1}^{n+1}{}' (\Lambda_j - \Lambda_i)) - e^{-\Lambda_{n+1} t} \sum_{j=1}^{n} (1 \Big/ \prod_{i=1}^{n+1}{}' (\Lambda_j - \Lambda_i)) \right]$$

..... (A9.43)

Comparing equations A9.38 and A9.43, it can be seen that the first n terms of the sum are already correctly given by the first sum in equation A9.43. If the final term ($j = n+1$) is also to be correct then the identity shown in equation A9.44 must be true.

$$\sum_{j=1}^{n} \left(1 \Big/ \prod_{i=1}^{n+1}{}' (\Lambda_j - \Lambda_i) \right) = -1 \Big/ \prod_{j=1}^{n} (\Lambda_{n+1} - \Lambda_j) \quad \text{..... (A9.44)}$$

Pathways containing 2 decays only

Consider the 2-link pathway (both decays) shown in Figure A9.2, where it can be seen that the quantity linking two nuclides is λ rather than σ as in Figure A9.1.

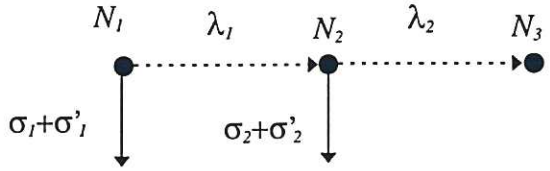

Figure A9.2. A 2-link pathway, consisting of decays only.

The solution of the set of differential equations for N_i is formally the same as above, if $\sigma_i \phi$ is replaced by λ_i. The solution for N_3 is given in equation A9.45.

$$N_3(t) = \frac{\lambda_1 \lambda_2 N_{10}}{(\Lambda_1 - \Lambda_2)} \left[(1 - e^{-\Lambda_2 t})/\Lambda_2 - (1 - e^{-\Lambda_1 t})/\Lambda_1 \right] \text{..... (A9.45)}$$

Considering the limit of equation A9.45 in both the long- and short-lived cases yields equations A9.46 and A9.47, respectively.

$$N_3(t) \xrightarrow{L} \lambda_1 \lambda_2 N_{10} t^2/2 \quad \text{..... (A9.46)}$$

$$N_3(t) \xrightarrow{S} N_{10} \quad \text{..... (A9.47)}$$

Thus the factor that can be deduced for the long-lived nuclide decaying is λt, and for a short lived nuclide it is 1.

Pathways containing an arbitrary number of decays

The general case of n+1 decay links can be solved by replacing $\sigma_i\phi$ by λ_i in equation A9.39. This is shown in equation A9.48.

$$N_{n+2}(t) = (-1)^{n+1} N_{10} \prod_{i=1}^{n+1} \lambda_i \cdot \sum_{j=1}^{n+1} \left((e^{-\Lambda_j t} - 1) / \Lambda_j \prod_{i=1}^{n+1}{}' (\Lambda_j - \Lambda_i) \right)$$

.....(A9.48)

Limits in arbitrary pathways

In the cases of two reactions or two decays the long-lived limits are shown in equations A9.26 and A9.46, and the short-lived limits in equations A9.27 and A9.47. In the general cases it should be possible using the same approach to find the limiting forms of equations A9.39 and A9.48. However, the algebra is very difficult and a set of identities similar to equation A9.44 is required. It is much simpler to apply the limits to the original equation A9.28 and solve this. In the long-lived limit $\Lambda_i t << 1$ and equation A9.28 can be simplified to give equation A9.49.

$$\frac{dN_{n+1}}{dt} = \sigma_n \phi N_n \quad \text{..... (A9.49)}$$

This can be integrated step by step, starting with the limiting form of equation A9.20, namely $N_1(t) = N_{10}$. To find the general solution a proof by induction can be used. Suppose that the form of $N_n(t)$ is given by equation A9.50. Then integrating the right hand side of equation A9.49 gives M as shown in equation A9.51. Comparing this with the form of equation A9.50 it can be seen that $M = N_{n+1}(t)$. Because this form is true for $n = 2$ (see equation A9.26), this argument shows it will be true for all $n \geq 2$.

$$N_n(t) = \prod_{i=1}^{n-1} \sigma_i \cdot \phi^{n-1} N_{10} t^{n-1} / (n-1)! \quad \text{..... (A9.50)}$$

$$M(t) = \prod_{i=1}^{n} \sigma_i \cdot \phi^n N_{10} \int_0^t \frac{t'^{n-1}}{(n-1)!} dt' = \prod_{i=1}^{n} \sigma_i \cdot \phi^n N_{10} t^n / n! \quad \text{(A9.51)}$$

The exact equation for the production of $N_{n+2}(t)$ is the same as the limiting form for the production of $N_{n+1}(t)$ as can be seen by comparing equations A9.24 and A9.49. Thus trivially the long-

lived limit for the final nuclide in an n+1 link pathway containing reactions is given in equation A9.52.

$$N_{n+2}(t) \xrightarrow{L} \prod_{i=1}^{n+1} \sigma_i \cdot \phi^{n+1} N_{10} t^{n+1} / (n+1)! \quad \text{(A9.52)}$$

In the short-lived limit then $\Lambda_i t >> 1$ and the differential can be set to zero. Equation A9.28 can be simplified to give equation A9.53.

$$N_{n+1} = \frac{\sigma_n \phi N_n}{\Lambda_{n+1}} \quad \text{(A9.53)}$$

This is easily solved to give equation A9.54.

$$N_{n+1}(t) = \prod_{i=1}^{n} \frac{\sigma_i}{\lambda_{i+1}} \cdot \phi^n N_1(t) \quad \text{(A9.54)}$$

The number of atoms of N_{n+2}, the final nuclide in the pathway (stable with no reactions) is calculated by integrating the equation equivalent to equation A9.24. This is shown in equation A9.55.

$$N_{n+2}(t) \xrightarrow{S} \sigma_{n+1} \phi \int_0^t N_{n+1}(t')dt' = \prod_{i=1}^{n+1} \left(\frac{\sigma_i}{\lambda_i} \right) \phi^{n+1} N_{10} \quad \text{(A9.55)}$$

Equations A9.52 and A9.55 are the general limiting forms of which equations A9.26 and A9.27 are special cases.

For the general case of a pathway containing decays, the corresponding limits of equation A9.48 are given in equations A9.56 and A9.57.

$$N_{n+2}(t) \xrightarrow{L} \prod_{i=1}^{n+1} \lambda_i \cdot N_{10} t^{n+1} / (n+1)! \quad \text{(A9.56)}$$

$$N_{n+2}(t) \xrightarrow{S} N_{10} \quad \text{(A9.57)}$$

Equations A9.56 and A9.57 are the general limiting forms of which equations A9.46 and A9.47 are special cases.

Pathways in which the final nuclide reacts and decays

In the derivations so far it has been assumed that the final nuclide in the pathway neither reacts or decays. In general this will not be true and it is necessary to determine what additional

factor would be introduced in both limits by allowing the constraint on the final nuclide to be removed.

Firstly assume that all the nuclides are long-lived. The limit of this case is trivially obtained from equation A9.50; there is no effect on the limit of the final long-lived nuclide.

Secondly assume that all the nuclides are short-lived. As can be seen from equation A9.38, setting the exponential of all terms (including the final one) to zero means that the limit for the number of atoms of the final nuclide is also zero (as expected physically since they have all decayed!). However, this is not very helpful and a physical argument is required.

The pathway for the production of a final nuclide will only need to be considered if the final nuclide is long enough lived to contribute significantly to radiological quantities. Thus the nuclide may be short-lived (compared to the irradiation time), but it is not so short-lived that all its atoms have decayed. Thus the number of atoms of the final nuclide must be in secular equilibrium with the previous nuclide and so not all the previous nuclides can be short-lived. Assume that all the nuclides in the pathway are long-lived except the final one. Thus, in secular equilibrium the number of atoms of the final nuclide is given by equation A9.58.

$$N_{n+2} = \frac{\sigma_{n+1}}{\Lambda_{n+2}} N_{n+1} \quad \text{..... (A9.58)}$$

In the long-lived limit N_{n+1} is given by equation A9.51. Substituting this value into equation A9.58 and rearranging yields equation A9.59.

$$N_{n+2} = \prod_{i=1}^{n+2} \sigma_i \phi^{n+1} N_{10} t^{n+1} / (n+1)! \Big/ (\lambda_{n+2} t / n+1) \quad \text{..... (A9.59)}$$

Equation A9.59 shows that in the short-lived limit for the final nuclide there is an additional factor of $(n+1)/\lambda_{n+2}t$ due to the final nuclide being short-lived rather than long-lived.

Summary of factors for each type of pathway link

The previous two sections show that for both long- and short-lived limits of the number of atoms of the final nuclide in the pathway, these are calculated by forming a product of factors, one for each link in the pathway, and multiplying this by the initial number of atoms of the first nuclide.

Table A9.3 lists these factors and also includes the additional factor that is determined by the half-life of the final nuclide.

Table A9.3. Factors for pathway links.

Type of link	Factor
Link is reaction from a long-lived nuclide	$\sigma\phi t$
Link is reaction from a short-lived nuclide	$\sigma\phi/\lambda$
Link is decay from a long-lived nuclide	λt
Link is decay from a short-lived nuclide	1
Final nuclide is long-lived	1
Final nuclide is short-lived	$n/(\lambda_{final}t)$

Note there is an additional numeric factor of $1/n_L!$, where n_L = number of long-lived links. n = total number of links.

FISPACT uncertainties

In the case that only uncertainties in the reaction cross sections are considered then the analysis above gives justification for the form of equation A9.9. If uncertainties in decay constants are also included then it is necessary to specify the type of each nuclide in the pathway since the final uncertainty will depend on whether each nuclide is long- or short-lived.

The notation L_r used in reference 31 for a reaction on a long-lived nuclide in a pathway, would be inconvenient to use in computer output. Therefore the notation shown in Table A9.4 is proposed to describe pathways.

Table A9.4. Notation for pathway description.

Symbol	Description	Reduced factor	Number of links
R	Link is reaction from a long-lived nuclide	σ	n_R
r	Link is reaction from a short-lived nuclide	σ/λ	n_r
D	Link is decay from a long-lived nuclide	λ	n_D
d	Link is decay from a short-lived nuclide	1	n_d
L	Final nuclide is long-lived	1	-
S	Final nuclide is short-lived	$1/\lambda$	-

The notation for one of the 4-link pathways with a final nuclide long-lived is written as [RRrD|L], where the symbols for the links are enclosed by '[..|', while the symbol for the final nuclide is enclosed by '|.]'. This notation is also convenient for displaying in the FISPACT output.

Table A9.4 also shows the 'reduced factor' for each type of link and final nuclide. This factor is obtained from the factors for links summarised in Table A9.3, but with the terms containing flux and numerical constants removed. This reduced factor is convenient since for a particular calculation both the irradiation time and the flux are constant for all pathways. The final column defines the number of each type of link in the pathway.

Thus, corresponding to equation A9.9, equation A9.60 can be written to express the dependence of the number of atoms on the character of the pathway.

$$N_{ij} = \beta' \prod_{k=1}^{n_R+n_r} \sigma_k \prod_{l=1}^{n_r} \left(\frac{1}{\lambda_l}\right) \prod_{m}^{n_D} \lambda_m \cdot \zeta / \lambda_{final} \quad \text{..... (A9.60)}$$

where $\zeta = 1$ if the final nuclide is short-lived and $\zeta = \lambda_{final}$ if the final nuclide is long-lived.

Thus equation A9.10 is modified as shown in equation A9.61 to reflect the changes due to the decay constant uncertainties. Note that the limit on the second summation contains both short-lived reactions and long-lived decays since the error terms for λ and $1/\lambda$ are identical.

$$\left(\frac{\Delta N_{ij}}{N_{ij}}\right)^2 = \sum_{k=1}^{n_R+n_r}\left(\frac{\Delta\sigma_k}{\sigma_k}\right)^2 + \sum_{m=1}^{n_r+n_D+\delta}\left(\frac{\Delta\lambda_m}{\lambda_m}\right)^2 \quad \text{.....(A9.61)}$$

where $\delta = 1$ if the final nuclide is short-lived and $\delta = 0$ if the final nuclide is long-lived.

In equations A9.15 and A9.18 one-group ('collapsed') cross sections are used. It is necessary for FISPACT to also process the uncertainty data given in the EAF uncertainty file before it can be used. This process is described in the next section.

Collapsing uncertainty data

The EAF uncertainty file contains values of the energy boundaries (*e.g.* E_V and E_H) and values of Δ^2 for each energy range. In the case of threshold reactions only one energy range is considered (threshold - 20 MeV) and so the shape of the neutron flux is unimportant. But for fission and capture three values are given and these must be combined taking into account the shape of the neutron spectrum.

The effective cross section ($\overline{\sigma}$) used by FISPACT is defined by equation A9.62.

$$\overline{\sigma} = \sum_i \sigma_i\phi_i \Big/ \sum_i \phi_i \quad \text{.....(A9.62)}$$

where

σ_i is the cross sections in group i

ϕ_i is the neutron flux in group i

and the sum is over all energy groups.

If Δ_i is the relative error of the cross section in a particular energy group then the error (ε_i) of a particular weighted group cross section is given by equation A9.63.

$$\varepsilon_i = \frac{\sigma_i\phi_i}{\sum_i \phi_i}\Delta_i \quad \text{.....(A9.63)}$$

The following two assumptions are made:

1. Errors in all the groups of a particular energy range are 100% correlated.
2. The errors in the three energy ranges are 0% correlated.

The first means that the error used for a particular energy range determines the position of the cross section curve - its shape is correct in that range, but its absolute position is uncertain. While the second implies that there are independent measurements in the various energy ranges.

Using assumption 1 the error in an energy range is given by equation A9.64.

$$\varepsilon_I = \frac{\Delta_I}{\sum_i \phi_i} \sum_{i \in S_I} \sigma_i \phi_i \quad \text{.....(A9.64)}$$

where

$I \in$ {Low, Medium, High}

S_I is the set of groups in the various energy ranges.

Assumption 2 means that the total error is given by equation A9.65.

$$\varepsilon^2 = \sum_I \varepsilon_I^2 \quad \text{.....(A9.65)}$$

The corresponding total relative error (Δ) is given by equation A9.66.

$$\Delta = \varepsilon / \overline{\sigma} \quad \text{.....(A9.66)}$$

The weighted cross section ($\overline{\sigma}_I$) in one of the energy regions is defined by equation A9.67.

$$\overline{\sigma}_I = \sum_{i \in S_I} \sigma_i \phi_i \Big/ \sum_i \phi_i \quad \text{.....(A9.67)}$$

Combining equations A9.64 - A9.67 the total relative error is shown by equation A9.68.

$$\Delta^2 = \sum_I \Delta_I^2 \left(\frac{\overline{\sigma}_I}{\overline{\sigma}} \right)^2 \quad \text{.....(A9.68)}$$

Equation A9.68 is used by FISPACT to collapse the uncertainty data for a particular neutron spectrum.

Appendix 10 - γ group structures

There are two gamma energy group structures used in FISPACT. The 24-group structure is the default, while the 22-group must be requested by the code word **GROUP**. Table A10.1 shows the values of the group boundaries for both structures.

Table A10.1. Energy group structure for the 24- and 22-group formats.

Group number	Energy range (MeV) 24 groups	Group number	Energy range (MeV) 22 groups
1	0.00 - 0.01	1	0.00 - 0.01
2	0.01 - 0.02	2	0.01- 0.10
3	0.02 - 0.05	3	0.10 - 0.20
4	0.05 - 0.10	4	0.20 - 0.40
5	0.10 - 0.20	5	0.40 - 1.00
6	0.20 - 0.30	6	1.00 - 1.50
7	0.30 - 0.40	7	1.50 - 2.00
8	0.40 - 0.60	8	2.00 - 2.50
9	0.60 - 0.80	9	2.50 - 3.00
10	0.80 - 1.00	10	3.00 - 3.50
11	1.00 - 1.22	11	3.50 - 4.00
12	1.22 - 1.44	12	4.00 - 4.50
13	1.44 - 1.66	13	4.50 - 5.00
14	1.66 - 2.00	14	5.00 - 5.50
15	2.00 - 2.50	15	5.50 - 6.00
16	2.50 - 3.00	16	6.00 - 6.50
17	3.00 - 4.00	17	6.50 - 7.00
18	4.00 - 5.00	18	7.00 - 7.50
19	5.00 - 6.50	19	7.50 - 8.00
20	6.50 - 8.00	20	8.00 - 10.00
21	8.00 - 10.00	21	10.00 - 12.00
22	10.00 - 12.00	22	12.00 - 14.00
23	12.00 - 14.00		
24	14.00 →		

Appendix 11 - Error messages

During the course of a FISPACT run the program can terminate prematurely if mistakes are made in the syntax of the code words in the **INPUT** file. If this happens then the **OUTPUT** file will contain one of the following error messages. If the message ends with a code word in square brackets ([ ]), then the user should consult the earlier sections to check the syntax and the allowed values of the parameters. If the message ends with a subroutine name in angle brackets (< >), then the error has occurred in the named subroutine. UKAEA should be contacted if a solution to the problem cannot be found.

Error Messages

1 or 2 required [DOSE]
Only 22 or 24 gamma groups can be specified.

69, 100, 172, 175 or 315 required for N2COLL [COLLAPSE]
The neutron spectrum ***MUST*** be in 69, 100, 172, 175 or 315 groups.

All nuclides must be fissionable [FISYIELD]
Specified nuclides ***MUST*** be fissionable actinides.

ATWO and CLEAR both used [ATWO]
Only one of these two code words can be used per case.

ATWO and CLEAR both used [CLEAR]
Only one of these two code words can be used per case.

Cannot find uncertainty - no library data [UNCERTAINTY]
There is no uncertainty data in the cross section library, so cannot work out error estimates only give pathway information.
IUNCER ***MUST*** be 0, 3 or 4.

Characters required for NEWNAM [NEWFILE]
File name ***MUST*** consist of characters.

Chemical symbol not recognised <CNVTXT>
The chemical symbol ***MUST*** represent one of the elements H - Fm and be in normal form *e.g.* 'AG'.

Chemical symbol not recognised <RENUCL>
The chemical symbol ***MUST*** represent one of the elements H - Fm.

Chemical symbol not recognised [MASS]
The chemical symbol ***MUST*** represent a naturally occurring element.

Chemical symbol not recognised [PARTITION]
The chemical symbol ***MUST*** represent one of the elements H - Fm and be entered in upper case.

Chemical symbol required <RENUCL>
Specify the nuclide identifier as 'AG108' not '108AG'.

Chemical symbol required [MASS]
A chemical symbol *e.g.* 'AG' ***MUST*** follow the code word.

Code word PULSE has not been used [ENDPULSE]
The code words **PULSE** and **ENDPULSE** ***MUST*** occur in a pair - cannot have **ENDPULSE** without a matching **PULSE**.

Code word required [ENFA]
A second code word ***MUST*** follow the code word.

Contribution must be in range 0 to 100% [DOMINANT]
A value between 0 and 100% ***MUST*** be used.

D or R required to specify link [PATH]
When specifying a pathway use an 'R' if the link is a reaction or a 'D' if it is a decay.

Daughter isotope not recognised <OVERID>
The daughter isotope specified after the **OVER** code word is not in the index of nuclides, check that the isotope has been correctly entered.

Daughter nuclide not in library [PATH]
The daughter nuclide specified in a particular pathway is not present in the decay or cross section libraries.

Daughter nuclide of reaction not in library <COL069>
The daughter nuclide of a reaction in the cross section library is not present in the decay library, has the correct decay library been used?

Daughter nuclide of reaction not in library <COL100>
The daughter nuclide of a reaction in the cross section library is not present in the decay library, has the correct decay library been used?

Daughter nuclide of reaction not in library <COL172>
The daughter nuclide of a reaction in the cross section library is not present in the decay library, has the correct decay library been used?

Daughter nuclide of reaction not in library <COL175>
The daughter nuclide of a reaction in the cross section library is not present in the decay library, has the correct decay library been used?

Daughter nuclide of reaction not in library <COL315>
The daughter nuclide of a reaction in the cross section library is not present in the decay library, has the correct decay library been used?

Decay library and index file not consistent <ENDFPR>
A nuclide appears in the decay library which is not present in the **INDEX** file, has the correct decay library been used?

Decay mode not allowed in library <ENDFP>
A decay mode unknown to FISPACT has been found in the decay library, has the correct decay library been used?

DECIN: Too many input errors
An error has occurred in one of the 'DECIN' functions (responsible for the processing of the **INPUT** file), check the input syntax.

File HALFUNC is not connected to stream 38 [UNCTYPE]
Check that the file **FILES** contains a valid file name on a line starting with stream 38.

Fractional error required for ERMAT [ERROR]
There is no uncertainty data in the cross section library, so the fractional error value ***MUST*** be specified for *ERMAT*.

FUEL and MASS both used [FUEL]
Only one of these two code words can be used per case.

FUEL and MASS both used [MASS]
Only one of these two code words can be used per case.

Group structures in GRPC and COLL incompatible [COLLAPSE]
The output group structure defined by **GRPCONVERT** and **COLLAPSE** ***MUST*** be compatible.

IGENER can takes values 0 or 1 [GENERIC]
The generic output is either on or off.

Incompatible input group structure [GRPCONVERT]
The output group structure defined by **GRPCONVERT** and **COLLAPSE** ***MUST*** be the same.

IPCWRT can takes values 0 or 1 [SEQUENTIAL]
The pseudo cross section output is either on or off.

ISEQUE can takes values 0 or 1 [SEQUENTIAL]
Sequential charged particle reactions are either considered or not.

Isomer appears stable <CHAINP>
One of the isomers that is to be included in the calculation by **LOOPS** appears to be stable, has the *TLOOP* parameter been sensibly set?

Isomer does not decay to gs <CHAINP>
One of the isomers that is to be included in the calculation by **LOOPS** does not decay back to the ground state nuclide on the pathway, so no loop is formed.

Isomer not in library <RENUCL>
The nuclide specified does not have an isomeric state in the current library, has the correct decay library been used?

Isomer not in library [FUEL]
The isomer specified is not in the decay library.

Isomer symbol not recognised <CNVTXT>
The isomer symbol ***MUST*** be either 'm' or 'n' and be in lower case.

Isomer symbol not recognised <RENUCL>
The isomer symbol ***MUST*** be either 'm' or 'n' in upper or lower case.

Isotope and daughter not recognised <OVERID>
The isotope specified after the **OVER** code word is not in the index of nuclides, check that the isotope has been correctly entered.

Isotope not recognised <OVERID>
The isotope specified after the **OVER** code word is not in the index of nuclides, check that the isotope has been correctly entered.

ITDEC: Invalid argument
An argument of one of the 'DECIN' functions (responsible for the processing of the **`INPUT`** file) is invalid. UKAEA should be contacted for advice.

JSTRM can only be 12, 17 or 20 [NEWFILE]
Only files connected to streams 12, 17 or 20 can be redefined.

LAMBDA or SIGMA required [SENSITIVITY]
If the sensitivity with respect to half-life is required then **LAMBDA *MUST*** follow the code word, else **SIGMA *MUST*** follow the code word.

LINA, TAPA or ARRAY required [ENFA]
The code word ***MUST*** be one of these three options.

M or N required for isomer [FUEL]
Specify isomer by 'M' for first or 'N' for second.

MONIT can takes values 0 or 1 [MONITOR]
The output of code words is either on or off.

NDSTRC can only be 69, 100, 172, 175 or 315 [GRPCONVERT]
The output group structure ***MUST*** be one of the 5 standard types.

NEAFVN can takes values 2, 3 or 4 [EAFVERSION]
Only versions 2, 3 or 4 of EAF are considered.

NESTRC can takes values 2 to 400 [GRPCONVERT]
The input group structure ***MUST*** have between 2 and 400 groups.

No neutron spectrum available <ENDFPR>
In order to process the fission yield data a **FLUXES** file ***MUST*** be available, check **FILES** to ensure that the name is correct.

No space before isomer label [OVER]
There ***MUST*** be no space between the atomic mass and the isomer label in a nuclide identifier.

No value for density if FUEL used [MASSIN]
Density ***MUST*** be specified if **FUEL** is used, it can be calculated only if **MASS** is used.

No wall loading or ID in input [GRPCONVERT]
There is either no data on the wall loading or no a text string describing the spectrum.

NPULSE can take values 2 to 500 [PULSE]
The value specified for the number of times to loop is invalid - it must be in the range 2 - 500.

Nuclide on pathway has different decay mode <CHAINP>
One of the pathway nuclides does not decay to the next nuclide in the pathway.

Nuclide on pathway has no reactions <CHAINP>
One of the pathway nuclides is followed by an 'R', however the nuclide is so short-lived that it has no cross section data in the library.

Nuclide on pathway is stable <CHAINP>
One of the pathway nuclides is followed by a 'D', however the nuclide is stable.

Number of fissionable parents <= 20 [FISCHOOSE]
Can only specify a maximum of 20 fissionable parents.

Numeric value required for C [LEVEL]
A numeric value ***MUST*** follow the code word.

Numeric value required for CONV [CONV]
A numeric value ***MUST*** follow the code word.

Numeric value required for CONVS [CONV]
A numeric value ***MUST*** follow the code word.

Numeric value required for DENSTY [DENSITY]
A numeric value ***MUST*** follow the code word.

Numeric value required for FLUX2 [FLUX]
A numeric value ***MUST*** follow the code word.

Numeric value required for FRACOK [UNCERTAINTY]
A numeric value ***MUST*** follow the code word.

Numeric value required for FRACWT [UNCERTAINTY]
A numeric value ***MUST*** follow the code word.

Numeric value required for GRSHOW [GRAPH]
A numeric value ***MUST*** follow the code word.

Numeric value required for GUNCRT [GRAPH]
A numeric value ***MUST*** follow the code word.

Numeric value required for IA [TAB1]
A numeric value representing the stream to connected the **TAB1** file ***MUST*** follow the code word.

Numeric value required for IARG [BREM]
A numeric value ***MUST*** follow the code word.

Numeric value required for IB [TAB2]
A numeric value representing the stream to connected the **TAB2** file ***MUST*** follow the code word.

Numeric value required for IC [TAB3]
A numeric value representing the stream to connected the **TAB3** file ***MUST*** follow the code word.

Numeric value required for ID [TAB4]
A numeric value representing the stream to connected the **TAB4** file ***MUST*** follow the code word.

Numeric value required for IGAMGP [GROUP]
A numeric value ***MUST*** follow the code word.

Numeric value required for IGENER [GENERIC]
A numeric value ***MUST*** follow the code word.

Numeric value required for INDX2 [MASS]
A numeric value ***MUST*** follow the code word.

Numeric value required for INSEN3 [SENSITIVITY]
A numeric value ***MUST*** follow the code word.

Numeric value required for INSEN4 [SENSITIVITY]
A numeric value ***MUST*** follow the code word.

Numeric value required for IPCWRT [SEQUENTIAL]
A numeric value ***MUST*** follow the code word.

Numeric value required for IPRPA [ROUTES]
A numeric value ***MUST*** follow the code word.

Numeric value required for ISEQUE [SEQUENTIAL]
A numeric value ***MUST*** follow the code word.

Numeric value required for IUNCER [UNCERTAINTY]
A numeric value ***MUST*** follow the code word.

Numeric value required for IUNCTY [UNCTYPE]
A numeric value ***MUST*** follow the code word.

Numeric value required for JSTRM [NEWFILE]
A numeric value ***MUST*** follow the code word.

Numeric value required for MAXXT [CONV]
A numeric value ***MUST*** follow the code word.

Numeric value required for MIND [MIND]
A numeric value ***MUST*** follow the code word.

Numeric value required for MONIT [MONITOR]
A numeric value ***MUST*** follow the code word.

Numeric value required for N [LEVEL]
A numeric value ***MUST*** follow the code word.

Numeric value required for N1 [FUEL]
A numeric value ***MUST*** follow the code word.

Numeric value required for N2COLL [COLLAPSE]
A numeric value ***MUST*** follow the code word.

Numeric value required for NCHO [FISCHOOSE]
A numeric value ***MUST*** follow the code word.

Numeric value required for NDOSE [DOSE]
A numeric value ***MUST*** follow the code word.

Numeric value required for NEAFVN [EAFVERSION]
A numeric value ***MUST*** follow the code word.

Numeric value required for NERROR [ERROR]
A numeric value ***MUST*** follow the code word.

Numeric value required for NDSTRC [GRPCONVERT]
A numeric value ***MUST*** follow the code word.

Numeric value required for NESTRC [GRPCONVERT]
A numeric value ***MUST*** follow the code word.

Numeric value required for NLINK [PATH]
A numeric value ***MUST*** follow the code word.

Numeric value required for NMAX [ROUTES]
A numeric value ***MUST*** follow the code word.

Numeric value required for NMAXB [UNCERTAINTY]
A numeric value ***MUST*** follow the code word.

Numeric value required for NMAXC [UNCERTAINTY]
A numeric value ***MUST*** follow the code word.

Numeric value required for NMAXR [UNCERTAINTY]
A numeric value ***MUST*** follow the code word.

Numeric value required for NOPT [GRAPH]
A numeric value ***MUST*** follow the code word.

Numeric value required for NPART [PARTITION]
A numeric value ***MUST*** follow the code word.

Numeric value required for NPULSE [PULSE]
A numeric value ***MUST*** follow the code word.

Numeric value required for NRESU [RESULT]
A numeric value ***MUST*** follow the code word.

Numeric value required for NUMG [GRAPH]
A numeric value ***MUST*** follow the code word.

Numeric value required for NYLD [FISYIELD]
A numeric value ***MUST*** follow the code word.

Numeric value required for PMIN [ROUTES]
A numeric value ***MUST*** follow the code word.

Numeric value required for T [TIME]
A numeric value ***MUST*** follow the code word.

Numeric value required for TLOOP [LOOPS]
A numeric value ***MUST*** follow the code word.

Numeric value required for TOTM [MASS]
A numeric value ***MUST*** follow the code word.

Numeric value required for WALL [WALL]
A numeric value ***MUST*** follow the code word.

Numeric value required for XDOM [DOMINANT]
A numeric value ***MUST*** follow the code word.

Numeric value required for XNSEN1 [SENSITIVITY]
A numeric value ***MUST*** follow the code word.

Numeric value required for XP [MASS]
A numeric value ***MUST*** follow the code word.

Numeric value required for XRESU [RESULT]
A numeric value ***MUST*** follow the code word.

Numeric value required for ZZZLVL [UNCERTAINTY]
A numeric value ***MUST*** follow the code word.

Only 5 levels of nesting allowed [PULSE]
When using the **PULSE**, **ENDPULSE** construction it is only possible to nest the construction 5 levels deep.

Parent nuclide of reaction not in library <COL069>
The parent nuclide of a reaction in the cross section library is not present in the decay library, has the correct decay library been used?

Parent nuclide of reaction not in library <COL100>
The parent nuclide of a reaction in the cross section library is not present in the decay library, has the correct decay library been used?

Parent nuclide of reaction not in library <COL172>
The parent nuclide of a reaction in the cross section library is not present in the decay library, has the correct decay library been used?

Parent nuclide of reaction not in library <COL175>
The parent nuclide of a reaction in the cross section library is not present in the decay library, has the correct decay library been used?

Parent nuclide of reaction not in library <COL315>
The parent nuclide of a reaction in the cross section library is not present in the decay library, has the correct decay library been used?

Parent nuclide not in library [PATH]
The parent nuclide of a reaction in a pathway is not present in the decay library.

Reaction for new uncertainty data not in library <INTERP>
The reaction specified is not in the cross section library. Check it has been entered correctly in **INPUT** file.

Reaction for new uncertainty data not in library <OUTERR>
The reaction specified is not in the cross section library. Check it has been entered correctly in **INPUT** file.

Reaction for new uncertainty data not in library <OUTPUT>
The reaction specified is not in the cross section library. Check it has been entered correctly in **INPUT** file.

Sub-library flagged as other than decay data <ENDFP>
The decay library being used is not in ENDF/B-V or -VI format, has the correct decay library been used?

This graph type not defined [GRAPH]
Five graph types (1 - 5) can be specified.

This version of FISPACT cannot handle half-life uncertainties [UNCTYPE]
If a version of FISPACT prior to 97 is used then including the **UNCTYPE** code word will generate this error message.

Too many alpha decays <OUTPUT>
More than five α decay modes found for a nuclide, has the correct decay library been used?

Too many beta decays <OUTPUT>
More than five β decay modes found for a nuclide, has the correct decay library been used?

Too many input nuclides <OUTERR>
The code words **MASS** or **FUEL** have been used to specify the material to be irradiated. Only 300 nuclides may be input, if **MASS** is used then there may be too many naturally occurring isotopes for the input elements. Reduce the number of input elements or nuclides.

Unable to open FILES from MAIN
The file **FILES** contains the names of all the other files required by the system, it was not available.

Uncertainty data not consistent with cross section data < COL069>
There are reactions in the uncertainty library that are not present in the cross section library, have the correct libraries been used?

Uncertainty data not consistent with cross section data < COL100>
There are reactions in the uncertainty library that are not present in the cross section library, have the correct libraries been used?

Uncertainty data not consistent with cross section data < COL172>
There are reactions in the uncertainty library that are not present in the cross section library, have the correct libraries been used?

Uncertainty data not consistent with cross section data < COL175>
There are reactions in the uncertainty library that are not present in the cross section library, have the correct libraries been used?

Uncertainty data not consistent with cross section data < COL315>
There are reactions in the uncertainty library that are not present in the cross section library, have the correct libraries been used?

Value for density must be given if FUEL used <MAIN>
Density ***MUST*** be specified if **FUEL** is used to specify the input material.

Appendix 12 - Sequential charged particle reactions

This appendix gives only a very brief summary of the theory developed by the group at KfK Karlsruhe for the treatment of sequential charged particle reactions (SCPR) in inventory calculations. Full details are given in reference 32.

A SCPR is a two-step process in which charged particles x are created in primary neutron-induced reactions A(n,x), followed by a charged particle induced reaction B(x,n)C producing the residual nucleus C. In general B ≠ A since the initial material may contain many different nuclides or B may be formed by transmutation of A. If this process is included it is then possible to form nuclides with atomic number Z+1 and Z+2 from a nuclide with atomic number Z. Note that with neutron-induced reactions, products with atomic numbers of Z, Z-1 and Z-2 can be formed directly. Neutron-induced reactions can form nuclides with atomic number Z+1 only by β^- decays. SCPR therefore make it possible to form nuclides that are not formed (or only in very small quantities) by neutron-induced reactions; and can therefore significantly alter the activation properties of a material.

Reference 32 shows how an expression for a 'pseudo' cross section can be derived which is formally identical to the effective cross section used by FISPACT. This is shown in equation A12.1.

$$\sigma_{x,C}^{pseudo} = \frac{1}{\Phi_n}\sum_{k=1}^{24}\sigma_{x,C}(E_{x_k})\sum_{A}\sum_{i=1}^{175}N_A\phi_n(E_{n_i})\sigma_{n,x}(E_{n_i})\sum_{j=k}^{24}f_{n,x}(E_{n_i},E_{x_j})\Delta E_{x_j}\Delta R_x(E_{x_k})$$

.....(A12.1)

where

$\phi_n(E_{n_i})$	is the neutron flux in the i th energy group
$\Phi_n = \sum_{i=1}^{175}\phi_n(E_{n_i})$	is the integrated neutron flux
N_A	is the number of atoms of the nuclide A
ΔE_{x_k}	is the k th charged particle energy step
$\sigma_{n,x}(E_{n_i})$	is the production cross section of charged particle x in the i th energy group

$\sigma_{x,C}(E_{x_k})$ is the production cross section of nuclide C in the k th energy group

$f_{n,x}(E_{n_i}, E_{x_k})$ is the normalised charged particle spectrum for neutron energy in the i th energy group and in the k th outgoing energy step

$\Delta R_x(E_{x_k})$ is the differential thickness of the surrounding material for charged particle of starting energy E_{x_k}

In the original work of KfK a separate code PCROSS[33] was written to calculate the pseudo cross sections for a particular material in a specified neutron spectrum. These pseudo cross sections were then merged with the collapsed cross sections and this new library used with FISPACT. This process has been simplified by building the PCROSS subroutines into FISPACT and giving the user the option to include SCPR by means of a code word.

FISPACT calculates the pseudo cross sections and inserts these in the correct order into the correct place in the internal data storage space (the `A()` array). The modified `A()` array is not written to a file so that there is no permanent effect on the data libraries. As the composition of a material changes during a run more nuclides will become available to act as targets for the charged particles.

Appendix 13 - Platform differences

This appendix explains how to install FISPACT and the EAF libraries on various computer systems. FISPACT is currently available on two computer platforms:

- 80x86/Pentium/Pentium II PC running Windows 95, Windows 98 or Windows NT 4.0
- UNIX workstation

The details for each system are given below.

Personal computer

FISPACT is supplied to users on a CD ROM. FISPACT-99 will run under Windows 95, Windows 98 or Windows NT4.0. The CD ROM contains the PC version of FISPACT, a run time file and the EAF library. The run time library is supplied by Salford Software.

To install:

1. Insert CD-Rom (assume drive D).
2. Install the FISPACT Windows Interface (see Appendix 15) by running `d:\fwi\setup`.
3. Install the Install_EASY application by running `d:\install_easy\setup`.
4. Run Install_EASY by clicking the Start | Programs | Install icon. Follow the onscreen instructions including the input of personal details.

The installation can be tested by carrying out the following steps:

1. Open the FISPACT Windows Interface by clicking the Start | Programs | fispactw icon.
2. Click the FISPACT item on the Run menu and FISPACT will carry out the calculation shown in the **`INPUT`** file. Note that all entries in **`FILES`** have been tailored to the user's system during installation.
3. Use the Help file for more details.

UNIX

The EASY-99 code package, including the inventory code FISPACT-99 and the EAF-99 libraries, is available on the following media:

1. ¼" DC 6150 Data cartridge tape (150 Mbytes, tar format).
2. D8-112 8 mm data tape (2.3 or 5.0 Gbytes commonly called 'Exabyte', tar format).
3. Magneto-optical disk (IBM RISC/6000 AIX file system) 512 or 1024 bytes/sector.
4. Magneto-optical disk 512 bytes/sector (tar on the raw device).
5. DAT 4mm data tape.
6. CD-ROM.

EASY-99 requires a minimum of 120 Mbytes of free disk space on the UNIX machine on which it will be installed.

The FISPACT program and the associated EAF libraries, under UNIX, needs to be setup in a certain fixed directory structure since the programme itself will look for files in definite places in the directory tree.

A README file is supplied that details the installation and the QA procedures as well as the necessary adaptations required for use on IBM AIX, SUN SUNos and Solaris, HP UX, Silicon Graphics IRIX, DEC Alpha OSF and PC Linux.

Appendix 14 - Standard test cases

The following input files constitute the set of standard test cases. This set covers all the code words and is supplied to users to enable them to confirm that a new installation is working correctly.

COLLAPSE

[typical case, for 100 groups]

```
COLLAPSE 100
FISPACT
* COLLAPSE EAF4.100 WITH FW EEF
END
* END OF RUN
```

WRITE

[typical case, for 175 groups using **TAPA** option]

```
SPEK
ENFA
* EAF_DEC4.OOX/EAF4.175.DATA/EEF121M.GPJ)
TAPA
FISPACT
* WRITE DATA TO ARRAY FILE.
END
* END OF RUN
```

PRINTLIB

[typical case, with option to print only cross sections]

```
AINP
FISPACT
* PRINTLIB OF FW EEF
PRINTLIB  0
END
* END OF PRINTLIB
```

Test1

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF TI EEF FW 1.0 MW/M2
MASS 1.0 1
TI 100.0
MIND 1.E5
GRAPH 5 1 1 1 2 3 4 5
WALL 1.00
ATOMS
LEVEL 100 1
TIME 2.5 YEARS
HAZA
HALF
ATWO
UNCERT 2
DOSE 1
ATOMS
LEVEL 20 1
FLUX 0.
ZERO
TIME 1 MINS ATOMS
TIME 1 HOURS ATOMS
TIME 1 DAYS ATOMS
TIME 7 DAYS ATOMS
TIME 1 YEARS ATOMS
END
* END
```

Test2

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF TI EEF FW 1.0 MW/M2
DENSITY 4.54
FUEL 5
TI46 1.00619E24
TI47 9.18148E23
TI48 9.28210E24
TI49 6.91755E23
TI50 6.79178E23
MIND 1.E5
GRAPH 3 0 0 1 2 3
FLUX 4.27701E14 ATOMS
LEVEL 100 1
TIME 2.5 YEARS
DOSE 1
ATOMS
LEVEL 20 1
FLUX 0.
ZERO
TIME 1 MINS ATOMS
TIME 1 HOURS ATOMS
TIME 1 DAYS ATOMS
TIME 7 DAYS ATOMS
WALL 1.0
LEVEL 100 1
DOSE 2 1
GROUP 1
NOSTAB
TIME 0.5 YEARS ATOMS
LEVEL 20 1
FLUX 0.
ZERO
TIME 1 YEARS SPECTRUM
END
* END
```

Test3

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF TI EEF FW 1.0 MW/M2
MASS 1.0 1
TI 100.0
DENSITY 19.254
MIND 1.E5
WALL 1.00 ATOMS
LEVEL 100 1
TIME 2.0 YEARS
HALF ATOMS
LEVEL 20 1
FLUX 0.
ZERO
NOCOMP
NOSTAB
TIME 1 ATOMS
LEVEL 100 1
FLUX 4.27701E14
TIME 0.5 YEARS ATOMS
LEVEL 20 1
FLUX 0.
ZERO
NOCOMP
NOSTAB
TIME 1.022 YEARS ATOMS
END
* END
```

Test4

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF TI EEF FW 1.0 MW/M2
MASS 1.0 1
TI 100.0
DENSITY 19.254
MIND 1.E5
WALL 1.00
ATOMS
HALF
HAZA
TAB1 22
TAB2 23
TAB3 24
TAB4 25
CONV 10 1E-2 1E-2
BREM 4 AR39 AR42 K42 CL38
UNCERT 4 0.98 0.01 5 3 12 5.E8 3
LEVEL 100 1
TIME 2.5 YEARS
ATOMS
LEVEL 20 1
FLUX 0.
ZERO
NOT1
NOT2
NOT3
NOT4
TIME 1.022 YEARS ATOMS
END
* END
```

Test5

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF TI EEF FW 1.0 MW/M2
DENSITY 4.54
FUEL 5
TI46 1.00619E24
TI47 9.18148E23
TI48 9.28210E24
TI49 6.91755E23
TI50 6.79178E23
MIND 1.E5
FLUX 4.27701E14
ATOMS
LEVEL 10000 1
TIME 2.5 YEARS
ROUTES TI46 SC44 5 1E13 0
ROUTES TI46 CA45 3 1E18 1
RESULT 2
SC44 1.01843E15
CA45 3.73063E20
END
* END
```

Test6

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF TI EEF FW 1.0 MW/M2
FUEL 5
TI46 1.00619E24
TI47 9.18148E23
TI48 9.28210E24
TI49 6.91755E23
TI50 6.79178E23
MIND 1.E5
FLUX 4.27701E14 ATOMS
LEVEL 10000 1
TIME 2.5 YEARS
PATH 3 TI46 R TI45 D SC45 R SC44M
PATH 1 TI46 R SC46
PATH 5 TI50 R TI51 D V51 R V52 D CR52 R CR51
ATOMS
END
* END
```

Test7

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF TI EEF FW 1.0 MW/M2
DENSITY 4.54
FUEL 5
TI46 1.00619E24
TI47 9.18148E23
TI48 9.28210E24
TI49 6.91755E23
TI50 6.79178E23
MIND 1.E5
FLUX 4.27701E14 ATOMS
LEVEL 100 5
SENSITIVITY SIGMA 1E-10 2 1
TI48 SC48
TI49 SC48
SC48
ERROR 2
TI48 SC48 0.5
TI49 SC49 0.2
TIME 2.5 YEARS ATOMS
END
* END
```

Test8

```
NOHEAD
AINP
FISPACT
* 1 PPM OF CO IN FE EEF FW 1.0 MW/M2
IRON
MASS 1.0 2
FE 99.9999
CO  0.0001
MIND 1.E5
WALL 1 ATOMS
LEVEL 100 1
TIME 2.5 YEARS
UNCERT 3 ATOMS
LEVEL 20 1
FLUX 0.
ZERO
TIME 0.1 YEARS ATOMS
TIME 0.9 YEARS ATOMS
END
* END
```

Test9

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF BE EEF FW 1.0 MW/M2
MASS 1.0 1
BE 100.0
MIND 1.E5
WALL 1.00
ATOMS
HALF
DOSE 1
LEVEL 100 1
TIME 0.5 YEARS
UNCERT 3
ATOMS
LEVEL 20 1
FLUX 0.
TIME 0.083 YEARS ATOMS
WALL 1.0
LEVEL 100 1
TIME 0.5 YEARS
UNCERT 0
ATOMS
LEVEL 20 1
FLUX 0.
TIME 0.083 YEARS ATOMS
WALL 1.0
LEVEL 100 1
TIME 0.5 YEARS
ATOMS
LEVEL 20 1
FLUX 0.
TIME 0.083 YEARS ATOMS
WALL 1.0
LEVEL 100 1
TIME 0.5 YEARS
ATOMS
LEVEL 20 1
FLUX 0.
TIME 0.083 YEARS ATOMS
WALL 1.0
LEVEL 100 1
TIME 0.5 YEARS
ATOMS
END
* END
```

Test10

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF BE EEF FW 1.0 MW/M2
MASS 1.0 1
BE 100.0
MIND 1.E5
WALL 1.00
ATOMS
OVER BE9
ACROSS BE10 1.4195E-4
OVER H3
ALAM 1.9455E8 1
HALF
DOSE 1
LEVEL 100 1
TIME 0.5 YEARS
UNCERT 3
ATOMS
LEVEL 20 1
FLUX 0.
UNCERT 0
ZERO
TIME 0.083 YEARS ATOMS
PARTITION 2
H   0.
HE  0.
TIME 0.083 YEARS ATOMS
END
* END
```

Test11

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF TI EEF 175 FW 1.0 MW/M2
MASS 1.0 1
TI 100.0
MIND 1.E5
GRAPH 5 1 1 1 2 3 4 5
WALL 1.00
ATOMS
LEVEL 100 1
TIME 2.5 YEARS
HAZA
HALF
ATWO
UNCERT 3
DOSE 1
ATOMS
LEVEL 20 1
FLUX 0.
ZERO
TIME 1 MINS ATOMS
TIME 1 HOURS ATOMS
TIME 1 DAYS ATOMS
TIME 7 DAYS ATOMS
TIME 1 YEARS ATOMS
END
* END
```

Test12

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF TI EEF FW 1.0 MW/M2
DENSITY 4.54
FUEL 5
TI46 1.00619E24
TI47 9.18148E23
TI48 9.28210E24
TI49 6.91755E23
TI50 6.79178E23
MIND 1.E5
FLUX 4.27701E14
ATOMS
LEVEL 100 5
SENSITIVITY SIGMA 1E-10 2 1
TI48 SC48
TI49 SC48
SC48
ERROR 2
TI48 SC48 -1
TI49 SC49 -1
TIME 2.5 YEARS
ATOMS
END
* END
```

Test13

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF FE + U EEF 175 FW 1.0 MW/M2
MASS 1.0 2
FE 99.9999
U   0.0001
MIND 1.E5
GRAPH 5 1 1 1 2 3 4 5
WALL 1.00
ATOMS
LEVEL 100 1
TIME 2.5 YEARS
HAZA
HALF
ATWO
UNCERT 2
DOSE 1
ATOMS
LEVEL 20 1
FLUX 0.
ZERO
TIME 1 MINS ATOMS
TIME 1 HOURS ATOMS
TIME 1 DAYS ATOMS
TIME 7 DAYS ATOMS
TIME 1 YEARS ATOMS
TIME 5000 YEARS ATOMS
END
* END
```

Test14

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF Ti EEF 175 FW 1.0 MW/M2
MASS 1.0 1
TI 100.0
MIND 1.E5
WALL 1.00
ATOMS
LEVEL 100 1
TIME 2.5 YEARS
HAZA
HALF
ATWO
DOMINANT 80.0
UNCERT 3
DOSE 1
ATOMS
LEVEL 20 1
FLUX 0.
ZERO
TIME 1 MINS ATOMS
TIME 1 HOURS ATOMS
TIME 1 DAYS ATOMS
TIME 7 DAYS ATOMS
TIME 1 YEARS ATOMS
END
* END
```

Test15

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF Ti EEF 175 FW 1.0 MW/M2
MASS 1.0 1
TI 100.0
MIND 1.E5
WALL 1.00
ATOMS
LEVEL 100 1
TIME 2.5 YEARS
HAZA
HALF
ATWO
<< Test case for comment >>
GENERIC 0
UNCERT 3
DOSE 1
ATOMS
LEVEL 20 1
FLUX 0.
ZERO
TIME 1 MINS ATOMS
TIME 1 HOURS ATOMS
<< Test case for comment >>
TIME 1 DAYS ATOMS
TIME 7 DAYS ATOMS
TIME 1 YEARS ATOMS
END
* END
```

Test16

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF Ti EEF 175 FW 1.0 MW/M2
MASS 1.0 1
TI 100.0
MIND 1.E5
GRAPH 3 1 1 1 2 3
WALL 1.00
ATOMS
LEVEL 100 1
SEQU 1 1
TIME 2.5 YEARS
HAZA
HALF
ATWO
UNCERT 3
DOSE 1
ATOMS
LEVEL 20 1
FLUX 0.
ZERO
TIME 1 MINS ATOMS
TIME 1 HOURS ATOMS
TIME 1 DAYS ATOMS
TIME 7 DAYS ATOMS
TIME 1 YEARS ATOMS
END
* END
```

Test17

```
NOHEAD
EAFV 4
AINP
FISPACT
* IRRADIATION OF Ti EEF 175 FW 1.0 MW/M2
MASS 1.0 1
TI 100.0
MIND 1.E5
GRAPH 3 1 1 1 2 3
WALL 1.00
ATOMS
LEVEL 100 1
SEQU 1 0
TIME 2.5 YEARS
HAZA
HALF
ATWO
UNCERT 3
DOSE 1
ATOMS
LEVEL 20 1
FLUX 0.
ZERO
TIME 1 MINS ATOMS
TIME 1 HOURS ATOMS
TIME 1 DAYS ATOMS
TIME 7 DAYS ATOMS
TIME 1 YEARS ATOMS
END
* END
```

Test18

```
NOHEAD
MONITOR 1
AINP
FISPACT
* IRRADIATION OF Fe EEF 175 FW 1.0 MW/M2
MASS 1.0 1
FE 100.0
MIND 1.E5
WALL 1.00
ATOMS
LEVEL 100 1
TIME 2.5 YEARS
HAZA
HALF
ATWO
UNCERT 2
SPECTRUM
PULSE 5
  LEVEL 20 1
  FLUX 0.
  TIME 1.0 HOUR SPECTRUM
  LEVEL 100 1
  WALL 1.0
  TIME 1.0 HOUR SPECTRUM
ENDPULSE
LEVEL 20 1
FLUX 0.
TIME 1.0 HOUR SPECTRUM
LEVEL 100 1
WALL 1.0
TIME 1.0 HOUR ATOMS
FLUX 0.0
ZERO
TIME 1 MINS ATOMS
TIME 1 HOURS ATOMS
TIME 1 DAYS ATOMS
TIME 7 DAYS ATOMS
TIME 1 YEARS ATOMS
END
* END
```

Test19

```
NOHEAD
MONITOR 1
AINP
FISPACT
* IRRADIATION OF Sc-45 EEF FW
DENSITY 2.989
FUEL 1
SC45 1.0E25
MIND 1.E5
FLUX 4.27701E14
LEVEL 10000 1
TIME 2.5 YEARS
LOOPS 20
PATH 2 SC45 R SC46 R SC47
PATH 3 SC45 R K42 D CA42 R AR39
PATH 3 SC45 R K42 D CA42 R CA41
ATOMS
END
* END
```

Test20

```
NOHEAD
MONITOR 1
AINP
FISPACT
* IRRADIATION OF Ti EEF 175 FW 1.0 MW/M2
MASS 1.0 1
TI 100.0
MIND 1.E5
WALL 1.00
ATOMS
LEVEL 100 1
TIME 2.5 YEARS
HAZA
HALF
ATWO
UNCERT 2
UNCTYPE 2
ATOMS
LEVEL 20 1
FLUX 0.
ZERO
TIME 1 MINS ATOMS
TIME 1 HOURS ATOMS
TIME 1 DAYS ATOMS
TIME 7 DAYS ATOMS
TIME 1 YEARS ATOMS
END
* END
```

Test21

```
NOHEAD
AINP
FISPACT
*PWR FUEL 3.1% U235 PWRDEAN
DENSITY 10.1
FUEL 2
U235 7.948E22
U238 2.453E24
MIND 1.E5
HAZA
HALF
GRAPH 5 1 1 1 2 3 4 5
FLUX 3.25E+14
ATOMS
LEVEL 20 8
TIME 30.4375 DAYS
TAB1 41
ATWO
DOSE 1
ATOMS
TIME 60.875 DAYS
ATOMS
TIME 91.3125 DAYS
ATOMS
TIME 182.625 DAYS
ATOMS
TIME 182.625 DAYS
ATOMS
TIME 182.625 DAYS
ATOMS
LEVEL 20 1
FLUX 0.
NOSTABLE
ZERO
TIME 60
ATOMS
TIME 1 DAYS ATOMS
TIME 29.4375 DAYS ATOMS
TIME 152.1875 DAYS ATOMS
TIME 182.625 DAYS ATOMS
TIME 2 YEARS ATOMS
TIME 2 YEARS ATOMS
TIME 5 YEARS ATOMS
END
* END
```

Test22

```
NOHEAD
EAFV 4
MONITOR 1
AINP
FISPACT
*PWR FUEL 3.1% U235 PWRDEAN
DENSITY 10.1
FUEL 2
U235 7.948E22
U238 2.453E24
MIND 1.E5
FISCHOOSE 5 U235 U238 PU239 PU240 PU242
HAZA
HALF
GRAPH 5 1 1 1 2 3 4 5
FLUX 3.25E+14
ATOMS
LEVEL 20 50
TIME 730.5 DAYS
UNCERT 2
TAB1 41
ATWO
DOSE 1
ATOMS
LEVEL 20 1
FLUX 0.
NOSTABLE
ZERO
TIME 60
ATOMS
TIME 1 DAYS ATOMS
TIME 29.4375 DAYS ATOMS
TIME 152.1875 DAYS ATOMS
TIME 182.625 DAYS ATOMS
TIME 2 YEARS ATOMS
TIME 2 YEARS ATOMS
TIME 5 YEARS ATOMS
END
* END
```

Test23

```
NOHEAD
MONITOR 1
AINP
FISPACT
*PWR FUEL 3.1% U235 PWRDEAN
DENSITY 10.1
FUEL 2
U235 7.948E22
U238 2.453E24
MIND 1.E5
FISYIELD 0
HAZA
HALF
FLUX 3.25E+14
LEVEL 20 50
TIME 730.5 DAYS
UNCERT 0
ATOMS
NOSORT
LEVEL 20 1
FLUX 0.
ZERO
TIME 60
ATOMS
TIME 1 DAYS ATOMS
TIME 29.4375 DAYS ATOMS
TIME 152.1875 DAYS ATOMS
TIME 182.625 DAYS ATOMS
TIME 2 YEARS ATOMS
TIME 2 YEARS ATOMS
TIME 5 YEARS ATOMS
END
* END
```

Test24

```
NOHEAD
MONITOR 1
AINP
FISPACT
*PWR FUEL 3.1% U235 PWRDEAN
DENSITY 10.1
FUEL 2
U235 7.948E22
U238 2.453E24
MIND 1.E5
FISYIELD 2 U235 PU239
HAZA
HALF
FLUX 3.25E+14
LEVEL 20 50
TIME 730.5 DAYS
UNCERT 0
ATOMS
NOSORT
LEVEL 20 1
FLUX 0.
ZERO
TIME 60
ATOMS
TIME 1 DAYS ATOMS
TIME 29.4375 DAYS ATOMS
TIME 152.1875 DAYS ATOMS
TIME 182.625 DAYS ATOMS
TIME 2 YEARS ATOMS
TIME 2 YEARS ATOMS
TIME 5 YEARS ATOMS
END
* END
```

Test25

```
NOHEAD
MONITOR 1
AINP
FISPACT
* IRRADIATION B4C LMJ FW 1mm thick
DENSITY 2.7
MASS 848.23   2
B 78.57
C 21.43
SEQUENTIAL 1 0
TAB4 44
MIND 1.E5
<< IRRADIATION HISTORY: 1 YEAR 12 SHOTS >>
HAZA
HALF
DOSE 1
SPECTRUM
<<-------------------->>
PULSE 11
  FLUX 1.02292E+22
  LEVEL 100 1
  TIME 1.0E-9    SPECTRUM
  LEVEL 20 1
  FLUX 0.0
  TIME 30. DAYS  SPECTRUM
ENDPULSE
<<-------------------->>
FLUX 1.02292E+22
LEVEL 100 1
TIME 1.0E-9    ATOMS
LEVEL 20 1
FLUX 0.
ZERO
UNCERT 2
NOSTABLE
TIME 1.0E-9    ATOMS
TIME 0.5       ATOMS
TIME 0.5       ATOMS
TIME 1 MINS    ATOMS
TIME 1 HOURS   ATOMS
TIME 5 HOURS   ATOMS
TIME 0.75 DAYS ATOMS
TIME 1.0 DAYS  ATOMS
TIME 1 DAYS    ATOMS
TIME 2 DAYS    ATOMS
TIME 2 DAYS    ATOMS
TIME 1 DAYS    ATOMS
TIME 1 DAYS    ATOMS
TIME 1 DAYS    ATOMS
TIME 1 DAYS    ATOMS
TIME 1 DAYS    ATOMS
TIME 5 DAYS    ATOMS
TIME 10 DAYS   ATOMS
TIME 10 DAYS   ATOMS
TIME 10 DAYS   ATOMS
TIME 10 DAYS   ATOMS
TIME 10 DAYS   ATOMS
TIME 50 DAYS   ATOMS
TIME 100 DAYS  ATOMS
TIME 252 DAYS  ATOMS
TIME 0.76923  YEARS  ATOMS
TIME 1 YEARS   ATOMS
TIME 3 YEARS   ATOMS
TIME 25 YEARS  ATOMS
END
* END
```

Test31

```
NOHEAD
AINP
FISPACT
*PWR FUEL 3.1% U235 PQY Paluel
DENSITY 10.1
FUEL 2
U235 7.948E22
U238 2.453E24
MIND 1.E5
HAZA
HALF
GRAPH 5 1 1 1 2 3 4 5
FLUX 3.25E+14
ATOMS
LEVEL 20 8
TIME 30.4375 DAYS
TAB1 41
ATWO
DOSE 1
ATOMS
TIME 60.875 DAYS
ATOMS
TIME 91.3125 DAYS
ATOMS
TIME 182.625 DAYS
ATOMS
TIME 182.625 DAYS
ATOMS
TIME 182.625 DAYS
ATOMS
LEVEL 20 1
FLUX 0.
NOSTABLE
ZERO
TIME 60
ATOMS
TIME 1 DAYS ATOMS
TIME 29.4375 DAYS ATOMS
TIME 152.1875 DAYS ATOMS
TIME 182.625 DAYS ATOMS
TIME 2 YEARS ATOMS
TIME 2 YEARS ATOMS
TIME 5 YEARS ATOMS
END
* END
```

Test32

```
NOHEAD
EAFV 4
MONITOR 1
AINP
FISPACT
*PWR FUEL 3.1% U235 PQY Paluel
DENSITY 10.1
FUEL 2
U235 7.948E22
U238 2.453E24
MIND 1.E5
FISCHOOSE 5 U235 U238 PU239 PU240 PU242
HAZA
HALF
GRAPH 5 1 1 1 2 3 4 5
FLUX 3.25E+14
ATOMS
LEVEL 20 50
TIME 730.5 DAYS
UNCERT 2
TAB1 41
ATWO
DOSE 1
ATOMS
LEVEL 20 1
FLUX 0.
NOSTABLE
ZERO
TIME 60
ATOMS
TIME 1 DAYS ATOMS
TIME 29.4375 DAYS ATOMS
TIME 152.1875 DAYS ATOMS
TIME 182.625 DAYS ATOMS
TIME 2 YEARS ATOMS
TIME 2 YEARS ATOMS
TIME 5 YEARS ATOMS
END
* END
```

Test41

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF TI EEF 172 FW 1.0 MW/M2
MASS 1.0 1
TI 100.0
MIND 1.E5
GRAPH 5 1 1 1 2 3 4 5
WALL 1.00
ATOMS
LEVEL 100 1
TIME 2.5 YEARS
HAZA
HALF
ATWO
UNCERT 3
DOSE 1
ATOMS
LEVEL 20 1
FLUX 0.
ZERO
TIME 1 MINS ATOMS
TIME 1 HOURS ATOMS
TIME 1 DAYS ATOMS
TIME 7 DAYS ATOMS
TIME 1 YEARS ATOMS
END
* END
```

Test42

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF TI EEF FW 1.0 MW/M2
DENSITY 4.54
FUEL 5
TI46 1.00619E24
TI47 9.18148E23
TI48 9.28210E24
TI49 6.91755E23
TI50 6.79178E23
MIND 1.E5
FLUX 4.27701E14
ATOMS
LEVEL 100 5
SENSITIVITY SIGMA 1E-10 2 1
TI48 SC48
TI49 SC48
SC48
ERROR 2
TI48 SC48 -1
TI49 SC49 -1
TIME 2.5 YEARS
ATOMS
END
* END
```

Test43

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF FE + U EEF 172 FW 1.0 MW/M2
MASS 1.0 2
FE 99.9999
U   0.0001
MIND 1.E5
GRAPH 5 1 1 1 2 3 4 5
WALL 1.00
ATOMS
LEVEL 100 10
TIME 2.5 YEARS
HAZA
HALF
ATWO
UNCERT 2
DOSE 1
ATOMS
LEVEL 20 1
FLUX 0.
ZERO
TIME 1 MINS ATOMS
TIME 1 HOURS ATOMS
TIME 1 DAYS ATOMS
TIME 7 DAYS ATOMS
TIME 1 YEARS ATOMS
TIME 5000 YEARS ATOMS
END
* END
```

Test44

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF Ti EEF 172 FW 1.0 MW/M2
MASS 1.0 1
TI 100.0
MIND 1.E5
WALL 1.00
ATOMS
LEVEL 100 1
TIME 2.5 YEARS
HAZA
HALF
ATWO
DOMINANT 80.0
UNCERT 3
DOSE 1
ATOMS
LEVEL 20 1
FLUX 0.
ZERO
TIME 1 MINS ATOMS
TIME 1 HOURS ATOMS
TIME 1 DAYS ATOMS
TIME 7 DAYS ATOMS
TIME 1 YEARS ATOMS
END
* END
```

Test45

```
NOHEAD
AINP
FISPACT
* IRRADIATION OF Ti EEF 172 FW 1.0 MW/M2
MASS 1.0 1
TI 100.0
MIND 1.E5
WALL 1.00
ATOMS
LEVEL 100 1
TIME 2.5 YEARS
HAZA
HALF
ATWO
<< Test case for comment >>
GENERIC 0
UNCERT 3
DOSE 1
ATOMS
LEVEL 20 1
FLUX 0.
ZERO
TIME 1 MINS ATOMS
TIME 1 HOURS ATOMS
<< Test case for comment >>
TIME 1 DAYS ATOMS
TIME 7 DAYS ATOMS
TIME 1 YEARS ATOMS
END
* END
```

spectra

```
GRPC 99 172
FISPACT
* SPECTRAL MODIFICATION  99 APOLLO - 172 XMAS
END
* END
```

Test51

```
NOHEAD
AINP
FISPACT
*PWR FUEL 3.1% U235 PQY Paluel
DENSITY 10.1
FUEL 2
U235 7.948E22
U238 2.453E24
MIND 1.E5
HAZA
HALF
GRAPH 5 1 1 1 2 3 4 5
FLUX 3.25E+14
ATOMS
LEVEL 20 8
TIME 30.4375 DAYS
TAB1 41
ATWO
DOSE 1
ATOMS
TIME 60.875 DAYS
ATOMS
TIME 91.3125 DAYS
ATOMS
TIME 182.625 DAYS
ATOMS
TIME 182.625 DAYS
ATOMS
TIME 182.625 DAYS
ATOMS
LEVEL 20 1
FLUX 0.
NOSTABLE
ZERO
TIME 60
ATOMS
TIME 1 DAYS ATOMS
TIME 29.4375 DAYS ATOMS
TIME 152.1875 DAYS ATOMS
TIME 182.625 DAYS ATOMS
TIME 2 YEARS ATOMS
TIME 2 YEARS ATOMS
TIME 5 YEARS ATOMS
END
* END
```

Test52

```
NOHEAD
MONITOR 1
AINP
FISPACT
*PWR FUEL 3.1% U235 PQY Paluel
DENSITY 10.1
FUEL 2
U235 7.948E22
U238 2.453E24
MIND 1.E5
FISCHOOSE 5 U235 U238 PU239 PU240 PU242
HAZA
HALF
GRAPH 5 1 1 1 2 3 4 5
FLUX 3.25E+14
ATOMS
LEVEL 20 50
TIME 730.5 DAYS
UNCERT 2
TAB1 41
ATWO
DOSE 1
ATOMS
LEVEL 20 1
FLUX 0.
NOSTABLE
ZERO
TIME 60
ATOMS
TIME 1 DAYS ATOMS
TIME 29.4375 DAYS ATOMS
TIME 152.1875 DAYS ATOMS
TIME 182.625 DAYS ATOMS
TIME 2 YEARS ATOMS
TIME 2 YEARS ATOMS
TIME 5 YEARS ATOMS
END
* END
```

Test60

```
NOHEAD
MONITOR 1
COLLAPSE 69
FISPACT
* THREE COLLAPSES
NEWFILE 20 FLUXES.02
NEWFILE 17 COLLAPX4.02
COLLAPSE 69
NEWFILE 20 FLUXES.03
NEWFILE 17 COLLAPX4.03
COLLAPSE 69
END
* END OF COLLAPSE
```

Test61

```
NOHEAD
MONITOR 1
SPEK
ENFA
* EAFDEC97/EAF97/spec_01
TAPA
FISPACT
* THREE SPECTRA
DENSITY 9.838
FUEL 6
U235  7.9991E20
U238  2.1149E22
O16   4.3795E22
O17   1.6682E19
O18   8.7798E19
PU239 1.0E4
HALF
MIND 1.0E8
UNCERT 0
FLUX 2.59032E+14 ATOMS
LEVEL 50 10
TIME 6.109E-06 DAYS SPECTRUM
NEWFILE 12 COLLAPX4.02
SPEK
ENFA
* EAFDEC97/EAF97/spec_02
ARRAY
FLUX 2.64634E+14
TIME 6.108994E0 DAYS SPECTRUM
NEWFILE 12 COLLAPX4.03
SPEK
ENFA
* EAFDEC97/EAF97/spec_03
ARRAY
FLUX 2.66930E+14
TIME 2.44410E+01 DAYS
ATOMS
LEVEL 50 1
FLUX 0.0
ZERO
TIME 1.00E2 ATOMS
TIME 9.00E2 ATOMS
TIME 9.00E3 ATOMS
TIME 9.00E4 ATOMS
TIME 9.00E5 ATOMS
TIME 9.00E6 ATOMS
END
* END OF MULTIPLE RUN
```

Test70

```
NOHEAD
MONITOR 1
AINP
FISPACT
* PURE IRON
DENSITY 7.874
MASS 1.0 1
FE 100.0
MIND 1.E5
HAZA
CLEAR
HALF
ATOMS
FLUX 1.0E15
LEVEL 100 1
TIME 1.0 YEARS ATOMS
LEVEL 20 1
FLUX 0.
ZERO
TIME 1 DAYS ATOMS
TIME 9 DAYS ATOMS
TIME 90 DAYS ATOMS
TIME 265.25 DAYS ATOMS
TIME 9 YEARS ATOMS
END
* END OF COLLAPSE
```

Test71

```
NOHEAD
MONITOR 1
AINP
FISPACT
* PURE IRON
DENSITY 7.874
MASS 1.0 1
FE 100.0
MIND 1.E5
HAZA
CLEAR
HALF
ATOMS
FLUX 1.0E12
LEVEL 100 1
TIME 1.0 YEARS
SPECTRUM
PULSE 150
  LEVEL 20 1
  FLUX 0.
  TIME 1.0 HOURS SPECTRUM
  LEVEL 100 1
  FLUX 1.0E15
  TIME 1.0 HOURS SPECTRUM
ENDPULSE
FLUX 0.
ZERO
TIME 1 DAYS ATOMS
TIME 9 DAYS ATOMS
TIME 90 DAYS ATOMS
TIME 265.25 DAYS ATOMS
TIME 9 YEARS ATOMS
TIME 90 YEARS ATOMS
TIME 900 YEARS ATOMSEND
* END OF MULTIPLE RUN
```

Test72

```
NOHEAD
MONITOR 1
AINP
FISPACT
* PURE IRON
DENSITY 7.874
MASS 1.0 1
FE 100.0
MIND 1.E5
HAZA
CLEAR
HALF
ATOMS
FLUX 1.0E12
LEVEL 100 1
TIME 1.0 YEARS
SPECTRUM
PULSE 10
  PULSE 10
    PULSE 5
      LEVEL 20 1
      FLUX 0.
      TIME 1.0 HOURS SPECTRUM
      LEVEL 100 1
      FLUX 1.0E15
      TIME 1.0 HOURS SPECTRUM
    ENDPULSE
  ENDPULSE
ENDPULSE
FLUX 0.
ZERO
TIME 1 YEARS ATOMS
END
* END OF COLLAPSE
```

Test73

```
NOHEAD
MONITOR 1
AINP
FISPACT
* IRRADIATION B4C LMJ FW 1mm thick
DENSITY 2.7
MASS 848.23   2
B 78.57
C 21.43
TAB4 44
MIND 1.E5
<< IRRADIATION HISTORY: 1 YEAR 12 SHOTS >>
HAZA
HALF
DOSE 1
SPECTRUM
<<------------------->>
PULSE 11
  FLUX 1.02292E+22
  LEVEL 100 1
  TIME 1.0E-9    SPECTRUM
  LEVEL 20 1
  FLUX 0.0
  TIME 30. DAYS  SPECTRUM
ENDPULSE
<<------------------->>
FLUX 1.02292E+22
LEVEL 100 1
TIME 1.0E-9    ATOMS
LEVEL 20 1
FLUX 0.
ZERO
UNCERT 2
NOSTABLE
TIME 1.0E-9    ATOMS
TIME 0.5       ATOMS
TIME 0.5       ATOMS
TIME 1 MINS    ATOMS
TIME 1 HOURS   ATOMS
TIME 5 HOURS   ATOMS
TIME 0.75 DAYS ATOMS
TIME 1.0 DAYS  ATOMS
TIME 1 DAYS    ATOMS
TIME 2 DAYS    ATOMS
TIME 2 DAYS    ATOMS
TIME 1 DAYS    ATOMS
TIME 1 DAYS    ATOMS
TIME 1 DAYS    ATOMS
TIME 1 DAYS    ATOMS
TIME 1 DAYS    ATOMS
TIME 5 DAYS    ATOMS
TIME 10 DAYS   ATOMS
TIME 10 DAYS   ATOMS
TIME 10 DAYS   ATOMS
TIME 10 DAYS   ATOMS
TIME 10 DAYS   ATOMS
TIME 50 DAYS   ATOMS
TIME 100 DAYS  ATOMS
TIME 252 DAYS  ATOMS
TIME 0.76923  YEARS  ATOMS
TIME 1 YEARS   ATOMS
TIME 3 YEARS   ATOMS
TIME 25 YEARS  ATOMS
END
* END
```

Test74

```
NOHEAD
MONITOR 1
AINP
FISPACT
* IRRADIATION LMJ CONCRETE
DENSITY 2.30
FUEL 3
K39     2.60886E+24
K40     3.27303E+20
K41     1.88275E+23
TAB1 41
TAB4 44
MIND 1.E5
LEVEL 100 1
<<-------------------->>
PULSE 5
FLUX 2.11598E+19
TIME 1.0E-9       ATOMS
FLUX 0.0
TIME 30 DAYS ATOMS
ENDPULSE
<<-------------------->>
FLUX 2.11598E+19
ATOMS
TIME 1.0E-9
HAZA
HALF
UNCERT 2
DOSE 1
ATOMS
LEVEL 20 1
FLUX 0.
ZERO
TIME 1.0E-9    ATOMS
TIME 1 DAYS    ATOMS
TIME 10 DAYS   ATOMS
TIME 10 DAYS   ATOMS
TIME 100 DAYS ATOMS
END
* END
```

Note that the various testcases are divided into several sets that use cross section data in the various group structures. Table A14.1 shows the details of the group structures used.

Table A14.1 Details of energy groups for testcases.

Energy structure	Tests
69 group	21 - 24, 60, 61
100 groups	1 - 10
172 groups (WIMS)	31, 32, 51, 52
172 groups (Vitamin J)	41 - 45
175 groups	11 - 20, 25
315 groups	70 - 74

Timings

To give some idea of the relative speeds of the code on various platforms the running times for the test cases can be compared. Table A14.2 shows running times for three platforms.

Table A14.2 Running times (seconds) on various platforms.

	RS/6000 3CT [a] (66 MHz)	Pentium Pro (200 MHz) [b]	Pentium Pro (266 MHz) PC [c]
Collapse [d]	11	10	48
Write [e]	62	28	200
Write [f]	4	2	12
Printlib [g]	4	1	8
Test 1	49	24	17
Test 2	50	20	15
Test 3	37	15	11
Test 4	57	32	22
Test 5	7	3	3
Test 6	37	14	10
Test 7	148	40	28
Test 8	25	11	8
Test 9	47	21	17
Test 10	17	9	7
Test 11	49	23	17
Test 12	149	41	28
Test 13	126	47	36
Test 14	46	21	15
Test 15	49	22	17
Test 16	94	60	38
Test 17	94	42	32
Test 18	102	46	35
Test 19	33	12	9
Test 20	49	22	17
Test 21	294	99	68
Test 22	638	292	211
Test 23	289	90	63
Test 24	284	91	63
Test 25	764	314	238
Test 31	293	92	73
Test 32	649	296	216
Test 41	49	23	18
Test 42	155	42	28
Test 43	135	52	36
Test 44	49	16	16
Test 45	49	20	17
Test 51	293	99	71
Test 52	649	299	217
Test 60	25	13	12
Test 61	248	95	73
Test 70	56	24	18
Test 71	1446	664	529
Test 72	5325	2341	1830
Test 73	202	97	79
Test 74	130	63	47

Notes

[a] AIX XL3.2.3 FORTRAN compiler (C compiler 3.1.3) running under AIX 4.1.5.

[b] Salford FTN77 for Win32 FORTRAN V4.02, running in a Windows NT4.0 command window in the foreground.

[c] Salford FTN77 FORTRAN V4.02, running in a Windows 95 DOS box in the foreground.

[d] 100-group library.

[e] Using **TAPA** option.

[f] Using **ARRAY** option.

[g] With *PRINT* parameter set to 2.

All runs performed with FISPACT-99 and EAF-99.

Appendix 15 - FISPACT Windows Interface

Introduction

The FISPACT Windows Interface, an interactive application, was originally developed to help users to prepare input files. It is now a fully featured 32-bit windows application that makes all aspects of running FISPACT easier. Note that even if the platform chosen to do the actual FISPACT runs is a UNIX workstation, some users may wish to use a PC to analyse the output.

The FISPACT Windows Interface is a standard MDI (Multiple Document Interface) having the following features:

- Input files can be viewed, edited and saved.
- New input files appropriate for various types of run can be constructed by filling in a series of dialog boxes.
- The connections to the input/output streams can be set up simply by a dialog box.
- An output file (of arbitrary size) can be viewed and searched.
- A summary of an output file, showing any of the total quantities (*e.g.* activity or γ dose rate) or values for a particular nuclide at each of the time intervals can be produced.
- The summary of total quantities can be written to a database file.
- The lists of dominant nuclides can be summarised.
- Pathway information can be summarised.
- Summary information can be placed on the clipboard for pasting to another application such as an Excel spreadsheet.
- A log/log plot can be displayed of any of the five possible FISPACT graphs (activity, heat, γ dose rate, ingestion or inhalation dose as functions of time).

- The graph can be printed on any Windows compatible printer with various options.
- The PC version of FISPACT can be run.
- A Windows Help file covering the application and containing much of the present manual is available.

Figure A15.1 shows a screen shot of the Interface with icons for the various child windows that can be opened - the **FILES** file, a graph and the summary of an **OUTPUT** file; a blank **INPUT** file is also shown. As with other Windows applications there is a menubar and toolbar (containing editing buttons) at the top of the window. Details of the various features are given below.

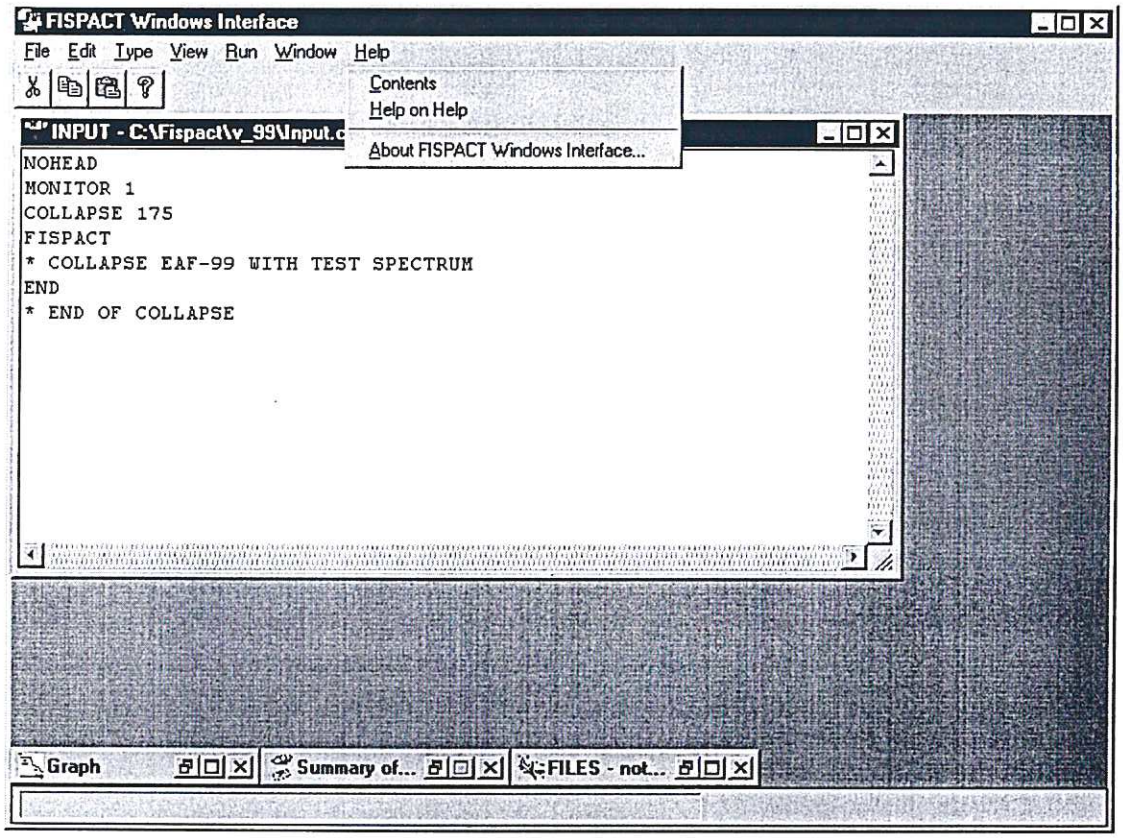

Figure A15.1. The main window of the FISPACT Windows Interface

Input files

A FISPACT run is specified by means of the **INPUT** file. The FISPACT Windows Interface allows existing input files to be opened and edited (using the cut, copy and paste tools) and saved. For the various categories of FISPACT runs listed below

input files can be prepared easily by entering data in a series of dialog boxes.

- Collapse cross section library.
- Process decay data and prepare an **ARRAY** file.
- Output a readable form of the nuclear data libraries (PRINTLIB).
- Inventory run.
- Generate pathways (either using the code words **PATHS** or **ROUTES**).

Connecting the various input and output streams to external files by means of the **FILES** file is also simplified by a dialog box.

Graph plotting

The code word **GRAPH** in a FISPACT input file does not physically plot a graph, it only writes the relevant data required for plotting (up to five) graphs to a file. This file then has to be processed by a separate package to produce hard copy. This process is extremely dependent on both the hardware and software available to the user. In order to make standard FISPACT graph plotting more accessible to users, the FISPACT Windows Interface includes the capability to display graphs and to print them on Windows supported printers.

Options are available on the menu to alter the appearance of the graph; adding error bars or an uncertainty band (if uncertainty data are included in the **GRAPH** file), adding gridlines and changing colours and sizes. For the γ dose rate graph the option to include/exclude the bremsstrahlung contribution is available, as is the option of adding lines to indicate the 'recycling' ($10\ mSvh^{-1}$) and 'hands-on' ($25\ \mu Svh^{-1}$) limits. Similar limits (the 'ILW/LLW' and 'IAEA non-radioactive' limits) can also be added to the activity plot. Figure A15.2 shows a typical graph with activity for a low activation steel plotted. The uncertainty band, activity limits and common times options have been selected.

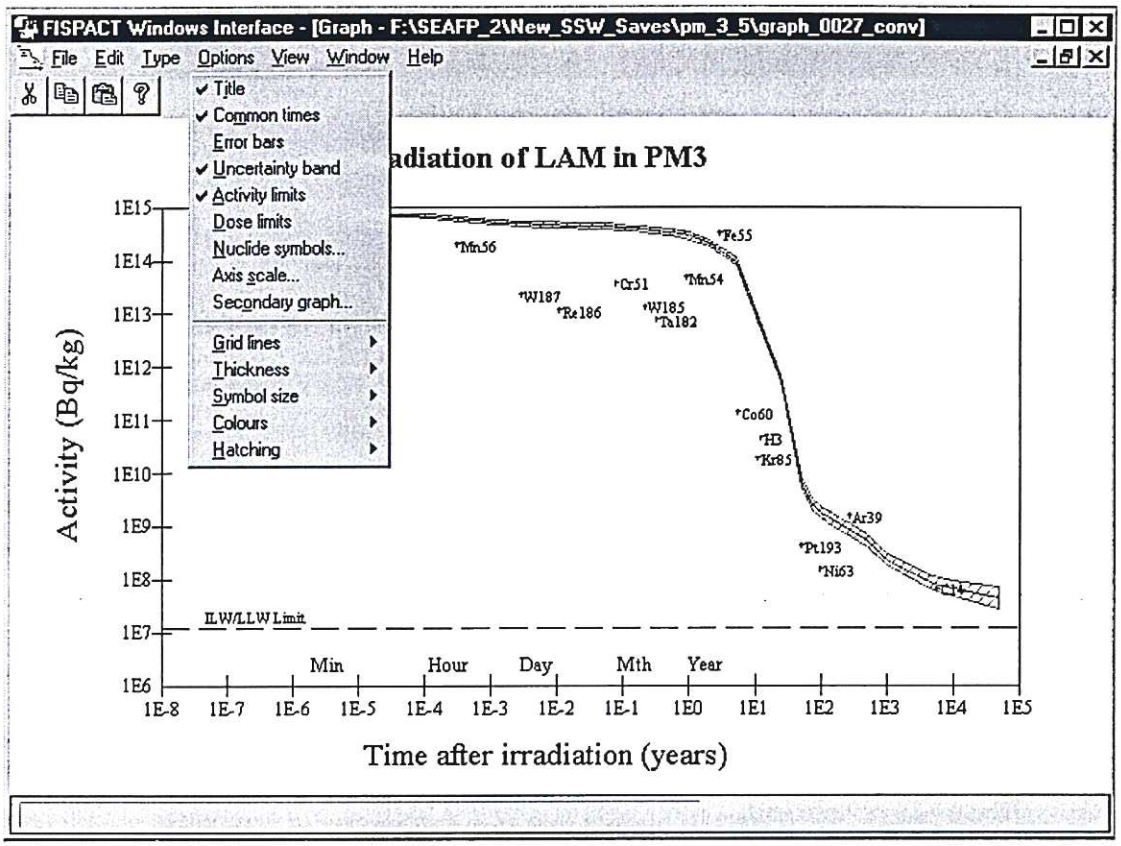

Figure A15.2. The graph window of the FISPACT Windows Interface

Summary of output files

The **OUTPUT** file corresponding, to say, the irradiation of an alloy with impurities, followed by a series of cooling times can be large (200 - 1000 kB) and extracting information can be time consuming using the **OUTPUT** file viewer. The FISPACT Windows Interface also allows the user to summarise the output, displaying the required total quantities (*e.g.* activity or γ dose rate) for each time interval in tabular form. This can then be copied to the clipboard and pasted into another application such as a spreadsheet, or written to a database file. The Microsoft Access database format (***.mdb**) is used for the database files; the FISPACT Windows Interface can create, open, view the structure of and add data to a database file.

The information about the dominant nuclides and the pathways responsible for their production for each time interval can also be summarised and presented in tabular form. This can then be copied to the clipboard for further use. Figure A15.3 shows a typical summary window.

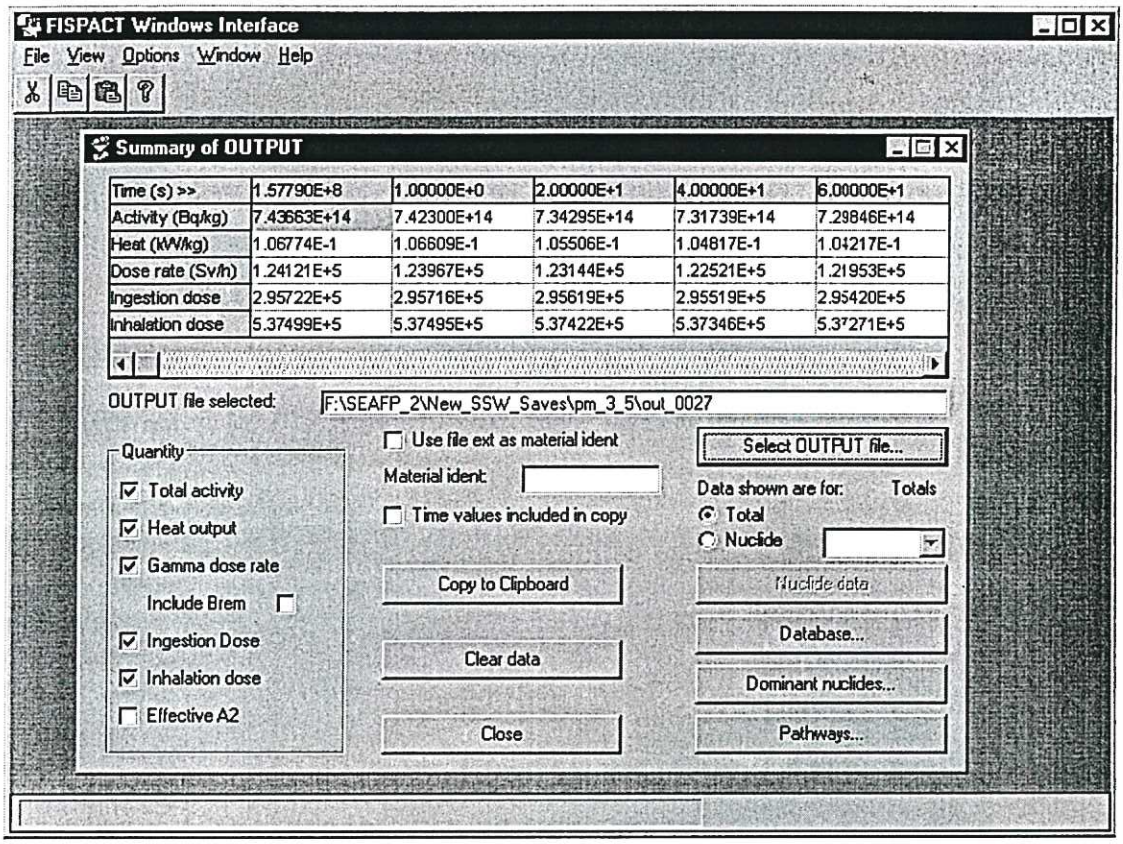

Figure A15.3. The summary window of the FISPACT Windows Interface

Running FISPACT

FISPACT can be run directly from the FISPACT Windows Interface, either in a visible command window or minimised. This is a very convenient way to carry out the calculation prior to analysing the output or plotting graphs.

If there is an error message similar to the one shown in Figure A15.4, then the FISPACT run has terminated abnormally. This is usually due to an incorrect file being specified in the **FILES** file. To aid in correcting this fault the 'Troubleshoot FISPACT...' item on the Run menu should be clicked. This brings up the dialog shown in Figure A15.5.

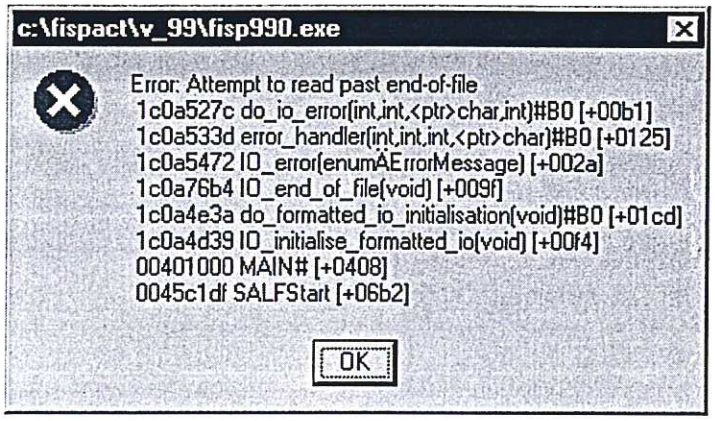

Figure A15.4. An error box displayed when a FISPACT run 'crashes'

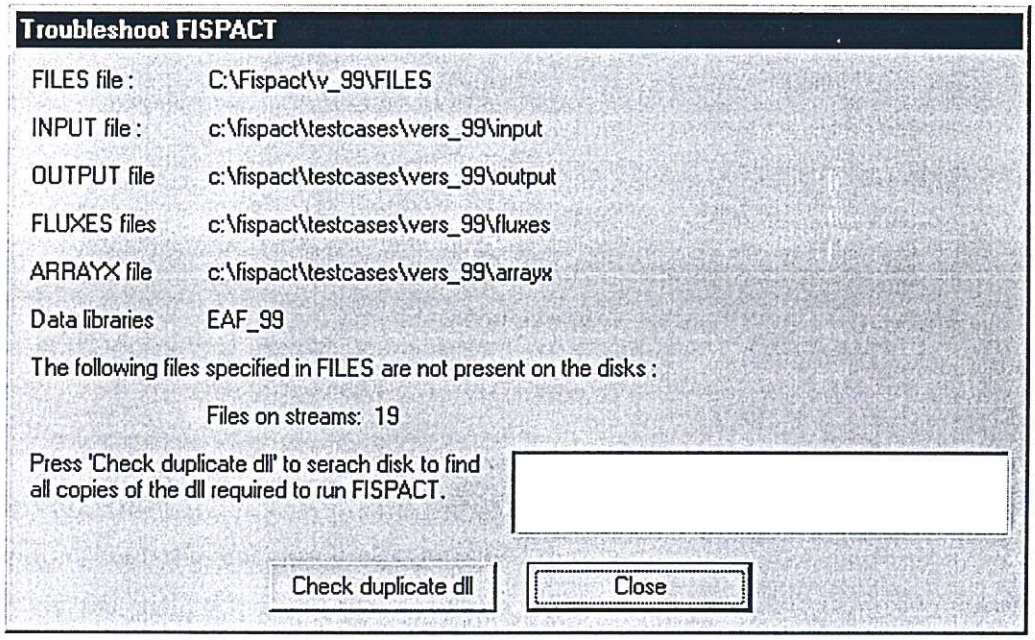

Figure A15.5. The Troubleshoot FISPACT dialog

The Troubleshoot FISPACT dialog shows the path and names of some of the specified files and checks whether any of the files specified in **FILES** are missing (or have zero size). In Figure A15.5 the file connected to stream 19 (the cross section library) is missing. If files such as the **INPUT** file are missing then FISPACT will terminated abnormally.

Help file

Windows allows the user to view information on the application by means of 'Help'. The user can view an index,

jump between topics, see 'pop-up' definitions of terms and use context sensitive help. The present version of the interface contains help on the FISPACT code words and error messages. Information on the interface (*e.g.* pictures of the dialog boxes) is also given. Note that when viewing a dialog in the application, help is available by pressing the 'F1' key. Figure A15.6 shows a typical help screen for a code word, note the underlined terms (*e.g.* HOURS) which enables a jump to another topic. Any dotted underlined terms, can be clicked and will give a definition of the term in a pop-up window.

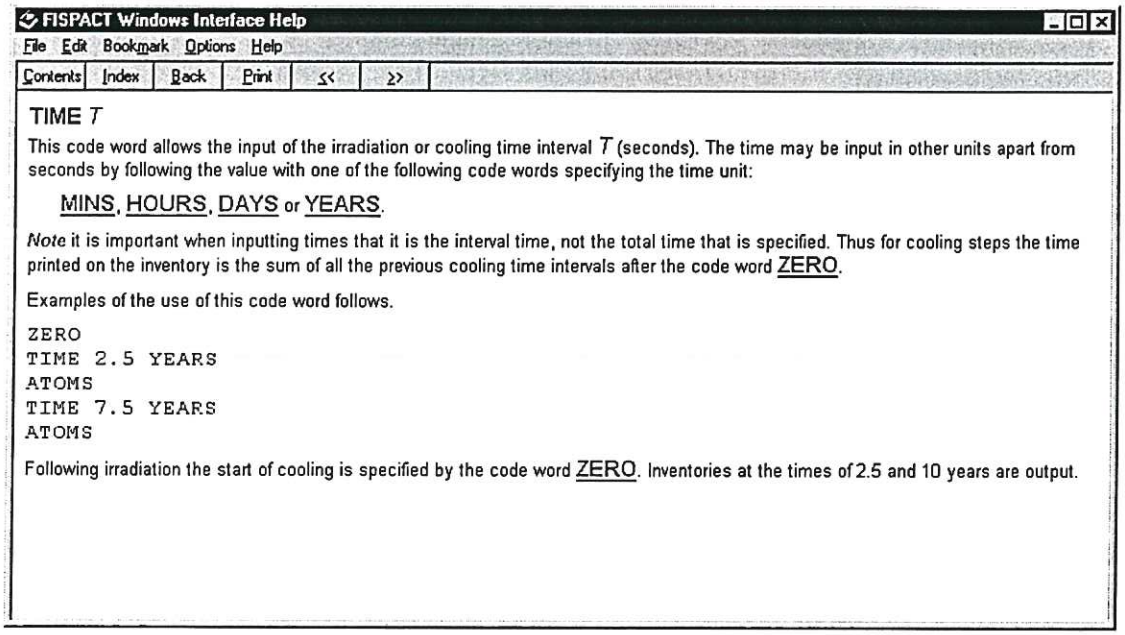

Figure A15.6. A Help topic of the FISPACT Windows Interface

Appendix 16 - Density and abundance data

All data on decay properties and cross sections are read in by FISPACT from external libraries. However, some basic physical quantities are held internally in FISPACT, primarily to enable the numbers of atoms of isotopes to be calculated when amounts of elements are input. These values are given in Table A16.1. The sources of the data are: Atomic weights and densities - reference 34, abundance - reference 35.

Table A16.1. Data held internally in FISPACT.

Atomic number	Atomic weight	Density (g cm^{-3})	Mass of first stable isotope	Abundance (%)
1	1.00794	0.0708	1	99.985, 0.015
2	4.002602	0.1221	3	0.000138, 99.999862
3	6.941	0.534	6	7.5, 92.5
4	9.01218	1.848	9	100.0
5	10.811	2.34	10	19.9, 80.1
6	12.011	2.1	12	98.9, 1.1
7	14.0067	0.808	14	99.634, 0.366
8	15.9994	1.14	16	99.762, 0.038, 0.2
9	18.998403	1.111	19	100.0
10	20.179	1.2015	20	90.51, 0.27, 9.22
11	22.98977	0.971	23	100.0
12	24.305	1.738	24	78.99, 10.0, 11.01
13	26.98154	2.6989	27	100.0
14	28.0855	2.33	28	92.23, 4.67, 3.10
15	30.97376	1.82	31	100.0
16	32.066	2.07	32	95.02, 0.75, 4.21, 0., 0.02
17	35.453	1.8956	35	75.77, 0., 24.23
18	39.948	1.6504	36	0.337, 0., 0.063, 0., 99.6
19	39.0983	0.862	39	93.2581, 0.0117, 6.7302
20	40.078	1.55	40	96.941, 0., 0.647, 0.135, 2.086, 0., 0.004, 0., 0.187
21	44.95591	2.989	45	100.0
22	47.88	4.54	46	8.0, 7.3, 73.8, 5.5, 5.4
23	50.9415	6.11	50	0.250, 99.750
24	51.9961	7.19	50	4.345, 0., 83.789, 9.501, 2.365
25	54.9380	7.44	55	100.0
26	55.847	7.874	54	5.8, 0., 91.72, 2.2, 0.28
27	58.9332	8.9	59	100.0
28	58.69	8.902	58	68.27, 0., 26.10, 1.13, 3.59, 0., 0.91
29	63.546	8.96	63	69.17, 0., 30.83
30	65.39	7.133	64	48.6, 0., 27.9, 4.1, 18.8, 0., 0.6
31	69.723	5.904	69	60.1, 0., 39.9
32	72.59	5.323	70	20.5, 0., 27.4, 7.8, 36.5, 0., 7.8
33	74.9216	5.73	75	100.0
34	78.96	4.79	74	0.9, 0., 9.0, 7.6, 23.6, 0., 49.7, 0., 9.2

Atomic number	Atomic weight	Density (g cm^{-3})	Mass of first stable isotope	Abundance (%)
35	79.904	3.12	79	50.69, 0., 49.31
36	83.80	2.6021	78	0.35, 0., 2.25, 0., 11.6, 11.5, 57.0, 0., 17.3
37	85.4678	1.532	85	72.165, 0., 27.835
38	87.62	2.54	84	0.56, 0., 9.86, 7.0, 82.58
39	88.9059	4.469	89	100.0
40	91.224	6.506	90	51.45, 11.22, 17.15, 0., 17.38, 0., 2.8
41	92.9064	8.57	93	100.0
42	95.94	10.22	92	14.84, 0., 9.25, 15.92, 16.68, 9.55, 24.13, 0., 9.63
43	0.	11.50		
44	101.07	12.41	96	5.52, 0., 1.88, 12.7, 12.6, 17.0, 31.6, 0., 18.7
45	102.9055	12.41	103	100.0
46	106.42	12.02	102	1.02, 0., 11.14, 22.33, 27.33, 0., 26.46, 0., 11.72
47	107.8682	10.50	107	51.839, 0., 48.161
48	112.41	8.65	106	1.25, 0., 0.89, 0., 12.49, 12.80, 24.13, 12.22, 28.73, 0., 7.49
49	114.82	7.31	113	4.3, 0., 95.7
50	118.710	5.75	112	0.97, 0., 0.65, 0.36, 14.53, 7.68, 24.22, 8.58, 32.59, 0., 4.63, 0., 5.79
51	121.75	6.691	121	57.3, 0., 42.7
52	127.60	6.24	120	0.096, 0., 2.6, 0.908, 4.816, 7.14, 18.95, 0., 31.69, 0., 33.80
53	126.9045	4.93	127	100.0
54	131.29	3.0589	124	0.10, 0., 0.09, 0., 1.91, 26.4, 4.1, 21.2, 26.9, 0., 10.4, 0., 8.9
55	132.9054	1.873	133	100.0
56	137.33	3.5	130	0.106, 0., 0.101, 0., 2.417, 6.592, 7.854, 11.23, 71.7
57	138.9055	6.145	138	0.09, 99.91
58	140.12	6.770	136	0.19, 0., 0.25, 0., 88.48, 0., 11.08
59	140.9077	6.773	141	100.0
60	144.24	7.008	142	27.13, 12.18, 23.80 ,8.3, 17.19, 0., 5.76, 0., 5.64
61	0.	7.264		
62	150.36	7.520	144	3.1, 0., 0., 15.0, 11.3, 13.8, 7.4, 0., 26.7, 0., 22.7
63	151.96	5.244	151	47.8, 0., 52.2
64	157.25	7.901	152	0.2, 0., 2.18, 14.8, 20.47, 15.65, 24.84, 0., 21.86
65	158.9254	8.230	159	100.0
66	162.50	8.551	156	0.06, 0., 0.1, 0., 2.34, 18.9, 25.5, 24.9, 28.2
67	164.9304	8.795	165	100.0
68	167.26	9.066	162	0.14, 0., 1.61, 0., 33.6, 22.95, 26.8, 0., 14.9
69	168.9342	9.321	169	100.0
70	173.04	6.903	168	0.13, 0., 3.05, 14.3, 21.9,

Atomic number	Atomic weight	Density (g cm^{-3})	Mass of first stable isotope	Abundance (%)
				16.12, 31.8, 0., 12.7
71	174.967	9.841	175	97.41, 2.59
72	178.49	13.31	174	0.162, 0., 5.206, 18.606, 27.297, 13.629, 35.1
73	180.9479	16.654	180	0.012, 99.988
74	183.85	19.3	180	0.13, 0., 26.3, 14.3, 30.67, 0., 28.6
75	186.207	21.02	185	37.4, 0., 62.6
76	190.2	22.57	184	0.02, 0., 1.58, 1.6, 13.3, 16.1, 26.4, 0., 41.0
77	192.22	22.42	191	37.3, 0., 62.7
78	195.08	21.45	190	0.01, 0., 0.79, 0., 32.9, 33.8, 25.3, 0., 7.2
79	196.9665	19.3	197	100.0
80	200.59	13.546	196	0.14, 0., 10.02, 16.84, 23.13, 13.22, 29.80, 0., 6.85
81	204.383	11.85	203	29.524, 0., 70.476
82	207.2	11.35	204	1.4, 0., 24.1, 22.1, 52.4
83	208.9804	9.747	209	100.0
84	0.	9.32		
85	0.	5.0		
86	0.	5.0		
87	0.	5.0		
88	0.	5.0		
89	0.	10.07		
90	232.0381	11.72	232	100.0
91	0.	15.37		
92	238.0289	18.95	234	0.0055, 0.720, 0., 0., 99.2745

Appendix 17 - FISPACT modifications

Changes made to the FISPACT source code in response to problems or to add new features following version 4.0 are described in Table A17.1. Note that a 'modification number' is used for each change made to the source code.

Table A17.1. List of FISPACT modifications.

Date	Problem	Solution	Modification numbers
18/5/95	Inconsistent values of tritium in summary at end of each time interval. Only seen when masses ≠ 1 kg used.	The *specific* tritium activity was stored and added to the *total* activity (not specific). So store the *total* activity for tritium.	555
19/5/95	Titles of final summary at end of run say *specific* values. The *total* values are shown, and this is probably most useful.	Change titles to show *total* values.	556
19/5/95	Would be useful to show total mass of material in final summary.	Add this feature.	557, 558
24/5/95	Output of neutron spectrum in Printlib is incorrect for XMAS (172) group structures.	Changes made in COL172 subroutine because only first 69 values of neutron spectrum written to COLLAPX file.	559,560
24/5/95	The printing of the different group structures does not distinguish between 172 and 175 groups.	This feature added.	561,562,563
24/5/95	When an array created by ENFA + ARRAY the new spectral data was input, but if the original data was in more groups then the old data values remain. This causes a problem in the Printlib output.	Changes made in the ENDFPR subroutine so SPECN() is reinitialised to -1 for those values where data are not read in.	564
12/6/95	The output γ spectrum in the 22 group format was missing data from the second group.	Changes made to the OUTPUT subroutine so all 22 groups output.	573
13/6/95	The output γ spectrum lists energy per group. It would	This feature added.	565 - 572, 574 - 577

Date	Problem	Solution	Modification numbers
	also be useful to show number of γs per group. These data should also be available in TAB4.		
12/7/95	The warning message that 'Ratio of Fission Products/Fissions differs from 2' is seen more often than expected.	An error was noted in CALC in the fission source term. This was corrected. Also the warning message is not appropriate if very small amounts of actinides are input. If actinides < 0.1% of input atoms then no warning.	578-580
17/7/95	In multiple irradiations of actinides the reported burnups and number of fissions are not correct.	Variables are being re-initialised in CALC. This must not be done, the initial number of fissionable nuclides must be stored in a common.	581-600
17/7/95	Warning about having multiple subintervals with actinides should only be given in an irradiation step.	Modify test for warning.	601
17/10/95	Index file now contains Fm isotopes, for these the ZA value requires an I7 format not an I6.	Format statements in COL069, COL100, COL172, COL175 and ENDFPR changed.	602-614
18/10/95	Groupwise files must contain the ZAI value in a 'coded' form for Fm isotopes.	Change made on COL069, COL100, COL172 and COL175.	615, 623-625
18/10/95	Format change from I6 to I7 required when reading A2 and Hazard files containing Fm isotopes and when outputting error data.	Changes made in A2INP, HAZINP and ENDFPR.	616-618
18/10/95	Need to initialise XSECT array.	Change made in COL069, COL100, COL172 and COL175.	619-622
23/10/95	Array overflow in INTERP.	More bremsstrahlung candidates, increase array dimensions from 400 to 450.	626
24/10/95	Array sizes for sequential charged particle too small.	Array sizes increased, some constants redefined.	627-636
14/11/95	For problems involving	This feature added by	637-645

Date	Problem	Solution	Modification numbers
	pulsed irradiation it would be useful to include a 'loop' facility in the FISPACT input file.	introducing the new code words PULSE and ENDPULSE.	
12/2/96	For problems involving actinides it would be useful to be able to switch off fission product production from specified actinides.	This feature added by introducing the new code word FISYIELD.	646-648, 653-655
12/2/96	Problem found when considering neutrons with only low energy (*e.g.* D-D spectrum). Cross section and uncertainty files 'get out of step' because so many of the collapsed cross sections are zero.	Change a constant from 20 to 30 in COL069, COL100, COL172 and COL175.	649-652
15/3/96	Problem with pathways for some actinide targets.	Incorrect use of the variable LIMIT1 in CHAINP.	656
15/3/96	The reaction (n,4n) is not correctly printed in the PRINTLIB output.	Changes made in INTERP and OUTP.	657-659
23/5/96	Printout of pseudo cross sections was not done properly if more than 1 subinterval defined.	Changes so that stream connected to LIN5 is properly closed.	660-662
23/10/96	A Macintosh version of FISPACT is required.	Modifications so that the Master file contains modifications for a Macintosh version.	663-688
24/10/96	Need to add the facility to include half-life as well as cross section uncertainties to the uncertainty estimation.	Add this feature.	689-712
29/10/96	Need to include the Build number and date into the code and the output when compiling a new version.	Add this feature.	713-717, 721, 727, 728
6/11/96	Noted that the ENDF codes for some of the more exotic decays are not treated correctly.	Changes made in ENDFP.	718-720,722-726
12/11/96	For runs where the neutron spectrum changes it would be useful to be able to change	This feature added by introducing the code word NEWFILE, which allows	729-734

Date	Problem	Solution	Modification numbers
	the name of the COLLAPX, ARRAYX and FLUXES files during the course of a run.	the name of the file on a stream given in FILES to be redefined.	
14/11/96	When using the OVER code word it was only possible to specify an isomer by 'm' or 'n' when it is a parent, for the daughter the FISPACT identification number is still required.	Corrected this in OVERID.	735, 736
14/11/96	PRINTLIB output contains the neutron fractions (in the three energy regions) in the reverse order.	Corrected this in INTERP.	737
16/12/96	FISYIELD and UNCTYP code words used code belonging to following code word.	Added the missing 'GO TO 100' statements in MAIN.	738, 739
9/1/97	SCPR not included if ROUTES used without a full inventory.	Using ROUTES now causes the pseudo cross sections to be calculated.	740 - 755
20/1/97	Some platforms require long pathnames for entries in FILES.	FILES array redefined to be CHARACTER*80.	756 - 762
20/1/97	The variable WOR not defined in MAIN.	WOR defined as CHARACTER*4.	763
20/1/97	Usage of the '±' character causes problems when printing on some platforms.	Replace by '+/-' or '+-'.	764 - 770
21/1/97	New data available for calculating γ dose rates.	Data read from stream 39 rather than taken from DATA statements. New algorithm used for point source.	771 - 787
29/1/97	FISPACT version number not printed correctly.	Change made in MAIN.	788, 789
3/2/97	Run time not correctly calculated in Mac version	Change type of TIME0 and TIME1 variables.	790 - 798
3/2/97	UNIX version had problems using NEWFILE code word.	Need to explicitly close the cross section library after collapsing.	799 - 802
4/2/97	UNIX version required change of name and addition of additional comment lines	Changes in MAIN, CLOCK and CLOKK.	803 - 805

Date	Problem	Solution	Modification numbers
5/2/97	Errors when reading spontaneous fission data	FNUBAR set to 0. A check made that decay is spontaneous fission.	806
5/2/97	PC label needs to be more general	Label changed to reflect new compiler version	807
1/7/97	Error when irradiating H or He	Additional test added to identify case where only nuclides 1-5 present.	808
1/7/97	Variables not initialised	DELB array correctly initialised	809
2/7/97	Inconsistencies between platforms	Some variables made double precision and checks made so that single precision don't underflow	810-818
2/7/97	Error due to undefined variable under certain conditions	ZDAU variable initialised correctly	819
13/10/98	Need to be able to read clearance data	Subroutine CLINP added	820
13/10/98	Modifications due to CLINP	Commons modified, variables added and output formats changed	821-860
14/10/98	Need to be able to read 315 group data files	Subroutine COL315 added	861
15/10/98	Modifications due to COL315	Commons modified, variables added and output formats changed	862-876
16/10/98	Error if more than 200 time intervals in case	Arrays storing summary data now act as buffers with earlier data discarded so that only data for the most recent 200 intervals shown	877
20/10/98	Modifications due to COL315	Defining F1, F2, F3 for 315 groups	878, 879
20/10/98	Group conversions need to include 315 as a standard	Change array dimensions, add new code in GRPCON	880-884
22/10/98	Errors after modifications	Variables in some commons not typed correctly	885, 886
2/11/98	Ensure no Y2K issues	Increase size of date string and make changes to system clock calls for all versions	887-946
5/11/98	Error if collapse with a zero spectrum	Additional test to trap cases where total flux is zero	947-952
10/12/98	Error when using PRINTLIB with 315 group spectrum	Correction made in COL315	953

Date	Problem	Solution	Modification numbers
10/12/98	Warning from UNIX compiler on a FORMAT statement in GRPCON	Extra ',' added to FORMAT statement	954
10/12/98	Error on UNIX when run SEQU case with multiple irradiations	Stream 19 not always closed, error seen under UNIX. Corrected.	955, 956

Users with problems are asked to supply the following information when reporting a bug:

- Version number of FISPACT and EAF libraries used.
- Computer platform used.
- Copy of input file.
- Copy of neutron spectrum.
- Details of error message given.

Appendix 18 - EASY documentation set

The FISPACT-99 User Manual forms part of the EASY documentation set. The complete set shown in Table A18.1 is available to commercial users of FISPACT, most of it is also available as the individual UKAEA reports shown in Table A18.2, in some cases these only contain a sample of the complete data where these are very extensive.

Table A18.1. Parts of the EASY Documentation Series.

EDS Report	Title
EDS-0	EASY-99: Overview
EDS-1	FISPACT-99: User manual
EDS-2	FISPACT-99: Qualification report
EDS-3	EAF-99: Data libraries
EDS-4	EASY-99: Processing system

Table A18.2. The composition of the EASY Documentation Series.

EDS Report	UKAEA report number	Ref.
EDS-0	*EASY-99: Overview*	36
EDS-1	FISPACT-99: User manual	-
EDS-2	*FISPACT-99: Validation (EDS-2a)*	2
	Selection of reports and papers	-
EDS-3	EAF-99: Cross section library	15
	EAF-99: Report file (EDS-3a)	17
	EAF-99: Decay data library	21
	EAF-99: Biological, clearance and transport libraries	25
EDS-4	SYMPAL: User guide	37
	SYMPAL: Utilities guide	38
	SAFEPAQ: User manual	39

Notes: documents in *italics* are not UKAEA reports. There is no report on the EAF-99 (n,γ) reactions, however reference 16 contains data for EAF-97. The processing reports in EDS-4 have not been modified for EAF-99.

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