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FISPACT-2005: User manual

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Abstract

FISPACT is the inventory code included in the European Activation System (EASY). A new version of FISPACT, FISPACT-2005, has been developed and this report is the User manual for the code. It explains the use of all the code words used in the input file to specify a FISPACT run and describes how all the data files are connected. A series of appendices covers the working of the code and the physical and mathematical details. Background information on the data files and extensive examples of input files suitable for various applications are included.

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Document modifications

The following procedure will be followed if the FISPACT-2005 user manual requires updating:

Each page carries the issue number and date; if a page does not show ‘*Issue 1*’ then there has been a modification which will be shown by strikethrough of the old prior to the new underlined text and by a sidebar in the margin, *e.g.*

This is just a demonstration of ~~the changes.~~ how the modifications are made.

In some cases it will be necessary to add new pages, and the page numbering will be changed by adding a, b... after the page number, *e.g.*:

Originally the page numbers were ... 26, 27, 28, If a new sheet is inserted after page 27 then the numbers will become:

... 26, 27, 27a, 27b, 28, ...

Users will be sent modified or additional pages, and these should be inserted based on the instructions which are given in the Modification List.

Modification List

Issue	Date	Modified Pages	New Pages	Removed Pages
Issue 1	23/12/04	None	None	None

The current issue of the manual is Issue 1.
The current version of FISPACT is 05.0/0, build 39.

Users are asked to notify UKAEA of any problems with FISPACT. New versions will attempt to remove bugs and add features in response to feedback from users. Appendix 17 gives details of changes in FISPACT made in response to particular problems.

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Disclaimer

Neither the authors nor UKAEA accept responsibility for consequences arising from any errors either in the present documentation or in the FISPACT code.

Contact person

Feedback on the use of FISPACT is welcomed. Please contact RA Forrest with comments or in case of problems.

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Introduction

FISPACT is an inventory code that has been developed for neutron induced activation calculations for materials in fusion devices. It is a powerful code that can answer the basic questions about the numbers of atoms and the activity in a material following neutron irradiation, and can also give details of the pathways by which these nuclides are formed. It can treat trace amounts of actinides that are able to fission, and includes the effects of sequential charged particle reactions. This manual describes version 2005 that represents the outcome of developments of the code during the last nineteen years. FISPACT was developed from the FISPIN¹ inventory code that was designed for fission reactor calculations and dealt in greater detail with inventories arising from the irradiated fuel in a reactor. FISPACT is complementary to FISPIN and has been designed for activation calculations; however, it can be used with any type of neutron spectrum and is not restricted to only fusion applications.

FISPACT is now used by many groups throughout Europe and has been adopted by the ITER project as the reference activation code. It is available on two computer platforms: UNIX workstations and IBM compatible personal computers running a Windows operating system. On the latter it can be used as part of the EASY User Interface which gives a 'user friendly' front end to the main task of 'number crunching'.

FISPACT uses external libraries of reaction cross sections and decay data for all relevant nuclides to calculate an inventory of nuclides produced as a result of the irradiation of a starting material with a flux of neutrons. The actual output quantities include the amount (number of atoms and grams), the activity (Bq), α -, β - and γ -energies (kW), γ dose-rate (Sv h⁻¹), the potential ingestion and inhalation doses (Sv), the legal transport limit (A₂ value), the clearance index and the half-life for each nuclide. Amounts and heat outputs are also given for the elements and the γ -ray spectrum for the material is listed as

well as various summed quantities, such as total activity and total dose-rate. At the end of each time interval the dominant nuclides (in terms of activity, heat, γ dose-rate, potential biological hazards and clearance index) and the pathway data for the production of these nuclides can be shown. The uncertainties in eight total radiological quantities can be calculated and output. As options, data files can be produced for subsequent use by other programs to plot graphs of the total responses as functions of elapsed time and selected blocks of output may be written to external data files.

FISPACT is a part of the European Activation System (EASY), and the current report should be viewed in parallel with the complete document set for EASY; this is discussed in detail in Appendix 18. It should be noted that the report on validation, which in releases prior to 2003 was a separate document² is now included as Appendix 19 of the current report. This contains a set of examples that confirm the correct processing of input data and cases where FISPACT results can be compared with analytical calculations. These tests can be run for each new version, as part of the quality assurance procedure.

Version summary

Version 1

Version 1 of FISPACT enabled inventories to be calculated, but it was not possible to correctly follow the production of the gases ^1H , ^2H , ^3H , ^3He and ^4He . These nuclides were only correctly counted if they arose as products via reactions such as $^3\text{He}(n,p)^3\text{H}$, *i.e.* the gas producing nuclide is written as the daughter nuclide. They can also arise as the outgoing projectile, *i.e.* the ‘p’ in the previous reaction is actually ^1H , but for these cases the gas producing nuclide was assumed to be lost from the system.

Version 2

Version 2 addressed the issue of gas production by storing both the cross section for the standard reaction *e.g.* $X(n,p)Y$ and for the reaction in the form $X(n,Y)^1\text{H}$. For the latter reaction the effective cross section is stored as a negative value in order to identify this type of reaction, and during the calculation this is converted back to a positive value before use. This meant that the array $A()$ in which all the nuclear data are stored had to be substantially increased in size and the convention has been adopted that the various files used for version 2 onwards have an ‘X’ appended to them for identification.

There was no need to alter existing data libraries when moving to version 2 but a new index file (**INDEX**) had to be used which repeated the five gas nuclides at the end, but with the ZA identifier indicating that the nuclide is a 3rd isomer. Thus ^1H is labelled as 10010 at the start and as 10013 when repeated at the end of the index. Gas production is also correctly followed in the pathway analysis so that the routes for the production of tritium can be calculated.

Dominant nuclides were given in a sorted list at the end of each time interval and the pathways for their production could be shown if required.

Version 3

Version 3 had two major new facilities. Firstly it could use the uncertainty data for each reaction, which became available as part of the European Activation File³ (EAF-3), and the pathway data routinely generated at the end of each time interval to calculate the uncertainty in the total radiological quantities (activity, heat, γ dose-rate and potential ingestion and inhalation hazards). Secondly EAF-3 contained cross sections for nuclides in the atomic number range 85 - 96 (actinides), including the fission channel. This version was able to use these data in conjunction with fission yield data (taken from JEF-2) to calculate the inventory of fission products if actinides were initially present as trace elements in the material.

Version 4

Version 4 includes the option of including sequential charged particle reactions as an additional mechanism for the production of activity. Details of this mechanism are given in Appendix 12. Two additional energy group structures (WIMS and XMAS) are treated, and in addition it is now possible to input the neutron spectrum in an arbitrary format and then convert to one of the 4 standard structures. A maximum of twenty (rather than 10) dominant nuclides can now be listed and the presentation of the pathway information has been improved. The decay data and fission yield data are based on JEF-2.2. Version 4 was designed to use EAF-4 data libraries (reference 4).

Version 97

Starting with FISPACT-97, the version number indicates the year of release of the new version. The main new features of FISPACT-97 were the ability to input the EAF-97 library and the use of half-life uncertainties in addition to cross section uncertainties to calculate the uncertainties on radiological quantities. Options to consider either source of uncertainty alone or both together could be defined in the input file. Note that the decay data library used should contain these uncertainty

data for all nuclides (as do EAF_DEC-97 - EAF_DEC-2005) if this new option is to be used.

The data on photon absorption used to calculate dose rates was updated. These are read from a file rather than being stored in the FISPACT code as in previous versions.

To aid the preparation of input files for cases with pulsed irradiation a simple loop construct was added. This enables all the code words between the start and finish of the loop to be repeated as many times as required.

In cases where actinides are relevant it is possible to specify which of these will produce fission products when they undergo fission. Such a facility allows all fission product production to be switched off or to be allowed for a particular set of actinides for detailed investigations of the contributions of individual nuclides.

Data on the higher actinides (Bk - Fm) were included in EAF-97 and FISPACT is able to treat these actinides in the same ways as the other actinides (At - Cm).

In most work modelling irradiations it is possible to assume that the neutron spectrum remains constant. However, in some cases it is required to allow for a change in the shape of the neutron spectrum. Rather than having to do a series of separate runs it was possible in FISPACT-97 to prepare **COLLAPX** files for each spectrum and during the run to change the **COLLAPX** file that is used as the run progresses.

Version 99

The main new features of FISPACT-99 were the ability to input the EAF-99 library, use of a new energy group structure (the TRIPOLI 315-group structure) and the use of clearance data to calculate a clearance index for the disposal of radioactive material. Several bugs were dealt with; the most important was to ensure that the summary at the end of the output could be printed for large numbers of time intervals. This change means that pulsed irradiations with large numbers of time intervals could be run successfully.

FISPACT does not use dates in the calculation of inventories, but does print out various times and dates in the output file. FISPACT-99 was designed for Y2K compliance and there have been no Y2K problems reported. Changes were made to the format of printing dates; these show 4 digits instead of 2 (1999 not 99). So long as the operating system and computer used to run FISPACT are Y2K compliant then FISPACT should introduce no Y2K issues.

Version 2001

The main new features of FISPACT-2001 are the ability to input the EAF-2001 library, calculation of dominant nuclides (and uncertainties) for three additional quantities, additional information output and the updating of physical constants and properties. Several bugs have been dealt with; the most important was to correct the gamma dose rate from a point source which was a factor of 10 too large in both FISPACT-97 and -99. Also the nuclides masses from the decay data file are now used, leading to more consistent mass calculations.

Version 2003

The main new features of FISPACT-2003 are the ability to input the EAF-2003 library and the inclusion of new reaction types (mostly in readiness for a future extension of the energy range of the data libraries).

Version 2005

The main new feature of FISPACT-2005 is the ability to input the EAF-2005 library which, in group form, extends to an energy of 55 MeV. This has involved most of the FISPACT arrays being significantly larger as the EAF-2005 library contains 62,637 reactions compared to only 12,617 in EAF-2003. There are many new reaction types (typically with thresholds above 20 MeV) and four new decay modes have been defined. The data for sequential charged particles also extends above 20 MeV, and can be used for runs using both 175 and 211 group libraries. Three additional charged particle

cross section files are available, which require additional entries in the **FILES** file. A bug that caused only some of the sequential charged particle data to be used was fixed, consequently if using EAF-2003 data the contribution from SCPR will be larger than when using FISPACT-2003. The calculation of the production of fission products in previous versions was also found to be lacking, changes have been made in FISPACT-2005 to correct this bug.

FISPACT-2005 has been tested running under the Windows 98, Windows NT4.0, Windows 2000 and Windows XP operating systems. It runs in an MS-DOS (Command) window, and there is a 32-bit version of the 'EASY-2005 User Interface'.

FISPACT-2005 can be run on a UNIX workstation running a variety of operating systems; however, there is no UNIX version of the 'EASY-2005 User Interface'.

The main features of FISPACT and the version that first included it are summarised in Table 1.

Table 1. Features of FISPACT.

Feature	Details	Comments
Cross section data	69 (WIMS) format.	New in version 3.
	100 (GAM-II) format.	
	172 (XMAS).	New in version 4.
	175 (VITAMIN-J) format.	New in version 2.
	315 (TRIPOLI) format	New in version 99.
Neutron spectrum	Arbitrary group structure can be used for neutron spectrum, internally converted to one of the standard structures.	New in version 4.
Decay data input	ENDF/B-V or -VI format.	External library enables changes to be easily made.
Gas production	H and He isotopes produced by <i>e.g.</i> (n,p) reactions properly included.	New in version 2.
Dose rate calculation	Surface contact dose from infinite slab.	
	Dose at arbitrary distance from a point source.	New in version 3.
Bremsstrahlung	The contribution of γ rays produced by energetic β particles can be included in the dose rate.	New in version 2.
Graphical output	Data produced in suitable format for processing by auxiliary program.	
γ spectrum	Output in 24 energy groups.	
	Output in 22 energy groups.	New in version 2.
Modification of library data	Particular cross sections or decay data can be modified for a run.	
	Uncertainty data can be modified.	New in version 3.
Dominant nuclides	The 'top 20' nuclides for activity, γ dose rate, heating and biological hazards listed for each time interval.	New in version 2, modified in version 4.
Sensitivity method	Option to calculate effect of a change of cross section or decay constant on the production of a nuclide.	New in version 2. Time consuming method to identify important reactions.
Pathway Method	Calculates the amount of a nuclide that is produced by a particular pathway, or calculates all pathways between a parent and daughter.	New in version 2. A fast method to identify important reactions - can be used routinely.
	Generic pathways can be output.	New in version 3.
Inclusion of actinides	Can treat actinide impurities (including fission) in same detail (<i>e.g.</i> pathways) as other nuclides.	New in version 3.
Uncertainties	An uncertainty file and the pathway method for the dominant nuclides enables uncertainty on activity, γ dose rate, heating and biological hazards to be calculated for each time interval.	New in version 3. Routine production of uncertainties is possible.
Sequential charged particle reactions	This method of activation can be included by inputting new data libraries.	New in version 4.
Comments	Comments can be inserted in the input file with the syntax <code><< comment >></code> .	New in version 3.
Monitoring the progress of a run	The progress of a run can be monitored by echoing the code words to the current window.	New in version 3.

Feature	Details	Comments
'Loop' construct in the input file.	If the irradiation consists of many repeated steps, the construction of the input file is made simpler by allowing some of the code words to be repeated.	New in version 97.
Fission product production can be switched off.	Fission product production from individual actinides can be controlled to aid in understanding the various pathways involving fission.	New in version 97.
Version available for 32-bit PC operating systems.	Windows 95 and Windows NT4.0 versions developed.	New in version 97.
New photon absorption data.	All dose rates are calculated using a set of photon absorption data. A new set is read from a file rather than being stored in the FISPACT code.	New in version 97.
Version available for the Macintosh platform.	Macintosh Power PC version developed. This platform is not supported in versions 99 or 2001.	New in version 97.
Half-life uncertainties.	The estimation of uncertainties of radiological quantities now includes the contribution of half-life uncertainties in addition to cross section uncertainties.	New in version 97.
Redefinition of file names during the course of a run.	The file names defined in FILES for streams 12, 17 and 20 can be changed during the course of a run. Useful if the neutron spectrum varies during the irradiation.	New in version 97.
Calculation of clearance index	Clearance data for radionuclides are available in EAF-99 and are read on stream 40. The clearance index for each nuclide and the total inventory are calculated if required.	New in version 99.
Dates made Y2K compliant	Years in dates shown at start and end of run are printed using 4 digits instead of 2 (1999 not 99).	New in version 99.
Dominant nuclides for additional quantities	The 'top 20' nuclides for clearance index and gamma and beta heats are listed for each time interval.	New in version 2001.
Uncertainties for additional quantities	Uncertainty estimates for clearance index and gamma and beta heats can be calculated for each time interval.	New in version 2001.
New summary table at end of case	A summary table containing data on beta and gamma heat and mean energy can be displayed at the end of case.	New in version 2001.
Updated physical constants	The values of the amu, the Avogadro constant, abundances and atomic masses have been updated.	New in version 2001.
New reaction types included	(n,3n α), (n,p α), (n,2n2 α), (n,d2 α), (n,t2 α), (n,nt2 α), (n,3 α), (n,n3 α) reactions defined	New in version 2003.
Cross section data	211 (VITAMIN-J+) format. 351 (TRIPOLI+) format	New in version 2005. New in version 2005.
Neutron spectrum	Arbitrary group structure can be converted to the new 211 or 351 group structures.	New in version 2005.
New decay modes	(n), (pp), ($\beta^- \beta^-$), ($\beta^- \text{SF}$) modes defined	New in version 2005.

Feature	Details	Comments
New reaction types included	(n,5n), (n,6n), (n,7n), (n,8n), (n,3p), (n,d α), (n,t α), (n,h α), (n,ph), (n,4n α), (n,5n α), (n,6n α), (n,7n α), (n,nt α), (n,2nt), (n,3nt), (n,4nt), (n,5nt), (n,6nt), (n,3n2 α), (n,4n2 α), (n,4np α) reactions defined	New in version 2005.
New charged particle reactions	(p,2n), (h,2n), (α ,2n) reactions defined	New in version 2005.
Sequential charged particle reactions at high energies	Sequential charged particle reactions can be included for runs using 175 and 211 group data	New in version 2005.

Use of FISPACT

Details of the installation of FISPACT and the data libraries and differences in running FISPACT on different platforms are discussed in Appendix 13. This section concentrates on the information that a user must assemble prior to using FISPACT and on introducing the code words that instruct FISPACT to carry out various types of calculation.

The user will require details of the material to be irradiated by neutrons, the times of irradiation and cooling and, most importantly, details of the neutron spectrum that is to be used. The spectrum must be available either in one of the standard energy structures used by FISPACT or in an arbitrary energy structure in which case the user must supply details of the energy boundaries. The standard energy structures are WIMS, GAM-II, XMAS, VITAMIN-J, VITAMIN-J+, TRIPOLI and TRIPOLI+. Cross section data in these seven energy structures are available for the EAF cross section library. Details of the energy boundaries of the seven standard structures are given in Appendix 1. One of the seven group format libraries is used to form the 1-group 'effective' cross sections that FISPACT requires by 'collapsing' the library with the neutron spectrum.

The physical theory and the numerical approximations employed to solve the set of differential equations are described in Appendix 2.

FISPACT is recommended to be used as part of the package of data and codes referred to as EASY (**E**uropean **A**ctivation **S**ystem). EASY has been developed as a self-consistent system of data libraries and code; with this the user is assured that data will be in the correct format and that data in the cross section and decay libraries are consistent with each other. The point-wise EAF library covers the energy range from thermal - 60 MeV, but the upper energy of the group structures are lower, the values are shown in brackets following each structure. WIMS (10 MeV), GAM-II (14.9 MeV), XMAS (19.6 MeV), VITAMIN-J (19.6 MeV), TRIPOLI (19.6 MeV), VITAMIN-J+

(55 MeV) and TRIPOLI+ (55 MeV). Appendix 6 describes the data libraries (*e.g.* cross section data, decay data, potential biological hazards, clearance data and legal transport data) of EASY in more detail.

The input file constructed by a user consists of a series of code words that fall into two categories. The first series ('preliminary') are concerned with library specification and the second ('main') give details of the materials and irradiation history. A separate file containing a list of file names and the various data streams (units) to which the input and output files are connected is also required.

The code words in both categories are described in the following sections in alphabetical order. The code words are shown in **BOLD** type with details of the various parameters that accompany some of them shown in an *ITALIC* font. If a parameter is optional, or only applicable under certain circumstances, it is enclosed in angle brackets (< >). If default values are assumed if the code word is *not* used, then these are shown after the parameters in curly brackets ({ }). Many of the code words consist of many characters, of which only the first four are read and so abbreviations may be used if wished. All the input is 'free format'; the user may include as many blanks (white space) between the words and parameters as desired so that the file is readable and easily understood.

So long as code words are input in the two categories there are usually no restrictions on the order or on repetition; where a certain form or order must be used the reader is warned in the text by the word **MUST**. Other typographical conventions that are used throughout the manual are the use of a bold **COURIER** font for file names and a `COURIER` font for actual computer commands. The code words in the input file tend to follow chronologically the course of the neutron irradiation and subsequent cooling with various options, such as file dumps, interspersed as required.

In this manual recommendations are made about suitable values of parameters. These recommendations refer to typical applications in fusion devices and reflect the experience gained by the authors in running FISPACT. The user should however give some thought to the values of parameters for his particular application, especially if this represents a neutron irradiation under very different conditions.

FISPACT is able to calculate the effects of irradiation of a wide range of actinides. This facility was introduced primarily to allow the naturally occurring actinides (U and Th) to be included in trace amounts in fusion relevant materials. The EAF libraries contain infinitely dilute cross sections, and so if actinides constitute a significant proportion of the input material then the data will not be physically representative since self-shielding and burn-up effects are not included.

Thus whilst it is possible to perform irradiations on pure actinides either to model fuel in a fission power station or in a transmutation device, the results will not be as exact as if a specialised fission reactor code such as FISPIN, were used. If knowledge of the changes in the neutron spectrum during irradiation is available then by using the **NEWFILE** code word some modelling of fuel burn-up is possible. Users are warned that FISPACT and EAF will only give approximate results for the irradiation of large amounts of actinides.

It is important to stress that FISPACT is controlled by means of a series of code words that are collected together in an **INPUT** file. These code words describe the type of the run, the material that is to be considered and what type of output is required. Many data files are required by FISPACT, and the location of these files on the users system must be defined; this is done by means of the **FILES** file (described in the following section). The results of the FISPACT run are written to the **OUTPUT** file. This general structure can be represented by the diagram shown in Figure 1.

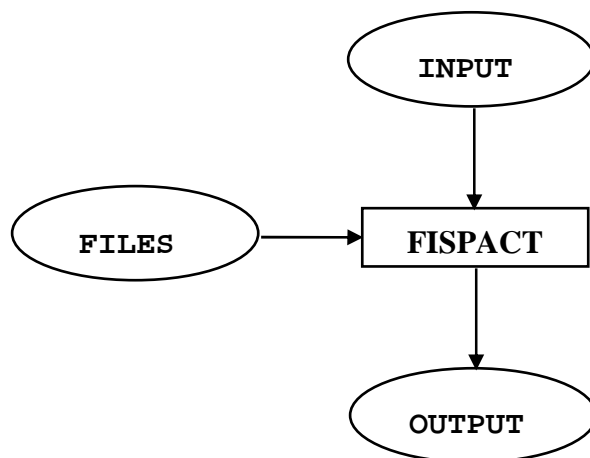


Figure 1. Overview of files used by FISPACT.

Users of FISPACT are recommended to build up a collection of input files for performing typical tasks, such as collapsing, producing a library printout and standard runs under varying conditions and to alter the **FILES** file so that the required **INPUT** file is used. Similarly several **FILES** files can be stored (for various libraries or tasks) and then these renamed so that the one to be used is named **FILES** and is located in the directory where the FISPACT executable resides.

Users are reminded that when specifying time intervals it is necessary to remember that the interval times are cumulative. Specifying times of 1 year, 5 years and 10 years will actually cause inventories to be calculated at 1 year, 6 years (1 + 5) and 16 years (1 + 5 + 10). Forgetting this point is responsible for many of the problems experienced by users.

Input/Output streams and files

The **FILES** file shows the locations of all the files that FISPACT requires for input of data and the conditions for a particular run and for output. FISPACT reserves streams 1-43 for this input/output. Table 2 gives the functions of the reserved streams, with the direction of data flow indicated by I (input) or O (output).

Table 2. Standard streams and generic file names.

Stream	Flow	Description	File Name
3	I	Energy group structure, neutron spectrum and wall loading for arbitrary group structure.	ARB_FLUX
4	I	List of all files and their stream numbers	FILES
5	I	System input	INPUT
6	O	System output	OUTPUT
7	I	Cross section uncertainties library	CROSSUNC
8	I	Links between fissionable nuclides and fission yields	ASSCFY
9	I	Fission yield library	FISSYLD
10	O	Graphical data output	GRAPH
11	I	A ₂ data	A2DATA
12	I	Collapsed cross section library	COLLAPX
13	I/O	Condensed library data	ARRAYX
14	I	Biological hazard data	HAZARDS
15	I/O	Summary of nuclides and isomers	SUMMARYX
16	I	Decay data	DECAY
17	O	Collapsed cross section library	COLLAPX
18	I	Index of materials in library	INDEX
19	I	Cross section library	CROSSEC
20	I/O	Neutron spectrum and wall loading	FLUXES
21	I	Range of proton in each element	STOP_PRO
22	I	Range of deuteron in each element	STOP_DEU
23	I	Range of alpha particle in each element	STOP_ALP
24	I	Range of triton in each element	STOP_TRI
25	I	Range of He-3 in each element	STOP_HE3
26	I	Cross section data for (p,n) reactions	XN_PN
27	I	Cross section data for (d,n) reactions	XN_DN
28	I	Cross section data for (α,n) reactions	XN_AN
29	I	Cross section data for (t,n) reactions	XN_TN
30	I	Cross section data for (h,n) reactions	XN_HN
31	I	Cross section data for (d,2n) reactions	XN_D2N
32	I	Cross section data for (t,2n) reactions	XN_T2N
33	I	Energy spectrum of emitted particles (part 1)	SPEC_1
34	I	Energy spectrum of emitted particles (part 2)	SPEC_2
35	I	Energy spectrum of emitted particles (part 3)	SPEC_3
36	I	Energy spectrum of emitted particles (part 4)	SPEC_4
37	I	Energy spectrum of emitted particles (part 5)	SPEC_5
38	I/O	Relative uncertainty values for nuclide half-lives	HALFUNC
39	I	Gamma absorption data	ABSORP
40	I	Clearance data	CLEAR
41	I	Cross section data for (p,2n) reactions	XN_P2N
42	I	Cross section data for (α,2n) reactions	XN_A2N
43	I	Cross section data for (h,2n) reactions	XN_H2N

The beginning of a typical **FILES** file is shown below:

```
03 d:\fispact\tests\v_2005\spectra
05 d:\fispact\tests\ss316_2.i
06 d:\fispact\tests\ss316_2.o
07 d:\eaf_data\eaf_2005\eaf_un_20050
08 d:\eaf_data\eaf_2005\eaf_asscfy_20050
09 d:\eaf_data\eaf_2005\eaf_fis_20050
10 ...
```

On each line the stream number is followed by the full pathname of the file on the user's system that is to be connected to the stream. The file names shown in column 4 of Table 2 are generic names that will be used in the text of this manual. Actual file names can be chosen as desired on a particular system. It is important to note that for printing via stream 6, the length of the line should be set to 165 characters. This is necessary to enable as much information as practical to be output on a line, so making the output compact and free of repetition. The **FILES** file **MUST** be located in the directory that contains the FISPACT executable.

If the user requires streams for external files *e.g.* specified by the **TABn** code words, then these should have values greater than 43. The name of the file is allocated automatically; the user only has to define the stream number. The **TABn** files are located in the directory that contains the FISPACT executable.

Note that the gamma absorption data (**ABSORP**) on stream 39 is required when FISPACT-2005 is run. Versions previous to FISPACT-97 contained an earlier set of data internally. Thus even if a version of EAF prior to EAF-97 (or a non-EAF library) is used as input then stream 39 **MUST** be connected to **ABSORP**.

The files **COLLAPX** and **ARRAYX** **MUST** exist (even if they are empty) at the locations stated in **FILES**. Other files will be created if they do not already exist.

Preliminary input

This section of the input file deals with the input and processing of library data and ends with the code word **FISPACT**. An important part of library processing is the ‘collapsing’ of the cross section library with a neutron spectrum. The user must construct a file (generic name **FLUXES**) containing the spectrum data. The format is not rigid, and the numbers can be stored in the file as, say, a single column or six columns as convenient. Note that the group flux values in the file **MUST** be entered starting with the highest energy group. Following the spectrum a single number is required - the wall loading (MW m^{-2}) corresponding to the particular neutron spectrum. If the user requires to use the **WALL** code word then this value is used to convert the wall loading parameter to a flux value. If only the **FLUX** code word is used, then a dummy value (such as 1.0) can be used. Following this, a line of text (up to 22 characters) identifying the spectrum is input. This text string is used as part of the library information for each subsequent inventory run.

Diagrams of the basic types of FISPACT runs are shown in Figures 2 - 4. In Figure 2 the cross section library (**CROSSEC**) is collapsed with the neutron spectrum (**FLUXES**) to produce the collapsed cross section library (**COLLAPX**). In Figure 3 the collapsed cross section library (**COLLAPX**) is now used as an input with the decay data library (**DECAY**) to produce the condensed library data (**ARRAYX**). Figure 4 shows a standard inventory calculation that used the condensed library data (**ARRAYX**) as input and produces an additional output - the **GRAPH** file that will be used for plotting a graph of the decay curve.

Note that in all cases the **FILES** file is used to show which input and output files are connected and the location of all the other standard files.

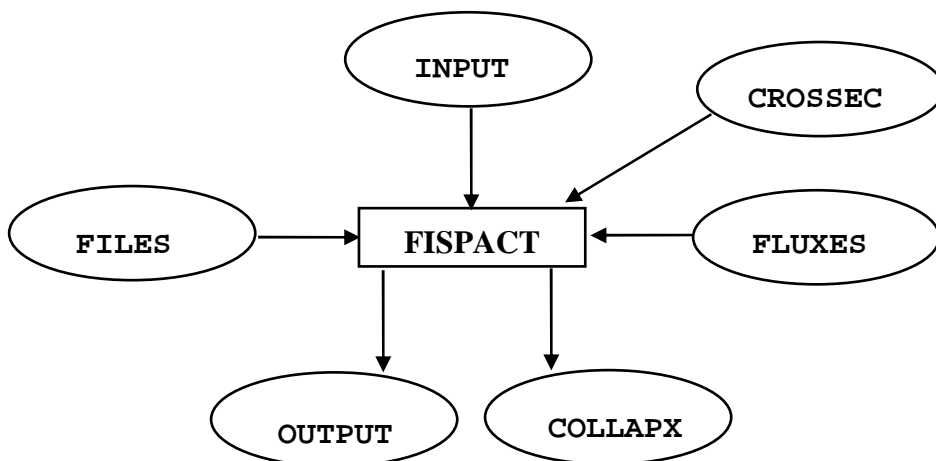


Figure 2. Files used by FISPACT to produce collapsed library.

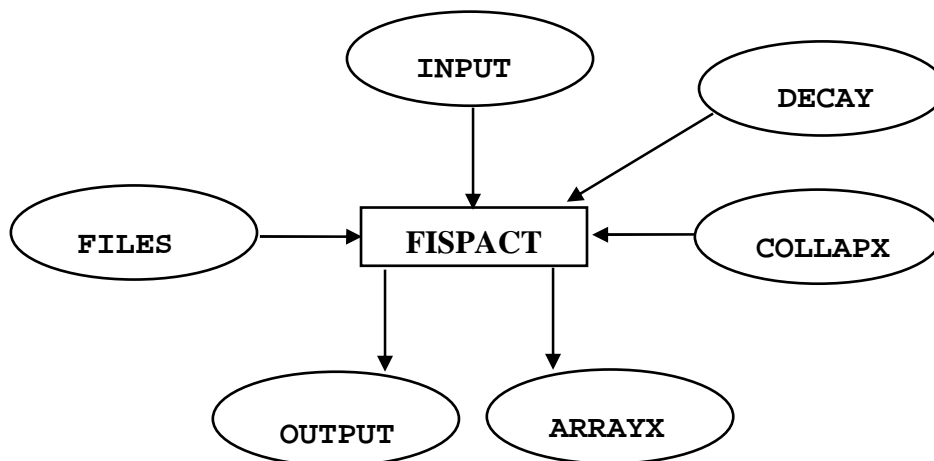


Figure 3. Files used by FISPACT to produce condensed library.

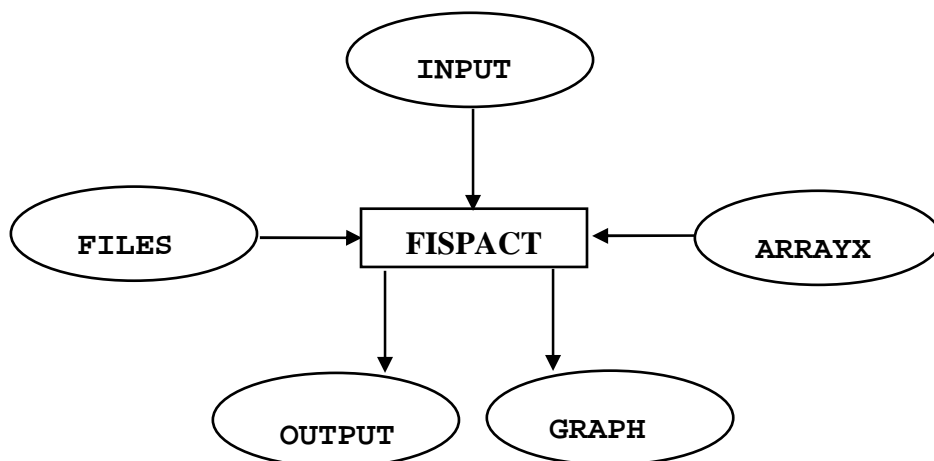


Figure 4. Files used by FISPACT for standard run.

AINPUT

This code word causes condensed library data to be read. The user is recommended to follow the standard procedure of collapsing the cross section library and writing the array file as separate runs. A subsequent inventory run would then always require this code word. It is possible to put all the above steps together in a single input file when this code word would not be required.

This code word is thus typically used in all inventory runs, an example of its use in an **INPUT** files follows.

```
AINPUT
FISPACT
* Irradiation of SS316 steel
...
```

COLLAPSE N2COLL

This code word causes FISPACT to read the cross section library in 69-, 100-, 172-, 175-, 211-, 315- or 351- group format (determined by *N2COLL* being 69, 100, 172, 175, 211, 315 or 351) and combines this with the neutron spectrum to produce a 1-group effective cross section library which is used directly in subsequent runs.

Note that if no uncertainty data exists in the library then the code word **NOERROR MUST** be used before the code word **COLLAPSE**.

An example of the use of this code word follows.

```
COLLAPSE 211
FISPACT
* Collapsing EAF_2005
...
```

The cross section library in 211 groups will be used with the neutron spectrum read from stream 20.

EAFVERSION NEAFV {6}

This code word **MUST** be used if a version of the European Activation File (EAF) cross section library prior to version 2005 is used. It **MUST** be used before the other code words **AINP** or **ENFA** as it determines the number of nuclides treated as fission products.

If version 'n.m' of EAF is used then *NEAFV* should be set to the value 'n'. Note that for EAF-97 and EAF-99 the value '4' should also be used. For EAF-2001 and EAF-2003 the value of 5 should be used. For EAF-2005 the default value of 6 should be used.

An example of the use of this code word follows.

```
EAFVERSION 5
AINPUT
FISPACT
* Irradiation of SS316 steel
```

The cross section library EAF-2003 or an **ARRAYX** file produced using this library is to be input.

ENFA*** TITLE**

This code word reads a title (beginning with an ‘*’ and containing a maximum of 72 characters). In versions prior to 3.0 the title had to contain relevant identifying data about the libraries used. FISPACT now automatically takes text strings from the **CROSSEC**, **FLUXES**, **DECAY** and **COLLAPX** files and uses these to construct the identification information that is stored in **ARRAYX**.

The user **MUST** include at least a single character, but it is still useful to put a sensible title to aid legibility of the output. This code word causes the decay library and the collapsed 1-group library to be input and processed and the condensed library data to be written to an external file.

One of the following code words **MUST** follow the title.

TAPA writes a summary file of nuclides and isomers,

ARRAY uses decay data from an existing **ARRAYX** file,

LINA reads an existing summary file [this option is included only for compatibility with **FISPIN**, it is not recommended].

Users preparing an **ARRAYX** file for a new decay data library **MUST** use **TAPA**. For subsequent runs when only the cross section library is different, then the code word **ARRAY** can be used. If this is done then the decay data is taken from the existing **ARRAYX** file rather than processed afresh from the **DECAY** file.

Note that there is no error checking that the **ARRAYX** file that is read is consistent with the cross sections and consequently an inappropriate use of this code word (*e.g.* using an **ARRAYX** corresponding to a different decay data library) would lead to a new **ARRAYX** file containing rubbish. However, when used carefully this option will make a large time saving (see Table A14.2) in the preparation of **ARRAYX** files.

An example of the use of this code word follows.

```
SPEK
ENFA
* EAF_2005,100-Group,zone 13
TAPA
FISPACT
* Write to ARRAYX file
...
```

FISPACT

*** *TITLE***

This code word reads a 72 character title (beginning with an ‘*’) containing information about the particular run. This title is also used to label the graphs, but for the graph title only the first 40 characters are used. Note that the text used for *TITLE* here is different from that text following **ENFA**.

Note that the code word does not trigger any action, it is only used as a convenient divider to separate the library input from the irradiation details.

SPEK

This code word calculates an approximate γ -spectrum for nuclides in the decay library which have no spectral data. Details about the approximate spectrum are given in Appendix 4. These nuclides are flagged by an ‘&’ in the standard output and in the output of library data produced in a run with the code word **PRINTLIB**.

Main input

This section follows the code word **FISPACT** and contains information about the particular material (elemental or isotopic composition and mass) and the irradiation history (times and flux values). Code words specifying options such as pathways, sensitivity coefficients or graphs are described in this section.

ATOMS

This code word starts the calculation of the inventory equations over the time interval specified and causes the results (isotopic, elemental, spectral, pathway and uncertainty) to be output. It is the standard method of producing output; other options are **SPECTRUM** and **RESULT**.

ATWO

This code word causes data on the legal limits of activity for transport of radioactive material to be input, for the calculations to include these data and for the results for individual nuclides and summed values to be output. Appendix 6 contains more information on these data values.

Note that both **ATWO** and **CLEAR MUST** not be used in a particular case.

BREMSSTRAHLUNG IARG**NUCLB(JJ) JJ=1, IARG**

This code word allows the input of the number (*IARG*) of nuclides and the identifiers (*NUCLB(JJ)*) for each of the nuclides. The identifier should be specified using the format 'TE129M'. When the output is printed, this code word causes the bremsstrahlung dose rate of each specified nuclide to be printed at the end of each time interval.

Note a maximum of 25 nuclides can be specified, and possible candidates, if EAF-2005 is the decay library used, are listed in Appendix 7.

An example of the use of this code word follows.

<pre>BREM 4 CL36 AR39 AR42 K42</pre>

In this case the bremsstrahlung contributions of ^{36}Cl , ^{39}Ar , ^{42}Ar and ^{42}K are calculated and output at the end of each time interval.

CLEAR

This code word causes data on the clearance data of radionuclides to be input, for the calculations to include these data and for the results for individual nuclides and summed clearance indices to be output. Appendix 6 contains more information on these data values.

Note that both **ATWO** and **CLEAR MUST** not be used in a particular case.

CONV MAXXT {10} CONV {2.0 10⁻³} CONVS {2.0 10⁻³}

This code word allows the user to alter the convergence limits used in the integrating routines. The number of iterations (*MAXXT*) can be set in the range 1-10 instead of using the default value of 10. The convergence limit (*CONV*) against which each nuclide is tested in the integrating routines for normal inventory calculations can be specified. The convergence limit for the integrating routines involving pathways is set by *CONVS*.

Note if a nuclide has not converged, then it is flagged on the printed output by a '?'. It should be noted that in the majority of cases the nuclides that are flagged as not converged are of little practical importance. The output values for nuclides that have not converged do not have the accuracy of the rest of the output and thus should be used with caution.

An example of the use of this code word follows.

```
CONV 5 0.005 0.01
```

This would allow a maximum of 5 iterations, and the inventory calculations attempt to get the agreement of each nuclide amount between iterations to within 0.5%, while for the pathway calculations an agreement of 1% is satisfactory.

CULTAB

This code word adds additional lines at the beginning and end of the **TAB** files, so that the files can be more easily processed by other computer programs. The data written are unchanged by the use of this code word, which is retained for consistency with previous versions.

DENSITY *DENSTY*

This code word enables the input of the density of the material undergoing neutron irradiation with the parameter *DENSTY* = density (g cm^{-3}). If this code word is used, then the total activity will also be output in units of Ci cm^{-3} in addition to the standard output in Bq kg^{-1} .

If **FUEL** is used to specify the input material for a run in which an inventory is calculated then the density **MUST** be specified.

An example of the use of this code word follows.

```
DENSITY 8.96
```

The density of the material specified by **MASS** or **FUEL** is 8.96 g cm^{-3} .

DOMINANT *XDOM* {98.0}

In versions of FISPACT prior to 3.1 pathways were calculated for all the dominant nuclides at a particular time interval. With some materials this meant that the calculational time was excessive and it was decided to reduce the number calculated by default and to give the user the ability to vary this. It is now possible to ignore the pathway information for some of the less important 'dominant nuclides' by specifying *XDOM*, which is the cumulative percentage contribution above which pathways are not calculated. The default value has been set at 98%.

An example of the use of this code word follows.

```
DOMINANT 90.0
```

In this case pathways are calculated for each dominant nuclide until the contribution made by the dominant nuclides to each of the radiological quantities is no more than 90.0%. Other dominant nuclides that contribute to the remaining 10% have no pathway information.

DOSE *NDOSE* {1} <*DIST*> {0}

In versions prior to 3.0 all dose rates were calculated for a semi-infinite slab of the material. This is still the default if the code word is not used or if *NDOSE* = 1, but if *NDOSE* = 2 then the calculations are done for a point source of 1 gm of material at a distance of *DIST* metres. *DIST* is not used for the semi-infinite slab as the contact dose rate is always assumed. The minimum distance is 0.3 m, if a smaller value is specified then *DIST* is set to 0.3 m and a message to this effect is printed.

Appendix 3 gives more details of the method of calculation for the two options described above.

An example of the use of this code word follows.

```
DOSE 2 1.0
```

In this case the dose due to a point source (1 g) of the irradiated material at a distance of 1 m is calculated.

END*** TITLE**

This code word terminates the input of data for a particular case. Another case can then be input by specifying more input data; unchanged data do not have to be input again. The text used in *TITLE* is arbitrary, except that at the end of the last case the first three characters after the '*' **MUST** be 'END'.

An example of the use of this code word follows.

```
END
*END of Fe run
```

In this case a line of text is entered after **END**.

ENDPULSE

This code word terminates the 'loop' construct that was started by **PULSE**. All code words between **PULSE** and **ENDPULSE** are repeated *NPULSE* times (*NPULSE* is the parameter following **PULSE**).

ERROR NERROR

*Parent(I) Daughter(I) ERMAT(I) I=1,
NERROR*

Inputs the number (*NERROR*) of reactions and the identifiers of the parent and daughter of each reaction and (optionally) the fractional error of the reaction cross section. In versions prior to 3.0, the user had to input a value of the fractional error, but this is now available from the EAF uncertainty file.

If data from the file are to be used then *ERMAT MUST* be set to -1.

Note that if no uncertainty data exists in the library then the fractional error **MUST** be input, using -1 will cause an error message to be printed.

This code word should only be used following the code word **SENSITIVITY** to give the error in the number of atoms of a nuclide due to the specified reactions; for routine calculations the uncertainty calculations are automatically performed by a simplified method. The maximum value that can be specified for *NERROR* is 50.

Examples of the use of this code word follow.

```
ERROR 2
  LI7 LI8 -1.0
  BE9 HE6 -1.0
```

Line 2 specifies that the reaction ${}^7\text{Li}(n,\gamma){}^8\text{Li}$ is to be considered. Line 3 specifies that the reaction ${}^9\text{Be}(n,\alpha){}^6\text{He}$ is to be considered.

The uncertainty for both reactions is obtained from the uncertainty file.

```
ERROR 2
  LI7 LI8 0.25
  BE9 HE6 0.6
```

Line 2 specifies that the reaction ${}^7\text{Li}(n,\gamma){}^8\text{Li}$ is to be considered.
 Line 3 specifies that the reaction ${}^9\text{Be}(n,\alpha){}^6\text{He}$ is to be considered.

The uncertainty for the first reaction is set at 25% and for the second 60%. The values in the uncertainty file are not used.

FISCHOOSE *NCHO* {2} *FISCHO(I)* *I* = 1, *NCHO* {U238 PU239}

When actinides are included as trace elements in a material then dominant nuclides that can be formed as a result of the fission of an actinide will be considered in the calculation of pathway information. Although uranium and thorium may have been the only actinides input, neutron induced reactions will create many other fissionable actinides and the user may wish to specify which of these actinides are considered as possible parents when calculating the pathways. By default only ${}^{238}\text{U}$ and ${}^{239}\text{Pu}$ are considered, but by increasing *NCHO* and specifying the identifiers of the actinides (*e.g.* 'AM242M') then other nuclides can be included.

Note that including many minor actinides will substantially increase the running time. In most cases minor actinides are unlikely to have significant impact on the total radiological quantities and so are unlikely to be part of the important pathways. Also this code word only affects the calculation of pathways, all actinides are considered during the calculation of inventories.

An example of the use of this code word follows.

```
FISCHOOSE 4 U238 PU239 PU240 PU242
```

In this case any pathways containing a fission reaction can only have one of the four actinides ${}^{238}\text{U}$, ${}^{239}\text{Pu}$, ${}^{240}\text{Pu}$ and ${}^{242}\text{Pu}$ as parent.

FISYIELD NYLD <SYMB(I) I=1,NYLD>

When actinides are included in the list of input elements then by default all the actinides will produce fission products when they fission. If *NYLD* = 0 then no fission products are produced from any of the actinides. If *NYLD* is a positive integer then only the actinides that are specified in the list of identifiers *SYMB* (e.g. 'AM242M') produce fission products. If *NYLD* is a negative integer then all actinides except those that are specified in the list of identifiers *SYMB* (e.g. 'AM242M') produce fission products.

This facility is included so that information on the irradiated actinides alone can be obtained. Also when investigating the properties of various actinides it may be useful to be able to restrict which of these produce fission products.

Note that for a complete inventory this code word should not be used.

Examples of the use of this code word follow.

```
FISYIELD 0
```

None of the actinides will produce any fission products when fissioned.

```
FISYIELD 2 U235 PU239
```

Only ²³⁵U and ²³⁹Pu will produce any fission products when they undergo fission.

```
FISYIELD -2 U238 AM241
```

All actinides except ²³⁸U and ²⁴¹Am will produce fission products when they undergo fission.

FLUX FLUX2

This code word enables the total energy integrated neutron flux ($\text{n cm}^{-2}\text{s}^{-1}$) to be specified for a particular time interval.

Note if several consecutive time intervals require the same flux value then it need only be entered once for these intervals.

Setting the total flux to zero gives a decay time-step.

The flux **MUST** be set to 0.0 before using the code word **ZERO**.

An example of the use of this code word follows.

FLUX 1.5E15

For this particular time interval a total flux of $1.5 \cdot 10^{15} \text{ n cm}^{-2}\text{s}^{-1}$ will be used.

FUEL N1

IS(J) ATOMS(J) J=1, N1

Inputs the number (*N1*) of nuclides and the identifier (*IS(J)*) and the number of atoms (*ATOMS(J)*) for each nuclide. The identifier can be specified either using the format 'TE129M' or by the material number.

Note the 'material number' is the identification given to the nuclide internally by FISPACT. Its value can be seen in the decay data part of the **PRINTLIB** output if required.

The specification of nuclides is essential if materials are to be irradiated which do not have the natural isotopic abundance. Appendix 16 gives the natural abundance of isotopes for each element used by FISPACT. If different values are required then **FUEL** should be used.

The total mass of input material is calculated from the amounts of the nuclides input.

Note that both **FUEL** and **MASS MUST** not be used in a particular case. If **FUEL** is used for a run in which an inventory is calculated then the density of the material **MUST** be specified using **DENSITY**.

An example of the use of this code word follows.

```
FUEL 2
  LI6 8.5E24
  LI7 1.5E24
```

In this case lithium highly enriched in the ⁶Li isotope is to be irradiated.

GENERIC *IGENER* {1}

In addition to the normal output of pathway data, there is a section showing generic pathway data. A generic pathway is one in which all instances of a link of type ‘Nuclide[isomer state m or n](IT)Nuclide[state g]’ is replaced by ‘Nuclide[state g]’. All pathways that when simplified in this fashion have the same form belong to the same generic pathway and the contribution of all the pathways are added to give the contribution of the generic pathway. The default is to always print the generic information, but it can be switched off by setting *IGENER* to 0.

More information on pathways is given in Appendix 8.

GRAPH NUMG GRSHOW GUNCRT*NOPT(I) I=1, NUMG*

This code word specifies what information is stored in the file **GRAPH** for subsequent post-processing. The number of graphs required (*NUMG*) is input, and for each graph an option number (*NOPT(I)*) is read. Allowable values for the options are:

- 1 Total Activity
- 2 Total γ dose rate
- 3 Total heat output
- 4 Ingestion dose
- 5 Inhalation dose

The parameter *GRSHOW* allows slightly different versions of the data file to be constructed. If *GRSHOW* = 0 then an output suitable for PC post-processing is obtained, if *GRSHOW* = 1 then the output might be more suitable for other platforms. The recommended method of producing graphs on a PC is to use the EASY User Interface; Appendix 15 gives details of the Interface and gives a screen shot of a typical graph. An example of a total dose rate output graph produced by a plotting package on a UNIX workstation is shown in Figure 5.

The third parameter *GUNCRT* allows the user to specify if uncertainty data should be (1) or not be (0) written to the **GRAPH** file. If the uncertainty data are written then the plotting routines can display the uncertainties on all five types of plots.

An example of the use of this code word follows.

```
GRAPH 3 0 1
      1 2 4
```

In this case data on activity, γ dose-rate and ingestion dose are written to a file in standard format (suitable for a processing by the EASY-2005 User Interface) with uncertainty data included, from this file three graphs can be subsequently plotted.

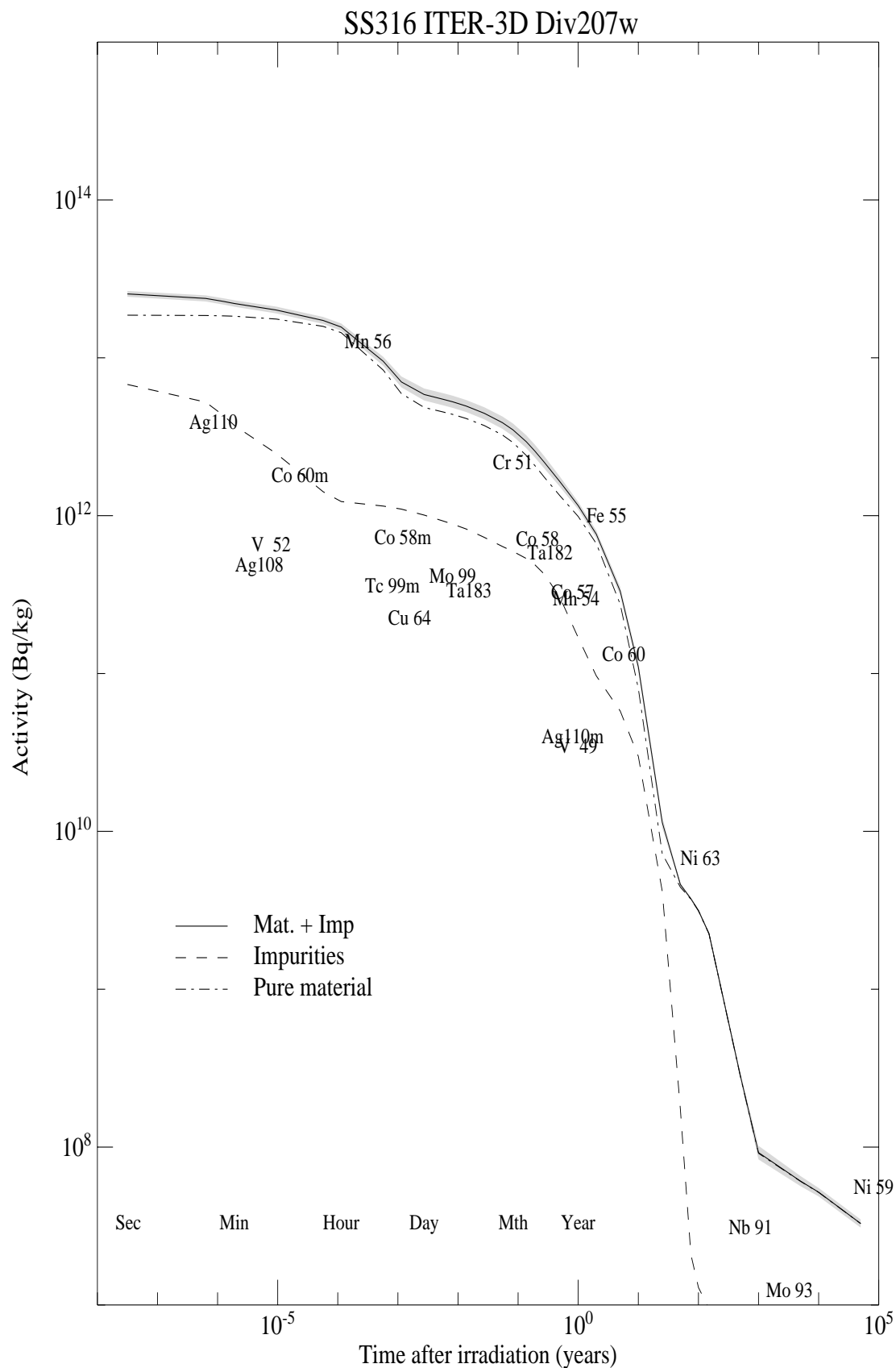


Figure 5. Graphical output produced using the PV-WAVE visualisation package (© Visual Numerics).

GROUP IGAMGP {0}

This code word allows details of the γ -spectrum to be input. The default ($IGAMGP = 0$) means that the γ -spectrum data are output in a 24-energy group structure. This structure is also used when processing the decay data and in the internal calculations.

However, if $IGAMGP = 1$ then the output is in the 22-group ‘Steiner’ energy structure. The values of the energy groups are shown in Appendix 10.

Note that the structure determined by $IGAMGP$ is also used when **TAB4** is specified to produce a file of the γ -spectrum data.

An example of the use of this code word follows.

GROUP 1

In this case data will be output in 22 energy groups.

GRPCONVERT *NESTRC NDSTRC*

This code word allows the user to read a neutron spectrum in an arbitrary number of groups (*NESTRC*) and instruct FISPACT to convert it into one of the seven standard structures. *NDSTRC* must therefore be 69, 100, 172, 175, 211, 315 or 351; using any other value will result in an error message. The user must prepare a file containing the following data and connect it to stream 3 in the **FILES** file.

- *NESTRC*+1 values representing the arbitrary energy boundaries starting with the highest energy.
- *NESTRC* values representing the flux values ($\text{n cm}^{-2}\text{s}^{-1}$) in each group starting with the high energy group.
- First wall loading (MWm^{-2})
- Text string (maximum of 100 characters) identifying the spectrum.

Note that each of the above groups of items should start on a new line in the file, but there should be no blank lines separating them.

The **OUTPUT** file will contain information about the conversion: what fraction of the input groups are included in each output group and details of the input and the output spectra.

The converted spectrum is written to the file connected to stream 20, this contains the standard information for a **FLUXES** file:

- *NDSTRC* values representing the flux values ($\text{n cm}^{-2}\text{s}^{-1}$) in each group starting with the high energy group.
- First wall loading (MWm^{-2})
- Text string (maximum of 100 characters) identifying the spectrum.

Note that although the text string can contain 100 characters only the first 22 will be used as the spectrum identifier, so these should provide an unambiguous description.

The conversion is done on an equal flux per unit lethargy basis; *e.g.* if one of the input groups is split into two or more groups in the converted spectrum then the fraction of neutrons in each output group is determined by the ratio of each lethargy interval of the output structure to the total lethargy interval of the input structure.

There is a restriction on the number of arbitrary energy groups - this **MUST** be greater than 2 and no more than 400.

An example of the use of this code word follows.

```
GRPCONVERT 99 172
```

In this case a spectrum in 99 groups is converted into the XMAS (172) group structure.

HALF

This code word causes the half-life of each nuclide to be printed in the output. The units are seconds, but if the nuclide is stable then the word 'Stable' is printed. If this code word is not used then an indication of the stable nuclides in the output can be seen in the 'flags' section to the right of the nuclide identifier.

HAZARDS

This code word causes data on potential ingestion and inhalation doses to be input and the dose due to individual nuclides to be printed in the output. See Appendix 6 for more details of the data stored in the library.

IRON

This code word should only be used for calculations where small quantities of impurities in an iron matrix are to be irradiated. In a run without this code word the activity of the impurities would probably be masked by the activity of the iron. In order to remove the 'background' this code word causes the iron matrix to be replaced by a matrix of ^{49}Fe (a stable pseudo-isotope with no neutron reactions) so that the printed inventories and dose rates refer only to the impurities.

An example of the use of this code word follows.

```
IRON  
MASS 1.0 2  
FE 99.9999  
AG 1.0E-4
```

In this run, corresponding to the irradiation of 1 ppm of silver impurity in iron, the output will be due only to the reactions on silver. However, the γ dose-rate will represent decays of silver isotopes in an iron matrix rather than in solid silver.

LEVEL C N

This code word allows the input of the two parameters which determine the nuclides that are in equilibrium (**C**) and the number of time subintervals (**N**) into which the irradiation time is divided.

This code word **MUST** be used for the first irradiation, but only needs to be used again for the remaining time intervals if the parameters need to be changed.

If the time interval is T seconds long then the nuclides with decay constant λ (s^{-1}) will be in equilibrium if $\lambda T > C$. These nuclides are flagged with an '*' in the printed output. For typical irradiations a value of $C = 100$ is recommended, while for cooling steps $C = 20$ should be used. Short-lived nuclides that are in equilibrium are calculated by an approximate method. Further details are given in Appendix 2. **Note** that very large values of **C MUST** be given in scientific notation.

Wherever possible the number of subintervals should be set to 1, to reduce computing time. However, if a particular integration gives the message 'Case not converged' then N can be increased. However, since the non-convergent nuclides are flagged in the output, it is easy to judge if the nuclides that have not converged are unimportant and whether the message can therefore be ignored.

For sensitivity calculations a value $N = 5$ is recommended.

If actinides are amongst the starting nuclides then a value $N = 5$ or 10 should be used, since the rate of fission of actinides is only updated at the end of each subinterval.

An example of the use of this code word follows.

```
LEVEL 100 1
TIME 2.5 YEARS
```

In this run, the time interval of 2.5 years is specified; this is not split into subintervals and all nuclides with half-lives < 6.3 days will be considered in equilibrium.

LOOPS *TLOOP*

In calculations of pathways the possibility of excitation of an isomer of a ground state nuclide on the pathway is not automatically considered. However, if the isomer half-life is short and it decays by an isomeric transition (back to the nuclide on the pathway) then it is important to be able to also include the isomer in the calculation.

TLOOP specifies the maximum half-life (seconds) of an isomer such that the reaction $X(n,n')X^*$ and subsequent decay $X^*(IT)X$ will be included in the calculation even though X^* is not on the pathway.

Pathways for the formation of the dominant nuclides that are calculated at the end of each time interval do include the isomers automatically. If **LOOPS** has not been used then the value of *TLOOP* is set to $T / 1000$ where T is the time interval specified by the **TIME** code word.

An example of the use of this code word follows.

```
LOOPS 20.0
```

In the case of the pathway $^{45}\text{Sc}(n,\gamma)^{46}\text{Sc}(n,\gamma)^{47}\text{Sc}$, there is an isomeric state $^{46\text{m}}\text{Sc}$ with half-life of 18.7 s. Using the code word as shown would mean that this isomer was included in the calculations. See Appendix 8 for more information on pathways.

MASS TOTM INDX2 $SYM(I) XP(I) I=1, INDX2$

This code word allows the input of the total mass *TOTM* (kg) and the number (*INDX2*) of elements in the material to be irradiated. For each element the chemical symbol *SYM(I)*, e.g. 'FE', and the percentage by weight, *XP(I)*, are then input. This code word enables elements to be input with the number of atoms of each isotope calculated by FISPACT using natural abundance data that are stored internally. The values used for natural abundance are given in Appendix 16.

This is the recommended method of inputting materials, except if special isotopic compositions are required.

Note that both **FUEL** and **MASS MUST** not be used in the same case in the input file.

Note it is not essential that the total of all elements is exactly 100%, however if the total was say 80% and 1 kg was specified for *TOTM*, then in fact only 800 g of material would be considered in the calculation. It is recommended to ensure that the total percentage of all elements equals 100%.

An example of the use of this code word follows.

```
MASS 1.0 7
      FE 65.255
      CR 18.0
      NI 12.015
      MO 2.4
      MN 1.8
      SI 0.5
      C 0.03
```

In this case the composition of a stainless steel (ignoring impurities and minor elements) is specified. 1 kg of the steel containing the seven listed elements is to be irradiated.

MIND *MIND* {1}

This code word allows the input of a parameter indicating the minimum number of atoms which is not set to zero during the integrations. It is usually not important to consider a few atoms of a nuclide. The default value is 1, but this means that an inventory with an extremely large number of unimportant nuclides will be generated, and it is recommended that a value such as 1.10^5 be used for the *MIND* parameter. It is possible to use a parameter value less than 1 if information on a wide range of nuclides is required.

Note that the value of *MIND* corresponds to the amount of material specified, it does not refer to number of atoms for a unit mass.

An example of the use of this code word follows.

```
MIND 1.0E5
```

In this case all nuclides with numbers of atoms $< 1.10^5$ are reset to zero during the calculation.

MONITOR *MONIT* {0}

The progress of a FISPACT run can be monitored by printing the various code words as they are read in the input file to the standard output. The default is not to print this information, but it can be switched on by setting *MONIT* to 1. **MONITOR** should appear near the start of the input file (but after **NOHEAD**, if that code word is used).

An example of the use of this code word follows.

```
MONITOR 1
```

In this case the code words in the input are echoed to standard output.

NEWFILE JSTRM NEWNAM

This code word allows a new file name to be specified for files connected to particular streams, thus overriding the name defined in **FILES**. **JSTRM** is the number of the stream; only streams 12, 17 or 20 can be chosen. **NEWNAM** is the new file name (a maximum of 12 characters can be used). Thus either the **FLUXES** or **COLLAPX** files may be redefined. **Note** that the new file **MUST** be in the same directory as the original file given in **FILES**.

This facility is included so that cases where the neutron spectrum changes significantly during the course of an irradiation can be modelled. If the neutron spectra at a series of irradiation times are known then it is possible to prepare the corresponding **COLLAPX** files prior to considering the irradiation. At suitable times during the total irradiation **NEWFILE** can be used with one of the calculated **COLLAPX** files. Thus if two different neutron fluxes exist and the collapsed files are **collapx.1** and **collapx.2**, then **collapx.1** is connected to stream 12 in **FILES** and the relevant portion of the **INPUT** file is as follows.

```
ENFA
* EAF_2005 with spectrum 1
ARRAY
FISPACT
* 1st part of irradiation
FLUX 1.3E15
LEVEL 50 1
TIME 1.0 YEARS SPECTRUM
NEWFILE 12 COLLAPX.2
ENFA
* EAF_2005 with spectrum 2
ARRAY
FISPACT
* 2nd part of irradiation
FLUX 1.4E15
TIME 1.0 YEARS ATOMS
...
```

In this example the formation of the **ARRAYX** file is followed by an irradiation for 1 year. The **SPECTRUM** code word is used so that the detailed inventory is not produced. The second **COLLAPX** file is specified by **NEWFILE** and the **ARRAYX** file is recalculated. The irradiation is then continued for a further 1 year (note that the flux value has also changed) and a detailed inventory produced by **ATOMS**.

NOCOMP

This code word causes the table of elemental compositions to be omitted from the inventory printout.

NOERROR

This code word stops uncertainty information from being used. It should be used if a cross section library with no uncertainty component is being collapsed, or if such a collapsed library is used with the **UNCERTAINTY** code word (this code word can still be used so long as only pathway data is required).

Note that if this code word is used with the **ERROR** code word then the user **MUST** supply values of the fractional error (*ERMAT*).

If an output of the data libraries is requested with the **PRINTLIB** code word, and no uncertainty data exist, then **NOERROR MUST** be used.

In all cases the code word **MUST** come near the top of the input file, before the code words **COLLAPSE**, **UNCERTAINTY**, **PRINTLIB** or **ERROR**.

NOFISS

This code word stops the fission yield data from being input and processed during the preparation of the **ARRAYX** file.

Note it should only be used if the cross section library contains no actinide fission cross sections.

NOHEAD

This code word stops the printing of the header and user information at the beginning of the output and is useful if it is required to reduce the printed output.

Note that if this code word is used it **MUST** be at the beginning of the input file and must not be preceded by any characters, not even blanks.

NOSORT

The default output includes a sorted list of the dominant nuclides where a maximum of 20 nuclides is shown. The nuclides are sorted by activity, heat, γ dose rate, ingestion dose, inhalation dose, β -heat, γ -heat and clearance index. The list can be removed by the use of this code word to reduce running time (although including the list only typically increases the running time by a few percent).

Note removing the dominant nuclide list also disables the output of pathways and uncertainty estimates that might have been requested by the **UNCERTAINTY** code word.

NOSTAB

Use of this code word inhibits the printing of any stable nuclides in the inventory and is useful when the inventory is large and it is required to save space.

NOT1

This code words switch off the output to the external files that was switched on by the **TAB1** code word. Both **TAB1** and **NOT1** can be used several times during a case to restrict the output as required.

NOT2

This code words switch off the output to the external files that was switched on by the **TAB2** code word. Both **TAB2** and **NOT2** can be used several times during a case to restrict the output as required.

NOT3

This code words switch off the output to the external files that was switched on by the **TAB3** code word. Both **TAB3** and **NOT3** can be used several times during a case to restrict the output as required.

NOT4

This code words switch off the output to the external files that was switched on by the **TAB4** code word. Both **TAB4** and **NOT4** can be used several times during a case to restrict the output as required.

OVER JA

This code word enables library data to be modified for a particular case. It can be called several times during an irradiation if required. *JA* specifies the nuclide that is to have data changed. The identifier can be specified either using the format 'TE129M' or by the material number.

Note the 'material number' is the identification given to the nuclide internally by FISPACT, its value can be seen in the decay data part of the **PRINTLIB** output if required.

It is followed by one of three code word options:

ACROSS JB

SIG(N) N=1, NGR

JB is the daughter of the reaction and *SIG(N)* is the new cross section (barns) for the *N*-th energy group. For all existing EAF libraries *NGR* = 1 (*NGR* is used to retain compatibility with FISPIN input). *JB* is specified in the same manner as *JA* above.

Note that if a fission reaction is specified then *JB* must be 0.

ALAM THALF INDX

THALF is the new half-life of the nuclide and *INDX* specifies the time unit:

- | | |
|---|---------|
| 1 | seconds |
| 2 | minutes |
| 3 | hours |
| 4 | days |
| 5 | years |

ERROR JB*ERRFCX*

JB is the daughter of the reaction and *ERRFCX* is the new error factor for the cross section.

Examples of the uses of this code word follow.

```
OVER BE9
    ACROSS HE6 1.05490E-2
```

Here the 1-group cross section for the reaction ${}^9\text{Be}(n,\alpha){}^6\text{He}$ is given the value 10.549 mb for all subsequent calculations in the run.

```
OVER C14
    ALAM 3000.0 5
```

Here the half-life of ${}^{14}\text{C}$ is given the value 3000.0 years for all subsequent calculations in the run.

```
OVER C14
    ERROR C13 1.10
```

Here the error factor for the ${}^{14}\text{C}(n,2n){}^{13}\text{C}$ reaction is set to 1.10 for all subsequent calculations in the run.

Note that the **ARRAYX** and **COLLAPX** files are not altered, so that in subsequent runs the cross section, half-life or error factor will revert to its original value.

Note a comment should not follow directly after **OVER** or **ACROSS**, **ALAM** or **ERROR**, ensure that at least one other code word is used before using a comment.

PARTITION *NPART**SYM(N) XPART(N) N=1, NPART*

This code word allows the material to be split or partitioned into two streams during an irradiation or cooling. The part that continues to be considered by the code consists of all elements *not* specified (*NPART* elements are specified) and the fractions *XPART(N)* of the specified elements *SYM(N)*. The stream containing the remainder is lost and cannot be followed any further by the code.

Typical uses of this code word might be to model recycling of irradiated material or the loss by diffusion of tritium from a material. In the first case **PARTITION** would be used after irradiation and cooling and would model the loss of volatile elements during re-fabrication. In the second case the irradiation might be split into several intervals and **PARTITION** used in each interval to model the loss of tritium.

An example of the use of this code word follows.

```
PARTITION 2
  AR 0.01
  K 0.20
```

In this case all elements except Ar and K remain unmodified, all Ar isotopes are reduced by a factor of 100 and all K isotopes are reduced to a fifth of their values before the code word was used.

PATH NLINK

INDXP(I) I = 1, NLINK+1

This code word allows a particular pathway consisting of *NLINK* reactions and decays to be specified. The (*NLINK*+1) nuclides in the pathway are input using the identifier (*e.g.* 'TE129M'), and in order to specify whether each link is a reaction or a decay an 'R' or a 'D' is placed between the identifiers.

This code word is only necessary if a special investigation of pathway information is needed. Pathway data can be generated automatically for all the dominant nuclides by using the **UNCERTAINTY** code word. **PATH** might be used for a particularly complicated pathway not generated automatically or to investigate nuclides only formed in small amounts.

Note when using this code word it is recommended that a standard inventory be produced first and the number of atoms of the daughter are specified in subsequent runs using the **RESULT** code word. No inventory then needs to be calculated for the runs investigating the pathways, making efficient interactive studies possible.

Note the maximum number of links that can be specified in a pathway is 20. See Appendix 8 for more details of pathways.

An example of the use of this code word follows.

PATH 5 TI48 R CA45 D SC45 R K42 D CA42 R CA41
--

The percentage of the daughter nuclide (^{41}Ca), that is formed by the pathway, $^{48}\text{Ti}(n,\alpha)^{45}\text{Ca}(\beta^-)^{45}\text{Sc}(n,\alpha)^{42}\text{K}(\beta^-)^{42}\text{Ca}(n,2n)^{41}\text{Ca}$ is given in the output.

PRINTLIB PRINT

This code word causes the output of the data libraries in a readable form. The output consists of five blocks of data, the contents of each are:

1. decay data, including fission yields if appropriate, for each nuclide
2. the branching ratios of decays for each radionuclide
3. the cross section data (including uncertainties) for each reaction in the specified neutron spectrum
4. nuclides which will give a bremsstrahlung contribution to the γ dose rate
5. the neutron spectrum used to collapse the cross section library

The value of the parameter *PRINT* determines which blocks are output.

- | | |
|----------|----------------------|
| 0 | All five blocks |
| 1 | Block 1 only |
| 2 | Blocks 2, 3, 4 and 5 |
| 3 | Block 5 only |

Note that if no uncertainty data exists in the library then the code word **NOERROR MUST** be used before **PRINTLIB**.

Note it is recommended that a separate FISPACT run, giving a library output and no inventory, be done for each decay data library and kept for reference.

An example of the use of this code word follows.

```
PRINTLIB 1
```

The library data for decays (half-lives, average energies, γ spectrum and fission yield) are output.

PULSE NPULSE

This code word is used to start the 'loop' construct in the **INPUT** file. *NPULSE* is the number of times that the code words between **PULSE** and **ENDPULSE** are repeated. It is possible to nest this pair of code words up to 5 deep, and the maximum value of *NPULSE* for any loop is 500.

This facility is included so that a series of identical pulses (off time + on time) can be represented easily in the input file.

An example of the use of this code word follows.

```
PULSE 5
  FLUX 0.0
  TIME 1.0 HOURS SPECTRUM
  FLUX 1.0E15
  TIME 1.0 HOURS SPECTRUM
ENDPULSE
FLUX 0.0
TIME 1.0 HOURS SPECTRUM
FLUX 1.0E15
TIME 1.0 HOURS ATOMS
```

At the end of the irradiation it is wished to include six hour-long pulses. Five of these are specified in the loop using **SPECTRUM** so that no detailed inventory is produced. The final pulse (end of irradiation) has a detailed inventory since **ATOMS** is used.

RESULT NRESU***SYM(I) X(I) I = 1, NRESU***

This code word is used when calculating pathways. The pathway output includes the percentage of the total amount of the daughter nuclide produced by a particular pathway. One way to obtain this total amount is to do an inventory prior to the pathway calculation. However, it is much easier to be able to do the inventory in a separate run and then manually to use results from that inventory and input them into the pathway calculation.

NRESU nuclides are specified and for each, the identifier *SYM(I)* (e.g. 'TE129M') and the number of atoms *X(I)* are specified.

If **ATOMS** or **SPECTRUM** is not present, then **RESULT** is necessary to start the pathway calculation and so **MUST** follow the code word **PATH** or **ROUTES**.

An example of the use of this code word follows.

RESULT 3
C14 1.356E19
N14 8.560E17
N15 7.568E12

The number of atoms of ¹⁴C, ¹⁴N and ¹⁵N produced in a standard inventory run are specified.

ROUTES PAR DAU NMAX PMIN IPRPA

In addition to specifying a particular pathway with the code word **PATH**, the code word **ROUTES** can be used. This will search for all pathways from the parent nuclide (*PAR*) to the daughter nuclide (*DAU*) with a maximum of *NMAX* links (reactions or decays).

The contribution of each pathway is calculated and if the number of daughter atoms is greater than *PMIN* the pathway and the contribution will be printed in the output.

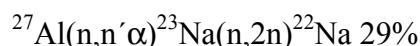
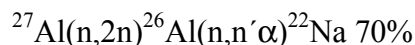
If *IPRPA* > 0 then each pathway found (irrespective of its contribution to the number of daughter atoms) will be listed prior to the pathway output. This option is only recommended if the output is not understood and the user wishes to check all the pathways calculated.

Note that **ROUTES MUST** come before the **RESULT** code word. **Note** the maximum number of links that can be specified is 8. See Appendix 8 for more details of pathways.

An example of the use of this code word follows.

```
ROUTES AL27 NA22 3 1.E10 0
RESULT 1
      NA22 1.0E15
```

In a spectrum corresponding to the first wall of a fusion device the output would typically be as shown below (more information on typical pathways is available in references 5 and 6):



The *PMIN* value was set so that it was 1.10^{-5} times the total amount of ^{22}Na formed in the irradiation (given after the **RESULT** code word), and with *IPRPA* set to 0 none of the many pathways tested (each with negligible contributions) were printed.

SENSITIVITY XSENS XNSEN1 INSEN3 INSEN4

Parent(I) Daughter(I) I=1, INSEN3

Nuclide(J) J=1, INSEN4

This code word allows sensitivity calculations to be performed. If *XSENS* = **LAMBDA** then the sensitivity coefficients with respect to decay constant are calculated.

If *XSENS* = **SIGMA** then the sensitivity coefficients with respect to cross section are calculated.

However, only one of these options can be specified for a case, the code word **MUST** not be input twice.

The cut-off value *XNSEN1* is the value below which sensitivity coefficients are not printed (a typical value might be $1. 10^{-10}$).

For each of the *INSEN4* nuclides specified the sensitivity of that nuclide to each of the *INSEN3* cross sections or decay constants is calculated. The maximum value of both *INSEN3* and *INSEN4* is 50.

If either *INSEN3* or *INSEN4* are set to -1, then the calculations are done for all cross sections or all nuclides.

It is not recommended that *INSEN3* be set to -1, as with a large library the computing time would be prohibitive. Setting *INSEN4* to -1 gives a large amount of output, but does not require much more time than typical to run.

Sensitivity calculations will be performed only for one time interval, so it is possible to follow the irradiation with cooling steps if these are needed. See Appendix 5 for further details of the sensitivity method.

Examples of the use of this code word follow.

```
SENSITIVITY SIGMA 1.E-10 2 3
  C12 C13
  C13 C14
  C13
  C14
  BE10
```

The sensitivity coefficients of the amounts of the three nuclides ^{13}C , ^{14}C and ^{10}Be to the values of the cross sections for the two reactions $^{12}\text{C}(n,\gamma)^{13}\text{C}$ and $^{13}\text{C}(n,\gamma)^{14}\text{C}$ are calculated.

```
SENSITIVITY LAMBDA 1.E-10 1 2
  C14 N14
  N14
  N15
```

The sensitivity coefficients of the amounts of the two nuclides ^{14}N and ^{15}N to the value of the half-life of the decay of ^{14}C to ^{14}N is calculated.

In both cases the coefficients are only printed if they are larger than $1.0 \cdot 10^{-10}$.

SEQN LNNM {175}

This code word allows the user to change the number of energy groups used for an inventory calculation including sequential charged particle reactions (SCPR). By default data in 175 groups is assumed, but for a spectrum with neutrons with energies above 20 MeV *LNNM* can be set to 211.

More details about SCPR are given in Appendix 12.

An example of the use of this code word follows.

```
SEQN 211
```

In this case 211 group data must be used for the inventory calculation.

SEQUENTIAL *ISEQUE* {0} *IPCWRT* {0}

This code word allows the user to include the effect of sequential charged particle reactions (SCPR) in the inventory calculations. By default SCPR are not considered, but if *ISEQUE* is set to 1 then the additional data libraries are read and the pseudo cross sections calculated. These pseudo cross sections are included with the standard collapsed cross sections in inventory calculations. The values of the pseudo cross sections can be seen if *IPCWRT* is set to 1 as this causes them to be included in the **OUTPUT** file.

In previous versions it is assumed that a neutron spectrum in 175 groups is available for calculations of the pseudo cross sections. In the current version a neutron spectrum in either 175 or 211 groups can be used. **ARRAYX** and **COLLAPX** files prepared with a neutron spectrum in 175 or 211 groups **MUST** be used with this code word.

More details about SCPR are given in Appendix 12.

An example of the use of this code word follows.

```
SEQUENTIAL 1 0
```

In this case sequential charged particle reactions will be included in the calculations, but the values of the pseudo cross sections are not displayed in the output.

SPECTRUM

This code word is an alternative to **ATOMS**. It suppresses the inventory, so that only the γ -spectrum and total values are printed for the time interval. It is useful if summary information is required for many time intervals, but the details of the individual nuclide contributions are not needed.

SPLIT *ISPLIT* {0}

This code word allows the display of an additional summary table at the end of the run. This summary table contains separate information on the heat production by beta and gamma radiation at each time interval to be output after the existing summary table. By default this new summary table is not printed, but it can be displayed if *ISPLIT* is set to 1. **Note** that if the new summary table is required then the code word **HAZARDS *MUST*** be used to ensure that uncertainties are correctly printed.

TAB1 *IA*

This code word causes the inventory data in columns 1 and 2 (number of atoms and grams of each nuclide) to be written to an external file (**TAB1**) via stream *IA*. Note that stream numbers greater than 43 ***MUST*** be used for all **TAB** files.

TAB2 *IB*

This code word causes the inventory data in columns 3 and 7 (activity (Bq) and dose rate (Sv h⁻¹) of each nuclide) to be written to an external file (**TAB2**) via stream *IB*. Note that stream numbers greater than 43 ***MUST*** be used for all **TAB** files.

TAB3 *IC*

This code word causes the inventory data in columns 8 and 9 (ingestion and inhalation dose (Sv) of each nuclide) to be written to an external file (**TAB3**) via stream *IC*. Note that stream numbers greater than 43 ***MUST*** be used for all **TAB** files.

TAB4 *ID*

This code word causes the gamma-ray spectrum (in MeV s⁻¹) in the 24-energy group format (or 22-group format if the **GROUP** parameter is 1) to be written to an external file (**TAB4**) via stream *ID*. In addition a second column showing the number of gammas per group is also given in **TAB4**. Note that stream numbers greater than 43 **MUST** be used for all **TAB** files.

TIME *T*

This code word allows the input of the irradiation or cooling time interval *T* (seconds). The time may be input in units other than seconds by following the value with one of the following code words specifying the time unit:

MINS, HOURS, DAYS or YEARS.

Note it is important when inputting times that it is the interval time, not the total time that is specified. Thus for cooling steps the time printed on the inventory is the sum of all the previous cooling time intervals after the code word **ZERO**.

Examples of the use of this code word follow.

```
ZERO
TIME 2.5 YEARS
ATOMS
TIME 7.5 YEARS
ATOMS
```

Following irradiation the start of cooling is specified by the code word **ZERO**. Inventories at the times of 2.5 and 10 years are output.

UNCERTAINTY *IUNCER* {0} < *FRACOK* {0.98} *FRACWT* {0.005} *NMAXB* {3} *NMAXR* {3} *NMAXC* {12} *ZZZLVL* {50.0} *IUNCER*>

This code word allows user control of the uncertainty estimates and pathway information that is calculated and/or output for each time interval. This is primarily specified by the parameter *IUNCER* {0}. The allowed values are:

- 0 No pathways or estimates of uncertainty are calculated or output
- 1 Only estimates of uncertainty are output (although all the pathway information has been calculated)
- 2 Both estimates of uncertainty and the pathway information are output
- 3 Only the pathway information is output.
- 4 Allows default values to be reset for a particular run. Particular values can be specified by the following parameters only for this value of *IUNCER*.

FRACOK {0.98} is the fraction of the daughter nuclide produced such that no further pathways with more links need to be considered.

FRACWT {0.005} is the fraction of the total contribution below which pathway contributions are not output.

NMAXB {3} is the maximum number of links allowed in pathways except where tritium is the final daughter. *NMAXB* **MUST** be in the range 1 - 5.

NMAXR {3} is the maximum number of links for tritium production. *NMAXR* **MUST** be in the range 1 - 6.

NMAXC {12} is the maximum number of links when only captures and β^- decays are considered in a pathway. *NMAXC* **MUST** be in the range 1 - 12.

ZZZLVL {50.0} is the first level parameter for calculation of the pathways.

IUNCER following all the other parameters allows values 0, 1, 2 or 3 to be input again so that after resetting the default values an actual calculation with the new values can be done.

Note if a time interval prior to the irradiation is specified then *IUNCER* **MUST** be set to 0 (or **UNCERTAINTY** not used) for this time interval.

Note if more than one irradiation time is considered in a run then *IUNCER* **MUST** be set to 0 for all time intervals except the first. If the uncertainty estimate is to be sensible for such a ‘pulsed’ irradiation then the initial irradiation should contain the majority of the neutron fluence. See Appendix 9 for more details on uncertainties and Appendix 20 for non-steady irradiations.

Note that very large values of *ZZZLVL* **MUST** be given in scientific notation.

Note the code word **UNCERTAINTY** **MUST** immediately proceed the code word **ATOMS**.

Note that if no uncertainty data exists in the cross section library then the valid values of *IUNCER* are only: 0, 3 or 4.

Examples of the use of this code word follow.

Omitting the code word will ensure that only inventory calculations are carried out, and should be the case if a fast scoping run or multiple irradiation periods are required.

```
UNCERT 2
```

This will ensure that in addition to the inventory calculations, the pathways to form the dominant nuclides and the uncertainty estimates are output. This is the standard use of the code word for a full investigation of activation.

```
UNCERT 4 0.95 0.01 4 6 10 100.0 2
```

This resets the default values and then carries out a full calculation.

UNCTYPE *IUNCTY* {1}

This code word allows the user to specify the type of uncertainty contributions to include when calculating the uncertainties of the radiological quantities. If *IUNCTY* is set to 1, or if the code word is not used then only the cross section uncertainties are used in the calculation of uncertainties.

If *IUNCTY* = 2 then only the half-life uncertainties taken from the decay data library are used in the calculation of uncertainties. If *IUNCTY* = 3 then both cross section and half-life uncertainties are used. Appendix 9 gives more details of the calculation of uncertainties.

Examples of the use of this code word follow.

```
UNCERT 2  
UNCTYPE 2
```

Uncertainty calculations will be done, but only using the half-life uncertainties. Cross sections are assumed to have no uncertainties. Such a calculation is useful to isolate the contribution (generally small) of half-life uncertainties.

```
UNCERT 2  
UNCTYPE 3
```

Uncertainty calculations will be done, but using both the cross section and half-life uncertainties.

WALL WALL

This code word allows the input of the total neutron first wall loading *WALL* in units of MW m⁻² for a fusion device. This is converted to a flux value by using data read from the neutron spectrum file. The neutron spectrum file (**FLUXES**) contains a value of the first wall loading, *e.g.* 4.15 MW m⁻². The energy integrated flux, *e.g.* 1.80 10¹⁵ n cm⁻²s⁻¹ which is the sum of neutrons in all the groups is calculated and equated to the wall loading during library processing.

Note that it is the user's responsibility to ensure that this wall loading is correct when the spectrum file is constructed. If a wall loading of 2.0 MW m⁻² was input then a flux value of (2.0 / 4.15) * 1.80 10¹⁵ n cm⁻²s⁻¹ would be used in the calculations. It is a convenient alternative to using **FLUX** for irradiation of first wall materials, but great care must be exercised if used for irradiations in other than first wall spectra (in these cases the flux specified for the region must be that which would be present if the first wall loading shown in the file was present on the first wall). It is recommended that **FLUX** is always used in preference to **WALL** unless the user has a run that makes its use essential.

ZERO

This code word is used to reset the time value to zero after an irradiation. After **ZERO** the output will show 'COOLING TIME' rather than 'TIME' in the title for the interval. The flux **MUST** be set to zero by the code word **FLUX** with parameter 0.0 prior to the use of **ZERO**. This code word **MUST** be used after an irradiation if the code word **GRAPH** is also used in the input file.

<< comment >>

In versions of FISPACT prior to 3.0 it was not possible to include any comment lines in the input file. This can now be done by enclosing the comment in double angle brackets (<< >>). Such a comment can be included anywhere in the input file that a code word would normally be used; however, it **MUST** not occur in the middle of a code word - parameter combination.

Examples of the use of this construction follow.

```
FLUX 1.2E14
<< This is the first wall flux >>
LEVEL 50 1
```

This is a correct usage of a comment.

```
FLUX << This is the first wall flux
>> 1.2E14
```

This is an incorrect usage of a comment.

Examples of preliminary input

There are basically three types of FISPACT runs, and the preliminary inputs are rather different.

1. Formation of a collapsed library from the full group cross section libraries and a specified neutron spectrum.
2. Reading and processing of the decay data and a collapsed library, to produce a condensed library (an **ARRAYX** file) which can optionally be followed by an inventory run.
3. Reading a condensed library and using this to perform an inventory run, a sensitivity analysis or an evaluation of pathways.

Examples are given for each type below.

```
COLLAPSE 175
FISPACT
* Collapse of EAF-2005(175), Zone 12
END
* END OF COLLAPSE
```

In this case a cross section library (EAF-2005) in 175-group format is collapsed with a neutron spectrum (identified as Zone 12).

```
SPEK
ENFA
* EAF_DEC-05,EAF-2005(100), Zone 13
TAPA
FISPACT
* Write to arrayx file
END
* END OF RUN
```

In this case there was no existing **ARRAYX** file produced from the current decay data (**EAF_DEC-2005**), so the **TAPA** option was used. By specifying **SPEK** any nuclides with no γ -spectral data had this synthesised approximately (this is recommended). The collapsed cross section file (**COLLAPX**), in this case for EAF-2005, in Zone 13, is read and added to **ARRAYX**.

```
SPEK
ENFA
* EAF_DEC-05,EAF-2005(175), Zone 15
ARRAY
FISPACT
* Write to arrayx file
END
* END of library run
```

In this case there was an existing **ARRAYX** file produced from the current decay data (**EAF_DEC-2005**), so the **ARRAY** option was used. By specifying **SPEK** any nuclides with no γ -spectral data had this synthesised approximately (this is recommended). The collapsed cross section file (**COLLAPX**), in this case for EAF-2005 in Zone 15, is read and substituted into the existing **ARRAYX** file.

```
AINPUT
FISPACT
* An inventory run
```

This is the standard start to an inventory calculation - see the following section for complete examples.

Examples of main input

Six examples of input data are given, in each case it is assumed that a condensed library (an **ARRAYX** file) is being used (see previous section). More examples are given in Appendix 14.

```
NOHEAD
AINPUT
FISPACT
* Produce PRINTLIB
PRINTLIB 0
END
* END of run
```

This run produces an output of the data libraries and it is recommended that this type of run be done to produce a reference document for a particular decay data library which can be used for subsequent work.

```
MONITOR 1
AINPUT
FISPACT
* Irradiation of 1 ppm of K in FE
MASS 1.0 2
K 1.E-4
FE 99.9999
BREM 1 BE10
MIND 1.E5
HAZA
ATWO
GRAPH 2 0 0 1 3
WALL 5.0
LEVEL 100 1
TIME 2.5 YEARS ATOMS
LEVEL 20 1
FLUX 0.0
ZERO
TIME 0.1 YEARS ATOMS
TIME 0.9 YEARS ATOMS
TIME 49.0 YEARS
ATOMS
END
* END of K irradiation
```

This case models the irradiation of 1 kg of iron containing 1 ppm of potassium in a first wall flux of 5 MW m^{-2} for 2.5 years. Progress of the run is included by using **MONITOR** with the

parameter 1. The **MIND** parameter is set to 10^5 , biological hazards and transport limits are required and a bremsstrahlung correction is output for ^{10}Be . Two graphs (total activity and total heat) in PC format with no uncertainty data are requested and the **LEVEL** parameters are set to 100 and 1 (1 subinterval and nuclides with half-life < 6.3 days are in equilibrium). After the irradiation, the inventory is printed by calling **ATOMS** and then the first **LEVEL** parameter is reduced to 20. The neutron flux is reduced to 0, the value of time reset to 0 by **ZERO**, three cooling times follow and inventories are printed for 0.1 years, 1 year and 50 years. The run is finished by **END**.

```

AINPUT
FISPACT
* C sensitivity calculations
MASS 10.0 1
C 100.
MIND 1.E5
HALF
FLUX 2.0E15
TAB1 45
LEVEL 100 5
SENS SIGMA 1.E-10 3 2
C12 C13
C13 C14
C13 BE10
C14
BE10
ERROR 3
C12 C13 -1
C13 C14 -1
C13 BE10 0.5
TIME 5.0 YEARS ATOMS
LEVEL 20 1
FLUX 0.0
NOT1
ZERO
TIME 5.0 YEARS SPECTRUM
TIME 95.0 YEARS ATOMS
END
* END of sensitivity calculations

```

This case models the irradiation of 10 kg of carbon in a flux of $2.0 \times 10^{15} \text{ n cm}^{-2} \text{ s}^{-1}$ for 5 years. The **MIND** parameter is set to 10^5 and half-lives are to be printed. A dump to an external file of the nuclide amounts is required using data stream 45. The **LEVEL** parameters are set to 100 and 5 (5 subintervals and

nuclides with half-life < 12.6 days are in equilibrium). The sensitivity of the nuclides ^{14}C and ^{10}Be to the cross sections $^{12}\text{C}(n,\gamma)$, $^{13}\text{C}(n,\gamma)$ and $^{13}\text{C}(n,\alpha)$ are required with a cut-off value of $1 \cdot 10^{-10}$. The fractional errors in the first two reactions are taken from the uncertainty file, while the third is input directly. These uncertainties are used to calculate the errors in the two nuclides previously specified.

After the irradiation, the inventory is printed by calling **ATOMS** and then the **LEVEL** parameters are reduced to 20 and 1 respectively and the value of time reset to 0 by **ZERO**. The neutron flux is reduced to 0 and the dump of data to the external file is stopped. Two cooling times of 5 and 100 years follow (the first only has summary information since **SPECTRUM** is used, meaning that the full inventory is omitted) and the run is finished by **END**.

```

AINPUT
FISPACT
* Pathways of Zn66 5MW/m2
FUEL 1
ZN66 2.56943E24
WALL 5.
LEVEL 100 1
TIME 2.5 YEARS
ROUTES ZN66 C060 6 1.E11 0
ROUTES ZN66 NI63 6 1.E16 0
PATHS 2
ZN66 R NI63 R FE60
PATHS 5
ZN66 R ZN67 R ZN68 R ZN69 D GA69 R GA70
RESULT 4
C060 1.62032E16
NI63 1.78082E21
FE60 2.02345E19
GA70 4.45689E12
END
* END of pathways run

```

This case has $2.56943 \cdot 10^{24}$ atoms of ^{66}Zn (**Note** that it is important to start with one isotope only, since we require the pathways from a parent isotope not an element) irradiated in a first wall flux of 5 MW m^{-2} for 2.5 years. The **LEVEL** parameters are set to 100 and 1. All the pathways with a maximum of 6 links between ^{66}Zn and ^{60}Co and ^{66}Zn and ^{63}Ni , and in addition the two specified pathways between ^{66}Zn and

^{60}Fe and ^{66}Zn and ^{70}Ga will be calculated. The **RESULT** code word enables the amounts of ^{60}Co , ^{63}Ni , ^{60}Fe and ^{70}Ga that were calculated in a previous inventory run to be input. The run is finished by **END**.

```
AINPUT
FISPACT
* Irradiation of C - EEF Zone 12
MASS 1.0 1
C 100.0
DENSITY 2.0
DOSE 2 5.0
GROUP 1
MIND 1.0E5
OVER BE9
ACROSS HE6 1.05490E-2
FLUX 1.5E15
LEVEL 50 1
TIME 2.5 YEARS
UNCERT 2
ATOMS
END
* END of over run
```

This case models the irradiation of 1 kg of carbon for 2.5 years in a flux of $1.5 \cdot 10^{15} \text{ n cm}^{-2} \text{ s}^{-1}$, with the cross section of the reaction $^9\text{Be}(n,\alpha)^6\text{He}$ set to 10.549 mb by the **OVER** code word. The density of carbon is input (2.0 g cm^{-3}) by the **DENSITY** code word, and the γ dose-rate output is requested for a point source (by following **DOSE** with 2) at a distance of 5 m, the spectral data is requested (by following **GROUP** with 1) in the 22-group format. The pathways and uncertainty estimates are requested (by following **UNCERT** with 2) after the inventory. **ATOMS** causes the inventory to be output and the run is ended by **END**.

```
AINPUT
FISPACT
* Pathways of Sc45
FUEL 1
SC45 1.0E25
FLUX 1.8E15
LEVEL 100 1
CONV 10 2.E-3 1E-2
TIME 2.5 YEARS
LOOPS 20.0
PATHS 2
SC45 R SC46 R SC47
RESULT 1
SC47 1.62032E19
END
* END of pathways run
```

This case models 1×10^{25} atoms of ^{45}Sc being irradiated for 2.5 years in a flux of $1.8 \times 10^{15} \text{ n cm}^{-2} \text{ s}^{-1}$. The convergence limit for the pathway calculation is reduced to 1% by the code word **CONV** and **LOOPS** is used to include any isomers with half-lives less than 20 seconds in the calculation. The pathway ($^{45}\text{Sc}(n,\gamma)^{46}\text{Sc}(n,\gamma)^{47}\text{Sc}$) specified by **PATHS** contains 2 reactions (the user must give the identifiers of three nuclides), and the total amount of the daughter nuclide (^{47}Sc) calculated in a previous run is given by the code word **RESULT**.

Interpretation of FISPACT output

The output from FISPACT consists of several distinct blocks that are described in detail below.

Header and user information

The header gives a banner version of the program name and the date of the version, this is followed by a box giving the version number and platform on which the run was done.

```
=====
=
= FISPACT VERSION 05.0/0  DECEMBER 2004 PC+Salford FTN77/32 =
=
=====
```

Depending on the platform being used the end part of the printed text will be:

PC+Salford FTN77/32	32-bit PC
UNIX	Various UNIX operating systems

This is followed by the current user information where any changes since the publication of this manual will be given.

Library information

In response to the code word **AINPUT** another box giving the library information is printed.

```
-----
L I B R A R Y   I N F O R M A T I O N
-----
COLLAPX from EAF-2005(0)211G and IFMIF test           on 09/12/04 using FISPACT 05.0/0
FISSION YIELD DATA FROM JEF-2.2 WEIGHTED BY ABOVE NEUTRON SPECTRUM
ARRAYX produced from EAF-2005           and above COLLAPX on 09/12/04 using FISPACT 05.0/0
OUTPUT produced by FISPACT 05.0/0 [Build 0039] dated 22/12/04
-----
```

This shows the name of the cross section library that was used for the collapsing, the date that it was produced and the version of FISPACT that was used. The origin of the fission yield data and the name of the decay data library and the date of production of the **ARRAYX** file follow. The actual build number is shown as an additional check of the version used to produce the output.

Nuclide inventory

Following the code word **FISPACT** the remainder of the input file is read and each code word and its parameters are printed out before the processing of the code word. Following **ATOMS** the number of iterations required for convergence is given.

```
.....
NUMBER OF ITERATIONS      6
.....
```

If convergence has not been reached then the following message is shown:

```
.....
CASE NOT PROPERLY CONVERGED, but if no "?" flags set then convergence
                                achieved for ALL printed isotopes.
.....
```

Prior to the inventory listing the following key is printed:

```
-----
] NB: IN FOLLOWING TABLES * MEANS ISOTOPE IS CALCULATED BY APPROXIMATE METHOD ]
]                               ? MEANS CONVERGENCE NOT REACHED FOR NUCLIDE   ]
]                               & MEANS GAMMA SPECTRUM IS APPROXIMATELY CALCULATED ]
]                               # MEANS NUCLIDE IS STABLE                       ]
]                               > MEANS NUCLIDE WAS PRESENT BEFORE IRRADIATION ]
-----
]
]
V
```

This key lists five single character flags that are printed immediately following each nuclide identifier. ‘*’ indicates that the nuclide has been calculated as if it were in equilibrium, increasing the first parameter following **LEVEL** will mean that fewer nuclides are labelled by this flag. ‘?’ is the convergence flag, any nuclide labelled by this has not been calculated accurately enough, decreasing the second parameter in **CONV** can remove the flag, but in most cases the nuclides are of no practical importance and any error can be ignored. ‘&’ indicates that no γ -spectral data were present in the decay data library and that the code word **SPEK** was used to approximately calculate a spectrum. If most of the γ dose-rate is produced from nuclides with this flag then the result should be treated with great caution. ‘#’ indicates that the nuclide is stable and ‘>’ indicates that this nuclide was present in the material input, specified by the **MASS** or **FUEL** code words.

The main output of this section follows - this is the details of the nuclides present at the end of the time interval. The time is shown in a title at the top, followed by the inventory.

```
* TIME INTERVAL 1 * * TIME IS 7.8894E+07 SECS OR 2.5000E+00 YEARS *
```

The inventory contains up to 11 columns of data (excluding the nuclide identifier and flags), and contains the number of atoms of the isotope, the mass of the isotope in grams, the activity in Bq, the β energy in kW, the α energy in kW, the γ energy in kW, the γ dose-rate in Sv h⁻¹, the ingestion dose in Sv, the inhalation dose in Sv, the ratio of the activity to the A₂ value or the clearance index and the half-life in seconds. The output of the last four columns depends on whether **HAZARDS**, **ATWO** or **CLEAR** and **HALF** are present in the input file.

NUCLIDE			ATOMS	GRAMS	Bq
H	1	#	2.80723E+20	4.662E-04	0.000E+00
H	3		1.35830E+20	6.767E-04	2.420E+11

b-Energy kW	a-Energy kW	g-Energy kW	DOSE RATE Sv/hr
0.000E+00	0.00E+00	0.000E+00	0.000E+00
2.212E-07	0.00E+00	0.000E+00	0.000E+00

INGESTION DOSE (Sv)	INHALATION DOSE (Sv)	Bq/A2 Ratio	HALF LIFE seconds
0.000E+00	0.000E+00	0.000E+00	Stable
4.113E+00	4.113E+00	6.052E-03	3.891E+08

When data for all the nuclides has been printed the total number of nuclides and the total number of nuclides not converged are output.

Summary and elemental inventory

The totals of the activity (in Curies and Becquerels) for the irradiated material, and the split of the activity between α , β and γ decays (**Note** that the value for γ decays includes only the isomeric transitions) follow. If **DENSITY** has been input, then the activity is given in both Bq kg⁻¹ and Ci cm⁻³. The total heat production in kW is also split into α , β and γ components, and the totals for potential ingestion and inhalation hazards are output. For all these quantities the values excluding tritium are

also given. If **ATWO** was input then the effective A_2 value for the material is output. If **CLEAR** was input then the clearance index for the material is output. The number of fissions and the burn-up of actinides are output; these are only non-zero if actinides are initially present. The initial mass in kg and the neutron flux in the interval are also included.

The composition of material by element is given next, the column headings for this are: number of atoms of the element, number of gram-atoms, number of grams, β heat output (Curie-MeV and kW), γ heat output (Curie-MeV and kW) and α heat output (Curie-MeV and kW).

Gamma spectrum

In this section the total energies (MeV s^{-1}) from α , β and γ radiations and the total number of spontaneous fission neutrons are listed followed by two columns giving the γ spectrum (MeV s^{-1} per group) and number of gammas per group ($\text{cm}^{-3}\text{s}^{-1}$) in either a 24- or 22- group form, depending on the parameter used for **GROUP**. The total dose rate is then given in one of two forms dependant on the **DOSE** parameter; these two outputs are for contact dose from a semi-infinite slab of the material:

```
DOSE RATE (PLANE SOURCE) FROM GAMMAS WITH ENERGY 0-20 MeV IS 2.67503E+05
Sieverts/hour ( 2.67503E+07 Rems/hour)
```

and for the dose from a point source at a specified distance.

```
DOSE RATE (1 g POINT SOURCE 1.0m) FROM GAMMAS WITH ENERGY 0-20MeV IS
1.16480E-03 Sieverts/hour ( 1.16480E-01 Rems/hour)
```

If most of the dose rate is produced by nuclides with approximate γ -spectra then the following warning message will be given:

```
*** WARNING : >20% OF DOSE FROM NUCLIDES WITH NO SPECTRAL DATA. TREAT
DOSE AND GAMMA SPECTRUM WITH CAUTION ***
```

Sensitivity output

If the code word **SENSITIVITY** is used in the input then the sensitivity output is given at this point. In the case of sensitivity with respect to cross section a part of the output is shown below. In the first column is given the reaction (*e.g.* ${}^7\text{Li}(n,\gamma){}^8\text{Li}$) that is varied, the second column gives the nuclide that is considered, column three gives $\partial N/\partial\sigma$ and column four the sensitivity coefficient $(\partial N/\partial\sigma)(\sigma/N)$. Using these sensitivity coefficients and uncertainty data for the cross sections, the errors in the nuclides specified by **ERROR** are then listed below.

WITH RESPECT TO CROSS-SECTIONS						
REACTION			NUCLIDE	dN/dx	(dN/dx)(x/N)	
Li 7 -->	Li 8	SENSITIVITY OF	He 6 =	-4.710E+30	-1.348E-09	
Li 7 -->	Li 8	"	Li 8 =	4.646E+34	2.711E-02	
Be 9 -->	Li 8	"	He 6 =	-1.609E+35	-2.450E-08	
Be 9 -->	Li 8	"	Li 8 =	2.228E+38	6.914E-02	
ERRORS IN NUCLIDE AMOUNTS						
NUMBER OF ATOMS OF	He 6 =	2.2765E+12 +/-	1.0984E+12	(+/- 4.8248E+01 %)		
NUMBER OF ATOMS OF	Li 8 =	1.1170E+09 +/-	4.7476E+08	(+/- 4.2502E+01 %)		
NUMBER OF ATOMS OF	C 14 =	5.2430E+18 +/-	6.5638E+13	(+/- 1.2519E-03 %)		
NUMBER OF ATOMS OF	Be 10 =	1.1034E+21 +/-	3.9654E+20	(+/- 3.5937E+01 %)		

Similar output is obtained if the sensitivity with respect to the half-life is requested.

Uncertainty estimates

At the end of each time interval the nuclides that contribute most to the activity, heat output, γ dose rate, potential ingestion and inhalation doses, clearance index and the beta and gamma heat outputs are calculated and a 'top twenty' given. For each of the eight quantities the top twenty nuclides may be different so that more than twenty dominant nuclides in total will be calculated. The residual after subtracting the contribution from the top ten is given as 'Rest', so that the user can judge if there are actually more than twenty significant nuclides. The contribution of each nuclide is given both absolutely and in

percentage terms. If there are less than twenty radionuclides then only data for these is given. The output of this list of dominant nuclides can be switched off by using the code word **NOSORT**, but this is not usually desirable as it removes the ability to calculate uncertainties or pathways.

If the first **UNCERTAINTY** parameter is 1 or 3, then the uncertainty estimates for the eight total radiological quantities are printed next. The title for this section identifies what types of uncertainties contribute to the estimates. The output for the activity is shown below:

```
Total Activity is 5.62518E+12 +/- 1.16E+12 Bq.      Error is 2.06E+01 % of
                                                    the total.
```

The uncertainty is given both absolutely and as a percentage of the total. Note that if no clearance data have been calculated then only seven sets of nuclides are output.

As noted above there are probably more than twenty top ten nuclides in total, and these are listed with the uncertainties in the following fashion: the number of atoms, the error in the number of atoms [shown as E(Atoms) in the output], similar columns for the other four total quantities and then a column giving the percentage error. Note that numbers of atoms for clearance index and beta and gamma heats are not shown.

Bremsstrahlung corrections

If the code word **BREMSSTRAHLUNG** is included in the input, then the contributions to the dose rate from the nuclides specified are given here. First details of the configuration (infinite plane or point source) are given, and then the data in the following form:

```
Bremsstrahlung dose rate from BE 10 is 7.97779E-13 Sv/h ( 7.97779E-11
Rems/h). This is 6.84908E-08% of the total dose rate.
```

The dose rate from the particular nuclide is given in units of both Sv h⁻¹ and Rems h⁻¹, and then the percentage contribution to the total dose rate is given. **Note** this total does *not* include

the bremsstrahlung corrections, but in the following line a total of the γ dose rate and all the bremsstrahlung corrections is given.

Pathway analysis

If the first parameter following the **UNCERTAINTY** code word is either 2 or 3, or the code words **PATHS** or **ROUTES** are used then pathway analysis information is output. A short key describing the way links are shown is given first.

The paths show REACTIONS as eg (n,p), REACTIONS where projectiles are followed as (n,X), REACTIONS of sequential charged particles as eg [p,n], DECAYS as eg (b-) and DECAYS forming He4 as (X) . Pathway type [...|.] shows type of link (R,r,D,d) and if final nuclide is (L)ong or (S)hort lived.

For standard reactions such as $^{48}\text{Ti}(n,p)^{48}\text{Sc}$, the use of (n,p) is obvious, although because of the lack of a Greek font 'a' is used for α and 'g' is used for γ . If the projectile is followed in order to calculate gas production, then the above reaction would be shown as (n,X) meaning $^{48}\text{Ti}(n,^{48}\text{Sc})^1\text{H}$. Decays are shown as (b-), (b+), (a) and (IT) meaning β^- , β^+ or ϵ , α and Isomeric Transition respectively. If it is required to follow the α to calculate the production of ^4He , then the decay is shown as (X). Sequential charged particle reactions are indicated in square brackets, [p,n] means that a proton from say a (n,p) reaction reacts with the nuclide emitting a neutron.

For each of the daughter nuclides specified by the code words or calculated as dominant nuclides the following typical output is given:

```

. . . . .
C12(n,a)Be9(n,d)Li8
This path contributes      7.657 % of total amount of Li 8 , pathway type is : [RR|S]

C12(n,d)B11(n,a)Li8
This path contributes      9.531 % of total amount of Li 8 , pathway type is : [RR|S]

C13(n,t)B11(n,a)Li8
This path contributes     79.429 % of total amount of Li 8 , pathway type is : [RR|S]

C12(n,a)Be9(n,t)Li7(n,g)Li8
This path contributes      3.294 % of total amount of Li 8 , pathway type is : [RRR|S]

There are    4 paths which contribute    99.912 % of the Li 8
. . . . .

```

The pathway is given with the contribution that it makes to the production of the nuclide, and the pathway 'type descriptor'. The type descriptor shows whether each link is a reaction (R, r) or decay (D, d) and whether the parent is long-lived (R, D) or short-lived (r, d). After the ' | ' the final nuclide is shown as long-lived (L) or short-lived (S). Following the individual pathways the sum of all (in this case four) of the pathways is given. If the parameters in the code words have been set up correctly then the total of the listed pathways should be close to 100%.

Following the pathways, information on the generic pathways is listed unless the **GENERIC** code word is used to switch it off.

The information in the sections above is repeated for each time interval, but note that some of the above are only applicable for the first irradiation period. A difference between irradiation and cooling intervals is that the title of all intervals where the flux has been set to 0.0 and the code word **ZERO** has been used will contain 'COOLING TIME' rather than 'TIME'. Following the end of the output for the various time intervals the code word **END** triggers the end of the case with details of the CPU time used, and then the run ends.

End of case summary

A new feature added in FISPACT 4.1 is a summary at the end of the case containing the total values for each time interval. The intervals are listed as 'irradiation steps' or 'cooling steps' in both the most appropriate unit (sec, min, days) and in years. Six columns present Activity (Bq), Dose rate (Sv/h), Heat output (kW), Ingestion dose (Sv), Inhalation dose (Sv) and Tritium activity (Bq). For all except the latter the estimated uncertainty is also given. Following this the mass of input material (kg) and the density (g cm^{-3}) are shown. **Note** that the summary values are shown for the total mass of material not for a unit mass. A maximum number of time intervals (200) can be printed in the summary. In cases where more than 200 time

intervals are considered only the final 150 - 200 time intervals are displayed, the earlier ones (usually not important for pulsing scenarios) are discarded.

A feature added in FISPACT-2001 is a second summary at the end of the case. The intervals are listed as 'irradiation steps' or 'cooling steps' in both the most appropriate unit (sec, min, days) and in years. Four columns present Beta Heat (kW), Gamma Heat (kW), Mean Beta Energy (MeV), and Mean Gamma Energy (MeV). For all quantities the estimated uncertainty is also given. **Note** that this summary table is only displayed if the **SPLIT** code word is used with its parameter set to 1.

PRINTLIB output

The PRINTLIB output contains five sections. Firstly a summary of the decay data for each nuclide is given, with thirteen nuclides listed per page. For each nuclide its internal identifier number, the decay constant λ (s^{-1}) and the half-life in appropriate units (for stable nuclides '*****' is printed) are given, followed by the number of spontaneous fission neutrons per second and the number of neutrons from (α,n) reactions (the latter value is always 0.0, and is included for compatibility with FISPIN, it can be ignored). The average energies for α , β and γ decays (shown as <ALPHA>, <BETA> and <GAMMA>) in MeV and the γ energy (MeV) in each of the 24 groups follow. The independent fission yield (%) from each of the fissionable nuclides is given for the first 1669 nuclides (1436 in EAF-2003, -2001, -99, -97, 1434 in EAF4.1 and 1190 in EAF3.1). The details of the neutron spectrum used to weight the fission yields are given, with the fraction of the neutrons > 5 MeV, (< 5 MeV and > 200 keV) and < 200 keV printed.

Fe 52m (b+)	Mn 52	8.000E+01	Fe 52m (IT)	Fe 52	2.000E+01
-------------	-------	-----------	-------------	-------	-----------

The second section gives the percentage branching ratio for each decay mode of the radionuclides. The parent and daughter

nuclides are given with a code representing the decay between them. These codes are:

(b+)	β^+ or electron capture	(b-)	β^- decay
(b-n)	β^- followed by neutron emission	(b-b-)	double β^- decay
(b+n)	β^+ followed by neutron emission	(b-a)	β^- followed by α emission
(b+p)	β^+ followed by proton emission	(b+a)	β^+ followed by α emission
(a)	α decay	(p)	proton emission
(n)	neutron emission	(pp)	double proton emission
(SF)	spontaneous fission	(IT)	isomeric transition
(b-SF)	β^- followed by spontaneous fission		

```
Be 9 (n,2n) Be 8 4.328E-03+-4.0E+00
```

The third section gives the cross section in barns (the effective cross section obtained by collapsing with the neutron spectrum) followed by the percentage error. Note that if there are no uncertainty data in the library then the code word **NOERROR** switches the output in this section to include only the cross section. The parent and daughter nuclides are given with a code representing the reaction between them. These codes are:

(n, g)	(n,γ)	(n, 2n)	(n,2n)
(n, 3n)	(n,3n)	(n, 4n)	(n,4n)
(n, 5n)	(n,5n)	(n, 6n)	(n,6n)
(n, 7n)	(n,7n)	(n, 8n)	(n,8n)
(n, n')	(n,n')	(n, p)	(n,p)
(n, d)	(n,d)+(n,n'p)	(n, t)	(n,t)+(n,n'd)+(n,2np)
(n, h)	(n, ³ He)+(n,n'2p)+(n,pd)	(n, a)	(n,α)+(n,n'h)+(n,tp)+(n,n'pd) +(n,2n2p)
(n, nt)	(n,n't)+(n,2nd)+(n,3np)	(n, 2nt)	(n,2nt)+(n,3nd)+(n,4np)
(n, 3nt)	(n,3nt)+(n,4nd)+(n,5np)	(n, 4nt)	(n,4nt)+(n,5nd)+(n,6np)
(n, 5nt)	(n,5nt)+(n,6nd)+(n,7np)	(n, 6nt)	(n,6nt)
(n, 2p)	(n,2p)	(n, 3p)	(n,3p)
(n, na)	(n,n'α)+(n,2nh)+(n,dt)+ (n,n'pt)+(n,3n2p)	(n, 2na)	(n,2nα)+(n,3nh)+(n,n'dt)+ (n,4n2p)
(n, 3na)	(n,3nα)+(n,4nh)+(n,5n2p)	(n, 4na)	(n,4nα)
(n, 5na)	(n,5nα)	(n, 6na)	(n,6nα)
(n, 7na)	(n,7nα)	(n, ph)	(n,ph)+(n,n'3p)
(n, pa)	(n,pα)+(n,dh)+(n,n'ph)	(n, da)	(n,dα)+(n,n'pα)+(n,n'dh)
(n, ha)	(n,hα)	(n, ta)	(n,tα)+(n,n'dα)+(n,n'th)+ (n,2npα)
(n, nta)	(n,n'tα)+(n,3npα)	(n4npa)	(n,4npα)
(n, 2a)	(n,2α)	(n, n2a)	(n,n'2α)+(n,3n2pα)
(n2n2a)	(n,2n2α)	(n3n2a)	(n,3n2α)
(n4n2a)	(n,4n2α)	(n, d2a)	(n,d2α)
(n, t2a)	(n,t2α)+(n,d2α)	(nnt2a)	(n,n't2α)
(n, 3a)	(n,3α)	(n, n3a)	(n,n'3α)
(n, F)	(n,fission)		

The fourth section lists the nuclides that produce bremsstrahlung radiation from energetic β particles. The user may choose nuclides from here for the input file, although the most important nuclides when EAF-2005 is used are summarised in Appendix 7.

The fifth section lists the neutron spectrum used to collapse the cross section library.

Appendix 1 - Cross section group structures

Seven standard group structures are used for the European Activation File and data in all these structures can be read into FISPACT. Table A1.1 lists the group structures for the five low- energy cases: WIMS (69), GAM-II (100), XMAS (172), VITAMIN-J (175) and TRIPOLI (315). This method of presentation makes it clear in which energy ranges particular structures have most groups and will therefore give a good representation of the cross sections. Table A1.2 lists part of the two high-energy structures, VITAMIN-J+ (211) and TRIPOLI+ (351), showing how these join to the low-energy ones. Users are advised to prepare neutron spectra for a particular application in one of these structures as appropriate.

Table A1.1 Energy group boundaries for the five low-energy standard structures.

GRP	TRIPOLI	GRP	VITAMIN-J	GRP	GAM-II	GRP	XMAS	GRP	WIMS
1	1.9640E+07	1	1.96403E+07			1	1.96403E+07		
2	1.7330E+07	2	1.73325E+07			2	1.73325E+07		
3	1.6910E+07	3	1.69046E+07						
4	1.6490E+07	4	1.64872E+07						
5	1.5680E+07	5	1.56831E+07						
6	1.4920E+07	6	1.49182E+07	1	1.49180E+07	3	1.49182E+07		
7	1.4550E+07	7	1.45499E+07						
8	1.4190E+07	8	1.41907E+07						
9	1.3840E+07	9	1.38403E+07			4	1.38403E+07		
10	1.3500E+07	10	1.34986E+07	2	1.34983E+07				
11	1.2840E+07	11	1.28403E+07						
		12	1.25232E+07						
12	1.2210E+07	13	1.22140E+07	3	1.22138E+07				
13	1.1620E+07	14	1.16183E+07			5	1.16183E+07		
14	1.1050E+07	15	1.10517E+07	4	1.10515E+07				
15	1.0510E+07	16	1.05127E+07						
16	1.0000E+07	17	1.00000E+07	5	9.99983E+06	6	1.00000E+07	1	1.00000E+07
17	9.5120E+06	18	9.51229E+06						
18	9.0480E+06	19	9.04837E+06	6	9.04822E+06				
19	8.6070E+06	20	8.60708E+06						
20	8.1870E+06	21	8.18731E+06	7	8.18717E+06	7	8.18731E+06		
21	7.7880E+06	22	7.78801E+06						
22	7.4080E+06	23	7.40818E+06	8	7.40806E+06				
23	7.0470E+06	24	7.04688E+06						
24	6.7030E+06	25	6.70320E+06	9	6.70309E+06	8	6.70320E+06		
25	6.5920E+06	26	6.59241E+06						
26	6.3760E+06	27	6.37628E+06						
27	6.0650E+06	28	6.06531E+06	10	6.06520E+06	9	6.06531E+06	2	6.06600E+06
28	5.7690E+06	29	5.76950E+06						
29	5.4880E+06	30	5.48812E+06	11	5.48802E+06	10	5.48812E+06		
30	5.2200E+06	31	5.22046E+06						
31	4.9660E+06	32	4.96585E+06	12	4.96577E+06				

GRP	TRIPOLI	GRP	VITAMIN-J	GRP	GAM-II	GRP	XMAS	GRP	WIMS
32	4.7240E+06	33	4.72367E+06						
33	4.4930E+06	34	4.49329E+06	13	4.49321E+06	11	4.49329E+06		
34	4.0660E+06	35	4.06570E+06	14	4.06562E+06				
35	3.6790E+06	36	3.67879E+06	15	3.67873E+06	12	3.67879E+06	3	3.67900E+06
36	3.3290E+06	37	3.32871E+06	16	3.32865E+06				
37	3.1660E+06	38	3.16637E+06						
38	3.0120E+06	39	3.01194E+06	17	3.01189E+06	13	3.01194E+06		
39	2.8650E+06	40	2.86505E+06						
40	2.7250E+06	41	2.72532E+06	18	2.72527E+06				
41	2.5920E+06	42	2.59240E+06						
42	2.4660E+06	43	2.46597E+06	19	2.46592E+06	14	2.46597E+06		
43	2.3850E+06	44	2.38513E+06						
44	2.3650E+06	45	2.36533E+06						
45	2.3460E+06	46	2.34570E+06						
46	2.3070E+06	47	2.30693E+06						
47	2.2310E+06	48	2.23130E+06	20	2.23126E+06	15	2.23130E+06	4	2.23100E+06
48	2.1220E+06	49	2.12248E+06						
49	2.0190E+06	50	2.01897E+06	21	2.01893E+06	16	2.01897E+06		
50	1.9210E+06	51	1.92050E+06						
51	1.8270E+06	52	1.82684E+06	22	1.82680E+06				
52	1.7380E+06	53	1.73774E+06						
53	1.6530E+06	54	1.65299E+06	23	1.65296E+06	17	1.65299E+06		
54	1.5720E+06	55	1.57237E+06						
55	1.4960E+06	56	1.49569E+06	24	1.49566E+06				
56	1.4230E+06	57	1.42274E+06						
57	1.3530E+06	58	1.35335E+06	25	1.35333E+06	18	1.35335E+06	5	1.35300E+06
58	1.2870E+06	59	1.28735E+06						
59	1.2250E+06	60	1.22456E+06	26	1.22454E+06	19	1.22456E+06		
60	1.1650E+06	61	1.16484E+06						
61	1.1080E+06	62	1.10803E+06	27	1.10801E+06	20	1.10803E+06		
62	1.0030E+06	63	1.00259E+06	28	1.00257E+06	21	1.00259E+06		
63	9.6160E+05	64	9.61672E+05						
64	9.0720E+05	65	9.07180E+05	29	9.07164E+05	22	9.07180E+05		
65	8.6290E+05	66	8.62936E+05						
66	8.2090E+05	67	8.20850E+05	30	8.20836E+05	23	8.20850E+05	6	8.21000E+05
67	7.8080E+05	68	7.80817E+05						
68	7.4270E+05	69	7.42736E+05	31	7.42723E+05				
69	7.0650E+05	70	7.06512E+05						
70	6.7210E+05	71	6.72055E+05	32	6.72044E+05				
71	6.3930E+05	72	6.39279E+05						
72	6.0810E+05	73	6.08101E+05	33	6.08090E+05	24	6.08101E+05		
73	5.7840E+05	74	5.78443E+05						
74	5.5020E+05	75	5.50232E+05	34	5.50223E+05	25	5.50232E+05	7	5.00000E+05
75	5.2340E+05	76	5.23397E+05						
		77	4.97871E+05	35	4.97862E+05	26	4.97871E+05		
76	4.5050E+05	78	4.50492E+05	36	4.50484E+05	27	4.50492E+05		
77	4.0760E+05	79	4.07622E+05	37	4.07615E+05	28	4.07622E+05		
78	3.8770E+05	80	3.87742E+05						
79	3.6880E+05	81	3.68832E+05	38	3.68825E+05				
80	3.3370E+05	82	3.33733E+05	39	3.33727E+05				
81	3.0200E+05	83	3.01974E+05	40	3.01968E+05	29	3.01974E+05	8	3.02500E+05
82	2.9850E+05	84	2.98491E+05						
83	2.9720E+05	85	2.97211E+05						
84	2.9450E+05	86	2.94518E+05						
85	2.8730E+05	87	2.87246E+05						
86	2.7320E+05	88	2.73237E+05	41	2.73232E+05	30	2.73237E+05		
87	2.4720E+05	89	2.47235E+05	42	2.47231E+05	31	2.47235E+05		
88	2.3520E+05	90	2.35177E+05						
89	2.2370E+05	91	2.23708E+05	43	2.23704E+05				
90	2.1280E+05	92	2.12797E+05						
91	2.0240E+05	93	2.02419E+05	44	2.02415E+05				
92	1.9250E+05	94	1.92547E+05						
93	1.8320E+05	95	1.83156E+05	45	1.83153E+05	32	1.83156E+05	9	1.83000E+05

GRP	TRIPOLI	GRP	VITAMIN-J	GRP	GAM-II	GRP	XMAS	GRP	WIMS
94	1.7420E+05	96	1.74224E+05						
95	1.6570E+05	97	1.65727E+05	46	1.65724E+05				
96	1.5760E+05	98	1.57644E+05						
97	1.5000E+05	99	1.49956E+05	47	1.49953E+05				
98	1.4260E+05	100	1.42642E+05						
99	1.3570E+05	101	1.35686E+05	48	1.35683E+05				
100	1.2910E+05	102	1.29068E+05						
101	1.2280E+05	103	1.22773E+05	49	1.22771E+05	33	1.22773E+05		
102	1.1680E+05	104	1.16786E+05						
103	1.1110E+05	105	1.11090E+05	50	1.11088E+05	34	1.11090E+05	10	1.11000E+05
104	9.8040E+04	106	9.80365E+04						
105	8.6520E+04	107	8.65170E+04	51	8.65155E+04				
106	8.2500E+04	108	8.25034E+04						
107	8.2300E+04					35	8.22975E+04		
108	7.9500E+04	109	7.94987E+04						
109	7.4990E+04								
110	7.2000E+04	110	7.20245E+04						
111	6.7380E+04	111	6.73795E+04	52	6.73783E+04	36	6.73795E+04	11	6.73400E+04
112	6.1730E+04								
113	5.6560E+04	112	5.65622E+04			37	5.51656E+04		
114	5.5170E+04								
115	5.2480E+04	113	5.24752E+04	53	5.24743E+04				
116	4.9390E+04								
117	4.6310E+04	114	4.63092E+04						
118	4.3590E+04								
119	4.0870E+04	115	4.08677E+04	54	4.08670E+04	38	4.08677E+04	12	4.08500E+04
120	3.6980E+04					39	3.69786E+04		
121	3.4310E+04	116	3.43067E+04						
122	3.1830E+04	117	3.18278E+04	55	3.18272E+04				
123	3.1620E+04								
124	3.0730E+04								
125	2.9850E+04								
126	2.9010E+04					40	2.92830E+04		
127	2.8500E+04	118	2.85011E+04						
128	2.8180E+04								
129	2.7380E+04					41	2.73944E+04		
130	2.7000E+04	119	2.70001E+04						
131	2.6610E+04								
132	2.6060E+04	120	2.60584E+04						
133	2.5850E+04								
134	2.5120E+04								
135	2.4790E+04	121	2.47875E+04	56	2.47871E+04	42	2.47875E+04	13	2.47800E+04
136	2.4410E+04								
137	2.4180E+04	122	2.41755E+04						
138	2.3580E+04	123	2.35786E+04						
139	2.3040E+04								
140	2.2390E+04								
141	2.1870E+04	124	2.18749E+04						
142	2.1130E+04								
143	2.0540E+04								
144	1.9950E+04								
145	1.9310E+04	125	1.93045E+04	57	1.93042E+04				
146	1.7780E+04								
147	1.6620E+04					43	1.66156E+04		
148	1.5850E+04								
149	1.5030E+04	126	1.50344E+04	58	1.50341E+04	44	1.50344E+04	14	1.50300E+04
150	1.3830E+04								
151	1.2730E+04								
152	1.1710E+04	127	1.17088E+04	59	1.17086E+04				
153	1.1140E+04					45	1.11378E+04		
		128	1.05946E+04						
154	1.0080E+04								
155	9.1190E+03	129	9.11882E+03	60	9.11866E+03	46	9.11882E+03	15	9.11800E+03

GRP	TRIPOLI	GRP	VITAMIN-J	GRP	GAM-II	GRP	XMAS	GRP	WIMS
156	8.2510E+03								
157	7.4660E+03					47	7.46586E+03		
158	7.1020E+03	130	7.10174E+03	61	7.10162E+03				
159	6.2670E+03								
160	5.5310E+03	131	5.53084E+03	62	5.53075E+03	48	5.53084E+03	16	5.53000E+03
161	5.0040E+03					49	5.00451E+03		
162	4.6430E+03								
163	4.3070E+03	132	4.30742E+03	63	4.30735E+03				
164	3.9810E+03								
165	3.7070E+03	133	3.70744E+03						
166	3.5480E+03					50	3.52662E+03	17	3.51900E+03
167	3.3550E+03	134	3.35463E+03	64	3.35457E+03	51	3.35463E+03		
168	3.1620E+03								
169	3.0350E+03	135	3.03539E+03						
170	2.8180E+03								
171	2.7470E+03	136	2.74654E+03						
172	2.6610E+03								
173	2.6130E+03	137	2.61259E+03	65	2.61254E+03				
174	2.4850E+03	138	2.48517E+03						
175	2.3710E+03								
176	2.2490E+03	139	2.24867E+03			52	2.24867E+03	18	2.23900E+03
177	2.1130E+03								
178	2.0350E+03	140	2.03468E+03	66	2.03465E+03	53	2.03468E+03		
179	1.7960E+03								
180	1.5850E+03	141	1.58461E+03	67	1.58458E+03				
181	1.5070E+03					54	1.50733E+03		
						55	1.43382E+03	19	1.42500E+03
182	1.3640E+03								
183	1.2340E+03	142	1.23410E+03	68	1.23407E+03	56	1.23410E+03		
184	1.1170E+03								
185	1.0100E+03					57	1.01039E+03		
186	9.6110E+02	143	9.61117E+02	69	9.61100E+02				
						58	9.14242E+02	20	9.06900E+02
187	8.4820E+02								
188	7.4850E+02	144	7.48518E+02	70	7.48505E+02	59	7.48518E+02		
189	7.0790E+02								
190	6.7730E+02					60	6.77287E+02		
191	6.3100E+02								
192	5.8300E+02	145	5.82947E+02	71	5.82937E+02				
193	5.1450E+02								
194	4.5400E+02	146	4.53999E+02	72	4.53991E+02	61	4.53999E+02		
195	3.9810E+02								
						62	3.71703E+02	21	3.67300E+02
196	3.5360E+02	147	3.53575E+02	73	3.53569E+02				
197	3.0430E+02					63	3.04325E+02		
198	2.7540E+02	148	2.75364E+02	74	2.75359E+02				
199	2.4300E+02								
200	2.1450E+02	149	2.14454E+02	75	2.14450E+02				
201	2.0400E+02					64	2.03995E+02		
202	1.7780E+02								
203	1.6700E+02	150	1.67017E+02	76	1.67014E+02				
204	1.5850E+02								
						65	1.48625E+02	22	1.48700E+02
205	1.3670E+02					66	1.36742E+02		
206	1.3010E+02	151	1.30073E+02	77	1.30070E+02				
207	1.1220E+02								
208	1.0130E+02	152	1.01301E+02	78	1.01299E+02				
209	9.1660E+01					67	9.16609E+01		
210	8.5280E+01								
211	7.8890E+01	153	7.88932E+01	79	7.88919E+01				
						68	7.56736E+01	23	7.55000E+01
212	7.0790E+01								
213	6.7900E+01					69	6.79041E+01		

GRP	TRIPOLI	GRP	VITAMIN-J	GRP	GAM-II	GRP	XMAS	GRP	WIMS
214	6.3100E+01								
215	6.1440E+01	154	6.14421E+01	80	6.14411E+01				
216	5.5590E+01					70	5.55951E+01		
						71	5.15780E+01		
217	5.0120E+01					72	4.82516E+01	24	4.80500E+01
218	4.7850E+01	155	4.78512E+01	81	4.78503E+01				
219	4.5520E+01					73	4.55174E+01		
220	3.9810E+01					74	4.01690E+01		
221	3.7270E+01	156	3.72665E+01	82	3.72659E+01	75	3.72665E+01		
222	3.3890E+01					76	3.37201E+01		
223	3.0510E+01					77	3.05113E+01		
224	2.9200E+01	157	2.90232E+01	83	2.90227E+01				
225	2.7920E+01					78	2.76077E+01	25	2.77000E+01
226	2.4980E+01					79	2.49805E+01		
227	2.2600E+01	158	2.26033E+01	84	2.26029E+01	80	2.26033E+01		
228	2.0450E+01								
229	1.9030E+01					81	1.94548E+01		
230	1.7600E+01	159	1.76035E+01	85	1.76031E+01				
231	1.6740E+01								
						82	1.59283E+01	26	1.59700E+01
232	1.5230E+01								
233	1.3710E+01	160	1.37096E+01	86	1.37093E+01	83	1.37096E+01		
234	1.2590E+01								
235	1.1220E+01					84	1.12245E+01		
236	1.0680E+01	161	1.06770E+01	87	1.06768E+01				
237	1.0000E+01					85	9.90555E+00	27	9.87700E+00
238	9.1900E+00					86	9.18981E+00		
239	8.9130E+00								
240	8.3150E+00	162	8.31529E+00	88	8.31515E+00	87	8.31529E+00		
241	7.9430E+00								
242	7.5240E+00					88	7.52398E+00		
243	7.0790E+00								
244	6.4760E+00	163	6.47595E+00	89	6.47584E+00				
245	6.1600E+00					89	6.16012E+00		
246	5.6230E+00					90	5.34643E+00		
247	5.0430E+00	164	5.04348E+00	90	5.04339E+00	91	5.04348E+00		
248	4.6700E+00								
249	4.4700E+00								
250	4.1290E+00					92	4.12925E+00		
						93	4.00000E+00	28	4.00000E+00
251	3.9280E+00	165	3.92786E+00	91	3.92779E+00				
252	3.3810E+00					94	3.38075E+00		
						95	3.30000E+00	29	3.30000E+00
253	3.0590E+00	166	3.05902E+00	92	3.05897E+00				
254	2.7680E+00					96	2.76792E+00		
						97	2.72000E+00		
						98	2.60000E+00	30	2.60000E+00
						99	2.55000E+00		
255	2.3720E+00	167	2.38237E+00	93	2.38233E+00				
256	2.3600E+00					100	2.36000E+00		
257	2.1300E+00					101	2.13000E+00		
						102	2.10000E+00	31	2.10000E+00
258	2.0200E+00					103	2.02000E+00		
259	1.9300E+00					104	1.93000E+00		
260	1.8550E+00	168	1.85539E+00	94	1.85536E+00				
261	1.8400E+00					105	1.84000E+00		
262	1.7550E+00					106	1.75500E+00		
263	1.6700E+00					107	1.67000E+00		
264	1.5900E+00					108	1.59000E+00		
265	1.5100E+00					109	1.50000E+00	32	1.50000E+00
						110	1.47500E+00		
266	1.4450E+00	169	1.44498E+00	95	1.44495E+00	111	1.44498E+00		

GRP	TRIPOLI	GRP	VITAMIN-J	GRP	GAM-II	GRP	XMAS	GRP	WIMS
267	1.4400E+00					112	1.37000E+00		
268	1.3700E+00					113	1.33750E+00		
269	1.3050E+00					114	1.30000E+00	33	1.30000E+00
270	1.2350E+00					115	1.23500E+00		
271	1.1700E+00					116	1.17000E+00		
272	1.1250E+00	170	1.12535E+00	96	1.12533E+00	117	1.15000E+00	34	1.15000E+00
273	1.1100E+00					118	1.12535E+00	35	1.12300E+00
274	1.0900E+00					119	1.11000E+00		
275	1.0800E+00					120	1.09700E+00	36	1.09700E+00
276	1.0700E+00								
277	1.0350E+00					121	1.07100E+00	37	1.07100E+00
278	1.0100E+00					122	1.04500E+00	38	1.04500E+00
279	9.8600E-01					123	1.03500E+00		
280	9.3000E-01					124	1.02000E+00	39	1.02000E+00
281	8.7640E-01	171	8.76425E-01	97	8.76410E-01	125	9.96000E-01	40	9.96000E-01
282	8.6000E-01					126	9.86000E-01		
283	7.9000E-01					127	9.72000E-01	41	9.72000E-01
284	7.0500E-01					128	9.50000E-01	42	9.50000E-01
285	6.8260E-01	172	6.82560E-01	98	6.82549E-01	129	9.30000E-01		
286	6.2500E-01					130	9.10000E-01	43	9.10000E-01
287	5.4000E-01					131	8.60000E-01		
288	5.3160E-01	173	5.31579E-01	99	5.31570E-01	132	8.50000E-01	44	8.50000E-01
289	4.8500E-01					133	7.90000E-01		
290	4.3300E-01					134	7.80000E-01	45	7.80000E-01
291	4.1400E-01	174	4.13994E-01	100	4.13987E-01	135	7.05000E-01		
292	3.9100E-01					136	6.25000E-01	46	6.25000E-01
293	3.5200E-01					137	5.40000E-01		
294	3.1450E-01					138	5.00000E-01	47	5.00000E-01
295	2.8250E-01					139	4.85000E-01		
296	2.4800E-01					140	4.33000E-01		
297	2.2000E-01					141	4.00000E-01	48	4.00000E-01
298	1.8900E-01					142	3.91000E-01		
299	1.6000E-01					143	3.50000E-01	49	3.50000E-01
300	1.3400E-01					144	3.20000E-01	50	3.20000E-01
301	1.1500E-01					145	3.14500E-01		
302	1.0000E-01	175	1.00001E-01			146	3.00000E-01	51	3.00000E-01
303	9.5000E-02					147	2.80000E-01	52	2.80000E-01
304	7.7000E-02					148	2.48000E-01	53	2.50000E-01
305	5.9000E-02					149	2.20000E-01	54	2.20000E-01
306	4.3000E-02					150	1.89000E-01		
						151	1.80000E-01	55	1.80000E-01
						152	1.60000E-01		
						153	1.40000E-01	56	1.40000E-01
						154	1.34000E-01		
						155	1.15000E-01		
						156	1.00001E-01	57	1.00000E-01
						157	9.50000E-02		
						158	8.00000E-02	58	8.00000E-02
						159	7.70000E-02		
						160	6.70000E-02	59	6.70000E-02
						161	5.80000E-02	60	5.80000E-02
						162	5.00000E-02	61	5.00000E-02
						163	4.20000E-02	62	4.20000E-02
						164	3.50000E-02	63	3.50000E-02

GRP	TRIPOLI	GRP	VITAMIN-J	GRP	GAM-II	GRP	XMAS	GRP	WIMS
307	3.2380E-02								
308	3.2000E-02								
309	3.0000E-02					165	3.00000E-02	64	3.00000E-02
						166	2.50000E-02	65	2.50000E-02
310	2.0000E-02					167	2.00000E-02	66	2.00000E-02
311	1.5000E-02					168	1.50000E-02	67	1.50000E-02
312	1.0000E-02					169	1.00000E-02	68	1.00000E-02
						170	6.90000E-03		
313	5.5000E-03					171	5.00000E-03	69	5.00000E-03
314	3.0000E-03					172	3.00000E-03		
315	1.1000E-04								
316	1.0000E-05	176	1.00000E-05	101	1.00000E-05	173	1.00000E-05	70	1.00000E-05

Table A1.2 Energy group boundaries for the two high-energy standard structures.

GRP	TRIPOLI+	GRP	TRIPOLI	GRP	VITAMIN-J	GRP	VITAMIN-J
1	5.5000E+07			1	5.5000E+07		
2	5.4000E+07			2	5.4000E+07		
3	5.3000E+07			3	5.3000E+07		
4	5.2000E+07			4	5.2000E+07		
5	5.1000E+07			5	5.1000E+07		
6	5.0000E+07			6	5.0000E+07		
7	4.9000E+07			7	4.9000E+07		
8	4.8000E+07			8	4.8000E+07		
9	4.7000E+07			9	4.7000E+07		
10	4.6000E+07			10	4.6000E+07		
11	4.5000E+07			11	4.5000E+07		
12	4.4000E+07			12	4.4000E+07		
13	4.3000E+07			13	4.3000E+07		
14	4.2000E+07			14	4.2000E+07		
15	4.1000E+07			15	4.1000E+07		
16	4.0000E+07			16	4.0000E+07		
17	3.9000E+07			17	3.9000E+07		
18	3.8000E+07			18	3.8000E+07		
19	3.7000E+07			19	3.7000E+07		
20	3.6000E+07			20	3.6000E+07		
21	3.5000E+07			21	3.5000E+07		
22	3.4000E+07			22	3.4000E+07		
23	3.3000E+07			23	3.3000E+07		
24	3.2000E+07			24	3.2000E+07		
25	3.1000E+07			25	3.1000E+07		
26	3.0000E+07			26	3.0000E+07		
27	2.9000E+07			27	2.9000E+07		
28	2.8000E+07			28	2.8000E+07		
29	2.7000E+07			29	2.7000E+07		
30	2.6000E+07			30	2.6000E+07		
31	2.5000E+07			31	2.5000E+07		
32	2.4000E+07			32	2.4000E+07		
33	2.3000E+07			33	2.3000E+07		
34	2.2000E+07			34	2.2000E+07		
35	2.1000E+07			35	2.1000E+07		
36	2.0000E+07			36	2.0000E+07		
37	1.9640E+07	1	1.9640E+07	37	1.9640E+07	1	1.9640E+07
38	1.7330E+07	2	1.7330E+07	38	1.7330E+07	2	1.7330E+07
n+36	...	n	...	n+36	...	n	...
338	1.0000E-01	302	1.0000E-01	211	1.0000E-01	175	1.0000E-01
n+36	...	n	...				
351	1.1000E-04	315	1.1000E-04				
352	1.0000E-05	316	1.0000E-05	212	1.0000E-05	176	1.0000E-05

Weighting spectra

Different weighting spectra are used depending upon which group structure is required and for which application (fusion or fission) the calculation needs to be performed. They are all generated at a temperature of 300 K.

The weighting spectra used to generate fission relevant libraries in the WIMS, XMAS and TRIPOLI group format from EAF point-wise data are as follows:

Energy range	Micro-flux weighting
$1.0 \cdot 10^{-5}$ - 0.2 eV	Maxwellian ($T = 0.0253$ eV)
0.2 eV - 0.82085 MeV	$1/E$
0.82085 MeV - E_{max}	Maxwellian fission spectrum ($T = 1.3539$ MeV)

The weighting spectra used to generate fusion relevant libraries in the VITAMIN-J, GAM-II and TRIPOLI group format from EAF point-wise data are as follows:

Energy range	Micro-flux weighting
$1.0 \cdot 10^{-5}$ - 0.414 eV	Maxwellian ($T = 0.0253$ eV)
0.414 eV - 12.52 MeV	$1/E$
12.52 - 15.68 MeV	Velocity exponential fusion peak ($E_f = 14.07$ MeV, $kT_f = 0.025$ MeV)
15.68 - 19.64 MeV	$1/E$

A flat weighting spectrum is used to generate special purpose libraries in the XMAS, VITAMIN-J, VITAMIN-J+, TRIPOLI and TRIPOLI+ group format from EAF point-wise data. Such libraries should be used to model cases where the neutron field is not produced by fission or DT fusion, but for example, from accelerator beam target interactions (e.g. IFMIF) or experimental devices. Such libraries also allow group-wise data to be plotted without weighting.

It is the user's responsibility to select the appropriate group-wise library depending on the type of activation calculations that will be made. The micro-flux weighting process can have significant impact on the cross sections, particularly for reactions with high thresholds.

Appendix 2 - Solution of the differential equations

The core task of FISPACT is the solution of a set of differential equations that describe the amounts of atoms of various nuclides present following the irradiation of a given material in a neutron field. The set of differential equations is given in equation A2.1.

$$\frac{dN_i}{dt} = -N_i(\lambda_i + \sigma_i\phi) + \sum_{j \neq i} N_j(\lambda_{ij} + \sigma_{ij}\phi) + S_i \dots\dots\dots(A2.1)$$

$$S_i = \sum_k N_k \sigma_k^f \phi Y_{ik}$$

where

N_i is the amount of nuclide i at time t

λ_i is the decay constant of nuclide i (s^{-1})

λ_{ij} is the decay constant of nuclide j producing i (s^{-1})

σ_i is the total cross section for reactions on i (cm^2)

σ_{ij} is the reaction cross section for reactions on j producing i (cm^2)

σ_k^f is the fission cross section for reactions on actinide k (cm^2)

ϕ is the neutron flux ($n\ cm^{-2}\ s^{-1}$)

S_i is the source of nuclide i from fission

Y_{ik} is the yield of nuclide i from the fission of nuclide k

The final term is only required if actinides are included in the initial material.

It is necessary to use an efficient method of solution of the set of equations in A2.1 since the total number of nuclides considered is over 1900. The method used in FISPACT (and in FISPIN from which it was developed) is that of Sidell⁷. This method is an extension of the Euler (first order Taylor series) which uses an exponential function of the step length.

Equation A2.2 shows the standard Euler solution and A2.3 the Sidell solution for the step time h .

$$N_i(t+h) = N_i(t) + h \left. \frac{dN_i}{dt} \right|_t \dots\dots\dots(A2.2)$$

$$N_i(t+h) = N_i(t) + \frac{(e^{\Lambda_i h} - 1)}{\Lambda_i} \left. \frac{dN_i}{dt} \right|_t \dots\dots\dots (A2.3)$$

where $\Lambda_i = (\lambda_i + \sigma_i \phi)$

The error in using A2.3 is lower than A2.2, but for stability of the solution it is still necessary that the time step be related to the reciprocal of the largest eigenvalue. For this reason a restriction is placed on the largest eigenvalue considered (some nuclides are considered in equilibrium). The number of steps in the computational solution of the Sidell method is greater than the Euler method, but not sufficiently to outweigh the advantages. The procedure is to split the irradiation time into two steps, perform the calculation, test the convergence of all the nuclides and, if the test fails then repeat with double the number of time steps. This procedure is continued until sufficient accuracy is achieved. The results at each stage are corrected using the results from the previous stage ('extrapolation') to improve the convergence of the solution.

Experience with this solution method in both FISPACT and FISPIN shows that it is both rapid to converge and able to give sufficient accuracy. The code implements a maximum number of iteration stages (10), but if convergence has not been achieved by then it is usually only for a very few 'unimportant' nuclides. The output flags these nuclides, thus enabling the worth of the particular 'non-converged' run to be judged.

It was mentioned above that there is a limit on the largest eigenvalue considered in the solution of the equations. This means that physically only nuclides with sufficiently long half-lives are calculated by the above method. The remainder are assumed to be in equilibrium, and thus their values can be written down immediately as shown in equation A2.4.

$$N_i^{equil} = \left\{ \sum_j N_j (\lambda_{ij} + \sigma_{ij} \phi) + S_i \right\} / (\lambda_i + \sigma_i \phi) \dots\dots\dots (A2.4)$$

The half-life at which nuclides are considered to be in equilibrium is under the control of the user. This is done by choosing the time interval (code word **TIME**) and the parameters following the **LEVEL** code word.

Appendix 3 - γ dose rate

In addition to the activity of irradiated materials, another measure of acceptability is the dose rate from emitted γ rays. FISPACT uses two approximate estimates of the γ dose rate - contact dose from the surface of a semi-infinite slab or dose at a given distance from a point source.

Contact γ dose rate

Equation A3.1 shows the formula used to calculate the γ dose rate at the surface of a semi-infinite slab of material, it is taken from Jaeger⁸.

$$D = 5.76 \cdot 10^{-10} \frac{B}{2} \sum_{i=1}^{24} \frac{\mu_a(E_i)}{\mu_m(E_i)} S_v(E_i) \dots\dots\dots(A3.1)$$

where

- D = surface γ dose rate (Sv h⁻¹)
- E_i = mean energy of the i th energy group
- μ_a = mass energy absorption coefficient (μ_{en}/ρ) of air (m² kg⁻¹)
- μ_m = mass energy attenuation coefficient (μ/ρ) of the material (m² kg⁻¹)
- B = build up factor (= 2)
- S_v = rate of γ emission (MeV kg⁻¹ s⁻¹)

The photon mass attenuation coefficient μ/ρ , and the mass energy-absorption coefficient μ_{en}/ρ for all elements with $Z = 1 - 100$ have been produced using the XGAM program from the National Institute of Standards and Technology⁹. The new data base covers energies of photons (X-ray, γ ray and bremsstrahlung) from 1 keV to 100 GeV and has been processed into a 24-group structure (1 keV - 20 MeV) identical to the FISPACT γ group structure. The present compilation is an extension of the recent calculations of Seltzer¹⁰, and is intended to replace the values given in Hubble¹¹ which were used in previous FISPACT versions. The present data differ from the Hubble set in the following respects:

1. The first 100 elements are included compared to the 40 selected elements previously covered.
2. All edge energies are included and identified and values of μ/ρ and μ_{en}/ρ are given just above and below each discontinuity to facilitate accurate interpolation.
3. Somewhat different values for the atomic photoeffect cross section have been used for $Z = 2 - 54$.
4. For compounds and mixtures, values for μ/ρ can now be obtained by simple addition, *i.e.* combining values for the elements according to their proportions by weight. Radiative losses are now included.
5. The total cross section per atom (σ_{tot}) which is related to μ/ρ can be written as the sum over contributions from the principal photon interactions:

$$\sigma_{\text{tot}} = \sigma_{\text{pe}} + \sigma_{\text{coh}} + \sigma_{\text{incoh}} + \sigma_{\text{pair}} + \sigma_{\text{trip}} + \sigma_{\text{phn}}$$

where σ_{pe} is the atomic photoeffect cross section, σ_{coh} and σ_{incoh} are the coherent (Rayleigh) and incoherent (Compton) scattering cross sections respectively, σ_{pair} and σ_{trip} are the cross sections for electron-positron production in the fields of the nucleus and the atomic electrons respectively and σ_{phn} is the photonuclear cross section. However, the latter contribution has been neglected as well as other less probable photon-atom interactions.

The library EAF_ABS-2005 contains μ/ρ [$\text{cm}^2 \text{g}^{-1}$] for all elements in increasing Z order, μ [m^{-1}] and μ_{en}/ρ [$\text{cm}^2 \text{g}^{-1}$] for air and the mean energies of the 24-group structure.

The value of μ_m for the material is calculated from the elemental values μ_{mj} using equation A3.2,

$$\mu_m = \sum_j f_j \mu_{mj} \dots\dots\dots(\text{A3.2})$$

where $f_j = (\text{mass of element } j) / (\text{total mass})$.

The value of S_v is calculated using equation A3.3:

$$S_\gamma = E_\gamma N_\gamma A(t) \dots\dots\dots(A3.3)$$

where

E_γ = energy of γ ray (MeV)

N_γ = number of quanta per decay

$A(t)$ = activity of material at time t (Bq kg⁻¹)

γ dose rate from point source

Equation A3.4 shows the standard formula (taken from reference 8) for calculation of the dose rate from a point source in air. In this section it is assumed that 1 g of material is present in the source.

$$D = 5.76 \cdot 10^{-10} \sum_{i=1}^{24} \frac{\mu_a(E_i)}{4\pi r^2} e^{-\mu(E_i)r} \frac{S_\gamma(E_i)}{1000} \dots\dots\dots(A3.4)$$

where

r = distance from source (m)

$\mu(E_i)$ = energy attenuation coefficient of air (m⁻¹)

The other symbols are as in equation A3.1.

Both equations A3.1 and A3.4 are approximations suitable for FISPACT calculations, but it is noted that they are not adequate for specific health physics problems.

Appendix 4 - Approximate γ spectral data

Wherever possible decay data from evaluated files such as JEF2.2 have been used to construct the decay data library (EAF_DEC-2005) used with FISPACT. However, for 223 unstable nuclides the file contains only the average γ energy - no data for the γ spectrum are available. Without the γ spectrum FISPACT is unable to calculate the γ dose rate contribution for these nuclides. In order to check if any of these nuclides are likely to significantly contribute to the total dose rate, the following method is used to calculate an approximate spectrum.

The maximum γ energy (E_m) for decays assumed in the method are given in Table A4.1.

Table A4.1 Maximum γ energies for various decay modes.

Decay mode	E_m
β^-	$2 \langle \beta \rangle$
β^+	5 MeV
α	0
Isomeric Transition	$\langle \gamma \rangle$

The intensity in the i -th group (I_i) is given by equation A4.1,

$$I_i = \frac{a \langle \gamma \rangle e^{-a\eta_{i-1}} - e^{-a\eta_i}}{E_m [1 - (1+a)e^{-a}]} \dots\dots\dots(\text{A4.1})$$

where

$$a = 14 \text{ (arbitrary constant)}$$

$$\eta_i = E_i / E_m$$

Appendix 5 - Sensitivity equations

An important feature of FISPACT is the ability to calculate sensitivity coefficients of nuclide quantities to either reaction cross section or decay constant. This development was done by Khursheed¹² and was based on the work of James¹³ who implemented a similar facility in FISPIN. This method relies on the quasi-linearity of the inventory equations (see Appendix 2). These are written in matrix form in equation A5.1,

$$\frac{d\mathbf{N}}{dt} = \mathbf{A}\mathbf{N} + \mathbf{S} \dots\dots\dots(\text{A5.1})$$

where

\mathbf{N} is a vector of nuclide quantities

\mathbf{S} is a vector of source of nuclides due to fissions

\mathbf{A} is matrix of terms involving cross sections and half-lives.

If x represents either λ or σ , then differentiating equation A5.1 with respect to x , and assuming that the order of differentiation can be exchanged, then equation A5.2 is obtained.

$$\frac{d}{dt} \left(\frac{\partial \mathbf{N}}{\partial x} \right) = \mathbf{A} \left(\frac{\partial \mathbf{N}}{\partial x} \right) + \frac{\partial \mathbf{A}}{\partial x} \mathbf{N} + \frac{\partial \mathbf{S}}{\partial x} \dots\dots\dots(\text{A5.2})$$

Equation A5.2 has the same form and the same matrix \mathbf{A} as equation A5.1, but now the source term \mathbf{S} is replaced by \mathbf{T} defined in equation A5.3.

$$\mathbf{T} = \frac{\partial \mathbf{A}}{\partial x} \mathbf{N} + \frac{\partial \mathbf{S}}{\partial x} \dots\dots\dots(\text{A5.3})$$

Thus in addition to calculating N_i in the inventory equations, a similar method is used to calculate the sensitivity coefficients defined in equations A5.4.

$$S(N_i; x) = \frac{x}{N_i} \frac{\partial N_i}{\partial x} \dots\dots\dots(\text{A5.4})$$

Appendix 6 - Data libraries

FISPACT requires connection to several data libraries before it can be used to calculate inventories. While any libraries in the correct format could be used, the development of FISPACT over the last few years has run in parallel with the development of the European Activation File and this library is the recommended source of cross section data. Together FISPACT and EAF make up the European Activation System (EASY) which is a complete package tailored for fusion applications. The following libraries are required:

- Cross section data for neutron induced reactions
- Uncertainty data for neutron induced reactions
- Decay data
- Fission yield data
- Biological hazard data
- Legal transport data
- Clearance data
- Gamma absorption data
- Charged particle ranges in materials
- Emitted particle spectral data (from neutron induced reactions)
- Charged particle cross section data

The last three libraries are only required if sequential charged particle effects are included. All the current libraries are described in more detail below.

EAF_XS-2005

EAF_XS is the point-wise cross section library. Data on 62,637 cross sections on 775 targets are held in a modified ENDF/B format. The basic criterion used to decide which nuclides to include as targets is that all nuclides with a half-life of greater than 0.5 day have cross section data. In the case of capture and fission cross sections the point-wise file has been processed from an evaluated file using NJOY¹⁴ to reconstruct the resonance region from resonance parameters. No self-shielding is included and the temperature for Doppler broadening is

300K. This library is available to users, but before it can be used by FISPACT it is necessary to process it into a particular group cross section format.

Reference 15 documents the EAF-2005 cross section library. There is no printed report on the capture cross sections for EAF-2005; however, reference 16 gives data for EAF-97, while reference 17 gives the complete listing of the EAF-99 REPORT file.

EAF_GXS-2005

Eleven group cross section libraries are available that can be used as input to FISPACT. The group boundaries of the WIMS (69), GAM-II (100), XMAS (172), VITAMIN-J (175), VITAMIN-J+ (211), TRIPOLI (315) and TRIPOLI+ (351) formats are listed in Appendix 1, where details of the micro-flux weighting spectra are also given. Note that three choices of weighting spectra are available for the TRIPOLI format. This is necessary because of the very different neutron spectra found in fission and fusion applications; in addition a flat-weighting library is available for other applications. Two choices of weighting spectra are available for the XMAS format: WIMS weighting and a flat-weighting. Two choices of weighting spectra are available for the VITAMIN-J format: standard VITAMIN-J weighting and a flat-weighting. A single weighting spectrum is available for WIMS, GAM-II, VITAMIN-J+ and TRIPOLI+. WIMS, XMAS and TRIPOLI are appropriate for fission applications, GAM-II, TRIPOLI and VITAMIN-J are appropriate for fusion applications, while VITAMIN-J+ and TRIPOLI+ are appropriate for IFMIF. For other applications, such as neutron sources, flat-weighting should be used.

EAF_UN-2005

A unique feature among activation libraries is the inclusion of an uncertainty file, EAF_UN, containing data for all cross sections. Reference 18 describes the uncertainty data for EAF 3.1 while reference 15 describes the modifications made for EAF-2005. The uncertainty data are very simplified, with no

covariance information; however the file enables FISPACT to give broad-brush estimates of uncertainties for fusion applications.

EAF_DEC-2005

In addition to cross sections the other basic quantities required by an inventory code are information on the decay properties (such as half-life) of all the nuclides considered. These data are available in the various evaluated decay data libraries. FISPACT is able to read the data directly in ENDF/B-V or -VI format; it requires no pre-processing to be done. EAF_DEC-2005 is based primarily on the JEF-2.2 radioactive decay data library¹⁹, with additional data from recent UK evaluations. However, not all of the 2192 nuclides that are needed are included in such sources. For these nuclides data are taken from sources such as Brown and Firestone²⁰ and ENDF/B-VI format files are constructed. Reference 21 documents the EAF_DEC-2005 library.

Care has been taken to ensure that EAF_XS and EAF_DEC are compatible. All nuclides (including isomeric states) that can be formed from the various reactions in EAF_XS are included so long as their half-lives are greater than 1 second. Some nuclides with shorter half-lives are included where it is felt that they are of particular importance. Short-lived (< 1 s) isomers which return to the ground state by an isomeric transition have no impact on activation calculations and most of these have been ignored.

EAF_FIS-2005

FISPACT requires fission yield data if actinides are included in the input materials. EAF_FIS is taken completely from the JEF-2.2 fission yield library and FISPACT reads the file (in ENDF/B-VI) format with no pre-processing. Only 19 of the 88 nuclides in EAF_XS which have fission cross sections have any fission yield data in JEF-2.2 at relevant energies. For the remainder a neighbouring fission yield is used. The file connected to stream 8 (see Table 2) contains these associations.

EAF_HAZ-2005

Activity is one quantity used to judge the potential hazard of an irradiated material. However, activity takes no account of the biological impact on human beings. To enable FISPACT to give some indication of the potential *biological* hazard of irradiated materials, a library of dose coefficients has been assembled which determine the dose received by a man over his lifetime (50 years) following the ingestion or inhalation of 1 Bq of activity of a particular radionuclide.

The basic sources for these data are reports published by ICRP²² and the NRPB²³. However, these sources primarily cover radionuclides generated by the fission power producing community and consequently only cover some of the nuclides that can arise in fusion applications. In order to extend the range of nuclides to all those in EAF_DEC it has been necessary to use an approximate method. Reference 24 describes how available data for an element are used with decay data for a nuclide to derive Committed Effective Doses per unit uptake for ingestion and inhalation for the nuclides with no data. In total 1134 nuclides have had data calculated approximately. Reference 25 documents the EAF_HAZ-2005 library.

EAF_A2-2005

Transport of radioactive material from place to place is governed by regulations set up by the IAEA. Reference 26 gives details of A_2 values for certain radionuclides. Using these values it is possible to work out how much of a particular mixture of radioactive materials can be packed into a type of container and safely transported. Data from this reference for the nuclides listed are transferred to EAF_A2, with the default prescription given in reference 26 used for all radionuclides not explicitly listed. Reference 25 documents the EAF_A2-2005 library. FISPACT can use these data to show the A_2 limit for individual nuclides and the effective A_2 value for the irradiated material.

EAF_CLEAR-2005

Disposal of radioactive material in special repositories is expensive. Regulations exist which determine activity levels for nuclides such that materials can be 'cleared' or disposed of as if they are not radioactive. Clearance data is being investigated by the IAEA and recommendations are available. Reference 27 gives details of suggested clearance values for certain radionuclides, while an earlier report (reference 28) gives a formula that allows values for other nuclides to be calculated. Data from these references for the nuclides listed are transferred to EAF_CLEAR, with the default prescription used for all radionuclides not explicitly listed. Reference 25 documents the EAF_CLEAR-2005 library. FISPACT can use these data to show the clearance index for individual nuclides and for the irradiated material.

EAF_STOP-2005

EAF_STOP is one of the data libraries assembled by UKAEA Culham to enable the effect of sequential charged particle reactions (SCPR) to be investigated. The data were generated using the code SRIM-2003²⁹. Details of this effect are given in Appendix 14, but the FZK report detailing the data used for previous EAF versions (reference 30) should be consulted for further details.

EAF_STOP contains the differential ranges for p, d, h (³He), t and α in all the elements from H to U. The term differential range at a particular energy defines the distance travelled by the particle in the material in losing 1 MeV of energy. Data are given from 0 to 60 MeV.

EAF_SPEC-2005

EAF_XS contains the cross section data for (n,x) reactions, while EAF_SPEC describes the energy distribution of the charged particles emitted in these reactions. This is the second of the libraries required for calculations with SCPR. The data are calculated by a theoretical model code (TALYS³¹) due to

the lack of experimental data. Thirty-nine input neutron energies are used and the outgoing charged particles are in 1 MeV bins covering the energy range 0-60 MeV.

EAF_XN-2005

EAF_XN describes the cross sections of p, d, h, t and α particles on 775 targets. Ten reactions types are considered: (p,n), (d,n), (t,n), (h,n), (α ,n), (p,2n), (d,2n), (t,2n), (h,2n) and (α ,2n). This is the third of the libraries required for calculations with SCPR. The data are calculated by a theoretical model code (TALYS³¹) due to the lack of experimental data. The data are given at 1 MeV intervals over the energy range 0-60 MeV.

EAF_ABS-2005

EAF_ABS-2005 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 Jarvis³² 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,

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

where

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

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,

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

where

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

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,

$$Z = \sum_j Z_j n_j \dots\dots\dots(A7.3)$$

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-2005 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.

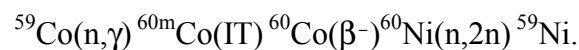
Nuclide	Half-life (y)	Parent	Branching ratio (%)
¹⁰ Be	1.60 10 ⁶		
³² P	330.0	³² Si	100.0
³⁶ Cl	3.07 10 ⁵		
³⁹ Ar	269.0		
⁴⁰ K	1.28 10 ⁹		
⁴² Ar	33.00		
⁴² K	33.00	⁴² Ar	100.0
⁸⁵ Kr	10.73		
⁸⁹ Sr	0.14		
⁹⁰ Sr	28.87		
⁹⁰ Y	28.87	⁹⁰ Sr	100.0
⁹¹ Y	0.16		
^{95m} Nb	0.18	⁹⁵ Zr	1.1
¹⁰⁶ Rh	1.01	¹⁰⁶ Ru	100.0
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
¹⁷⁰ Tm	0.35		
¹⁸⁶ Re	2.00 10 ⁵	^{186m} Re	100.0
¹⁸⁸ Re	0.19	¹⁸⁸ W	100.0
¹⁹²ⁿ Ir	241.0		
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	7365.0	²⁴³ Am	100.0
²⁴³ Pu	1.60 10 ⁷	²⁴⁷ Cm	100.0
²⁴² Am	141.0	^{242m} Am	99.6
²⁴⁵ Am	0.88	²⁴⁹ Bk	1.4 10 ⁻³
²⁵¹ Cf	898.0		
²⁵⁴ Es	0.75		

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 :



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.

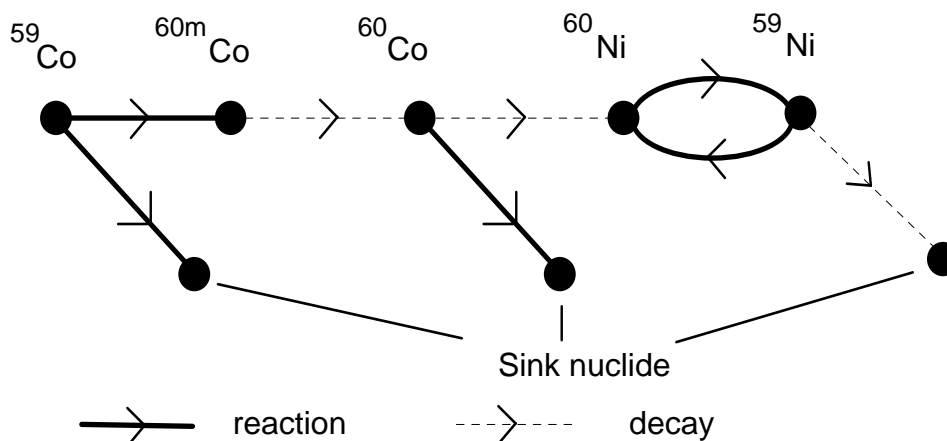
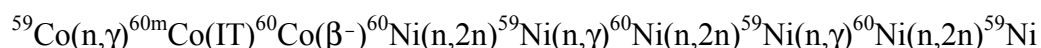


Figure A8.1. Diagram of a pathway from ^{59}Co to ^{59}Ni .

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 link 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 $^{59}\text{Ni}(n,\gamma)^{60}\text{Ni}$ 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 $^{60\text{m}}\text{Co}$ 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.



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.

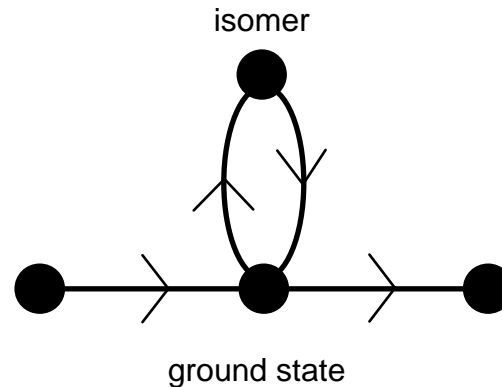


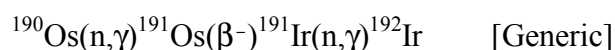
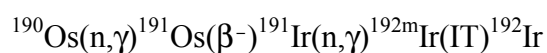
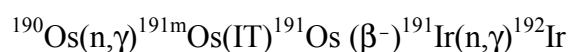
Figure A8.2. Detail of a diagram for a pathway containing an isomer loop.

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.



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. See Appendix 20 for more discussion of non-steady irradiations.

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-2005 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-2005

Since EAF_XS-2005 contains data up to an energy of 60 MeV, all non-threshold reactions (capture, fission and some (n,p), (n, α) reactions) have 4 rather than 3 uncertainty values in the file. The energy regions are defined in Table A9.1. Threshold reactions contain 2 uncertainty values if the threshold is below 20 MeV.

Table A9.1. Definition of uncertainty energy regions.

Low energy region	Medium energy region	High energy region	Extended energy region
$1.0 \cdot 10^{-5} \text{ eV} - E_V$	$E_V - E_H$	$E_H - 20 \text{ MeV}$	20 – 60 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	Extended energy region
Capture	10	2	1.5	1.5
Fission	5	2	2.0	2.0

In EAF-2005 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 that 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 eight radiological quantities (activity, heating, γ dose rate, potential ingestion hazard, potential inhalation hazard, clearance index and beta and gamma heat outputs) 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 noted³³ that the quantities $\log(\sigma_{\text{expt}} / \sigma_{\text{calc}})$

were approximately normally distributed and that the best representation of error limits on σ_{calc} were $\sigma_{\text{calc}} f$ 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.

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

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.

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

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

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

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

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

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.

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

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.

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

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.

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

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

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

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.

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

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

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

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

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

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

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

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

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

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

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

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

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

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 that 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

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

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

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

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 34.

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.

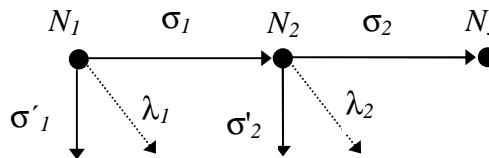


Figure A9.1. A 2-link pathway, consisting of reactions only.

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.

$$\frac{dN_1}{dt} = -\lambda_1 N_1 - (\sigma_1 + \sigma'_1)\phi N_1 = -\Lambda_1 N_1 \dots\dots\dots(A9.19)$$

The solution is given in equation A9.20.

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

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

$$\frac{dN_2}{dt} = -\lambda_2 N_2 - (\sigma_2 + \sigma'_2)\phi N_2 + \sigma_1 \phi N_1 = -\Lambda_2 N_2 + \sigma_1 \phi N_{10} e^{-\Lambda_1 t} \dots\dots\dots(A9.21)$$

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

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

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

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

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

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

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

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

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 : $10^{15} \text{ cm}^{-2}\text{s}^{-1}$, 10^{-25} cm^2 and 10^8 s . When a nuclide has a half-life of 1 s then $\lambda = 0.693$, $\lambda \gg \phi(\sigma + \sigma')$ and $\lambda \gg T^{-1}$. When a nuclide has a half-life of 1000 y then $\lambda = 2.196 \cdot 10^{-11}$, $\lambda \ll \phi(\sigma + \sigma')$ and $\phi(\sigma + \sigma') \ll T^{-1}$.

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

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

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

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

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 .

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

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.

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

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.

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

$$\begin{aligned} p\hat{N}_{n+1} &= -\Lambda_{n+1}\hat{N}_{n+1} + \sigma_n \phi \hat{N}_n \\ \Rightarrow \hat{N}_{n+1}(p) &= \frac{\sigma_n \phi}{p + \Lambda_{n+1}} \hat{N}_n(p) \dots\dots\dots (A9.31) \end{aligned}$$

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

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

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

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

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

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

In order to obtain the expression for $N_{n+1}(t)$ it is necessary to use the inverse Laplace transform that 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.

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

The value of c can be set to zero, since all poles in the transform are for $\text{Real}(z) < 0$ (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.

$$R(-\Lambda_j) = \frac{\phi^n N_{10} \prod_{i=1}^n \sigma_i \cdot e^{-\Lambda_j t}}{\prod_{i=1}^{n+1} (\Lambda_i - \Lambda_j)} \dots\dots\dots(A9.36)$$

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

$$\sum R = \phi^n N_{10} \prod_{i=1}^n \sigma_i \cdot \sum_{j=1}^{n+1} \left(\frac{e^{-\Lambda_j t}}{\prod_{i=1}^{n+1} (\Lambda_i - \Lambda_j)} \right) \dots\dots\dots(A9.37)$$

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.

$$N_{n+1}(t) = (-1)^n N_{10} \phi^n \prod_{i=1}^n \sigma_i \cdot \sum_{j=1}^{n+1} \left(\frac{e^{-\Lambda_j t}}{\prod_{i=1}^{n+1} (\Lambda_j - \Lambda_i)} \right) \dots\dots\dots(A9.38)$$

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.

$$N_{n+2}(t) = (-1)^{n+1} N_{10} \phi^{n+1} \prod_{i=1}^{n+1} \sigma_i \cdot \sum_{j=1}^{n+1} \left(\frac{(e^{-\Lambda_j t} - 1)/\Lambda_j}{\prod_{i=1}^{n+1} (\Lambda_j - \Lambda_i)} \right) \dots\dots\dots(A9.39)$$

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.

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

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

$$N_{n+1}(t) = (-1)^{n-1} N_{10} \phi^n \prod_{i=1}^n \sigma_i \cdot e^{-\Lambda_{n+1} t} \sum_{j=1}^n \left(\int e^{-(\Lambda_j - \Lambda_{n+1}) t} dt \right) / \prod_{i=1}^n (\Lambda_j - \Lambda_i) \dots\dots\dots(A9.41)$$

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

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

$$N_{n+1}(t) = (-1)^n N_{10} \phi^n \prod_{i=1}^n \sigma_i \cdot \left[\sum_{j=1}^n (e^{-\Lambda_j t} / \prod_{i=1}^{n+1} (\Lambda_j - \Lambda_i)) - e^{-\Lambda_{n+1} t} \sum_{j=1}^n (1 / \prod_{i=1}^{n+1} (\Lambda_j - \Lambda_i)) \right] \dots\dots\dots(A9.43)$$

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.

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

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.

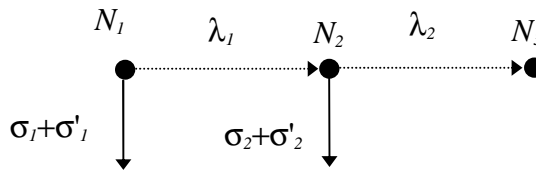


Figure A9.2. A 2-link pathway, consisting of decays only.

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

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

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

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

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

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.

$$N_{n+2}(t) = (-1)^{n+1} N_{10} \prod_{i=1}^{n+1} \lambda_i \cdot \sum_{j=1}^{n+1} \left((e^{-\Lambda_j t} - 1) / \Lambda_j \prod_{i=1}^{n+1} (\Lambda_j - \Lambda_i) \right) \dots\dots\dots (A9.48)$$

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 $\Lambda_i t \ll 1$ and equation A9.28 can be simplified to give equation A9.49.

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

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 $n \geq 2$.

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

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

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.

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

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

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

This is easily solved to give equation A9.54.

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

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.

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

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.

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

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

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 nor 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.

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

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.

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

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	$n / (\lambda_{\text{final}} t)$

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 34 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.

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

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.

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

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 , E_H and 20 MeV) and values of Δ^2 for each energy range. In the case of threshold reactions with threshold energy > 20 MeV only one energy range is considered (threshold - 60 MeV) and so the shape of the neutron flux is unimportant. But for other threshold reactions two values are given, while for non-threshold reactions four values are given and these must be combined taking into account the shape of the neutron spectrum.

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

$$\bar{\sigma} = \frac{\sum_i \sigma_i \phi_i}{\sum_i \phi_i} \dots\dots\dots(A9.62)$$

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.

$$\epsilon_i = \frac{\sigma_i \phi_i}{\sum_i \phi_i} \Delta_i \dots\dots\dots(A9.63)$$

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.

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

where

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

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.

$$\varepsilon^2 = \sum_I \varepsilon_I^2 \dots\dots\dots (A9.65)$$

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

$$\Delta = \varepsilon / \bar{\sigma} \dots\dots\dots (A9.66)$$

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

$$\bar{\sigma}_I = \sum_{i \in S_I} \sigma_i \phi_i / \sum_i \phi_i \dots\dots\dots (A9.67)$$

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

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

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, 211, 315 or 351 required for N2COLL
[COLLAPSE]

The neutron spectrum **MUST** be in 69, 100, 172, 175, 211, 315 or 351 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 <CNVTEXT>

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 <COL211>

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?

Daughter nuclide of reaction not in library <COL351>

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.

ISPLIT can takes values 0 or 1 [SPLIT]
Additional summary table is 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 <CNVTEXT>
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.

LNNM can take values of 175 or 211 [SEQNUMBER]

Data with either 175 or 211 groups **MUST** be used.

M or N required for isomer [FUEL]

Specify isomer by 'M' for first or 'N' for second.

MONIT can take values 0 or 1 [MONITOR]

The output of code words is either on or off.

NDSTRC can only be 69, 100, 172, 175, 211, 315 or 351 [GRPCONVERT]

The output group structure **MUST** be one of the 7 standard types.

NEAFVN can take values 2, 3, 4, 5 or 6 [EAFVERSION]

Only versions 2, 3, 4, 5 or 6 of EAF are considered.

NESTRC can take 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 ISPLIT [SPLIT]

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 LNNM [SEQNUMBER]

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 <COL211>

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 of reaction not in library <COL351>

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 dominant nuclides, JNUMB > 200. <OUTERR>
The run requires a total of more than 200 dominant nuclides. Either simplify the run or contact UKAEA for assistance.

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 < COL211>

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?

Uncertainty data not consistent with cross section data < COL351>

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 35.

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 35 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.

$$\sigma_{x,C}^{pseudo} = \frac{1}{\Phi_n} \sum_{k=1}^{24} \sigma_{x,C}(E_{x_k}) \sum_A \sum_{i=1}^{175} N_A \phi_n(E_{n_i}) \sigma_{n,x}(E_{n_i}) \sum_{j=k}^{24} f_{n,x}(E_{n_i}, E_{x_j}) \Delta E_{x_j} \Delta R_x(E_{x_k}) \dots\dots\dots (A12.1)$$

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

$\sigma_{x,C}(E_{xk})$	is the production cross section of nuclide C in the k th energy group
$f_{n,x}(E_{ni}, E_{xk})$	is the normalised charged particle spectrum for neutron energy in the i th energy group and in the k th outgoing energy step
$\Delta R_x(E_{xk})$	is the differential thickness of the surrounding material for charged particle of starting energy E_{xk}

Note that in equation A12.1 sums are over 175 groups, since version 2005, 211 group data can be used as well as 175.

In the original work of KfK a separate code PCROSS³⁶ 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-IV PC running Windows 98, Windows NT 4.0, Windows 2000 or Windows XP.
- UNIX workstation

The details for each system are given below.

Personal computer

FISPACT is supplied to users on a CD ROM. FISPACT-2005 will run under Windows 98, Windows NT4.0, Windows 2000 or Windows XP. 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 EASY User Interface (see Appendix 15) by running `d:\easy05ui\setup`.
3. Install the Install_EASY application by running `d:\install_easy\setup`.
4. Run Install_EASY by clicking the Start | Programs | Install EASY menu item. Follow the onscreen instructions including the input of personal details.

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

1. Open the EASY-2005 User Interface by clicking the Start | Programs | EASY-2005 User Interface menu item.
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-2005 code package, including the inventory code FISPACT-2005 and the EAF-2005 libraries, is available on the following media:

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

EASY-2005 requires a minimum of 500 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, Solaris, HP UX, Silicon Graphics IRIX, 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 6
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 6
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 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

```

Test26

```

NOHEAD
AINP
FISPACT
* Aluminium
MASS 1.57E-05 1
AL 100.0
MIND 1
SPLIT 1
UNCERT 2
UNCTYPE 3
DOMINANT 100.0
HAZA
HALF
CLEAR
LEVEL 100 1
FLUX 4.725E+08
TIME 600 ATOMS
LEVEL 20 1
FLUX 0.0
ZERO
TIME 123 ATOMS
TIME 29 ATOMS
TIME 154 ATOMS
TIME 30 ATOMS
TIME 269 ATOMS
TIME 30 ATOMS
TIME 271 ATOMS
TIME 30 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 6
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 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

```

Test81 - Test86 *Identical to Test11 - Test16***Test87**

```

NOHEAD
EAFV 6
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
SEQN 211
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

```


Test88 – Test90 *Identical to Test18 – Test20*

Test95

```

NOHEAD
MONITOR 1
AINP
FISPACT
* IRRADIATION B4C LMJ FW 1mm thick
DENSITY 2.7
MASS 848.23 2
B 78.57
C 21.43
SEQN 211
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 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

```

Test96 *Identical to Test26*

Test100-Test104 *Identical to Test70-Test74*

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, 26
211 groups	81 - 90, 95, 96
315 groups	70 - 74
351 groups	100 - 104

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 four platforms.

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

	AMD Athlon (2800+) [a]	Pentium III (800 MHz) [b]	XEON (3.2 GHz) [c]	Pentium IV (2.66 GHz) [d]
Collapse [e]	3	4	2	2
Write [f]	6	7	2	3
Write [g]	1	1	1	1
Printlib [h]	1	1	1	1
Test 1	2	8	1	2
Test 2	2	7	1	2
Test 3	2	5	1	1
Test 4	2	7	1	1
Test 5	1	1	1	1
Test 6	2	5	1	1
Test 7	7	14	3	4
Test 8	1	4	1	1
Test 9	3	7	1	1
Test 10	1	3	1	1
Test 11	3	7	1	2
Test 12	6	14	3	4
Test 13	7	18	4	4
Test 14	2	7	2	2
Test 15	3	7	2	2
Test 16	22	35	9	12
Test 17	17	29	6	15
Test 18	6	16	3	4
Test 19	2	5	1	1
Test 20	2	7	2	2
Test 21	14	28	6	8
Test 22	24	74	14	16
Test 23	13	24	7	8

	AMD Athlon (2800+) [a]	Pentium III (800 MHz) [b]	XEON (3.2 GHz) [c]	Pentium IV (2.66 GHz) [d]
Test 24	13	24	6	6
Test 25	173	248	59	150
Test 26	2	7	1	1
Test 31	15	27	6	8
Test 32	24	74	14	17
Test 41	3	7	1	2
Test 42	7	14	4	4
Test 43	9	22	4	5
Test 44	3	7	1	1
Test 45	3	7	2	2
Test 51	14	29	6	7
Test 52	24	75	14	17
Test 60	9	11	3	4
Test 61	18	25	7	9
Test 70	3	8	2	2
Test 71	76	234	37	45
Test 72	283	834	143	170
Test 73	11	33	5	6
Test 74	7	23	4	4
Test 81	5	14	2	2
Test 82	9	18	4	5
Test 83	12	30	4	6
Test 84	3	11	2	2
Test 85	4	14	2	2
Test 86	34	85	12	23
Test 87	33	73	11	23
Test 88	11	30	5	6
Test 89	3	5	2	2
Test 90	4	14	2	3
Test 95	223	193	70	194
Test 96	4	10	2	2
Test 100	3	9	2	2
Test 101	162	415	75	90
Test 102	109	278	50	61
Test 103	14	39	6	7
Test 104	51	164	20	24

Notes

- [a] GNU g77 FORTRAN v3.3.3 running under Redhat linux.
 - [b] Salford FTN77 for Win32 FORTRAN V4.02, running in a Windows NT4.0 command window in the foreground.
 - [c] Salford FTN77 for Win32 FORTRAN V4.02, running in a Windows XP command window in the foreground.
 - [d] Salford FTN77 FORTRAN V4.02, running in a Windows 2000 command window in the background.
 - [e] 100-group library.
 - [f] Using **TAPA** option.
 - [g] Using **ARRAY** option.
 - [h] With *PRINT* parameter set to 2.
- All runs performed with FISPACT-2005 and EAF-2005.

Appendix 15 – EASY User Interface

Introduction

The EASY User Interface, an interactive application, was originally developed (it was called FISPACT Windows Interface) 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 EASY User 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 and 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.
- EASY decay data can be viewed interactively.
- EASY multi-group cross section data can be viewed interactively.
- Neutron spectra used by FISPACT can be stored and plotted.
- 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 an icon for one of the various child windows that can be opened - an **INPUT** file is shown. Behind the summary window a part of a graph window is visible. As with other Windows applications there is a menubar and toolbar (containing fifteen buttons giving the user quick access to the most important features) at the top of the window. Details of the various features are given below.

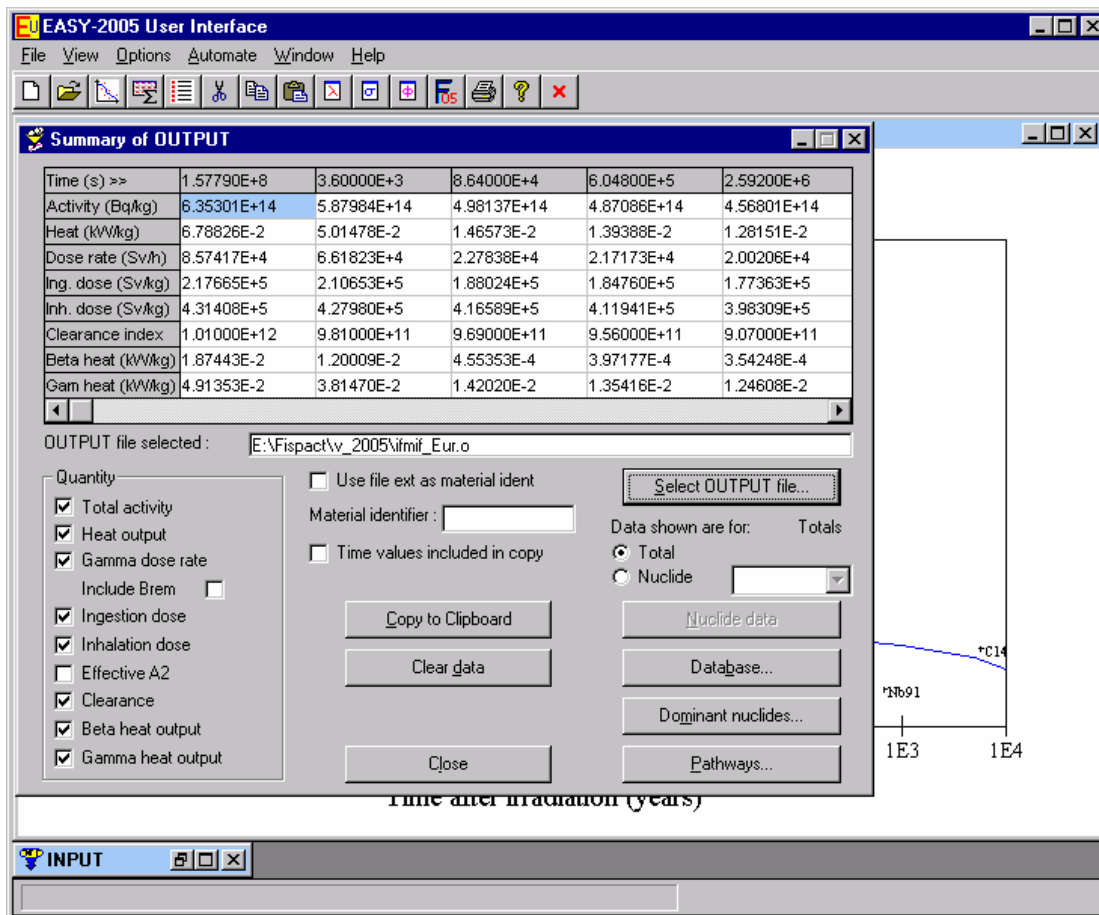


Figure A15.1. The main window of the EASY User Interface.

Input files

A FISPACT run is specified by means of the **INPUT** file. The EASY User 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 EASY User 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 mSv h^{-1}) and ‘hands-on’ ($25 \text{ } \mu\text{Sv h}^{-1}$) 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 Eurofer steel plotted. The uncertainty band and common times options have been selected.

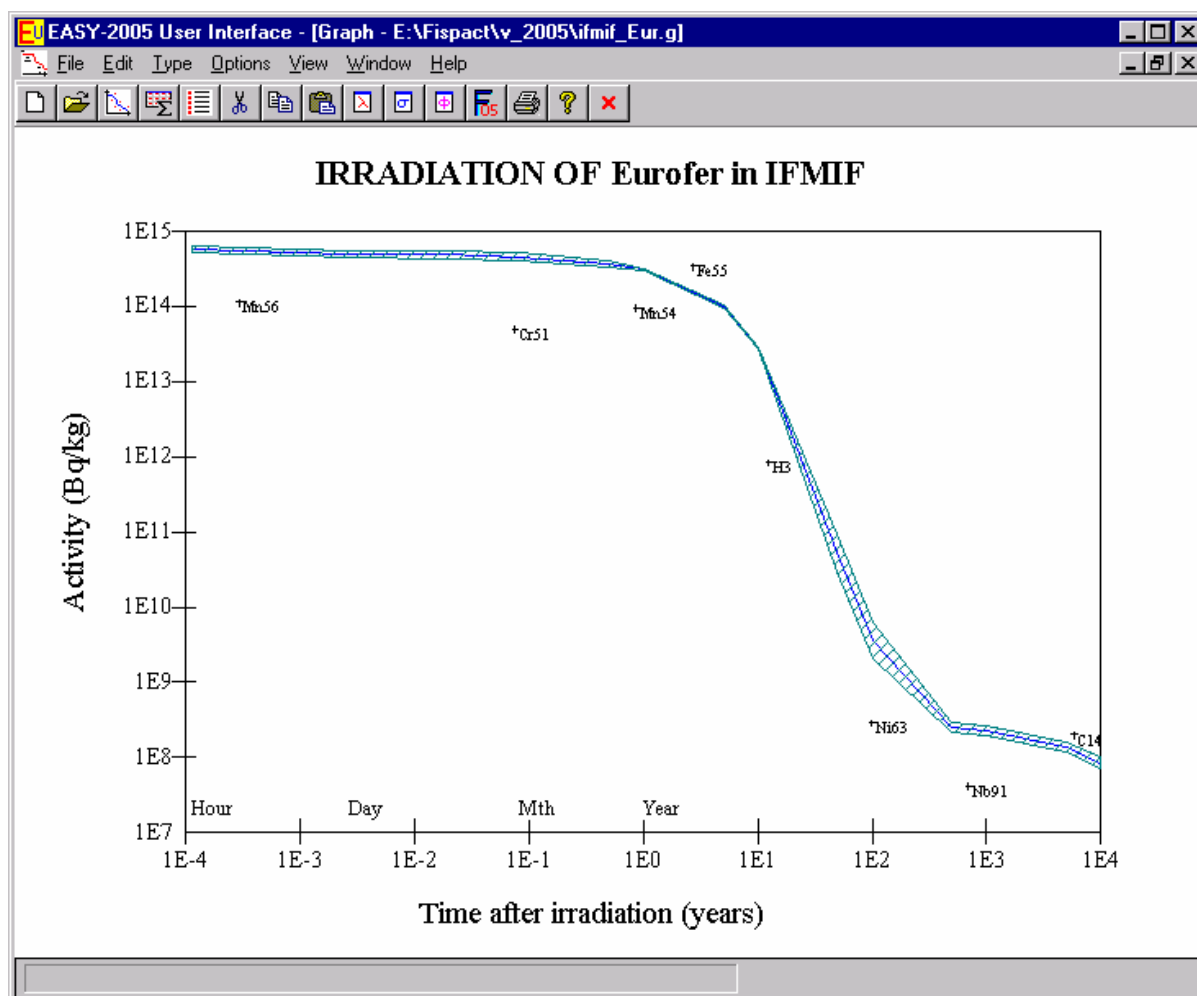


Figure A15.2. The graph window of the EASY User Interface.

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 - 2000 kB) and extracting information can be time consuming using the **OUTPUT** file viewer. The EASY User 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 EASY User 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 A15.1 shows a typical summary window, while Figure A15.3 shows a summary of the dominant nuclides for activity.

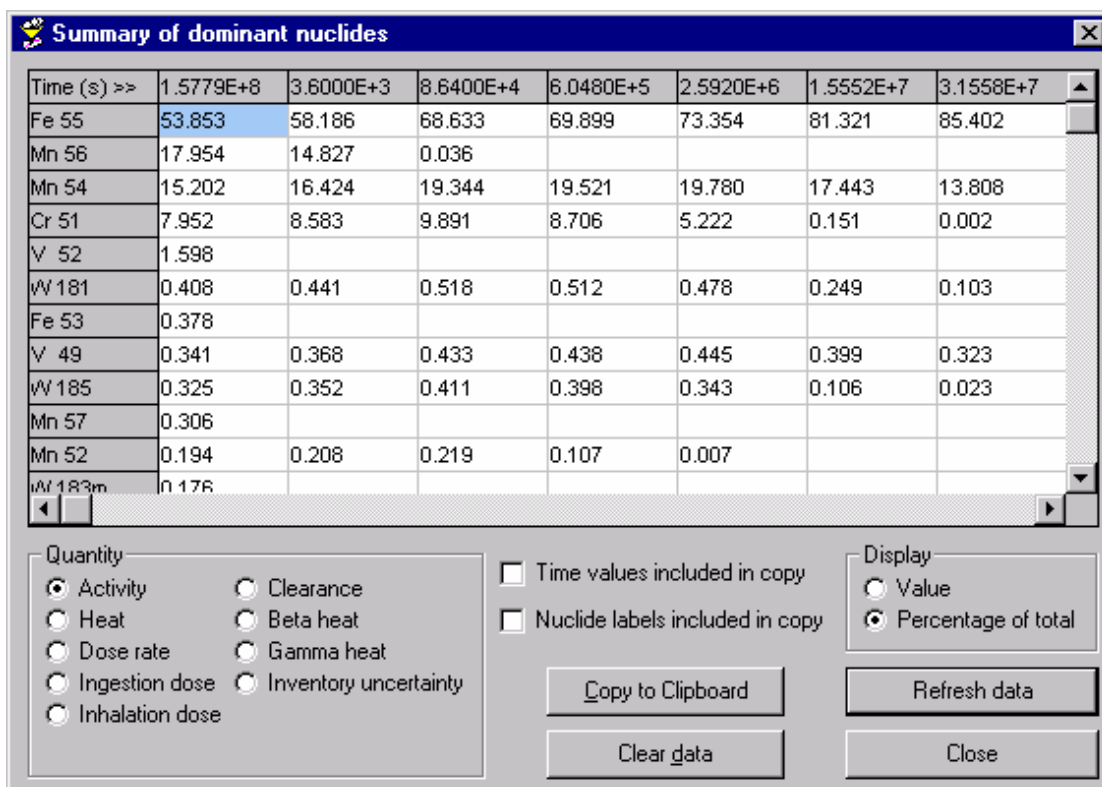


Figure A15.3. The summary of dominant nuclides window.

Running FISPACT

FISPACT can be run directly from the EASY User 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.

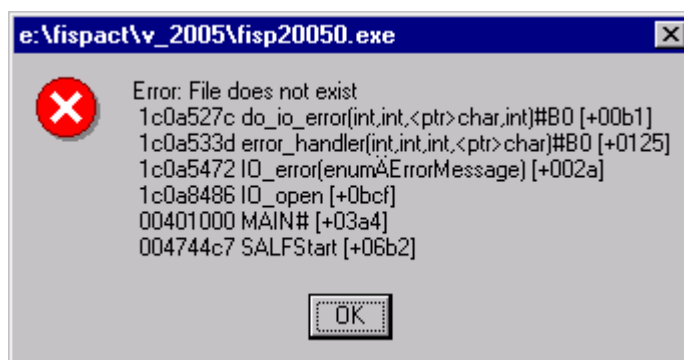


Figure A15.4. An error box displayed when a FISPACT run ‘crashes’.

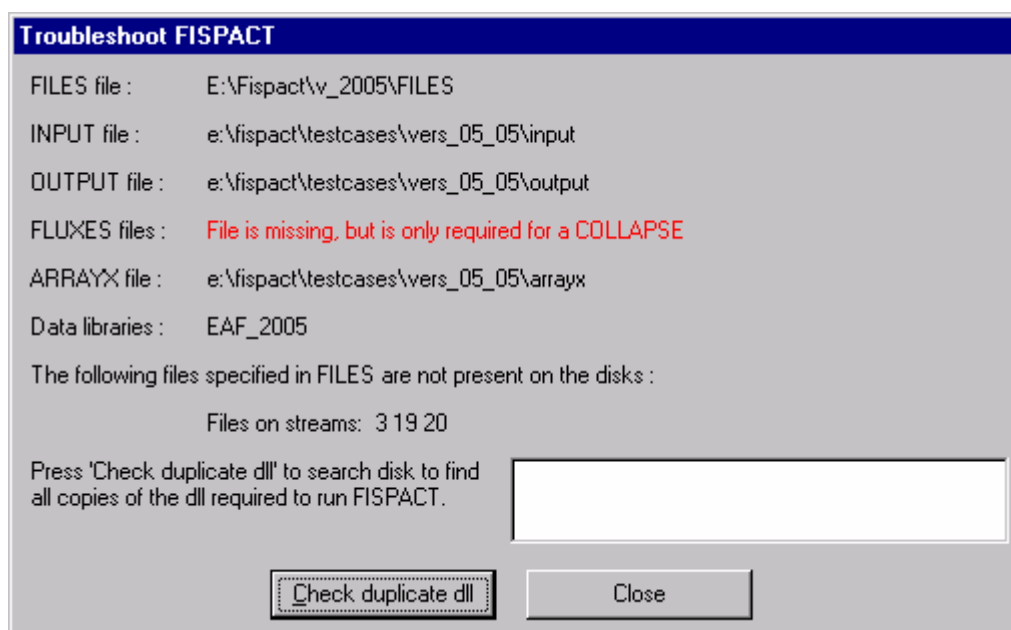


Figure A15.5. The Troubleshoot FISPACT dialog.

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 files connected to streams 3 (arbitrary spectrum), 19 (cross section library) and 20 (neutron spectrum) are missing. If files such as the **INPUT** file are missing then FISPACT will terminated abnormally.

EAF decay data

A new feature in the EASY User Interface since version 2001 is the ability to view EAF decay data. Clicking on the ninth toolbar button in the main window (Figure A15.1) displays the EAF-2005 decay data window shown in Figure A15.6. The

required nuclide is entered in the Nuclide text box and all the decay data from EAF_DEC-2005 are displayed as well as biological hazard, transport and clearance data. Note that the units of half-life and energy can be changed to give convenient numbers. Clicking on the Photon lines tab enables the γ - and X-ray lines to be displayed, and these can be plotted using the fourth toolbar button. The many options and facilities of this window are fully explained in the Help file.

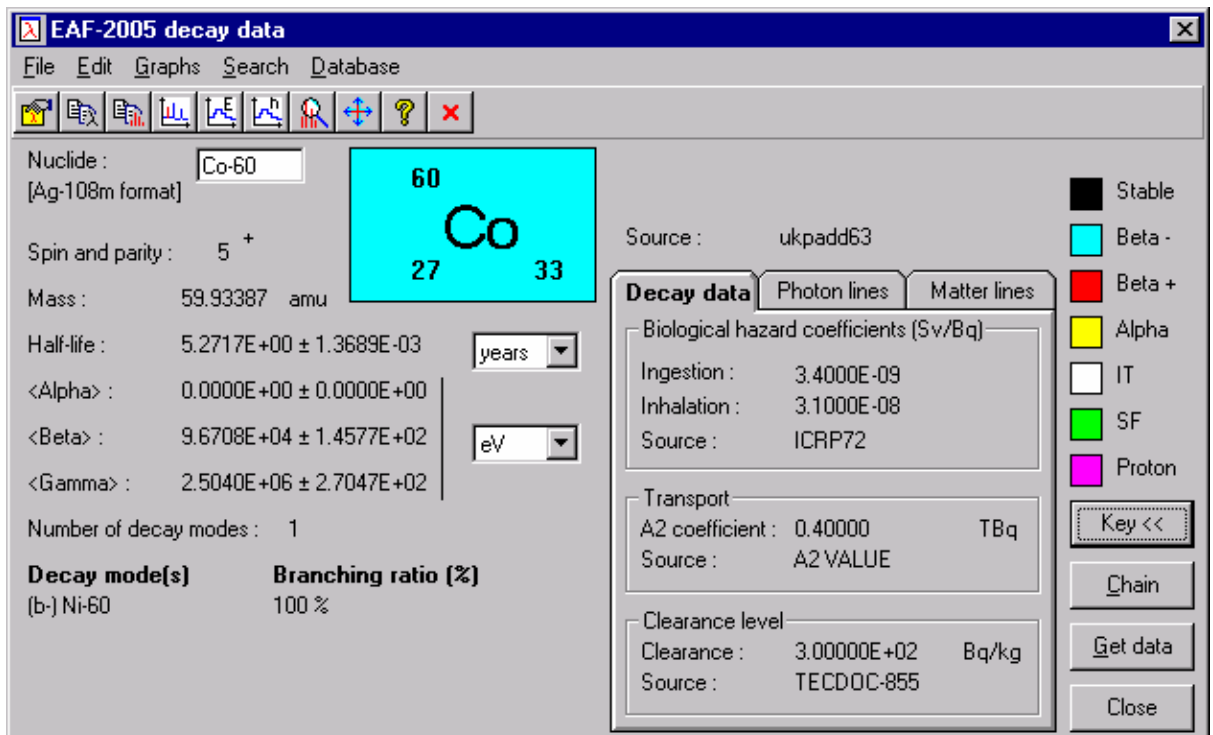


Figure A15.6. The EAF-2005 decay data window.

EAF group cross section data

Another new feature in the EASY User Interface since version 2001 is the ability to view EAF group cross section data. Clicking on the tenth toolbar button in the main window (Figure A15.1) displays the EAF-2005 group cross section data window shown in Figure A15.7. The required database is selected (one of the eleven EAF-2005 multi-group libraries), any neutron spectra of the correct structure are shown and selecting one displays the Reaction Rate graph at the bottom right of the window. A target nuclide is entered in the Target

nuclide text box and a reaction chosen and the summary values are displayed at the bottom left of the window.

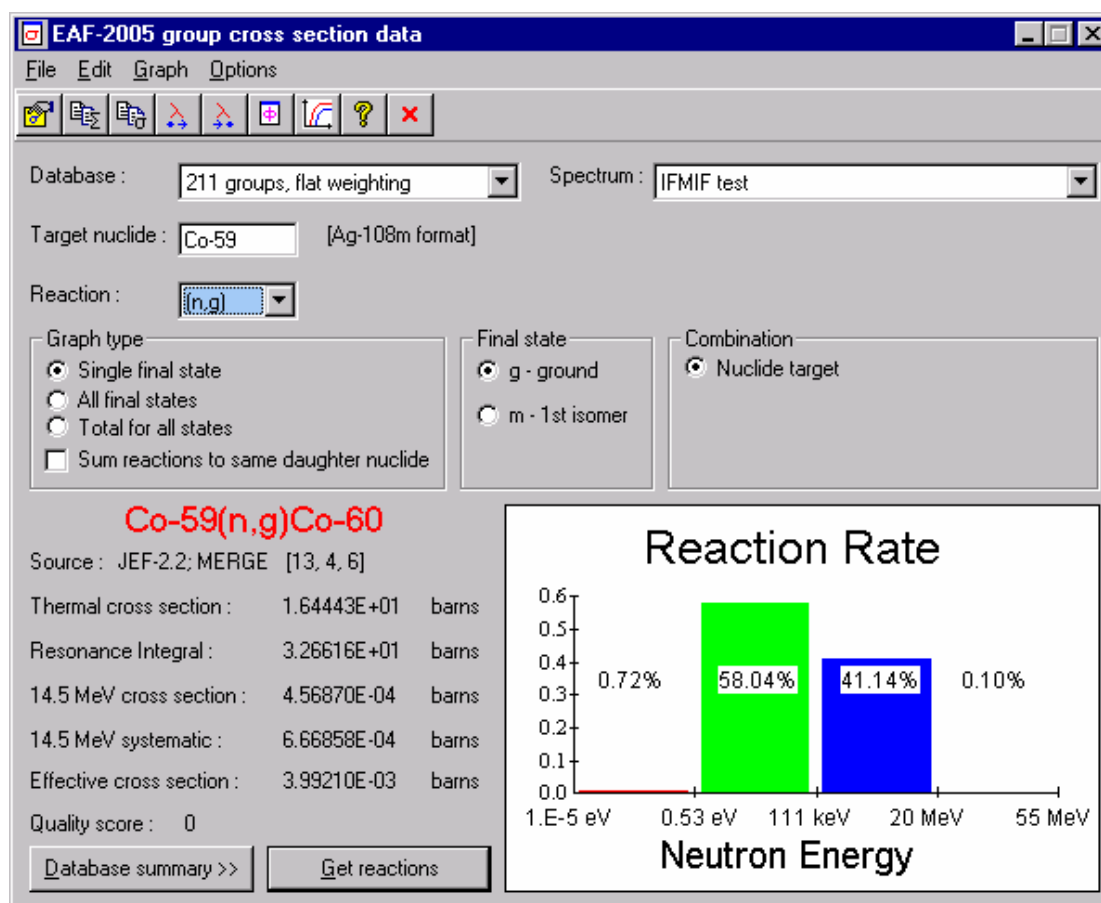


Figure A15.7. The EAF-2005 group cross section data window.

The cross section data can be plotted using the seventh toolbar button. The many options and facilities of this window are fully explained in the Help file.

Neutron spectra

Neutron spectra are central to all FISPACT calculations. The EASY User Interface enables neutron spectra to be stored, referenced and plotted. Clicking on the eleventh toolbar button in the main window (Figure A15.1) displays the Neutron spectra window shown in Figure A15.8. This displays the spectra that are stored in the database and gives information about the one selected in the list box. This spectrum can be plotted and further spectra can be added to the database (standard FISPACT **FLUXES** files are read). A spectrum can be

written out from the database in standard FISPACT format in order to carry out a FISPACT run. The spectra database thus acts as a useful repository of spectra, ensuring that they don't get 'lost'.

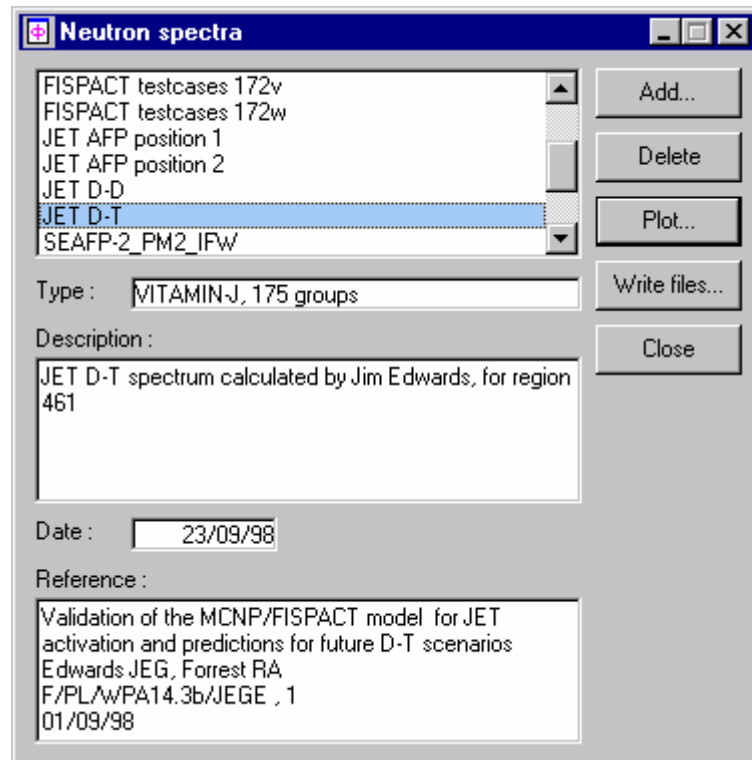


Figure A15.8. The Neutron spectra window.

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. The present document gives only a very brief introduction to the usage of the application, for full details the Help file should be used. Figure A15.9 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.

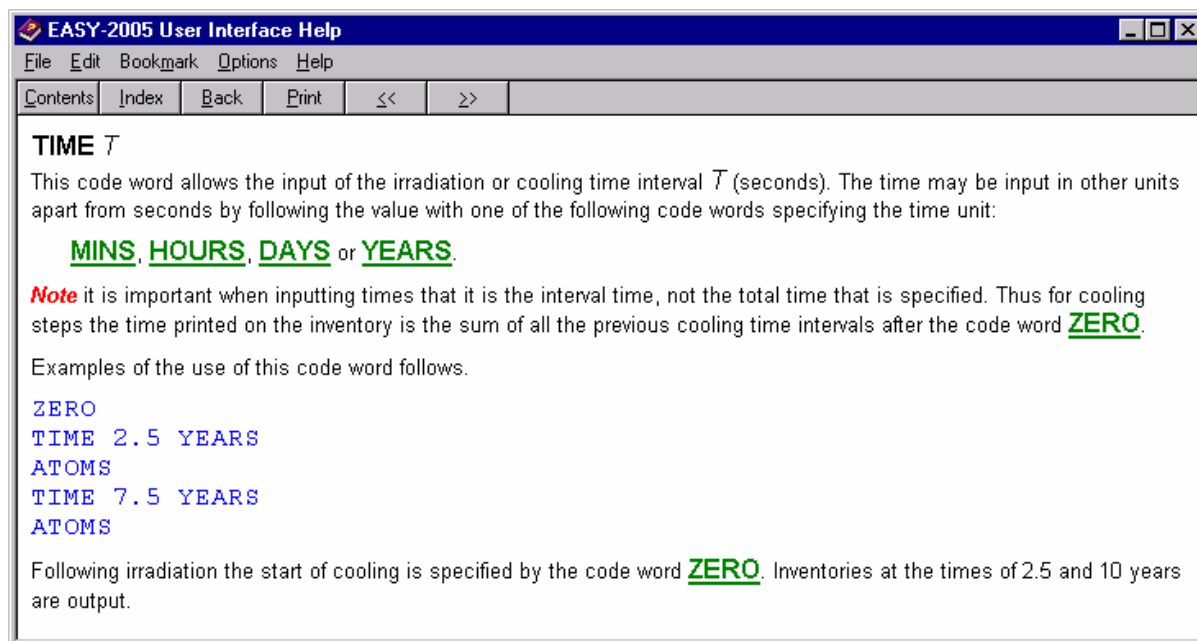


Figure A15.9. A Help topic of the EASY User Interface.

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 from references 37 and 38.

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	0.000137, 99.999863
3	6.941	0.534	6	7.59, 92.41
4	9.012182	1.848	9	100.0
5	10.811	2.34	10	19.8, 80.2
6	12.011	2.1	12	98.89, 1.11
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	20.1797	1.2015	20	90.48, 0.27, 9.25
11	22.98977	0.971	23	100.0
12	24.305	1.738	24	78.99, 10.0, 11.01
13	26.981539	2.6989	27	100.0
14	28.0855	2.33	28	92.23, 4.683, 3.087
15	30.973761	1.82	31	100.0
16	32.065	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	0.3365, 0., 0.0632, 0., 99.6003
19	39.0983	0.862	39	93.2581, 0.0117, 6.7302
20	40.078	1.55	40	96.94, 0., 0.647, 0.135, 2.09, 0., 0.004, 0., 0.187
21	44.95591	2.989	45	100.0
22	47.867	4.54	46	8.25, 7.44, 73.72, 5.41, 5.18
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	54.938049	7.44	55	100.0
26	55.845	7.874	54	5.845, 0., 91.754, 2.119, 0.282
27	58.9332	8.9	59	100.0
28	58.6934	8.902	58	68.077, 0., 26.223, 1.14, 3.634, 0., 0.926
29	63.546	8.96	63	69.17, 0., 30.83
30	65.39	7.133	64	48.63, 0., 27.9, 4.1, 18.75, 0., 0.62
31	69.723	5.904	69	60.108, 0., 39.892
32	72.64	5.323	70	20.37, 0., 27.31, 7.76, 36.73, 0., 7.83
33	74.9216	5.73	75	100.0
34	78.96	4.79	74	0.89, 0., 9.37, 7.63, 23.77, 0., 49.61, 0., 8.73

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., 2.28, 0., 11.58, 11.49, 57.0, 0., 17.3
37	85.4678	1.532	85	72.17, 0., 27.83
38	87.62	2.54	84	0.56, 0., 9.86, 7.0, 82.58
39	88.90585	4.469	89	100.0
40	91.224	6.506	90	51.45, 11.22, 17.15, 0., 17.38, 0., 2.8
41	92.90638	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	5.54, 0., 1.87, 12.76, 12.6, 17.06, 31.55, 0., 18.62
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	112.411	8.65	106	1.25, 0., 0.89, 0., 12.49, 12.80, 24.13, 12.22, 28.73, 0., 7.49
49	114.818	7.31	113	4.29, 0., 95.71
50	118.710	5.75	112	0.97, 0., 0.66, 0.34, 14.54, 7.68, 24.22, 8.59, 32.58, 0., 4.63, 0., 5.79
51	121.76	6.691	121	57.21, 0., 42.79
52	127.60	6.24	120	0.09, 0., 2.55, 0.89, 4.74, 7.07, 18.84, 0., 31.74, 0., 34.08
53	126.90447	4.93	127	100.0
54	131.293	3.0589	124	0.095, 0., 0.089, 0., 1.91, 26.4, 4.071, 21.232, 26.909, 0., 10.436, 0., 8.857
55	132.90545	1.873	133	100.0
56	137.327	3.5	130	0.106, 0., 0.101, 0., 2.417, 6.592, 7.854, 11.232, 71.698
57	138.9055	6.145	138	0.09, 99.91
58	140.115	6.770	136	0.185, 0., 0.251, 0., 88.45, 0., 11.114
59	140.90765	6.773	141	100.0
60	144.24	7.008	142	27.2, 12.2, 23.8, 8.3, 17.2, 0., 5.7, 0., 5.6
61	0.	7.264		
62	150.36	7.520	144	3.07, 0., 0., 14.99, 11.24, 13.82, 7.38, 0., 26.75, 0., 22.75
63	151.965	5.244	151	47.81, 0., 52.19
64	157.25	7.901	152	0.2, 0., 2.18, 14.8, 20.47, 15.65, 24.84, 0., 21.86
65	158.92534	8.230	159	100.0
66	162.50	8.551	156	0.06, 0., 0.1, 0., 2.34, 18.91, 25.51, 24.9, 28.18
67	164.93032	8.795	165	100.0
68	167.259	9.066	162	0.139, 0., 1.601, 0., 33.503, 22.869, 26.978, 0., 14.91
69	168.93421	9.321	169	100.0

Atomic number	Atomic weight	Density (g cm ⁻³)	Mass of first stable isotope	Abundance (%)
70	173.04	6.903	168	0.13, 0., 3.04, 14.28, 21.83, 16.13, 31.83, 0., 12.76
71	174.967	9.841	175	97.41, 2.59
72	178.49	13.31	174	0.16, 0., 5.26, 18.6, 27.28, 13.62, 35.08
73	180.9479	16.654	180	0.012, 99.988
74	183.84	19.3	180	0.12, 0., 26.5, 14.31, 30.64, 0., 28.43
75	186.207	21.02	185	37.4, 0., 62.6
76	190.23	22.57	184	0.02, 0., 1.59, 1.6, 13.29, 16.21, 26.36, 0., 40.93
77	192.217	22.42	191	37.3, 0., 62.7
78	195.08	21.45	190	0.014, 0., 0.782, 0., 32.967, 33.832, 25.242, 0., 7.163
79	196.96655	19.3	197	100.0
80	200.59	13.546	196	0.15, 0., 9.97, 16.87, 23.1, 13.18, 29.86, 0., 6.87
81	204.3833	11.85	203	29.524, 0., 70.476
82	207.2	11.35	204	1.4, 0., 24.1, 22.1, 52.4
83	208.98038	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	232.03805	11.72	232	100.0
91	0.	15.37		
92	238.02891	18.95	234	0.0054, 0.7204, 0., 0., 99.2742

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 \neq 1 kg used.	The <i>specific</i> tritium activity was stored and added to the <i>total</i> activity (not specific). So store the <i>total</i> activity for tritium.	555
19/5/95	Titles of final summary at end of run say <i>specific</i> values. The <i>total</i> values are shown, and this is probably most useful.	Change titles to show <i>total</i> 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 also be useful to show number of γ s per group. These data should also be available in TAB4.	This feature added.	565 - 572, 574 - 577
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

Date	Problem	Solution	Modification numbers
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	Group-wise 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 pulsed irradiation it would be useful to include a 'loop' facility in the FISPACT input file.	This feature added by introducing the new code words PULSE and ENDPULSE.	637-645
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 (<i>e.g.</i> 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

Date	Problem	Solution	Modification numbers
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 the name of the COLLAPX, ARRAYX and FLUXES files during the course of a run.	This feature added by introducing the code word NEWFILE, which allows the name of the file on a stream given in FILES to be redefined.	729-734
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
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	810-818

Date	Problem	Solution	Modification numbers
		precision and checks made so that single precision don't underflow	
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
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
24/7/00	Dominant nuclides for three additional quantities	Additional arrays and extra printing	957-970, 973-981
22/8/00	Final page of PRINTLIB does not contain '&'	Additional line added when printing	971
23/8/00	Point dose rate too large by a factor 10	Factor of 10 needed to correct following a change of units in FISPACT-97	972, 982-984
25/8/00	Incorrect MT value used for (n,2np) reactions, because of error in SYMPAL	MT corrected, but to ensure back compatibility it was necessary to introduce new EAFV value	985-997
3/10/00	All atomic masses held as integer values	AWR values from decay data read and held in floating point variables	998-1002, 1004, 1006-1015, 1017-1022, 1024-1028
5/10/00	Physical constants require updating	Avogadro constant changed from 6.02204459E+23 to 6.0221367E+23. amu changed from 1.66056559E-27 to 1.6605402E-27	1003, 1005, 1016, 1023
4/1/01	Additional summary table showing	Table implemented	1029-1037,

Date	Problem	Solution	Modification numbers
	heat output split into beta and gamma contributions		1043-1054
5/1/01	Units of quantities in uncertainty output incorrectly shown as per kg	Format statements changed	1038-1041
5/1/01	FISPACT-2001 not recognised as a recent version when reading uncertainty options	Check on VSIDNT changed, now all versions since FISPACT-2 correctly recognised	1042
8/1/01	Values of atomic weights and abundances need to be updated	Changes implemented	1055, 1056
24/1/01	Clock routines for UNIX streamlined	CLOCK and CLOKK routines modified	1057-1064
1/6/01	Error when all elements are input and fission is included	Size of ERR increased, test on value of JNUMB	1065
1/6/01	Some rare reactions did not contribute to gas production	New MT numbers defined and effect on gas production made consistent	1066-1109
20/6/01	Differences between PC and UNIX outputs	Inconsistent treatment of variable types in PC version. Many variables made Double precision by default	1110-1280
25/6/01	Gamma Becquerel value in OUTPUT is not consistent for all decays	All decay modes made consistent	1281-1283
12/7/01	Incorrect output of some generic pathways	Sizes of IGNU and GPATH arrays increased	1284-1289
2/10/01	Generic pathways starting with unstable nuclide could cause crash	Correct initialisation of Y(0)	1290-1291
4/12/01	Generic pathways resulting from n(IT)m(IT)g links not correctly handled	ISIGN2 introduced	1292-1293
28/8/03	Need to be able to read 211 group data files	Subroutine COL211 added	1294, 1464
1/9/03	Need to be able to read 351 group data files	Subroutine COL351 added	1295, 1465
4/9/03	Larger number of nuclides in index	Fe-48 now the fictional nuclide	1296, 1297
4/9/03	Larger number of reactions	Increase size of many arrays	1298-1433, 1452-1461
2/10/03	Decay library contains n decay mode	Add this decay mode	1434, 1462, 1463
2/10/03	Many new reaction types	Add definitions for these reactions	1435
2/10/03	Gas production caused by new reactions	Add these reactions	1436-1451
24/10/03	Changes required in existing COLnnn routines	Make the changes	1466-1509
27/10/03	GRPCON must consider 211 and 351 groups	Add these options	1510-1515
19/4/04	Problem found with production of fission products	Change algorithm for source term	1516-1522
25/10/04	The section MF=1, MT=452 in new decay files causes a crash	Read this format properly	1523-1525
25/10/04	Decay files containing extended energy release data causes a crash	Read this format properly	1526-1527
26/10/04	Exotic decay modes in decay file cause a crash	Define (pp), ($\beta^-\beta^-$), (β^-SF) modes	1528-1543

Date	Problem	Solution	Modification numbers
3/11/04	Need to include effect of SCPR for high energy data	New code word SEQNUMBER and additions to existing routines	1544-1571
4/11/04	New types of charged particle data	Dimension of FILES increased to 43	1572-1576
4/11/04	Include new charged particle reactions in pathways	Define these new reactions	1577-1584
5/11/04	Charged particle libraries contain data for Fm	Allow for 7 digits in INDEX file to describe nuclide	1585
5/11/04	More charged particle data	Increase array dimensions	1586-1593
8/11/04	Printing of charged particle data in output inconsistent	Change [P,N] to [p,n] etc	1594
8/11/04	Increased number of target nuclides	Adjust ICPN array and add IYCP array	1595-1613
9/11/04	Charged particle data includes isomers	New INCPNT array	1614-1637
7/12/04	Problems using 175 data with a high energy library	New array EXTRA, track carefully number of energy groups used	1638-1664
9/12/04	Use of PULSE code word with an old version of EAF causes a crash	Line of code added in error many years ago, but no effect except under these conditions. Removed.	1665
15/12/04	Problem found when using spectrum with only low energy neutrons.	Increase constants in all COLnnn routines	1666-1679
15/12/04	Some BREM candidates not output in PRINTLIB.	FORMAT statements for 1 or 2 nuclides per line.	1680-1685
16/12/04	Problems when collapsing with a 351 group spectrum	Dimensions of arrays increased to same values used in COL211	1686-1691
22/12/04	Fe-49 not required for EAF-2005 so it can be fictional nuclide	Remove changes introduced in 1296 and 1297 and in other COLnnn routines	1992, 1693

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-2005 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-2005: Overview
EDS-1	FISPACT-2005: User manual
EDS-2	FISPACT-2005: Qualification report
EDS-3	EAF-2005: Data libraries
EDS-4	EASY-2005: Processing system

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

EDS Report	UKAEA report number	Ref.
EDS-0	EASY-2005: Overview	39
EDS-1	FISPACT-2005: User manual	-
EDS-2	<i>Selection of reports and papers</i>	-
EDS-3	EAF-2005: Cross section library	15
	EAF-2005: Decay data library	21
	EAF-2005: Biological, clearance and transport libraries	25
EDS-4	SYMPAL: User guide	40
	SYMPAL: Utilities guide	41
	SAFEPAQ: User manual	42
	SAFEPAQ-II: User manual	43

Notes: documents in *italics* are not UKAEA reports. There is no report on the EAF-2005 (n, γ) reactions, however reference 16 contains data for EAF-97. There is no EAF-2005 Report file; however reference 17 contains data for EAF-99. The first three processing reports in EDS-4 are of historical interest only for EAF-2005. The FISPACT-99 validation report (reference 2) was available as a separate document.

Appendix 19 – Validation

Introduction

A series of test cases for FISPACT is discussed in Appendix 14. These test cases cover the various code words and by comparing with the outputs from previous versions ensure that a new version of FISPACT is behaving correctly. However, to fully test a new version it is necessary that the validity of the code is checked by comparing particular outputs with the original input data libraries to show that these data are input and processed correctly. The numerical method employed by FISPACT can also be validated by comparing with cases where analytical results are available. This Appendix details a set of tests to provide this validation; it consists of two main parts: the first that considers the data processing and the second that considers the comparison with analytical calculations.

To test FISPACT-2005 the data of EAF-97 can be used; there is no need to update the input data to EAF-2005 since the comparison is against analytical values. Note that much of the EAF-97 data are modified (as described in the following) to enable analytical results to be obtained.

Data library processing

Prior to any activation calculations FISPACT has to read in the nuclear data libraries and output the processed data in a format that can be used for future calculations. This section considers the various types of processing and compares the samples of the input data with those reported in the **PRINTLIB** output that contains the nuclear data in readable form.

Decay library processing

¹¹Be decay data

The EAF-97 decay data library contains the data for ¹¹Be shown in Table 1. The EAF-97 fission yield library (JEF-2.2) contains data for ¹¹Be shown in Table 2. FISPACT stores the nuclear

data in internal arrays, but in order to view the data used for a particular case a run using the code word **PRINTLIB** can be used to produce output in a format suitable for viewing. The part of the **PRINTLIB** output for ^{11}Be is shown in Table 3.

When FISPACT reads the gamma spectrum data it converts the discrete data into binned data that conforms to the internal energy structure. The calculations for the ^{11}Be data are given in Table 4.

FISPACT uses a weighted fission yield, this is calculated by taking the yield data at the various neutron energies (typically 0.0253 eV, 400 keV and 14 MeV) and multiplying by the fraction of neutrons in the relevant energy range (< 200 keV, 200 keV - 5 MeV and > 5 MeV) and summing. The **PRINTLIB** output for a particular neutron spectrum gives the fractions as 0.4120, 0.3871 and 0.2009, respectively. The calculation of the weighted yield is given in Table 5.

Table 1. Data for ^{11}Be in decay library.

Quantity	Value
Half-life	$1.38100 \cdot 10^1 \text{ s}$
E_β	$4.64731 \cdot 10^6 \text{ eV}$
E_γ	$1.41878 \cdot 10^6 \text{ eV}$
E_α	$3.62726 \cdot 10^4 \text{ eV}$
Decay mode 1	β^- 97%
Decay mode 2	β^- - α 3%
γ spectrum data	8 discrete lines
Normalisation factor	0.33
(Energy, Relative Intensity) ₁	$1.7722 \cdot 10^6 \text{ eV}, 8.48485 \cdot 10^{-3}$
(Energy, Relative Intensity) ₂	$2.1248 \cdot 10^6 \text{ eV}, 1.00000 \cdot 10^0$
(Energy, Relative Intensity) ₃	$2.8931 \cdot 10^6 \text{ eV}, 2.81818 \cdot 10^{-3}$
(Energy, Relative Intensity) ₄	$4.6663 \cdot 10^6 \text{ eV}, 6.06061 \cdot 10^{-2}$
(Energy, Relative Intensity) ₅	$5.0193 \cdot 10^6 \text{ eV}, 1.42424 \cdot 10^{-2}$
(Energy, Relative Intensity) ₆	$5.8518 \cdot 10^6 \text{ eV}, 6.45455 \cdot 10^{-2}$
(Energy, Relative Intensity) ₇	$6.7905 \cdot 10^6 \text{ eV}, 1.36667 \cdot 10^{-1}$
(Energy, Relative Intensity) ₈	$7.9747 \cdot 10^6 \text{ eV}, 5.27273 \cdot 10^{-2}$

Table 2. Fission yield library data for ^{11}Be .

Fissioning nuclide	Energy (eV)	Independent yield
^{235}U	$2.53 \cdot 10^{-2}$	$3.4639 \cdot 10^{-7}$
^{235}U	$4.00 \cdot 10^5$	0.0
^{235}U	$1.40 \cdot 10^7$	0.0
^{239}Pu	$2.53 \cdot 10^{-2}$	$7.7526 \cdot 10^{-7}$
^{239}Pu	$4.00 \cdot 10^5$	0.0

Table 3. FISPACT PRINTLIB output data for ^{11}Be .

Quantity	Value
Half-life	$1.3810 \cdot 10^1 \text{ s}$
<ALPHA>	$3.627 \cdot 10^{-2} \text{ MeV}$
<BETA>	$4.647 \cdot 10^0 \text{ MeV}$
<GAMMA>	$1.419 \cdot 10^0 \text{ MeV}$
Decay mode 1	(b-) 97%
Decay mode 2	(b-a) 3%
γ energy in GROUPS 1 - 13 (0 - 1.66 MeV)	0.0 MeV
γ energy in GROUP 14 (1.66 - 2.0 MeV)	$4.962 \cdot 10^{-3} \text{ MeV}$
γ energy in GROUP 15 (2.0 - 2.5 MeV)	$7.012 \cdot 10^{-1} \text{ MeV}$
γ energy in GROUP 16 (2.5 - 3.0 MeV)	$2.691 \cdot 10^{-3} \text{ MeV}$
γ energy in GROUP 17 (3.0 - 4.0 MeV)	0.0 MeV
γ energy in GROUP 18 (2.5 - 3.0 MeV)	$9.333 \cdot 10^{-2} \text{ MeV}$
γ energy in GROUP 19 (5.0 - 6.5 MeV)	$1.482 \cdot 10^{-1} \text{ MeV}$
γ energy in GROUP 20 (6.5 - 8.0 MeV)	$4.450 \cdot 10^{-1} \text{ MeV}$
γ energy in GROUPS 21 - 24 (8.0 MeV \rightarrow)	0.0 MeV
Weighted fission yield from ^{235}U	$1.427 \cdot 10^{-5} \%$
Weighted fission yield from ^{239}Pu	$3.194 \cdot 10^{-5} \%$

Table 4. Binning of ^{11}Be γ spectrum data to FISPACT structure.

GROUP	Expression	Result (MeV)
14	$1.7722 \cdot 10^6 \times 8.48485 \cdot 10^{-3} \times 0.33$	$4.96216 \cdot 10^{-3}$
15	$2.1248 \cdot 10^6 \times 1.0 \times 0.33$	$7.01184 \cdot 10^{-1}$
16	$2.8931 \cdot 10^6 \times 2.81818 \cdot 10^{-3} \times 0.33$	$2.69058 \cdot 10^{-3}$
18	$4.6663 \cdot 10^6 \times 6.06061 \cdot 10^{-2} \times 0.33$	$9.33261 \cdot 10^{-2}$
19	$(5.0193 \cdot 10^6 \times 1.42424 \cdot 10^{-2} + 5.8518 \cdot 10^6 \times 6.45455 \cdot 10^{-2}) \times 0.33$	$1.48234 \cdot 10^{-1}$
20	$(6.7905 \cdot 10^6 \times 1.36667 \cdot 10^{-1} + 7.9747 \cdot 10^6 \times 5.27273 \cdot 10^{-2}) \times 0.33$	$4.45012 \cdot 10^{-1}$

Table 5. Calculation of weighted fission yields.

Fissioning nuclide	Expression	Result (MeV)
²³⁵ U	$3.4637 \cdot 10^{-7} \times 0.4120 \times 100.0$	$1.4270 \cdot 10^{-5}$
²³⁹ Pu	$7.7526 \cdot 10^{-7} \times 0.4120 \times 100.0$	$3.1941 \cdot 10^{-5}$

Looking at various parts of the previous tables it can be seen that:

- Comparison between Table 1, row 1 and Table 3, row 1 shows agreement for half-life.
- Comparison between Table 1, row 2 and Table 3, row 3 shows agreement for β energy.
- Comparison between Table 1, row 3 and Table 3, row 4 shows agreement for γ energy.
- Comparison between Table 1, row 4 and Table 3, row 2 shows agreement for α energy.
- Comparison between Table 1, row 5 and Table 3, row 5 shows agreement for mode 1.
- Comparison between Table 1, row 6 and Table 3, row 6 shows agreement for mode 2.
- Comparison between Table 4 and Table 3, rows 7 - 15 shows agreement for the γ spectrum.
- Comparison between Table 5 and Table 3, rows 16 - 17 shows agreement for the fission yields.

Collapsing cross sections

FISPACT reads neutron induced cross section libraries in one of five energy group structures. The folding of this energy dependant cross section with the neutron spectrum for a particular situation generates an effective (or collapsed) cross section for each reaction. FISPACT also needs to use a single cross section value for the reaction from a parent to a daughter, while the data libraries often contain more than one cross section entry for a particular pair of parent and daughter nuclides. This is because, for example, the $A(n,n'p)B$ and $A(n,d)B$ reactions both produce the same daughter nuclide. The library keeps these reactions separate because the first produces ¹H from the proton, while the second produces ²H from the

deuteron. The method that FISPACT uses to keep track of these secondary gas products is to include further cross section values in the **COLLAPX** file for $A(n,X)^1H$ and $A(n,X)^2H$. These cross section values are stored with a negative sign so that it is possible to avoid double counting when summing the cross sections (only sum positive values) but when considering gas production the absolute value of the cross section is used.

The output of this processing is stored in the **COLLAPX** file which contains parent, daughter and cross section values. To validate the collapsing of the cross section library it is necessary to do several calculations and compare with values from a **COLLAPX** file. Appendix 14 describes the **COLLAPX** files for each type of group library; the 100-group neutron spectrum is used here for the validation.

In the validation report for FISPACT-99² a listing of the procedure that was used to calculate the collapsed values was given. This is not repeated for this Appendix. The collapsed cross section ($\bar{\sigma}$) is calculated as indicated by equation 1, where σ_i are the group averaged cross sections and ϕ_i the corresponding group flux.

$$\bar{\sigma} = \sum_i \sigma_i \phi_i / \sum_i \phi_i \dots\dots\dots(1)$$

Table 6 presents a small part of the **COLLAPX** file for EAF-97 in the 100-group spectrum. The nuclides corresponding to these ID numbers are shown in Table 7. Table 8 presents the relevant reactions present in the EAF-97 library with the calculated collapsed.

Table 6. A portion of the COLLAPX file for 100-group neutron spectrum.

Parent ID	Daughter ID	Cross section (b)
20	8	2.52861E-02
20	21	1.06530E-02
20	16	8.04049E-03
20	1918	-1.45158E-02
20	15	8.73429E-03
20	1919	-2.15873E-02
20	14	4.56114E-02
20	1920	-2.62832E-02
20	9	8.17455E+01
20	1922	-8.17708E+01

Table 7. A selection of FISPACT ID numbers for the EAF-97 library.

ID	Nuclide
8	⁶ Li
9	⁷ Li
14	⁸ Be
15	⁹ Be
16	¹⁰ Be
20	¹⁰ B
21	¹¹ B
1918	¹ H
1919	² H
1920	³ H
1922	⁴ He

Table 8. A selection of reactions from the EAF-97 library.

Reaction	Collapsed cross section (b)
¹⁰ B(n,n'α)	2.52861E-02
¹⁰ B(n,n'p)	2.75172E-03
¹⁰ B(n,n'd)	1.56047E-02
¹⁰ B(n,2n'p)	3.72359E-03
¹⁰ B(n,γ)	1.06530E-02
¹⁰ B(n,p)	8.04049E-03
¹⁰ B(n,d)	5.98257E-03
¹⁰ B(n,t)	2.62831E-02
¹⁰ B(n,h)	0.00000E+00
¹⁰ B(n,α)	8.17455E+01

In order to compare Tables 6 and 8 it is necessary to combine the values for various reactions given in Table 8 to produce the

values used in the FISPACT **COLLAPX** file (Table 6). Table 9 gives these calculations and column 4 can be directly compared with column 3 of Table 6, showing agreement.

Table 9. Combining effective cross sections to give values in FISPACT form.

Daughter ID	Reaction combinations	Expression	Result (b)
8	(n,n'α)	2.52861E-02	2.52861E-02
21	(n,γ)	1.06530E-02	1.06530E-02
16	(n,p)	8.04049E-03	8.04049E-03
1918	-[(n,n'p) + (n,2n'p) + (n,p)]	-(2.75172E-03 + 3.72359E-03 + 8.04049E-03)	-1.45158E-02
15	(n,d) + (n,n'p)	5.98257E-03 + 2.75172E-03	8.73429E-03
1919	-[(n,n'd) + (n,d)]	-(1.56047E-02 + 5.98257E-03)	-2.158727E-02
14	(n,t) + (n,n'd) + (n,2n'p)	2.62831E-02 + 1.56047E-02 + 3.72359E-03	4.561139E-02
1920	-(n,t)	-2.62831E-02	-2.62831E-02
9	(n,α)	8.17455E+01	8.17455E+01
1922	-[(n,n'α) + (n,α)]	-(2.52861E-02 + 8.17455E+01)	-8.1770786E1

Decay tests

A series of simple decays from a single starting nuclide is considered. In these cases there is an analytical solution which can be calculated using the standard solutions of the Bateman equations⁴⁴. A procedure was written (see reference 2) which uses as input a file which contains the half-lives of all relevant nuclides, a starting number of atoms and a series of times at which numbers of atoms and the total activity are to be calculated. It was coded so that numbers of atoms less than 1.0 were written in the output as 0.0. The procedure used double precision variables and was tested against a hand calculator for various cases.

Data on half-lives were extracted from the decay data library (EAF_DEC-97), and compared against the values shown in the FISPACT **PRINTLIB** output. Decays were chosen to cover a wide range of nuclide half-lives, to have either a single daughter or a chain of daughters and to have different decay

modes. Isomeric states, either as the initial nuclide or as daughters, and decay branching were also investigated. The method for dealing with branched decays is as follows.

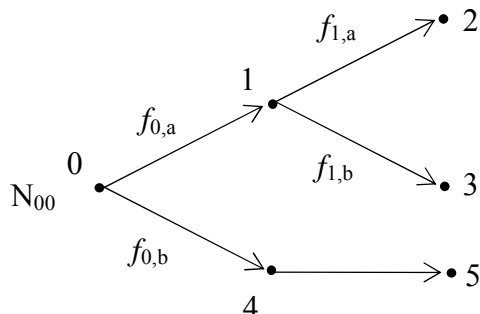


Figure A19.1. A general series of decays that includes branching.

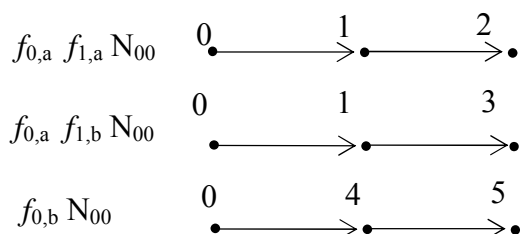


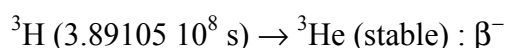
Figure A19.2. The series of linear pathways equivalent to Figure 1.

A particular branched decay is shown in Figure A19.1, where the nuclides are labelled by numbers and the branching fractions are indicated by the symbols $f_{i,n}$ where i labels the parent nuclide and n label the decays (a,b,...). It is assumed that at time 0, there are N_{00} atoms of nuclide 0 present. This series of decays is equivalent to Figure A19.2, where the starting numbers of atoms of nuclide 0 for each of the parallel pathways is given. Each pathway is a decay chain that can be solved by the Bateman method, and the total number of atoms of each type then found by suitable additions of the values for each pathway.

The calculation for each nuclide contains a table showing the comparison between the analytical results (labelled by A) and the FISPACT results (labelled by F). The number of atoms of each nuclide (N) and the total activity for all relevant nuclides (A) are given at a series of decay times. For each nuclide the

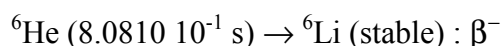
FISPACT column contains the value of $(N_F - N_A) / N_A$ which has the largest absolute value over the considered times, and the time where the maximum value occurred is indicated by the shading. The FISPACT input files for all the tests are given in the Annex.

³H decay (test_d1)



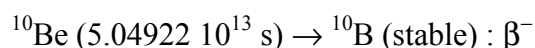
Decay times (s)	N _A (H-3)	N _F (H-3)	N _A (He-3)	N _F (He-3)	A _A (Total)	A _F (Total)
3.15576E+07	9.45335E+19	9.45335E+19	5.46654E+18	5.46654E+18	1.68401E+11	1.684008E+11
1.57788E+08	7.54967E+19	7.54967E+19	2.45033E+19	2.45033E+19	1.34489E+11	1.344889E+11
3.15576E+08	5.69975E+19	5.69975E+19	4.30025E+19	4.30025E+19	1.01535E+11	1.015346E+11
4.73364E+08	4.30312E+19	4.30312E+19	5.69688E+19	5.69687E+19	7.66553E+10	7.665525E+10
6.31152E+08	3.24871E+19	3.24871E+19	6.75129E+19	6.75128E+19	5.78722E+10	5.787216E+10
9.46728E+08	1.85168E+19	1.85168E+19	8.14832E+19	8.14827E+19	3.29857E+10	3.298567E+10
1.26230E+09	1.05542E+19	1.05541E+19	8.94458E+19	8.94451E+19	1.88011E+10	1.880099E+10
1.57788E+09	6.01558E+18	6.01558E+18	9.39844E+19	9.39835E+19	1.07161E+10	1.071609E+10
3.15576E+09	3.61872E+17	3.61873E+17	9.96381E+19	9.96421E+19	6.44635E+08	6.446356E+08
Max. diff. (%)		-0.00095		0.00401		-0.00059

⁶He decay (test_d2)

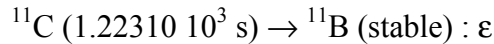


Decay times (s)	N _A (He-6)	N _F (He-6)	N _A (Li-6)	N _F (Li-6)	A _A (Total)	A _F (Total)
1.00000E-02	9.91459E+19	9.91459E+19	8.54076E+17	8.54081E+17	8.50418E+19	8.504232E+19
5.00000E-02	9.58019E+19	9.58019E+19	4.19806E+18	4.19808E+18	8.21735E+19	8.217401E+19
1.00000E-01	9.17801E+19	9.17801E+19	8.21987E+18	8.21992E+18	7.87239E+19	7.872428E+19
5.00000E-01	6.51243E+19	6.51242E+19	3.48757E+19	3.48758E+19	5.58600E+19	5.586019E+19
1.00000E+00	4.24118E+19	4.24116E+19	5.75882E+19	5.75885E+19	3.63785E+19	3.637848E+19
5.00000E+00	1.37225E+18	1.37221E+18	9.86278E+19	9.86306E+19	1.17704E+18	1.177015E+18
1.00000E+01	1.88306E+16	1.88297E+16	9.99812E+19	9.99873E+19	1.61519E+16	1.615115E+16
1.50000E+01	2.58403E+14	2.58384E+14	9.99997E+19	9.99967E+19	2.21644E+14	2.216282E+14
Max. diff. (%)		-0.00735		0.00610		-0.00713

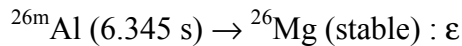
¹⁰Be decay (test_d3)



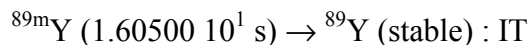
Decay times (s)	N _A (Be-10)	N _F (Be-10)	N _A (B-10)	N _F (B-10)	A _A (Total)	A _F (Total)
1.57788E+13	8.05245E+19	8.05245E+19	1.94755E+19	1.94755E+19	1.10543E+06	1.105425E+06
3.15576E+13	6.48420E+19	6.48420E+19	3.51580E+19	3.51580E+19	8.90138E+05	8.901383E+05
4.73364E+13	5.22137E+19	5.22137E+19	4.77863E+19	4.77862E+19	7.16780E+05	7.167798E+05
6.31152E+13	4.20449E+19	4.20449E+19	5.79551E+19	5.79551E+19	5.77184E+05	5.771836E+05
1.57788E+14	1.14626E+19	1.14626E+19	8.85374E+19	8.85391E+19	1.57356E+05	1.573560E+05
3.15576E+14	1.31391E+18	1.31391E+18	9.86861E+19	9.86915E+19	1.80370E+04	1.803705E+04
6.31152E+14	1.72635E+16	1.72635E+16	9.99827E+19	9.99913E+19	2.36990E+02	2.369900E+02
9.46728E+14	2.26826E+14	2.26826E+14	9.99998E+19	9.99999E+19	3.11382E+00	3.113828E+00
1.57788E+15	3.91580E+10	3.91582E+10	1.00000E+20	9.99999E+19	5.37553E-04	5.375559E-04
Max. diff. (%)		0.00051		0.00860		0.00054

¹¹C decay (test_d4)

Decay times (s)	N _A (C-11)	N _F (C-11)	N _A (B-11)	N _F (B-11)	A _A (Total)	A _F (Total)
3.00000E+02	8.43653E+19	8.43653E+19	1.56347E+19	1.56347E+19	4.78109E+16	4.781094E+16
6.00000E+02	7.11750E+19	7.11750E+19	2.88250E+19	2.88250E+19	4.03358E+16	4.033584E+16
1.20000E+03	5.06589E+19	5.06589E+19	4.93411E+19	4.93410E+19	2.87091E+16	2.870905E+16
1.80000E+03	3.60565E+19	3.60565E+19	6.39435E+19	6.39434E+19	2.04337E+16	2.043368E+16
3.60000E+03	1.30007E+19	1.30007E+19	8.69993E+19	8.69997E+19	7.36766E+15	7.367663E+15
7.20000E+03	1.69018E+18	1.69018E+18	9.83098E+19	9.83135E+19	9.57846E+14	9.578471E+14
1.80000E+04	3.71390E+15	3.71392E+15	9.99963E+19	1.00002E+20	2.10472E+12	2.104725E+12
3.60000E+04	1.37931E+11	1.37932E+11	1.00000E+20	1.00002E+20	7.81673E+07	7.816770E+07
5.40000E+04	5.12262E+06	5.12266E+06	1.00000E+20	1.00002E+20	2.90306E+03	2.903082E+03
7.20000E+04	1.90249E+02	1.90251E+02	1.00000E+20	1.00002E+20	1.07817E-01	1.078180E-01
Max. diff. (%)		0.00105		0.00570		0.00093

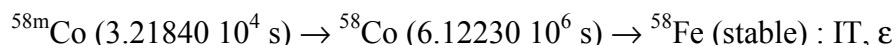
^{26m}Al decay (test_d5)

Decay times (s)	N _A (Al-26m)	N _F (Al-26m)	N _A (Mg-26)	N _F (Mg-26)	A _A (Total)	A _F (Total)
2.00000E+00	8.03735E+19	8.03735E+19	1.96265E+19	1.96265E+19	8.78024E+18	8.780241E+18
5.00000E+00	5.79138E+19	5.79138E+19	4.20862E+19	4.20861E+19	6.32668E+18	6.326675E+18
1.50000E+01	1.94243E+19	1.94243E+19	8.05757E+19	8.05767E+19	2.12197E+18	2.121969E+18
2.50000E+01	6.51491E+18	6.51492E+18	9.34851E+19	9.34865E+19	7.11709E+17	7.117093E+17
5.00000E+01	4.24441E+17	4.24441E+17	9.95756E+19	9.95817E+19	4.63672E+16	4.636727E+16
1.00000E+02	1.80150E+15	1.80151E+15	9.99982E+19	9.99516E+19	1.96801E+14	1.968019E+14
1.50000E+02	7.64630E+12	7.64634E+12	1.00000E+20	9.99522E+19	8.35305E+11	8.353091E+11
2.50000E+02	1.37748E+08	1.37749E+08	1.00000E+20	9.99522E+19	1.50480E+07	1.504814E+07
Max. diff. (%)		0.00073		-0.04780		0.00093

^{89m}Y decay (test_d6)

Decay times (s)	N _A (Y-89m)	N _F (Y-89m)	N _A (Y-89)	N _F (Y-89)	A _A (Total)	A _F (Total)
5.00000E+00	8.05789E+19	8.05789E+19	1.94211E+19	1.94211E+19	3.47994E+18	3.479938E+18
1.00000E+01	6.49295E+19	6.49296E+19	3.50705E+19	3.50704E+19	2.80410E+18	2.804095E+18
1.50000E+01	5.23195E+19	5.23195E+19	4.76805E+19	4.76805E+19	2.25951E+18	2.259508E+18
2.00000E+01	4.21585E+19	4.21585E+19	5.78415E+19	5.78415E+19	1.82069E+18	1.820686E+18
5.00000E+01	1.15402E+19	1.15402E+19	8.84598E+19	8.84615E+19	4.98382E+17	4.983821E+17
1.00000E+02	1.33175E+18	1.33175E+18	9.86682E+19	9.86736E+19	5.75141E+16	5.751412E+16
2.00000E+02	1.77357E+16	1.77357E+16	9.99823E+19	9.99908E+19	7.65945E+14	7.659470E+14
3.00000E+02	2.36195E+14	2.36196E+14	9.99998E+19	9.99997E+19	1.02005E+13	1.020053E+13
Max. diff. (%)		0.00042		0.00850		0.00029

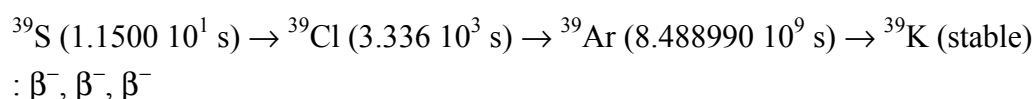
^{58m}Co decay (test_d7)



Decay times (s)	N _A (Co-58m)	N _F (Co-58m)	N _A (Co-58)	N _F (Co-58)	N _A (Fe-58)	N _F (Fe-58)
7.20000E+03	8.56358E+19	8.56358E+19	1.43582E+19	1.43582E+19	6.00415E+15	6.00415E+15
1.80000E+04	6.78639E+19	6.78639E+19	3.21013E+19	3.21013E+19	3.48311E+16	3.48312E+16
3.60000E+04	4.60551E+19	4.60551E+19	5.38211E+19	5.38211E+19	1.23822E+17	1.23822E+17
8.64000E+04	1.55548E+19	1.55549E+19	8.39128E+19	8.39129E+19	5.32307E+17	5.32308E+17
8.64000E+05	8.29197E+11	8.29201E+11	9.11605E+19	9.11608E+19	8.83951E+18	8.83964E+18
1.72800E+06	6.87568E+03	6.87575E+03	8.26655E+19	8.26658E+19	1.73345E+19	1.73347E+19
3.45600E+06	0.00000E+00	0.00000E+00	6.79766E+19	6.79769E+19	3.20234E+19	3.20236E+19
5.18400E+06	0.00000E+00	0.00000E+00	5.58978E+19	5.58980E+19	4.41022E+19	4.41024E+19
6.91200E+06	0.00000E+00	0.00000E+00	4.59653E+19	4.59655E+19	5.40347E+19	5.40350E+19
8.64000E+06	0.00000E+00	0.00000E+00	3.77977E+19	3.77978E+19	6.22023E+19	6.22026E+19
1.72800E+07	0.00000E+00	0.00000E+00	1.42115E+19	1.42116E+19	8.57885E+19	8.57893E+19
2.59200E+07	0.00000E+00	0.00000E+00	5.34340E+18	5.34342E+18	9.46566E+19	9.46576E+19
4.32000E+07	0.00000E+00	0.00000E+00	7.55387E+17	7.55391E+17	9.92446E+19	9.92468E+19
Max. diff. (%)		0.00102		0.00070		0.00222

Decay times (s)	A _A (Total)	A _F (Total)
7.20000E+03	1.84597E+15	1.845965E+15
1.80000E+04	1.46522E+15	1.465219E+15
3.60000E+04	9.97982E+14	9.979819E+14
8.64000E+04	3.44505E+14	3.445054E+14
8.64000E+05	1.03209E+13	1.032095E+13
1.72800E+06	9.35912E+12	9.359153E+12
3.45600E+06	7.69609E+12	7.696120E+12
5.18400E+06	6.32857E+12	6.328591E+12
6.91200E+06	5.20404E+12	5.204060E+12
8.64000E+06	4.27933E+12	4.279347E+12
1.72800E+07	1.60899E+12	1.608992E+12
2.59200E+07	6.04962E+11	6.049647E+11
4.32000E+07	8.55225E+10	8.552292E+10
Max. diff. (%)		0.00049

³⁹S decay (test_d8)

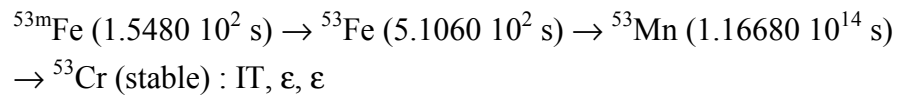


Decay times (s)	N _A (S-39)	N _F (S-39)	N _A (Cl-39)	N _F (Cl-39)	N _A (Ar-39)	N _F (Ar-39)
5.00000E+00	7.39805E+19	7.39805E+19	2.60053E+19	2.60053E+19	1.41885E+16	1.41885E+16
1.00000E+01	5.47312E+19	5.47312E+19	4.52171E+19	4.52171E+19	5.16878E+16	5.16878E+16
1.50000E+01	4.04904E+19	4.04904E+19	5.94032E+19	5.94032E+19	1.06405E+17	1.06405E+17
5.00000E+01	4.91105E+18	4.91105E+18	9.43808E+19	9.43808E+19	7.08158E+17	7.08158E+17
1.00000E+02	2.41184E+17	2.41184E+17	9.80404E+19	9.80406E+19	1.71837E+18	1.71838E+18
5.00000E+02	8.16092E+06	8.16099E+06	9.04443E+19	9.04301E+19	9.55568E+18	9.55363E+18
1.00000E+03	0.00000E+00	0.00000E+00	8.15198E+19	8.15070E+19	1.84802E+19	1.84768E+19
2.00000E+03	0.00000E+00	0.00000E+00	6.62256E+19	6.62152E+19	3.37744E+19	3.37685E+19
5.00000E+03	0.00000E+00	0.00000E+00	3.55071E+19	3.55016E+19	6.44928E+19	6.44823E+19
1.00000E+04	0.00000E+00	0.00000E+00	1.25641E+19	1.25621E+19	8.74358E+19	8.74217E+19
5.00000E+04	0.00000E+00	0.00000E+00	3.08787E+15	3.08740E+15	9.99965E+19	9.99814E+19
1.00000E+05	0.00000E+00	0.00000E+00	9.50208E+10	9.50064E+10	9.99992E+19	9.99811E+19
Max. diff. (%)		0.00086		-0.01570		-0.02145

Decay times (s)	N _A (K-39)	N _F (K-39)	A _A (Total)	A _F (Total)
5.00000E+00	1.95399E+06	1.97855E+06	4.46448E+18	4.464480E+18
1.00000E+01	1.47216E+07	1.47479E+07	3.30824E+18	3.308244E+18
1.50000E+01	4.65072E+07	4.65182E+07	2.45285E+18	2.452848E+18
5.00000E+01	1.15401E+09	1.15403E+09	3.15617E+17	3.156171E+17
1.00000E+02	6.09647E+09	6.09649E+09	3.49077E+16	3.490771E+16
5.00000E+02	1.91968E+11	1.91910E+11	1.87923E+16	1.878938E+16
1.00000E+03	7.67422E+11	7.67251E+11	1.69380E+16	1.693535E+16
2.00000E+03	2.92239E+12	2.92183E+12	1.37602E+16	1.375807E+16
5.00000E+03	1.53464E+13	1.53439E+13	7.37760E+15	7.376447E+15
1.00000E+04	4.71565E+13	4.71488E+13	2.61055E+15	2.610142E+15
5.00000E+04	3.68830E+14	3.68780E+14	6.49757E+11	6.496562E+11
1.00000E+05	7.77088E+14	7.77031E+14	8.18493E+09	8.183448E+09
Max. diff. (%)		1.25692		-0.01811

This case shows a significant difference (1.26 %) between the FISPACT and analytical calculations for ³⁶K at 5 s decay time. However, note that the number of atoms is very small and that with increasing decay time the differences get less significant.

^{53m}Fe decay (test_d9)

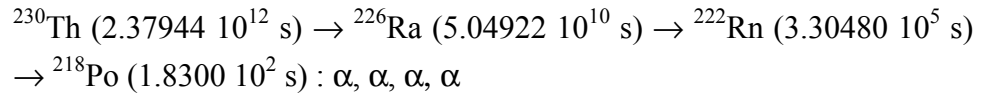


Decay times (s)	N _A (Fe-53m)	N _F (Fe-53m)	N _A (Fe-53)	N _F (Fe-53)	N _A (Mn-53)	N _F (Mn-53)
6.00000E+01	7.64402E+19	7.64402E+19	2.25847E+19	2.25847E+19	9.75146E+17	9.75146E+17
1.20000E+02	5.84310E+19	5.84310E+19	3.80818E+19	3.80818E+19	3.48717E+18	3.48717E+18
1.80000E+02	4.46648E+19	4.46648E+19	4.82994E+19	4.82994E+19	7.03579E+18	7.03580E+18
3.00000E+02	2.60981E+19	2.60981E+19	5.80480E+19	5.80480E+19	1.58540E+19	1.58540E+19
6.00000E+02	6.81110E+18	6.81110E+18	5.37789E+19	5.37789E+19	3.94100E+19	3.94100E+19
9.00000E+02	1.77757E+18	1.77757E+18	3.97422E+19	3.97420E+19	5.84803E+19	5.84814E+19
1.20000E+03	4.63910E+17	4.63911E+17	2.74793E+19	2.74791E+19	7.20568E+19	7.20582E+19
1.50000E+03	1.21072E+17	1.21072E+17	1.85560E+19	1.85559E+19	8.13229E+19	8.13243E+19
1.80000E+03	3.15974E+16	3.15975E+16	1.24189E+19	1.24191E+19	8.75495E+19	8.75499E+19
2.40000E+03	2.15213E+15	2.15213E+15	5.51677E+18	5.51686E+18	9.44811E+19	9.44817E+19
3.00000E+03	1.46584E+14	1.46584E+14	2.44430E+18	2.44438E+18	9.75556E+19	9.75557E+19
3.60000E+03	9.98395E+12	9.98399E+12	1.08255E+18	1.08259E+18	9.89174E+19	9.89174E+19
7.20000E+03	9.96793E+05	9.96801E+05	8.16646E+15	8.16603E+15	9.99918E+19	9.99948E+19
1.08000E+04	0.00000E+00	0.00000E+00	6.16046E+13	6.16014E+13	9.99999E+19	9.99983E+19
2.16000E+04	0.00000E+00	0.00000E+00	2.64455E+07	2.64442E+07	1.00000E+20	9.99983E+19
4.32000E+04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.00000E+20	9.99983E+19
8.64000E+04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.00000E+20	9.99983E+19
1.72800E+05	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.00000E+20	9.99983E+19
Max. diff. (%)		0.00080		-0.00527		0.00300

Decay times (s)	N _A (Cr-53)	N _F (Cr-53)	A _A (Total)	A _F (Total)
6.00000E+01	1.11022E+05	1.19244E+05	3.72935E+17	3.729348E+17
1.20000E+02	8.88178E+05	8.77086E+05	3.13333E+17	3.133328E+17
1.80000E+02	2.73115E+06	2.72775E+06	2.65562E+17	2.655624E+17
3.00000E+02	1.07914E+07	1.07933E+07	1.95660E+17	1.956602E+17
6.00000E+02	6.03517E+07	6.03401E+07	1.03504E+17	1.035036E+17
9.00000E+02	1.48437E+08	1.48415E+08	6.19100E+16	6.190978E+16
1.20000E+03	2.65499E+08	2.65477E+08	3.93808E+16	3.938055E+16
1.50000E+03	4.02700E+08	4.02692E+08	2.57322E+16	2.573208E+16
1.80000E+03	5.53546E+08	5.53529E+08	1.70003E+16	1.700059E+16
2.40000E+03	8.79619E+08	8.79593E+08	7.49873E+15	7.498858E+15
3.00000E+03	1.22260E+09	1.22249E+09	3.31882E+15	3.318944E+15
3.60000E+03	1.57308E+09	1.57293E+09	1.46962E+15	1.46962E+15
7.20000E+03	3.70698E+09	3.70662E+09	1.10861E+13	1.108551E+13
1.08000E+04	5.84556E+09	5.84555E+09	8.36297E+10	8.362547E+10
2.16000E+04	1.22614E+10	1.22613E+10	6.29958E+05	6.299463E+05
4.32000E+04	2.50930E+10	2.50927E+10	5.94058E+05	5.940479E+05
8.64000E+04	5.07564E+10	5.07556E+10	5.94058E+05	5.940479E+05
1.72800E+05	1.02083E+11	1.02081E+11	5.94058E+05	5.940479E+05
Max. diff. (%)		7.40574		-0.00532

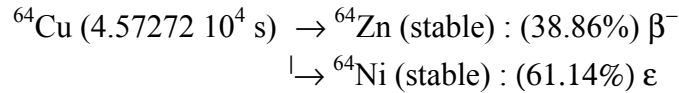
This case shows a significant difference (7.41 %) between the FISPACT and analytical calculations for ⁵³Cr at 60 s decay time. However, note that the number of atoms is very small and that with increasing decay time the differences get less significant.

²³⁰Th decay (test_d10)



Decay times (s)	N _A (Th-230)	N _F (Th-230)	N _A (Ra-226)	N _F (Ra-226)	N _A (Rn-222)	N _F (Rn-222)
1.00000E+12	7.47286E+19	7.47286E+19	1.62013E+18	1.62013E+18	1.06041E+13	1.06041E+13
2.00000E+12	5.58437E+19	5.58437E+19	1.21071E+18	1.21071E+18	7.92428E+12	7.92433E+12
3.00000E+12	4.17312E+19	4.17312E+19	9.04744E+17	9.04744E+17	5.92170E+12	5.92174E+12
4.00000E+12	3.11852E+19	3.11852E+19	6.76103E+17	6.76103E+17	4.42521E+12	4.42524E+12
5.00000E+12	2.33043E+19	2.33043E+19	5.05242E+17	5.05243E+17	3.30690E+12	3.30692E+12
6.00000E+12	1.74149E+19	1.74150E+19	3.77561E+17	3.77561E+17	2.47120E+12	2.47122E+12
1.00000E+13	5.43088E+18	5.43089E+18	1.17743E+17	1.17743E+17	7.70648E+11	7.70653E+11
5.00000E+13	4.72446E+13	4.72448E+13	1.02427E+12	1.02428E+12	6.70405E+06	6.70408E+06
Max. diff. (%)		0.00057		0.00098		0.00081

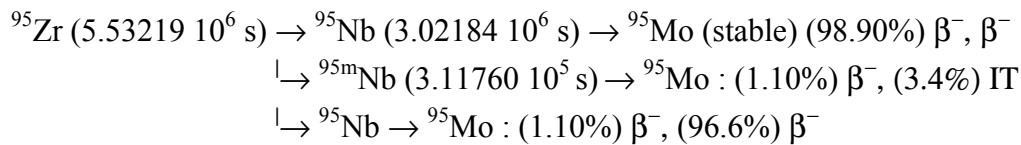
Decay times (s)	N _A (Po-218)	N _F (Po-218)	A _A (Total)	A _F (Total)
1.00000E+12	5.87189E+09	5.88199E+09	8.84916E+07	8.8530E+07
2.00000E+12	4.38799E+09	4.39554E+09	6.61287E+07	6.6160E+07
3.00000E+12	3.27908E+09	3.28472E+09	4.94170E+07	4.9440E+07
4.00000E+12	2.45041E+09	2.45043E+09	3.69287E+07	3.6927E+07
5.00000E+12	1.83116E+09	1.83117E+09	2.75963E+07	2.7597E+07
6.00000E+12	1.36840E+09	1.36841E+09	2.06223E+07	2.0622E+07
1.00000E+13	4.26738E+08	4.26741E+08	6.43111E+06	6.4300E+06
5.00000E+13	3.71230E+03	3.71232E+03	5.59458E+01	5.5940E+01
Max. diff. (%)		0.17206		0.04733

⁶⁴Cu decay (test_d11)

Decay times (s)	N _A (Cu-64)	N _F (Cu-64)	N _A (Zn-64)	N _F (Zn-64)	N _A (Ni-64)	N _F (Ni-64)
1.80000E+04	7.61207E+19	7.61207E+19	9.27949E+18	9.27949E+18	1.45998E+19	1.45998E+19
3.60000E+04	5.79436E+19	5.79437E+19	1.63431E+19	1.63431E+19	2.57133E+19	2.57132E+19
5.40000E+04	4.41071E+19	4.41071E+19	2.17200E+19	2.17199E+19	3.41729E+19	3.41729E+19
7.20000E+04	3.35746E+19	3.35747E+19	2.58129E+19	2.58129E+19	4.06125E+19	4.06124E+19
1.72800E+05	7.28497E+18	7.28498E+18	3.60291E+19	3.60301E+19	5.66860E+19	5.66876E+19
4.32000E+05	1.43242E+17	1.43242E+17	3.88043E+19	3.88057E+19	6.10524E+19	6.10546E+19
8.64000E+05	2.05182E+14	2.05183E+14	3.88599E+19	3.88502E+19	6.11399E+19	6.11246E+19
1.29600E+06	2.93907E+11	2.93908E+11	3.88600E+19	3.88502E+19	6.11400E+19	6.11246E+19
1.72800E+06	4.20998E+08	4.21001E+08	3.88600E+19	3.88502E+19	6.11400E+19	6.11246E+19
Max. diff. (%)		0.00071		-0.02522		-0.02519

Decay times (s)	A _A (Total)	A _F (Total)
1.80000E+04	1.15386E+15	1.153862E+15
3.60000E+04	8.78328E+14	8.783278E+14
5.40000E+04	6.68590E+14	6.685895E+14
7.20000E+04	5.08935E+14	5.089352E+14
1.72800E+05	1.10428E+14	1.104280E+14
4.32000E+05	2.17131E+12	2.171308E+12
8.64000E+05	3.11022E+09	3.110227E+09
1.29600E+06	4.45513E+06	4.455155E+06
1.72800E+06	6.38161E+03	6.381658E+03
Max. diff. (%)		0.00075

This test considers the treatment of decay branching by FISPACT. The branching ratios are taken from the decay data library. There is excellent agreement with the analytical calculations (two Bateman calculations).

⁹⁵Zr decay (test_d12)

The branching in this series of decays means that three Bateman calculations were carried out.

Decay times (s)	N _A (Zr-95)	N _F (Zr-95)	N _A (Nb-95)	N _F (Nb-95)	N _A (Nb-95m)	N _F (Nb-95m)
5.00000E+04	9.93755E+19	9.93755E+19	6.14462E+17	6.14462E+17	6.50115E+15	6.50115E+15
1.00000E+05	9.87549E+19	9.87549E+19	1.21874E+18	1.21874E+18	1.22777E+16	1.22777E+16
5.00000E+05	9.39275E+19	9.39275E+19	5.69544E+18	5.69544E+18	4.00890E+16	4.00891E+16
1.00000E+06	8.82238E+19	8.82238E+19	1.04522E+19	1.04522E+19	5.08443E+16	5.08444E+16
2.00000E+06	7.78344E+19	7.78344E+19	1.75687E+19	1.75687E+19	5.03606E+16	5.03615E+16
3.00000E+06	6.86685E+19	6.86685E+19	2.21402E+19	2.21402E+19	4.50258E+16	4.50267E+16
4.00000E+06	6.05819E+19	6.05819E+19	2.48127E+19	2.48128E+19	3.97879E+16	3.97887E+16
5.00000E+06	5.34476E+19	5.34477E+19	2.60884E+19	2.60884E+19	3.51094E+16	3.51101E+16
6.00000E+06	4.71536E+19	4.71536E+19	2.63534E+19	2.63534E+19	3.09756E+16	3.09762E+16
8.00000E+06	3.67017E+19	3.67017E+19	2.49620E+19	2.49621E+19	2.41097E+16	2.41100E+16
1.00000E+07	2.85665E+19	2.85665E+19	2.22418E+19	2.22419E+19	1.87656E+16	1.87659E+16
5.00000E+07	1.90234E+17	1.90234E+17	2.27795E+17	2.27797E+17	1.24967E+14	1.25025E+14
1.00000E+08	3.61888E+14	3.61889E+14	4.35724E+14	4.35726E+14	2.37729E+11	2.37739E+11
Max. diff. (%)		0.00028		0.00046		0.04641

Decay times (s)	N _A (Mo-95)	N _F (Mo-95)	A _A (Total)	A _F (Total)
5.00000E+04	3.54592E+15	3.54591E+15	1.26065E+13	1.260649E+13
1.00000E+05	1.41038E+16	1.41038E+16	1.26802E+13	1.268019E+13
5.00000E+05	3.36946E+17	3.36946E+17	1.31641E+13	1.316405E+13
1.00000E+06	1.27317E+18	1.27318E+18	1.35644E+13	1.356442E+13
2.00000E+06	4.54657E+18	4.54656E+18	1.38940E+13	1.389400E+13
3.00000E+06	9.14630E+18	9.14628E+18	1.37823E+13	1.378232E+13
4.00000E+06	1.45655E+19	1.45655E+19	1.33705E+13	1.337051E+13
5.00000E+06	2.04289E+19	2.04288E+19	1.27588E+13	1.275883E+13
6.00000E+06	2.64621E+19	2.64621E+19	1.20219E+13	1.202182E+13
8.00000E+06	3.83121E+19	3.83121E+19	1.03779E+13	1.037787E+13
1.00000E+07	4.91729E+19	4.91729E+19	8.72274E+12	8.722740E+12
5.00000E+07	9.95818E+19	9.95820E+19	7.63643E+10	7.636481E+10
1.00000E+08	9.99992E+19	9.99994E+19	1.45816E+08	1.458174E+08
Max. diff. (%)		0.00079		0.00096

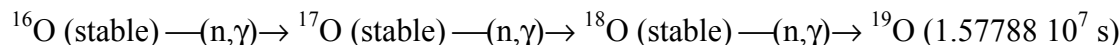
The agreement between the FISPACT and the analytical calculations for this reasonably complex decay chain demonstrates the validity of the method used in FISPACT.

Reaction tests

It is much more difficult to make direct comparison of FISPACT calculations with analytical calculations for cases that model a neutron irradiation. This is because the non-zero cross sections for pairs of reactions such as (n,γ) and (n,2n) mean that it is not possible to start at the initial nuclide and solve the differential equations for each nuclide in the chain sequentially. Indeed, if it were easy to make analytical solutions then there would be no need for a numerical code such as FISPACT! However, by using the FISPACT facility to overwrite data for a particular run it is possible to consider

some simplified pathways that can be solved analytically. Three cases are considered, and one of these is the pathway that was considered in the IAEA Benchmark⁴⁵.

Oxygen reactions (test_r1)



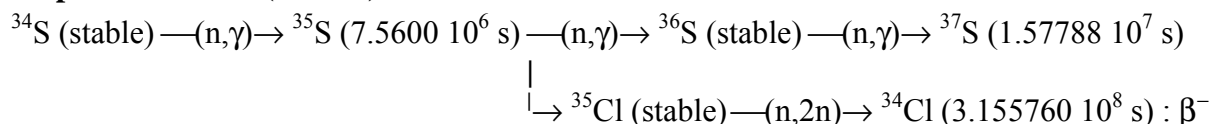
Cross section libraries contain many reactions on the oxygen isotopes other than the capture reactions. For this simplified pathway all these cross sections are set to zero by means of the **OVER** code word in the input file. Note that the correct half-life of ¹⁹O is 26.91 s, but with such a short half-life all the ¹⁹O atoms will have already decayed by the end of the 1 y irradiation; to avoid this the half-life is altered to 0.5 y.

The values of the cross sections used for the calculations are included in the table below.

Nuclide	Reaction	Cross section (b)	N _A	N _F	diff. (%)
O-16	(n,γ)	6.60189E-05	9.99998E+19	9.99998E+19	0.00000
O-17	(n,γ)	1.18499E-04	2.08340E+14	2.08339E+14	0.00048
O-18	(n,γ)	5.42613E-05	3.89555E+08	3.89546E+08	-0.00205
O-19	-	-	1.62633E+02	1.62549E+02	-0.00052

This pathway is particularly simple since all the nuclides (apart from the final one) are stable. Only a single Bateman calculation is required, and agreement even for the final nuclide is impressive.

Sulphur reactions (test_r2)

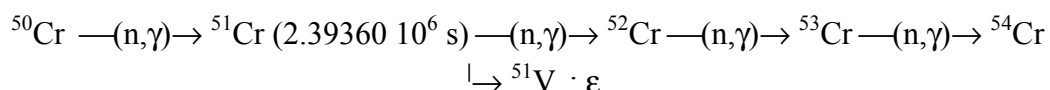


The correct half-lives of ³⁷S and ³⁴Cl are 4.99 m and 1.256 s respectively, but to ensure sensible numbers of atoms after the 1 y irradiation these half-lives are set to 0.5 and 10 y, respectively. The values of the cross sections used for the calculations are included in the table below.

Nuclide	Reaction	Cross section (b)	N_A	N_F	diff. (%)
S-34	(n, γ)	6.58663E-03	9.99794E+19	9.99792E+19	-0.00016
S-35	(n, γ)	5.64830E-03	6.78468E+15	6.78464E+15	-0.00056
S-36	(n, γ)	5.83017E-03	8.62295E+11	8.62290E+11	-0.00058
S-37	-	-	4.44595E+07	4.44598E+07	0.00067
Cl-34	-	-	5.02308E+10	5.02304E+10	-0.00080
Cl-35	(n,2n)	2.92143E-04	1.39982E+16	1.39981E+16	-0.00071

This pathway is more complicated since ³⁵S is radioactive and therefore the reactions and decays compete, giving a branched pathway that requires two Bateman calculations.

Chromium reactions (test_r3)



In the above diagram all the nuclides are stable except ⁵¹Cr. In addition to the reactions shown, other reactions on ⁵⁰Cr, ⁵¹Cr, ⁵²Cr and ⁵³Cr are possible. The values of the cross sections have been changed so that they agree with the values used in the benchmark calculation. The values chosen can be seen in the FISPACT input file in the Annex. In addition various half-lives and cross sections have been changed so that the numbers of atoms of each chromium nuclide are determined solely by the pathway shown above.

The values of the cross sections used for the calculations are included in the table below.

Nuclide	Reaction	Cross section (b)	N_A	N_F	diff. (%)
Cr-50	(n, γ)	1.36187E-2	9.90825E+24	9.90825E+24	0.00000
Cr-51	(n, γ)	2.51242E-2	1.69666E+21	1.69666E+21	0.00000
Cr-52	(n, γ)	5.26653E-3	4.37656E+18	4.37656E+18	0.00000
Cr-53	(n, γ)	1.49953E-2	1.19852E+15	1.19852E+15	0.00000
Cr-54	-	-	6.29661E+11	6.29661E+11	0.00000

Two Bateman calculations are required in this case. The agreement between FISPACT and the analytical solution demonstrates the validity of the methods used in FISPACT.

Annex: FISPACT input files

test_d1

```
NOHEAD
MONITOR 1
EAFV 4
AINP
FISPACT
* DECAY OF H-3
FUEL 1
  H3 1.0E20
DENSITY 8.988E-5
MIND 1.E5
GRAPH 1 0 1 1
UNCERT 0
LEVEL 100 1
FLUX 0.0
ZERO
TIME 1.0 YEARS ATOMS
TIME 4.0 YEARS ATOMS
TIME 5.0 YEARS ATOMS
TIME 5.0 YEARS ATOMS
TIME 5.0 YEARS ATOMS
TIME 10.0 YEARS ATOMS
TIME 10.0 YEARS ATOMS
TIME 10.0 YEARS ATOMS
TIME 50.0 YEARS ATOMS
END
* END
```

test_d2

```
NOHEAD
MONITOR 1
EAFV 4
AINP
FISPACT
* DECAY OF HE-6
FUEL 1
  HE6 1.0E20
DENSITY 1.785E-4
MIND 1.E5
GRAPH 1 0 1 1
UNCERT 0
LEVEL 100 1
FLUX 0.0
ZERO
TIME 0.01 ATOMS
TIME 0.04 ATOMS
TIME 0.05 ATOMS
TIME 0.4 ATOMS
TIME 0.5 ATOMS
TIME 4.0 ATOMS
TIME 5.0 ATOMS
TIME 5.0 ATOMS
END
* END
```

test_d3

```

NOHEAD
MONITOR 1
EAFV 4
AINP
FISPACT
* DECAY OF BE-10
FUEL 1
  BE10 1.0E20
DENSITY 1.848
MIND 1.E5
GRAPH 1 0 1 1
UNCERT 0
LEVEL 100 1
FLUX 0.0
ZERO
TIME 5.0E5 YEARS ATOMS
TIME 5.0E5 YEARS ATOMS
TIME 5.0E5 YEARS ATOMS
TIME 5.0E5 YEARS ATOMS
TIME 3.0E6 YEARS ATOMS
TIME 5.0E6 YEARS ATOMS
TIME 1.0E7 YEARS ATOMS
TIME 1.0E7 YEARS ATOMS
TIME 2.0E7 YEARS ATOMS
END
* END

```

test_d4

```

NOHEAD
MONITOR 1
EAFV 4
AINP
FISPACT
* DECAY OF C-11
FUEL 1
  C11 1.0E20
DENSITY 1.9
MIND 1.0
GRAPH 1 0 1 1
UNCERT 0
LEVEL 100 1
FLUX 0.0
ZERO
TIME 5.0 MINS ATOMS
TIME 5.0 MINS ATOMS
TIME 10.0 MINS ATOMS
TIME 10.0 MINS ATOMS
TIME 30.0 MINS ATOMS
TIME 1.0 HOURS ATOMS
TIME 3.0 HOURS ATOMS
TIME 5.0 HOURS ATOMS
TIME 5.0 HOURS ATOMS
TIME 5.0 HOURS ATOMS
END
* END

```

test_d5

```
NOHEAD
MONITOR 1
EAFV 4
AINP
FISPACT
* DECAY OF AL-26M
FUEL 1
  AL26M 1.0E20
DENSITY 2.6989
MIND 1.E5
GRAPH 1 0 1 1
UNCERT 0
LEVEL 100 1
FLUX 0.0
ZERO
TIME 2.0 ATOMS
TIME 3.0 ATOMS
TIME 10.0 ATOMS
TIME 10.0 ATOMS
TIME 25.0 ATOMS
TIME 50.0 ATOMS
TIME 50.0 ATOMS
TIME 100.0 ATOMS
END
* END
```

test_d6

```
NOHEAD
MONITOR 1
EAFV 4
AINP
FISPACT
* DECAY OF Y-89M
FUEL 1
  Y89M 1.0E20
DENSITY 4.469
MIND 1.0
GRAPH 1 0 1 1
UNCERT 0
LEVEL 100 1
FLUX 0.0
ZERO
TIME 5.0 ATOMS
TIME 5.0 ATOMS
TIME 5.0 ATOMS
TIME 5.0 ATOMS
TIME 30.0 ATOMS
TIME 50.0 ATOMS
TIME 100.0 ATOMS
TIME 100.0 ATOMS
END
* END
```

test_d7

```

NOHEAD
MONITOR 1
EAFV 4
AINP
FISPACT
* DECAY OF CO-58M
FUEL 1
  CO58M 1.0E20
DENSITY 8.90
MIND 1.0
GRAPH 1 0 1 1
UNCERT 0
LEVEL 100 1
FLUX 0.0
ZERO
TIME 2.0 HOURS ATOMS
TIME 3.0 HOURS ATOMS
TIME 5.0 HOURS ATOMS
TIME 14.0 HOURS ATOMS
TIME 9.0 DAYS ATOMS
TIME 10.0 DAYS ATOMS
TIME 20.0 DAYS ATOMS
TIME 20.0 DAYS ATOMS
TIME 20.0 DAYS ATOMS
TIME 20.0 DAYS ATOMS
TIME 100.0 DAYS ATOMS
TIME 100.0 DAYS ATOMS
TIME 200.0 DAYS ATOMS
END
* END

```

test_d8

```

NOHEAD
MONITOR 1
EAFV 4
AINP
FISPACT
* DECAY OF S-39
FUEL 1
  S39 1.0E20
DENSITY 2.07
MIND 1.0
GRAPH 1 0 1 1
UNCERT 0
LEVEL 100 1
FLUX 0.0
ZERO
TIME 5.0 ATOMS
TIME 5.0 ATOMS
TIME 5.0 ATOMS
TIME 35.0 ATOMS
TIME 50.0 ATOMS
TIME 400.0 ATOMS
TIME 500.0 ATOMS
TIME 1000.0 ATOMS
TIME 3000.0 ATOMS
TIME 5000.0 ATOMS
TIME 40000.0 ATOMS
TIME 50000.0 ATOMS
END
* END

```

test_d9

```
NOHEAD
MONITOR 1
EAFV 4
AINP
FISPACT
* DECAY OF FE-53M
FUEL 1
  FE53M 1.0E20
DENSITY 7.874
MIND 1.0
OVER MN53
  ALAM 1.16680E14 1
GRAPH 1 0 1 1
UNCERT 0
LEVEL 100 1
FLUX 0.0
ZERO
TIME 1.0 MINS ATOMS
TIME 1.0 MINS ATOMS
TIME 1.0 MINS ATOMS
TIME 2.0 MINS ATOMS
TIME 5.0 MINS ATOMS
TIME 5.0 MINS ATOMS
TIME 5.0 MINS ATOMS
TIME 5.0 MINS ATOMS
TIME 5.0 MINS ATOMS
TIME 5.0 MINS ATOMS
TIME 10.0 MINS ATOMS
TIME 10.0 MINS ATOMS
TIME 10.0 MINS ATOMS
TIME 1.0 HOURS ATOMS
TIME 1.0 HOURS ATOMS
TIME 3.0 HOURS ATOMS
TIME 6.0 HOURS ATOMS
TIME 12.0 HOURS ATOMS
TIME 1.0 DAYS ATOMS
END
* END
```

test_d10

```
NOHEAD
MONITOR 1
EAFV 4
AINP
FISPACT
* DECAY OF TH-230
FUEL 1
  TH230 1.0E20
DENSITY 11.72
MIND 1.E3
GRAPH 1 0 1 1
UNCERT 0
LEVEL 100 1
FLUX 0.0
ZERO
TIME 1.0E12 ATOMS
TIME 1.0E12 ATOMS
TIME 1.0E12 ATOMS
TIME 1.0E12 ATOMS
TIME 1.0E12 ATOMS
TIME 1.0E12 ATOMS
TIME 4.0E12 ATOMS
TIME 4.0E13 ATOMS
END
* END
```

test_d11

```

NOHEAD
MONITOR 1
EAFV 4
AINP
FISPACT
* DECAY OF CU-64
FUEL 1
  CU64 1.0E20
DENSITY 8.96
MIND 1.0
GRAPH 1 0 1 1
UNCERT 0
LEVEL 100 1
FLUX 0.0
ZERO
TIME 5.0 HOURS ATOMS
TIME 5.0 HOURS ATOMS
TIME 5.0 HOURS ATOMS
TIME 5.0 HOURS ATOMS
TIME 28.0 HOURS ATOMS
TIME 3.0 DAYS ATOMS
TIME 5.0 DAYS ATOMS
TIME 5.0 DAYS ATOMS
TIME 5.0 DAYS ATOMS
END
* END

```

test_d12

```

NOHEAD
MONITOR 1
EAFV 4
AINP
FISPACT
* DECAY OF ZR-95
FUEL 1
  ZR95 1.0E20
DENSITY 6.506
MIND 1.0E5
GRAPH 1 0 1 1
UNCERT 0
LEVEL 120 1
FLUX 0.0
ZERO
TIME 5.0E4 ATOMS
TIME 5.0E4 ATOMS
TIME 4.0E5 ATOMS
TIME 5.0E5 ATOMS
TIME 1.0E6 ATOMS
TIME 1.0E6 ATOMS
TIME 1.0E6 ATOMS
TIME 1.0E6 ATOMS
TIME 1.0E6 ATOMS
TIME 1.0E6 ATOMS
TIME 2.0E6 ATOMS
TIME 2.0E6 ATOMS
TIME 4.0E7 ATOMS
TIME 5.0E7 ATOMS
END
* END

```

test_r1

```
NOHEAD
MONITOR 1
EAFV 4
AINP
FISPACT
* Simplified reactions on O-16
FUEL 1
  O16 1.0E20
DENSITY 0.001429
<< 1918 = H-1 >>
<< 1919 = H-2 >>
<< 1920 = H-3 >>
<< 1922 = He-4 >>
OVER O16
  ACROSS O17 6.60189E-5
  ACROSS C13 0.0
  ACROSS C12 0.0
  ACROSS N16 0.0
  ACROSS N15 0.0
  ACROSS 1918 0.0
  ACROSS 1919 0.0
  ACROSS 1922 0.0
OVER O17
  ACROSS O18 1.18499E-4
  ACROSS O16 0.0
  ACROSS C13 0.0
  ACROSS N17 0.0
  ACROSS N16 0.0
  ACROSS N15 0.0
  ACROSS C14 0.0
  ACROSS 1918 0.0
  ACROSS 1919 0.0
  ACROSS 1920 0.0
  ACROSS 1922 0.0
OVER O18
  ACROSS O19 5.42613E-5
  ACROSS O17 0.0
  ACROSS O16 0.0
  ACROSS C14 0.0
  ACROSS N18 0.0
  ACROSS N16 0.0
  ACROSS C15 0.0
  ACROSS 1918 0.0
  ACROSS 1920 0.0
  ACROSS 1922 0.0
OVER O19
  ALAM 0.5 5
MIND 1.0
HALF
DOMINANT 100.0
UNCERT 3
LEVEL 100 1
FLUX 1.0E15
TIME 1.0 YEARS
ATOMS
END
* END
```


test_r2

```
NOHEAD
MONITOR 1
EAFV 4
AINP
FISPACT
* Simplified reactions on S-34
FUEL 1
  S34 1.0E20
DENSITY 2.07
<< 1918 = H-1 >>
<< 1919 = H-2 >>
<< 1920 = H-3 >>
<< 1921 = He-3 >>
<< 1922 = He-4 >>
<< 121 = Cl-34m >>
OVER S34
  ACROSS S35 6.58663E-3
  ACROSS S33 0.0
  ACROSS SI30 0.0
  ACROSS P34 0.0
  ACROSS P33 0.0
  ACROSS P32 0.0
  ACROSS SI32 0.0
  ACROSS SI31 0.0
  ACROSS 1918 0.0
  ACROSS 1919 0.0
  ACROSS 1920 0.0
  ACROSS 1921 0.0
  ACROSS 1922 0.0
OVER S35
  ACROSS S36 5.64830E-3
  ACROSS S34 0.0
  ACROSS SI31 0.0
  ACROSS P35 0.0
  ACROSS P34 0.0
  ACROSS P33 0.0
  ACROSS SI32 0.0
  ACROSS 1918 0.0
  ACROSS 1919 0.0
  ACROSS 1920 0.0
  ACROSS 1922 0.0
OVER S36
  ACROSS S37 5.83017E-3
  ACROSS S35 0.0
  ACROSS SI32 0.0
  ACROSS P36 0.0
  ACROSS P35 0.0
  ACROSS P34 0.0
  ACROSS SI33 0.0
  ACROSS 1918 0.0
  ACROSS 1919 0.0
  ACROSS 1920 0.0
  ACROSS 1922 0.0
OVER S37
  ALAM 0.5 5
OVER CL35
  ACROSS CL34 2.92143E-4
  ACROSS 121 0.0
  ACROSS P31 0.0
  ACROSS CL36 0.0
  ACROSS S35 0.0
  ACROSS S34 0.0
  ACROSS S33 0.0
  ACROSS P33 0.0
  ACROSS P32 0.0
  ACROSS P34 0.0
  ACROSS 1918 0.0
  ACROSS 1919 0.0
  ACROSS 1920 0.0
  ACROSS 1921 0.0
  ACROSS 1922 0.0
OVER CL34
  ALAM 10.0 5
MIND 1.0
HALF
DOMINANT 100.0
UNCERT 3
```

```

LEVEL 100 1
FLUX 1.0E15
TIME 1.0 YEARS
ATOMS
END
* END

```

test_r3

```

NOHEAD
MONITOR 1
EAFV 4
AINP
FISPACT
* Simplified reactions on Cr-50
FUEL 1
  CR50 1.0E25
DENSITY 7.19
<< 1918 = H-1 >>
<< 1919 = H-2 >>
<< 1920 = H-3 >>
<< 1921 = He-3 >>
<< 1922 = He-4 >>
OVER CR50
  ACROSS CR49 0.0
  ACROSS TI46 0.0
  ACROSS TI47 0.0
  ACROSS TI48 0.0
  ACROSS TI49 0.0
  ACROSS CR51 1.36187E-2
  ACROSS V50 3.37120E-2
  ACROSS V49 3.28852E-2
  ACROSS 1918 -6.52733E-2
  ACROSS 1919 -1.32379E-3
  ACROSS 1921 0.0
  ACROSS 1922 0.0
OVER CR51
  ACROSS CR50 0.0
  ACROSS TI47 0.0
  ACROSS TI50 0.0
  ACROSS CR52 2.51242E-2
  ACROSS V51 3.11597E-2
  ACROSS V50 3.80524E-3
  ACROSS V49 1.29794E-4
  ACROSS TI49 2.36955E-7
  ACROSS TI48 8.43151E-3
  ACROSS 1918 -3.38729E-2
  ACROSS 1919 -1.09204E-3
  ACROSS 1920 -1.29794E-4
  ACROSS 1921 -2.36955E-7
  ACROSS 1922 -8.43151E-3
  ALAM 2.3936E6 1
OVER CR52
  ACROSS CR51 0.0
  ACROSS TI48 0.0
  ACROSS V52 0.0
  ACROSS TI50 0.0
  ACROSS TI51 0.0
  ACROSS CR53 5.26653E-3
  ACROSS V51 8.62371E-3
  ACROSS TI49 3.94947E-3
  ACROSS 1918 -7.71701E-3
  ACROSS 1919 -9.06704E-4
  ACROSS 1921 0.0
  ACROSS 1922 -3.94947E-3
OVER CR53
  ACROSS CR52 0.0
  ACROSS TI49 0.0
  ACROSS V53 0.0
  ACROSS V52 0.0
  ACROSS TI51 0.0
  ACROSS TI50 0.0
  ACROSS TI52 0.0
  ACROSS CR54 1.49953E-2
  ACROSS V51 6.37435E-5
  ACROSS 1918 0.0
  ACROSS 1919 0.0
  ACROSS 1920 -6.37435E-5
  ACROSS 1921 0.0
  ACROSS 1922 0.0

```

```
OVER CR54
  ACROSS CR53 0.0
  ACROSS TI50 0.0
  ACROSS CR55 0.0
  ACROSS V54 0.0
  ACROSS V53 0.0
  ACROSS V52 0.0
  ACROSS TI51 0.0
  ACROSS 1918 0.0
  ACROSS 1919 0.0
  ACROSS 1920 0.0
  ACROSS 1922 0.0
OVER V52
  ALAM 1.0E25 1
OVER V53
  ALAM 1.0E25 1
OVER V54
  ALAM 1.0E25 1
OVER MN53
  ALAM 1.0E25 1
OVER MN54
  ACROSS CR54 0.0
  ALAM 1.0E25 1
OVER MN55
  ACROSS CR54 0.0
OVER FE55
  ACROSS CR54 0.0
OVER FE57
  ACROSS CR54 0.0
OVER FE58
  ACROSS CR54 0.0
MIND 1.0
HALF
DOMINANT 100.0
UNCERT 3
LEVEL 100 1
FLUX 3.64099E15
TIME 1.0 YEARS
ATOMS
END
* END
```

Appendix 20 – Non-steady irradiation

Introduction

Modelling the irradiation history for a FISPACT calculation requires considerable understanding of the physics of the situation and the way in which FISPACT works. Although several recommendations about non-steady or pulsed irradiations are made in the body of this document, they are gathered together here with some additional background information.

Modelling an irradiation

Most irradiation histories that correspond to realistic devices will be non-steady. This is because devices must be switched on and off for maintenance and because of unforeseen circumstances. Also neutron sources cannot be expected to operate for long periods of time without fluctuation. The simplest approach to modelling such a situation is to use a continuous flux of neutrons for the total time of irradiation (T) such that the fluence in the model is the same as the measured fluence. This simple approach conserves both the fluence and the irradiation time. This will be adequate in many situations (*e.g.* if waste management issues are being studied) especially if the times of interest for the inventories are long compared to T . However, if the inventories at short times after the end of the irradiation are needed (as for safety studies) then the amounts of short-lived radionuclides need to be accurately calculated.

Consider the cases of short- and long-lived radionuclides (time scales are always considered relative to T) formed by a reaction on a target that is initially present. The long-lived nuclide will build up in a linear fashion during the irradiation as the long half-life means that little will have decayed. In contrast, the short-lived nuclide will initially rise linearly, but then saturate as equilibrium between formation and decay (secular equilibrium) is reached. Thus at the end of the irradiation (assuming that it is steady prior to shut-down) the effect of

fluctuations of flux near the start will have little effect, the long-lived nuclide will build up when ever the flux is present, while the short-lived nuclide will reach equilibrium quickly after a change in flux. Thus the inventory at the end of the irradiation is very insensitive to changes in flux at the start.

If there are changes in flux near the end of the irradiation, this will affect levels of the short-lived nuclides dramatically, having an off period followed by a 10 times higher pulse at the end of irradiation will give approximately 10 times more nuclide than a steady flux that lasts 10 times as long (fluence conserved). Thus modelling the irradiation carefully at the end of the irradiation is crucial, while careful modelling at the start is unimportant.

Thus the recommendation about a non-steady irradiation is to model in detail the final time before shut-down, for example by using the correct on/off details with variable fluxes. For the rest of the irradiation (the bulk of it after the start) use a continuous flux such that the irradiation time and the fluence are conserved. Further discussion of this is given in references 46 and 47.

Implications for FISPACT

FISPACT is able to model non-steady irradiations of arbitrary complexity. Indeed the loop construct (**PULSE** and **ENDPULSE**) was specifically added to aid such calculations. However, bearing in mind the conclusions of the previous section there would be little to be gained from using all of say 10,000 equal pulses, it would be preferable to use a steady irradiation for 9,990 of them and consider only the final 10 in detail. This saves time in setting up the input file, time in calculation and in the size of the output.

However, there is one important area in which the modelling of the irradiation is crucial when calculating pathways and uncertainties. The method used by FISPACT in the routine calculation of uncertainties stores the values of the inventory at

the end of the first irradiation period. These values are then used at latter times when long-lived nuclides become dominant and so contribute in the uncertainty calculation. It is therefore important that the first irradiation period should contain the bulk of the fluence so that an accurate calculation of uncertainties is possible. Using a short on pulse at the beginning of the irradiation would mean that completely wrong uncertainty estimates would be calculated. This reinforces the conclusion of the previous section:

Use a steady flux for all but the last few (5 – 10) on/off intervals. Conserve total irradiation time and fluence.

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