CCFE-R(11)11 Issue 6
June 2014

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This work was funded by the RCUK Energy Programme under grant EP/I501045.

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Date of Issue: 4 August 2014			Issue number: 6
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Executive Summary

FISPACT-II is an inventory code capable of performing modelling of activation, transmutations and burn-up induced by neutron, proton, alpha, deuteron or gamma particles incident on matter. It is a completely new inventory code initially designed to be a functional replacement for FISPACT-2007, but now extended to have substantially more capability.

FISPACT-II is written in object fortran and has full dynamic memory allocation. It has improved algorithms for the ode solver, pathways, uncertainty and sensitivity calculations. All these can be used in multi-pulse irradiation calculations, including those where the flux spectrum changes from pulse to pulse. It can now read ENDF-style data libraries in addition to the EAF libraries, and the present version uses the latest TALYS-based TENDL-2011, TENDL-2012 and TENDL-2013 evaluated nuclear data libraries together with probability table data from CALENDF for including self-shielding in the calculations. These libraries allow additional projectiles and nuclides to be included, and make possible additional kerma, dpa and appm diagnostics.

This document is its User Manual. It first outlines what calculations the code performs and how the code differs from FISPACT-2007. It has a 'getting-started' section to provide a basic introduction to new users. It explains the use and provides examples of all the keywords used in the input file to specify a FISPACT-II run and describes how all the data files are connected. It introduces the test cases provided with the code and gives a guide to interpreting the physical output and logging output from the code. It also introduces subsidiary programs for printing output and for compressing the ENDF cross-section libraries.

Three appendices are provided; the first outlines the physical and mathematical models implemented in the code. The second summarises the EAF nuclear data used by the code, giving background information on the data files and examples of neutron spectra suitable for various applications. The final appendix describes the ENDF data forms introduced in Version 2 of the code.

Revision History

Revision	Date	Issued by	Comment
0.0	28 October 2010	J G Morgan	Initial Template
1.0	1 December 2010	J W Eastwood	Partial document for alpha release
1.1	10 May 2011	J W Eastwood	Revised and expanded for 1-00-beta release
1.2	21 September 2011	J W Eastwood	Revised and expanded for Release 1-00
2.1	14 March 2012	J W Eastwood	Revised and expanded for Release 2-00
2.2	18 July 2012	J W Eastwood	Minor corrections for Release-2-00-01
2.3	27 September 2012	J W Eastwood	Minor corrections for Release-2-00-02
2.4	31 May 2013	J W Eastwood	Revised and expanded for Release-2-10-00
2.5	30 June 2014	J W Eastwood	Revised and expanded for Release-2-20-00
2.6	4 Aug 2014	J W Eastwood	Revised for Release-2-20-01

CVS document source revision

```
Name: Release-2-20-01
RCSfile: sd7.tex,v
Revision: 1.74
Author: jim
Date: 2014/08/08 10:07:01
```

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1 Introduction

This document contains guidance and reference material for users of FISPACT-II.

FISPACT-II is a completely new inventory code designed to be a functional replacement for FISPACT-2007 [1]. This new code is written in object-style Fortran 95 [2, 3, 4, 5, 6, 7], and has extended physical models and improved numerical algorithms compared to the old code. Users familiar with the old code will be able for most cases to use the new code with their existing control input files. Some new keywords have been added to deal with the new capabilities, and some of the old keywords have become obsolete. The differences between FISPACT-II and FISPACT-2007 that are relevant to the user are listed in Section 3 below.

This version of the user manual refers to the Version 2.20 release of FISPACT-II. There have been three major versions of the code:

Version 0 was a direct functional replacement for FISPACT-2007. It differed in that it used improved algorithms and was written in object Fortran 95. The data encapsulation, together with full dynamic memory allocation provided a robust and flexible platform for the new capabilities introduced in the later versions to be built on.

It used the same user input files and was designed to use the European Activation File (EAF-2007 [8, 9, 10] and EAF-2010 [11, 12, 13]) data sets for cross-section, decay, fission, and radiological quantities and was extensively validated and cross-checked against FISPACT-2007. Discrepancies in the results from the two codes have been shown to arise from the increased number of reactions and improved numerical methods employed in the new code.

Version 1 began the process of extending the activation-transmutation prediction capability whilst maintaining the validation heritage of FISPACT-2007. New pathways and new monte-carlo sensitivity capabilities were introduced to extend both pathways and sensitivity calculations to multi-pulse irradiation cases. The reading and processing of CALENDF [14] probability table data was introduced in the calculation of cross-section collapse to include self-shielding effects in the inventory calculations.

Version 2 The major change introduced in Release 2.0 of FISPACT-II was the addition of the reading and processing of alternative ENDF-format library data sets. This caused a major overhaul of the data input parts of the software and a huge expansion of the number of nuclides and reactions that can be treated; better fission yield data and cross-section data in more energy groups up to higher energies can now be used (see Appendix C on page 195). This version can also handle more irradiating projectiles (γ, n, p, d, α) and provides additional diagnostic outputs (kerma, dpa and gas appm rates) if the ENDF-format library contains the required input data.

Features added in Release 2.10 are self-shielding using the universal sigmoid curve approximation (c.f., Appendix A.4.4), processing of covariances between different reactions, extended pathways analysis features, handling additional isomeric states and the capability to use the TENDL-2012 library data.

The present release (Release 2.20) includes ENDFB-VII.1, JEFF 3.2 and JENDL 4.0 nuclear data libraries and the capability to read and process them. It can compress these and the TENDL libraries to allow faster collapse calculations. There is a new interface module that allows inventories to computed for multiple flux spectra and returned to a calling program. There is also a separate FISPACT_MP program that allows inventory calculations to be performed for simulataneous irradiation by several different projectiles [15].

Included with the FISPACT-II Version 2.20 distribution are over 270 test input files per library that exercise the code options and datasets. FISPACT-II has been compiled using Intel, Oracle, gfortran and g95 Fortran compilers and has been shown to give the same results (apart from roundoff errors) on Unix, Linux, Mac-OS and Windows machines.

1.1 Structure of the Document

Section 2 contains a brief summary of what FISPACT-II does, and Section 3 summarises the differences from FISPACT-2007.

Section 4 provides an introductory guide to the new user by walking through some simple example runs of FISPACT-II, the data for which may be found in the `getting_started` subdirectory of the test data tree provided with the code. It also describes how to speed up calculations by using compressed ENDF libraries and reduced nuclide indexes.

Section 5 on page 44 contains a summary of all the keywords that users may use in the run control files. Section 6 shows where to find examples of uses of these keywords in input files and the resulting output files in the `fispQA2010` and `fispQA` test directories.

A guide to interpreting the output from FISPACT-II is given in Section 7 on page 99.

The first appendix (page 133) expands on the details of the model used in the code, and the decay, reaction and spectrum types recognised by the software. The second appendix (page 169) summarises the EAF library data. The final appendix (page 195) summarises the ENDF library data that can be read by Version 2 of the code.

2 What FISPACT-II Does

FISPACT-II is a practical activation-transmutation engineering prediction tool. The four principal tasks that it undertakes are

1. extraction, reduction and storage of nuclear and radiological data from the EAF or ENDF library files;
2. construction and solution of the rate equations to determine the time evolution of the inventory in response to different irradiation scenarios. These scenarios include
   (a) a cooling-only calculation;
   (b) a single irradiation pulse followed by cooling;
   (c) multiple irradiation pulses where only flux amplitudes change, followed by cooling;
   (d) multi-step irradiation where flux amplitude, flux spectra and cross-sections may change, followed by cooling.
3. computation and output of derived radiological quantities;
4. subsidiary calculations to identify the key reactions and decays, and to assess the quality of the predictions. The four main subsidiary items are
   (a) pathways analysis;
   (b) uncertainty calculations from pathways;
   (c) reduced model calculations;
   (d) monte-carlo sensitivity and uncertainty calculations.

These items are described further in the following subsections.

2.1 Library Data Preparation

The library preparation task comprises reading and 'collapsing' the cross-section data, reading, 'condensing' and storing the decay data and fission data, and storing the regulatory radiological data (potential biological hazards, clearance data and legal transport data).

FISPACT-II constructs 'effective' cross-sections by 'collapsing' the energy dependent cross-sections in the EAF or ENDF libraries, i.e., taking the weighted average over energy of the cross-section weighted by the irradiating projectile flux (Equation (10) on page 134), where the projectiles may be neutrons, protons, deuterons, alpha particles or gamma rays. The collapse process differs slightly depending on the data libraries used:

EAF The cross-section data in the EAF-2010 library come in 9 different energy group structures and the most appropriate choice depends on the application and the energy spectrum of the irradiating flux (see Appendices B.1 and B.2). Provided with the EAF library are a number of sample projectile flux spectra for specific

applications in energy groups that match the cross-section energy groups (see Appendix B.3). FISPACT-II can also take user-defined spectra specified in arbitrary groups and convert them into a suitable form to match the cross-section energy groups. Uncertainties in the cross-sections are available only as variances in fewer (up to five) energy groups and are assumed to be uncorrelated. These are 'collapsed' and stored for use in evaluating uncertainties and sensitivities (see.Appendices B.1 and B.2.5).

ENDF The cross-section data in the TENDL-2013 data sources come in two group structures, the CCFE(709) group scheme for neutron induced cross-sections and the CCFE(162) group scheme for p, d, α and γ-induced reactions. The cross-sections are collapsed in the same manner as is used for the EAF data, but the cross-section uncertainties are found using the ENDF-6 [16] LB=5 covariance data in the manner described in Appendix A.2. The EAF cross-section and uncertainty data for the 616-group structure have been converted to the same format to provide Verification and Validation for the new data input and processing.

A preliminary ENDF data compression step can be used (c.f., Section 4.8) to provide a binary version of the ENDF data that gives a much faster collapse calculation.

The effect of self-shielding on collapsed cross-sections may be introduced using either the probability table method or the universal sigmoid curve method.

In the 'condensing' task, decay constants, branching ratios and discrete decay spectra are read from the EAF (Appendix B.4) or ENDF (Appendix C.5) decay data files. The γ and X-ray lines are used to construct 24-group spectra for use in computing gamma doses from the inventories. In cases where the γ spectrum data are not available, then approximate spectra may be constructed for the purpose of estimating gamma doses (see the **SPEK** keyword and Appendix A.10.3). For the EAF data, fission yield data for actinides where data are available are read from the EAF fission yield library, and for the remainder a neighbouring fission yield is used as specified by the fission association file (Appendix B.5). More extensive fission yield data for more nuclides are available in the TENDL-2013 data in the ENDF library and so the fission association and surrogate daughter schemes are not used for these new data.

The twenty-four decay types, ten spectrum types and ninety reaction types recognised by FISPACT-II when reading the EAF and ENDF library data are summarised in Tables 10, 11 and 12 in Appendix A. The additional seven `MT` values for total cross-sections for gas production, eight for kerma and four for dpa that may appear in the TENDL-2013 data sets are listed in Table 13. Other `MT` values that are recognised by the code but are silently ignored are listed in Table 14. The mapping of reaction `MT` numbers to the CALENDF group `MT` numbers implemented in FISPACT-II are summarised in Table 15.

Printed summaries of the related library data may be output using the **PRINTLIB**

keyword (see page 77).

2.2 Inventory Calculation

Library data preparation provides the cross-sections and decay constants needed to construct the coefficients for the rate equations. The rate equations describe the transmutation of the initial inventory by nuclear reactions induced by the projectiles and by spontaneous radioactive decay (see Appendix A). The inventory calculation then proceeds by

1. setting the physical initial conditions of the target;
2. setting the output selections;
3. specifying the subsidiary calculations;
4. computing the irradiation steps;
5. performing the subsidiary calculations;
6. computing the cooling steps;
7. computing summary data.

Output is written as it becomes available at each step.

The sequence of steps performed in the calculation follows the sequence of steps specified in the user's `input` file controlling the run. The duration of a step is specified by the user, and typically ranges from fractions of a second to many years. During each step, the irradiating flux amplitude, cross-sections and decay rates are kept constant. Also, it is assumed that the imposed projectile flux is not modified by the reactions and decays in the target material. In consequence, the rate equations are linear and have constant coefficients for each step. The material is homogeneous, infinite and infinitely dilute (but in some circumstances, self-shielding can be accommodated in the model) and the description of the evolution of the nuclide numbers is reduced to a stiff set of ordinary differential equations (see Appendix A.1 on page 133). Unlike FISPACT-2007 [1], FISPACT-II does not use the equilibrium approximation for short-lived nuclides and includes the evolution of actinide sources in the rate equations. The core engine of the FISPACT-II stiff-ode solver is the LSODES package [17].

If the inventory calculation includes irradiation, then the first step must have a non-zero irradiating flux amplitude. The rate equation coefficients in subsequent steps may be changed in one or more of the following ways

- changing the flux amplitude;

- changing the library cross-section data (e.g., to take account of temperature effects);
- changing the flux spectrum;

The end of the irradiation (heating) phase is signalled by the **ZERO** keyword in the user input file, and it is this keyword that triggers the subsidiary pathways and sensitivity calculations as well as resetting the elapsed time to zero.

The cooling phase is a sequence of steps the same as the irradiation phase, although the projectile flux amplitude is usually, but not necessarily, set to zero and must be zero for the first cooling step (The purpose of cooling steps with irradiation is to provide flexibility in the range of applicability of pathways analysis and graphical output).

The principal output of an inventory calculation step is the inventory of nuclides at the end of the step.

Secondary outputs are derived from the inventory, the choice of which is controlled by a number of the keywords described later in this manual (see Section 5.3 on page 87 and Appendix A).

2.3 Subsidiary Calculations

The standard inventory calculation employing EAF-2010 library data uses all 2233 nuclides and 66256 reactions that are catalogued in these libraries. If the TENDL-2011, TENDL-2012 and TENDL-2013 library data are used, the number of nuclides increases to 3873 with a corresponding increase in the number of reactions. The dominant nuclides at the end of a sequence of irradiation pulses can be readily identified from lists of nuclides ordered by various radiological quantities derived from the inventory. These lists do not show which dominant nuclide arose from which initial target nuclide, and by what path.

The subsidiary calculations in FISPACT-II provide tools for the user to probe the reactions and decays in detail. Unlike FISPACT-2007, pathways and sensitivity analyses can be undertaken for a series of irradiation pulses rather than for just a single irradiation pulse. Pathways calculations can be to arbitrary depths, and automatically identify loops that make significant differences to the contribution of the paths on which they lie.

The pathways calculation identifies how much of the inventory of each of the dominant nuclides came from which initial nuclide, and by what chains (and loops) of reactions and decays. Specific routes and paths can be probed independently from the dominant nuclide lists, and specific cross-sections and decay rates can be changed to assess their effects.

A reduced list of nuclides can be generated from the pathways information and full inventory calculations can be undertaken on the reduced set of nuclides and reactions to check whether all important reactions and decays are included.

Uncertainty estimates can be made by combining the pathways information with uncertainty data for cross-sections and decay rates.

Sensitivity calculations provide a complementary method of identifying important reactions, providing uncertainty estimates and for quantifying how the uncertainty in the final amount of a nuclide depends on the uncertainty of specific reactions.

3 Differences from FISPACT-2007

Many keywords in the FISPACT-2007 control input file have been retained in FISPACT-II to provide a substantial degree of backwards compatibility. In many cases the new code will run with existing control input files. Some new keywords have been added to deal with the new capabilities of FISPACT-II, and some of the old keywords have become obsolete. Where a keyword no longer works as before, the new code will issue a warning or fatal error message.

3.1 New Features

The new and extended features of FISPACT-II are:

Additional projectiles: five projectiles may now be used (n, p, d, α and γ);

Additional reactions: 90 reaction types are now recognised;

Additional nuclides and elements Elements up to Z=111 are recognised, and the new libraries contain 3873 nuclides;

ENDF format data libraries Capability to read and process TENDL-2011, TENDL-2012 and TENDL-2013 cross-section, uncertainty, decay and fission yield libraries;

Self-shielding: Probability table data generated by CALENDF can now be used in conjunction with the 616 energy group EAF and the 709 energy group TENDL-2013 cross-section data for neutron induced reactions to model dilution effects in the computation of collapsed cross-sections (c.f., Appendix A.4.3). Alternatively, The universal sigmoid curve method for approximating self-shielding can be employed using the MF = 2 data in the TENDL-2013 files (c.f., Appendix A.4.4);

Additional decay types: a total of 24 decay types are now recognised; 7 single decay and 17 multiple particle decay modes;

Input file syntax checking: Checking of the correctness of the `input` file and detailed error reporting has been added to aid the development and testing of new `input` control files (see Section 4.7);

Additional PRINTLIB output: it is now possible to specify the output of photon and material spectral lines;

Kerma, dpa and gas appm Additional cross-section data in the TENDL-2013 cross-section data files are read and processed to permit the output of derived rates of kinetic energy release, displacements per atom and generation rates of gas atoms;

New stiff-ode solver: the solution of the inventory equations is now based on the LSODES package. There is no equilibrium approximation and the time dependence of actinide inventories is treated in full;

New pathways analysis: graph-theory-based tree-searching methods are now used to identify significant pathways, removing the restrictions of the previous methods. All loops and paths are automatically included if their contribution is above the user-specified thresholds, and searches can be made to arbitrary depths. Pathways analysis works for single and multi-pulse irradiation phases and changing cross-sections. Information on all reactions between a given parent and daughter is available and is displayed by pathways output;

Covariance data Reaction cross-section data for different reactions can be read from the TENDL-2013 files and used to produce collapsed covariances and correlations;

New sensitivity analysis: the local derivative sensitivity analysis calculation implemented in FISPACT-2007 that was only applicable for single irradiation pulses has been replaced by a Monte-Carlo sensitivity calculation that works for single and multi-pulse irradiation phases and changing cross-sections;

New reduced nuclide set: runs with subsets of the nuclides in the EAF or ENDF libraries can be undertaken;

Encapsulated data: FISPACT-II is written using an object-based modular code design, including built-in error-logging and code-timing objects. Consequently, the user will observe some differences in the output, particularly the improved reporting of errors and warnings.

Dynamical memory allocation is used throughout, so the same code works for all the data sets irrespective of their sizes.

`files` file changes: Filename mnemonics can be used as an alternative to unit numbers to link external filenames to FISPACT-II input and output streams, and comments can be included in the `files` file. Repeated entries for the same stream name are read into a queue of external filenames, which are used in sequence. (See the **GETXS** keyword below.)

A summary of the physical models and algorithms is given in Appendix A. A more complete treatment of the model, algorithms, architectural design and software specification is given in References [3, 4, 5, 18, 19, 20].

3.2 Obsolete Features

There is very little reliable data for the treatment of sequential charged particle reactions and so this feature has been disabled in the new code to simplify the user interface.

The new algorithms for integrating the rate equations and for computing pathways have led to a number of related keywords (e.g., **LEVEL**, **CONV**, **DOMINANT**, **LOOPS**) becoming redundant. See the following section for details.

3.3 Keyword Changes

All the FISPACT-2007 keywords are recognised by the new program, but where their use has changed error and warning messages are written to the log file. Most obsolete keywords can be ignored by the new code or are replaced with their new equivalents, so that runs of FISPACT-II can still be conducted with historical `input` files.

Note that the new keyword reader will recognise a truncated keyword if three or more leading letters of the keyword given uniquely identify it. The reader will *not* recognise keywords that have extra letters at the end (e.g., **NOFISSION** will not be recognised as **NOFISS**). The following list gives a summary of the changes in keywords.

CLOBBER is a new keyword that allows existing output files to be overwritten. By default, FISPACT-II terminates with a fatal error rather than overwriting an existing output file.

COLLAPSE still works, but is deprecated; use **GETXS** instead.

CONV is now obsolete and its use generates a warning message instructing users to use **TOLERANCE** instead.

COVARIANCE is a new keyword used to instruct FISPACT-II to read and condense covariances between different reactions.

DOMINANT is now obsolete; use **UNCERTAINTY** and **SORTDOMINANT** instead to control dominant nuclide output.

EAFVERSION is now used to distinguish between EAF and ENDF format data libraries; version 8 causes reading of the new-style ENDF library files, while 7 or less causes the reading of EAF libraries (EAF-2007 and EAF-2010 data).

ENFA still works, but is deprecated; use **GETDECAY** instead.

ERROR The **ERROR** sub-keyword of keyword **OVER** has been replaced by **ADCROSS** to avoid conflict with the keyword **ERROR** used in sensitivity calculations.

GETDECAY is a replacement for **ENFA** and its subordinate keywords **TAPA**, **ARRAY** and **LINA**.

GETXS is a replacement for the **COLLAPSE** and **NEWFILE** keywords.

GRAPH now has an additional option to write output suitable for gnuplot.

INDEXPATH has been added to allow the user to create a reduced nuclide index file containing only those nuclides that lie on pathways from the initial inventory nuclides to the dominant nuclides at the end of the irradiation phase.

LOOPS is now obsolete and its use generates a warning message to use the updated **UNCERTAINTY** keyword instead.

LOOKAHEAD is a new keyword used to fine-tune pathways calculations.

MCSAMPLE has been added to control parameters for the Monte-Carlo sampling used in sensitivity calculations.

MCSEED has been added to allow users to specify the pseudo-random number sequence for sensitivity calculations.

MIND now affects only the inventory output, not the calculation.

NEWFILE is now obsolete and is ignored, apart from generating a warning message. Its functionality has been implemented with the **GETXS** keyword in association with multiple cross-section files in the `files` file.

NOHEAD has been replaced by **NOHEADER**.

NOSTAB has been replaced by **NOSTABLE**.

OVER now accepts an alternative name of **ADCROSS** for the subordinate keyword **ERROR** and a new subordinate keyword **ADLAM** for the input of a new error factor for the half-life.

PATHRESET is a new keyword that allows pathways calculations to be repeated at times after the initial pathways calculation at the end of the irradiation phase.

PROBTABLE is a new keyword that causes the probability table data to be read and used for the nuclides specified by the **SSFCHOOSE** keyword.

SAVELINES is a new keyword that causes spectral lines to be read from the decay file and stored. It is needed if the new **PRINTLIB** 5 option to print decay lines is used.

SEQNUMBER has no effect apart from generating a warning message.

SEQUENTIAL has no effect apart from generating a warning message.

SORTDOMINANT is a new keyword to control the uncertainty calculations and their display in the output file.

SSFCHOOSE is a new keyword used to specify the nuclides for which the self-shielding factors are computed.

SSFDILUTION is a new keyword to provide expert control of dilution values used in applying the self-shielding corrections.

SSFFUEL is a new keyword used to specify directly the mixture of nuclides to be used in the self-shielding calculations.

SSFGEOMETRY is a new keyword that allows thin and thick target geometry information to be input for use in conjunction with the universal sigmoid curve approximation for self-shielding.

SSFMASS is a new keyword used to specify indirectly the mixture of nuclides to be used in the self-shielding calculations.

TABn now accepts arbitrary Fortran unit numbers, which are ignored. The unit numbers actually used are chosen internally and are reported in the log file.

TIME now accepts an optional keyword **SECS** for the time units.

TOLERANCE is a new keyword used to introduce convergence parameters for the LSODES solver used to compute the inventories.

UNCERTAINTY has a changed option to set numerical parameters relevant to the improved pathways calculation. The new option is introduced by a value of -1 for the first parameter and use of the previous value of 4 for this parameter now generates a fatal error message. (The meanings of values 0–3 for the first parameter are unchanged.)

USEFISSION is a new keyword that causes fission reactions specified by the **FISYIELD** keyword and for which yield data are available to be self-consistently included in the matrix describing the inventory equations. It should be used whenever actinides (or other heavy elements that are transmuted to actinides) are specified in the target material. Its absence leads to a much faster calculation which remains accurate when actinides are not present or produced.

4 Getting Started

4.1 Introduction

The user interface of FISPACT-II differs from that of FISPACT-2007 primarily in the use of command line arguments in running the program and the availability of more user-friendly mnemonics and comments in the `files` file. Users of FISPACT-2007 will need to make very few changes in the way in which they work to transfer to the new code, and will benefit from the improved physical and numerical models the new code offers.

This section provides a simple step-by-step guide to running FISPACT-II for those unfamiliar with the old code.

The new code follows the sequence used by its predecessors. It has four stages to the prediction of inventories:

1. process the library data;
    - collapse cross-section data
    - condense decay and fission data
    - print summary of library data
2. set initial conditions;
3. run irradiation (heating) phases;
4. run cooling phases;

All of these stages can be undertaken in a single run of FISPACT-II, but the library data processing produces intermediate binary files that can be reused for many inventory calculations. However, in this introduction we shall separate the parts of the library processing (item 1) from the inventory calculation (items 2-4).

To run FISPACT-II, go to the directory in which the run input files are and type

```
fispact <fileroot>
```

or

```
fispact <fileroot> <files>
```

where it is assumed that FISPACT-II has been installed and is on the user's path. `<fileroot>` is the name root of all the user input and output files for a run of the code. The input file has the name `<fileroot>.i`, and the output files have names `<fileroot>.<ext>`, where the list extensions is given in Table 1. Thus, for example, if the input file is called `example.i`, then the run

Table 1: Filename extensions for user input and output files.

extension	unit name	description
.i	input	The run control file
.out	output	The main output file
.log	runlog	The logging and error output file
.gra	graph	The graphical data output file
.plt	gnuplot	The gnuplot plot command file
.sens	sens	The raw sensitivity data output file
.tab1	tab1	Number of atoms and grams of each nuclide table
.tab2	tab2	Activity and dose rate of each nuclide table
.tab3	tab3	Ingestion and inhalation dose of each nuclide table
.tab4	tab4	Gamma spectrum table

Table 2: Mapping of internal unit names to external EAF library files.

unit name	unit number	EAF library file
absorp	39	Element gamma absorption data
ind_nuc	18	Index of materials included in run
ind_nuco	49	Output file for reduced index of materials from pathways
crossec	19	Cross-section library
crossunc	7	Cross-section fractional uncertainties library
decay	16	Decay data
fissyld	9	Fission yield data
asscfy	8	Links between fissionable nuclides and fission yields
a2data	11	A2 transport data
clear	40	Clearance data
hazards	14	Biological hazards data

```
fispact example
```

would generate the output file `example.out`, the log file `example.log`, and so forth.

When FISPACT-II is run with only the single argument, `<fileroot>`, then the program looks (in the order given) for files in the present working directory with the name '`files`', '`Files`', or '`FILES`'. The first one found is used[1] and if none of them is found, then the program will flag a fatal error to the log file and close down.

If the filename of the `files` file is given as a second argument, then a file of name `<files>` will be used.

In order to work through the following examples, copy the FISPACT-II `test` tree into your own work space. In the test directory is a sub-directory `getting_started` with

[1] Users of Mac-OS and Windows systems should avoid having more than one 'files' file in a directory because of problems with the lack of case-consciousness.

Table 3: Mapping of internal unit names to external CALENDF and ENDF directories of library files.

unit name	unit number	Library directory (CALENDF or ENDF)
prob_tab	51	Probability table data
xs_endf	52	Resonance, cross-section and covariance data
dk_endf	53	Decay and its uncertainty data
fy_endf	54	Fission yield data
xs_endfb	55	Binary compressed cross-section and covariance data

Table 4: Mapping of internal unit names to external flux files and to intermediate cross-section and decay files.

unit name	unit number	description of file
arb_flux	3	Energy group structure, projectile spectrum and wall loading for arbitrary group structure.
fluxes	20	Projectile spectrum and wall loading for a standard group structure.
arrayx	13	Input and output condensed decay library.
collapxi	12	Input collapsed cross-section library.
collapxo	17	Output collapsed cross-section library.

all the files needed for you to perform the runs described in the following subsections. In getting_started, there is a files file that contains the following:

```
# gamma attenuation data
absorp  ../EAF2007data/eaf_abs_20070

# index of nuclides to be included
ind_nuc  ../EAF2010data/eaf_index_20100

# Library cross-section and uncertainty data
# neutron induced GAM-II (100 group) library
crossec  ../EAF2010data/eaf_n_gxs_100_fus_20100
crossunc  ../EAF2010data/eaf_un_20100

# fluxes
fluxes  EEF_first_wall_fluxes

# collapsed cross-section data (in and out)
collapxi  collapsed_cross_section_data
collapxo  collapsed_cross_section_data

# Library decay data
decay  ../EAF2010data/eaf_dec_20100.001
```

```
# Library fission  data
asscfy  ../EAF2010data/eaf_n_asscfy_20100
fissyld  ../EAF2007data/eaf_n_fis_20070

# condensed decay and fission data (in and out)
arrayx  condensed_decay_and_fission_data


# Library regulatory data
hazards  ../EAF2010data/eaf_haz_20100
clear  ../EAF2010data/eaf_clear_20100
a2data  ../EAF2010data/eaf_a2_20100
```

The purpose of the `files` file is to provide a mapping of the unit names used within the program to the names of the EAF library and to other input/output data files used by the program but whose names are not constructed from `<fileroot>`. Tables 2, 3 and 4 summarise the file names and the files they map to. The file numbers are aliases for the file names that provide backwards compatibility with FISPACT-2007 `FILES` files.

The ENDF-6 format input data libraries use a single file for each parent nuclide, where the file name is related to the nuclide name. In this case the entry in the `files` file gives the name of the library directory in which the separate data files for each nuclide are stored. Table 3 lists the internal unit names and numbers that are used to map to the nuclide data in the cases of the probability table data and the ENDF format data for cross-sections, decays and fission yields.

4.2 Cross-section Collapse

The EAF and ENDF libraries contain cross-sections as functions of the energy of the incoming projectile. For the example we are considering here (`eaf_n_gxs_100_fus_20100`) the incoming projectile is the neutron; this is the default, but other projectiles may be selected using the **PROJECTILE** keyword. FISPACT-II reduces each of these cross-sections to a single value by taking an average weighted by the spectrum of the incoming projectile flux ('collapsing', see Equation (24) on page 140). The input file in the `getting_started` directory that instructs FISPACT-II to collapse the cross-sections and the cross-section uncertainties is `collapse.i`:

```
<< -----collapse cross-section data----- >>
GETXS 1 100
FISPACT
* COLLAPSE 100_99 WITH FW EEF
<< print summary of collapsed cross-sections >>
PRINTLIB  4
```

```
END
* END OF RUN
```

The first argument (*1*) of the **GETXS** keyword tells the program to collapse cross-sections and uncertainties from the EAF library files connected to the `crossec` and `crossunc` file unit names and write the collapsed values to the file connected to `collapxo`. The second argument specifies that the 100 group (GAM-II) energy bins should be used.

NOTE: You must ensure that the correct projectile and the correct number of energy groups are specified as there is no information in the EAF library files for the program to check that consistent values are chosen.

The ENDF-format alternative to the EAF library does contain internal information about the projectile and energy group boundaries. If this library is used, consistency checking is possible and the new code will issue a fatal error message if discrepancies are found.

The **FISPACT** keyword enters a labelling line and marks the end of the library preparation section of the input control file. The **PRINTLIB 4** line causes a summary of the collapsed cross-sections to be printed. The **END** keyword marks the end of the input.

To perform the collapse, type

```
fispact collapse
```

You should see the output

```
collapse: cpu time = 0.472     secs.   No errors/warnings
```

where the cpu time will be changed to that appropriate to your computer.

You will find that new files `collapse.log`, `collapse.out` and `collapsed_cross_section_data` have appeared in the present working directory. The first two are text files, and the third is a binary file of data that can be used as input for later runs.

The log file contains a summary of the files linked to the program, monitoring echo of the keywords and actions, a list of the files used and a summary of the cpu times.

The output file contains the header summary, the collapsed cross-sections and uncertainties, run identification information and a summary of the files used.

If you type `fispact collapse` again, you will get output

```
collapse:--------- FATAL ERROR --------- run terminated, for details see runlog file, collapse.log
```

Inspection of `collapse.log` in this case will reveal the error message:

```
Log   : file unit name = output
Log   : file name = collapse.out
00001: Fatal   : files_m:files_open: 9:
       cannot open new file for writing
```

The run failed because the repeat run tried to write output to an existing file. The error reporting first gives the internal file name (`output`) and the file to which it is connected (`collapse.out`). The error message has a number (`00001`), a severity (`Fatal`) a record of from where it was issued (module `files_m`, subprogram `files_open`, point `9`) and a brief explanation of the error. FISPACT-II is designed to avoid accidental overwriting of existing output files. To run the program with the fileroot `collapse` all the output files `collapse.<ext>` (see Table 1) and the `collapxo` file must first be moved away or deleted. If you prefer the default option of overwriting old run data used by FISPACT-2007, then you can add the **CLOBBER** keyword to the top of the input file.

Figure 1 shows the input and output files used in a collapse run, where the file unit names are mapped to real files according to the specifications in the `files` file. In cases where self-shielding using the probability table method is included, there are additional inputs through the `prob_tab` file unit.

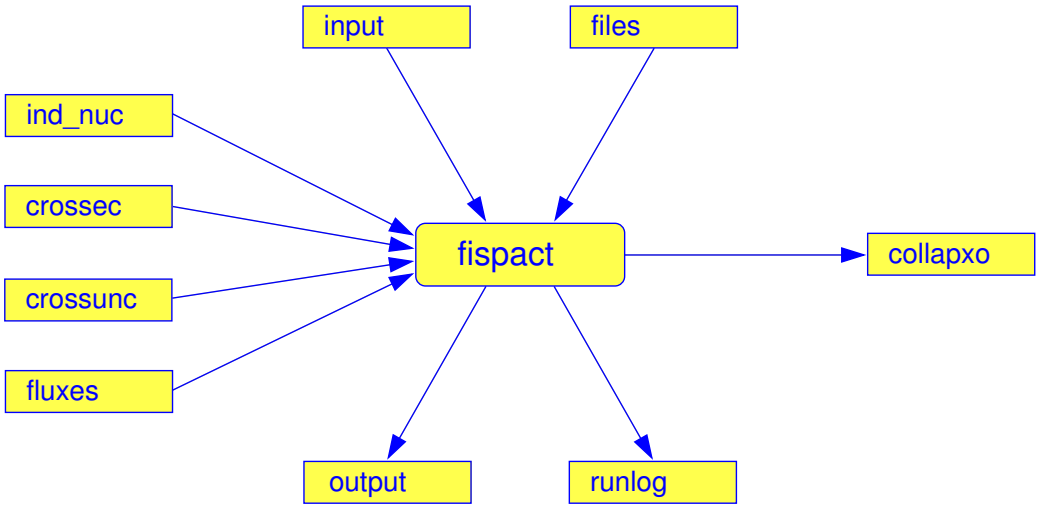

Figure 1: The files used by FISPACT-II in the cross-section collapse run example. The `files` file maps the internal file names shown in the figure to the actual files used by the run.

4.3 Decay Data Condense

The next stage is to condense the decay and fission data. The input file for this is `condense.i`:

```
<< -----condense decay data----- >>
NOHEADER
SPEK
GETDECAY 1
FISPACT
* DEC_99.00X/100_99/EEF121M.GP)
END
* END OF RUN
```

The **NOHEADER** keyword suppresses the heading information in the output. **SPEK** causes approximate γ-spectra to be generated for nuclides in the decay library that have no spectral data. **GETDECAY** *1* causes the decay data to be read from the EAF library files connected to `decay` by the `files` file. (Note that when a library file has the extension `.001` then the program will search the library directory for files with the same root and extensions `.002`, `.003`, etc. and add them to the input queue.) Keyword **FISPACT** marks the end of the library processing section of the input and **END** marks the end of input.

To do the run to condense the decay data, type

```
fispact condense
```

and you should get at the terminal window a message of the form

```
condense: cpu time = 0.639     secs.   No errors/warnings
```

and the program will have generated ascii output files `condense.log`, `condense.out` and binary file `condensed_decay_and_fission_data`.

Figure 2 shows the input and output files used in the condense run example, where the file unit names are mapped to real files according to the specifications in the `files` file. Note that a summary of the files used and their mapping is written to the output and log files for all runs to provide a quality record.

4.4 Library Summary Printing

The library summary print example `print_lib` uses the binary files containing cross-section and decay data generated by the `collapse` and `condense` runs above:

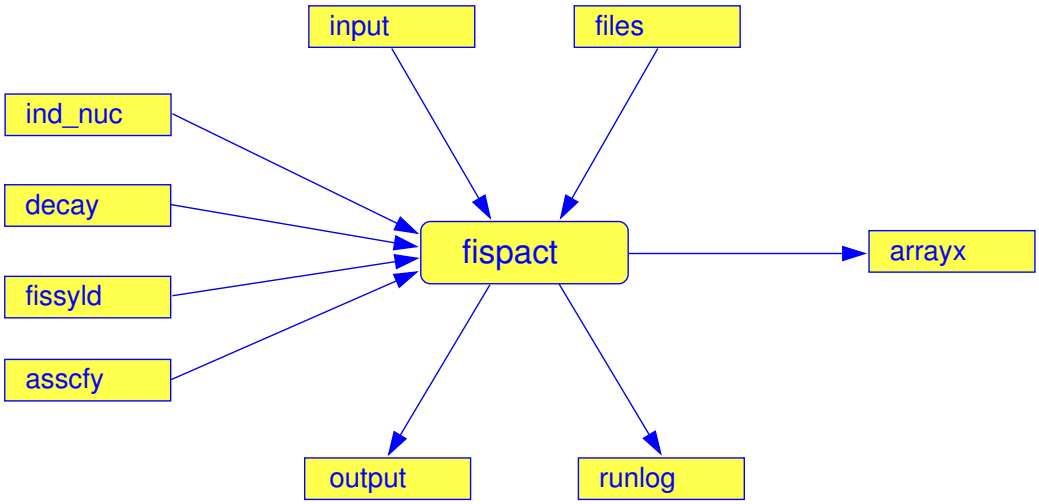

Figure 2: The files used by FISPACT-II in the decay and fission data condense run example.

```
<< print library data summary >>
NOHEADER
<< read condensed cross-section and collapsed decay data >>
GETXS 0
GETDECAY 0
FISPACT
* PRINTLIB OF FW EEF
<< print library data summary selection 0 >>
PRINTLIB  0
END
* END OF PRINTLIB
```

The keywords **GETXS** and **GETDECAY** with *0* arguments respectively instruct FISPACT-II to read cross-section and decay data from the binary files mapped to `collapxi` and `arrayx`. See the definition of **PRINTLIB** on page 77 for details of the tables printed.

To generate `print_lib.out`, type

```
fispact print_lib
```

To convert the Fortran carriage control characters 0 and 1 to line-feed and form-feed in the output file and print the results to the default printer set for the `a2ps` command, type

```
fisprint print_lib.out
```

4.5 Inventory Calculation

The example file for the inventory calculation is `inventory.i`. The first part reads in the collapsed and condensed data as for the `print_lib` example:

```
<< -----set initial switches and get nuclear data----- >>
NOHEAD
MONITOR 1
GETXS 0
GETDECAY 0
FISPACT
* IRRADIATION OF TI EEF FW 1.0 MW/M2
```

The **MONITOR 1** keyword causes the input keywords to be echoed to the terminal; for those keywords that cause actions, a summary of the actions is also echoed to the terminal.

The second part specifies the initial conditions. In this case the **MASS** keyword specifies 1 kg of one element (Ti), and the number of atoms of each isotope of Ti is computed from internal tables of natural abundances.

```
<< -----set initial conditions----- >>
MASS 1.0 1
Ti 100.0
FLUX 4.27701E+14
MIND 1.E5
GRAPH 2 2 1 1 4
UNCERT 2
ATOMS
HAZARDS
HALF
ATWO
```

The **FLUX** keyword specifies the energy integrated neutron flux ($\mathrm{cm}^{-2}\,\mathrm{s}^{-1}$). The next two keywords are output selectors. The **MIND** keyword gives the threshold inventory for a nuclide to be displayed in the output tables. The **GRAPH** keyword causes the generation of a gnuplot data and gnuplot command file for plotting total activity and ingestion dose during the cooling period.

The **UNCERTAINTY** keyword causes pathways analysis to be undertaken for the irradiation period, and for uncertainties to be output. The **ATOMS** keyword leads to the initial state being printed to the output file. The remaining three keywords are output selectors to control the output printed for each time interval of the calculation. In this case the selections are: output of ingestion and inhalation doses (**HAZARDS**), half lives (**HALF**) and transport limits (**ATWO**).

The remainder of the file specifies the irradiation and cooling phases of the inventory calculation. In this example, an irradiation phase of 2.5 years is specified.

```
<< -----irradiation phase----- >>
TIME 2.5 YEARS
ATOMS
```

The cooling phase is started by the **ZERO** keyword. This resets the time origin, causes the pathways analysis to be performed over all the steps preceding it, and initiates the saving of data for the graphs. ***NOTE:*** *there must be at least* ***two*** *cooling steps for the graph output to be plotted.*

NOTE: *there must be no more than one* ***ZERO*** *keyword in an input file, but there may be irradiation as well as cooling steps after the* ***ZERO*** *keyword.*

```
<< -----cooling phase----- >>
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
```

To run the inventory calculation, type:

```
fispact inventory
```

This should cause the output shown below to appear at the terminal window. The settings keywords are simply echoed, but the action keywords (in this example **ATOMS**, **ZERO** and **END**) list the actions they initiate. The final line gives cpu timing and a summary of the number of errors or warnings issued.

```
 MONITOR 1
 GETXS 0
 GETDECAY 0
 FISPACT
 * IRRADIATION OF TI EEF FW 1.0 MW/M2
  load cross-sections
  load decay data
  collapse fission yields
  run reset cross-section
 MASS 1.0 1
```

```
TI 100.0
FLUX 4.27701E+14
MIND 1.E5
GRAPH 2 2 1
1
4
UNCERTAINTY 2
ATOMS
 load initial values
 run output inventory
HAZARDS
 load hazards data
HALF
ATWO
 load a2 data
TIME 2.5
 fill rate equation matrix for cooling
 fill rate equation matrix for irradiation
 start pathstep recording
 initialise dominant analysis
YEARS
ATOMS
 run add rateeq for pathways
 run irradiation init
 run irradiation step
 run add pathstep
 run output inventory
FLUX 0.
ZERO
TIME 1
MINS
ATOMS
 run pathways initialisation
 run pathways uncertainty
 run cooling step
 run add pathstep
 run output inventory
 run pathways uncertainty
TIME 1
HOURS
ATOMS
 run cooling step
 run add pathstep
 run output inventory
 run pathways uncertainty
TIME 1
DAYS
ATOMS
 run cooling step
 run add pathstep
 run output inventory
 run pathways uncertainty
TIME 7
DAYS
ATOMS
 run cooling step
```

```
 run add pathstep
 run output inventory
 run pathways uncertainty
TIME 1
YEARS
ATOMS
 run cooling step
 run add pathstep
 run output inventory
 run pathways uncertainty
END
* END
 run output summary
 run closedown
 deallocate and closedown
inventory:cpu time = 0.379     secs.   No errors/warnings
```

The files `inventory.log`, `inventory.out`, `inventory.gra` and `inventory.plt` are also created by this run.

To convert the `inventory.gra` file to a postscript output file, type

```
gnuplot inventory.plt
```

Figure 3 shows the first page of the resulting plots.

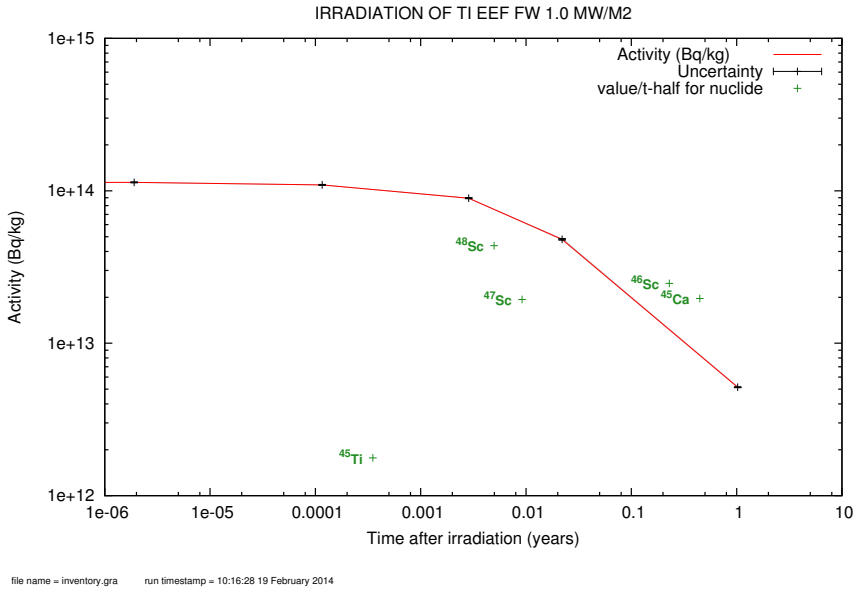

Figure 3: The total activity graph produced by the `inventory` run.

Figure 4 shows the input and output files used in the inventory run example, where the file unit names are mapped to real files according to the specifications in the `files`

file.

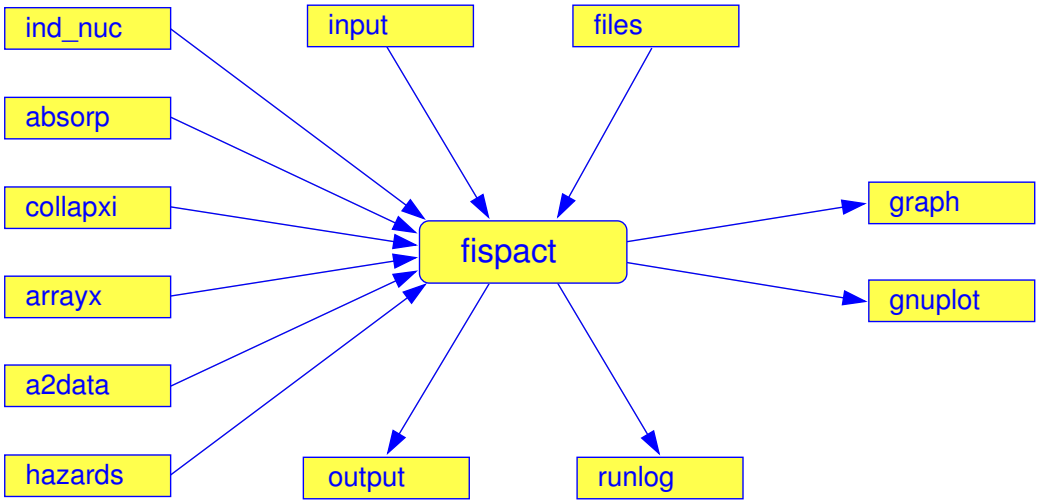

Figure 4: The files used by FISPACT-II in the inventory run example.

An explanation of the contents of the output file may be found in Section 7.1

4.6 ENDF-format Library Data

The ENDF-format of library data are provided in directories containing separate files for each nuclide. These directories are made available to FISPACT-II by including the stream names `prob_tab`, `xs_endf`, `dk_endf` and `fy_endf` in the `files` file, as listed in Table 3.

FISPACT-II is directed to use these new libraries by including the **EAFVERSION** keyword with argument *8* near the head of the `input` file, before the **GETXS** keyword, for example:

```
<< -----collapse cross section data----- >>
EAFVERSION 8
GETXS 1 162
```

then the remainder of the `input` file is unchanged. The number of energy groups must be consistent with the library data; currently 162 and 709 energy group libraries are provided in ENDF format, together with a translation of the EAF 616 group data into ENDF format.

If the cross-section data collapse and decay data condense are undertaken in separate runs of FISPACT-II it is necessary to include the **EAFVERSION** *8* command in both runs to obtain both new cross-section data and new decay data. This allows

the flexibility of using old cross-section data with new decay data and vice versa. If the **GETXS** *1* and **GETDECAY** *1* commands appear in the same input file, then **EAFVERSION** should appear at most once and the cross-section data and decay data are either both ENDF format or both EAF format.

The file connection diagram for a collapse run using the ENDF format data is obtained by replacing the crossec and crossunc streams in Figure 1 by the single input stream xs_endf. Similarly, the ENDF format file connection diagram for a condense run is obtained from Figure 2 by respectively replacing the decay and fissyld streams by dk_endf and fy_endf and by removing the asscfy stream (Fission yield associations are not used with the new TENDL-2011, TENDL-2012 and TENDL-2013 data.).

4.7 Developing New input Files

The above examples give an initial guide on how to use FISPACT-II to undertake inventory calculations. Examining the sets of test cases in directories fispQA2010 and fispQA (see Section 6) together with the definitions and usage examples of the keywords (see Section 5) provide further guidance on how to use the keywords in the input files to specify the desired calculations.

FISPACT-II offers the user more help in developing new input files than FISPACT-2007 does because it has new input file syntax checking and error reporting. This is illustrated by the erroneous example test142a input file. It is in the subdirectory Tst_input_errors of directory fispQA2010 and is shown below:

```
<< -----get nuclear data----- >>
CLOBBER
NOHEAD
MONITOR 1
GETXS 0
GETDECAY 0
FISPACT
* IRRADIATION OF TI EEF FW 1.0 MW/M2
<< -----set initial conditions----- >>
DENSITY 4.54
FUEL 4
Ti46 1.00619E24
Ti47 9.18148E23
Ti48 9.28210E24
Ti49 6.91755E23
Ti60 6.79178E23
MIND 1.E5
GRAPH 3 2 0 1 2 3
FLUX 4.27701E14
TOLERANCE 1 1.0E8 2.0e-3
UNCERT 3
SENSITIVITY SIGMA 1E-10 2 1
Ti48 Sc48
```

```
Ti49 Sc48
Sc48
ATOMS
DOSE 1 1.0

<< -----irradiation phase----- >>
TIME 2.5 YEARS
ATOMS

<< -----cooling phase-----
FLUX 0.
ZERO
TIME 1 MIN ATOMS
TIME 1 HOURS ATOMS
TIME 1 DAYS ATOMS
TIME 7 DAYS ATOMS

END
* END
```

The syntax checker tries to report as many errors as it can in one pass, but interaction of errors may lead to more than one test run being needed to locate all the syntax errors. The **CLOBBER** and **MONITOR** keywords are included at the top of the `input` file to help in the debugging of the input file. **CLOBBER** is used to eliminate the need to clear up the files generated by failed tests before reruns are undertaken. **MONITOR** with argument 1 indicates how far the run has gone, and in the case of failure helps identify where things have gone wrong. Once problems are ironed out, then it is recommended that these keywords are removed from the input file; **CLOBBER** allows the accidental overwriting of output files, and **MONITOR** duplicates information that can be obtained from the `runlog` file in production runs.

Executing the command

```
fispact test142a
```

generates the following output

```
ERROR in INPUT file
Unexpected eof encountered while reading the input file.
Check for missing closing >> on comment string beginning on line  33
test142a:------- FATAL ERROR --------- run terminated, for details see runlog file, test142a.log
```

Inspection of line 33 indeed reveals that the closing >> of the comment is missing, and this caused the remainder of the input file to be treated as a comment. Adding this missing comment closure, saving the input file as `test142b.i` and rerunning `fispact` then generates the error messages:

```
ERROR in INPUT file
```

```
keyword FUEL has too many arguments
Line number =  16 token = Ti60
Skipping to next keyword.

ERROR in INPUT file
keyword DOSE has too many arguments
Line number =  27 token = 1.0
Skipping to next keyword.

ERROR in INPUT file
Abbreviated keyword MIN matches 2 keywords
Detected on line number =  36
Skipping to next keyword

Input syntax errors. Run terminating.
test142b:---------FATAL ERROR --------- run terminated, for details see runlog file, test142b.log
```

This run has generated three syntax error messages for the file `test142b.i`.

The first error is on line 16. Inspection of the **FUEL** keyword on line 11 shows that it specifies four nuclides, whereas five are listed, with the fifth on line 16. To correct this, change the `4` to `5` on line 11.

After detecting an error, the syntax checker attempts to recover by skipping the tokens in the input stream until the next keyword is detected and then continuing the checking. This *may* (as in this example) provide the opportunity to correct more than one error using the output of one run, depending on the effectiveness of the recovery.

The second error detected is for **DOSE**. This is an instance of a keyword that has a variable number of arguments. If you consult Section 5.2.7 on page 60 you will see that if the first argument of **DOSE** has value one, then the second argument should not be present. Deleting the second argument `1.0` corrects this error.

The final error arises because of keyword ambiguity. A minimum of three characters are needed for a keyword, provided the abbreviation is unique. The `MIN` on line 36 could be an abbreviation for either **MIND** or **MINS**, and so an error message is issued. It is clear from the context on line 36 that the keyword should be **MINS**, and so adding an `S` fixes this error.

The run is always terminated with a fatal error message if errors in the input file are detected. Correcting all three of the errors detected for `test142b.i` gives input file `test142c.i` and rerunning produces:

```
ERROR in INPUT file
Detected at argument  10 on line  16 of keyword FUEL on line  11.
Argument value is Ti60. Expected argument type is nuclide name.
Unrecognised nuclide argument

Input syntax errors. Run terminating.
test142c:-------- FATAL ERROR --------- run terminated, for details see runlog file, test142c.log
```

The error has occurred because FISPACT-II does not have the nuclide `Ti60` in its index of nuclides. This example of finger trouble, where `6` was entered instead of `5`, could not be detected by the earlier run because the context of the token 'Ti60' was corrupted by the previously incorrect argument count given with the **FUEL** keyword.

Going to line 16, changing the `6` to `5` gives a syntactically correct input file. Deleting the **CLOBBER** and **MONITOR** keywords, saving the input file as `test142.i` and rerunning gives the concise terminal output that signifies a successful run:

```
test142:   cpu time =  2.11     secs.   No errors/warnings
```

(provided that the `collapx` and `arrayx` files have already been prepared by running `collapx.i` and `arrayx.i`.)

This example and further illustrations of messages generated by `input` file errors may be found in the subdirectory `Tst_input_errors` of `fispQA2010`.

4.8 Compressed ENDF Library Files

The TENDL nuclear data libraries are large – they contain many gigabytes of data. If a sequence of FISPACT-II runs uses the same incident particle spectrum, then the time for a single collapse run may be spread over many runs by using a preliminary collapse run (c.f., Section 4.2). However, if the sequence of runs uses different flux spectra in each run, then the computational time for the collapses becomes significant, particularly if data are accessed across a network. To speed up calculations in these cases, three capabilities have been added to FISPACT-II. The first, described in this section, is to preprocess the ENDF libraries and store only those data by FISPACT-II in a single compressed binary file. The second is to store the cross-sections versus energy in FISPACT-II and then perform a number of collapses without re-reading the ENDF data. The third approach to speedup is to use a reduced master index as described in the next section.

A separate executable `compress_xs_endf` is used to convert the ASCII ENDF libraries into a compressed binary file. It has up to five arguments, in the following order:

1. the fileroot name used to construct binary output and log file names (default `compress_xs_endf`);
2. the projectile – a letter that denotes the projectile used for the reaction data. Valid values are n, p, d, a, g (default `n`);
3. the bin-size: number of energy bins in cross-section data. For the present TENDL data this make take values 709 or 162 (default `709`);

4. the save type: This takes a value 0-5 that specifies what data are to be saved (default `1`);
5. the name of files file (default `files`).

The save types are

0 cross-section only
1 cross-section and variance
2 cross-section, variance and covariance
3 resonances and cross-section
4 resonances, cross-section and variance
5 resonances, cross-section, variance and covariance

Any other value defaults to 1. For most applications cross-sections only or cross-sections and variance (neutron irradiation) are sufficient. Covariance data are only available for neutron irradiation and are only needed if the **COVARIANCE** keyword is being used. The resonance data are only used if the **SSFGEOMETRY** keyword is to be used.

An example of the use of `compress_xs_endf` that creates a binary compressed library `tal2013-n.bin` containing 709-group cross-sections, variance and covariance data for neutron irradiating flux using the TENDL2013 library is as follows:

```
compress_xs_endf tal2013-n n 709 2
```

The fifth argument is not present and so will take its default value `files`. This file must contain the mappings for `ind_nuc` and for `xs_endf`. For example:

```
# index of nuclides to be included
ind_nuc  ../../ENDFdata/TENDL2013data/tendl13_decay12_index

# Library cross section data
xs_endf ../../ENDFdata/TENDL2013data/tal2013-n/gxs-709
```

Only those nuclides listed in the `ind_nuc` file are included in the compressed library.

The input files for collapse calculations using the compressed ENDF libraries differ from those using the full ASCII libraries only in that the **GETXS** has first argument -1 rather than 1, and the `files` file contains a mapping for the compressed library:

```
# Compressed library cross-section data
xs_endfb tal2013-n.bin
```

Typically, the compressed library is about one quarter of the size of the full ASCII library, and collapse calculations are typically a factor four faster. Further reductions in file size and execution times can be realised using a reduced nuclide index.

4.9 Reduced Nuclide Index

TENDL-2013 contains 3875 nuclides. In most applications, only a small number of these nuclides are significant. Those that are not can be left out of the activation or transmutation calculation without affecting the quality of the physics predictions. Omitting the unimportant nuclides leads to much faster FISPACT-II calculations and smaller data files. FISPACT-II has a simple mechanism for excluding unwanted nuclides; only those nuclide listed in the `ind_nuc` master index file are included in the calculation. Keeping only significant nuclides can reduce the computation time for collapse calculations and inventory by one or two orders of magnitude, and can reduce the computation time of larger Monte-Carlo sensitivity calculations by several orders of magnitude.

The reduced index can be created by hand editing the full nuclide index to retain only the light gas nuclides and those in the region of Z-A space around the target materials being studied. Alternatively, a reduced index can be automatically generated from a full calculation with pathways analysis by including the **INDEXPATH** keyword in the input file.

5 Control File Keywords

A run of FISPACT-II is controlled by a sequence of commands given in a user-supplied `input` file as illustrated in the previous section. Each command is introduced by a keyword which may be followed by integer, real or character-string parameters. Some commands require further data to be supplied in records of the file following the keyword. Some commands are followed by subordinate keywords which cannot be used independently of their parent keyword.

The keywords belong to one of two classes distinguished by their effect on the calculation. Some keywords provide settings such as logical flags and numerical values, while others cause FISPACT-II to perform actions. Depending on the context, the effect of an action keyword may be immediate, or its action may be added to a queue and its execution deferred.

The `input` file is divided into three sections:

1. library data preparation—reading and processing the physical and regulatory data supplied in a library of files;

Table 5: Pages on which the Keywords recognised by FISPACT-II are defined.

page	keyword	page	keyword	page	keyword
73	ACROSS	73	ADCROSS	73	ADLAM
23	AINPUT	73	ALAM	23	ARRAY
59	ATOMS	59	ATWO	59	BREMSSTRAHLUNG
59	CLEAR	47	CLOBBER	47	COLLAPSE
23	CONV	47	COVARIANCE	60	CULTAB
82	DAYS	60	DENSITY	23	DOMINANT
60	DOSE	23	EAFVERSION	61	END
88	ENDPULSE	23	ENFA	61	ERROR
62	FISCHOOSE	48	FISPACT	62	FISYIELD
63	FLUX	64	FUEL	48	FULLXS
65	GENERIC	48	GETDECAY	49	GETXS
65	GRAPH	67	GROUP	50	GRPCONVERT
67	HALF	69	HAZARDS	82	HOURS
69	INDEXPATH	69	IRON	23	LEVEL
23	LINA	51	LOGLEVEL	69	LOOKAHEAD
23	LOOPS	70	MASS	71	MCSAMPLE
71	MCSEED	72	MIND	82	MINS
51	MONITOR	23	NEWFILE	72	NOCOMP
52	NOERROR	52	NOFISS	52	NOHEADER
72	NOSORT	73	NOSTABLE	73	NOT1
73	NOT2	73	NOT3	73	NOT4
73	OVER	91	PARTITION	75	PATH
92	PATHRESET	77	PRINTLIB	52	PROBTABLE
53	PROJECTILE	93	PULSE	93	RESULT
78	ROUTES	54	SAVELINES	82	SECS
79	SENSITIVITY	23	SEQNUMBER	23	SEQUENTIAL
80	SORTDOMINANT	80	SPECTRUM	54	SPEK
80	SPLIT	54	SSFCHOOSE	55	SSFDILUTION
56	SSFFUEL	56	SSFGEOMETRY	57	SSFMASS
81	TAB1	82	TAB2	82	TAB3
82	TAB4	23	TAPA	82	TIME
82	TOLERANCE	83	UNCERTAINTY	85	UNCTYPE
86	USEFISSION	86	WALL	82	YEARS
96	ZERO				

2. initial conditions—specifying physical, numerical and housekeeping conditions for a calculation;

3. inventory calculation phase—specifying a sequence of timesteps including one or more irradiation steps optionally separated by cooling steps, with further cooling steps optionally following the final irradiation step.

The first section is terminated by the **FISPACT** keyword and this triggers the execution of the library data preparation actions which have been queued prior to the occurrence of the **FISPACT** keyword. The actions are queued in the correct order to ensure that any dependences between them are respected.

The initial conditions section of the `input` file is terminated by the first occurrence of the **TIME** keyword, or exceptionally the **END** keyword for a run that does not involve any inventory calculations. FISPACT-II requires that all initial condition settings are declared before the inventory calculation is started and so there are more restrictions on the placing of keywords in the `input` file than in FISPACT-2007. Consequently, some older files may need minor editing before they can be reused.

The final, inventory calculation section of the `input` file is terminated by the **END** keyword; any further content in the file is ignored. FISPACT-II attaches more significance to the **ZERO** keyword than did FISPACT-2007. **ZERO** may now occur at most once and it triggers the calculation of pathways, routes, sensitivities and uncertainties.

The relevant keywords for each section of the control input file are presented in alphabetical order in the following three sub-sections. A further sub-section describes miscellaneous input constructs. Table 5 gives a complete list of the keywords together with the pages on which they are defined.

The notation used in the sub-subsection headings defining the keywords is as follows:

1. keywords are displayed in bold font;

2. arguments are in lower case italics;

3. default values of arguments assumed by the program if the keyword is not used are displayed in curly brackets {...};

4. arguments that are present only for certain values of earlier arguments are displayed in angle brackets <...>.

Some keywords may appear in more than one section of the `input` file. In these cases, the full descriptions of the keywords are placed in the first subsection below where the keywords are permitted. Summary descriptions are repeated in other subsections where the keywords are permitted, and any context-specific details are noted.

5.1 Library Data Preparation

The first section of the input file deals with the input and processing of library data and with initial output settings. It is terminated with the keyword **FISPACT**.

5.1.1 CLOBBER

In order to prevent accidental loss of data, the default action of FISPACT-II is to terminate with a fatal error if output files of the same names as specified in the current run already exist in the present working directory. This keyword allows existing output files to be overwritten without any error messages from the program.

5.1.2 COVARIANCE

If this keyword is present, a collapse run will compute collapsed covariances between different reactions if covariance data are available in the reaction data files. Tables of the collapsed covariances and correlations may be printed using the *print* = 4 option with the **PRINTLIB** keyword.

5.1.3 EAFVERSION *neafv* {7}

This keyword is used to select the format of the nuclear data libraries to be read. It is not needed if the EAF-2007 or EAF-2010 libraries are to be used. *neafv* is an integer indicating the EAF library version. For backwards compatibility, the default value of *neafv* is 7, indicating the EAF-2007 or EAF-2010 libraries. The new value of 8 is used to indicate the ENDF-format libraries that are now an alternative to EAF. Note that FISPACT-II has not been validated for earlier versions of the EAF library than EAF-2007.

EAFVERSION must be used before the **FISPACT** keyword as it determines which input streams from the `files` file are used to read the nuclear data.

This keyword may also be used in the initial conditions and inventory calculation sections of the `input` file if the cross-sections or decay rates are to be changed during the course of a run; see Sections 5.2.8 and 5.3.2.

An example of the use of this keyword is

```
EAFVERSION 8
NOERROR
PROJ 2
GETXS 1 162
```

```
FISPACT
* TENDL-2011 gxs-162: deuteron   1 MeV - 200 MeV
```

The 162-group ENDF format cross-section library for a deuteron projectile is to be read.

5.1.4 FISPACT
**** Title***

This keyword 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 keyword is the divider that separates the library input from the initial conditions and irradiation sequence details. It is the action keyword that triggers the execution of the queued actions from the library data preparation section of the `input` file.

5.1.5 FULLXS

This keyword causes the full, energy-dependent group cross-sections to be stored when the cross-section library data are being collapsed.

5.1.6 GETDECAY *libdecay*

This keyword has one integer parameter *libdecay* which is set to zero to read decay data from an existing condensed decay library (`arrayx` file), or to one to condense decay and fission data from the EAF or ENDF library files specified in the `files` file.

For example, to get cross-section data from a collapsed library and decay data from a condensed library:

```
GETXS 0
GETDECAY 0
FISPACT
* Irradiation of SS316 steel
...
```

5.1.7 GETXS *libxs* <*ebins* >

This keyword has two integer parameters. If the first parameter *libxs* is set to zero, then the second parameter should be omitted, and cross-section data are read from the existing collapsed library (`collapx` file) specified in the `files` file. If *libxs* is 1, then the second parameter *ebins* gives the number of energy bins to be used in collapsing the cross-section data from the EAF or ENDF library files and `fluxes` or `arb_flux` files specified in the `files` file. If *libxs* is -1, then the ENDF data are read from the compressed binary version of the ENDF data stored in the file specified by `xs_endfb` in the `files` file. The value *libxs* = -1 is not valid for EAF libraries. For information on the preparation of the compressed binary ENDF data files see Section 4.8 on page 42.

The **GETXS** keyword may also be used in the initial conditions and inventory calculation phases for handling time-dependent projectile spectra and temperature changes in cross-sections (see pages 65 and 88).

The number of energy groups *ebins* **must** be consistent with the number of groups in the supplied library file. The permitted numbers of groups for cross-section data are currently

EAF-2010	66	69	100	172	175	211	315	351	616
ENDF	162	616	709						

Each set of energy-dependent cross-sections is then combined in a weighted sum with the supplied projectile spectrum to produce a one-group effective cross-section library which is used directly in subsequent runs.

Note that if no uncertainty data are supplied in the library (as for the deuteron and proton induced reactions) then the keyword **NOERROR** ***must*** be used.

An example of the use of this keyword is

```
GETXS 1 211
FISPACT
* Collapsing EAF_2007
...
```

Note that the format of the EAF-2010 and earlier cross-section libraries does not embed the number of energy groups or the group boundaries in the library file, so it is not possible to confirm the consistency of the specified *ebins* with the cross-sections being used. If they are not consistent, erroneous results may be calculated without any warning from FISPACT-II.

5.1.8 GRPCONVERT *nestrc ndstrc*

This keyword allows the user to read a neutron (or other projectile) spectrum in an arbitrary number of groups (*nestrc*) and instruct FISPACT-II to convert it into one of the presently-allowed eleven standard structures. *ndstrc* **must** therefore be 66, 69, 100, 162, 172, 175, 211, 315, 351, 616, or 709; using any other value will result in an error message. The user must prepare a file containing the following data and connect it to the `arb_flux` input stream in the `files` file:

- *nestrc*+1 values representing the arbitrary energy boundaries starting with the highest energy.
- *nestrc* values representing the flux values ($\mathrm{cm}^{-2}\,\mathrm{s}^{-1}$) in each group starting with the high-energy group.
- First wall loading ($\mathrm{MW}\,\mathrm{m}^{-2}$)
- 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 the `fluxes` stream named in the `files` file; this contains the standard information for a `fluxes` file:

- *ndstrc* values representing the flux values ($\mathrm{cm}^{-2}\,\mathrm{s}^{-1}$) in each group starting with the high-energy group.
- First wall loading ($\mathrm{MW}\,\mathrm{m}^{-2}$)
- 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 particles 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.

An example of the use of this keyword is

```
GRPCONVERT 99 172
```

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

5.1.9 LOGLEVEL *level* {2}

The error logging module in FISPACT-II provides error messages identifying the point in the code from which the message is issued, together with information identifying its severity and its nature. In some cases, values are output before the error message for further clarification.

Six error severities are defined by the value of *level*:

0 fatal error
1 serious error
2 error warning
3 error information
4 debug information
5 logging info

The default is to write messages for severity 2 (error warning) and higher. The **LOGLEVEL** keyword allows the amount of information written to the `runlog` file to be varied. For example

```
LOGLEVEL 4
```

will cause extra information to be output that may help identifwaqy the cause of problems.

LOGLEVEL may appear repeatedly throughout the `input` file to increase or decrease the amount of diagnostic information as required.

5.1.10 MONITOR *monit* {0}

The progress of a FISPACT-II run can be monitored by printing the various keywords as they are read in the input file and reporting the actions they initiate to the standard output. The default is not to print this information, but it can be switched on by setting *monit* to 1. For both settings of *monit*, the keywords and their actions are written to the `runlog` file.

An example of the use of this keyword is

```
MONITOR 1
```

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

5.1.11 NOERROR

This keyword 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** keyword. (This keyword can still be used so long as only pathway data are required.)

Note that if this keyword is used with the **ERROR** keyword then the user **must** supply values of the fractional error (*ermat*).

If output of the data libraries is requested with the **PRINTLIB** keyword, and no uncertainty data exist, then **NOERROR must** be used.

In all cases the keyword **must** come near the top of the input file, before the keyword **FISPACT**.

5.1.12 NOFISS

This keyword stops the fission yield data from being input and processed during the preparation of the `arrayx` file. It causes substantial speedup of the calculation, but will cause errors in the inventory predictions if fission is important. It is advisable not to use this keyword if the initial inventory contains actinides.

5.1.13 NOHEADER

This keyword stops the printing of the header and user information at the beginning of the output and is useful to reduce the amount of printed output.

5.1.14 PROBTABLE *multxs* {0} *usepar* {1}

This keyword causes the probability tables to be read for the nuclides specified by the elements listed by the **SSFCHOOSE** keyword.

The self-shielding is applied to the existing cross-section value as a multiplicative factor if *multxs* is set to 1. If it is set to zero, then the cross-section values in the energy

groups for which there are probability table data are replaced with apportionment determined from the EAF or ENDF library data.

The second argument defines the way in which the self-shielding factors (SSF) are computed:

***usepar* = 0** use the total cross-section to calculate one SSF for each nuclide and apply this factor to all relevant cross-sections;

***usepar* = 1** use macro-partial cross-sections to calculate a separate SSF for each macro-partial and apply it to relevant reactions contributing to that macro-partial.

If the 616-group infinitely-dilute cross-sections in the EAF data library and the CALENDF probability table data were fully consistent, these two methods of calculation would give the same answers. However, the EAF data do not contain the elastic scattering cross-sections, and so cannot give the correct total cross-section. The CALENDF probability tables do give the correct total cross-sections, but only provide cross-sections for sets of macro-partials, and so have to use the EAF data to apportion the cross-sections when they are used to replace EAF values when self-shielding is included. The replacement option is the recommended one, but both options are included so that the user can assess the uncertainty of the effective collapsed self-shielding factor. An expert mode that allows fine-tuning of the dilution factors is provided using the **SSFDILUTION** keyword.

See Appendix A.4.3 for a more detailed explanation of the alternative calculations performed, and Section 7.4 for an illustration of including self-shielding in the computation of the effective collapsed cross-section data.

At present, the probability table data are available only for the 616 and 709 energy group structures for neutrons. Attempts to use this keyword with other projectiles or cross-section datasets with other than the 616 or 709 energy group structure will cause FISPACT-II to terminate with a fatal error.

The TENDL-2011, TENDL-2012 and TENDL-2013 709 group data for neutron projectiles do contain elastic scattering cross-section data, and so both choices of *multxs* should give very similar results if these are used in conjunction with probability table data.

5.1.15 PROJECTILE *nproj* {1}

This keyword defines the incoming particle for the activation calculations. This keyword **must** be used if a library other than a neutron-activation one is used.

At present, cross-section uncertainty data are known only for neutron-induced reactions, so if *nproj* is not 1, then the **NOERROR** keyword **must** also be used.

For a gamma library *nproj* should be set to '5', for a deuteron library *nproj* should be set to '2', for a proton library *nproj* should be set to '3' and for an alpha library *nproj* should be set to '4'. A neutron library uses the default value of '1'.

An example of the use of this keyword in the collapse of a deuteron library is

```
MONITOR 1
PROJ 2
NOERROR
GETXS 1 211
FISPACT
* COLLAPSE EAF_20070 WITH IFMIF
END
* END OF RUN
```

5.1.16 SAVELINES

This keyword causes the spectral line energies and intensities to be stored when the decay library data are being condensed.

Note that the spectral lines output option chosen with the **PRINTLIB** 5 command will produce spectral line output only if the **SAVELINES** command is used as described above.

5.1.17 SPEK

This keyword causes the calculation of an approximate γ spectrum for nuclides in the decay library which have no spectral data. These nuclides are flagged by an '&' in the inventory output and in the output of library data produced in a run with the keyword **PRINTLIB**.

5.1.18 SSFCHOOSE *ncho* {0} *nprint* {0} *sym(j), j=1, ncho*

This keyword is used to specify the nuclides for which the self-shielding factors are computed using the probability table data (see Appendix A.4.3 on page 144).

ncho gives the number of element or nuclide names that follow the keyword. The symbols *sym* may either be element names (e.g., Ti) or nuclide names (e.g., W182). If an element name is given, then all the naturally occurring isotopes of that element are included in the list of nuclides to which the self-shielding correction is to be applied.

nprint is by default 0, in which case it prints the list of probability table data files and the nuclide mixture. If it is set to 1, then it additionally prints total and partial cross-sections and dilutions versus energy bin for all the nuclides to which self-shielding is being applied.

The following is an example of a collapse run where probability table corrections are included for all the naturally occurring isotopes of titanium and tungsten in a mixture of titanium, tungsten and iron.

```
GETXS 1 616
PROBTAB 1 0
SSFCHOOSE 2 0
Ti W
FISPACT
* COLLAPSE EAF_616_FLT WITH PROBABILITY TABLE CORRECTIONS
MASS 1.0 3
TI 85.0
W 10.0
Fe 5.0
END
* END OF RUN
```

5.1.19 SSFDILUTION *nnuc* *nucname(j) num(j)* *grp(i,j) dilution(i,j), i=1,num(j), j=1, nnuc*

This keyword adds further user control to that provided by the **SSFCHOOSE** keyword.

If **SSFCHOOSE** is used with argument *nprint* set to 1, then the computed dilutions versus energy bin are printed for each nuclide. These dilutions are computed using the formulae given in Appendix A.4.3. If the user wishes to override these values, then he may do so using the **SSFDILUTION** keyword.

The first argument *nnuc* lists the number of nuclides for which dilution values are to be specified. For each nuclide *j*, the nuclide name *nucname(j)* and the number of table entries *num(j)* are given, followed by a list of *num(j)* pairs of energy group indices *grp* and dilution cross-section values *dilution* in barns.

In this example the dilution for ^{182}W is set to 100 and 80 barns respectively in energy groups 300 and 301, and the dilution for ^{184}W is set to 2.5 and 10 barns in groups 194 and 200.

```
SSFDILUTION 2
W182 2
300 100.0 301 80.0
```

```
W184 2
194 2.5
200 10.0
```

5.1.20 SSFFUEL *n1* *is(j) atoms(j) j=1, n1*

This keyword allows the input of the number, *n1* of nuclides and the identifier, *is(j)* and the number of atoms, *atoms(j)* for each nuclide that is to be used in the self-shielding calculation. The identifier should be a nuclide name with the format of a chemical symbol followed by an atomic mass number, e.g. 'W184'.

The specification of nuclides is essential if the materials specified do not have the natural isotopic abundance. If different values are required then **SSFFUEL** should be used.

Note that **SSFFUEL** and **SSFMASS must not** both be used in a particular case.

An example of the use of this keyword is

```
SSFFUEL 4
W182 1.34834187E+22
W183 7.27597094E+21
W184 1.55899050E+22
W186 1.44654079E+22
```

In this case tungsten with the ^{180}W isotope removed is to be used in the self-shielding calculation.

The **SSFFUEL** keyword in this section applies to the collapse calculation initiated by the **FISPACT** keyword. The keyword may also appear in the inventory calculation section in conjunction with further **GETXS** keywords.

5.1.21 SSFGEOMETRY *type length1* <*length2* >

This keyword introduces the use of the "universal sigmoid curve" model of self-shielding [21, 22, 23] to account approximately for the reduction of the neutron flux by cross-section resonances.

The first integer parameter *type* defines the type of target geometry and the following one or two real parameters specify the size of the target, in units of cm. Permitted values of *type* are 1–4, with interpretations as follows

type	Target shape	*length1*	*length2*
1	foil	thickness	*(not used)*
2	wire	radius	*(not used)*
3	sphere	radius	*(not used)*
4	cylinder	radius	height

where foil targets are taken to be of infinite transverse extent and wires are taken to be infinitely long.

The self-shielding factors are calculated using the resolved resonances of the nuclides specified with the **SSFFUEL** keyword, or indirectly using the **SSFMASS** keyword. In the latter case, the natural abundance data stored internally in FISPACT-II are used to calculate the numbers of atoms of the individual nuclides.

For foil (*type* = 1) or wire (*type* = 2) targets, the numbers of atoms specified are interpreted as being per unit area or length, respectively.

Note that **SSFGEOMETRY** and **PROBTABLE must not** both be used in a particular case.

An example of the use of this keyword is

```
SSFMASS 0.000193 1
 W 100.0
SSFGEOMETRY 1 0.01
```

In this case pure tungsten is specified. A foil 0.1 mm thick containing 0.193 gcm^{-2} of tungsten with the five stable isotopes in their natural abundances is to be used in the self-shielding calculation.

The **SSFGEOMETRY** keyword in this section applies to the collapse calculation initiated by the **FISPACT** keyword. The keyword may also appear in the inventory calculation section in conjunction with further **GETXS** keywords.

5.1.22 SSFMASS *totm indx2* *sym(i) xp(i) i=1, indx2*

This keyword allows the input of the total mass *totm* (kg) and the number (*indx2*) of elements in the material to be used in the self-shielding calculation. For each element the chemical symbol *sym(i)*, e.g. 'W', and the percentage by weight, *xp(i)*, are then read. This keyword enables elements to be input with the number of atoms of each isotope calculated by FISPACT-II using natural abundance data that are stored internally. If an element whose natural abundances are not known is selected, then FISPACT-II will issue a fatal error message. Computations for these cases **must** use the **SSFFUEL** keyword.

The **SSFMASS** keyword is the recommended method of inputting materials, unless special isotopic compositions are required.

An example of the use of this keyword is

```
SSFMASS 1.0 1
 W 100.0
```

In this case pure tungsten is specified. 1 kg of tungsten containing the five stable isotopes in their natural abundances is to be used in the self-shielding calculation.

Note that **SSFFUEL** and **SSFMASS must not** both be used in the same case in the input file.

It is not essential that the total of all elements is exactly 100%. However, it is recommended that the user ensures that the total percentage of all elements equals 100%.

The **SSFMASS** keyword in this section applies to the collapse calculation initiated by the **FISPACT** keyword. The keyword may also appear in the inventory calculation section in conjunction with further **GETXS** keywords.

5.2 Initial Conditions

This section of the input file follows the keyword **FISPACT**. If an inventory calculation is to follow, this section **must** contain information about the particular material (elemental or isotopic composition and mass) and the initial conditions for the irradiation history (the first timestep and flux value).

Keywords that control the initialisation of the rate equation solution process **must** be placed in this section.

If pathways calculations are to be performed, this section **must** also contain the keywords that initialise the pathway calculations. Similarly, the keywords used for sensitivity calculations **must** also be placed in this section.

Keywords that set the flux amplitude should be used in this section, but may also occur in the inventory calculation section.

Most output selection keywords **must** also be placed in this section, although some may also occur in the inventory calculation section.

The **ATOMS** or **SPECTRUM** keywords may appear in this section to produce output describing the initial inventory before irradiation.

The initial conditions section is terminated by the first occurrence of the **TIME** keyword, which sets the first timestep and causes the start of the solution of the inventory

equations. Exceptionally, the section may also be terminated by the **END** keyword for runs that do not require an inventory calculation.

5.2.1 ATOMS

When it is used in the initial conditions section of the `input` file, this keyword causes the initial inventory to be printed to the `output` file. This keyword may also be used in the inventory calculation section of the `input` file; see Section 5.3.1.

5.2.2 ATWO

This keyword causes data on the legal limits of activity for transport of radioactive material to be read, the calculations to include these data to be performed and the results for individual nuclides and summed values to be output for all timesteps.

5.2.3 BREMSSTRAHLUNG *iarg* *nuclb(j) j=1, iarg*

This keyword allows the input of the number, *iarg* of nuclides and the identifiers, *nuclb(j)* for each of the nuclides. The identifier should be specified using the format 'Te129m'. When the output is generated, this keyword causes the bremsstrahlung dose rate of each specified nuclide to be printed at the end of each time interval.

An example of the use of this keyword is

```
BREM 4
CL36 AR39 AR42 K42
```

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.

5.2.4 CLEAR

This keyword causes information on the clearance data of radionuclides to be input, the calculations to include these data to be performed and the results for individual nuclides and summed clearance indices to be output at all timesteps.

5.2.5 CULTAB

This keyword inserts additional lines at the beginning and end of the `tab` files, so that the files can be processed more easily by other computer programs. The data written are unchanged by the use of this keyword, which is retained for consistency with earlier FISPACT versions.

5.2.6 DENSITY *densty*

This keyword enables the input of the density of the material undergoing irradiation. The parameter *densty* should be given in units of $\mathrm{g\,cm^{-3}}$. If this keyword is used, then the total activity will also be output in units of $\mathrm{Ci\,cm^{-3}}$ in addition to the standard output in $\mathrm{Bq\,kg^{-1}}$. 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 keyword is

```
DENSITY 8.96
```

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

5.2.7 DOSE *ndose* {1} <*dist*> {0}

Dose rates are calculated for a semi-infinite slab of the material. This is the default if the keyword is not used or if $ndose = 1$, but if $ndose = 2$ then the calculations are done for a point source of 1 g 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.

An example of the use of this keyword is

```
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.

The **DOSE** keyword **must not** appear more than once in an input file.

5.2.8 EAFVERSION *neafv* {7}

This keyword may also appear in the library data preparation section of the `input` file; see Section 5.1.3.

EAFVERSION must be used before the keywords **GETXS** or **GETDECAY** to which it refers, as it determines which input streams from the `files` file are used to read the nuclear data.

5.2.9 END
**** Title***

This keyword terminates the input of data for a particular run. It is the final keyword that is read from the `input` file and the remainder of the file is ignored. The text used in *Title* is arbitrary and must be preceded by the `*`.

An example of the use of this keyword is

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

5.2.10 ERROR *nerror*
parent(i) daughter(i) ermat(i) i=1, nerror

This keyword 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 of FISPACT prior to 3.0, the user had to input a value of the fractional error, but this is now available from the EAF or ENDF uncertainty files.

If data from the uncertainty file are to be used then *ermat* **must** be set to -1. If the keyword is absent, then all *ermat* values default to -1.

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

This keyword should only be used following the keyword **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. Parent-daughter pairs listed must also appear in the **SENSITIVITY** list.

An example of the use of this keyword is

```
ERROR 2
 Li7 Li8 -1.0
 Be9 He6 -1.0
```

Line 2 specifies that the reaction ^{7}Li(n,γ)^{8}Li is to be considered. Line 3 specifies that the reaction ^{9}Be(n,α)^{6}He is to be considered. The uncertainty for both reactions is obtained from the uncertainty file.

5.2.11 FISCHOOSE *ncho fischo(i) i = 1, ncho*

FISCHOOSE affects the choice of actinides included in the pathways analysis, *not* the actinides included in the activation calculation. **USEFISSION** and **FISYIELD** are the keywords to use to alter the treatment of actinides in the activation calculation.

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 and decay 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 all actinides are considered, but by setting *ncho* and specifying the identifiers of the actinides the user can limit the nuclides to be included.

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 keyword only affects the calculation of pathways, all actinides are considered during the calculation of inventories (unless the use of other keywords indicates otherwise).

An example of the use of this keyword is

```
FISCHOOSE 4 U238 Pu239 Pu240 Pu242
```

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

5.2.12 FISYIELD *nyld <symb(i) i=1,|nyld|>*

When actinides are included in the list of input elements and **USEFISSION** is specified, then by default only U235, U238 and Pu239 will produce fission products when they undergo 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 fissionable isotopes that have no fission yield data in the selected library do *not* undergo fission.

Examples of the use of this keyword are

```
FISYIELD 0
```

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

```
FISYIELD 2 U235 Pu239
```

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

```
FISYIELD -2 U238 Am241
```

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

5.2.13 FLUX *flux2*

This keyword enables the total energy-integrated projectile flux (in $\mathrm{cm}^{-2}\,\mathrm{s}^{-1}$) to be specified for a particular time interval.

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

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

The flux **must** be set to a strictly positive value before the first irradiation step.

The flux **must** be set to zero before using the keyword **ZERO**.

An example of the use of this keyword is

```
FLUX 1.5E15
```

For the next time interval a total flux of 1.5×10^{15} n cm^{-2} s^{-1} will be used and this will also be used for subsequent time intervals until countermanded by a further **FLUX** keyword.

5.2.14 FUEL *n1* *is(j) atoms(j) j=1, n1*

This keyword allows the input of the number, *n1* of nuclides and the name, *is(j)* and the number of atoms, *atoms(j)* for each nuclide. The name is specified using the format 'Te129m'.

The specification of nuclides is essential if the materials to be irradiated do not have the natural isotopic abundance. 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 **FUEL** and **MASS must not** both 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 keyword is

```
FUEL 2
 Li6 8.5E24
 Li7 1.5E24
```

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

5.2.15 FULLXS

This keyword may also be used in the library data preparation section of the `input` file; see Section 5.1.5.

For it to be effective it must be specified before the cross-section libraries are collapsed, i.e., before the **GETXS** keyword with arguments *1 ebins*.

5.2.16 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 contributions of all the pathways are added to give the contribution of the generic pathway. The default is always to print the generic information, but it can be switched off by setting *igener* to 0.

5.2.17 GETXS *libxs* <*ebins* >

This keyword may also appear in the library data preparation section of the `input` file; see Section 5.1.7.

When this keyword is used in the initial conditions section of the `input` file, its actions are performed immediately, so all settings that are to apply to the reading of new cross-sections **must** be declared before the use of **GETXS**.

5.2.18 GRAPH *numg grshow guncrt nopt(i) i=1, numg*

This keyword 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. If *grshow* = 2 then a `.gra` file is written in a form suitable for gnuplot and a `.plt` file containing gnuplot commands to plot the graphs is also written. For example, issuing the command

```
gnuplot test81.plt
```

will create the file `test81.gra.ps` from `test81.gra`. An example of an activity output graph produced by this command on a Linux workstation is shown in Fig. 5.

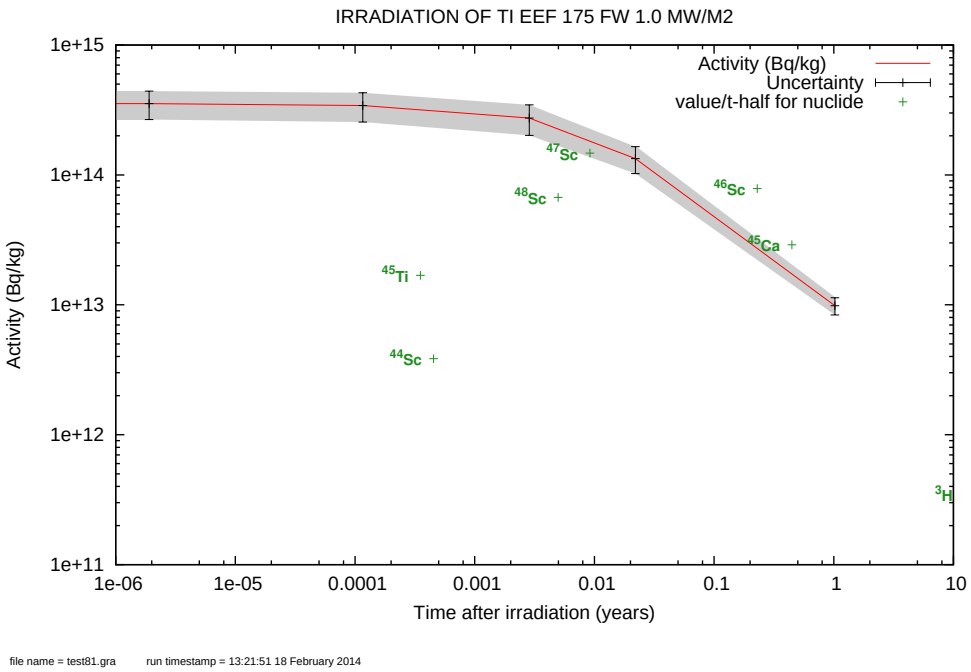

Figure 5: Graphical output produced using the gnuplot visualisation package.

The third parameter *guncrt* allows the user to specify if uncertainty data should be (1) or should 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.

The axes are scaled automatically in the gnuplot `.plt` file. The minimum time is set to the start of the logarithmic decade in which the first cooling step is displayed. The value of the radiological quantity at the start of the cooling time ($t = 0$) is plotted on the ordinate of this graph. The graph command will fail if there is not at least one cooling step.

If different display options are required, then the user may edit the `*.plt` files to match their preferences.

An example of the use of this keyword is

```
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 with uncertainty data included. From this file three graphs can subsequently be plotted.

5.2.19 GROUP *igamgp* {0}

This keyword specifies the binning of the discrete photon spectral lines into histograms for use in the γ-dose computations and **PRINTLIB** output. The same bins are used for the approximate γ spectra generated when the **SPEK** keyword is used in the condense phase of the library data processing.

The default ($igamgp = 0$) means that the γ-spectrum data are output in a 24-energy group structure.

However, if $igamgp = 1$ then the output is in the 22-group 'Steiner' energy structure.

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 keyword is

```
GROUP 1
```

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

Table 6 summarises the energy group structures for the 24- and 22-group formats.

5.2.20 GRPCONVERT *nestrc ndstrc*

This keyword may also be used in the library data preparation section of the `input` file; see Section 5.1.8.

5.2.21 HALF

This keyword causes the half-life of each nuclide to be printed in the output at all timesteps. The units are seconds, but if the nuclide is stable then the word 'Stable' is printed. If this keyword 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.

Table 6: The Gamma spectrum energy group structures for the 24- and 22-group formats.

24 Group		**22 Group**	
Group number	Energy range (MeV)	Group number	Energy range (MeV)
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 $\rightarrow$		

5.2.22 HAZARDS

This keyword causes data on potential ingestion and inhalation doses to be read and the dose due to individual nuclides to be printed in the output at all timesteps.

5.2.23 INDEXPATH

This keyword causes the index of nuclides that lie on the significant pathways to be written to the `ind_nuco` channel if a pathways calculation is selected (see also Section 5.2.59 on the **UNCERTAINTY** keyword).

5.2.24 IRON

This keyword should be used only for calculations where small quantities of impurities in an iron matrix are to be irradiated. In a run without this keyword the activity of the impurities would probably be masked by the activity of the iron. In order to remove the "background" this keyword causes the iron matrix to be replaced by a matrix of a fictitious stable nuclide with no induced reactions so that the printed inventories and dose rates refer only to the impurities.

An example of the use of this keyword is

```
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.

5.2.25 LOGLEVEL *level* {2}

See Section 5.1.9 on page 51 for more information.

5.2.26 LOOKAHEAD

This keyword is used for fine-tuning of the pathways and uncertainty calculations. If it is present then the pathways and uncertainty calculations do a look-ahead over the entire cooling phase and add any dominant nuclides that appear in the late-time

dominant nuclide lists to the list of target nuclides created at the **ZERO** time for use in the pathways calculation.

This keyword should be used with care as it may lead to slow calculations or even code failure through heap exhaustion because of large numbers of target nuclides in the pathways calculation. For further discussion on this see the **UNCERTAINTY** keyword on page 83.

Examples of the use of the **LOOKAHEAD** keyword may be found in `fispQA/-Tst_709/test127.i` and `fispQA2010/Tst_211/test79.i`.

5.2.27 MASS *totm indx2* *sym(i) xp(i) i=1, indx2*

This keyword 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 read. This keyword enables elements to be input with the number of atoms of each isotope calculated by FISPACT-II using natural abundance data that are stored internally. If an element whose natural abundances are not known is selected, then FISPACT-II will issue a fatal error message. Computations for these cases **must** use the **FUEL** keyword.

The **MASS** keyword is the recommended method of inputting materials, unless special isotopic compositions are required.

An example of the use of this keyword is

```
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.

Note that **FUEL** and **MASS must not** both 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 only 800 g of material would be considered in the calculation. It is recommended that the user ensures that the total percentage of all elements equals 100%.

5.2.28 MCSAMPLE *distrib* {1} *nsamples* {10} *lb* {-3.0} *ub* {3.0}

This keyword is used in conjunction with the **SENSITIVITY** keyword to change the sampling used in the Monte-Carlo calculation. In the Monte-Carlo calculation, values of cross-sections are randomly selected from a distribution with a mean and standard deviation given by the value and uncertainty specified. The first argument, *distrib*, is an integer that specifies the distribution to be used:

1 log-normal
2 normal
3 uniform
4 log-uniform

nsamples is the number of Monte-Carlo samples per parent-daughter pair specified by **SENSITIVITY**. *lb* and *ub* give the cutoffs for the log-normal and normal distributions. For the log-normal distribution, these define the range in multiples of the standard deviation from the logarithm of the mean at which the logarithm of the sample is accepted. For the normal distribution, they define the range in multiplies of the standard deviation from the mean at which the sample is accepted. *lb* and *ub* are not used for the uniform and log-uniform distributions.

5.2.29 MCSEED *dim seed(i), i=1,dim*

This keyword is provided to allow repeatable selections of pseudo-random numbers to be made by specifying the random number seed. FISPACT-II uses the intrinsic Fortran 95 random number generator, and the dimension of the seed depends on the compiler used. *dim* is the dimension of the seed array, and *seed(i)* are the *dim* integers to seed the pseudo-random number generator. An example of the use of this keyword is

```
MCSEED 8 437395160 1404128605 572505362 -1187264075 454383258 525702629 973594203 1758310677
```

The value of *dim* may be found by looking at the log file for a run undertaken without this keyword. For example, a run using FISPACT-II compiled using the Intel Fortran compiler gave the log message

```
run sensitivity
Log  : dimension of seed array =            2
Log  :              seed value =    502091259
Log  :              seed value =          493
```

In this case, two integer values are needed to get reproducible pseudo-random numbers.

5.2.30 MIND *mind* {1}

This keyword allows the input of a parameter indicating the minimum number of atoms which are regarded as significant for the output of the inventory. It is usually not important to consider a few atoms of a nuclide. The default value is 1, but this means that inventory tables with an extremely large number of unimportant nuclides will be output, and it is recommended that a value such as 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.

A request for a small *mind* will produce meaningful results only if the *atol* parameter of the **TOLERANCE** keyword is also set to a suitable small value, less than the value of *mind*.

An example of the use of this keyword is

```
MIND 1.0E5
```

In this case all nuclides with numbers of atoms $< 10^5$ are omitted from the inventory output.

5.2.31 NOCOMP

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

5.2.32 NOSORT

The default output includes a sorted list of the dominant nuclides where a maximum of *topx* {10} 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 keyword to reduce running time, although including the list typically increases the running time by only a few percent.

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

5.2.33 NOSTABLE

Use of this keyword 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. This keyword may also be used in the inventory calculation section of the `input` file.

5.2.34 NOT1

This keyword switches off the output to the external file that was switched on by the **TAB1** keyword. Both **TAB1** and **NOT1** may be used several times during a run to restrict the output as required.

5.2.35 NOT2

This keyword switches off the output to the external file that was switched on by the **TAB2** keyword. Both **TAB2** and **NOT2** may be used several times during a run to restrict the output as required.

5.2.36 NOT3

This keyword switches off the output to the external file that was switched on by the **TAB3** keyword. Both **TAB3** and **NOT3** may be used several times during a run to restrict the output as required.

5.2.37 NOT4

This keyword switches off the output to the external file that was switched on by the **TAB4** keyword. Both **TAB4** and **NOT4** may be used several times during a run to restrict the output as required.

5.2.38 OVER *ja*

This keyword 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 using the format 'Te129m'[2].

The **OVER** keyword is followed by one of four keyword options:

[2]Note that the nuclide name specification is not case conscious, so Te129m or TE129M or te129m or tE129M, etc. could equally well be used.

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 and ENDF libraries $ngr = 1$. (*ngr* is used to retain backward compatibility.) *jb* is specified in the same manner as *ja* above.

Note that if a fission reaction is required then *jb* should be either `Fission` or `0`.

ALAM *thalf units*

thalf is the new half-life of the nuclide and *units* specifies the time unit:

SECS	1	seconds
MINS	2	minutes
HOURS	3	hours
DAYS	4	days
YEARS	5	years

The units are specified either by name (SECS, MINS, etc.) or by number (1, 2, etc)

ADCROSS *jb*
errfcx

jb is the daughter of the reaction and *errfcx* is the new error factor for the cross-section.

ADLAM *dthalf*

dthalf is the new error factor for the half-life.

Examples of the uses of the **OVER** keyword are:

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

Here the 1-group cross-section for the reaction ^{9}Be(n,α)^{6}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}C is given the value 3000.0 years for all subsequent calculations in the run.

```
OVER C14
 ADCROSS C13 1.10
```

Here the error factor for the ^{14}C(n,2n)^{13}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 that the **OVER** keyword **must** occur after the **GETXS** and **GETDECAY** keywords that obtain the library data to be modified.

5.2.39 PATH *nlink*
indxp(i) i = 1, nlink+1

This keyword allows a particular pathway consisting of *nlink* reactions and decays to be specified. The (*nlink*+1) nuclides in the pathway are input using their identifiers (e.g. 'Te129m'). For backwards compatibility the 'R' and 'D' have been retained, but are not used. Any character (e.g., 'X') could be used instead. All reactions and decays between a given parent and daughter nuclide are retained, and the path calculation gives a breakdown of the percentage of the inventory of the daughter due to each reaction and decay that leads to it from the specified parent.

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

Path inventories are calculated over all the timesteps until the **ZERO** keyword is encountered.

It is possible when using this keyword to produce first a standard inventory and then the numbers of atoms of the daughters are specified in subsequent runs using the **RESULT** keyword. No inventory then needs to be calculated for these runs investigating the pathways.

An example of the use of this keyword is

```
PATH 3
Ti46 R Ti45 D Sc45 R Sc44m
```

This generated the output

```
Target nuclide Sc 44m     5.060% of inventory given by  1 path
--------------------

path  1   5.060% Ti 46 ---(R)--- Ti 45 ---(b)--- Sc 45 ---(R)--- Sc 44m---(S)---
                  100.00%(n,2n)   100.00%(b+)     100.00%(n,2n)
                                    0.00%(n,p)
```

i.e., 5.06% of the daughter nuclide ^{44m}Sc was formed from ^{46}Ti along the path ^{46}Ti(n,2n)^{45}Ti(β^+)^{45}Sc(n,2n)^{44m}Sc.
A very small percentage ($< 0.005\%$) of ^{45}Ti was transmuted to ^{45}Sc by the (n,p) reaction (MT=103).

5.2.40 PATHRESET *showpathways*

For inventory calculations with long cooling times, the dominant nuclides at late times may not be significant at the end of the irradiation phase, and this leads to poor estimates for the uncertainties. One remedy for this is to use the **LOOKAHEAD** keyword. In some instances, particularly where there are actinides in the source material, the look-ahead approach may lead to excessively large numbers of target nuclides in the pathways calculations.

The **PATHRESET** keyword provides an alternative means of including late-time dominant nuclides. Its inclusion leads to the pathways calculation being repeated in the cooling phase and this causes the late time dominant nuclides to be included in the uncertainty calculations. There are three values for the *showpathways* argument:

-1 display pathways for a target nuclide for which pathways have not been displayed at earlier times;

0 do not display pathways, but use the pathways in uncertainty estimates;

1 display pathways for all dominant nuclides at each pathways reset.

If the **PATHRESET** keyword is included in the initial conditions section of the input file, then pathways are recalculated at each step where there are new target nuclides, and all occurrences of the **PATHRESET** keyword in the inventory calculation phase are ignored. The recommended usage of this keyword is to use it where required in the cooling phase of the inventory calculation (c.f., Section 5.3.17 on page 92)

5.2.41 PRINTLIB *print*

This keyword causes the printing of the data libraries in a readable form. The output consists of seven blocks of data, the contents of which 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 projectile spectrum
4. nuclides which will give a bremsstrahlung contribution to the γ dose rate
5. the projectile spectrum used to collapse the cross-section library
6. the photon and particle decay spectral lines energy and intensity for unstable nuclides
7. a list giving the library source of the ENDF cross-section data file for each nuclide (ENDF library input only).

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

0 Blocks 1-5
1 Block 1 only
2 Blocks 2, 3, 4 and 5
3 Block 5 only
4 Block 3 to extra significant figures in two-column format, with the collapsed dpa and kerma cross-sections added
5 Block 6
6 Block 7

Note that if no uncertainty data exist in the library then the keyword **NOERROR must** be used before **PRINTLIB**.

Note that it is recommended that a separate FISPACT-II 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 keyword is

```
PRINTLIB 1
```

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

5.2.42 PROBTABLE *multxs* {0} *usepar* {1}

The primary use of this keyword is in the library data preparation section of the `input` file; see Section 5.1.14. Its use here is in conjunction with a subsequent **GETXS** keyword.

5.2.43 ROUTES *par dau nmax pmin iprpa*

As an alternative to specifying a particular pathway with the keyword **PATH**, the keyword **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.

The parameter *iprpa* must be 0 or 1. It is not used by FISPACT-II, but is retained for backwards compatibility with FISPACT-2007. If output from more pathways is required, then increase *nmax* and decrease *pmin*.

The **ZERO** or **RESULT** keyword initiates the calculation of the routes over all the time intervals before its occurrence.

An example of the use of this keyword is

```
ROUTES Ti46 Sc44 5 1E14 0
RESULT 1
 Sc44 1.00621E15
```

The output for a run using these commands gave:

```
                R O U T E S   A N A L Y S I S   F O R   I R R A D I A T I O N   P H A S E
                ================================================================================

 no of steps        =      1
 irradiation time   =  7.88940E+07 secs
 flux               =  4.27701E+14 n/cm**2/s
 path floor         =  9.93829E+00% of target inventory
 loop floor         =  1.00000E+00% of path inventory
 max depth          =    5    (maximum number of edges between source and target)

 Source Nuclides
  Ti 46

 Target Nuclides
  Sc 44
```

```
Target nuclide Sc 44     43.147% of inventory given by  3 paths
--------------------

path  1  19.768% Ti 46 ---(R)--- Sc 45 ---(R)--- Sc 44 ---(S)---
                    98.16%(n,np)   100.00%(n,2n)
                     1.84%(n,d)

path  2  12.392% Ti 46 ---(R)--- Sc 45 ---(R)--- Sc 44m---(b)--- Sc 44 ---(S)---
                    98.16%(n,np)   100.00%(n,2n)   100.00%(IT)
                     1.84%(n,d)                      0.00%(n,n)

path  3  10.987% Ti 46 ---(R)--- Sc 45m---(d)--- Sc 45 ---(R)--- Sc 44 ---(S)---
                    96.62%(n,np)   100.00%(IT)     100.00%(n,2n)
                     3.38%(n,d)

                 G E N E R I C    R O U T E S   F O R   I R R A D I A T I O N   P H A S E
                 ================================================================================

Target nuclide Sc 44     43.147% of inventory given by  1 path
--------------------

path  1  43.147% Ti 46 ---(R)--- Sc 45 ---(R)--- Sc 44 ---(S)---
This generic pathway is the sum of  3 pathways
```

The `path floor` is *pmin* as a percentage of the number of atoms of the target nuclide (^{44}Sc) and `max_depth` is set by *nmax*. For an interpretation of the output, see page 111.

5.2.44 SENSITIVITY *xsens xnsen1 insen3 insen4 parent(i) daughter(i) i=1, insen3 nuclide(j) j=1, insen4*

This keyword allows sensitivity calculations to be performed. The sensitivity Monte-Carlo calculation is undertaken over all the irradiation steps and is initiated by the **ZERO** keyword. Time dependent flux amplitude, flux spectra and cross-sections are permitted in sensitivity runs.

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 keyword **must not** be input twice. In the current version the *LAMBDA* option is not available.

The cut-off value *xnsen1* is the magnitude of the correlation coefficient (≤ 1.0) value below which results are not printed. A typical value may be 0.8.

The independent variables for the monte-carlo calculations are the reactions defined by *insen3* parent-daughter pairs. To include fission use the name `Fission` or number `0` for the daughter nuclide name.

For each of the *insen4* nuclides specified the sensitivity of that nuclide to each of the *insen3* cross-sections or decay constants is calculated.

If *insens4* is set to zero, then the merged list of dominant nuclides (i.e., all nuclides that appear on any of the dominant lists) is used as the nuclide list.

See Appendix A.11 on page 156 for further details of the sensitivity method, and Section 7.1.9 on page 109 for a description of the output produced.

Example

```
SENSITIVITY SIGMA 0.8 2 1
Ti48 Sc48
Ti49 Sc48
Sc48
```

Parameters for the Monte-Carlo calculation may be reset using the **MCSAMPLE** and **MCSEED** keywords. If *insens4*=0, then the number of nuclides displayed may be controlled by the **SORTDOMINANT** keyword.

5.2.45 SORTDOMINANT *topxx* {20} *topx* {20}

This keyword controls the uncertainty calculations and their display in the output file. *topxx* nuclides are included in the dominant list used for uncertainty calculations and *topx* of them are displayed in the output file. *topx* **must** be less than or equal to *topxx*.

5.2.46 SPECTRUM

This keyword is an alternative to **ATOMS**. It suppresses the inventory output, so that only the γ spectrum and total values are printed. When it is used in the initial conditions section of the `input` file, this summary applies to the initial inventory. This keyword may also be used in the inventory calculation section of the `input` file; see Section 5.3.21.

5.2.47 SPLIT *isplit* {0}

This keyword 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 and is 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 keyword **HAZARDS must** be used to ensure that uncertainties are correctly printed.

5.2.48 SSFCHOOSE *ncho* {0} *nprint* {0}
sym(j), j=1, ncho

The primary use of this keyword is in the library data preparation section of the `input` file; see Section 5.1.18. In this section it will apply to the actions of the next occurrence of the **GETXS** keyword.

5.2.49 SSFDILUTION *nnuc*
nucname(j) num(j)
grp(i,j) dilution(i,j), i=1,num(j), j=1, nnuc

The primary use of this keyword is in the library data preparation section of the `input` file; see Section 5.1.19. In this section it will apply to the actions of the next occurrence of the **GETXS** keyword.

5.2.50 SSFFUEL *n1*
is(j) atoms(j) j=1, n1

The primary use of this keyword is in the library data preparation section of the `input` file; see Section 5.1.20. In this section it will apply to the actions of the next occurrence of the **GETXS** keyword.

5.2.51 SSFGEOMETRY *type length1 <length2 >*

The primary use of this keyword is in the library data preparation section of the `input` file; see Section 5.1.21. In this section it will apply to the actions of the next occurrence of the **GETXS** keyword.

5.2.52 SSFMASS *totm indx2*
sym(i) xp(i) i=1, indx2

The primary use of this keyword is in the library data preparation section of the `input` file; see Section 5.1.22. In this section it will apply to the actions of the next occurrence of the **GETXS** keyword.

5.2.53 TAB1 *ia*

This keyword causes the inventory data in columns 1 and 2, the number of atoms and grams of each nuclide, to be written to an external file (`TAB1`). Note that the stream

number *ia* is now ignored. Both **NOT1** and **TAB1** may be used several times during a run to restrict and restore the output as required.

5.2.54 TAB2 *ib*

This keyword causes the inventory data in columns 3 and 7, the activity (Bq) and dose rate ($\mathrm{Sv\,h^{-1}}$) of each nuclide, to be written to an external file (`TAB2`). Note that the stream number *ib* is now ignored. Both **NOT2** and **TAB2** may be used several times during a run to restrict and restore the output as required.

5.2.55 TAB3 *ic*

This keyword causes the inventory data in columns 8 and 9, the ingestion and inhalation dose (Sv) of each nuclide, to be written to an external file (`TAB3`). Note that the stream number *ic* is now ignored. Both **NOT3** and **TAB3** may be used several times during a run to restrict and restore the output as required.

5.2.56 TAB4 *id*

This keyword causes the gamma-ray spectrum (in $\mathrm{MeV\,s^{-1}}$) in the 24-energy group format (or 22-group format if the **GROUP** parameter is 1) to be written to an external file (`TAB4`). In addition a second column showing the number of gammas per group is also given in `TAB4`. Note that the stream number *id* is now ignored. Both **NOT4** and **TAB4** may be used several times during a run to restrict and restore the output as required.

5.2.57 TIME *t*

When used in the initial conditions section of the `input` file, this keyword sets the first time interval t for the inventory calculation, terminates the initial conditions section and triggers the processing of any keyword actions that may have been queued. The time interval is specified in seconds by default, but the value of the time may be followed by one of the following keywords
SECS, **MINS**, **HOURS**, **DAYS** or **YEARS**
so that time units other than seconds may be used.

5.2.58 TOLERANCE *itol atol* {10^4} *rtol* {2×10^{-3}}

This keyword is used to set absolute (*atol*) and relative (*rtol*) tolerances that are passed to the LSODES solver to control the convergence of the solution. If $itol = 0$

the tolerances are applied to the main inventory calculation and if *itol* = 1 they are applied to pathways calculations. The keyword may be used twice to adjust both pairs of tolerances. If the keyword is used twice or more for a given *itol*, then the last values specified will be used.

The *atol* parameter is significant in relaxing the accuracy requirement on the results for the minor constituents of an inventory and to avoid excessive demands on the solver. If accurate results *are* required for minor constituents of the inventory, indicated by the setting of a small *mind* parameter, then *atol* should be reduced as well.

An example of the use of this keyword is

```
TOLERANCE 0 5.0E3 1.0E-3
```

In this case the absolute and relative tolerances for the main inventory calculation are reduced by a factor of two compared with the default values. See Appendix A.14.4 for more information.

5.2.59 UNCERTAINTY *iuncer* {0} <*path_floor* {0.005} *loop_floor* ↘ →{0.01} *max_depth* {10} iuncer >

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

−1 resets default values for a particular run and permits other values to be specified by the following parameters, which can be present only for this value of *iuncer*.

0 no pathways or estimates of uncertainty are calculated or output;

1 only estimates of uncertainty are output (although all the pathway information is calculated);

2 both estimates of uncertainty and the pathway information are output;

3 only the pathway information is output;

4 now generates a fatal error message.

path_floor {0.005} All pathways contributing more than the *path_floor* fraction of the inventory of the final (target) nuclide are retained.

loop_floor {0.01} All loops that increase the inventory contribution of the path they are on by a fraction greater than the *loop_floor* are retained.

max_depth {10} is the maximum number of links in a path from a source nuclide to a target nuclide.

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 any use of the keyword **UNCERTAINTY** to change the default settings for the pathways calculation **must** precede the first occurrence of the keywords **ATOMS** or **SPECTRUM**.

Note that if no uncertainty data exist in the cross-section library then the valid values of *iuncer* are only −1, 0 or 3.

Omitting the keyword will ensure that only inventory calculations are carried out, and should be done if a fast scoping run is required.

Examples of the use of this keyword are

```
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 keyword for a full investigation of activation.

```
UNCERT -1 0.001 0.005 10 2
```

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

The target nuclides included in a pathways calculation are by default selected by merging the dominant nuclide lists at the end of the irradiation phase. The number of nuclides included in the merged list is controlled by the *topxx* argument of the **SORTDOMINANT** keyword (see page 80).

The number of nuclides selected by the default *topxx*, and the pruning of the pathways search tree caused by the default *path_floor*, *loop_floor* and *max_depth* values usually lead to a quick and accurate pathways and uncertainty calculation. However, even the pruned tree search is subject to combinatorial growth, and so in some cases computational times may become excessive or the available heap storage may become exhausted. Balanced against this is the need to keep sufficient pathways to ensure that important reaction and decay chains are identified and included. If excessive time for pathways calculations is encountered, then try using larger *path_floor* and *loop_floor*

values and smaller *max_depth* and *topxx* values to get faster calculations, and then use different values to assess convergence.

Inventory calculations which have long cooling times pose a particular problem, in that dominant nuclide in late cooling times may be insignificant at the end of the irradiation phase. A symptom of this problem are uncertainties that drop to zero at late times because the pathways to the late-time dominant nuclides are not included in the uncertainty calculation. If the loss of accuracy is due to only a few late-time dominant nuclides, then the **LOOKAHEAD** (Section 5.2.26) keyword provides a simple means of including all the late-time dominant nuclides. In some cases, particularly when there are actinides in the material, then **LOOKAHEAD** leads to a slow computation because too many nuclides get included in the pathways calculation. The **PATHRESET** (Section 5.3.17) keyword provides an alternative in these cases. This keyword causes the pathways calculation to be redone for the dominant nuclides at the time interval preceding the keyword, and by reducing *topxx* and increasing the number of occurrences of **PATHRESET** combinatorial growth can be avoided whilst retaining important pathways at each time step. Uncertainty estimates that are printed for both the old and new set of pathways at the points where **PATHRESET** are used indicate whether the reset is needed to achieve convergence of the error estimate.

A description and examples of the uncertainty and pathways output generated by using this keyword may be found in Sections 7.1.10, 7.1.11 and 7.1.12. Appendices A.12 and A.13 outline the methods of calculation.

5.2.60 UNCTYPE *iuncty* {1}

This keyword 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 keyword 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.

Examples of the use of this keyword are

```
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.

5.2.61 USEFISSION

This keyword causes fission reactions for which fission yield data are stored in the fission yield library to be self-consistently included in the matrix describing the inventory equations. It should be used in conjunction with **FISYIELD** whenever actinides (or other heavy elements that are transmuted to actinides) are specified in the target material. When it is absent, all fission reactions are omitted from the inventory equations, leading to much faster calculations which remain accurate when there are no actinides in the initial inventory and none is produced.

If there are actinides in the initial inventory and the **USEFISSION** keyword has not been used, then warning messages are written to both the `output` and `runlog` files.

5.2.62 WALL *wall*

This keyword allows the input of the total neutron first wall loading *wall* in units of $\mathrm{MW\,m^{-2}}$ 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. $4.15\,\mathrm{MW\,m^{-2}}$. The energy integrated flux, e.g. $1.80 \times 10^{15}\,\mathrm{n\,cm^{-2}\,s^{-1}}$, which is approximated by 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 $2.0\,\mathrm{MW\,m^{-2}}$ was input then a flux value of $(2.0/4.15) \times 1.80 \times 10^{15}\,\mathrm{n\,cm^{-2}\,s^{-1}}$ would be used in the calculations.

WALL is a convenient alternative to using **FLUX** for the irradiation of first wall materials, but great care must be exercised if it used for irradiations with 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.

It should be noted that the wall loading describes the power that impinges on the first wall, *not* what is actually absorbed by it. In this sense the wall loading represents a convenient, but not fundamental, parameter. The power carried by the neutron flux

impinging upon the first wall is related to the 14 MeV neutron current not flux. If one works out the heating power of 14 MeV neutrons it is found that a current C, of $4.44 \times 10^{13}\,\mathrm{n\,cm^{-2}\,s^{-1}}$ is equivalent to $1\,\mathrm{MW\,m^{-2}}$. The relationship between 14 MeV neutron current and flux depends upon the source and first wall geometry and will vary from plant to plant.

5.3 Inventory Calculation Phase

This section of the input file is introduced by the first occurrence of the **TIME** keyword that triggers the start of the solution of the inventory equations. The inventory calculation has one or more irradiation steps, optionally interleaved with cooling steps and terminated by the occurrence of the keyword **ZERO**, optionally followed by one or more cooling steps.

5.3.1 ATOMS

This keyword starts the solution of the inventory equations over the time interval specified and causes the results (isotopic, elemental, spectral) to be output. After the **ZERO** keyword, it also causes pathways and uncertainty results to be output. It is the standard method of producing output; other options are **SPECTRUM** and **RESULT**. The time step is set to zero after the completion of the output, and so **must** be reset in subsequent steps using the **TIME** keyword. This keyword may also be used in the initial conditions section of the `input` file; see Section 5.3.1.

5.3.2 EAFVERSION *neafv* {7}

The primary use of this keyword is in the library data preparation section of the `input` file; see Section 5.1.3.

In this section, **EAFVERSION must** be used before the keyword **GETXS** to which it refers, as it determines which input streams from the `files` file are used to read the nuclear data.

5.3.3 END
**** Title***

This keyword may also be used in the initial conditions sections of the `input` file; see Section 5.2.9.

5.3.4 ENDPULSE

This keyword terminates a "loop" construct that was started by **PULSE**. The actions for all keywords between **PULSE** and **ENDPULSE** are repeated *npulse* times, where *npulse* is the parameter following **PULSE**.

5.3.5 FLUX *flux2*

This keyword may also be used in the initial conditions section of the `input` file; see Section 5.2.13.

5.3.6 FULLXS

This keyword may also be used in the library data preparation section of the `input` file; see Section 5.1.5.

5.3.7 GETXS *libxs* <*ebins* >

This keyword must be used in the library preprocessing section (see page 49) to collapse cross-sections or to input previously collapsed cross-sections.

It may be also used in the inventory calculation phase to compute new collapsed cross-sections where the projectile spectrum changes significantly during the course of an irradiation, or where the dependence of cross-sections on energy changes significantly due to temperature changes.

When **GETXS** is used in the inventory calculation section of the `input` file, its actions are performed immediately, so all settings that are to apply to the reading of new cross-sections **must** be declared before the use of **GETXS**.

If the projectile spectra at a series of irradiation times are known, then it is possible to prepare the corresponding `collapx` files prior to the inventory calculation. An input file that would achieve this is

```
GETXS 1 69 << first collapse >>
SPEK
GETDECAY 1 << condense decay data >>
FISPACT
* THREE COLLAPSES AND CONDENSE
GETXS 1 69 << second collapse >>
GETXS 1 69 << third collapse >>
END
* END OF COLLAPSE
```

The cross-section files and flux files for each of these collapses are specified in the order in which they are used in the `files` file:

```
...
# first collapse
#input
fluxes  FLUXES.01
crossec  ../../EAF2007data/eaf_n_gxs_069_fis_20070
crossunc  ../../EAF2007data/eaf_un_20070
#output
collapxo  COLLAPX.01

# second collapse
#input
fluxes  FLUXES.02
crossec  ../../EAF2007data/eaf_n_gxs_069_fis_20070
crossunc  ../../EAF2007data/eaf_un_20070
#output
collapxo  COLLAPX.02

# third collapse
#input
fluxes  FLUXES.03
crossec  ../../EAF2007data/eaf_n_gxs_069_fis_20070
crossunc  ../../EAF2007data/eaf_un_20070
#output
collapxo  COLLAPX.03
...
```

The inventory run using these collapsed cross-sections uses **GETXS** in the input file to replace the collapsed cross-sections as required:

```
<< physical data from condensed library >>
GETXS 0 << get cross section from first COLLAPX.01 file in files >>
GETDECAY 0 << get decay data from ARRAYX >>
FISPACT
...
<< first part  using COLLAPX.01 >>
TIME 6.109E-06 DAYS
SPECTRUM

<< second part  using COLLAPX.02 >>
GETXS 0
FLUX 2.64634E+14
TIME 6.108994E0 DAYS
SPECTRUM

<< third part using COLLAPX.03 >>
GETXS 0
FLUX 2.66930E+14
TIME 2.44410E+01 DAYS
```

```
ATOMS
...
```

where now the `files` file contains the queue of collapsed cross-section files, with one `collapxi` for each **GETXS** *0* in the input file:

```
# collapsed cross-sections queue
collapxi  COLLAPX.01
collapxi  COLLAPX.02
collapxi  COLLAPX.03
```

Complete examples of this usage are given in the test directory `fispQA2010/Tst_burn`.

5.3.8 GRPCONVERT *nestrc ndstrc*

The primary use of this keyword is in the library data preparation section of the `input` file; see Section 5.1.8. Its use in the inventory section is in conjunction with **GETXS**.

5.3.9 LOGLEVEL *level* {2}

See Section 5.1.9 on page 51 for more information.

5.3.10 NOSTABLE

This keyword may also be used in the initial conditions section of the `input` file; see Section 5.2.33.

5.3.11 NOT1

This keyword may also be used in the initial conditions section of the `input` file; see Section 5.2.34.

5.3.12 NOT2

This keyword may also be used in the initial conditions section of the `input` file; see Section 5.2.35.

5.3.13 NOT3

This keyword may also be used in the initial conditions section of the `input` file; see Section 5.2.36.

5.3.14 NOT4

This keyword may also be used in the initial conditions section of the `input` file; see Section 5.2.37.

5.3.15 OVER *ja*

This keyword may also be used in the initial conditions section of the `input` file; see Section 5.2.38.

5.3.16 PARTITION *npart*
sym(n) xpart(n) n=1, npart

This keyword 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 keyword 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 keyword is

```
PARTITION 2
 Ar 0.01
 K  0.20
```

In this case all elements except argon and potassium remain unmodified, all argon isotopes are reduced by a factor of 100 and all potassium isotopes are reduced to a fifth of their values before the keyword was used.

5.3.17 PATHRESET *showpathways*

For inventory calculations with long cooling times, the dominant nuclides at late times may not be significant at the end of the irradiation phase, and this leads to poor estimates for the uncertainties. One remedy for this is to use the **LOOKAHEAD** keyword. In some instances, particularly where there are actinides in the source material, the look-ahead approach may lead to excessively large numbers of target nuclides in the pathways calculations at the end of the irradiation phase, and this may cause slow calculations and in some cases exhaustion of available heap storage.

The **PATHRESET** keyword provides an alternative means of including late-time dominant nuclides. Its inclusion after the **ZERO** keyword leads to the pathways calculation being repeated at the cooling step immediately before its occurrence. It can be included as often as required. This causes the late-time dominant nuclides to be included in the uncertainty calculations. There are three values for the *showpathways* argument:

-1 display pathways for a target nuclide for which pathways have not been displayed at earlier times;

0 do not display pathways, but use the pathways in uncertainty estimates;

1 display pathways for all dominant nuclides at each pathways reset.

An example of the use of this keyword is

```
TIME 6.8E10 ATOMS
PATHRESET 0
TIME 2.2E11 ATOMS
```

For further discussion on this see the **UNCERTAINTY** keyword on page 83.

Examples of its use may be found in `fispQA/Tst_709/test128.i` and `fispQA2010/-Tst_211/test80.i`.

5.3.18 PROBTABLE *multxs* {0} *usepar* {1}

The primary use of this keyword is in the library data preparation section of the `input` file; see Section 5.1.14. Its use here is in conjunction with a subsequent **GETXS** keyword.

5.3.19 PULSE *npulse*

This keyword is used to start the "loop" construct in the `input` file. *npulse* is the number of times that the keywords between **PULSE** and **ENDPULSE** are repeated. Using FISPACT-II it is possible to nest this pair of keywords to an arbitrary depth, and there is now no limit on *npulse* for any loop.

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

An example of the use of this keyword is

```
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 (the end of the irradiation) has a detailed inventory since **ATOMS** is used.

5.3.20 RESULT *nresu*
sym(i) x(i) i =1, nresu

This keyword 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 perform an inventory run prior to the pathway calculation. However, it is much easier to be able to get the inventory from 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 keyword **PATH** or **ROUTES**.

An example of the use of this keyword is

```
RESULT 3
 C14 1.356E19
 N14 8.560E17
 N15 7.568E12
```

The numbers of atoms of ^{14}C, ^{14}N and ^{15}N obtained from a standard inventory run are specified.

5.3.21 SPECTRUM

This keyword is an alternative to **ATOMS**. It suppresses the inventory output, 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. This keyword may also be used in the initial conditions section of the `input` file; see Section 5.2.46.

5.3.22 SSFCHOOSE *ncho* {0} *nprint* {0}
sym(j), j=1, ncho

The primary use of this keyword is in the library data preparation section of the `input` file; see Section 5.1.18. In this section it will apply to the actions of the next occurrence of the **GETXS** keyword.

5.3.23 SSFDILUTION *nnuc*
nucname(j) num(j)
grp(i,j) dilution(i,j), i=1,num(j), j=1, nnuc

The primary use of this keyword is in the library data preparation section of the `input` file; see Section 5.1.19. In this section it will apply to the actions of the next occurrence of the **GETXS** keyword.

5.3.24 SSFFUEL *n1*
is(j) atoms(j) j=1, n1

The primary use of this keyword is in the library data preparation section of the `input` file; see Section 5.1.20. In this section it will apply to the actions of the next occurrence of the **GETXS** keyword.

5.3.25 SSFGEOMETRY *type length1 <length2 >*

The primary use of this keyword is in the library data preparation section of the `input` file; see Section 5.1.21. In this section it will apply to the actions of the next occurrence of the **GETXS** keyword.

5.3.26 SSFMASS *totm indx2*
sym(i) xp(i) i=1, indx2

The primary use of this keyword is in the library data preparation section of the `input` file; see Section 5.1.22. In this section it will apply to the actions of the next occurrence of the **GETXS** keyword.

5.3.27 TAB1 *ia*

This keyword may also be used in the initial conditions section of the `input` file; see Section 5.2.53.

5.3.28 TAB2 *ib*

This keyword may also be used in the initial conditions section of the `input` file; see Section 5.2.54.

5.3.29 TAB3 *ic*

This keyword may also be used in the initial conditions section of the `input` file; see Section 5.2.55.

5.3.30 TAB4 *id*

This keyword may also be used in the initial conditions section of the `input` file; see Section 5.2.56.

5.3.31 TIME *t*

This keyword allows the input of the irradiation or cooling time interval t (in seconds by default). The value of the time may be followed by one of the following keywords

SECS, **MINS**, **HOURS**, **DAYS** or **YEARS**
so that time units other than seconds may be used.

Note that it is important when inputting times that it is the interval time, not the total elapsed 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 keyword **ZERO**.

Examples of the use of this keyword are

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

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

5.3.32 WALL *wall*

This keyword may also be used in the initial conditions section of the `input` file; see Section 5.2.62.

5.3.33 ZERO

This keyword 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. It also sets the flux to zero, but the **FLUX** keyword should also be used.

This keyword **must** be used after an irradiation if the keyword **GRAPH** is also used in the input file.

This keyword initiates the calculation and output of pathways (as specified by the **UNCERTAINTY**, **ROUTES** or **PATH** keyword in the initialisation phase). If neither **ZERO** nor **RESULT** keywords are present, then no pathways information will be output.

NOTE: Irradiation steps can be specified after the **ZERO** keyword has been specified if so desired. This allows one to investigate pathways for a subset of the irradiation steps or to get graphical output for irradiation steps.

5.4 Miscellaneous

Comments can now be placed throughout the input file.

5.4.1 <<comment >>

Comments may be included anywhere (apart from within the text input lines beginning with *) enclosed by double angle brackets (<< >>). These comments may cover several lines of the input file.

An example of the use of this construction is

```
ATOMS
<< -----irradiation phase----- >>
TIME 2.5 YEARS
```

6 Test Cases: fispQA2007, fispQA2010, fispQA2012 and fispQA

Supplied with the FISPACT-II software are 110 test input files in the `fispQA2007` directory, 185 test input files in the `fispQA2010` directory, 256 test input files in the `fispQA2012` and 270 test input files in the `fispQA` directory together with test output and log files to illustrate the running of FISPACT-II for a variety of irradiation and cooling scenarios, using all the different EAF and ENDF library files and illustrating the use of all the keywords listed in Section 5. The tests are grouped according to the cross-section libraries used. (Directory `Tst_100` uses the 100-group GAM-II cross-section data, and so forth).

The `fispQA2007` tests are based on the test set that was distributed with FISPACT-2007. These are included to show the compatibility with the old-style `files` and `INPUT` files. The `fispQA2010` directory repeats some of the 2007 tests using the new format `files` file and input control files, and adds new tests for the new capabilities and data libraries that were added for Versions 0 and 1 of FISPACT-II. We *strongly* recommend that you do NOT use the obsolete old-style input files, but instead use corresponding new-style files that can be found in the later fispQA directories.

The `fispQA` test set provides tests that use the new ENDF format libraries introduced in Version 2 for cross-sections, fission yields and decay, and the new CALENDF output files for the probability tables used in calculating self-shielding.

Note that some of the test cases issue warnings and some terminate with fatal error messages. The purpose of these test cases is to illustrate the

errors that are issued if obsolescent keywords are used, or if keywords are used incorrectly in the input file.

To find examples of the use of a particular keyword, go to the `fispQA2010` or `fispQA` directory and use `grep` to search for the keyword, for example **UNCERTAINTY**:

```
.../fispQA2010> grep UNCER Tst_*/*.i
Tst_066/test112.i:UNCERT 2
Tst_066/test113.i:UNCERT 0
...
Tst_100/test4.i:UNCERT -1 1.0E-4 1.0E-2 20 3
Tst_100/test8.i:UNCERT 3
Tst_100/test9.i:UNCERT 3
Tst_100/test9.i:UNCERT 0
Tst_172v/test32.i:UNCERT 2
...
```

One can then go to the relevant test directory, e.g., `Tst_100` and view the input files, `files` and say `test8.i`, to see the context of the use of the keyword, and then view what the result of running that case is by looking in the `Tst_100/testresults` directory for the output files `test8.log`, `test8.out`, etc.

In addition to providing a useful guide to using FISPACT-II these test cases provide a check on whether your installation is working correctly. In each of the test directories is a script `fisprun` that runs all the test cases in the directory. The results generated by executing this script should match those in the `testresults` directory, apart from run timestamp, minor roundoff discrepancies and (for sensitivity calculations only) differences arising from different random numbers. ***So if you see error messages from your runs, check against the reference data to see if that is what is expected!***

Test input cases for standard collapse, condense and inventory runs including pathways and uncertainties are covered in the 'Getting Started' section (page 26). Examples of different ways of using the code are illustrated in the `fispQA2010` and `fispQA` directories. For example, in `fispQA2010` see

`test37`	for sensitivity calculation
`test18`	for multi-pulse irradiation
`test65`	for time dependent collapsed cross-sections
`test97/8`	for reduced nuclide set calculations
`test5`	for **ROUTES** investigation
`test6`	for **PATH** calculation
`test8`	for **IRON** calculation
`test10`	for **OVER** calculation

The subdirectories of directory `fispQA` illustrates features added in Version 2.20. Directories `Tst_162alpha`, `Tst_162deut`, `Tst_162gamm`, and `Tst_162prot` respectively contain

illustrations of calculations using the TENDL-2013 libraries for α, d, γ, and p projectiles. The `Tst_709pt` directory illustrates the combination of the CALENDF probability table data with the TENDL-2013 709 group cross-section data for neutron irradiation to add self-shielding corrections to the collapsed cross-sections. The `Tst_709uc` directory illustrates the use of the alternative universal sigmoid curve approximation for self-shielding corrections. The `Tst_709` directory contains some sample inventory runs using different 709 group library data. Further tests using the different ENDF libraries are in the `Tst_709lib` directory. The `Tst_709cern` directory contains examples where the **LOOKAHEAD** and **PATHRESET** keywords are used to capture pathways for late-time dominant nuclides. The `Tst_709mc` directory contains examples of the use of the Monte-Carlo sensitivity calculation. `Tst_binxs` illustrates the use of compressed binary files derived from the ENDF data libraries to speed up calculations. `Tst_709fns` gives examples of the validation calculations for decay heat[24] and `Tst_pulse` contains examples of validation tests using pulse irradiation of actinides.

7 Interpretation of Output

All FISPACT-II runs have two main output files; `output` containing the physical results of the calculation and `runlog` containing error reporting and logging information.

7.1 The Inventory Run `output` File

The layout of `output` has been designed to follow closely that of FISPACT-2007. Unless stated otherwise, the following excerpts are taken from the inventory run described in Section 4.5.

7.1.1 Header and run information

The `output` file always begins with a header identifying the version of the code and the CVS repository export Tag for the Release version. If the **NOHEADER** keyword is absent, this header is followed by a summary of the information given in Section 3 of this manual.

```
================================================================================
|                                                                              |
|                          F I S P A C T - I I                                 |
|                          -------------------                                 |
|                                                                              |
|                 Transmutation-Activation Inventory Code                      |
|                  United Kingdom Atomic Energy Authority                      |
|                                  and                                         |
```

```
|                      Culham Electromagnetics Limited                          |
|                                                                               |
|                           Release 2.20 June 2014                            |
|                    Authors: James Eastwood and Guy Morgan                     |
|            Copyright (c) 2009-14, UK Atomic Energy Authority and              |
|                      Culham Electromagnetics Limited.                         |
|                                                                               |
=================================================================================

---------------------------------------------------------------------------------
Source CVS Tag: $Name:  $
---------------------------------------------------------------------------------
```

Printed after the header information is the box containing unique identifying information for the run.

```
=================================================================================================
|                                                                                               |
|                    R U N   I D E N T I F I C A T I O N   I N F O R M A T I O N                |
|                                                                                               |
| INITIAL CROSS SECTION DATA                                                                    |
| Collapsed library timestamp: 18:16:44 2 August 2014                                           |
| EAF source library label:    EAF-2010 100Gp THE EUROPEAN ACTI                                 |
| FLUX file label:             EEF FW NORM. 1MW/M2 GAM-II TOT=4                                 |
|                                                                                               |
| DECAY DATA                                                                                    |
| Condensed library timestamp: 18:16:45 2 August 2014                                           |
| EAF source library label:    EAF-2010                                                         |
|                                                                                               |
| THIS RUN                                                                                      |
| timestamp:                   18:16:47 2 August 2014                                           |
| fileroot :                   test1                                                            |
| name of FILES file:          files                                                            |
| FISPACT title:               * IRRADIATION OF TI EEF FW 1.0 MW/M2                             |
|                                                                                               |
| See the test1.log file                                                                        |
| and summary details at the end of this file for further information on files used by this run |
|                                                                                               |
=================================================================================================
```

Note that only the initial cross-section data are identified. For runs where the cross-section data change further information on EAF source and flux files is displayed at the end of the `output` file. There are no platform-specific messages, as FISPACT-II is written in standard-conforming Fortran, and the same source is used for Unix, Linux, Mac-OS and Windows versions.

Occurrences of the **ATOMS** keyword in the input file cause the output at the end of the step of

1. table keys (first **ATOMS** only);
2. the time line;
3. iron information (if the **IRON** keyword used, see `fispQA2010 test8` for an example);
4. the inventory, comprising

(a) the heading line;
(b) a line for each nuclide with non-negligible inventory (see **MIND** keyword);
(c) nuclide table totals;
(d) inventory summary.

5. inventory by element (if **NOCOMP** is not used);
6. gamma spectra;
7. gamma-dose totals;
8. dominant nuclides (if **NOSORT** is not used);
9. Bremsstrahlung corrections (if the **BREMSSTRAHLUNG** keyword is used, see `fispQA2010 test4` for an example);

7.1.2 Table key

Prior to the first inventory tables output initiated by the **ATOMS** keyword the following key is printed:

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

This key lists four single character flags that are printed immediately following each nuclide identifier. (Note that the * that was present in FISPACT-2007 output has been dropped, as the equilibrium approximation is not used in the FISPACT-II solver.)

? is the convergence flag whose presence indicates a nuclide with larger uncertainty in its inventory. It is set if the error for the nuclide is greater that 1.5 times the rms norm error set by the `rtol` and `atol` flags (see Appendix A.14);

& indicates that no γ-spectral data were present in the decay data library and that the keyword **SPEK** was used to calculate a spectrum approximately (see Appendix A.10.3). 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;

> indicates that this nuclide was present in the material input, specified by the **MASS** or **FUEL** keyword.

7.1.3 Time line and nuclide inventory

The time line is printed at the start of the output produced at the end of an integration step initiated by the **ATOMS** or **SPECTRUM** keyword. It displays the time interval number, the step length and the total elapsed time. The **ZERO** keyword causes the elapsed time counter to be reset to zero, and the word `COOLING` to be added to the time line.

```
 * * * * TIME INTERVAL   2 * * * * * * * * * * TIME IS   7.8894E+07 SECS OR  2.5000E+00 YEARS * * * * * * ELAPSED TIME IS   2.500 y
NUCLIDE        ATOMS          GRAMS          Bq       b-Energy    a-Energy   g-Energy    DOSE RATE   INGESTION  INHALATION     Bq/A2
                                                          kW          kW         kW         Sv/hr      DOSE(Sv)    DOSE(Sv)      Ratio

H   1    #  8.11507E+21   1.358E-02   0.000E+00   0.000E+00   0.00E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
H   2    #  3.39818E+20   1.137E-03   0.000E+00   0.000E+00   0.00E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
H   3       1.92678E+17   9.650E-07   3.432E+08   3.139E-10   0.00E+00   0.000E+00   0.000E+00   1.442E-02   8.924E-02   8.581E-06
He  3    #  5.62944E+15   2.819E-08   0.000E+00   0.000E+00   0.00E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
He  4    #  2.57627E+21   1.712E-02   0.000E+00   0.000E+00   0.00E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
Si 28    #  3.37819E+05   1.569E-17   0.000E+00   0.000E+00   0.00E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
```

The inventory contains up to eleven columns of data (excluding the nuclide identifier and flags) giving values at the end of the step indicated by the time line. The first seven of these are always printed, and their contents are defined in Table 7. In that table

$A_{r,i}$ = atomic weight of isotope i (amu)
N_A = Avogadro constant (mol^{-1})
$E_{\beta,i}$ = β decay energy for isotope i (eV)
$E_{\alpha,i}$ = α decay energy for isotope i (eV)
$E_{\gamma,i}$ = γ decay energy for isotope i (eV)
C_1 = conversion from eV to kJ ($= 10^{-3}e$)

Note that the atomic weights read from the `eaf_decay` file are in units of neutron masses, but these are converted and stored internally in amu. Note also that the column headings `b-Energy`, `a-Energy` and `g-Energy` used by FISPACT-2007 are retained, despite the fact that the columns contain powers (kW).

The remaining four columns are specified by using the **HAZARDS**, **CLEAR**, **ATWO** and **HALF** keywords. The contents of these columns are defined in Table 8. Note that the clearance index is defined as a dimensionless quantity in FISPACT-II rather than as a quantity of dimension mass (kg) as used in FISPACT-2007 so different results will be seen for input masses different from 1 kg. In that table

e_i^{ing}, e_i^{inh} = factors to convert activity of an ingested or inhaled nuclide into the dose (in Sv) received by an average person over 50 years. These factors are tabulated in `eaf_hazards`.

Table 7: Entries in columns 1-7 of the inventory output table.

column	description	value	units
1	number of atoms	N_i	
2	mass	$N_i A_{r,i}/N_A$	g
3	activity	$A_i = N_i\lambda_i$	Bq
4	β-power	$A_i E_{\beta,i} C_1$	kW
5	α-power	$A_i E_{\alpha,i} C_1$	kW
6	γ-power	$A_i E_{\gamma,i} C_1$	kW
7	dose rate	Eq.(58) or Eq.(61)	$\mathrm{Sv\,h^{-1}}$

L_i = specific activity (in Bq kg^{-1}) below which a material is given clearance for disposal. Values of L_i are tabulated in `eaf_clear`.
m_{tot} = total mass of material (kg)
$A_{2,i}$ = activity level for safe transport. Values of $A_{2,i}$ in TBq are tabulated in `eaf_a2`.
C_2 = conversion factor from TBq to Bq ($= 10^{12}$)

Table 8: Keywords and the entries that they cause to be printed in columns 8-11 of the inventory output table.

keyword	description	value	units
HAZARDS	ingestion dose	$A_i e_i^{ing}$	Sv
	inhalation dose	$A_i e_i^{inh}$	Sv
CLEAR	clearance index	$A_i/(m_{tot}L_i)$	
ATWO	transport index	$A_i/(A_{2,i}C_2)$	
HALF	half-life	$\lambda_i^{-1}\log_e 2$ or 'Stable'	s

See Appendix B.6 and References[13, 25] for more details on the hazards, clearance and transport (A2) data.

7.1.4 Inventory step summary

The step summary appears after the table of values for individual nuclides. The first line contains the number of nuclides N_n printed in the preceding table and the remaining lines give sums over nuclides of various diagnostic quantities. The first three of these lines contain

1. the total activity in curies

$$\texttt{TOTAL CURIES} = C_3 \sum_{i=1}^{N_n} A_i$$

where $C_3 = 1/(3.7 \times 10^{10})$ is the conversion factor from Bq to Ci.

2. the total alpha power in Ci-MeV

$$\texttt{TOTAL ALPHA} = 10^{-6} C_3 \sum_{i=1}^{N_n} A_i E_{\alpha,i}$$

   where the 10^{-6} is the conversion factor from eV to MeV

3. the total beta power in Ci-MeV

$$\texttt{TOTAL BETA} = 10^{-6} C_3 \sum_{i=1}^{N_n} A_i E_{\beta,i}$$

4. the total gamma power in Ci-MeV

$$\texttt{TOTAL GAMMA} = 10^{-6} C_3 \sum_{i=1}^{N_n} A_i E_{\gamma,i}$$

```
 TOTAL NUMBER OF NUCLIDES PRINTED IN INVENTORY =   87

 TOTAL CURIES    TOTAL ALPHA    TOTAL BETA     TOTAL GAMMA
                 CURIE-MeV      CURIE-MeV      CURIE-MeV
 3.38027E+03    3.72537E-13    5.92195E+02    5.48191E+03
```

The next line splits the total activity into parts associated with α, β and γ decays according to their decay type (c.f., Table 10 on page 138). Activity from decays with type IRT = 4 is assigned to the ALPHA BECQUERELS total, activity from those with IRT = 1, 11, 16, 17, 20, 2, 14, 19 is assigned to the BETA BECQUERELS total and from those with IRT = 3 to GAMMA BECQUERELS. Activity from decays with IRT = 12 or 13 is split between the α and β totals, and activity from decays with IRT = 15 is split between the α and γ totals. Note that this definition of the split is different from that used in FISPACT-2007.

```
 ALPHA BECQUERELS = 5.153452E-22  BETA BECQUERELS = 1.133988E+14  GAMMA BECQUERELS = 1.167103E+13

 TOTAL ACTIVITY FOR ALL MATERIALS     1.25070E+14 Bq
                                       6.50837E+01 Ci/cc          DENSITY   1.93E+01 gm/cc
 TOTAL ACTIVITY EXCLUDING TRITIUM     1.25070E+14 Bq
                                       6.50835E+01 Ci/cc

 TOTAL ALPHA HEAT PRODUCTION          2.20867E-18 kW
 TOTAL BETA  HEAT PRODUCTION          3.51057E-03 kW
 TOTAL GAMMA HEAT PRODUCTION          3.24971E-02 kW             TOTAL HEAT PRODUCTION 3.60076E-02 kW

 INITIAL TOTAL MASS OF MATERIAL       1.00000E+00 kg             TOTAL HEAT EX TRITIUM 3.60076E-02 kW

 TOTAL MASS OF MATERIAL               1.00006E+00 kg
 NEUTRON  FLUX DURING INTERVAL        4.27701E+14 n/cm**2/s

 NUMBER OF FISSIONS                   0.00000E+00                BURN-UP OF ACTINIDES  0.00000E+00 %

 INGESTION  HAZARD FOR ALL MATERIALS  1.38528E+05 Sv/kg
 INHALATION HAZARD FOR ALL MATERIALS  3.06441E+05 Sv/kg

 INGESTION  HAZARD EXCLUDING TRITIUM  1.38528E+05 Sv/kg
 INHALATION HAZARD EXCLUDING TRITIUM  3.06441E+05 Sv/kg
```

The TOTAL ACTIVITY FOR ALL MATERIALS item gives total activity in Bq, and the TOTAL ACTIVITY EXCLUDING TRITIUM is the total with tritium activity excluded. The HEAT PRODUCTION items are the sums over all materials of the respective α-, β- and γ-powers, the total of these three powers, and the total with the contribution of tritium decay excluded.

The NUMBER OF FISSIONS is a count of the change of the number of nuclides that may undergo fission from the number in the the initial inventory. These nuclides are identified as those with the MT = 18 reaction on their list of reactions (c.f., Table 12 on page 140). BURN-UP OF ACTINIDES gives the percentage of the initial number of fissionable nuclides that have been burnt up.

Note that NUMBER OF FISSIONS may become negative if, for example, there are no nuclides with MT=18 initially but ones are created by irradiation of the initial inventory. All nuclides with MT=18 reactions are counted, even if their reactions are excluded because **USEFISSION** is absent, or reactions are excluded by the **FISYIELD** keyword or reactions are excluded because their fission yield data are not available.

The remaining items in the summary list depend upon the use of the **ATWO**, **CLEAR** and **HAZARDS** keywords, and on whether the **DENSITY** keyword was used.

If the **ATWO** keyword is used in the input file, then table items TOTAL Bq/A2 RATIO and EFFECTIVE A2 are displayed, where

$$\texttt{TOTAL Bq/A2 RATIO} = \sum_{i=1}^{N_n} \left(\frac{A_i}{A_{2,i} C_2} \right)$$

and EFFECTIVE A2 is the ratio of the total activity to (TOTAL Bq/A2 RATIO).

If the **CLEAR** keyword is used in the input file, then the A2 values are replaced by

$$\texttt{CLEARANCE INDEX} = \sum_{i=1}^{N_n} \left(\frac{A_i}{M_{tot} L_i} \right)$$

The **HAZARDS** keyword causes the total ingestion and inhalation doses, and the total doses excluding the contribution from tritium to be printed.

The **DENSITY** keyword causes the density (in $\mathrm{g\,cm^{-3}}$) to be printed.

The following output fragment is from Tst_709/test120 using TENDL-2013 data that contains kerma, dpa and appm cross-sections (see Table 13). These output appear at this point in the output only for irradiation steps where there is a non-zero flux amplitude.

```
 Total Displacement Rate (n,Ddiss) =  6.21857E+17 Displacements/sec  =  5.76667E-08 Displacements Per Atom/sec  =  1.81982E+00 DPA/year
 Total Displacement Rate (n,Dinel) =  2.13196E+18 Displacements/sec  =  1.97703E-07 Displacements Per Atom/sec  =  6.23903E+00 DPA/year
 Total Displacement Rate (n,Del  ) =  3.12211E+18 Displacements/sec  =  2.89522E-07 Displacements Per Atom/sec  =  9.13662E+00 DPA/year
```

```
Total Displacement Rate (n,Dtot ) =  7.11931E+18 Displacements/sec  =  6.60194E-07 Displacements Per Atom/sec  =  2.08342E+01 DPA/year

KERMA RATE (n,Kktot) =  5.37761E+22 eV/sec = 8.61588E+00 kW/kg = 6.78414E-02 kW/cm^3
KERMA RATE (n,Kphot) =  4.97704E+22 eV/sec = 7.97409E+00 kW/kg = 6.27880E-02 kW/cm^3
KERMA RATE (n,Kfiss) =  0.00000E+00 eV/sec = 0.00000E+00 kW/kg = 0.00000E+00 kW/cm^3
KERMA RATE (n,Kinel) =  1.55007E+22 eV/sec = 2.48348E+00 kW/kg = 1.95549E-02 kW/cm^3
KERMA RATE (n,Knone) =  5.65720E+22 eV/sec = 9.06384E+00 kW/kg = 7.13687E-02 kW/cm^3
KERMA RATE (n,Kel  ) =  5.05826E+20 eV/sec = 8.10422E-02 kW/kg = 6.38127E-04 kW/cm^3
KERMA RATE (n,Ktot ) =  5.70779E+22 eV/sec = 9.14488E+00 kW/kg = 7.20068E-02 kW/cm^3

GAS   RATE (n,Xa   ) =  7.47206E+13 atoms per sec =  6.92906E-06 appm/sec
GAS   RATE (n,Xh   ) =  1.50099E+08 atoms per sec =  1.39191E-11 appm/sec
GAS   RATE (n,Xt   ) =  3.20388E+09 atoms per sec =  2.97105E-10 appm/sec
GAS   RATE (n,Xd   ) =  1.16080E+13 atoms per sec =  1.07644E-06 appm/sec
GAS   RATE (n,Xp   ) =  4.15739E+14 atoms per sec =  3.85527E-05 appm/sec
```

The displacements per atom (DPA) for a single element is given by [26, Eq.(90)]. For mixtures of elements with different lattice displacement energies, the total displacements rate, D_{tot} may be estimated using the ratio of the mean total available energy to the mean displacement energy:

$$D_{tot} = e_d \phi \sum_{i=1}^{N_n} N_i \bar{d}_i / 2\bar{E}_d \tag{1}$$

where ϕ is the flux amplitude in $\mathrm{cm}^{-2}\,\mathrm{s}^{-1}$, N_i is the number of atoms of nuclide i and $\bar{d}_i$ is the collapsed dpa reaction cross-section in eV-cm^2. The constant e_d is the DPA efficiency factor and is set to 80% [26, p. 2757]. A list of the dpa cross-sections recognised by FISPACT-II is given in Table 13.

The mean atomic displacement energy $\bar{E}_d$ is given by

$$\bar{E}_d = \sum_{i=1}^{N_n} N_i E_d(Z_i) / \sum_{i=1}^{N_n} N_i \tag{2}$$

Z_i is the atomic number of nuclide i and E_d are atomic displacement energies (in eV) taken from Table II of Reference[26], with the exception of the value 55 eV used for tungsten (see Table 9).

Alternatively, the displacement rate may be estimated using the mean of the displacement rates of the constituents:

$$D_{tot} = e_d \phi \sum_{i=1}^{N_n} N_i \bar{d}_i / 2E_d(Z_i) \tag{3}$$

Both options have been evaluated and have been shown to give similar results. Equation (3) is used in the present version of FISPACT-II.

The displacements per atom is given by dividing this by the total number of atoms:

$$\texttt{DPA RATE} = D_{tot} / \sum_{i=1}^{N_n} N_i \tag{4}$$

Table 9: Atomic displacement energies used to compute DPA. E_d is 25 eV for all other elements.

Element	E_d in eV	Element	E_d in eV
Be	31	Co	40
C	31	Ni	40
Mg	25	Cu	40
Al	27	Zr	40
Si	25	Nb	40
Ca	40	Mo	60
Ti	40	Ag	60
V	40	Ta	90
Cr	40	W	53
Mn	40	Au	30
Fe	40	Pb	25

The kinetic energy released in materials rates are given by

$$\texttt{KERMA RATE} = \phi \sum_{i=1}^{N_n} \bar{\kappa}_i \tag{5}$$

where $\bar{\kappa}_i$ is the collapsed kerma cross-section for one of the kerma cross-sections listed in Table 13. Specific values of this energy per kilogram and per cm^3 are obtained by scaling the total kerma using the initial mass and density.

Gas production rates (in s^{-1}) are given by

$$\texttt{GAS RATE} = \phi \sum_{i=1}^{N_n} N_i \bar{\sigma}_i^{gas} \tag{6}$$

where $\bar{\sigma}_i^{gas}$ is the collapsed total gas production cross-section in cm^2. A list of the total gas production cross-sections recognised by the code is given in Table 13 on page 143. If there is gas production from decays, then there will be corresponding rates (e.g., `GAS RATE (a decay)`) printed.

If any of the kerma, dpa or gas appm rates are zero, then their production rates are not printed.

The final part of the summary output table is the gas atoms parts per million for the five secondary gas nuclides:

```
APPM OF H   1    =   644.46
APPM OF H   2    =   26.987
APPM OF H   3    =  0.15302E-01
APPM OF He  3    =  0.44706E-03
APPM OF He  4    =   204.59
```

7.1.5 Elemental inventory

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

COMPOSITION OF MATERIAL BY ELEMENT

		ATOMS	GRAM-ATOMS	GRAMS	BETA CURIES-MeV	BETA kW	GAMMA CURIES-MeV	GAMMA kW	ALPHA CURIES-MeV	ALPHA kW
1	H	8.4551E+21	1.4040E-02	1.4718E-02	5.2945E-05	3.1385E-10	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	He	2.5763E+21	4.2780E-03	1.7123E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
14	Si	3.2358E+09	5.3732E-15	1.6928E-13	1.7214E-08	1.0204E-13	1.8729E-08	1.1102E-13	0.0000E+00	0.0000E+00
15	P	2.4013E+09	3.9875E-15	1.2675E-13	3.5813E-08	2.1229E-13	9.9559E-08	5.9016E-13	0.0000E+00	0.0000E+00

7.1.6 Gamma spectrum

In this section the total powers ($\mathrm{MeV\,s^{-1}}$) from α, β and γ radiations and the total number of spontaneous fission neutrons are listed followed by two columns giving the γ spectrum ($\mathrm{MeV\,s^{-1}}$ per group) and number of gammas per group ($\mathrm{cm^{-3}\,s^{-1}}$) in either a 24- or 22-group form, depending on the parameter used for **GROUP**.

GAMMA SPECTRUM AND ENERGIES/SECOND

NEUTRONS PER SECOND ARISING FROM SPONTANEOUS FISSION		0.00000E+00	Calculated density (g/cc)	4.54
POWER FROM ALPHA PARTICLES (MeV per Second)		1.37839E-02		
POWER FROM BETA PARTICLES (MeV per Second)		2.19112E+13		
TOTAL GAMMA POWER FROM ACTIVATION (MeV per Second)		2.02831E+14	Total gammas (per cc per second)	9.51308E+11
GAMMA RAY POWER FROM ACTIVATION DECAY MeV/s	(0.00- 0.01 MeV)	6.05782E+09	Gammas per group (per cc per second)	5.50050E+09
	(0.01- 0.02 MeV)	1.88216E+08		5.69668E+07
	(0.02- 0.05 MeV)	9.93236E+05		1.28837E+05
	(0.05- 0.10 MeV)	8.71468E+02		5.27528E+01
	(0.10- 0.20 MeV)	3.10646E+12		9.40223E+10
	(0.20- 0.30 MeV)	2.36863E+10		4.30143E+08
	...			
	...			
	(10.00-12.00 MeV)	0.00000E+00		0.00000E+00
	(12.00-14.00 MeV)	0.00000E+00		0.00000E+00
	(14.00-20.00 MeV)	0.00000E+00		0.00000E+00

The total dose rate is then given in one of two forms depending on the **DOSE** parameter; these two outputs are for contact dose from a semi-infinite slab of the material (`PLANE SOURCE`, see Equation (58) on page 153)) and for the dose from a point source at a specified distance (`POINT SOURCE`, see Equation (61) on page 154).

DOSE RATE (PLANE SOURCE) FROM GAMMAS WITH ENERGY 0-20 MeV IS 5.63098E+04 Sieverts/hour (5.63098E+06 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 ***
```

7.1.7 Dominant nuclides

At each step the inventory is sorted into descending order of radiological quantities and tables of nuclides at the tops of these lists are printed (see, **SORTDOMINANT** keyword). In all cases, dominant nuclides, as measured by activity, total heat production, dose rate, gamma heating and beta heating are displayed. If the **HAZARDS** keyword is used, nuclides are also sorted by ingestion and inhalation dose, and **CLEAR** adds columns with sorting by clearance index.

```
                                                                DOMINANT NUCLIDES
                                                                -----------------

  NUCLIDE   ACTIVITY    PERCENT  NUCLIDE     HEAT      PERCENT  NUCLIDE  DOSE RATE    PERCENT  NUCLIDE  INGESTION    PERCENT  ..
              (Bq)      ACTIVITY             (kW)       HEAT             (Sv/hr)     DOSE RATE           (Sv)       INGESTION ..
    Total   1.2507E+14             Total   3.6006E-02             Total   5.6310E+04             Total   1.3853E+05            ..
1   Sc 48   4.3656E+13  34.91E+00  Sc 48   2.4964E-02  69.33E+00  Sc 48   4.1357E+04  73.45E+00  Sc 48   7.4216E+04  53.57E+00 ..
2   Sc 46   2.4682E+13  19.73E+00  Sc 46   8.3894E-03  23.30E+00  Sc 46   1.3625E+04  24.20E+00  Sc 46   3.7023E+04  26.73E+00 ..
3   Ca 45   1.9657E+13  15.72E+00  Sc 47   8.4082E-04  23.35E-01  Sc 50   5.4522E+02  96.83E-02  Ca 45   1.3956E+04  10.07E+00 ..
4   Sc 47   1.9369E+13  15.49E+00  Sc 50   4.6108E-04  12.81E-01  Ti 45   3.2266E+02  57.30E-02  Sc 47   1.0459E+04  75.50E-01 ..
```

7.1.8 Bremsstrahlung correction

If the **BREMSSTRAHLUNG** keyword is used, then the Bremsstrahlung correction to the gamma dose is calculated using either plane or point source formulae (see Appendix A.10.4 for details) and are printed as shown below for `test4`.

```
                --- THE BREMSSTRAHLUNG CORRECTIONS ARE CALCULATED FOR AN INFINITE PLANE SOURCE ---

Bremsstrahlung dose rate from  Ar 39  is 1.96842E-07 Sv/h  ( 1.96842E-05 Rems/h). This is  3.49951E-10% of the total dose rate.
```

7.1.9 Sensitivity output

The **SENSITIVITY** keyword causes the generation of summary sensitivity output in the `output` file and full details are sent to the `sens` output file to allow further post-processing. The summary output for `test35` is shown below.

The first part of the sensitivity output summarises the irradiation steps over which the sensitivity calculation is performed (i.e., all steps before the **ZERO** keyword in the `input` file.) In the summary output for `test35` shown below, there is only one irradiation step, but more generally a table of the steps is displayed (c.f., pathways output below). This is followed by a summary of the number of sample calculations,

the number of parent-daughter pairs, the number of nuclides to be output and the type of analysis.

```
                    S E N S I T I V I T Y   A N A L Y S I S   F O R   I R R A D I A T I O N   P H A S E
                    ================================================================================

no of steps        =      1
irradiation time   =  7.88940E+07 secs
flux               =  4.27701E+14 n/cm**2/s

Number of samples  =      400
Number of pd edges =        4
Number of nuclides =        7
Sensitivity to cross-section errors
```

Next are tables of the parent-daughter pair properties, a list of the nuclides whose sensitivities are being evaluated and the type of distribution (and distribution cutoff) assumed for the Monte-Carlo calculations.

```
Base cross section data
index          parent                      daughter              sigma      sigma_unc
    i   zai    nuc_no  name     i   zai    nuc_no  name          cm**2
   1  220460     233   Ti 46      210460     219   Sc 46      0.39039E-25  0.35942E-01
   2  220460     233   Ti 46      210461     220   Sc 46m     0.10142E-25  0.35942E-01
   3  220480     235   Ti 48      210480     222   Sc 48      0.11049E-25  0.87272E-02
   4  220480     235   Ti 48      210470     221   Sc 47      0.15312E-26  0.54053E-02

Output nuclides
   j    zai    nuc_no  name
   1  210460     219   Sc 46
   2  210470     221   Sc 47
   3  210480     222   Sc 48
   4  210490     223   Sc 49
   5  210500     224   Sc 50
   6  200450     205   Ca 45
   7  220450     232   Ti 45
Normal, x cutoff = [ -3.0000    ,  3.0000    ] std dev
```

The summary output tables give the input and output mean and fractional standard deviations of reaction (or decay) rates and the resulting output inventory means and fractional uncertainties. The final summary output tables give values of the Pearson correlation coefficients that are above the threshold specified by the keyword argument *xnsens1* (See also Appendix A.11 on page 156).

```
   i  sigma_base sigma_unc_base  sigma_mean   sigma_unc
   1  3.90391E-26  3.59421E-02  3.87468E-26  3.38911E-02
   2  1.01424E-26  3.59421E-02  1.01360E-26  3.47551E-02
   3  1.10489E-26  8.72720E-03  1.10302E-26  8.60142E-03
   4  1.53124E-27  5.40532E-03  1.52796E-27  5.36675E-03

   j   atoms_base   atoms_mean    atoms_unc
   1  2.50290E+20  2.49955E+20  2.46164E-02
   2  7.99801E+18  7.99665E+18  1.68690E-03
   3  9.91006E+18  9.90588E+18  8.55649E-03
   4  9.87505E+15  9.87505E+15  2.77468E-06
   5  9.19707E+13  9.19707E+13  6.54647E-12
   6  3.99705E+20  3.99705E+20  3.81181E-06
   7  2.75193E+16  2.75193E+16  6.16791E-06

Correlation coefficients
  j\i       1           2           3           4
    1  9.66468E-01   - - - -     - - - -     - - - -
    2   - - - -      - - - -     - - - -    9.99810E-01
    3   - - - -      - - - -    1.00000E+00   - - - -
    4   - - - -      - - - -    9.99993E-01   - - - -
```

```
5   - - - -      - - - -      - - - -    -9.99911E-01
6   - - - -      - - - -    -9.60898E-01   - - - -
7 -9.66478E-01   - - - -      - - - -      - - - -
```

7.1.10 Uncertainty estimates

Sensitivity analysis provides uncertainties from an ensemble of calculations. A faster approach is to use a sum of squares estimate from the errors in reactions on the pathways from the initial inventory to the dominant nuclides at the end of the irradiation phase (see Appendix A.13). The uncertainty estimates of the form shown in the next output extract are computed from pathways for an **UNCERTAINTY** keyword parameter of 1 or 3. Presented first for each of the dominant nuclide categories are total values and their uncertainties:

```
                                                UNCERTAINTY ESTIMATES (cross sections only)
                                                -------------------------------------------

Uncertainty estimates are based on pathway analysis for the irradiation phase
Total Activity is          1.25070E+14  +/-   8.52E+11  Bq.        Error is   6.81E-01 % of the total.

Total Heat Production is   3.60059E-02  +/-   3.09E-04  kW.        Error is   8.60E-01 % of the total.

Total Gamma Dose Rate is   5.63098E+04  +/-   5.04E+02  Sv/hr.     Error is   8.95E-01 % of the total.

Total Ingestion Dose is    1.38528E+05  +/-   1.17E+03  Sv.        Error is   8.45E-01 % of the total.

Total Inhalation Dose is   3.06441E+05  +/-   4.40E+03  Sv.        Error is   1.44E+00 % of the total.

Total Gamma Heat Prod is   3.24955E-02  +/-   2.90E-04  kW.        Error is   8.92E-01 % of the total.

Total Beta Heat Prod is    3.51040E-03  +/-   3.07E-05  kW.        Error is   8.74E-01 % of the total.
```

This is followed by a table showing values and uncertainties for the dominant nuclides:

```
Nuclide     Atoms     E(Atoms)  Activity E(Activity)   Heat     E(Heat)  Dose Rate E(Dose Rate) Ingest   E(Ingest)  ...
Sc 48    9.90164E+18  8.60E+16  4.366E+13  3.79E+11  2.496E-02  2.17E-04  4.136E+04  3.59E+02  7.422E+04  6.45E+02  ...
Sc 46    2.57782E+20  6.68E+18  2.468E+13  6.40E+11  8.389E-03  2.18E-04  1.363E+04  3.53E+02  3.702E+04  9.60E+02  ...
Sc 47    8.09046E+18  1.21E+17  1.937E+13  2.89E+11  8.408E-04  1.26E-05  1.827E+02  2.73E+00  1.046E+04  1.56E+02  ...
Sc 50    8.82538E+13  2.33E+12  5.968E+11  1.57E+10  4.611E-04  1.22E-05  5.452E+02  1.44E+01  1.552E+03  4.09E+01  ...
...
```

Note that uncertainties that drop to zero are usually indicate that important pathways are being ignored. The **SORTDOMINANT**, **LOOKAHEAD** and **PATHRESET** keywords can be used to deal with this problem (c.f., Section 5.2.59).

7.1.11 Pathways

Pathways analysis is initiated by the **UNCERTAINTY** keyword, and is performed over all steps preceding the **ZERO** keyword (the irradiation phase). The initial pathways output summarises the steps over which the pathways calculations are performed, and the criteria used in pruning the tree search for paths. The example below (from

test65) shows three irradiation steps, each with a different time interval, flux amplitude and neutron spectrum (as indicated by the rateeq number). In examples where the flux amplitudes vary but the same collapsed cross-sections are used throughout (e.g., test18), the rateeq number remains unchanged:

```
                    P A T H W A Y   A N A L Y S I S   F O R   I R R A D I A T I O N   P H A S E
                    ================================================================================

 number of steps    =      3
 irradiation time   =  2.63952E+06 secs

 step     start        end          delta-t       flux     rateeq
number     sec          sec            sec         n/cm^2/s  number
     2  0.00000E+00  5.27818E-01  5.27818E-01  2.59032E+14    1
     3  5.27818E-01  5.27818E+05  5.27817E+05  2.64634E+14    2
     4  5.27818E+05  2.63952E+06  2.11170E+06  2.66930E+14    3

 path floor    =  5.00000E-01% of target inventory
 loop floor    =  1.00000E+00% of path inventory
 max depth     =   10    (maximum number of edges between source and target)
```

Pathways are given in order of decreasing dominance of target nuclide as ordered in the dominant nuclide tables above. Pathways are retained if they contribute more than the path floor percentage of the number of target atoms given by the full rate equation solution for the time interval. Loops are retained in a pathway if they contribute more than the loop floor percentage of the number of target atoms created along the pathway. The max depth is the maximum number or parent-daughter pairs (edges) that are considered in a path. Pathways are analysed between the nuclides of the initial material being irradiated (source nuclides) and the target nuclides. The target nuclides are those on the merged dominant nuclides list at the end of the irradiation. If the LOOKAHEAD keyword is used, then nuclides that appear on the merged dominant nuclide list at later steps in the cooling phase are added to the list. The number of target nuclides included in the calculation may be altered by changing the value of topxx using the SORTDOMINANT keyword.

```
Source Nuclides
 Ti 46      Ti 47      Ti 48      Ti 49      Ti 50

Target Nuclides
 Sc 48      Sc 46      Sc 47      Sc 50      Ca 45      Ti 45      Sc 49      Ti 51      Ca 47      Sc 46m
 Ar 42      Sc 45m     Sc 44      Ar 41      Sc 50m     Ar 39      V  52      K  42      Sc 44m     K  43
 H   3
```

The pathways calculation prints lists of all significant paths and loops ordered by target nuclide. The first line for each target nuclide gives the nuclide name and the percentage of the total number of atoms given by the number of significant paths shown. The first line for each pathway identifies a path or loop, gives its number and its respective percentage contribution to the target nuclide inventory. The remainder of the line gives the nuclides on the path (or loop) from source to target, and the type of graph edge joining them. Edge types (r,R), (d,D) and (b,B) respectively denote reaction, decay and combined reaction and decay edges from short (lower case) and long lived (upper case) parents. L and S denote short and long lived target nuclides. Short-lived nuclides have half lives less than the time interval and long-lived have half lives greater.

```
Target nuclide Sc 44     99.557% of inventory given by  8 paths
--------------------

path  1  20.048% Ti 46 ---(R)--- Sc 45 ---(R)--- Sc 44 ---(S)---
                    98.16%(n,np)   100.00%(n,2n)
                     1.84%(n,d)

path  2  12.567% Ti 46 ---(R)--- Sc 45 ---(R)--- Sc 44m---(b)--- Sc 44 ---(S)---
                    98.16%(n,np)   100.00%(n,2n)   100.00%(IT)
                     1.84%(n,d)                      0.00%(n,n)

path  3  11.143% Ti 46 ---(R)--- Sc 45m---(d)--- Sc 45 ---(R)--- Sc 44 ---(S)---
                    96.62%(n,np)   100.00%(IT)     100.00%(n,2n)
                     3.38%(n,d)
```

Shown below each edge is a list giving the percentage contributions that each reaction and decay make towards the total rate for the edge for primary products. If the edge daughter is a secondary then the isomeric state of the primary product of the reaction or decay is also displayed. Significant loops are displayed directly after their path, with the percentages of their part of the total path percentage.

7.1.12 Generic pathways

All pathways differing only by an isomeric decay (IT) edge are regarded as the same generic pathway and are shown in the generic pathways list. Individual pathways with details of the reactions and decays on each edge may be found by referring to the individual pathways. The generic pathway (path) displays a path number, the percentage of the target nuclide atoms generated along the pathway and the source to target edges. Below each path is a statement of the number of individual pathways combined to create the generic pathway.

```
Target nuclide Sc 46     97.564% of inventory given by  3 paths
--------------------

path  1  87.893% Ti 46 ---(R)--- Sc 46 ---(S)---
This generic pathway is the sum of  2 pathways

path  2   9.124% Ti 47 ---(R)--- Sc 46 ---(S)---
This generic pathway is the sum of  2 pathways
```

7.1.13 Run summary

At the end of a run, tables are printed containing the total values for each time interval. The intervals are listed as 'Irradiation Phase' or 'Cooling Phase' in the most appropriate unit (sec, min, days) and cumulatively 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.

If the **SPLIT** keyword is used with parameter 1, then a second summary table containing Beta Heat (kW), Gamma Heat (kW), Mean Beta Energy (MeV), and Mean

Gamma Energy (MeV) is printed. For all quantities the estimated uncertainty is also given.

```
          Time       Cumulative   Activity               Dose rate              Heat output            Ingestion dose        ...
         (step)       (Years)      (Bq)                   (Sv/h)                 (kW)                   (Sv)                  ...
-----Irradiation Phase-----
Irradn    2.500 y     2.50E+00   1.25E+14 +/-    0.7%   5.63E+04 +/-    0.9%   3.60E-02 +/-    0.9%   1.39E+05 +/-    0.8% ...
-----Cooling Phase-----
Cooling   1.000 m     1.90E-06   1.14E+14 +/-    0.7%   5.61E+04 +/-    0.9%   3.57E-02 +/-    0.9%   1.38E+05 +/-    0.8% ...
Cooling   1.000 h     1.16E-04   1.09E+14 +/-    0.7%   5.49E+04 +/-    0.9%   3.45E-02 +/-    0.9%   1.35E
Cooling   1.000 d     2.85E-03   8.94E+13 +/-    0.8%   4.16E+04 +/-    1.0%   2.61E-02 +/-    1.0%   1.10E+05 +/-    1.0% ...
Cooling   7.000 d     2.20E-02   4.81E+13 +/-    1.3%   1.47E+04 +/-    2.2%   9.44E-03 +/-    2.2%   5.39E+04 +/-    1.7% ...
Cooling   1.000 y     1.02E+00   5.15E+12 +/-    0.8%   6.22E+02 +/-    2.6%   4.32E-04 +/-    2.3%   4.59E+03 +/-    1.0% ...

 Mass of material input =  1.0000E+00 kg.

 Total irradiation time =  7.889400E+07 s
 Total fluence          =  3.374304E+22 n/cm2
 Mean flux              =  4.277010E+14 n/cm2/s
 Number of on-times     =    1

ispact run time=                0.37894     secs
```

The final section of the `output` file contains QA information that displays a list of all the external files used during the run, and run timestamps.

```
-----------------------------------------------------------------
Files that have been opened during this run.
-----------------------------------------------------------------
The numbers after the unit names are the internal unit numbers.

input( 5)       inventory.i
graph(10)       inventory.gra
a2data(11)      ../EAF2010data/eaf_a2_20100
collapxi(12)    collapsed_cross_section_data
arrayx(13)      condensed_decay_and_fission_data
hazards(14)     ../EAF2010data/eaf_haz_20100
gnuplot(15)     inventory.plt
ind_nuc(18)     ../EAF2010data/eaf_index_20100
output(38)      inventory.out
absorp(39)      ../EAF2007data/eaf_abs_20070
runlog(48)      inventory.log
-----------------------------------------------------------------


    Run timestamp:17:11:57 25 July 2011

    Current time: 17:11:58 25 July 2011
```

7.2 The Inventory Run `runlog` File

The `runlog` file contains the run monitoring and error logging data from a FISPACT-II run. The first part gives the name of the log file, the run timestamp, the `files` file name, the fileroot and a list of the file mappings specified in the `files` file.

```
LOG FILE: inventory.log

16:03:10 22 May 2013

Log  : FILES file = files
```

```
Log  : fileroot   = inventory


-----------------------------------------------------------------
Files specified by the FILES file and fileroot for this run.
-----------------------------------------------------------------
The numbers after the unit names are the internal unit numbers.

input( 5)       inventory.i
crossunc( 7)    ../EAF2010data/eaf_un_20100
asscfy( 8)      ../EAF2010data/eaf_n_asscfy_20100
...
```

A copy of the run monitoring information (see **MONITOR** keyword) is written to the runlog. Settings keywords are simply echoed, and action keywords (e.g., **ATOMS**) are followed by summary messages for the actions they initiate.

```
NOHEADER
MONITOR 1
GETXS 0
GETDECAY 0
FISPACT
* IRRADIATION OF TI EEF FW 1.0 MW/M2
 load cross-sections
 load decay data
 collapse fission yields
 run reset cross-section
MASS 1.0 1
TI 100.0
FLUX 4.27701E+14
MIND 1.E5
GRAPH 2 2 1
1
4
UNCERTAINTY 2
ATOMS
 load initial values
 run output inventory
HAZARDS
 load hazards data
HALF
ATWO
 load a2 data
TIME 2.5
 fill rate equation matrix for cooling
 fill rate equation matrix for irradiation
 start pathstep recording
 initialise dominant analysis
 test for gas, kerma and dpa data
YEARS
ATOMS
 run add rateeq for pathways
```

```
 run irradiation init
 run irradiation step
 run add pathstep
 run output inventory
FLUX 0.
ZERO
TIME 1
MINS
ATOMS
 run pathways initialisation
 run pathways uncertainty
 run cooling step
 run add pathstep
 run output inventory
 run pathways uncertainty
TIME 1
HOURS
ATOMS
 run cooling step
 run add pathstep
 run output inventory
 run pathways uncertainty
TIME 1
DAYS
ATOMS
 run cooling step
 run add pathstep
 run output inventory
 run pathways uncertainty
TIME 7
DAYS
ATOMS
 run cooling step
 run add pathstep
 run output inventory
 run pathways uncertainty
TIME 1
YEARS
ATOMS
 run cooling step
 run add pathstep
 run output inventory
 run pathways uncertainty
END
* END
 run output summary
 run closedown
 deallocate and closedown
```

The QA information on files used that was written to the `output` file is also written for cross-reference to the `runlog` file, followed by a cpu timing summary of the major program components:

```
Log  :                 fispact run time  =  0.37094     secs
Log  :                 rateeq_init_flux  =   0.0000     secs
Log  :                rateeq_irrad_step  =  0.10199     secs
Log  :                 rateeq_cool_step  =  0.77989E-01 secs
Log  :            output_inventory_step  =  0.13996E-01 secs
Log  :                    pathways_step  =  0.80988E-01 secs
Log  :                sensitivity_step  =   0.0000     secs


 Error Summary
-------------
 total number of errors/warnings   =      0
 number of serious errors/warnings =      0
16:03:10 22 May 2013

END OF LOG FILE
```

In runs where errors are flagged, output of the following form (taken from `test10`) is displayed

```
00001: Warning: output_m: output_inventory: 1:
       >20% of dose from nuclides with no spectral data
```

The first line is the error message identifier. It comprises five fields, each terminated by a colon. These fields are

1 error number
2 error severity
3 module
4 subprogram
5 point

There are six error severities, only three of which are of concern to users:

Fatal	Close down immediately
Serious	Close down if 10 or more serious errors
Warning	Flag information to user

The module, subprogram and point identifiers uniquely identify the line in the code from which the error message was issued. Each error message has between one and three lines of descriptive information.

In some cases, values relevant to error messages are output in the lines preceding the error message. These take the form `Log : name = value`:

```
Log  : projectile =            2
00001: Fatal  : rundata_m:read_lib_keys: 7:
```

```
       NOERROR keyword needed for projectile /=1

FATAL ERROR - run terminated
```

7.3 The Printlib Run `output` File

The printlib output consists of the six blocks of data illustrated below. These are selected by the **PRINTLIB** keyword as described in Section 5.2.41 on page 77.

7.3.1 Decay data

The summary of the decay data for each nuclide is printed 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 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 then given.

At the end of this section, details of the neutron spectrum used to weight the fission yields are given, showing the fraction of the neutrons in different energy ranges (see Appendix A.5).

```
MAT. NUMBER           1          2          3          4          5          6      ...

 ISOTOPE           H   1      H   2      H   3      He  3      He  4      He  6     ...

 LAMBDA          0.000E+00  0.000E+00  1.781E-09  0.000E+00  0.000E+00  8.577E-01  ...

 HALF-LIFE       *********  *********   12.330 y  *********  *********  808.100ms  ...

 SP.FISS n/s     0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  ...
 (a,n) n         0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  ...
 <ALPHA>         0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  ...
 <BETA>          0.000E+00  0.000E+00  5.707E-03  0.000E+00  0.000E+00  1.561E+00  ...
 <GAMMA>         0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  5.644E-03  ...
 GAMMA GROUP  1  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  5.547E-06  ...
 GAMMA GROUP  2  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  1.591E-05  ...
 ...
 ...
 GAMMA GROUP 23  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  ...
 GAMMA GROUP 24  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  ...

 Th232 FIS YIELD 1.751E-03  5.350E-04  7.633E-03  0.000E+00  1.107E-01  0.000E+00  ...
 U 233 FIS YIELD 3.289E-03  9.337E-04  1.409E-02  0.000E+00  2.079E-01  2.153E-03  ...
```

```
...
...
Cm244 FIS YIELD  3.828E-03  1.170E-03  1.910E-02  0.000E+00  2.420E-01  0.000E+00  ...
Cm245 FIS YIELD  3.607E-03  1.102E-03  1.850E-02  0.000E+00  2.280E-01  0.000E+00  ...
...
...
    Fraction of neutrons < 200 keV = 0.4120, fraction of neutrons > 200 keV and < 5...
```

7.3.2 Branching ratios

The second block gives percentage branching ratios 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 summarised in Table 10 on page 138.

```
                                    P E R C E N T A G E    B R A N C H I N G    R A T I O S

 H   3   (b-)   He  3  1.000E+02      He  6   (b-)   Li  6  1.000E+02      Li  5    (p)   He  4  1.000E+02  ...
 Li  9   (b-)   Be  9  5.050E+01      Li  9  (b-n)   Be  8  4.950E+01      Be  6   (pp)   He  4  1.000E+02  ...
 Be  8    (a)   He  4  1.000E+02      Be 10   (b-)   B  10  1.000E+02      Be 11   (b-)   B  11  9.700E+01  ...
 Be 12   (b-)   B  12  1.000E+02      Be 13    (n)   Be 12  1.000E+02      B   8  (b+a)   He  4  1.000E+02  ...
 B  12   (b-)   C  12  9.842E+01      B  12  (b-a)   Be  8  1.580E+00      B  13   (b-)   C  13  9.972E+01  ...
 B  14   (b-)   C  14  1.000E+02      B  15   (b-)   C  15  6.000E+00      B  15  (b-n)   C  14  9.360E+01  ...
 C   9   (b+)   B   9  6.000E+01      C   9  (b+p)   Be  8  2.300E+01      C   9  (b+a)   Li  5  1.700E+01  ...
 C  11   (b+)   B  11  1.000E+02      C  14   (b-)   N  14  1.000E+02      C  15   (b-)   N  15  1.000E+02  ...
 C  16  (b-n)   N  15  9.790E+01      C  17   (b-)   N  17  7.160E+01      C  17  (b-n)   N  16  2.840E+01  ...
 ...
 ...
```

7.3.3 Cross-sections

The third section gives the effective cross-section obtained by collapsing with the neutron spectrum followed by the percentage error obtained by collapsing the cross-section uncertainties. Note that if there are no uncertainty data in the library then the keyword **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. The cross-section codes are listed in Table 12 on page 140 and the diagnostic cross-section codes are given in Table 13 on page 143.

```
                                    C R O S S    S E C T I O N S    I N    B A R N S

                    The cross section for the specified reaction is given in barns, followed by the error in percent.

H   1 n,g      H   2  7.147E-03+-1.0E+01  H   2 n,2n     H   1  3.322E-02+-1.6E+00  H   2 n,g      H   3  1.523E-05+-1.0E+01  ...
H   3 n,3n     H   1  3.902E-04+-1.1E+00  He  3 n,g      He  4  2.493E-05+-3.6E+01  He  3 n,p      H   3  1.142E+02+-5.0E+01  ...
Li  6 n,2na    H   1  1.453E-02+-2.4E+01  Li  6 n,nd     He  4  9.076E-02+-2.1E+01  Li  6 n,g      Li  7  8.524E-04+-9.3E+00  ...
Li  6 n,t      He  4  2.049E+01+-1.0E+01  Li  7 n,2n     Li  6  9.857E-03+-1.6E+00  Li  7 n,na     H   3  6.166E-02+-2.1E+01  ...
Li  7 n,np     He  6  3.861E-04+-2.9E+00  Li  7 n,g      Li  8  9.816E-04+-8.2E+00  Li  7 n,d      He  6  1.784E-03+-2.9E+00  ...
Be  7 n,g      Be  8  1.573E-03+-1.9E+02  Be  7 n,p      Li  7  8.204E+02+-5.0E+01  Be  7 n,d      Li  6  2.113E-02+-2.9E+01  ...
Be  7 n,2p     He  6  1.572E-03+-9.5E+00  Be  9 n,2n     Be  8  1.128E-01+-3.1E+00  Be  9 n,g      Be 10  1.667E-04+-9.6E+00  ...
...
...
```

7.3.4 Bremsstrahlung candidates

The fourth section contains the table of Bremsstrahlung candidates using the criteria described in Appendix A.10.4. The user may select nuclides from this table for input with the **BREMSSTRAHLUNG** keyword.

```
                                    B R E M S S T R A H L U N G   C A N D I D A T E S

NUCLIDE       AV BETA (MeV)  AV GAMMA (MeV)    NUCLIDE       AV BETA (MeV)  AV GAMMA (MeV)    NUCLIDE       AV BETA (MeV)...

HALF LIFE < 1 DAY
He   6       1.5613E+00     5.6441E-03        Li   8       6.2046E+00     3.2983E-02        Li   9       5.6963E+00    ...
Be  11       4.6473E+00     1.4188E+00        Be  12       5.6150E+00     0.0000E+00        B   12       6.3084E+00    ...
B   13       6.2783E+00     3.1353E-01        B   14       7.0847E+00     5.9363E+00        N   12       7.7285E+00    ...
N   17       1.6978E+00     4.4508E-02        O   19       1.7096E+00     1.0046E+00        O   20       1.1974E+00    ...
F   20       2.4673E+00     1.6447E+00        F   21       2.3418E+00     5.5687E-01        F   23       2.9705E+00    ...
...
...
```

7.3.5 Projectile spectrum

This table shows the energy bin boundaries and the flux in each bin for the neutron spectrum used to collapse the cross section library. The available energy groups are tabulated in Appendix B.1.

```
                          N E U T R O N     S P E C T R U M

    Group    Upper         Lower         Flux          Group    Upper         Lower         Flux
    index    energy        energy                      index    energy        energy

      1  1.491800E+07  1.349830E+07  6.97424E+13         51  8.651550E+04  6.737830E+04  7.02505E+12
      2  1.349830E+07  1.221380E+07  3.88579E+12         52  6.737830E+04  5.247430E+04  5.20028E+12
      3  1.221380E+07  1.105150E+07  1.16576E+12         53  5.247430E+04  4.086700E+04  5.39238E+12
     ...
     48  1.356830E+05  1.227710E+05  3.67138E+12         98  6.825490E-01  5.315700E-01  9.00249E+11
     49  1.227710E+05  1.110880E+05  3.06565E+12         99  5.315700E-01  4.139870E-01  8.25430E+11
     50  1.110880E+05  8.651550E+04  6.20848E+12        100  4.139870E-01  1.000000E-05  7.09818E+12

  Spectrum type is GAM-II
  flux spectrum_identifier is  EEF FW NORM. 1MW/M2 GAM-II TOT=4.277E+14
```

7.3.6 Decay spectral lines

Decay spectral lines are listed for unstable nuclides. The decay type (Table 10 on page 138) and spectrum type (Table 11 on page 139), line energy and line intensity for all unstable nuclides are displayed where data are available (see keyword **SAVE-LINES**). For unstable nuclides without data, the text `no spectral data` is displayed.

```
                  D E C A Y   R A D I A T I O N   D I S C R E T E   S P E C T R A

NUCLIDE NUCLIDE NUCLIDE SPECTRUM   DECAY  LINE ENERGY    INTENSITY
  NAME     ZAI   NUMBER   TYPE      TYPE     (eV)           (eV)
 H   3    10030     3   beta        (b-)  1.85710E+04  1.85710E+04
 He  6    20060     6   beta        (b-)  3.50700E+06  3.50700E+06
 Li  5    30050     7   no spectral data
```

```
Li  8    30080    10   beta        (b-)  1.29650E+07  1.29650E+07
                       alpha        (a)  1.56600E+06  1.56600E+06
Li  9    30090    11   beta        (b-)  2.32000E+06  9.28000E+04
                       beta        (b-)  5.67000E+06  8.50500E+04
                       beta        (b-)  1.08300E+07  1.08300E+06
                       beta        (b-)  1.11770E+07  3.80018E+06
                       beta        (b-)  1.36060E+07  6.87103E+06
Be  6    40060    12   no spectral data
...
```

7.4 Probability Table Collapse Run

The cross-section collapse with probability table data to compute the self-shielding factor and the effective collapsed cross-sections differs from the standard collapse (c.f., Section 4.2) in that

1. a mapping for the probability table data directory must be added to the `files` file:

   ```
   # Library probability tables for self-shielding
   prob_tab  ../../PTdata/tp294
   ```

2. the reading of the probability table data must be activated by including the **PROBTABLE** keyword in the library preparation section of the `input` file.

3. the set of parent nuclides (or elements) to which the self-shielding factor is to be applied is specified by the **SSFCHOOSE** keyword.

4. the mixture of nuclides to be included in the dilution computation must be specified using either the **SSFMASS** of **SSFFUEL** keywords. Note that the values specified for these may be different from the **MASS** or **FUEL** mixtures specified in the inventory run. This gives the user the flexibility to manipulate the dilutions, but in general, one should specify the same mixture for the inventory run as is used for the collapse run. If subsequent collapses are requested by **GETXS** keywords then additional **SSFFUEL** or **SSFMASS** keywords will be needed for them.

To illustrate the usage, we consider the following input file for a cross-section collapse calculation using probability table data:

```
GETXS 1 616
PROBTAB 1 1
SSFCHOOSE 4 0
W182 W183 W184 W186
SSFFUEL 4
W182 1.34834187E+22
W183 7.27597094E+21
W184 1.55899050E+22
```

```
W186 1.44654079E+22
FISPACT
* COLLAPSE EAF_616_FLT with PT for W
END
* END OF RUN
```

The first keyword specifies collapse of the 616 energy group EAF cross-section data (the EAF group structure for which probability table data are presently available). The second activates the reading of probability table data to compute self-shielding factors and the use of partial cross-sections to compute self-shielding factors with the infinite dilution values in the EAF library being replaced rather than scaled.

The **SSFCHOOSE** keyword specifies 4 entries on the list and suppresses detailed printing (0). The subsequent line (or lines) list the elements or nuclides. In this case they are four isotopes of tungsten.

The **SSFFUEL** keyword specifies the mixture. In this case all the nuclides in the mixture are in the apply list of **SSFCHOOSE**, but in general the apply list will contain a subset of the nuclides in the mixture.

The output from a run using this dataset has the labelling and heading information, followed by the probability table data initialisation output that specifies the method of calculation chosen and the source data directory for the probability table data:

```
PROBABILITY TABLE INITIALISATION
================================

Self shielding factors are computed using partial cross-sections

Library infinite dilution values are replaced by self-shielded probability table values

Probability table data directory: ../../PTdata/tp294/

Temperature =  294K
```

Printed next is a list of the parent nuclides to which the self-shielding factor correction is applied and the name of the files containing the probability table data used:

```
Probability Table Application List
----------------------------------
Nuclide     Data File
W 182       W182-294.tpe
W 183       W183-294.tpe
W 184       W184-294.tpe
W 186       W186-294.tpe
```

and then a summary of the material mixture used in the dilution calculation:

```
 Material Mixture List
 ---------------------
 Nuclide     Percentage
 W 182       26.534
 W 183       14.319
 W 184       30.680
 W 186       28.467
```

A full list of collapsed cross-sections can be obtained using **PRINTLIB**. The collapse run simply summarises the reactions whose cross-sections are changed by self-shielding. The table for this example is as follows:

```
 P R O B A B I L I T Y  T A B L E  C H A N G E S  T O  C R O S S - S E C T I O N S
 ================================================================================

  The EAF/TENDL infinitely dilute values (old sigma) are replaced by the probability
table effective cross-section (new sigma).
  The effective self-shielding factor is the ratio of new to old value

  parent     daughter     mt cal-mt    old sigma     new sigma     self shielding
  nuclide    nuclide                    barns         barns         factor (%)
  W 182      W 183       102   101    2.10385E+00   4.99375E-01        23.74
  W 182      W 183m      102   101    3.14997E-01   7.52384E-02        23.89
  W 182      Hf179       107   101    7.26039E-05   7.25547E-05        99.93
  W 182      Hf179m      107   101    7.78139E-06   7.76192E-06        99.75
  W 182      Hf179n      107   101    2.85923E-07   2.85918E-07       100.00
  W 183      W 184       102   101    3.41600E+00   1.06712E+00        31.24
  W 183      Hf180       107   101    8.04463E-05   7.73309E-05        96.13
  W 183      Hf180m      107   101    3.92752E-06   3.92574E-06        99.95
  W 184      W 185       102   101    4.42228E-01   1.35932E-01        30.74
  W 184      W 185m      102   101    9.81381E-04   6.06302E-04        61.78
  W 184      Hf181       107   101    5.28951E-05   5.28901E-05        99.99
  W 186      W 187       102   101    3.12173E+00   1.68884E+00        54.10
  W 186      Hf183       107   101    3.14859E-05   3.14858E-05       100.00
```

For fission (MT=18) and other (MT=5), the daughter nuclide names are respectively replaced by ‘fission’ and ’other’.

7.5 Universal Curve Self-Shielding Collapse Run

The cross-section collapse using the universal sigmoid curve approximation to compute the self-shielding factor and the effective collapsed cross-sections differs from the standard collapse (c.f., Section 4.2) in that:

1. The `files` file must specify an ENDF-format cross-section library that includes MF = 2 resolved resonance range data.

2. The **SSFGEOMETRY** keyword must be added to the `input` file to trigger the use of this self-shielding model.

3. The target shape and size must be specified with arguments to **SSFGEOMETRY**.

4. The mixture of nuclides whose resonances are to be included in the calculation of the self-shielding factors must be specified using either the **SSFMASS** of **SSFFUEL** keywords. Note that the values specified for these may be different from the **MASS** or **FUEL** mixtures specified in the inventory run. This gives the user the flexibility to manipulate the self-shielding factors, but in general, one should specify the same mixture for the inventory run as is used for the collapse run. If subsequent collapses are requested by **GETXS** keywords then additional **SSFFUEL** or **SSFMASS** keywords will be needed for them.

To illustrate the usage, we consider the following input file for a cross-section collapse calculation using probability table data:

```
EAFVERSION 8
GETXS 1 709
SSFGEOMETRY 1 0.8
SSFFUEL 4
W182 1.34834187E+22
W183 7.27597094E+21
W184 1.55899050E+22
W186 1.44654079E+22
FISPACT
* COLLAPSE tal2011-n/gxs-709 with universal curve SSF for a foil
END
* END OF RUN
```

The first keyword specifies that an ENDF-format cross-section library is to be read from the directory indicated by `xs_endf` in the `files` file and the second keyword specifies collapse of the 709 energy group cross-section data. The **SSFGEOMETRY** keyword activates the universal sigmoid curve self-shielding approximation and indicates that a foil target 8 mm thick is to be irradiated. The **SSFFUEL** keyword specifies the mixture of nuclides whose resonances are to be used to calculate the self-shielding factors.

The output from a run using this dataset has the labelling and heading information for this self-shielding approximation, followed by the list of the parent nuclides that provide resonances for the calculation of the self-shielding factors:

```
S I G M O I D  C U R V E  S E L F  S H I E L D I N G  C H A N G E S  T O  C R O S S - S E C T I O N S
=============================================================================================

Target geometry set by the SSFGEOMETRY keyword: foil with thickness 8.00000E-01 cm
```

```
Target mass and inventory numbers of atoms refer to unit foil area.


The self shielding factors are calculated from the resonances of the materials specified with the SSFFUEL or SSFMASS keywords.

Material Mixture List
---------------------
Nuclide     Atoms percent
W 182       26.534
W 183       14.319
W 184       30.680
W 186       28.467
```

A full list of collapsed cross-sections can be obtained using **PRINTLIB**. The collapse run simply summarises the reactions whose cross-sections are changed significantly by self-shielding (reduced to less than 90% of their infinitely-dilute values.) The table for this example starts as follows:

```
The EAF/TENDL infinitely dilute values (old sigma) are replaced by the sigmoid curve effective cross-sections (new sigma).
The effective self-shielding factor is the ratio of new to old values. Factors greater than 90.00% are omitted from the table.

parent   daughter  mt  old sigma    new sigma    self shielding    parent   daughter  mt  old sigma    new sigma    self shielding
nuclide  nuclide        barns        barns       factor (%)       nuclide  nuclide        barns        barns       factor (%)
Na 22    Na 22      2  1.51796E+00  1.20106E+00      79.12        Cl 36    Cl 37    102  2.96858E-03  1.87209E-03      63.06
Ar 37    Ar 38    102  2.77255E-03  2.29233E-03      82.68        K  37    K  38    102  9.93047E-04  8.05455E-04      81.11
K  37    K  38m   102  2.13898E-03  1.71960E-03      80.39        K  38    K  39    102  3.26196E-03  2.71234E-03      83.15
K  42    K  43    102  6.93336E-03  5.29917E-03      76.43        K  43    K  44    102  3.77911E-03  3.36584E-03      89.06
K  44    K  45    102  3.63969E-03  3.14525E-03      86.42        Sc 42m   Sc 43    102  6.13298E-03  5.04557E-03      82.27
Sc 43    Sc 44    102  9.22430E-03  5.78151E-03      62.68        Sc 43    Sc 44m   102  7.72141E-04  5.84122E-04      75.65
Sc 44    Sc 45    102  4.83744E-03  3.01304E-03      62.29        Sc 44    Sc 45m   102  6.10641E-03  3.57961E-03      58.62
Sc 44m   Sc 45    102  1.27846E-02  7.33443E-03      57.37        Sc 44m   Sc 45m   102  8.44849E-04  5.33646E-04      63.16
Sc 46    Sc 47    102  1.25279E-02  9.22951E-03      73.67        Sc 46m   Sc 47    102  1.62702E-02  1.10540E-02      67.94
Sc 47    Sc 48    102  4.77165E-03  4.16265E-03      87.24        Ti 45    Ti 46    102  1.07775E-02  7.33420E-03      68.05
V  47    V  48    102  7.30012E-03  5.35352E-03      73.33        V  48    V  49    102  8.70205E-03  6.86722E-03      78.91
V  49    V  50    102  9.25513E-03  7.54519E-03      81.52        V  50    V  51    102  3.84027E-02  3.28603E-02      85.57
Cr 49    Cr 50    102  6.73542E-03  5.26221E-03      78.13        Mn 50m   Mn 51    102  6.84192E-03  5.66382E-03      82.78
Mn 51    Mn 52    102  1.29548E-03  1.10514E-03      85.31        Mn 51    Mn 52m   102  5.71788E-03  4.56122E-03      79.77
Mn 55    Mn 56    102  1.10650E-02  9.75274E-03      88.14        Mn 56    Mn 57    102  7.37615E-03  6.27235E-03      85.04
Mn 57    Mn 58    102  1.05890E-03  9.27035E-04      87.55        Mn 58    Mn 59    102  6.04988E-03  5.28837E-03      87.41
Mn 58m   Mn 59    102  9.83010E-03  8.05237E-03      81.92        Mn 59    Mn 60    102  1.84688E-03  1.62945E-03      88.23
Mn 59    Mn 60m   102  6.33656E-03  5.70209E-03      89.99        Fe 53    Fe 54    102  4.97518E-03  4.19275E-03      84.27
Fe 53m   Fe 54    102  4.70607E-03  3.83581E-03      81.51        Co 54m   Co 55    102  4.58414E-03  4.06991E-03      88.78
...      ...      ...  ...          ...              ...          ...      ...      ...  ...          ...              ...
```

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References

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APPENDICES

A The Model

A.1 The Rate Equations

FISPACT-II follows the evolution of the inventory of nuclides in a target material that is irradiated by a time-dependent projectile flux, where the projectiles may be neutrons, protons, deuterons, α-particles or γ-rays. The material is homogeneous, infinite and infinitely dilute and the description of the evolution of the nuclide numbers is reduced to the stiff-ode set of rate equations [27]:

$$\frac{dN_i}{dt} = \sum_j (\lambda_i^j + \sigma_i^j \phi^{int}(t)) N_j \tag{7}$$

where

N_i = number of nuclide i at time t

ϕ^{int} = projectile flux ($\mathrm{cm}^{-2}\mathrm{s}^{-1}$)

for $j \neq i$:

λ_i^j = decay constant of nuclide j producing i (s^{-1})

σ_i^j = reaction cross-section for reactions on j producing i (cm^2)

for $j = i$:

$-\lambda_j^j$ = total decay constant of nuclide j (s^{-1})

$-\sigma_j^j$ = total cross-section for reactions on j (cm^2)

The processes described by Equation (7) may be interpreted in terms of a directed graph, with vertices corresponding to nuclides and edges giving the flow from parent to daughter nuclides via a decay process or an induced reaction. Figure 6 schematically presents a fragment of this graph. Graph theoretic methods are used to construct pathways (see Section A.12 on page 158).

The total flow out from vertex j by decay is equal to the total flow into other vertices i:

$$\lambda^j = -\lambda_j^j = \sum_{i \neq j} \lambda_i^j \tag{8}$$

Similarly, the balances of the flows by projectile-induced reactions give

$$\sigma^j = -\sigma_j^j = \sum_{i \neq j} \sigma_i^j \tag{9}$$

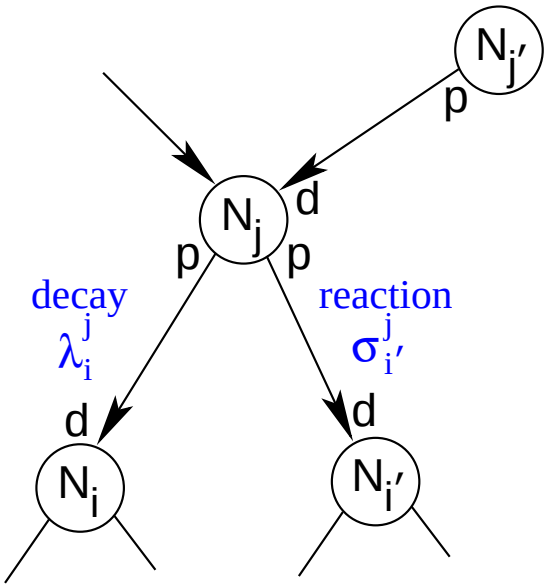

Figure 6: Directed graph representation of reactions and decays: The flow from the parent nuclide at vertex j to the daughter nuclide at vertex i along the directed edge ji is given by the sum of decay and reaction flows.

To maintain correct accounting, decays or reactions leading to daughter nuclides not included in the set being considered are assigned to a fictitious 'sink' nuclide, and secondary decay products are assigned to the appropriate gas nuclides.

Reaction cross-sections depend on the projectile energy, and the source data for cross-sections give values for a set of energy groups. In the code, an effective ('collapsed') cross-section is computed as an average cross-section weighted by projectile fluxes in each energy group:

$$\sigma_i^j = \sum_k \tilde{\sigma}_i^j(E_k)\phi_n(E_k) / \sum_k \phi_n(E_k) \tag{10}$$

where $\tilde{\sigma}_i^j(E_k)$ is the cross-section at projectile energy group k, $\phi_n(E_k)$ is the integrated projectile flux in energy group k, and the sums are over all energy groups k.

A consequence of the modelling assumptions underlying FISPACT-II is that the imposed projectile flux is not modified by the reactions and decays in the target material. Then the decay rates and cross-sections appearing in Equation (7) are all independent of the nuclide numbers N_j and the equation can be rewritten compactly as

$$\frac{d\mathbf{N}}{dt} = \mathsf{A}\mathbf{N} \tag{11}$$

where the matrix A is independent of the inventory $\mathbf{N}$. In FISPACT-II the projectile flux is constant during each time interval, so that A is also piecewise-constant in time.

Furthermore, the matrix A is sparse. Its sparsity pattern gives the adjacency matrix [28] and its components give weighting factors for constructing the digraphs [29]

used for pathways analysis. The `ind_nuc` file in the EAF-2010 library contains 2233 distinct nuclides, so A has a size of 2234×2234, including the 'sink' nuclide. However, there are only approximately 120 000 non-zero elements in A. If actinides are not relevant to a calculation, the fission reactions can be omitted and about 42 000 elements of A remain non-zero. This number drops to less than 5 000 during cooling periods when only decays are required. These properties of the system matrix are relevant to the method of solution described in Section A.14 below.

A.2 Data Collapse

The reaction data input to FISPACT-II are the projectile flux spectrum, cross-sections, induced fission yields and covariances tabulated in energy groups, where in general the cross-section data are tabulated at much smaller energy intervals than the fission yield or covariance data. These data are 'collapsed' using flux spectrum weighting into energy independent values for use in the inventory calculations.

Consider the collapsed cross-section $\bar{X}$ and its uncertainty Δ that are used in FISPACT-II. The input data for $\bar{X}$ are cross-sections X_i and the projectile flux [3]ϕ_i in energy groups $i \in [1, N]$.

ϕ_i is the flux ($\mathrm{cm}^{-2}\mathrm{s}^{-1}$) in energy range E_i to E_{i+1}, and we use it to define the weight for group i as

$$W_i = \phi_i / \sum_{i=1}^{N} \phi_i \tag{12}$$

The collapsed cross-section (c.f., Eq. (10)) $\bar{X}$ is given by

$$\bar{X} = \sum_{i=1}^{N} W_i X_i \tag{13}$$

Covariances for cross-sections X_i and Y_j grouped in energy bins $i \in [1, N_X]$, $j \in [1, N_Y]$ are $Cov(X_i, Y_j)$. The collapsed covariance arising from these is given by

$$Cov(\bar{X}, \bar{Y}) = \sum_{i=1}^{N_X} \sum_{j=1}^{N_Y} W_i W_j Cov(X_i, Y_j) \tag{14}$$

$Cov(\bar{X}, \bar{Y})$ is not presently used in FISPACT-II, but is planned to be used in future in the monte-carlo sensitivity calculations. The case of interest at present is that where reactions X and Y are the same, and then the collapsed variance is given by

$$var = Cov(\bar{X}, \bar{X}) = \sum_{i,j=1}^{N} W_i W_j Cov(X_i, X_j) \tag{15}$$

[3] If fluxes are in different energy groups, then the **GRPCONVERT** keyword can be used to remap them to the appropriate groups (c.f., Section 5.1.8on page 50).

For EAF data, the uncertainty is defined at the three standard deviation point:

$$\Delta = 3\sqrt{var}/\bar{X} \tag{16}$$

and for the TENDL-2013 data, it is defined as

$$\Delta = \sqrt{var}/\bar{X} \tag{17}$$

The covariance data are less complete than the cross-section data. Each covariance data energy group contains several cross-section energy groups, and in some cases the data in different energy groups are assumed to be uncorrelated.

The covariance data in the EAF and TENDL-2013 libraries that FISPACT-II recognises are the ENDF [16] NI-type data with LB=1, 5, 6 or 8. The projection operator S_i^k maps cross-section energy bins to covariance energy bins as illustrated in Figure 7.

$$S_i^k = \begin{cases} 1 & \text{bin i in bin k} \\ 0 & \text{otherwise} \end{cases} \tag{18}$$

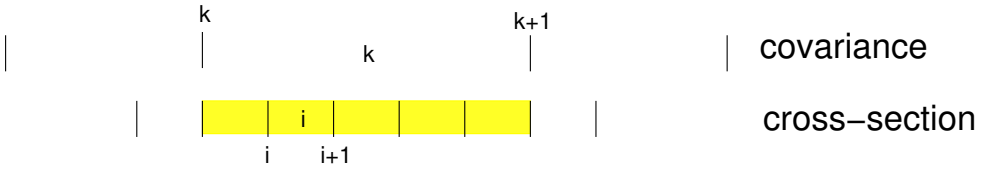

Figure 7: Projection operator S_i^k maps cross-section energy bins to covariance energy bins. The shaded energy bins have $S_i^k = 1$, and all others have $S_i^k = 0$

Using S_i^k, the formula used to construct estimates of the covariance matrix from the library data are as follows:

$$LB = 1: \quad Cov(X_i, X_j) = \sum_{k=1}^{M} S_i^k S_j^k F_k X_i X_j \tag{19}$$

$$LB = 5: \quad Cov(X_i, Y_j) = \sum_{k=1}^{M} \sum_{k'=1}^{M} S_i^k S_j^{k'} F_{kk'} X_i Y_j \tag{20}$$

$$LB = 6: \quad Cov(X_i, Y_j) = \sum_{k=1}^{M} \sum_{k'=1}^{M'} S_i^k S_j^{k'} F_{kk'} X_i Y_j \tag{21}$$

$$LB = 8: \quad Cov(X_i, X_j) = \sum_{k=1}^{M} S_i^k S_j^k 1000 F_k \quad (Koning) \tag{22}$$

$$(or = \sum_{k=1}^{M} S_i^k \delta_{ij} 1000 F_k) \tag{23}$$

The LB=1 case (Equation (19) is the one that applies to the computation of Δ for the EAF data. Covariances are described by a fraction for each k bin and the different k bins are assumed to be uncorrelated.

The LB = 5, 6, and 8 cases appear in the TENDL-2013 libraries. The LB = 5 data for X and Y referring to the same reaction are used to compute Δ, and are assumed to have LS=0. The LB = 6 data give cross-correlations between collapsed cross-sections. These are read but not used in the present version of the code. The LB = 8 data are produced from the same source as the LB = 5 data for $X = Y$, with some of the cross-correlations discarded and use definitions different from those in the ENDF manual [16]. FISPACT-II reads and discards these data.

A.3 Decay Modes

The code will allow 27 decay modes by which the parent nuclide j can decay to daughter nuclide i. These are listed in Table 10. The index `IRT` is the index used in the code. The index `RTYP` is the ENDF-6 reaction type code used for reaction product code `MT` = 457 [16, Sec. 8.3, page 8.5]. (The table also includes two unused `IRT` codes and another to indicate an unknown decay mode, so the maximum `IRT` is 26.) The decay constant λ_i^j appearing in Equation (7) is the sum of the decay constants for the transmutation of nuclide j to i. In terms of the directed graph, the edge shown in Figure 6 corresponds to the combination of a subset of 23 possible decay edges from j to i.

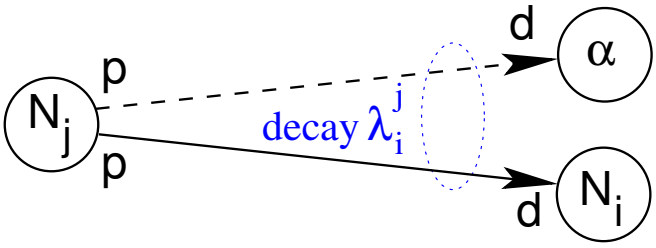

Figure 8: Decay processes (e.g., α-decay) may produce secondary gas nuclides that are included in the inventory calculation.

Some of the decay modes listed in Table 10 have secondary gas nuclides that are included in the inventory calculation, and the number of these is `NSEC` and their names are included in the right hand column of the table. This is illustrated in Figure 8. The primary reaction leads to a secondary edge in the directed graph, and other products from these decays are regarded as debris that is ignored. When there are gas nuclide secondaries, then a secondary edge from nuclide j to the gas nuclide is associated with the decay from j to i. There may be 0, 1 or 2 secondaries associated with a decay type; see Table 10 for details.

A.3.1 Heating

Heating from decay is computed using the average decay energies for light particles, electromagnetic radiation and heavy particles that are included in the data in the `decay` file.

Table 10: Decay Types (MT=457) recognised by the code. The column labelled 'Code' is the description used in output from FISPACT-II, NSEC is the number of secondaries and 'Secs' is an abbreviation for 'Secondaries'.

IRT	RTYP	Description	ΔZ	ΔA	Code	NSEC	Secs
1	1	β^- decay	1	0	b-	0	
2	2	β^+ decay or electron capture	−1	0	b+	0	
3	3	isomeric transition (IT)	0	0	IT	0	
4	4	α decay	−2	−4	a	1	^{4}He
5	5	neutron emission	0	−1	n	0	
6	6	spontaneous fission (SF)	−999	−999	SF	0	
7	7	proton emission	−1	−1	p	1	^{1}H
8	8	not used	0	0	0		
9	9	not used	0	0	0		
10	10	unknown	0	0	0		
11	1.5	β^- decay + neutron emission	1	−1	b-n	0	
12	1.4	β^- decay + α emission	−1	−4	b-a	1	^{4}He
13	2.4	β^+ decay + α emission	−3	−4	b+a	1	^{4}He
14	2.7	β^+ decay + proton emission	−2	−1	b+p	1	^{1}H
15	3.4	IT followed by α emission	−2	−4	IT+a	1	^{4}He
16	1.1	double β^- decay	2	0	b-b-	0	
17	1.6	β^- decay followed by SF	−999	−999	b-SF	0	
18	7.7	double proton emission	−2	−2	pp	2	^{1}H ^{1}H
19	2.2	double β^+ or electron capture	−2	0	b+b+	0	
20	1.55	β^- and double neutron emission	1	−2	b-2n	0	
21	1.555	β^- and triple neutron emission	1	−3	b-3n	0	
22	1.5555	β^- and quadruple neutron emission	1	−4	b-4n	0	
23	5.5	double neutron emission	0	−2	2n	0	
24	5.55	triple neutron emission	0	−3	3n	0	
25	2.77	β^+ decay + double proton emission	−3	−2	b+2p	2	^{1}H ^{1}H
26	2.777	β^+ decay + triple proton emission	−4	−3	b+3p	3	^{1}H ^{1}H ^{1}H
27	2.6	β^+ decay followed by SF	−999	−999	b+SF	0	

Table 11: Decay Radiation Types (MT=457) recognised by FISPACT-II The column headed 'Code' is the description used in output from FISPACT-II.

STYP	Radiation Type		Code
0	γ	gamma rays	gamma
1	β^-	beta rays	beta
2	ec,(β^+)	electron capture and/or positron emission	ec, beta+
3		not known	not known
4	α	alpha particles	alpha
5	n	neutrons	n
6	SF	spontaneous fission fragments	SF
7	p	protons	p
8	e^-	"discrete electrons"	e-
9	x	X-rays and annihilation radiation	x

A.3.2 Gamma spectrum

A 22- or 24-group histogram is generated by nearest grid point binning of the intensities of discrete gamma and X-ray lines (STYP= 0 or 9) contained in the data from the decay file.

A.3.3 Neutron yield

The spontaneous fission neutron yield (STYP=5) is accumulated using the decay yields contained in the decay file.

A.4 Neutron Activation

The main application of the code is to neutron activation calculations. In these the transmutation of a nuclide j to another nuclide i (and in some cases additional secondaries) may result from:

1. one of the decay processes listed in Table 10
2. one of the neutron-induced reactions listed in Table 12

The output for the induced reaction produced by FISPACT-II uses the code n for the neutron projectile and g, n, p, d, t, h, a respectively for products γ, N, T, h, α when printing output.

Decay processes are described in Section A.3 above. There are three special cases in the list of neutron-induced reactions:

Elastic scattering (MT=2 in Table 12). This special case is where the projectile z elastically scatters from the target nuclide and is designated (z, E);

Other reactions (MT=5 in Table 12). The set of reactions labelled as "other reactions" is a special case and is designated (z, O) for projectile z;

Fission (MT=18 in Table 12). The neutron-induced fission reaction (n, F) is a special case, and is treated below in Section A.5.

The total effective cross-section σ_i^j used in Equation (7) is obtained by summing the contributions from the different reactions.

$$\sigma_i^j = \sum_{mt} \left(\sigma_i^j((n, \{prod\})_{mt}) + \sum_{k \neq i} s_i \sigma_k^j((n, \{s_i i, \ldots\})_{mt}) \right) \tag{24}$$

where $\sigma_i^j((n, \{prod\})_{mt})$ is the cross-section for the production of nuclide i from nuclide j through the neutron induced-reaction with code mt as summarised in Table 12; these data are tabulated in file crossec. The second sum in Equation (24) is the production of secondary gas nuclide i from the reaction producing nuclide k from j, where s_i is the number of secondaries of nuclide i per reaction.

Table 12: Neutron induced reactions recognised by the code.

Projectile	Products	MT	ΔZ	ΔA	NSEC	Secondaries		
n	total	1	0	0	0			
n	E	2	0	0	0			
n	nonel	3	0	0	0			
n	n	4	0	0	0			
n	O	5			0			
n	2nd	11	−1	−3	1	^{2}H		
n	2n	16	0	−1	0			
n	3n	17	0	−2	0			
n	F	18			0			
n	nα	22	−2	−4	1	^{4}He		
n	n3α	23	−6	−12	3	^{4}He	^{4}He	^{4}He
n	2nα	24	−2	−5	1	^{4}He		
n	3nα	25	−2	−6	1	^{4}He		
n	np	28	−1	−1	1	^{1}H		
n	n2α	29	−4	−8	2	^{4}He	^{4}He	
n	2n2α	30	−4	−9	2	^{4}He	^{4}He	
n	nd	32	−1	−2	1	^{2}H		
n	nt	33	−1	−3	1	^{3}H		
n	nh	34	−2	−3	1	^{3}He		
n	nd2α	35	−5	−10	3	^{2}H	^{4}He	^{4}He
n	nt2α	36	−5	−11	3	^{3}H	^{4}He	^{4}He

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Projectile	Products	MT	ΔZ	ΔA	NSEC	Secondaries		
n	4n	37	0	−3	0			
n	2np	41	−1	−2	1	^{1}H		
n	3np	42	−1	−3	1	^{1}H		
n	n2p	44	−2	−2	2	^{1}H	^{1}H	
n	nαp	45	−3	−5	2	^{1}H	^{4}He	
n	γ	102	0	1	0			
n	p	103	−1	0	1	^{1}H		
n	d	104	−1	−1	1	^{2}H		
n	t	105	−1	−2	1	^{3}H		
n	h	106	−2	−2	1	^{3}He		
n	α	107	−2	−3	1	^{4}He		
n	2α	108	−4	−7	2	^{4}He	^{4}He	
n	3α	109	−6	−11	3	^{4}He	^{4}He	^{4}He
n	2p	111	−2	−1	2	^{1}H	^{1}H	
n	pα	112	−3	−4	2	^{1}H	^{4}He	
n	t2α	113	−5	−10	3	^{3}H	^{4}He	^{4}He
n	d2α	114	−5	−9	3	^{2}H	^{4}He	^{4}He
n	pd	115	−2	−2	2	^{1}H	^{2}H	
n	pt	116	−2	−3	2	^{1}H	^{3}H	
n	dα	117	−3	−5	2	^{2}H	^{4}He	
n	5n	152	0	−4	0			
n	6n	153	0	−5	0			
n	2nt	154	−1	−4	1	^{3}H		
n	tα	155	−3	−6	2	^{3}H	^{4}He	
n	4np	156	−1	−4	1	^{1}H		
n	3nd	157	−1	−4	1	^{2}H		
n	ndα	158	−3	−6	2	^{2}H	^{4}He	
n	2npα	159	−3	−6	2	^{1}H	^{4}He	
n	7n	160	0	−6	0			
n	8n	161	0	−7	0			
n	5np	162	−1	−5	1	^{1}H		
n	6np	163	−1	−6	1	^{1}H		
n	7np	164	−1	−7	1	^{1}H		
n	4nα	165	−2	−7	1	^{4}He		
n	5nα	166	−2	−8	1	^{4}He		
n	6nα	167	−2	−9	1	^{4}He		
n	7nα	168	−2	−10	1	^{4}He		
n	4nd	169	−1	−5	1	^{2}H		
n	5nd	170	−1	−6	1	^{2}H		
n	6nd	171	−1	−7	1	^{2}H		
n	3nt	172	−1	−5	1	^{3}H		
n	4nt	173	−1	−6	1	^{3}H		

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Projectile	Products	MT	ΔZ	ΔA	NSEC	Secondaries		
n	5nt	174	−1	−7	1	^{3}H		
n	6nt	175	−1	−8	1	^{3}H		
n	2nh	176	−2	−4	1	^{3}He		
n	3nh	177	−2	−5	1	^{3}He		
n	4nh	178	−2	−6	1	^{3}He		
n	3n2p	179	−2	−4	2	^{1}H	^{1}H	
n	3n2α	180	−4	−10	2	^{4}He	^{4}He	
n	3npα	181	−3	−7	2	^{1}H	^{4}He	
n	dt	182	−2	−4	2	^{2}H	^{3}H	
n	npd	183	−2	−3	2	^{1}H	^{2}H	
n	npt	184	−2	−4	2	^{1}H	^{3}H	
n	ndt	185	−2	−5	2	^{2}H	^{3}H	
n	nph	186	−3	−4	2	^{1}H	^{3}He	
n	ndh	187	−3	−5	2	^{2}H	^{3}He	
n	nth	188	−3	−6	2	^{3}H	^{3}He	
n	ntα	189	−3	−7	2	^{3}H	^{4}He	
n	2n2p	190	−2	−3	2	^{1}H	^{1}H	
n	ph	191	−3	−3	2	^{1}H	^{3}He	
n	dh	192	−3	−4	2	^{2}H	^{3}He	
n	hα	193	−4	−6	2	^{3}He	^{4}He	
n	4n2p	194	−2	−5	2	^{1}H	^{1}H	
n	4n2α	195	−4	−11	2	^{4}He	^{4}He	
n	4npα	196	−3	−8	2	^{1}H	^{4}He	
n	3p	197	−3	−2	3	^{1}H	^{1}H	^{1}H
n	n3p	198	−3	−3	3	^{1}H	^{1}H	^{1}H
n	3n2pα	199	−4	−8	3	^{1}H	^{1}H	^{4}He
n	5n2p	200	−2	−6	2	^{1}H	^{1}H	

A.4.1 Other reactions: gas, heat and damage

The neutron induced cross-section set of Table 12 has been extended and complemented by a further set of diagnostic reactions of technological importance in the design and assessment of nuclear power systems. These are listed in Table 13. For MT ={201–207}, the z denotes any projectile (γ, n, d, p, α) and X is a positive integer. There may be other products from the reaction but these are not displayed. Data for these reactions are included in the new TENDL-2013 libraries, and are summarised in the printlib cross-section output tables.

The NJOY [26] modules GASPR and HEATR can be used on a properly filled evaluation to generate gas production reactions, heat production cross-sections and radiation damage energy production. Heating is described by the Kerma (Kinetic Energy Release in Materials) coefficient and the damage caused by irradiation is described by

Table 13: Additional MT numbers for Gas production, Dpa and Kerma assessment.

MT	Description
201	(z,Xn) Total neutron production
202	(z,Xγ) Total gamma production
203	(z,Xp) Total proton production
204	(z,Xd) Total deuteron production
205	(z,Xt) Total triton production
206	(z,Xh) Total helion (^{3}He) production
207	(z,Xα) Total alpha particle production
301	Kerma total (eV-barns)
302	Kerma elastic
303	Kerma non-elastic (all but MT=2)
304	Kerma inelastic (MT={51-91})
318	Kerma fission (MT=18 or MT= {19, 20, 21, 38})
401	Kerma disappearance (MT={102-120})
403	Kerma for protons
407	Kerma for alphas
442	Total photon (eV-barns)
443	Total kinematic kerma (high limit)
444	Dpa total (eV-barns)
445	Dpa elastic (MT=2)
446	Dpa inelastic (MT={51-91})
447	Dpa disappearance (MT={102-120})

Table 14: Additional MT numbers for reactions that are silently ignored.

MT	Description
19	(n,f) First chance fission reaction
20	(n,nf) Second chance fission reaction
21	(n,2nf) Third chance fission reaction
38	(n,3nf) Fourth chance fission reaction
46–101	(z,n$_i$) Neutron production with residuals in excited states
110	Unassigned
118–150	Various p, d, t, α reactions
221	unassigned
251-253	scattering of neutron
402	energy release parameter
600–849	Various proton production reactions
851–859	Lumped reaction covariances
875–891	Various double neutron productions

Dpa (displacements per atom). The resulting dataset can be defined in terms of an MT number, and may be read into FISPACT-II and used in subsidiary calculations during inventory runs to quantify the damage to materials caused by neutron irradiation. See the end of Section 7.1.4 for a description of the output of kerma, dpa and appm rates.

A.4.2 Ignored reactions

The new ENDF style libraries of cross-section data may contain MT values not included in Tables 12 and 13. Data for the MT numbers shown in Table 14 are silently ignored. Data for any other MT encountered cause warning messages to be issued.

A.4.3 Self-shielding of resonant channels using probability tables

The probability tables keyword in FISPACT-II (see Section 5.1.14) allows probability table data generated by CALENDF [30, 14] to be used to model dilution effects in the computation of the collapsed effective cross-sections. CALENDF provides data in five sets of macro-partial cross-sections: The CALENDF set MT numbers (cal-mt) are defined in Table 15. The sum of these macro-partial cross-sections gives the total cross-section in each energy group over the resonance regions covered.

Table 15: CALENDF MT number.

cal-mt	description	MT in set
2	elastic scattering	2
101	absorption (no outgoing neutron)	102 103 107
18	fission total	18
4	inelastic scattering (emitting one neutron)	4 11
15	multiple neutron production (excluding fission)	5 16 17 37

The data provided by CALENDF are cross-section and probability values depending on four parameters:

$$\sigma(x,n) \equiv \sigma(p,g,x,n) \tag{25}$$
$$P(x,n) \equiv P(p,g,x,n) \tag{26}$$

where
p = parent nuclide number,
g = energy group number,
x = macro-partial (or total) index,
n = quadrature index,

In the expressions below, we suppress the explicit display of dependence of cross-section on the parent nuclide p and energy group g except in the formulae for dilution. The

infinite dilution ($d = \infty$) cross-section for a given parent, energy group and component is

$$\sigma(x, d = \infty) = \frac{1}{E_{max} - E_{min}} \int_{E_{min}}^{E_{max}} \sigma(E)\, dE = \sum_{n=1}^{N} P(x, n)\sigma(x, n) \tag{27}$$

When a nuclide is a part of a homogenous mixture of nuclides, then the effective cross-sections in the resonance regions are reduced, and are parameterised using the dilution cross-section d [31, 32, 33, 30]:

$$\sigma(x, d) = \frac{\sum_{n=1}^{N} P(x, n)\sigma(x, n)/(\sigma_t(n) + d)}{\sum_{n=1}^{N} P(x, n)/(\sigma_t(n) + d)} \tag{28}$$

where the total cross-section is given by the sum of the macro-partials:

$$\sigma_t(n) = \sum_{x=1}^{X} \sigma(x, n) \tag{29}$$

The total cross-section for nuclide p in energy group g at dilution d is given by

$$\sigma^{tot}(d) = \sum_{x=1}^{X} \sigma(x, d_p) \tag{30}$$

The probability table data from CALENDF are used in conjunction with the 616 energy group cross-section data in the EAF library or the 709 group data in the TENDL-2013 library. In the following discussion, we use the term 'library' or 'LIB' to refer to either the EAF of TENDL-2013 cross-section data as appropriate. The dilution computed using the CALENDF data is applied either as scaling factors to the library cross-section data or as replacements over the energy ranges for which the probability table data are available. (This is selected using the *multxs* argument to the **PROBTABLE** keyword). If the CALENDF and library data were fully self-consistent, then the same self-shielding would be obtained for both choices of *multxs*, but the absence of elastic scattering cross-section in the EAF data lead to some differences. For either choice of *multxs*, either partial or total scaling may be applied.

Scaling applied to LIB data: Scaling is applied to the library data in one of two ways depending on the *usepar* argument to the **PROBTABLE** keyword (see Section 5.1.14 on page 52).

If the partial self-shielding scaling factor option is chosen, then the cross-section for nuclide p in energy group g and for `MT` value y belonging to the macro-partial group x is scaled according to

$$\sigma^{new}(y, d) = \sigma^{LIB}(y) \left(\frac{\sigma(x, d)}{\sigma(x, d = \infty)} \right) \tag{31}$$

and for the total scaling factor

$$\sigma^{new}(y,d) = \sigma^{LIB}(y)\left(\frac{\sigma^{tot}(d)}{\sigma^{tot}(d=\infty)}\right) \tag{32}$$

The dilution $d(p,g)$ for a given nuclide p and energy group g is computed using a weighted sum over all the nuclides, $q = 1, Q$ in the mixture. The fraction f_q of the mixture is nuclide q. Nuclides in the mixture may or may not be included in the list of nuclides to which the self-shielding correction is to be applied. Nuclides to which self-shielding corrections are applied must be in the mixture list. The first approximation is given using the total cross-sections from the cross-section library:

$$d^{(0)}(p,g) = \sum_{\substack{q=1 \\ p\neq q}}^{Q} \frac{f_q \sigma^{LIB-tot}(q,g)}{f_p} \tag{33}$$

where

$$\sigma^{LIB-tot}(p,g) = \sum_{y=1}^{Y} \sigma^{LIB}(p,g,y) \tag{34}$$

Over the energy range for which the probability table data are available for those nuclides in the mixture for which self-shielding corrections are being applied, the approximation given by Eq. (33) is iteratively refined using

$$S^{(i)}(g) = \sum_{q=1}^{Q} f_q \sigma^{LIB-tot}(q,g)\left(\frac{\sigma^{tot}(q,g,d^{(i)}(q,g))}{\sigma^{tot}(q,g,\infty)}\right) \tag{35}$$

$$d^{(i+1)}(p,g) = \frac{S^{(i)}(g)}{f_p} - \sigma^{LIB-tot}(p,g)\left(\frac{\sigma^{tot}(p,g,d^{(i)}(p,g))}{\sigma^{tot}(p,g,\infty)}\right) \tag{36}$$

Replacement of LIB data: If there is only one reaction `MT` in the CALENDF macro-partial group, then the replacement formulae would be given by replacing the σ^{LIB} values in the above equations by the infinite dilution cross-sections obtained from the CALENDF data. When there is more than one reaction in the macro-partial set, then the dilution effect has to be apportioned according to the LIB reaction cross-sections.

If the partial self-shielding scaling factor option is chosen, then the cross-section for nuclide p in energy group g and for `MT` value y belonging to the macro-partial group x is given by

$$\sigma^{new}(y,d_p) = \sigma(x,d_p)\left(\frac{\sigma^{LIB}(y)}{\sum_{y'\in x}\sigma^{LIB}(y')}\right) \tag{37}$$

and for the total scaling factor

$$\sigma^{new}(y,d_p) = \sigma(x,\infty)\left(\frac{\sigma^{LIB}(y)}{\sum_{y'\in x}\sigma^{LIB}(y')}\right)\left(\frac{\sigma^{tot}(d_p)}{\sigma^{tot}(\infty)}\right) \tag{38}$$

The initial values of the dilutions are given by Equations (33) and (34) and the iterative refinements where CALENDF probability table data are available are given by

$$S^{(i)}(g) = \sum_{q=1}^{Q} f_q \sigma^{tot}(q, g, d^{(i)}(q, g)) \tag{39}$$

$$d^{(i+1)}(p, g) = \frac{S^{(i)}(g)}{f_p} - \sigma^{tot}(p, g, d_p^{(i)}) \tag{40}$$

The set of nuclides for which the self-shielding correction is calculated is specified by the **SSFCHOOSE** keyword. The set of nuclides included in the mixture for computing the dilution cross-section is specified by either the **SSFMASS** or **SSFFUEL** keyword. Nuclides included in the **SSFCHOOSE** keyword list that are not included in the in mixture will cause a fatal error message to be issued by the program.

The values of dilution given by Equation (36) or (40) may be overridden using the **SSFDILUTION** keyword (Section 5.1.19).

Tables of the energies, cross-sections, dilutions and self-shielding factors are printed for each of the nuclides to which the self-shielding correction is applied.

The final diagnostic table gives the collapsed cross-sections with ($\sigma^{new}(p, y)$)and without ($\sigma^{LIB}(p, y)$) the self-shielding correction. Also printed is the effective self-shielding factor for the collapsed cross-section:

$$ssf(p, y) = \frac{\sigma^{new}(p, y)}{\sigma^{LIB}(p, y)} \tag{41}$$

A.4.4 Self-shielding of resonant channels, using the universal curve model

Starting from Release 2.10, FISPACT-II provides a second method of accounting for self shielding in thick targets with a variety of geometries. This can be used as an alternative to the probability table method described in the previous section; it is not possible to use both descriptions of self shielding simultaneously.

In a series of papers [21, 22, 23], the authors Martinho, Gonçalves and Salgado described a "universal sigmoid curve" model of self shielding to account for the reduction of the neutron flux by cross-section resonances in the context of neutron activation analysis. They based their development on earlier experimental and theoretical work by Baumann [34].

The Martinho et al [21] model initially described the effect of a single resonance peak in a pure target consisting of a single nuclide. The self-shielding factor G_{res} is approximated as a simple function of a single dimensionless length parameter that depends on the physical size and shape of the target as well as the peak cross-section at the resonance and the resonance widths for elastic scattering and radiative capture.

The final form of the model [23] accommodates a group of isolated resonances of a pure target, and the target geometry could be a foil, wire, sphere or cylinder of finite height.

This model has been generalised further and applied to the mixture of nuclides required for a FISPACT-II calculation.

The FISPACT-II user invokes this model of self shielding by using the **SSFGEOMETRY** keyword to define the type and dimensions of the target, as detailed in Table 16.

Table 16: The types of target geometry recognised by FISPACT-II.

Identifier	**Type**	**Dimension(s)**	**Effective length (y)**
1	foil	thickness (t)	$y = 1.5t$
2	wire	radius (r)	$y = 2r$
3	sphere	radius (r)	$y = r$
4	cylinder	radius (r), height (h)	$y = 1.65rh/(r + h)$

In more detail, the initial form of the model [21] that accounts for the effect of a single resonance in a pure target containing a single nuclide defines a dimensionless parameter

$$z = \Sigma_{tot}(E_{res})y\sqrt{\frac{\Gamma_\gamma}{\Gamma}} \tag{42}$$

that depends on the physical length y, the macroscopic cross-section $\Sigma_{tot}(E_{res})$ at the energy E_{res} of the resonance peak, the resonance width Γ_γ for radiative capture and the total resonance width Γ. Then the self-shielding factor is

$$G_{res}(z) = \frac{A_1 - A_2}{1 + (z/z_0)^p} + A_2 \tag{43}$$

where the parameters defining this "universal sigmoid curve" are

$$A_1 = 1.000 \pm 0.005 \tag{44}$$
$$A_2 = 0.060 \pm 0.011 \tag{45}$$
$$z_0 = 2.70 \pm 0.09 \tag{46}$$
$$p = 0.82 \pm 0.02 \tag{47}$$

These parameters were determined empirically by Martinho et al [21] by fitting to a set of points generated by performing Monte-Carlo simulations with the MCNP code for a variety of targets of different shapes, sizes and compositions. Six nuclides that exhibit strong resonances were used individually, not as mixtures.

The model was then extended by Martinho et al [22], who defined an effective length y for cylinders of finite height, but a more significant extension was provided by Salgado et al [23], who defined an average $\langle G_{res} \rangle$ by assigning weights to each resonance

and forming an average of the individual G_{res} factors calculated for each resonance individually. The weight of resonance i is

$$w_i = \left(\frac{\Gamma_\gamma}{E_{res}^2} \cdot \frac{g\Gamma_n}{\Gamma} \right)_i \tag{48}$$

where

Γ_n is the neutron scattering width;

g is the statistical factor, $(2J+1)/(2(2I+1))$;

J is the spin of the resonance state;

I is the spin of the target nucleus.

Then the effective self-shielding factor is

$$\langle G_{res} \rangle = \frac{\sum_i w_i G_{res}(z_i)}{\sum_i w_i} \tag{49}$$

where each z_i is calculated from Eq. (42) using the effective length of the target, y and the resonance parameters for resonance i.

This model has been generalised further in two ways to make it suitable for application in FISPACT-II.

First, the average self-shielding factor is computed from the resonance parameters given in the resolved resonance range defined in the ENDF File 2 data for a subset of the nuclides specified with the **SSFFUEL** or **SSFMASS** keywords. It is assumed that the resonances for the mixture of nuclides are separated in energy sufficiently for them not to overlap significantly.

Note that TENDL-2012 uses a unique approach to create parameters for resolved statistical resonances for a large number of isotopes that did not have any. This method invokes global average parameters from the different systematics and from the TALYS reaction code [35]. These parameters are then used by either the CALENDF code or by the R-matrix code AVEFIT. Statistical resonance parameters are then obtained from zero up to the first excited level, reflecting the average resonance parameters coming from compound model calculations. Above the first inelastic level, grouped inelastic cross sections with local fluctuations are obtained. This method complements the measured resonance parameters, or provides a resolved resonance range when measurements do not existing. In between these two cases, statistical resonance parameters are adjusted to integral measurements when available. This method, which has been successfully applied to all isotopes living longer than one second, has been used to populate resonance range of the TENDL-2012 libraries [36].

The cross-section at a resonance peak is not supplied in the ENDF data. The simple expression provided by Fröhner [Eq. (186)][37] is used to supply this information.

Secondly, $\langle G_{res} \rangle$ is made energy dependent by taking averages separately for each energy bin used for the group-wise cross-sections, including only those resonances with peaks in the relevant energy bin. Then this array of energy-dependent self-shielding factors is applied to each energy-dependent cross-section before the cross-section collapse.

The principle underlying this model of self shielding is that the resonances perturb the spectrum of the applied neutron flux. Consequently, the self shielding factors should modify the cross-sections for all reactions. However, the effect of self shielding varies from reaction to reaction because of the differing energy dependencies of the cross-sections.

A.5 Fission

The EAF libraries have very little induced fission yield data and relatively few nuclides. At most, the fission yield data is in three energy ranges, and an extrapolation procedure is used to fill in missing data. To assess the effects of fission of actinides without fission yield data, fission associations were defined using the `asscfy` data stream so that actinides without fission yield data use the data of a nuclide with similar properties. Surrogate daughters were introduced to fill in where daughter nuclides are not included. Subsection A.5.1 describes these.

The new TENDL-2013 ENDF libraries have fission yield data for many more nuclides, and these data are tabulated in energy bins in the same manner as for cross-sections and covariances. With data available for many more nuclides, the fission association and surrogate daughter algorithms are not applied. The new treatment of fission yield is described below in Subsection A.5.2

A.5.1 EAF data

Projectile-induced fission yield data are available in three projectile energy ranges:

thermal	under 200 keV
fast	between 200 keV and 5 MeV
high	over 5 MeV

The boundary energies are $E_{hf} = 5\,\text{MeV}$ and $E_{ft} = 200\,\text{keV}$. It is assumed that there is a maximum of one fission yield fraction in each of these energy ranges for a given projectile, parent and daughter fragment.

The algorithm for infilling unknown values is:

- If yields for the thermal, fast and high energy projectiles, Y_t, Y_f and Y_h are known then these are used.

- If only one value Y is known, then set $Y_t = Y_f = Y_h = Y$.
- If only Y_t and Y_h are known, set $Y_f = (Y_t + Y_h)/2$, and if values for Y_t or Y_h are unknown, then set them to Y_f.

A single fission yield factor for use in the inventory equations is obtained by collapsing the available data in a manner similar to that used for cross-sections (Equation (10)). Fluxes in the thermal, fast and high energy groups are found by summing fluxes in the narrower groups used for the cross-sections.

A simple nearest-grid-point algorithm for this is as follows. Let ϕ_i be the flux in the cross-section energy group that lies between energies E_i and E_{i+1} (data are in decreasing energy order, and $1 \leq i < i_{max}$), then the group energy is $\bar{E}_i = (E_i + E_{i+1})/2$. Let i_{hf} and i_{ft} be the largest i for which $\bar{E}_i \geq E_{hf}$ and $\bar{E}_i \geq E_{ft}$, respectively, then

$$\phi_h = \sum_{i=1}^{i_{hf}-1} \phi(E_i) \tag{50}$$

$$\phi_f = \sum_{i=i_{hf}}^{i_{ft}-1} \phi(E_i) \tag{51}$$

$$\phi_t = \sum_{i=i_{ft}}^{i_{max}} \phi(E_i) \tag{52}$$

$$\phi^{int} = \phi_h + \phi_f + \phi_t \tag{53}$$

and the collapsed fission yield is given by

$$Y = (\phi_h Y_h + \phi_f Y_f + \phi_t Y_t)/\phi^{int} \tag{54}$$

In terms of the description of the reaction network as a directed graph, each fission reaction gives rise to many edges in the graph connecting the fissionable parent nuclide to all of its possible fission products. The effective reaction cross-section needed to calculate the flow along each edge of the graph is simply the fission cross-section multiplied by the appropriate fission yield.

To make up for the lack of data on fission for many actinides, a surrogate daughter algorithm is used. This is in addition to the use of associated fission yield data. The surrogate daughter algorithm replaces fission product daughters not known to the program with similar nuclides that are known. The algorithm works as follows:

- If the daughter fission product is in the list of nuclides known to the program, then assign the fission yield to that daughter.
- If the daughter is not listed, then assign its yield to the first nuclide encountered in the list of nuclides with the same A, and the same or larger Z.
- If neither of the above cases is satisfied, then assign the yield to the 'sink' nuclide.

A.5.2 ENDF data

The fission yield data, like the covariance data, are on coarser energy grids than the flux and cross-sections. To collapse the fission yield, the weights are calculated using

$$W_k = \sum_{i=1}^{N} S_i^k \phi_i / \sum_{i=1}^{N} \phi_i \tag{55}$$

where there are $k \in [1, K]$ fission yield energy groups. The yields are collapsed using

$$Y = \sum_{k=1}^{K} W_k Y_k \tag{56}$$

The variance of the collapsed fission yield is given by

$$var = \sum_{k=1}^{K} (W_k F_k)^2 \tag{57}$$

where F_k are the tabulated 1σ errors in the ENDF file. The fractional uncertainty is $\Delta = \sqrt{var}/Y$. In the present version of the FISPACT-II the fission yield uncertainty is not used.

A.6 Gamma Activation

The set of reactions allowed for gamma activation is identical to the set of 90 reactions for neutron activation. The table for these reactions can be obtained by replacing the projectile n by γ, and decreasing all the values of ΔA by 1 in Table 12.

A.7 Proton Activation

The set of reactions allowed for proton activation is identical to the set of 90 reactions for neutron activation. The table for these reactions can be obtained by replacing the projectile n by p, and increasing all the values of ΔZ by 1 in Table 12.

A.8 Deuteron Activation

The set of reactions allowed for deuteron activation is identical to the set of 90 reactions for neutron activation. The table for these reactions can be obtained by replacing the projectile n by d, and increasing all the values of ΔZ by 1 and all the values of ΔA by 1 in Table 12.

A.9 Alpha Activation

The set of reactions allowed for alpha particle activation is identical to the set of 90 reactions for neutron activation. The table for these reactions can be obtained by replacing the projectile n by α, and increasing all the values of ΔZ by 2 and all the values of ΔA by 3 in Table 12.

A.10 Gamma Radiation

In addition to the activity of irradiated materials, another measure of acceptability is the dose rate from emitted γ rays. FISPACT-II uses two approximate estimates of the γ dose rate due to irradiation by neutrons: contact dose from the surface of a semi-infinite slab or dose at a given distance from a point source. For both measures, the contribution of high-energy β-particle bremsstrahlung to the total dose rate can be significant, and this may be output using the **BREMSSTRAHLUNG** keyword. The formulae used for these are discussed in the following sub-subsections.

A.10.1 Contact gamma-dose rate

Equation (58) shows the formula used to calculate the γ dose rate at the surface of a semi-infinite slab of material, it is taken from Jaeger [38]:

$$D = C\frac{B}{2}\sum_{i=1}^{N_\gamma}\frac{\mu_a(E_i)}{\mu_m(E_i)}S_\gamma(E_i) \tag{58}$$

where
D = surface γ dose rate (Sv h^{-1})
N_γ = number of energy groups in the γ spectrum histogram
E_i = mean energy of the i-th energy group (c.f., Table 6 on page 68)
μ_a = mass energy absorption coefficient (μ_{en}/ρ) of air (m^2 kg^{-1})
μ_m = mass energy attenuation coefficient (μ/ρ) of the material (m^2 kg^{-1})
B = build up factor (= 2)
S_γ = rate of γ emission (MeV kg^{-1} s^{-1})
$C = 3.6 \times 10^9|e|$ converts (MeV kg^{-1} s^{-1}) to (Sv h^{-1})

The EAF library file `absorp` (see Section B.7) contains μ/ρ [cm^2 g^{-1}] for all elements in increasing Z order, μ [m^{-1}] and μ_{en}/ρ [cm^2 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} provided by the `absorp` data file using

$$\mu_m = \sum_j f_j \mu_{mj} \tag{59}$$

where f_j = (mass of element j)/(total mass).

The value of the emission rate S_γ is calculated using

$$S_\gamma(E_i) = I_i A(t) \tag{60}$$

where I_i is the intensity of energy group i (MeV) and $A(t)$ is the specific activity of material at time t (Bq kg^{-1}). If discrete spectral line data are available, then I_i is obtained by summing the contributions from spectral lines in energy group i read from the `decay` data files. If data are not available, then an approximate value may be computed as described below in Section A.10.3.

A.10.2 Gamma dose rate from point source

Equation (61) shows the standard formula (taken from Reference[38]) for calculation of the dose rate from a point source in air.

$$D = C \sum_{i=1}^{N_\gamma} \frac{\mu_a}{4\pi r^2} e^{-\mu(E_i)r} m_s S_\gamma(E_i) \tag{61}$$

where C, N_γ, μ_a, S_γ are as defined above for Equation (58), and
m_s = mass of source (kg)
r = distance from source (m)
$\mu(E_i)$ = energy attenuation coefficient of air (m^{-1})

Both Equations (58) and (61) are approximations suitable for FISPACT-II calculations, but it is noted that they may not be adequate for specific health physics problems.

A.10.3 Approximate gamma spectrum

Wherever possible decay data from JEFF-3.1 files [39] have been used to construct the decay data library (`decay` – see Appendix B.4) used with FISPACT-II. Intensity in a spectrum energy group is computed from the sum of intensities of discrete spectral lines lying in the energy group. However, for 254 unstable nuclides the file contains only the average γ energy - no data for the γ spectrum are available. Without the γ spectrum FISPACT-II is unable to calculate the γ dose rate contribution for these nuclides. In order to check if any of these nuclides are likely to contribute significantly to the total dose rate, the following method is used to calculate an approximate spectrum (see **SPEK** keyword on page 54).

The maximum γ energies (E_m) for decays assumed in the method are given in Table 17.

The intensity in the i-th group (I_i) is given by

$$I_i = \frac{a\langle\gamma\rangle}{E_m} \left(\frac{e^{-a\eta_{i-1}} - e^{-a\eta_i}}{1 - (1+a)e^{-a}} \right) \tag{62}$$

Table 17: Maximum γ energies for various decay modes.

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

where $a = 14$ (arbitrary constant)
$\eta_i = E_i/E_m$

Gamma doses for approximate spectra are found using the intensity from Equation (62) to find the emission rate (Equation (60)), and then using this rate in Equation (58) or (61) as appropriate.

A.10.4 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-II uses a similar approach to Jarvis [40] who considers γ emission from a mono-energetic electron.

The energy distribution of γ rays emitted by a mono-energetic electron in a matrix of charge Z is given by

$$dN = \begin{cases} aZ\left(\frac{E_0-E}{E}\right)dE & 0 \leq E < E_0 \\ 0 & E \geq E_0 \end{cases} \tag{63}$$

where
dN = number of γ-rays with energy E (keV)
E_0 = energy of electron (keV)
$a = 2.76 \times 10^{-6}$ (keV^{-1})

Integrating Equation (63) over the energy bins give the number of γ-rays associated with that bin. There are three cases:

$$N(i) = \begin{cases} aZ[E_0 \log(E_{i+1}/E_i) - (E_{i+1} - E_i)] & E_0 \geq E_{i+1} \\ aZ[E_0 \log(E_0/E_i) - (E_0 - E_i)] & E_{i+1} > E_0 > E_i \\ 0 & E_0 \leq E_i \end{cases} \tag{64}$$

where E_i and E_{i+1} are the lower and upper energy bounds of group i. The intensity for group i is given by

$$I_i = N(i)(E_i + E_{i+1})/2 \tag{65}$$

The bremsstrahlung corrections to gamma doses are found using the intensity from this equation to find the emission rate (Equation (60)), and then using this rate in Equation (58) or (61) as appropriate.

The above discussion is valid only for mono-energetic 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 (64) is calculated from

$$Z = \sum_j Z_j f_j \tag{66}$$

where Z_j = atomic number of the j-th element and f_j = atomic fraction of the j-th element (i.e., number of atoms of j / total number of atoms).

A.10.5 Bremsstrahlung candidates

Only a subset of all the nuclides in the decay library needs to be considered for bremsstrahlung production. Nuclides may make a contribution to the γ dose rate because of bremsstrahlung emission from energetic β particles.

The following criteria are applied by the code to the EAF decay library (Appendix B.4) to give the nuclides displayed by the **PRINTLIB** *4* keyword option:

- 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 is radioactive with a half-life $\leq 5.0 \times 10^{16}$ years;
- the nuclide has an average β-energy >average γ-energy;
- the nuclide has an average β-energy $> 0.145\,\mathrm{MeV}$.

A.11 Monte-Carlo Sensitivity Estimation

FISPACT-II uses a Monte-Carlo approach to sensitivity analysis. A series S of inventory calculations is performed with the set of I independent variables $\{X_i^s;\ i = 1, \ldots, I;\ s = 1, \ldots, S\}$ chosen from distributions with means $\langle X_i \rangle$ and standard deviations $\langle \Delta X_i \rangle$. These runs produce a set of J dependent variables $\{Y_j^s;\ j = 1, \ldots, J;\ s = 1, \ldots, S\}$. In the present context, the independent variables are cross-sections and their uncertainties or decay constants and their uncertainties. The dependent variables are the numbers of atoms of nuclides j or some related radiological quantity.

The implementation of this scheme uses the **SENSITIVITY** keyword to initialise the collecting of data within the main inventory calculation. The keyword **ZERO** causes the series of S runs with different independent variables to be undertaken to compute, process and output the set $\{Y_j^s\}$. The default distribution is taken to be log-normal, but other options are possible. (See keyword **MCSAMPLE** on page 71).

Any sequence of irradiation pulses, changes in cross-section, etc. that are possible with FISPACT-II can be used in the sensitivity calculations. The code performs the base calculation with full output, then repeats S times the sequence of steps with different sets $\{X_i^s\}$. The results of the base calculation are not included in the sensitivity calculation.

Sensitivity calculations provide both uncertainty and sensitivity output. Summary uncertainty output of means $\bar{X}_i$ and $\bar{Y}_j$ and standard deviations ΔX_i and ΔY_j are sent to the `output` file:

$$\bar{X}_i = \frac{1}{S}\sum_{s=1}^{S} X_i^s \tag{67}$$

$$\Delta X_i = \sqrt{\frac{1}{S-1}\sum_{s=1}^{S}[(X_i^s)^2 - \bar{X}_i^2]} \tag{68}$$

$$\bar{Y}_j = \frac{1}{S}\sum_{s=1}^{S} Y_j^s \tag{69}$$

$$\Delta Y_j = \sqrt{\frac{1}{S-1}\sum_{s=1}^{S}[(Y_j^s)^2 - \bar{Y}_j^2]} \tag{70}$$

Differences $(\bar{X}_i - \langle X_i \rangle)$ and $(\Delta X_i - \langle \Delta X_i \rangle)$ give a measure as to how well the sample set matches the distribution, and as S increases these two differences should tend to zero[4]. Similarly $\bar{Y}_j$ should tend to the value of the base calculation, and ΔY_j gives the uncertainty in the dependent variable resulting from uncertainties in the independent variables.

The sensitivity of dependent quantity Y_j on independent variable X_i is assessed using the Pearson product-moment correlation coefficient

$$r_{ij} = \frac{\sum_s X_i^s Y_j^s - S\bar{X}_i\bar{Y}_j}{(S-1)\Delta X_i \Delta Y_j} \tag{71}$$

The magnitude of r_{ij} is less than one, and a magnitude close to one indicates strong linear correlation. Values of r_{ij} close to $+1$ will be found for reactions or decays on principal pathways leading to nuclide j, and values close to -1 are expected for reactions or decays acting as sinks on pathways.

The best-fit line relating Y_j to X_i is given by

$$\frac{Y_j - \bar{Y}_j}{\Delta Y_j} = r_{ij}\left(\frac{X_i - \bar{X}_i}{\Delta X_i}\right) \tag{72}$$

[4]This is not strictly true; the sample standard deviation will be systematically smaller than the input value because of the truncation of the tails of the distributions for normal and log-normal distributions.

FISPACT-II writes tables of means, standard deviations and correlation coefficients to `output`, and writes the raw data $\{X_i^s,\ Y_j^s;\ i = 1, \ldots, I;\ j = 1, \ldots, J;\ s = 1, \ldots, S\}$ to file `sens` for post-processing by the user.

A.12 Pathways

The reaction network illustrated in Figure 6 may be described either by the rate equations (Eq. (7)) or as the sum of paths and loops, which we refer to as pathways. The inventory of a given nuclide computed using the rate equations can equivalently be found by a linear superposition of contributions of flows along the pathways to that nuclide.

Pathways are used in FISPACT-II to aid interpretation and to estimate uncertainties. If we know the inventory at the start and end of an irradiation (or cooling) period, then pathways analysis may be used to identify the most significant chains of reactions and decays in transmuting the initial inventory to the dominant nuclides in the final inventory of the step.

Key aspects of pathways analysis are methods for searching directed graphs (or *di-graphs*) of the form illustrated in Figure 6 to identify routes from a parent to a chosen descendant, and the assembly and solution of rate equations for chosen subsets of nuclides on the pathway to get the flow along the pathway.

In the directed graph, nuclides correspond to the vertices of the graph. A parent nuclide is connected to a daughter nuclide by a graph edge. Associated with the edge is a flow rate given by the sum of the rates of all reactions and the decay that take the parent to the daughter. This flow rate is given by the off-diagonal elements of the rate equation matrix. The flow rate from parent j to daughter i is given by the element A_i^j in row i and column j of matrix A of Equation (11).

We use the following definitions:

path A path is a chain of *different* nuclides connecting the source nuclide to the target nuclide;

loop A loop is a closed chain of *different* nuclides connecting a nuclide to itself. Loops formed by the cyclic permutation of the nuclides in the loop are considered to be the same loop;

pathway A pathway is the combination of a *single* path with zero or more loops.

These are illustrated in Figure 9.

The full directed graph has one vertex per nuclide, and one edge for each off-diagonal term in the rate equations. The EAF-2010 data have 2233 vertices (nuclides) and

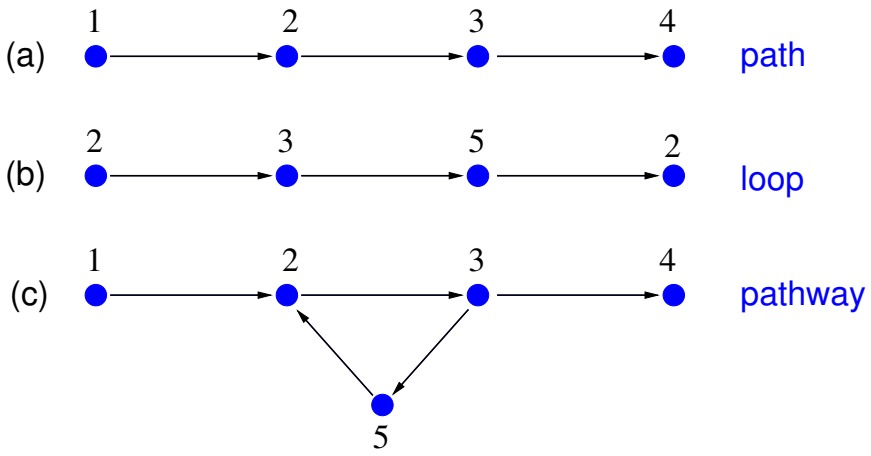

Figure 9: (a) A path is a linear chain of nuclides connected by edges, (b) a loop is a cyclic chain of nuclides and (c) a pathway is the combination of a single path with zero or more loops.

approximately 120 000 edges (non-zero elements in A). If fission can be omitted this reduces to about 42 000, and for a cooling period this drops to less than 5 000 (c.f., Section A.1). The brute-force approach to finding paths by examining all the paths to descendants of a given source nuclide for these numbers of edges rapidly becomes impracticable because of the combinatorial explosion of the number of alternatives to be examined as path lengths increase. FISPACT-II uses a much faster technique based on iteration on a single-visit tree, where the tree is pruned using edge weighting to reduce the number of graph edges to be retained in the search for significant pathways [41].

The weights are computed using coefficients of the rate equation matrix A, and are used to eliminate paths and loops as follows:

- Each edge on a path has weight ≤ 1. If the product of the weights along a path falls below the path threshold, then the path is discarded.
- Each edge on a loop has weight ≤ 1. The weight of the loop, W_l is the product of the edge weights around the loop. If $W_l/(1-W_l)$ falls below the loop threshold, then the loop is discarded.

The retained paths are significant paths, and the retained loops are significant loops. Significant paths and significant loops are combined to give pathways. Loops are added to paths according to the following criteria:

1. the loop has one or more nuclides in common with the path;
2. when the loop is added to the path, it does not create a second path to the target (this is to avoid double counting of paths);

3. when the loop is added to the path, the fractional increase in the target inventory due to the path is greater than the loop floor.

The resulting pathway is discarded as not significant if the fraction of the target inventory due to the pathway (i.e., the path and its loops) is below the path floor.

The pruning weights are computed from the coefficients of the rate equation matrix. The formulae used for single and for multiple pulse irradiation are those derived in [41].

A.12.1 Algorithm

Pathways are calculated from a single source nuclide to multiple target nuclides, and then they are sorted into target nuclide order for output.

For each source nuclide, lists of paths and loops ordered in decreasing importance are found. Parent to daughter rather than daughter to parent data ordering is used to simplify the extraction of adjacency information and of reaction rates from the compact storage structure used to store the rate equation matrix coefficients.

The computation of the significant paths and loops for a given source nuclide uses a five step process designed to prune unnecessary searches and thereby reduce computational effort:

Step 1: build a breadth-first search (BFS) tree representation of the digraph that visits as parents only once all significant nuclides that are descendants of the source nuclide. Significant nuclides are ones that are descendants of the source nuclide that may be reached by a path whose weight is above the `path_floor` threshold.

Step 2: repeatedly search the BFS tree of Step 1 to find all graph edges that lie on paths from the source nuclide to the target nuclide, or lie on loops that intersect these paths.

Step 3: build a 'brute force' BFS tree using those edges that survive step 2 and extract from this paths and loops that have one or more nuclides on one of the paths to the targets. A branch of the tree is terminated when

- a loop is found
- the weight of the path is below `path_floor`
- the length of the path reaches `max_depth`

Building of the tree terminates when there are no more parent nuclides in the digraph queue.

Step 4: prune loops, retaining only those loops where the weight of the loop is above `loop_floor` and the combination of loops and path give a single candidate pathway whose weight bound is above `path_floor`.

Step 5: integrate the rate equations for candidate pathways to get the actual weight of the path, storing pathways above the `path_floor` threshold in decreasing weight order, and discarding those pathways below the threshold.

A.13 Uncertainty Estimates

The pathways analysis is used to identify the pathways from the initial inventory nuclides to the (target) dominant nuclides at the end of the irradiation phase, together with the number of atoms created at target nuclide t due to the reaction and decay chain along path p to that nuclide. These, together with uncertainties in the reaction cross-sections and decay half lives associated with the edges of the pathways are used in FISPACT-II to provide estimates of the uncertainties.

Given a set of target nuclides S_t, then the uncertainty in some radiological quantity Q, where

$$Q = \sum_{t \in S_t} q_t \tag{73}$$

is given by ΔQ, where

$$(\Delta Q)^2 = \sum_{t \in S_t} \left(\frac{\Delta N_t}{N_t} \right)^2 q_t^2 \tag{74}$$

and N_t is the number of atoms of target nuclide t formed from the initial inventory, and ΔN_t is the error in N_t.

ΔN_t will be computed from the pathways inventories and the fractional squared error Δ_{tp}^2 in the number of atoms of target nuclide t formed along pathway p to that target. If we let the set of pathways to target t be S_p, then we may write

$$S_p = (\cup_{a \in S_{sa}} S_a) \cup S_o \tag{75}$$

where S_p is the set of pathways leading to target t, S_a is the subset of these pathways where the pathway starts from the fission of actinide source nuclide a and S_o is the set of other pathways. S_{sa} is the subset of set S_s of source nuclides that are actinides. The reason for the split in Eq. (75) is that the pathways arising from the fission of source actinide a are treated as correlated, and other pathways are treated as uncorrelated. The formula used to compute ΔN_t is

$$(\Delta N_t)^2 = \sum_{p \in S_o} \Delta_{tp}^2 N_{tp}^2 + \sum_{a \in s_{sa}} \left(\sum_{p \in S_a} |\Delta_{tp}| N_{tp} \right)^2 \tag{76}$$

where N_{tp} is the number of atoms of target t formed along path p to that target. Δ^2_{tp} is given by

$$\Delta^2_{tp} = \sum_{e \in S_e} \sum_{r \in S_r} \left[\frac{R_r(\Delta\sigma_r/\sigma_r)}{R_e} \right]^2 + \sum_{e \in D_e} \left[\frac{\Delta\tau_e}{\tau_e} \right]^2 \tag{77}$$

where
S_e is the set of edges on pathway p;
S_r is the set of reactions on edge e;
R_r is the pulse averaged reaction rate of reaction r;
R_e is the total pulse averaged reaction rate on edge e;
$\Delta\sigma_r/\sigma_r$ is the fractional uncertainty in the cross-section for reaction r;
D_e is the set of edges on pathway p where the parent nuclide is long-lived or where the parent is short-lived and the daughter nuclide is the target nuclide of the path. A short lived nuclide is one whose half life is less than the time interval of the irradiation pulse sequences;
$\Delta\tau_e/\tau_e$ is the fractional uncertainty in the half life of the parent nuclide on the edge.

The total reaction rate for the edge is the sum of the reaction rates for the parent-daughter nuclides on the edge:

$$R_e = \sum_{r \in S_r} R_r \tag{78}$$

Let there be J time intervals in the irradiation phase, and let the time of interval $j \in [1, J]$ be Δt_j and the flux amplitude be ϕ_j. In addition, assume that there are I different collapsed cross-sections, with cross-section $i \in [1, I]$ being the value used for pulses $j = J_i \ldots J_{i+1}$ ($J_1 = 1$ and $J_{I+1} = J$), then

$$R_r = (\sum_{i=1}^{I} \sigma_r^i \sum_{j=J_i}^{J_{i+1}} \phi_j \Delta t_j)/T_J \tag{79}$$

where

$$T_J = \sum_{j=1}^{J} \Delta t_j \tag{80}$$

In the case of fission reactions, σ_r^i is replaced by $\sigma_r^i f_r$, where f_r is the fission yield for the reaction product corresponding to the daughter nuclide on the edge.

A.14 Method of Solution of Rate Equations

The rate equations (11) and subsets of the rate equations used for pathway calculations are all specific examples of first-order systems of odes with the general form

$$\frac{dy_i}{dt} = F_i(\{y_j\}, t) \tag{81}$$

with initial conditions

$$y_i(t = 0) = y_{i,0} \text{ given} \tag{82}$$

for $1 \leq i, j \leq N$. These initial value problems can be solved to give $\{y_i(t)\}$ using numerical methods.

A.14.1 Properties of the equations

The rate equations (11) are linear because at the level of approximation used in FISPACT-II the reaction rates and decay constants are independent of the current inventory, being determined purely by intrinsic physical properties of the nuclides and also the imposed external projectile flux is assumed not to be modified by the presence of the target material.

Each reaction or decay typically produces a single principal daughter nuclide and a few secondary products, although fission reactions are an exception. Even with fissions included, less than 3% of the matrix elements of the system matrix A in Equation (11) are non-zero. Without fissions this proportion drops to about 0.8%. This sparsity is very significant for numerical approaches to the solution.

In principle, Equation (11) can be solved in closed form for each time interval during which A is constant. Introduce a matrix S to define a similarity transformation which diagonalises A and rewrite Equation (11) as

$$\frac{d(\mathsf{SN})}{dt} = (\mathsf{SAS}^{-1})(\mathsf{SN}) \tag{83}$$

where

$$\mathsf{SAS}^{-1} = \mathrm{diag}(\mu_1, \mu_2, \ldots, \mu_n) \tag{84}$$

and μ_i are the eigenvalues of A.

Note that the probability of A having repeated eigenvalues is vanishingly small since the elements of A are derived from physical data. Hence A is diagonalisable, the matrix S exists and the additional complexity of the Jordan normal form is not required.

Then the solution is

$$\mathsf{SN}(t) = \mathrm{diag}[\exp(\mu_1 t), \exp(\mu_2 t), \ldots, \exp(\mu_n t)]\mathsf{SN}(0) \tag{85}$$

for $t \in [0, T]$, a time interval during which A is constant. The extension to piecewise-constant A can be found in the obvious way by evaluating S and the eigenvalues for each interval and concatenating intervals with a rotation of the solution vector after the endpoint of each interval.

Unfortunately, this analysis does not represent a practical method of solution because the process of calculating the eigenvalues is numerically intensive, destroys the sparsity structure of the matrix, and is subject to the possibility of extreme ill-conditioning. However, the eigenvalues are useful in identifying the properties of the matrix A, as now described.

Table 18: The largest decay rates in the EAF library.

Range of λ (s^{-1})	Nuclides
$21 \leq \log_{10}\lambda < 22$	^{5}Li, ^{11}N, ^{15}F
$20 \leq \log_{10}\lambda < 21$	^{6}Be
$19 \leq \log_{10}\lambda < 20$	^{16}F
$18 \leq \log_{10}\lambda < 19$	none
$17 \leq \log_{10}\lambda < 18$	^{9}B
$16 \leq \log_{10}\lambda < 17$	none
$15 \leq \log_{10}\lambda < 16$	^{8}Be
$10 \leq \log_{10}\lambda < 15$	none
$9 \leq \log_{10}\lambda < 10$	^{13}Be
$7 \leq \log_{10}\lambda < 9$	none
$6 \leq \log_{10}\lambda < 7$	^{212}Po, ^{213}At, ^{214}At, ^{214}Rn

A study was performed by extracting the matrix A from FISPACT-II and using it in a testbed program which did perform the eigenvalue calculation by employing the library routine `GEEVX` from the LAPACK library. A cooling step provides information on the decays in isolation, whereas an irradiation step with unit flux provides the sum of the decay-rate matrix and the cross-section matrix.

The eigenvalue analysis of the decay-rate matrix highlights the presence in the EAF library of a few nuclides with very rapid decays, as listed in Table 18.

These very large decay rates ensure that all practical FISPACT-II calculations with the full inventory for many applications are always stiff. This remark applies as much to laser fusion applications with nanosecond irradiation pulses as it does to magnetic confinement applications with irradiation times of years.

However, when subsets of the nuclides are used in pathways calculations the reduced set of equations may not be stiff.

A.14.2 The choice of solver

It can be seen from the previous section that the key characteristics of the system of inventory equations are that they are linear, stiff and sparse.

A web search reveals several suitable solvers, but it appears that only one can be obtained with built-in efficient handling of sparse systems. This is the package LSODE [17, 42, 43] written at Lawrence Livermore Laboratory.

The variant of LSODE usually used in FISPACT-II is the double-precision version with efficient handling of sparse Jacobian matrices, called DLSODES, although on some platforms the single-precision version SLSODES may provide sufficient accuracy. This software is presented as a set of Fortran 77 library routines with an interface defined by

the subroutine argument list of the top-level driver routine. The present development treats DLSODES and SLSODES as "black boxes" and no significant modifications to their internal details have been made. In the following, these two variants of the solver will be referred to collectively as 'LSODES'.

The use by the solver of the sparsity structure of the matrix describing the rate equations is very significant practically since it yields a reduction in running time by a large factor because during the calculation LSODE performs many solutions of linear systems of equations derived from the matrix, which for general matrices requires $\mathcal{O}(N^3)$ arithmetic operations.

The stiffness of the system of equations limits the choice of numerical method. LSODES uses the backward differentiation formula method, also known as Gear's method. When the equations are not stiff, other methods are feasible and LSODES uses an implicit Adams method. For simplicity of implementation, FISPACT-II always calls on LSODES to apply Gear's method; there is no easy, rapid way of determining whether or not a system of equations is stiff, so an automatic selection of method does not seem to be possible. A limited number of tests reveals that LSODES still performs well on a small non-stiff reaction network typical of a pathway calculation. The automatic error control (see Section A.14.4 below) ensures that the results of Gear's method remain accurate, although LSODES may well be more efficient, using fewer internal timesteps, if the Adams method had been used instead.

LSODES performs the solution of stiff systems of equations without recourse to the equilibrium approximation that was used in earlier versions of FISPACT. All nuclides are followed dynamically and those with a rapid transient response automatically adjust to have near-equilibrium inventories.

A.14.3 The interface to the solver

Some of the complexity of the interface to LSODES arises because of the limitations in Fortran 77 concerning fixed-size arrays which must be defined at compile time. These limitations can be overcome with the dynamic memory allocation features now available in Fortran 95. The present development provides a Fortran 95 wrapper for the old Fortran 77 code with a simplified interface and automatic circumvention of LSODES error reports caused only by inadequately-sized workspace arrays.

Most of the details concerning the operation of LSODES can be encapsulated in a way that is consistent with the object-oriented approach adopted for the present development. However, it is necessary to provide a description of the sparsity structure of the system matrix A in a specific manner tailored to the requirements of LSODES. Also, the user program needs to provide subprograms that give LSODES values of the driving function $\{F_i(\{y_j\}, t)\}$ and its Jacobian $J_{ij} = \partial F_i / \partial y_j$. The subroutine argument lists of these user-supplied routines are defined by the internal details of LSODES and cannot be changed.

LSODES was written at a time when computers had much smaller main memories than present machines and the code improves memory efficiency by overlaying floating-point and integer workspace. Correct operation of the code requires knowledge of the ratio of the sizes of the storage units for floating-point numbers and integers. The authors of LSODES expected their users to be aware of this ratio on their computing platforms and this number is hard-wired into the code (as supplied) in two places. Users had to edit the source before using the code.

FISPACT-II improves the portability of the solver by automatically determining the required ratio of floating-point to integer storage sizes, using standard Fortran 95 intrinsic functions. The argument list of the driving routine for LSODES has been extended to pass this ratio to the relevant points in the solver and the hard-wired data statements have been removed.

The precision of the floating-point computations in FISPACT-II is controlled by using a specific real kind in all declarations to achieve a floating-point precision of 15 decimal places. [5]

This approach to floating-point precision is not compatible with the Fortran 77 code of LSODES which uses default `REAL` and `DOUBLE PRECISION` declarations in the single and double-precision versions, respectively.

FISPACT-II uses Fortran 95 intrinsic functions to determine the precision provided by default `REAL` and `DOUBLE PRECISION` floating-point variables and chooses the one that provides 15 decimal places. Unusually, a platform may achieve this precision with default `REAL` and on such a platform FISPACT-II would automatically use SLSODES rather than DLSODES.

A.14.4 Error estimation and step control

The LSODES solver controls the accuracy of its calculations by refining its internal timesteps to satisfy a criterion placed on its estimate of the error. Estimates are produced separately for each component of the solution vector, but these are combined into a single measure of the error using a root-mean-square norm.

The acceptance criterion is based on the sum of relative and absolute tolerances, so that for the dominant nuclides in a FISPACT-II calculation the error is determined by the chosen `rtol` parameter, while for the minor nuclides the tolerance is relaxed by the addition of the `atol` parameter. This avoids the problems that would occur for a pure relative error estimate in the case of zero or very small inventories.

The solver returns the error estimates of the individual components of the solution vector to its calling program. This information is used in FISPACT-II to flag the

[5] This is usually double precision on byte-oriented platforms. Exceptionally, if a specific platform cannot achieve 15 decimal places of precision, FISPACT-II will not compile.

nuclides with larger than usual error estimates. The criterion for flagging outlying nuclides is that the estimate should exceed the specified tolerance by a factor of more than the dimensionless parameter `err_factor` which is set in the code to 1.5.

The solver sets an array of logical convergence flags which are used by the output module to place '?' markers in the inventory output. This provides the equivalent of the markers used in the output from FISPACT-2007.

Specifically, LSODES computes a vector

$$w_i = rtol\, y_i + atol \tag{86}$$

from the solution vector, where the parameters `rtol` and `atol` are provided by the user through the **TOLERANCE** keyword. The weights w_i are used with the local estimates of the component-wise errors, e_i to compute

$$D = \left[\frac{1}{N} \sum_{i=1}^{N} \frac{e_i}{w_i} \right]^{1/2} \tag{87}$$

D is used as a single measure of acceptability; if $D > 1$ then LSODES refines its internal timesteps until a satisfactory D is obtained.

Users should be aware that LSODES works with local errors. Estimation of the global error is much harder and in common with many numerical methods, LSODES does not attempt this error estimation. Consequently, users should set `rtol` and `atol` cautiously.

A.14.5 Runtime error reporting

FISPACT-II traps any error returns from LSODES and reports them to the user with the same error logging system used elsewhere in the code. Extensive testing of FISPACT-II demonstrates that LSODES is robust and no abnormal returns from it should be expected.

Exceptionally, the abnormal error returns that may be encountered are listed in Table 19.

A fuller explanation of the meanings of these error returns may be found in the extensive comments at the head of the source files `dlsodes.f` and `slsodes.f`.

Table 19: The abnormal error returns from LSODES.

ISTATE	Brief explanation	User action
-7	sparse solver problem (should not happen)	Report error to developers
-6	zero variable with pure relative error control	rerun with `atol` $\neq 0$
-5	repeated convergence failures (bad Jacobian?)	Report error to developers
-4	repeated error test failures (bad input?)	Report error to developers
-3	illegal input	Report error to developers
-2	requested accuracy too great	rerun with larger `rtol` and/or `atol`
-1	excessive work (too many internal steps)	rerun with larger `rtol` and/or `atol`

B EAF Library Data

FISPACT-II 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 code has been designed to use the European Activation File and this library is the recommended source of cross-section data. The following libraries are required:

- Cross-section data for projectile-induced reactions, where the projectile defaults to neutron, or may be one of the other four options given using the **PROJECTILE** keyword, and the energy group structure is one of those listed in Appendix B.1
- Uncertainty data for neutron-induced reactions
- Projectile spectrum data. These may be one of the 'standard' `fluxes` files provided with the library (see Appendix B.3), or may be a user-generated one (see page 50).
- Decay data
- Fission yield data for projectile-induced reactions, where the projectile may be neutron, deuteron or proton
- Biological hazard data
- Legal transport data
- Clearance data
- Gamma absorption data

The libraries are described in more detail below. It is a user's choice to select from the 2003, 2005, 2007 or 2010 library versions.

B.1 Cross-section Group Structure

There are nine standard group structures are used for the European Activation File and two standard group structures in the ENDF format; data in all these structures can be read into FISPACT-II.

Table 20 lists the group structures for the five original cases with upper energy limits of 20 MeV:

Name	Number of groups
WIMS	69
GAM-II	100
XMAS	172
VITAMIN-J	175
TRIPOLI	315

The method of presentation in Table 20 is designed to make clear in which energy ranges particular structures have most groups and will therefore give a good representation of the cross-sections. Each group energy displayed (in eV) is the maximum energy of the group, with the minimum being given by the upper energy of the next group. The final entries are the minimum energy of the final group.

Table 21 lists the two original high-energy structures: VITAMIN-J+ (211 groups) and TRIPOLI+ (351 groups), which are still limited to 55 MeV and below. Table 21 omits the lower-energy groups below 20 MeV which are the same as the VITAMIN-J and TRIPOLI groups.

A further four group structures have been added to provide an increased upper energy bounds of 200 MeV and 1 GeV, to allow the addition of α and γ-induced reactions and to provide for more precise modelling of reaction thresholds and the resonance ranges. These additional groups are:

Name	Number of groups
LANL	66
CCFE	162
LLNL	616
CCFE	709

The CCFE (162) structure was introduced for studies of charged-particle projectiles and γ-induced activation and transmutation. The CCFE (709) group structure is an engineered extension of the LLNL (616) structure. It has 50 tally bins per energy decade, equally spaced in the logarithm of the energy between 10^{-5} eV and 10 MeV, and thereafter bins with appropriately chosen equally-spaced boundaries in energy up to 1 GeV.

Table 20: Energy group boundaries for the five low-energy standard structures.

TRIPOLI (315)		**VITAMIN-J (175)**		**GAMM-II (100)**		**XMAS (172)**		**WIMS (69)**	
grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
1	1.9640E+7	1	1.9640E+7			1	1.9640E+7		
2	1.7330E+7	2	1.7333E+7			2	1.7333E+7		
3	1.6910E+7	3	1.6905E+7						
4	1.6490E+7	4	1.6487E+7						
5	1.5680E+7	5	1.5683E+7						
6	1.4920E+7	6	1.4918E+7	1	1.4918E+7	3	1.4918E+7		

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TRIPOLI (315)		**VITAMIN-J (175)**		**GAMM-II (100)**		**XMAS (172)**		**WIMS (69)**	
grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
7	1.4550E+7	7	1.4550E+7						
8	1.4190E+7	8	1.4191E+7						
9	1.3840E+7	9	1.3840E+7			4	1.3840E+7		
10	1.3500E+7	10	1.3499E+7	2	1.3498E+7				
11	1.2840E+7	11	1.2840E+7						
		12	1.2523E+7						
12	1.2210E+7	13	1.2214E+7	3	1.2214E+7				
13	1.1620E+7	14	1.1618E+7			5	1.1618E+7		
14	1.1050E+7	15	1.1052E+7	4	1.1052E+7				
15	1.0510E+7	16	1.0513E+7						
16	1.0000E+7	17	1.0000E+7	5	9.9998E+6	6	1.0000E+7	1	1.0000E+7
17	9.5120E+6	18	9.5123E+6						
18	9.0480E+6	19	9.0484E+6	6	9.0482E+6				
19	8.6070E+6	20	8.6071E+6						
20	8.1870E+6	21	8.1873E+6	7	8.1872E+6	7	8.1873E+6		
21	7.7880E+6	22	7.7880E+6						
22	7.4080E+6	23	7.4082E+6	8	7.4081E+6				
23	7.0470E+6	24	7.0469E+6						
24	6.7030E+6	25	6.7032E+6	9	6.7031E+6	8	6.7032E+6		
25	6.5920E+6	26	6.5924E+6						
26	6.3760E+6	27	6.3763E+6						
27	6.0650E+6	28	6.0653E+6	10	6.0652E+6	9	6.0653E+6	2	6.0660E+6
28	5.7690E+6	29	5.7695E+6						
29	5.4880E+6	30	5.4881E+6	11	5.4880E+6	10	5.4881E+6		
30	5.2200E+6	31	5.2205E+6						
31	4.9660E+6	32	4.9659E+6	12	4.9658E+6				
32	4.7240E+6	33	4.7237E+6						
33	4.4930E+6	34	4.4933E+6	13	4.4932E+6	11	4.4933E+6		
34	4.0660E+6	35	4.0657E+6	14	4.0656E+6				
35	3.6790E+6	36	3.6788E+6	15	3.6787E+6	12	3.6788E+6	3	3.6790E+6
36	3.3290E+6	37	3.3287E+6	16	3.3287E+6				
37	3.1660E+6	38	3.1664E+6						
38	3.0120E+6	39	3.0119E+6	17	3.0119E+6	13	3.0119E+6		
39	2.8650E+6	40	2.8651E+6						
40	2.7250E+6	41	2.7253E+6	18	2.7253E+6				
41	2.5920E+6	42	2.5924E+6						
42	2.4660E+6	43	2.4660E+6	19	2.4659E+6	14	2.4660E+6		
43	2.3850E+6	44	2.3851E+6						
44	2.3650E+6	45	2.3653E+6						
45	2.3460E+6	46	2.3457E+6						
46	2.3070E+6	47	2.3069E+6						
47	2.2310E+6	48	2.2313E+6	20	2.2313E+6	15	2.2313E+6	4	2.2310E+6
48	2.1220E+6	49	2.1225E+6						
49	2.0190E+6	50	2.0190E+6	21	2.0189E+6	16	2.0190E+6		
50	1.9210E+6	51	1.9205E+6						
51	1.8270E+6	52	1.8268E+6	22	1.8268E+6				
52	1.7380E+6	53	1.7377E+6						
53	1.6530E+6	54	1.6530E+6	23	1.6530E+6	17	1.6530E+6		
54	1.5720E+6	55	1.5724E+6						
55	1.4960E+6	56	1.4957E+6	24	1.4957E+6				
56	1.4230E+6	57	1.4227E+6						
57	1.3530E+6	58	1.3534E+6	25	1.3533E+6	18	1.3534E+6	5	1.3530E+6

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TRIPOLI (315)		**VITAMIN-J (175)**		**GAMM-II (100)**		**XMAS (172)**		**WIMS (69)**	
grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
58	1.2870E+6	59	1.2874E+6						
59	1.2250E+6	60	1.2246E+6	26	1.2245E+6	19	1.2246E+6		
60	1.1650E+6	61	1.1648E+6						
61	1.1080E+6	62	1.1080E+6	27	1.1080E+6	20	1.1080E+6		
62	1.0030E+6	63	1.0026E+6	28	1.0026E+6	21	1.0026E+6		
63	9.6160E+5	64	9.6167E+5						
64	9.0720E+5	65	9.0718E+5	29	9.0716E+5	22	9.0718E+5		
65	8.6290E+5	66	8.6294E+5						
66	8.2090E+5	67	8.2085E+5	30	8.2084E+5	23	8.2085E+5	6	8.2100E+5
67	7.8080E+5	68	7.8082E+5						
68	7.4270E+5	69	7.4274E+5	31	7.4272E+5				
69	7.0650E+5	70	7.0651E+5						
70	6.7210E+5	71	6.7206E+5	32	6.7204E+5				
71	6.3930E+5	72	6.3928E+5						
72	6.0810E+5	73	6.0810E+5	33	6.0809E+5	24	6.0810E+5		
73	5.7840E+5	74	5.7844E+5						
74	5.5020E+5	75	5.5023E+5	34	5.5022E+5	25	5.5023E+5	7	5.0000E+5
75	5.2340E+5	76	5.2340E+5						
		77	4.9787E+5	35	4.9786E+5	26	4.9787E+5		
76	4.5050E+5	78	4.5049E+5	36	4.5048E+5	27	4.5049E+5		
77	4.0760E+5	79	4.0762E+5	37	4.0762E+5	28	4.0762E+5		
78	3.8770E+5	80	3.8774E+5						
79	3.6880E+5	81	3.6883E+5	38	3.6883E+5				
80	3.3370E+5	82	3.3373E+5	39	3.3373E+5				
81	3.0200E+5	83	3.0197E+5	40	3.0197E+5	29	3.0197E+5	8	3.0250E+5
82	2.9850E+5	84	2.9849E+5						
83	2.9720E+5	85	2.9721E+5						
84	2.9450E+5	86	2.9452E+5						
85	2.8730E+5	87	2.8725E+5						
86	2.7320E+5	88	2.7324E+5	41	2.7323E+5	30	2.7324E+5		
87	2.4720E+5	89	2.4724E+5	42	2.4723E+5	31	2.4724E+5		
88	2.3520E+5	90	2.3518E+5						
89	2.2370E+5	91	2.2371E+5	43	2.2370E+5				
90	2.1280E+5	92	2.1280E+5						
91	2.0240E+5	93	2.0242E+5	44	2.0242E+5				
92	1.9250E+5	94	1.9255E+5						
93	1.8320E+5	95	1.8316E+5	45	1.8315E+5	32	1.8316E+5	9	1.8300E+5
94	1.7420E+5	96	1.7422E+5						
95	1.6570E+5	97	1.6573E+5	46	1.6572E+5				
96	1.5760E+5	98	1.5764E+5						
97	1.5000E+5	99	1.4996E+5	47	1.4995E+5				
98	1.4260E+5	100	1.4264E+5						
99	1.3570E+5	101	1.3569E+5	48	1.3568E+5				
100	1.2910E+5	102	1.2907E+5						
101	1.2280E+5	103	1.2277E+5	49	1.2277E+5	33	1.2277E+5		
102	1.1680E+5	104	1.1679E+5						
103	1.1110E+5	105	1.1109E+5	50	1.1109E+5	34	1.1109E+5	10	1.1100E+5
104	9.8040E+4	106	9.8037E+4						
105	8.6520E+4	107	8.6517E+4	51	8.6516E+4				
106	8.2500E+4	108	8.2503E+4						
107	8.2300E+4					35	8.2298E+4		
108	7.9500E+4	109	7.9499E+4						

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TRIPOLI (315)		**VITAMIN-J (175)**		**GAMM-II (100)**		**XMAS (172)**		**WIMS (69)**	
grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
109	7.4990E+4								
110	7.2000E+4	110	7.2025E+4						
111	6.7380E+4	111	6.7380E+4	52	6.7378E+4	36	6.7380E+4	11	6.7340E+4
112	6.1730E+4								
113	5.6560E+4	112	5.6562E+4						
114	5.5170E+4					37	5.5166E+4		
115	5.2480E+4	113	5.2475E+4	53	5.2474E+4				
116	4.9390E+4								
117	4.6310E+4	114	4.6309E+4						
118	4.3590E+4								
119	4.0870E+4	115	4.0868E+4	54	4.0867E+4	38	4.0868E+4	12	4.0850E+4
120	3.6980E+4					39	3.6979E+4		
121	3.4310E+4	116	3.4307E+4						
122	3.1830E+4	117	3.1828E+4	55	3.1827E+4				
123	3.1620E+4								
124	3.0730E+4								
125	2.9850E+4								
126	2.9010E+4					40	2.9283E+4		
127	2.8500E+4	118	2.8501E+4						
128	2.8180E+4								
129	2.7380E+4					41	2.7394E+4		
130	2.7000E+4	119	2.7000E+4						
131	2.6610E+4								
132	2.6060E+4	120	2.6058E+4						
133	2.5850E+4								
134	2.5120E+4								
135	2.4790E+4	121	2.4788E+4	56	2.4787E+4	42	2.4788E+4	13	2.4780E+4
136	2.4410E+4								
137	2.4180E+4	122	2.4176E+4						
138	2.3580E+4	123	2.3579E+4						
139	2.3040E+4								
140	2.2390E+4								
141	2.1870E+4	124	2.1875E+4						
142	2.1130E+4								
143	2.0540E+4								
144	1.9950E+4								
145	1.9310E+4	125	1.9305E+4	57	1.9304E+4				
146	1.7780E+4								
147	1.6620E+4					43	1.6616E+4		
148	1.5850E+4								
149	1.5030E+4	126	1.5034E+4	58	1.5034E+4	44	1.5034E+4	14	1.5030E+4
150	1.3830E+4								
151	1.2730E+4								
152	1.1710E+4	127	1.1709E+4	59	1.1709E+4				
153	1.1140E+4					45	1.1138E+4		
		128	1.0595E+4						
154	1.0080E+4								
155	9.1190E+3	129	9.1188E+3	60	9.1187E+3	46	9.1188E+3	15	9.1180E+3
156	8.2510E+3								
157	7.4660E+3					47	7.4659E+3		
158	7.1020E+3	130	7.1017E+3	61	7.1016E+3				
159	6.2670E+3								

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TRIPOLI (315)		**VITAMIN-J (175)**		**GAMM-II (100)**		**XMAS (172)**		**WIMS (69)**	
grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
160	5.5310E+3	131	5.5308E+3	62	5.5308E+3	48	5.5308E+3	16	5.5300E+3
161	5.0040E+3					49	5.0045E+3		
162	4.6430E+3								
163	4.3070E+3	132	4.3074E+3	63	4.3074E+3				
164	3.9810E+3								
165	3.7070E+3	133	3.7074E+3						
166	3.5480E+3					50	3.5266E+3	17	3.5190E+3
167	3.3550E+3	134	3.3546E+3	64	3.3546E+3	51	3.3546E+3		
168	3.1620E+3								
169	3.0350E+3	135	3.0354E+3						
170	2.8180E+3								
171	2.7470E+3	136	2.7465E+3						
172	2.6610E+3								
173	2.6130E+3	137	2.6126E+3	65	2.6125E+3				
174	2.4850E+3	138	2.4852E+3						
175	2.3710E+3								
176	2.2490E+3	139	2.2487E+3			52	2.2487E+3	18	2.2390E+3
177	2.1130E+3								
178	2.0350E+3	140	2.0347E+3	66	2.0347E+3	53	2.0347E+3		
179	1.7960E+3								
180	1.5850E+3	141	1.5846E+3	67	1.5846E+3				
181	1.5070E+3					54	1.5073E+3		
						55	1.4338E+3	19	1.4250E+3
182	1.3640E+3								
183	1.2340E+3	142	1.2341E+3	68	1.2341E+3	56	1.2341E+3		
184	1.1170E+3								
185	1.0100E+3					57	1.0104E+3		
186	9.6110E+2	143	9.6112E+2	69	9.6110E+2				
						58	9.1424E+2	20	9.0690E+2
187	8.4820E+2								
188	7.4850E+2	144	7.4852E+2	70	7.4851E+2	59	7.4852E+2		
189	7.0790E+2								
190	6.7730E+2					60	6.7729E+2		
191	6.3100E+2								
192	5.8300E+2	145	5.8295E+2	71	5.8294E+2				
193	5.1450E+2								
194	4.5400E+2	146	4.5400E+2	72	4.5399E+2	61	4.5400E+2		
195	3.9810E+2								
						62	3.7170E+2	21	3.6730E+2
196	3.5360E+2	147	3.5358E+2	73	3.5357E+2				
197	3.0430E+2					63	3.0433E+2		
198	2.7540E+2	148	2.7536E+2	74	2.7536E+2				
199	2.4300E+2								
200	2.1450E+2	149	2.1445E+2	75	2.1445E+2				
201	2.0400E+2					64	2.0400E+2		
202	1.7780E+2								
203	1.6700E+2	150	1.6702E+2	76	1.6701E+2				
204	1.5850E+2								
						65	1.4863E+2	22	1.4870E+2
205	1.3670E+2					66	1.3674E+2		
206	1.3010E+2	151	1.3007E+2	77	1.3007E+2				
207	1.1220E+2								

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TRIPOLI (315)		**VITAMIN-J (175)**		**GAMM-II (100)**		**XMAS (172)**		**WIMS (69)**	
grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
208	1.0130E+2	152	1.0130E+2	78	1.0130E+2				
209	9.1660E+1					67	9.1661E+1		
210	8.5280E+1								
211	7.8890E+1	153	7.8893E+1	79	7.8892E+1				
						68	7.5674E+1	23	7.5500E+1
212	7.0790E+1								
213	6.7900E+1					69	6.7904E+1		
214	6.3100E+1								
215	6.1440E+1	154	6.1442E+1	80	6.1441E+1				
216	5.5590E+1					70	5.5595E+1		
						71	5.1578E+1		
217	5.0120E+1								
						72	4.8252E+1	24	4.8050E+1
218	4.7850E+1	155	4.7851E+1	81	4.7850E+1				
219	4.5520E+1					73	4.5517E+1		
220	3.9810E+1					74	4.0169E+1		
221	3.7270E+1	156	3.7267E+1	82	3.7266E+1	75	3.7267E+1		
222	3.3890E+1					76	3.3720E+1		
223	3.0510E+1					77	3.0511E+1		
224	2.9200E+1	157	2.9023E+1	83	2.9023E+1				
225	2.7920E+1					78	2.7608E+1	25	2.7700E+1
226	2.4980E+1					79	2.4981E+1		
227	2.2600E+1	158	2.2603E+1	84	2.2603E+1	80	2.2603E+1		
228	2.0450E+1								
229	1.9030E+1					81	1.9455E+1		
230	1.7600E+1	159	1.7604E+1	85	1.7603E+1				
231	1.6740E+1								
						82	1.5928E+1	26	1.5970E+1
232	1.5230E+1								
233	1.3710E+1	160	1.3710E+1	86	1.3709E+1	83	1.3710E+1		
234	1.2590E+1								
235	1.1220E+1					84	1.1225E+1		
236	1.0680E+1	161	1.0677E+1	87	1.0677E+1				
237	1.0000E+1					85	9.9056E+0	27	9.8770E+0
238	9.1900E+0					86	9.1898E+0		
239	8.9130E+0								
240	8.3150E+0	162	8.3153E+0	88	8.3152E+0	87	8.3153E+0		
241	7.9430E+0								
242	7.5240E+0					88	7.5240E+0		
243	7.0790E+0								
244	6.4760E+0	163	6.4760E+0	89	6.4758E+0				
245	6.1600E+0					89	6.1601E+0		
246	5.6230E+0					90	5.3464E+0		
247	5.0430E+0	164	5.0435E+0	90	5.0434E+0	91	5.0435E+0		
248	4.6700E+0								
249	4.4700E+0								
250	4.1290E+0					92	4.1293E+0		
						93	4.0000E+0	28	4.0000E+0
251	3.9280E+0	165	3.9279E+0	91	3.9278E+0				
252	3.3810E+0					94	3.3808E+0		
						95	3.3000E+0	29	3.3000E+0
253	3.0590E+0	166	3.0590E+0	92	3.0590E+0				

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TRIPOLI (315)		VITAMIN-J (175)		GAMM-II (100)		XMAS (172)		WIMS (69)	
grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
254	2.7680E+0					96	2.7679E+0		
						97	2.7200E+0		
						98	2.6000E+0	30	2.6000E+0
						99	2.5500E+0		
255	2.3720E+0	167	2.3824E+0	93	2.3823E+0				
256	2.3600E+0					100	2.3600E+0		
257	2.1300E+0					101	2.1300E+0		
						102	2.1000E+0	31	2.1000E+0
258	2.0200E+0					103	2.0200E+0		
259	1.9300E+0					104	1.9300E+0		
260	1.8550E+0	168	1.8554E+0	94	1.8554E+0				
261	1.8400E+0					105	1.8400E+0		
262	1.7550E+0					106	1.7550E+0		
263	1.6700E+0					107	1.6700E+0		
264	1.5900E+0					108	1.5900E+0		
265	1.5100E+0					109	1.5000E+0	32	1.5000E+0
						110	1.4750E+0		
266	1.4450E+0	169	1.4450E+0	95	1.4450E+0	111	1.4450E+0		
267	1.4400E+0								
268	1.3700E+0					112	1.3700E+0		
						113	1.3375E+0		
269	1.3050E+0					114	1.3000E+0	33	1.3000E+0
270	1.2350E+0					115	1.2350E+0		
271	1.1700E+0					116	1.1700E+0		
						117	1.1500E+0	34	1.1500E+0
272	1.1250E+0	170	1.1254E+0	96	1.1253E+0	118	1.1254E+0	35	1.1230E+0
273	1.1100E+0					119	1.1100E+0		
						120	1.0970E+0	36	1.0970E+0
274	1.0900E+0								
275	1.0800E+0								
276	1.0700E+0					121	1.0710E+0	37	1.0710E+0
						122	1.0450E+0	38	1.0450E+0
277	1.0350E+0					123	1.0350E+0		
						124	1.0200E+0	39	1.0200E+0
278	1.0100E+0								
						125	9.9600E-1	40	9.9600E-1
279	9.8600E-1					126	9.8600E-1		
						127	9.7200E-1	41	9.7200E-1
						128	9.5000E-1	42	9.5000E-1
280	9.3000E-1					129	9.3000E-1		
						130	9.1000E-1	43	9.1000E-1
281	8.7640E-1	171	8.7643E-1	97	8.7641E-1				
282	8.6000E-1					131	8.6000E-1		
						132	8.5000E-1	44	8.5000E-1
283	7.9000E-1					133	7.9000E-1		
						134	7.8000E-1	45	7.8000E-1
284	7.0500E-1					135	7.0500E-1		
285	6.8260E-1	172	6.8256E-1	98	6.8255E-1				
286	6.2500E-1					136	6.2500E-1	46	6.2500E-1
287	5.4000E-1					137	5.4000E-1		
288	5.3160E-1	173	5.3158E-1	99	5.3157E-1				
						138	5.0000E-1	47	5.0000E-1

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TRIPOLI (315)		**VITAMIN-J (175)**		**GAMM-II (100)**		**XMAS (172)**		**WIMS (69)**	
grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
289	4.8500E-1					139	4.8500E-1		
290	4.3300E-1					140	4.3300E-1		
291	4.1400E-1	174	4.1399E-1	100	4.1399E-1				
						141	4.0000E-1	48	4.0000E-1
292	3.9100E-1					142	3.9100E-1		
293	3.5200E-1					143	3.5000E-1	49	3.5000E-1
						144	3.2000E-1	50	3.2000E-1
294	3.1450E-1					145	3.1450E-1		
						146	3.0000E-1	51	3.0000E-1
295	2.8250E-1					147	2.8000E-1	52	2.8000E-1
296	2.4800E-1					148	2.4800E-1	53	2.5000E-1
297	2.2000E-1					149	2.2000E-1	54	2.2000E-1
298	1.8900E-1					150	1.8900E-1		
						151	1.8000E-1	55	1.8000E-1
299	1.6000E-1					152	1.6000E-1		
						153	1.4000E-1	56	1.4000E-1
300	1.3400E-1					154	1.3400E-1		
301	1.1500E-1					155	1.1500E-1		
302	1.0000E-1	175	1.0000E-1			156	1.0000E-1	57	1.0000E-1
303	9.5000E-2					157	9.5000E-2		
						158	8.0000E-2	58	8.0000E-2
304	7.7000E-2					159	7.7000E-2		
						160	6.7000E-2	59	6.7000E-2
305	5.9000E-2								
						161	5.8000E-2	60	5.8000E-2
						162	5.0000E-2	61	5.0000E-2
306	4.3000E-2								
						163	4.2000E-2	62	4.2000E-2
						164	3.5000E-2	63	3.5000E-2
307	3.2380E-2								
308	3.2000E-2								
309	3.0000E-2					165	3.0000E-2	64	3.0000E-2
						166	2.5000E-2	65	2.5000E-2
310	2.0000E-2					167	2.0000E-2	66	2.0000E-2
311	1.5000E-2					168	1.5000E-2	67	1.5000E-2
312	1.0000E-2					169	1.0000E-2	68	1.0000E-2
						170	6.9000E-3		
313	5.5000E-3								
						171	5.0000E-3	69	5.0000E-3
314	3.0000E-3					172	3.0000E-3		
315	1.1000E-4								
316	1.0000E-5	176	1.0000E-5	101	1.0000E-5	173	1.0000E-5	70	1.0000E-5

Table 21: Energy group boundaries for the two 55 MeV high-energy standard structures.

TRIPOLI+ (351)		**TRIPOLI (315)**		**VITAMIN-J+ (211)**		**VITAMIN-J (175)**	
grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
1	5.5000E+7			1	5.5000E+7		
2	5.4000E+7			2	5.4000E+7		
3	5.3000E+7			3	5.3000E+7		

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

Table 22: Energy group boundaries for the LANL 66 group structure.

LANL 66 group structure							
grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
1	2.5000E+7	18	3.0200E+5	35	2.7540E+2	52	8.0000E-2
2	2.0000E+7	19	1.8320E+5	36	1.6700E+2	53	6.7000E-2
3	1.6905E+7	20	1.1110E+5	37	1.0130E+2	54	5.8000E-2
4	1.4918E+7	21	6.7380E+4	38	6.1440E+1	55	5.0000E-2
5	1.0000E+7	22	4.0870E+4	39	3.7270E+1	56	4.2000E-2
6	6.0650E+6	23	2.5540E+4	40	2.2600E+1	57	3.5000E-2

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LANL 66 group structure							
grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
7	4.9658E+6	24	1.9890E+4	41	1.3710E+1	58	3.0000E-2
8	3.6788E+6	25	1.5030E+4	42	8.3150E+0	59	2.5000E-2
9	2.8650E+6	26	9.1190E+3	43	5.0430E+0	60	2.0000E-2
10	2.2313E+6	27	5.5310E+3	44	3.0590E+0	61	1.5000E-2
11	1.7377E+6	28	3.3550E+3	45	1.8550E+0	62	1.0000E-2
12	1.3534E+6	29	2.8400E+3	46	1.1250E+0	63	5.0000E-3
13	1.1080E+6	30	2.4040E+3	47	6.8300E-1	64	2.0000E-3
14	8.2085E+5	31	2.0350E+3	48	4.1400E-1	65	1.0000E-3
15	6.3928E+5	32	1.2340E+3	49	2.5100E-1	66	5.0000E-4
16	4.9790E+5	33	7.4850E+2	50	1.5200E-1	67	1.0000E-5
17	3.8870E+5	34	4.5400E+2	51	1.0000E-1		

Table 23: Energy group boundaries for the CCFE 162 group structure.

CCFE 162 group structure							
grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
1	1.0000E+9	42	2.0000E+7	83	3.8750E+6	123	5.7500E+5
2	9.6000E+8	43	1.9000E+7	84	3.7500E+6	124	5.5000E+5
3	9.2000E+8	44	1.8000E+7	85	3.6250E+6	125	5.2500E+5
4	8.8000E+8	45	1.7000E+7	86	3.5000E+6	126	5.0000E+5
5	8.4000E+8	46	1.6000E+7	87	3.3750E+6	127	4.7500E+5
6	8.0000E+8	47	1.5000E+7	88	3.2500E+6	128	4.5000E+5
7	7.6000E+8	48	1.4000E+7	89	3.1250E+6	129	4.2500E+5
8	7.2000E+8	49	1.3000E+7	90	3.0000E+6	130	4.0000E+5
9	6.8000E+8	50	1.2000E+7	91	2.8750E+6	131	3.7500E+5
10	6.4000E+8	51	1.1000E+7	92	2.7500E+6	132	3.5000E+5
11	6.0000E+8	52	1.0000E+7	93	2.6250E+6	133	3.2500E+5
12	5.6000E+8	53	9.8000E+6	94	2.5000E+6	134	3.0000E+5
13	5.2000E+8	54	9.6000E+6	95	2.3750E+6	135	2.8000E+5
14	4.8000E+8	55	9.4000E+6	96	2.2500E+6	136	2.6000E+5
15	4.4000E+8	56	9.2000E+6	97	2.1250E+6	137	2.4000E+5
16	4.0000E+8	57	9.0000E+6	98	2.0000E+6	138	2.2000E+5
17	3.6000E+8	58	8.8000E+6	99	1.8750E+6	139	2.0000E+5
18	3.2000E+8	59	8.6000E+6	100	1.7500E+6	140	1.8000E+5
19	2.8000E+8	60	8.4000E+6	101	1.6250E+6	141	1.6000E+5
20	2.4000E+8	61	8.2000E+6	102	1.5000E+6	142	1.4000E+5
21	2.0000E+8	62	8.0000E+6	103	1.3750E+6	143	1.2000E+5
22	1.8000E+8	63	7.8000E+6	104	1.2500E+6	144	1.0000E+5
23	1.6000E+8	64	7.6000E+6	105	1.1250E+6	145	9.5000E+4
24	1.4000E+8	65	7.4000E+6	106	1.0000E+6	146	9.0000E+4
25	1.2000E+8	66	7.2000E+6	107	9.7500E+5	147	8.5000E+4
26	1.0000E+8	67	7.0000E+6	108	9.5000E+5	148	8.0000E+4
27	9.0000E+7	68	6.8000E+6	109	9.2500E+5	149	7.5000E+4
28	8.0000E+7	69	6.6000E+6	110	9.0000E+5	150	7.0000E+4
29	7.0000E+7	70	6.4000E+6	111	8.7500E+5	151	6.5000E+4
30	6.0000E+7	71	6.2000E+6	112	8.5000E+5	152	6.0000E+4
31	5.5000E+7	72	6.0000E+6	113	8.2500E+5	153	5.5000E+4
32	5.4000E+7	73	5.8000E+6	114	8.0000E+5	154	5.0000E+4
33	5.0000E+7	74	5.6000E+6	115	7.7500E+5	155	4.5000E+4
34	4.5000E+7	75	5.4000E+6	116	7.5000E+5	156	4.0000E+4
35	4.0000E+7	76	5.2000E+6	117	7.2500E+5	157	3.5000E+4

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CCFE 162 group structure							
grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
36	3.5000E+7	77	5.0000E+6	118	7.0000E+5	158	3.0000E+4
37	3.0000E+7	78	4.8000E+6	119	6.7500E+5	159	2.5000E+4
38	2.8000E+7	79	4.6000E+6	120	6.5000E+5	160	2.0000E+4
39	2.6000E+7	80	4.4000E+6	121	6.2500E+5	161	1.5000E+4
40	2.4000E+7	81	4.2000E+6	122	6.0000E+5	162	1.0000E+4
41	2.2000E+7	82	4.0000E+6				

Table 24: Energy group boundaries for the LLNL 616 group structure.

LLNL 616 group structure							
grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
1	2.0000E+7	155	1.7378E+4	309	1.4454E+1	463	1.2023E-2
2	1.9953E+7	156	1.6596E+4	310	1.3804E+1	464	1.1482E-2
3	1.9055E+7	157	1.5849E+4	311	1.3183E+1	465	1.0965E-2
4	1.8197E+7	158	1.5136E+4	312	1.2589E+1	466	1.0471E-2
5	1.7378E+7	159	1.4454E+4	313	1.2023E+1	467	1.0000E-2
6	1.6596E+7	160	1.3804E+4	314	1.1482E+1	468	9.5499E-3
7	1.5849E+7	161	1.3183E+4	315	1.0965E+1	469	9.1201E-3
8	1.5136E+7	162	1.2589E+4	316	1.0471E+1	470	8.7096E-3
9	1.4454E+7	163	1.2023E+4	317	1.0000E+1	471	8.3176E-3
10	1.3804E+7	164	1.1482E+4	318	9.5499E+0	472	7.9433E-3
11	1.3183E+7	165	1.0965E+4	319	9.1201E+0	473	7.5858E-3
12	1.2589E+7	166	1.0471E+4	320	8.7096E+0	474	7.2444E-3
13	1.2023E+7	167	1.0000E+4	321	8.3176E+0	475	6.9183E-3
14	1.1482E+7	168	9.5499E+3	322	7.9433E+0	476	6.6069E-3
15	1.0965E+7	169	9.1201E+3	323	7.5858E+0	477	6.3096E-3
16	1.0471E+7	170	8.7096E+3	324	7.2444E+0	478	6.0256E-3
17	1.0000E+7	171	8.3176E+3	325	6.9183E+0	479	5.7544E-3
18	9.5499E+6	172	7.9433E+3	326	6.6069E+0	480	5.4954E-3
19	9.1201E+6	173	7.5858E+3	327	6.3096E+0	481	5.2481E-3
20	8.7096E+6	174	7.2444E+3	328	6.0256E+0	482	5.0119E-3
21	8.3176E+6	175	6.9183E+3	329	5.7544E+0	483	4.7863E-3
22	7.9433E+6	176	6.6069E+3	330	5.4954E+0	484	4.5709E-3
23	7.5858E+6	177	6.3096E+3	331	5.2481E+0	485	4.3652E-3
24	7.2444E+6	178	6.0256E+3	332	5.0119E+0	486	4.1687E-3
25	6.9183E+6	179	5.7544E+3	333	4.7863E+0	487	3.9811E-3
26	6.6069E+6	180	5.4954E+3	334	4.5709E+0	488	3.8019E-3
27	6.3096E+6	181	5.2481E+3	335	4.3652E+0	489	3.6308E-3
28	6.0256E+6	182	5.0119E+3	336	4.1687E+0	490	3.4674E-3
29	5.7544E+6	183	4.7863E+3	337	3.9811E+0	491	3.3113E-3
30	5.4954E+6	184	4.5709E+3	338	3.8019E+0	492	3.1623E-3
31	5.2481E+6	185	4.3652E+3	339	3.6308E+0	493	3.0200E-3
32	5.0119E+6	186	4.1687E+3	340	3.4674E+0	494	2.8840E-3
33	4.7863E+6	187	3.9811E+3	341	3.3113E+0	495	2.7542E-3
34	4.5709E+6	188	3.8019E+3	342	3.1623E+0	496	2.6303E-3
35	4.3652E+6	189	3.6308E+3	343	3.0200E+0	497	2.5119E-3
36	4.1687E+6	190	3.4674E+3	344	2.8840E+0	498	2.3988E-3
37	3.9811E+6	191	3.3113E+3	345	2.7542E+0	499	2.2909E-3
38	3.8019E+6	192	3.1623E+3	346	2.6303E+0	500	2.1878E-3
39	3.6308E+6	193	3.0200E+3	347	2.5119E+0	501	2.0893E-3
40	3.4674E+6	194	2.8840E+3	348	2.3988E+0	502	1.9953E-3

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LLNL 616 group structure

grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
41	3.3113E+6	195	2.7542E+3	349	2.2909E+0	503	1.9055E-3
42	3.1623E+6	196	2.6303E+3	350	2.1878E+0	504	1.8197E-3
43	3.0200E+6	197	2.5119E+3	351	2.0893E+0	505	1.7378E-3
44	2.8840E+6	198	2.3988E+3	352	1.9953E+0	506	1.6596E-3
45	2.7542E+6	199	2.2909E+3	353	1.9055E+0	507	1.5849E-3
46	2.6303E+6	200	2.1878E+3	354	1.8197E+0	508	1.5136E-3
47	2.5119E+6	201	2.0893E+3	355	1.7378E+0	509	1.4454E-3
48	2.3988E+6	202	1.9953E+3	356	1.6596E+0	510	1.3804E-3
49	2.2909E+6	203	1.9055E+3	357	1.5849E+0	511	1.3183E-3
50	2.1878E+6	204	1.8197E+3	358	1.5136E+0	512	1.2589E-3
51	2.0893E+6	205	1.7378E+3	359	1.4454E+0	513	1.2023E-3
52	1.9953E+6	206	1.6596E+3	360	1.3804E+0	514	1.1482E-3
53	1.9055E+6	207	1.5849E+3	361	1.3183E+0	515	1.0965E-3
54	1.8197E+6	208	1.5136E+3	362	1.2589E+0	516	1.0471E-3
55	1.7378E+6	209	1.4454E+3	363	1.2023E+0	517	1.0000E-3
56	1.6596E+6	210	1.3804E+3	364	1.1482E+0	518	9.5499E-4
57	1.5849E+6	211	1.3183E+3	365	1.0965E+0	519	9.1201E-4
58	1.5136E+6	212	1.2589E+3	366	1.0471E+0	520	8.7096E-4
59	1.4454E+6	213	1.2023E+3	367	1.0000E+0	521	8.3176E-4
60	1.3804E+6	214	1.1482E+3	368	9.5499E-1	522	7.9433E-4
61	1.3183E+6	215	1.0965E+3	369	9.1201E-1	523	7.5858E-4
62	1.2589E+6	216	1.0471E+3	370	8.7096E-1	524	7.2444E-4
63	1.2023E+6	217	1.0000E+3	371	8.3176E-1	525	6.9183E-4
64	1.1482E+6	218	9.5499E+2	372	7.9433E-1	526	6.6069E-4
65	1.0965E+6	219	9.1201E+2	373	7.5858E-1	527	6.3096E-4
66	1.0471E+6	220	8.7096E+2	374	7.2444E-1	528	6.0256E-4
67	1.0000E+6	221	8.3176E+2	375	6.9183E-1	529	5.7544E-4
68	9.5499E+5	222	7.9433E+2	376	6.6069E-1	530	5.4954E-4
69	9.1201E+5	223	7.5858E+2	377	6.3096E-1	531	5.2481E-4
70	8.7096E+5	224	7.2444E+2	378	6.0256E-1	532	5.0119E-4
71	8.3176E+5	225	6.9183E+2	379	5.7544E-1	533	4.7863E-4
72	7.9433E+5	226	6.6069E+2	380	5.4954E-1	534	4.5709E-4
73	7.5858E+5	227	6.3096E+2	381	5.2481E-1	535	4.3652E-4
74	7.2444E+5	228	6.0256E+2	382	5.0119E-1	536	4.1687E-4
75	6.9183E+5	229	5.7544E+2	383	4.7863E-1	537	3.9811E-4
76	6.6069E+5	230	5.4954E+2	384	4.5709E-1	538	3.8019E-4
77	6.3096E+5	231	5.2481E+2	385	4.3652E-1	539	3.6308E-4
78	6.0256E+5	232	5.0119E+2	386	4.1687E-1	540	3.4674E-4
79	5.7544E+5	233	4.7863E+2	387	3.9811E-1	541	3.3113E-4
80	5.4954E+5	234	4.5709E+2	388	3.8019E-1	542	3.1623E-4
81	5.2481E+5	235	4.3652E+2	389	3.6308E-1	543	3.0200E-4
82	5.0119E+5	236	4.1687E+2	390	3.4674E-1	544	2.8840E-4
83	4.7863E+5	237	3.9811E+2	391	3.3113E-1	545	2.7542E-4
84	4.5709E+5	238	3.8019E+2	392	3.1623E-1	546	2.6303E-4
85	4.3652E+5	239	3.6308E+2	393	3.0200E-1	547	2.5119E-4
86	4.1687E+5	240	3.4674E+2	394	2.8840E-1	548	2.3988E-4
87	3.9811E+5	241	3.3113E+2	395	2.7542E-1	549	2.2909E-4
88	3.8019E+5	242	3.1623E+2	396	2.6303E-1	550	2.1878E-4
89	3.6308E+5	243	3.0200E+2	397	2.5119E-1	551	2.0893E-4
90	3.4674E+5	244	2.8840E+2	398	2.3988E-1	552	1.9953E-4
91	3.3113E+5	245	2.7542E+2	399	2.2909E-1	553	1.9055E-4
92	3.1623E+5	246	2.6303E+2	400	2.1878E-1	554	1.8197E-4

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LLNL 616 group structure

grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
93	3.0200E+5	247	2.5119E+2	401	2.0893E-1	555	1.7378E-4
94	2.8840E+5	248	2.3988E+2	402	1.9953E-1	556	1.6596E-4
95	2.7542E+5	249	2.2909E+2	403	1.9055E-1	557	1.5849E-4
96	2.6303E+5	250	2.1878E+2	404	1.8197E-1	558	1.5136E-4
97	2.5119E+5	251	2.0893E+2	405	1.7378E-1	559	1.4454E-4
98	2.3988E+5	252	1.9953E+2	406	1.6596E-1	560	1.3804E-4
99	2.2909E+5	253	1.9055E+2	407	1.5849E-1	561	1.3183E-4
100	2.1878E+5	254	1.8197E+2	408	1.5136E-1	562	1.2589E-4
101	2.0893E+5	255	1.7378E+2	409	1.4454E-1	563	1.2023E-4
102	1.9953E+5	256	1.6596E+2	410	1.3804E-1	564	1.1482E-4
103	1.9055E+5	257	1.5849E+2	411	1.3183E-1	565	1.0965E-4
104	1.8197E+5	258	1.5136E+2	412	1.2589E-1	566	1.0471E-4
105	1.7378E+5	259	1.4454E+2	413	1.2023E-1	567	1.0000E-4
106	1.6596E+5	260	1.3804E+2	414	1.1482E-1	568	9.5499E-5
107	1.5849E+5	261	1.3183E+2	415	1.0965E-1	569	9.1201E-5
108	1.5136E+5	262	1.2589E+2	416	1.0471E-1	570	8.7096E-5
109	1.4454E+5	263	1.2023E+2	417	1.0000E-1	571	8.3176E-5
110	1.3804E+5	264	1.1482E+2	418	9.5499E-2	572	7.9433E-5
111	1.3183E+5	265	1.0965E+2	419	9.1201E-2	573	7.5858E-5
112	1.2589E+5	266	1.0471E+2	420	8.7096E-2	574	7.2444E-5
113	1.2023E+5	267	1.0000E+2	421	8.3176E-2	575	6.9183E-5
114	1.1482E+5	268	9.5499E+1	422	7.9433E-2	576	6.6069E-5
115	1.0965E+5	269	9.1201E+1	423	7.5858E-2	577	6.3096E-5
116	1.0471E+5	270	8.7096E+1	424	7.2444E-2	578	6.0256E-5
117	1.0000E+5	271	8.3176E+1	425	6.9183E-2	579	5.7544E-5
118	9.5499E+4	272	7.9433E+1	426	6.6069E-2	580	5.4954E-5
119	9.1201E+4	273	7.5858E+1	427	6.3096E-2	581	5.2481E-5
120	8.7096E+4	274	7.2444E+1	428	6.0256E-2	582	5.0119E-5
121	8.3176E+4	275	6.9183E+1	429	5.7544E-2	583	4.7863E-5
122	7.9433E+4	276	6.6069E+1	430	5.4954E-2	584	4.5709E-5
123	7.5858E+4	277	6.3096E+1	431	5.2481E-2	585	4.3652E-5
124	7.2444E+4	278	6.0256E+1	432	5.0119E-2	586	4.1687E-5
125	6.9183E+4	279	5.7544E+1	433	4.7863E-2	587	3.9811E-5
126	6.6069E+4	280	5.4954E+1	434	4.5709E-2	588	3.8019E-5
127	6.3096E+4	281	5.2481E+1	435	4.3652E-2	589	3.6308E-5
128	6.0256E+4	282	5.0119E+1	436	4.1687E-2	590	3.4674E-5
129	5.7544E+4	283	4.7863E+1	437	3.9811E-2	591	3.3113E-5
130	5.4954E+4	284	4.5709E+1	438	3.8019E-2	592	3.1623E-5
131	5.2481E+4	285	4.3652E+1	439	3.6308E-2	593	3.0200E-5
132	5.0119E+4	286	4.1687E+1	440	3.4674E-2	594	2.8840E-5
133	4.7863E+4	287	3.9811E+1	441	3.3113E-2	595	2.7542E-5
134	4.5709E+4	288	3.8019E+1	442	3.1623E-2	596	2.6303E-5
135	4.3652E+4	289	3.6308E+1	443	3.0200E-2	597	2.5119E-5
136	4.1687E+4	290	3.4674E+1	444	2.8840E-2	598	2.3988E-5
137	3.9811E+4	291	3.3113E+1	445	2.7542E-2	599	2.2909E-5
138	3.8019E+4	292	3.1623E+1	446	2.6303E-2	600	2.1878E-5
139	3.6308E+4	293	3.0200E+1	447	2.5119E-2	601	2.0893E-5
140	3.4674E+4	294	2.8840E+1	448	2.3988E-2	602	1.9953E-5
141	3.3113E+4	295	2.7542E+1	449	2.2909E-2	603	1.9055E-5
142	3.1623E+4	296	2.6303E+1	450	2.1878E-2	604	1.8197E-5
143	3.0200E+4	297	2.5119E+1	451	2.0893E-2	605	1.7378E-5
144	2.8840E+4	298	2.3988E+1	452	1.9953E-2	606	1.6596E-5

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LLNL 616 group structure							
grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
145	2.7542E+4	299	2.2909E+1	453	1.9055E-2	607	1.5849E-5
146	2.6303E+4	300	2.1878E+1	454	1.8197E-2	608	1.5136E-5
147	2.5119E+4	301	2.0893E+1	455	1.7378E-2	609	1.4454E-5
148	2.3988E+4	302	1.9953E+1	456	1.6596E-2	610	1.3804E-5
149	2.2909E+4	303	1.9055E+1	457	1.5849E-2	611	1.3183E-5
150	2.1878E+4	304	1.8197E+1	458	1.5136E-2	612	1.2589E-5
151	2.0893E+4	305	1.7378E+1	459	1.4454E-2	613	1.2023E-5
152	1.9953E+4	306	1.6596E+1	460	1.3804E-2	614	1.1482E-5
153	1.9055E+4	307	1.5849E+1	461	1.3183E-2	615	1.0965E-5
154	1.8197E+4	308	1.5136E+1	462	1.2589E-2	616	1.0471E-5
						617	1.0000E-5

Table 25: Energy group boundaries for the CCFE 709 group structure.

CCFE 709 group structure							
grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
1	1.0000E+9	179	4.1687E+5	357	1.1482E+2	535	3.1623E-2
2	9.6000E+8	180	3.9811E+5	358	1.0965E+2	536	3.0200E-2
3	9.2000E+8	181	3.8019E+5	359	1.0471E+2	537	2.8840E-2
4	8.8000E+8	182	3.6308E+5	360	1.0000E+2	538	2.7542E-2
5	8.4000E+8	183	3.4674E+5	361	9.5499E+1	539	2.6303E-2
6	8.0000E+8	184	3.3113E+5	362	9.1201E+1	540	2.5119E-2
7	7.6000E+8	185	3.1623E+5	363	8.7096E+1	541	2.3988E-2
8	7.2000E+8	186	3.0200E+5	364	8.3176E+1	542	2.2909E-2
9	6.8000E+8	187	2.8840E+5	365	7.9433E+1	543	2.1878E-2
10	6.4000E+8	188	2.7542E+5	366	7.5858E+1	544	2.0893E-2
11	6.0000E+8	189	2.6303E+5	367	7.2444E+1	545	1.9953E-2
12	5.6000E+8	190	2.5119E+5	368	6.9183E+1	546	1.9055E-2
13	5.2000E+8	191	2.3988E+5	369	6.6069E+1	547	1.8197E-2
14	4.8000E+8	192	2.2909E+5	370	6.3096E+1	548	1.7378E-2
15	4.4000E+8	193	2.1878E+5	371	6.0256E+1	549	1.6596E-2
16	4.0000E+8	194	2.0893E+5	372	5.7544E+1	550	1.5849E-2
17	3.6000E+8	195	1.9953E+5	373	5.4954E+1	551	1.5136E-2
18	3.2000E+8	196	1.9055E+5	374	5.2481E+1	552	1.4454E-2
19	2.8000E+8	197	1.8197E+5	375	5.0119E+1	553	1.3804E-2
20	2.4000E+8	198	1.7378E+5	376	4.7863E+1	554	1.3183E-2
21	2.0000E+8	199	1.6596E+5	377	4.5709E+1	555	1.2589E-2
22	1.8000E+8	200	1.5849E+5	378	4.3652E+1	556	1.2023E-2
23	1.6000E+8	201	1.5136E+5	379	4.1687E+1	557	1.1482E-2
24	1.5000E+8	202	1.4454E+5	380	3.9811E+1	558	1.0965E-2
25	1.4000E+8	203	1.3804E+5	381	3.8019E+1	559	1.0471E-2
26	1.3000E+8	204	1.3183E+5	382	3.6308E+1	560	1.0000E-2
27	1.2000E+8	205	1.2589E+5	383	3.4674E+1	561	9.5499E-3
28	1.1000E+8	206	1.2023E+5	384	3.3113E+1	562	9.1201E-3
29	1.0000E+8	207	1.1482E+5	385	3.1623E+1	563	8.7096E-3
30	9.0000E+7	208	1.0965E+5	386	3.0200E+1	564	8.3176E-3
31	8.0000E+7	209	1.0471E+5	387	2.8840E+1	565	7.9433E-3
32	7.5000E+7	210	1.0000E+5	388	2.7542E+1	566	7.5858E-3
33	7.0000E+7	211	9.5499E+4	389	2.6303E+1	567	7.2444E-3
34	6.5000E+7	212	9.1201E+4	390	2.5119E+1	568	6.9183E-3
35	6.0000E+7	213	8.7096E+4	391	2.3988E+1	569	6.6069E-3

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CCFE 709 group structure

grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
36	5.8000E+7	214	8.3176E+4	392	2.2909E+1	570	6.3096E-3
37	5.6000E+7	215	7.9433E+4	393	2.1878E+1	571	6.0256E-3
38	5.4000E+7	216	7.5858E+4	394	2.0893E+1	572	5.7544E-3
39	5.2000E+7	217	7.2444E+4	395	1.9953E+1	573	5.4954E-3
40	5.0000E+7	218	6.9183E+4	396	1.9055E+1	574	5.2481E-3
41	4.8000E+7	219	6.6069E+4	397	1.8197E+1	575	5.0119E-3
42	4.6000E+7	220	6.3096E+4	398	1.7378E+1	576	4.7863E-3
43	4.4000E+7	221	6.0256E+4	399	1.6596E+1	577	4.5709E-3
44	4.2000E+7	222	5.7544E+4	400	1.5849E+1	578	4.3652E-3
45	4.0000E+7	223	5.4954E+4	401	1.5136E+1	579	4.1687E-3
46	3.8000E+7	224	5.2481E+4	402	1.4454E+1	580	3.9811E-3
47	3.6000E+7	225	5.0119E+4	403	1.3804E+1	581	3.8019E-3
48	3.4000E+7	226	4.7863E+4	404	1.3183E+1	582	3.6308E-3
49	3.2000E+7	227	4.5709E+4	405	1.2589E+1	583	3.4674E-3
50	3.0000E+7	228	4.3652E+4	406	1.2023E+1	584	3.3113E-3
51	2.9000E+7	229	4.1687E+4	407	1.1482E+1	585	3.1623E-3
52	2.8000E+7	230	3.9811E+4	408	1.0965E+1	586	3.0200E-3
53	2.7000E+7	231	3.8019E+4	409	1.0471E+1	587	2.8840E-3
54	2.6000E+7	232	3.6308E+4	410	1.0000E+1	588	2.7542E-3
55	2.5000E+7	233	3.4674E+4	411	9.5499E+0	589	2.6303E-3
56	2.4000E+7	234	3.3113E+4	412	9.1201E+0	590	2.5119E-3
57	2.3000E+7	235	3.1623E+4	413	8.7096E+0	591	2.3988E-3
58	2.2000E+7	236	3.0200E+4	414	8.3176E+0	592	2.2909E-3
59	2.1000E+7	237	2.8840E+4	415	7.9433E+0	593	2.1878E-3
60	2.0000E+7	238	2.7542E+4	416	7.5858E+0	594	2.0893E-3
61	1.9800E+7	239	2.6303E+4	417	7.2444E+0	595	1.9953E-3
62	1.9600E+7	240	2.5119E+4	418	6.9183E+0	596	1.9055E-3
63	1.9400E+7	241	2.3988E+4	419	6.6069E+0	597	1.8197E-3
64	1.9200E+7	242	2.2909E+4	420	6.3096E+0	598	1.7378E-3
65	1.9000E+7	243	2.1878E+4	421	6.0256E+0	599	1.6596E-3
66	1.8800E+7	244	2.0893E+4	422	5.7544E+0	600	1.5849E-3
67	1.8600E+7	245	1.9953E+4	423	5.4954E+0	601	1.5136E-3
68	1.8400E+7	246	1.9055E+4	424	5.2481E+0	602	1.4454E-3
69	1.8200E+7	247	1.8197E+4	425	5.0119E+0	603	1.3804E-3
70	1.8000E+7	248	1.7378E+4	426	4.7863E+0	604	1.3183E-3
71	1.7800E+7	249	1.6596E+4	427	4.5709E+0	605	1.2589E-3
72	1.7600E+7	250	1.5849E+4	428	4.3652E+0	606	1.2023E-3
73	1.7400E+7	251	1.5136E+4	429	4.1687E+0	607	1.1482E-3
74	1.7200E+7	252	1.4454E+4	430	3.9811E+0	608	1.0965E-3
75	1.7000E+7	253	1.3804E+4	431	3.8019E+0	609	1.0471E-3
76	1.6800E+7	254	1.3183E+4	432	3.6308E+0	610	1.0000E-3
77	1.6600E+7	255	1.2589E+4	433	3.4674E+0	611	9.5499E-4
78	1.6400E+7	256	1.2023E+4	434	3.3113E+0	612	9.1201E-4
79	1.6200E+7	257	1.1482E+4	435	3.1623E+0	613	8.7096E-4
80	1.6000E+7	258	1.0965E+4	436	3.0200E+0	614	8.3176E-4
81	1.5800E+7	259	1.0471E+4	437	2.8840E+0	615	7.9433E-4
82	1.5600E+7	260	1.0000E+4	438	2.7542E+0	616	7.5858E-4
83	1.5400E+7	261	9.5499E+3	439	2.6303E+0	617	7.2444E-4
84	1.5200E+7	262	9.1201E+3	440	2.5119E+0	618	6.9183E-4
85	1.5000E+7	263	8.7096E+3	441	2.3988E+0	619	6.6069E-4
86	1.4800E+7	264	8.3176E+3	442	2.2909E+0	620	6.3096E-4
87	1.4600E+7	265	7.9433E+3	443	2.1878E+0	621	6.0256E-4

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CCFE 709 group structure

grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
88	1.4400E+7	266	7.5858E+3	444	2.0893E+0	622	5.7544E-4
89	1.4200E+7	267	7.2444E+3	445	1.9953E+0	623	5.4954E-4
90	1.4000E+7	268	6.9183E+3	446	1.9055E+0	624	5.2481E-4
91	1.3800E+7	269	6.6069E+3	447	1.8197E+0	625	5.0119E-4
92	1.3600E+7	270	6.3096E+3	448	1.7378E+0	626	4.7863E-4
93	1.3400E+7	271	6.0256E+3	449	1.6596E+0	627	4.5709E-4
94	1.3200E+7	272	5.7544E+3	450	1.5849E+0	628	4.3652E-4
95	1.3000E+7	273	5.4954E+3	451	1.5136E+0	629	4.1687E-4
96	1.2800E+7	274	5.2481E+3	452	1.4454E+0	630	3.9811E-4
97	1.2600E+7	275	5.0119E+3	453	1.3804E+0	631	3.8019E-4
98	1.2400E+7	276	4.7863E+3	454	1.3183E+0	632	3.6308E-4
99	1.2200E+7	277	4.5709E+3	455	1.2589E+0	633	3.4674E-4
100	1.2000E+7	278	4.3652E+3	456	1.2023E+0	634	3.3113E-4
101	1.1800E+7	279	4.1687E+3	457	1.1482E+0	635	3.1623E-4
102	1.1600E+7	280	3.9811E+3	458	1.0965E+0	636	3.0200E-4
103	1.1400E+7	281	3.8019E+3	459	1.0471E+0	637	2.8840E-4
104	1.1200E+7	282	3.6308E+3	460	1.0000E+0	638	2.7542E-4
105	1.1000E+7	283	3.4674E+3	461	9.5499E-1	639	2.6303E-4
106	1.0800E+7	284	3.3113E+3	462	9.1201E-1	640	2.5119E-4
107	1.0600E+7	285	3.1623E+3	463	8.7096E-1	641	2.3988E-4
108	1.0400E+7	286	3.0200E+3	464	8.3176E-1	642	2.2909E-4
109	1.0200E+7	287	2.8840E+3	465	7.9433E-1	643	2.1878E-4
110	1.0000E+7	288	2.7542E+3	466	7.5858E-1	644	2.0893E-4
111	9.5499E+6	289	2.6303E+3	467	7.2444E-1	645	1.9953E-4
112	9.1201E+6	290	2.5119E+3	468	6.9183E-1	646	1.9055E-4
113	8.7096E+6	291	2.3988E+3	469	6.6069E-1	647	1.8197E-4
114	8.3176E+6	292	2.2909E+3	470	6.3096E-1	648	1.7378E-4
115	7.9433E+6	293	2.1878E+3	471	6.0256E-1	649	1.6596E-4
116	7.5858E+6	294	2.0893E+3	472	5.7544E-1	650	1.5849E-4
117	7.2444E+6	295	1.9953E+3	473	5.4954E-1	651	1.5136E-4
118	6.9183E+6	296	1.9055E+3	474	5.2481E-1	652	1.4454E-4
119	6.6069E+6	297	1.8197E+3	475	5.0119E-1	653	1.3804E-4
120	6.3096E+6	298	1.7378E+3	476	4.7863E-1	654	1.3183E-4
121	6.0256E+6	299	1.6596E+3	477	4.5709E-1	655	1.2589E-4
122	5.7544E+6	300	1.5849E+3	478	4.3652E-1	656	1.2023E-4
123	5.4954E+6	301	1.5136E+3	479	4.1687E-1	657	1.1482E-4
124	5.2481E+6	302	1.4454E+3	480	3.9811E-1	658	1.0965E-4
125	5.0119E+6	303	1.3804E+3	481	3.8019E-1	659	1.0471E-4
126	4.7863E+6	304	1.3183E+3	482	3.6308E-1	660	1.0000E-4
127	4.5709E+6	305	1.2589E+3	483	3.4674E-1	661	9.5499E-5
128	4.3652E+6	306	1.2023E+3	484	3.3113E-1	662	9.1201E-5
129	4.1687E+6	307	1.1482E+3	485	3.1623E-1	663	8.7096E-5
130	3.9811E+6	308	1.0965E+3	486	3.0200E-1	664	8.3176E-5
131	3.8019E+6	309	1.0471E+3	487	2.8840E-1	665	7.9433E-5
132	3.6308E+6	310	1.0000E+3	488	2.7542E-1	666	7.5858E-5
133	3.4674E+6	311	9.5499E+2	489	2.6303E-1	667	7.2444E-5
134	3.3113E+6	312	9.1201E+2	490	2.5119E-1	668	6.9183E-5
135	3.1623E+6	313	8.7096E+2	491	2.3988E-1	669	6.6069E-5
136	3.0200E+6	314	8.3176E+2	492	2.2909E-1	670	6.3096E-5
137	2.8840E+6	315	7.9433E+2	493	2.1878E-1	671	6.0256E-5
138	2.7542E+6	316	7.5858E+2	494	2.0893E-1	672	5.7544E-5
139	2.6303E+6	317	7.2444E+2	495	1.9953E-1	673	5.4954E-5

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CCFE 709 group structure

grp	energy(eV)	grp	energy(eV)	grp	energy(eV)	grp	energy(eV)
140	2.5119E+6	318	6.9183E+2	496	1.9055E-1	674	5.2481E-5
141	2.3988E+6	319	6.6069E+2	497	1.8197E-1	675	5.0119E-5
142	2.2909E+6	320	6.3096E+2	498	1.7378E-1	676	4.7863E-5
143	2.1878E+6	321	6.0256E+2	499	1.6596E-1	677	4.5709E-5
144	2.0893E+6	322	5.7544E+2	500	1.5849E-1	678	4.3652E-5
145	1.9953E+6	323	5.4954E+2	501	1.5136E-1	679	4.1687E-5
146	1.9055E+6	324	5.2481E+2	502	1.4454E-1	680	3.9811E-5
147	1.8197E+6	325	5.0119E+2	503	1.3804E-1	681	3.8019E-5
148	1.7378E+6	326	4.7863E+2	504	1.3183E-1	682	3.6308E-5
149	1.6596E+6	327	4.5709E+2	505	1.2589E-1	683	3.4674E-5
150	1.5849E+6	328	4.3652E+2	506	1.2023E-1	684	3.3113E-5
151	1.5136E+6	329	4.1687E+2	507	1.1482E-1	685	3.1623E-5
152	1.4454E+6	330	3.9811E+2	508	1.0965E-1	686	3.0200E-5
153	1.3804E+6	331	3.8019E+2	509	1.0471E-1	687	2.8840E-5
154	1.3183E+6	332	3.6308E+2	510	1.0000E-1	688	2.7542E-5
155	1.2589E+6	333	3.4674E+2	511	9.5499E-2	689	2.6303E-5
156	1.2023E+6	334	3.3113E+2	512	9.1201E-2	690	2.5119E-5
157	1.1482E+6	335	3.1623E+2	513	8.7096E-2	691	2.3988E-5
158	1.0965E+6	336	3.0200E+2	514	8.3176E-2	692	2.2909E-5
159	1.0471E+6	337	2.8840E+2	515	7.9433E-2	693	2.1878E-5
160	1.0000E+6	338	2.7542E+2	516	7.5858E-2	694	2.0893E-5
161	9.5499E+5	339	2.6303E+2	517	7.2444E-2	695	1.9953E-5
162	9.1201E+5	340	2.5119E+2	518	6.9183E-2	696	1.9055E-5
163	8.7096E+5	341	2.3988E+2	519	6.6069E-2	697	1.8197E-5
164	8.3176E+5	342	2.2909E+2	520	6.3096E-2	698	1.7378E-5
165	7.9433E+5	343	2.1878E+2	521	6.0256E-2	699	1.6596E-5
166	7.5858E+5	344	2.0893E+2	522	5.7544E-2	700	1.5849E-5
167	7.2444E+5	345	1.9953E+2	523	5.4954E-2	701	1.5136E-5
168	6.9183E+5	346	1.9055E+2	524	5.2481E-2	702	1.4454E-5
169	6.6069E+5	347	1.8197E+2	525	5.0119E-2	703	1.3804E-5
170	6.3096E+5	348	1.7378E+2	526	4.7863E-2	704	1.3183E-5
171	6.0256E+5	349	1.6596E+2	527	4.5709E-2	705	1.2589E-5
172	5.7544E+5	350	1.5849E+2	528	4.3652E-2	706	1.2023E-5
173	5.4954E+5	351	1.5136E+2	529	4.1687E-2	707	1.1482E-5
174	5.2481E+5	352	1.4454E+2	530	3.9811E-2	708	1.0965E-5
175	5.0119E+5	353	1.3804E+2	531	3.8019E-2	709	1.0471E-5
176	4.7863E+5	354	1.3183E+2	532	3.6308E-2		
177	4.5709E+5	355	1.2589E+2	533	3.4674E-2		
178	4.3652E+5	356	1.2023E+2	534	3.3113E-2		

B.1.1 Weighting spectra

Different micro-flux weighting spectra are used depending upon which group structure is required and for which application the calculation needs to be performed. The weighting spectra are usually generated at a temperature of 294 K, however higher temperatures, 574 K and 824 K have also been prepared.

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 spectrum
1.0×10^{-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)

It is important not to have any fusion peak in order not to bias the high-threshold reactions such as (n, Xn). One may also keep in mind that the fission spectrum has a tail that extends well above 10 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 spectrum
1.0×10^{-5} – 0.414 eV	Maxwellian ($T = 0.0253$ eV)
0.414 eV – 12.52 MeV	$1/E$
12.52 MeV – 15.68 MeV	Velocity exponential fusion peak ($E_f = 14.07$ MeV, $kT_f = 0.025$ MeV)
15.68 MeV – 19.64 MeV	$1/E$

A flat weighting spectrum is used to generate multi-purpose libraries from EAF point-wise data in the various group formats, and in these cases the finer the structure the better. Such libraries could be used to model cases where the neutron field is not similar to one described above, 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-transmutation calculations that will be made. The micro-flux weighting process can have a significant impact on the cross-sections.

B.2 Cross-section Data

This section gives a brief summary of the cross-section libraries. For more information, see References [8, 9, 11].

B.2.1 Groupwise neutron induced: eaf_n_gxs

Many group cross-section libraries in EAF format are available for the neutron-induced library that can be used as input to FISPACT-II. The group boundaries of the LANL (66), WIMS (69), GAM-II (100), CCFE (142), XMAS (172), VITAMIN-J (175), VITAMIN-J+ (211), TRIPOLI (315), TRIPOLI+ (351), LLNL (616) and CCFE (709) formats are listed in Appendix B.1, where details of the micro-flux weighting spectra are also given. Note that three choices of weighting spectra are available for the most general formats. This is necessary because of the very different neutron spectra found in pure

fission or fusion applications; in addition a flat-weighting library is available for the other applications. The group boundaries of the LANL (66), WIMS (69), XMAS (172) and TRIPOLI (315) structures are appropriate for fission applications. The group boundaries of the GAM-II (100), VITAMIN-J (175) and TRIPOLI (315) structures are appropriate for fusion applications. The VITAMIN-J+ (211) and TRIPOLI+ (351) group structures cater for applications where the neutron flux may extend to 55 MeV. The LLNL (616), up to 20 MeV, and CCFE (709), up to 1 GeV, group structures cover all applications and energy ranges. The CCFE (162) group structure caters for all the charged particle (deuteron, proton, alpha) and gamma libraries up to 1 GeV.

B.2.2 Probability tables

The LLNL (616) and CCFE (709) neutron-induced cross-section libraries are also provided with a set of probability tables that cover the resolved and unresolved resonance ranges of any evaluations that contain a resonance parameters file. The CALENDF-2010 [14] code provides those probability tables in the energy range from 0.1 eV up to the end of the unresolved resonance range.

B.2.3 Groupwise deuteron induced: eaf_d_gxs

The deuteron-induced cross-section library is available in two group structures that can be used as input to FISPACT-II. These are the VITAMIN-J+ (211) and CCFE (142) formats, the group boundaries of which are listed in Tables 21 and 23. Only flat-weighting libraries are available, which are suitable for most applications.

B.2.4 Groupwise proton induced: eaf_p_gxs

The proton-induced cross-section library is available in two group structures that can be used as input to FISPACT-II. These are the VITAMIN-J+ (211) and CCFE (142) formats, the group boundaries of which are listed in Tables 21 and 23. Only flat-weighting libraries are available, which are suitable for most applications.

B.2.5 Uncertainty: eaf_un

A unique feature among activation libraries is the inclusion of an uncertainty file, `eaf_un`, containing data for all neutron-induced cross-sections. Reference [44] describes the uncertainty data for EAF 3.1 while reference [12] describes the modifications made for EAF-2010. The uncertainty data are greatly simplified but complete; no covariance information is provided. However the file enables FISPACT-II to give broad-brush estimates of uncertainties.

B.3 Neutron Flux Sample Data

The collapsed cross-sections depend strongly on the nature of the projectile spectra, and so it is important to use the appropriate spectrum together with the appropriately-weighted cross-section data.

The majority of neutron-application spectra stem from light-water assemblies, mock-ups or reactors where the integral responses are strongly, if not solely, influenced by the energy ranges of the fission spectra and thermal maxwellian. Fusion spectra that have been obtained from magnetic confinement (MCF) or inertial confinement fusion (ICF) present typical D-D 2.5 MeV, or D-T 14 MeV peaks sometimes accompanied by a higher-energy tail, but also showing rather different slowing-down profiles. Accelerator-driven beam spectra are important in their role in nuclear data acquisition and materials research, but also for medical therapeutic and diagnostic applications.

In essence the particle spectrum profile, through the collapsing process, emphasises the energy region of most importance for each application. Transferring data from one application or energy range to another should be done with great care as it can easily lead to misleading and inappropriate numerical results.

Illustrations of typical spectral profiles are given in Figures 10–12, which show plots of the neutron fluxes for the following assemblies:

1. Magnetic confinement fusion, EEF study (Figure 10(a))
2. Light water reactor, Paluel (Figure 10(b))
3. Fast breeder reactor, Phénix (Figure 10(c))
4. Fast breeder reactor, Superphénix (Figure 10(d))
5. Inertial confinement fusion, NIF ignited (Figure 10(e))
6. Californium-252 fission (Figure 10(f))
7. International Criticality Safety Benchmark Experiment, Bigten (Figure 11(a))
8. JAEA Fusion Neutron Source D-T (Figure 11(b))
9. ENEA Frascati Neutron Generator D-T (Figure 11(c))
10. TU Dresden D-T (Figure 11(d))
11. IFMIF D-Li (Figure 11(e))
12. CERN H4IRRAD (Figure 11(f))
13. Magnetic confinement fusion, ITER D-T (Figure 12(a))
14. Magnetic confinement fusion, ITER D-D (Figure 12(b))

It is clear that in each of these typical spectra the integral responses are most influenced by the energy region where the profile peaks. However it is important not to overlook the upper or lower tails. For instance, there is more neutron flux above 15 MeV in a fission environment, due to the high-energy tail of the fission spectrum, than in a pure MCF D-T fusion-only environment.

B.4 Decay Data: eaf_dec

In addition to cross-sections the other basic quantities required by an inventory code are data 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-II is able to read the data directly in ENDF-6 format; it requires no pre-processing to be done, although file debugging has always been found necessary. `eaf_dec_20100` is based primarily on the JEFF-3.1.1 [39] and JEFF-2.2 [45] radioactive decay data libraries, with additional data from the most recent UK evaluations. However, not all of the 2233 nuclides that are needed are included in such sources. For these nuclides data are taken from sources such as Brown and Firestone [46] and ENDF-6 format files have been constructed. Reference [12] documents the `eaf_dec_20100` 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 usually have no impact on activation calculations and most of these have been ignored.

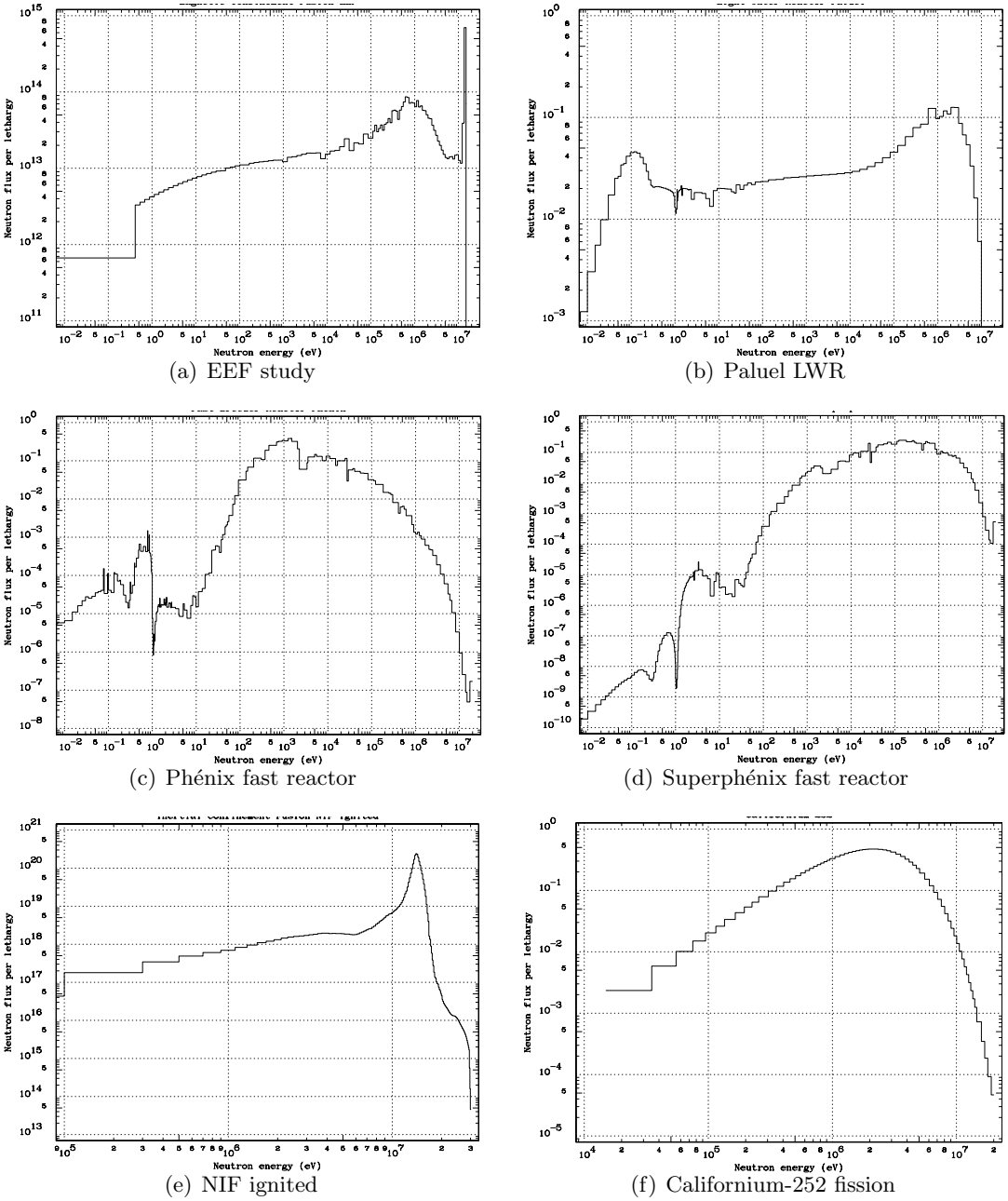
B.5 Fission Yield Data

B.5.1 Neutron: eaf_n_fis and eaf_n_asscfy

FISPACT-II requires fission yield data if actinides are included in the input materials. `eaf_n_fis` is taken completely from the JEFF-3.1.1 [39] fission yield library and FISPACT-II reads the file in ENDF-6 format with no pre-processing. Only 19 of the 102 nuclides in `eaf_n_xs` which have fission cross-sections have any fission yield data in JEFF-3.1.1 at relevant energies. For the remainder a neighbouring fission yield is used. For the EAF-2010 library, the file `eaf_n_asscfy_20100` connected to the stream `asscfy` contains these associations.

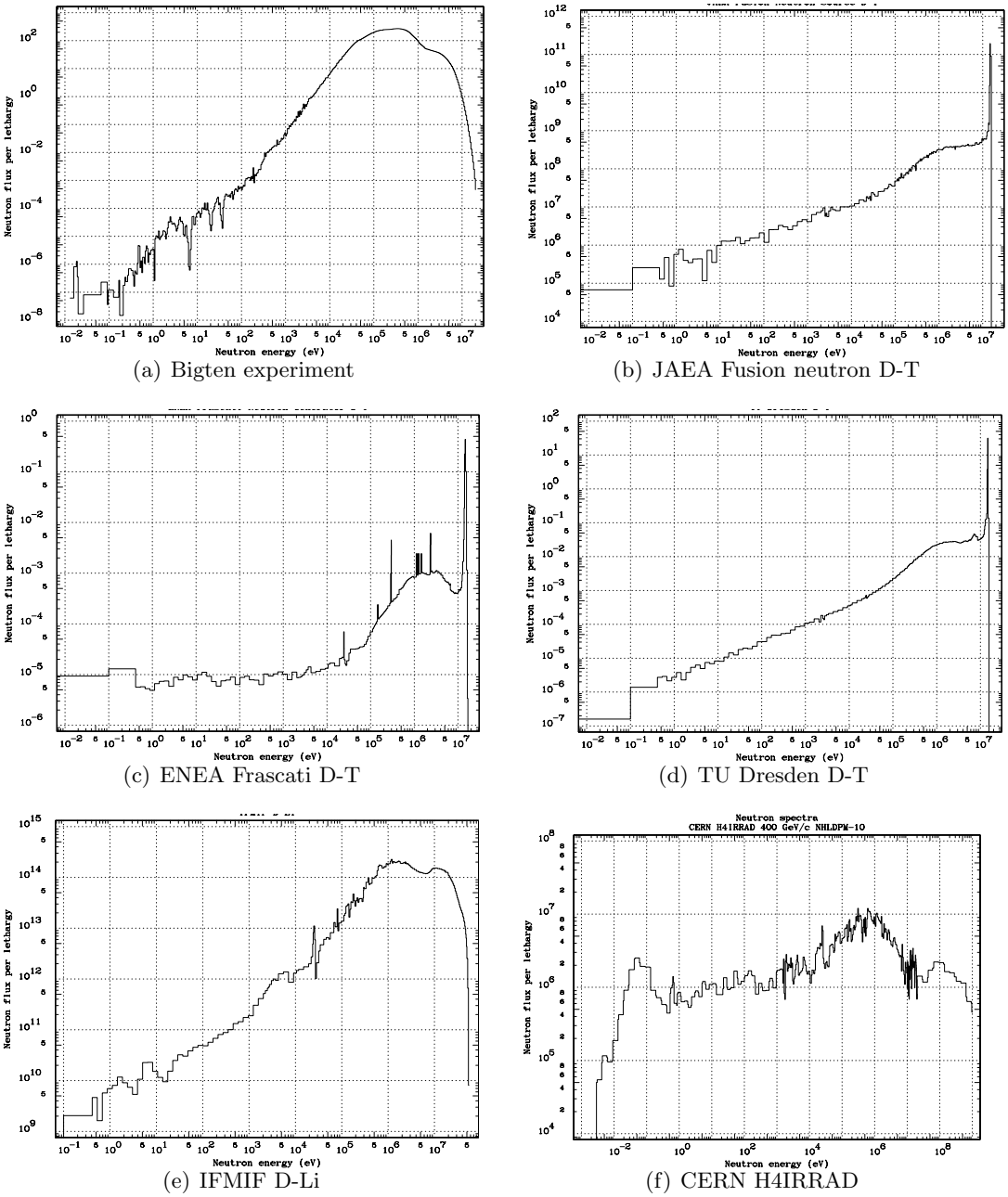
B.5.2 Deuteron: eaf_d_fis and eaf_d_asscfy

`eaf_d_fis` is taken completely from the UKFY-4.0 fission yield library [47] and FISPACT-II reads the file in ENDF-6 format with no pre-processing. Only 19 of the 90 nuclides



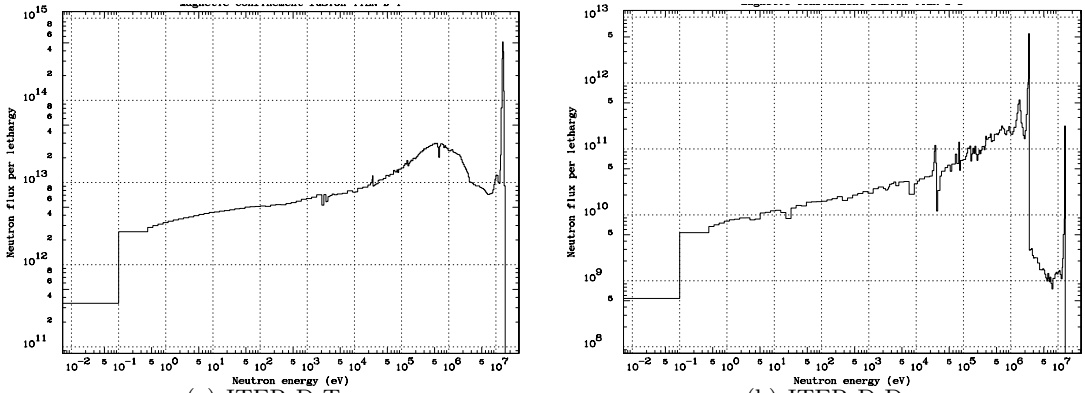
(a) EEF study
(b) Paluel LWR
(c) Phénix fast reactor
(d) Superphénix fast reactor
(e) NIF ignited
(f) Californium-252 fission

Figure 10: Sample neutron spectra.



(a) Bigten experiment
(b) JAEA Fusion neutron D-T
(c) ENEA Frascati D-T
(d) TU Dresden D-T
(e) IFMIF D-Li
(f) CERN H4IRRAD

Figure 11: Sample neutron spectra.



(a) ITER D-T (b) ITER D-D

Figure 12: Magnetic confinement fusion neutron spectra.

in `eaf_d_xs` which have fission cross-sections have any fission yield data in UKFY-4.0 at relevant energies. For the remainder a neighbouring fission yield is used. For the EAF-2010 library, the file `eaf_d_asscfy_20100` connected to the stream `asscfy` contains these associations.

B.5.3 Proton: eaf_p_fis and eaf_p_asscfy

`eaf_p_fis` is taken completely from the UKFY-4.0 fission yield library and FISPACT-II reads the file in ENDF/B-VI format with no pre-processing. Only 19 of the 90 nuclides in `eaf_p_xs` which have fission cross-sections have any fission yield data in UKFY-4.0 at relevant energies. For the remainder a neighbouring fission yield is used. For the EAF-2010 library, the file `eaf_p_asscfy_20100` connected to the stream `asscfy` contains these associations.

B.6 Radiological Data

B.6.1 Biological hazard index: eaf_haz

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-II 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 the ICRP [48, 49] and the NRPB [50, 51]. 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 the EAF decay library it has been necessary to use an approximate method. Reference [52] 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 1209 nuclides have had data calculated approximately. References [13, 25] document the `eaf_haz` library.

B.6.2 Legal transport index: eaf_a2

Transport of radioactive material from place to place is governed by regulations set up by the IAEA. Reference [53] gives details of A2 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 [25] used for all radionuclides not explicitly listed. References [13, 25] document the `eaf_a2` libraries. FISPACT-II can use these data to show the A2 limit for individual nuclides and the effective A2 value for the irradiated material.

B.6.3 Clearance index: eaf_clear

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 are being investigated by the IAEA and recommendations are available. Reference [54] gives details of suggested clearance values for certain radionuclides, while an earlier report (reference [55]) 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. References [13, 25] document the `eaf_clear` libraries. FISPACT-II can use these data to show the clearance index for individual nuclides and for the irradiated material.

B.7 Absorption Data: eaf_abs

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 Technology [56] The database 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-II γ group structure. The present compilation follows that used in FISPACT-2007, and is an extension of the calculations of Seltzer [57]. It replaces the values given in Hubble [58] which were used in earlier 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:

$$\sigma_{tot} = \sigma_{pe} + \sigma_{coh} + \sigma_{incoh} + \sigma_{pair} + \sigma_{trip} + \sigma_{phn} \tag{88}$$

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 `eaf_abs` file 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 shown in Table 6 on page 68.

C TENDL Library Data

FISPACT-II requires connection to several nuclear data libraries and forms before it can be used to calculate inventories. While any libraries in the correct ENDF-6 format could be used (c.f, Appendices D-F below) , the development of FISPACT-II over the last few years has run in parallel with the development of the TALYS-based Evaluated Nuclear Data Library TENDL project and those European libraries are the recommended source of cross section data forms. Together FISPACT-II and TENDL's nuclear data forms make up the European Activation System-II (EASY-II) that is a complete package tailored for all application needs: nuclear fission and fusion, nuclear fuel cycle, accelerator physics, isotope production, material characterisation, storage and life cycle, earth exploration, astrophysics, homeland security and more. The following data libraries are required:

1. Cross section data for neutron, proton, deuteron, alpha and gamma-induced reactions;
2. Fission yields data for neutron, proton, deuteron, alpha and gamma-induced reactions;
3. Variance-covariance data for neutron-induced reactions;
4. Probability tables data for neutron-induced reactions in the resonance energy ranges;
5. Decay data;
6. Radiological data:
   - Biological hazard data;
   - Legal transport data;
   - Clearance data.

To streamline, simplify and control any feature of all the nuclear data assimilation processes, the code development philosophy has been to follow in all aspects as much as possible the format described in the ENDF-6 format manual [16]. Three processing codes are used in sequence and in parallel to produce, process, check, and compare the nuclear data forms: NJOY12-021, PREPRO-2013 and CALENDF-2010. All the processing steps cannot be handled by only one or even two of those unique processing codes, a combination of the three is needed to extract the data forms that are the most useful in all applications. A schematic of the processing sequences is shown in Figure 13.

Further details of the data assimilation processes and its history can be found in Reference[59]. TENDL-2011 and TENDL-2012 processed data forms differ in some respects [35, 36]. This is due to enhancements made in the original ENDF-6 compliant TENDL data format and the way the files are processed. This is particularly noticeable in the partials kerma and dpa outputted from TENDL-2012 and the more complete usage made of the variance-covariance information contained in this library.

C.1 Cross-section Data

The principal sources of cross-section data are the different generations of the TALYS-based Evaluated Nuclear Data Libraries. The TENDL-2013 [60] is the latest recommended evaluated data source for use in any type of nuclear technology applications. The principal advances of this new library are in the unique target coverage, 2434 nuclides; the upper energy range, 200 MeV; variance-covariance information for all nuclides; and the extension to cover all important projectiles: neutron, proton, deuteron, alpha and gamma, and last but not least the proven capacity of this type of library

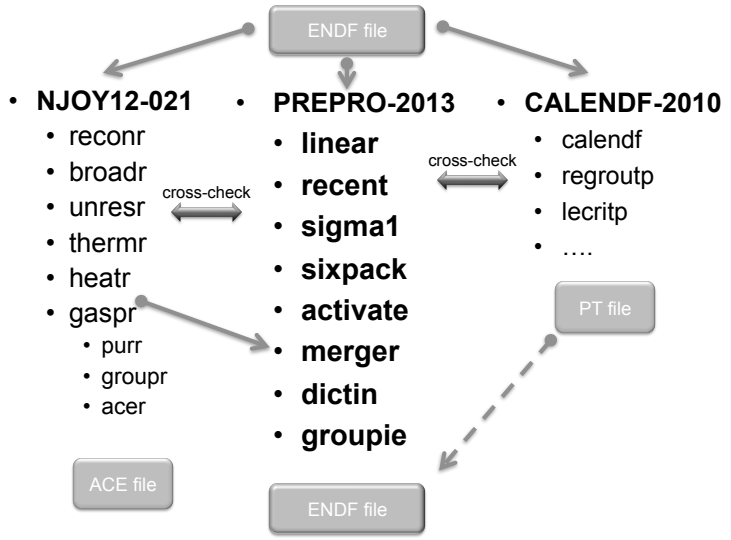


Figure 13: A schematic of the processing sequence using NJOY, PREPRO and CALENDF.

to transfer regularly to technology the feedbacks of extensive validation, verification and benchmark activities from one release to the next. TENDL-2013 is the fifth generation of such a library and as such has benefited from the previous releases since TENDL-2008, but also from the EAF-2007, and EAF-2010 V&V processes [24, 61].

The cross-section data are provided adequately in two universal group structures: a CCFE (709) scheme for the neutron-induced cross-sections and a CCFE (162) scheme for the non-resonant p, d, α and γ-induced cross-sections. The data format used is fully compliant with the ENDF-6 manual specification handled on an isotopic basis and so allows many existing utility codes further to manipulate, visualise or check any aspects of the pre-processed files. The data files are produced using a complex but robust, complementary sequence of modules of the processing codes NJOY12-021 and PREPRO-2013 [62]. During the processing outputs from verification and validation steps are regularly taken in order to establish the validity of all computed derived data. To be able to account for Doppler broadening effects the processed files are given at three temperatures: 293.6, 600 and 900 degree Kelvin.

Data for a small small number of nuclides are taken from sources different from TENDL. Table 26 lists those nuclides from different sources in the TENDL-2013 library.

Table 26: Non TENDL evaluations in TENDL-2013

nuclide	source	date	evaluators
5-B-10	LANL	APR06	G.M.Hale, P.G.Young
5-B-11	LANL	MAY89	P.G.Young
4-Be-9	LLNL, LANL	OCT09	G.Hale, Perkins et al, Frankle
6-C-0	JAERI	AUG83	K. Shibata
9-F-19	CNDC, ORNL	OCT03	Z.X.Zhao, C.Y.Fu,D .C.Larson, Leal+
1-H-1	LANL	OCT05	G.M.Hale
1-H-2	LANL	FEB97	P.G.Young, G.M.Hale, M.B.Chadwick
1-H-3	LANL	NOV01	G.M.Hale
2-He-3	LANL	MAY90	G.Hale, D.Dodder, P.Young
2-He-4	LANL	SEP10	G.Hale
3-Li-6	LANL	APR06	G.M.Hale, P.G.Young
3-Li-7	LANL	AUG88	P.G.Young
7-N-14	LANL	JUN97	M.B.Chadwick, P.G.Young
7-N-15	LANL	SEP83	E.Arthur, P.Young, G.Hale
8-O-16	LANL	DEC05	Hale, Young, Chadwick, Caro, Lubitz

C.2 Fission Yield Data

The fission yield data need to be provided for each actinide and incident particle. The files are supplied in an ENDF-6 format and are read by FISPACT-II with no further processing. The default library provided is based on the JEFF-3.1.1 library for neutron-induced fission. Only 19 of the many nuclides that have fission have any fission yield data in JEFF-3.1.1 and these cover only a reduced energy range. For the remainder the UKFY4.2 [63] library then further extends the range before a neighbouring fission yield is used. This UKFY4.2 library using Wahl's systematics is also used for all other particle induced fission yields.

C.3 Variance and Covariance

Above the upper energy of the resolved resonance range, for each of the 2434 isotopes a Monte Carlo method in which the covariance data come from uncertainties of the nuclear model calculations is used. A complete description of the procedure is given in Reference [64]. For all isotopes, the initial "best" set of results is produced by a TALYS-1.4 [65] calculation with an adjusted input parameter set. This set of results is stored in ENDF 'files' MF-3 to MF-10. Next, for each isotope, many TALYS runs with random nuclear model parameters are performed, which are used to generate uncertainties and correlations. As well as correlation within the same reaction channels, correlation between reaction channels is included. All information on cross-section covariance is stored in the MF-33 format, starting at the end of the resonance range up to 200 MeV. Short-range, self-scaling variance components are also specified for each `MT` type.

The data format used to store the variance-covariance information has been made fully compliant with the ENDF-6 format description and the files are read directly by FISPACT-II without any further processing.

C.4 Probability Tables

The CALENDF nuclear data processing system is used to convert the evaluation defining the cross-sections in ENDF-6 format (i.e., the resonance parameters, both resolved and unresolved) into forms useful for applications. Those forms used to describe neutron cross-section fluctuations correspond to "cross-section probability tables", based on Gauss quadratures and effective cross-sections. The CALENDF-2010 [14] code provides those probability tables in the energy range from 0.1 eV up to the end of the resolved or the unresolved resonance range. Probability table data in 709 (or 616) group formats are provided for 2143 isotopes of the TENDL-2013 library. These data are used to model dilution effects from channel, isotopic or elemental interferences. To account for Doppler broadening effects the tables are given at three temperatures: 293.6, 600 and 900 degree Kelvin.

C.5 Decay Data

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 a handful of evaluated decay data libraries. FISPACT-II is able to read the data directly in ENDF-6 format; it requires no pre-processing to be done. The now well verified and validated eaf_dec_2010 library based primarily on the JEFF-3.1.1 and JEF-2.2 radioactive decay data libraries, with additional data from the latest UK evaluations, UKPADD6.10 contain 2233 nuclides. However, to handle the extension in incident particle type, energy range and number of targets many more are needed. A new 3873-nuclide decay library dec_2012 has been assembled from eaf_dec_2010 complemented with all of JEFF-3.1.1 and a handful of ENDF/B-VII.1 decay files. See Reference [66] for more details.

There remain compatibility issues between the isomer definitions arising from the cross-section library, through the RIPL-3 database and the newly assembled decay library. Historical incompatibilities in isomeric state number (g, m, n, o, ...) and energy levels between radionuclide daughter products of reactions and the associated decay data files will need to be addressed in a future release.

C.6 Radiological Data

The radiological data for the increased number of nuclides present in the TENDL-2013 data are computed in the same manner as described for the EAF data (see

Appendix B.6 on page 193). The new hazards, clearance and transport data are respectively for 3647, 3873 and 3872 nuclides, compared to 2006, 2233 and 2233 for the EAF data. For further details see Reference [67].

D ENDF-B.VII.1 Library Data

The Cross Section Evaluation Working Group (CSEWG) released the ENDF/B-VII.1 library [68] on 22 December 2011. The ENDF/B-VII.1 library is the US latest recommended evaluated nuclear data file for use in nuclear science and technology applications, and incorporates advances made in the five years since the release of ENDF/B-VII.0, including: many new evaluation in the neutron sublibrary (423 in all) and over 190 of these contain covariances, new fission product yields for 31 isotopes and a greatly expanded decay data sublibrary for 3817 radionuclides.

For more details, visit http://www.nndc.bnl.gov/endf/b7.1/.

E JENDL-4.0 Library Data

The purpose of JENDL-4.0 [69] is to provide a Japanese standard library for fast breeder reactors, thermal reactors, fusion neutronics and shielding calculations, and other applications. The data libraries used have been updated to the JENDL-4.0u level of August 2013 for both the neutron reaction and fission yields sublibrary. JENDL FP Decay Data File 2011 [70] contains decay data of 1284 FP nuclides (of which 142 nuclides are stable) that includes recent TAGS (Total Absorption Gamma-ray Spectroscopy) information.

For more details, visit http://wwwndc.jaea.go.jp/jendl/j40/j40.html.

F JEFF-3.2 Library Data

The Joint Evaluated Fission and Fusion File is an evaluated library produced via an international collaboration of Data Bank member countries co-ordinated by the JEFF Scientific Co-ordination Group, under the auspices of the NEA Data Bank. The new JEFF-3.2 general purpose library has been released on March 5, 2014 in ENDF-6 format and contains incident neutron data for 472 nuclides or elements from 1-H-1 to 100-Fm-255.

for more details, visit https://www.oecd-nea.org/dbforms/data/eva/evatapes/jeff_32/.