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MASTER

Flux Weighted Group Cross Sections Based on the ACTLMFE Data File

Robert J. Howerton

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Lawrence Livermore Laboratory

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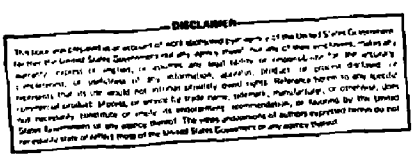
Robert J. Howerton

University of California
Lawrence Livermore Laboratory
Livermore, California 94550

ABSTRACT

A code GPC calculates flux-weighted group cross sections for up to 200 groups weighted by a flux with up to 200 entries from the ACTLMFE data file which is an ASCII form of the LLNL ACTL neutron activation cross section library.



Introduction

I have received requests from the controlled fusion community for flux-averaged group cross sections based on the LLNL ACTL[1] library of neutron-induced activation cross sections to be used in a post-processing code with calculated fluxes from a neutron transport code. The objective is to calculate activations induced in a region by the calculated neutron fluxes, with no further transport. To fulfill these requests and to make it possible for others to make similar calculations for arbitrary group structures and weighting spectra, I have written a code, GPC, that calculates the desired quantities for up to 200 groups and with weighting spectra with up to 200 entries. To accommodate those who wish to use the code at other installations I have converted the ACTL library to an ASCII form (ACTL.MFE) from its machine-dependent binary form. If anyone wishes to use the code with another library, he needs only to convert the other library to the format described below. A word of caution is appropriate. The ACTL data files and the weighting flux representations are assumed to be linearly interpolable in energy. While this restriction may be a slight burden in preparing the input, it greatly simplifies handling the data, especially since it allows analytic integration using the von Holdt-Howerton theorem[2] for the integration of the product of linear functions.

General Organization of GPC

The code GPC (Source Code GPCS) is interactive and, in its current form, is therefore designed to be operated from a console by the user. The user is asked by the code to supply the name of the input file that contains the group boundary and weighting flux information. Next, the code asks for the name to be assigned to the output file. (It is assumed that the name of the library is ACTLMFE.) Finally, the range of target nuclei for which group cross sections are required is requested. The group boundaries and weighting flux array are read from the appropriate files. The cross section file is then read to find the nuclei which meet the range criteria. Having found a nucleus that meets the criterion, the cross sections are read for the first reaction. If the threshold of the reaction is greater than the greatest group boundary, the reaction is ignored and the interrogation of the data file continues until a reaction is found that meets the input criteria.

The code then merges the group bourdary energies into the flux array, interpolating to obtain the flux values at the group boundaries. The energies of the cross sections for the reaction under consideration are then merged into the flux- group-boundary array and the flux is interpolated. Following that, the combined flux- group-boundary energies are merged into the cross section array and the cross sections are interpolated. The result of the merging processes is two arrays with identical energies; one is the weighting flux array and the other the cross section array.

For each group, two analytic integrals over energy are then done; the first is the integral of the product of the cross section by the weighting flux and the second is the integral of the weighting flux. The quotient of the first to the second is the desired quantity, i.e. the flux-weighted cross section for the group. After all group cross sections are calculated for the reaction, the resulting array is written into the output file. The procedure is then repeated until the range of desired nuclei is covered. As soon as the code finds a ZA (1000 x Z + A) value greater than the upper limit of the input range, the calculation is terminated. This, of course, implies that the data file must be organized in ascending ZA value, as is the ACTLMFE file.

The code is simple and fast. The entire ACTLMFE library was run for a 21 group, 51 flux-entry problem and required 8.4 seconds for 1210 reactions on the CRAY-1 computer.

INPUT

Two files are required for input. One contains the group boundary specification and the weighting flux specification. From the nature of the problem it is clear that the weighting flux must span the energy range of the group boundaries. The second input file is the library of cross section data (ACTLMFE).

The file containing the group boundaries and weighting flux may have any name of eight characters or less. The code asks for the name of the file. It's format is:

Record No.	Col.		Format
1	1-3	Number of group boundaries (NG)	i3
2 to as needed	1-66	Group Boundaries in ascending energies (MeV)	6E11.4
Next	1-3	Number of energy-flux pairs (NF)	i3
Next + 1 to as needed	1-66	Energy-flux pairs, three to a record in ascending energies (MeV, barns)	6E11.4

The format of the ACTLMFE data file is:

Record	Col.		Format
1	1-6	ZA (1000 x Z + A)	i6
	7-13	Ignore	7x
	14-24	Mass of Target (amu)	E11.4
	25-35	Ignore	11x
	36-46	Level of Target (MeV)	E11.4
	47	Ignore	1x
	48-58	Half-Life of Target (Sec.)	E11.4
2	1-2	Reaction Identifier Number (C*)	i2
	3-8	Ignore	6x
	9-20	Q-Value of Reaction (MeV)	E12.4
	21-32	ZA of Product	E12.4
	33-44	Level of Product (MeV)	E12.4
	45-56	Half-Life of Product (Sec)	E12.4

*See Appendix A

Record	Col.		Format
3	1-3	Number of Energy-Cross Section Pairs (NP)	i3
3 et seq	1-66	(EN(K), CS(K), K = 1, NP) where EN is energy in MeV and CS is cross section in barns	6E11.4
After the last line of EN, CS pairs	72	Reaction separator sentinel = 1	71x, i1

The above pattern is repeated for each reaction. The last reaction in ACTINFE is 240 U (N,γ) i.e. ZA of Target = 92240, C=46

OUTPUT

The code interrogates the user to obtain a name (eight characters or less) for the output file. A file of 100000 words is created and subsequently shrunk to the needed size when the program exits. The output file is 80 Column ASCII character records (card-image). The format is:

Record	Col.		Format
Group Definition			
1	1-3	Number of Group Boundaries (NG)	i3
2...	1-66	Group Boundaries from greatest to least (MEV)	6E11.4
Weighting Flux Definition			
1	1-3	Number of Pairs of Energy-Flux Entries	i3
2...	1-66	Energy-flux pairs in decreasing energy (MeV, Flux)	6E11.4

Record	Col.		Format
Group Cross Sections			
1	1-6	ZA (1000 I + A) of Target	i6
	7-13	Ignore	7x
	14-24	Mass of Target (amu)	E11.4
	25-35	Ignore	11x
	36-46	Level of Target (MEV)	E11.4
	47	Ignore	1x
	48-58	Half-Life of Target (Sec.) (Half-Life = 10^{50} means stable)	E11.4
2	1-2	Reaction Identifier No. (C*)	i2
	3-8	Ignore	6x
	9-20	Q-Value of Reaction (MeV)	E12.4
	21-32	ZA of Product	E12.4
	33-44	Level of Product (MeV)	E12.4
	45-56	Half-Life of Product (Sec.) (Half-Life = 10^{50} means stable)	E.12.4
3	1-66	NG-1 Group Cross Sections from greatest energy group to least energy group (barns)	6E11.4
After each Group Cross Section set			
	72	Separator record, has a 1 in Col. 72	71x, i1

The above pattern of group cross sections is repeated for all reactions that were processed.

*See Appendix A

Summary

The source code GPCS can be compiled to produce the object code GPC. GPC produces flux-weighted group cross sections for an arbitrary group structure of up to 200 groups. The weighting flux may be specified for as many as 200 neutron energies. The library of neutron cross sections must be in the format described above for the ACTLMFE data file.

When GPC was run on the CRAY 1 computer it required 8.4 seconds to process 1210 reactions into 21 group cross sections weighted by a flux with fifty-one entries.

For LLNL users two compiled versions of GPC are available via XPORT.

```
RD   .415600:RUBY:GPC              (7600 version)
RD   .415600:RUBY:CRAYGPC          (CRAY 1 version)
```

Likewise LLNL users may obtain an 8 bit ASCII form of ACTLMFE by the following XPORT command:

```
RD   .415600:RUBY:ACTLMFE
```

This file may be used on the 7600 after conversion (using TRIX AC) to 6 bit ASCII.

Non-LLNL users may obtain a copy of the source program and the ACTLMFE file upon request to the author.

Appendix A

The following are the two-digit integers used to designate reactions. These follow the ENDL convention.

C	Reaction
11	(n,n'γ)
12	(n,2n)
13	(n,3n)
14	(n,4n)
15	(n,f)
20	(n,n'p)
21	(n,pn')
22	(n,n'd)
23	(n,n'2α)
24	(n,n't)
25	(n,n' ^{3}He)
26	(n,n'α)
27	(n,n'3α)
28	(n,n't2α)
29	(n,2np)
40	(n,p)
41	(n,d)
42	(n,t)
43	(n,t2α)
44	(n, ^{3}He)
45	(n,α)
46	(n,γ)

References

1. M. A. Gardner and R. J. Howerton, ACTL: Evaluated Neutron Activation Cross Section Library - Evaluation Techniques and Reaction Index, UCRL-50400, Vol. 18 (1978).

2. R. E. von Holdt and R. J. Howerton, Mathematics of Computations XVII, No. 84, 419 (1963).