UCRL--53262

DE82 016132

ORLIB: A Computer Code that Produces One-Energy Group, Time- and Spatially-Averaged Neutron Cross Sections

J. A. Blink

R. E. Dye

J. R. Kimlinger

Manuscript Date: December 1981

DISCLAIMER

This report was prepared for the U.S. Government by Lawrence Livermore National Laboratory, which is managed by the University of California for the U.S. Department of Energy. The U.S. Government is authorized to reproduce and distribute reprints for government purposes not withstanding any copyright notation that may appear hereon. It is understood that any copyright in any material in this report belongs to the individual author(s) and/or to the U.S. Government. The U.S. Government is authorized to reproduce and distribute reprints for government purposes not withstanding any copyright notation that may appear hereon. The U.S. Government is authorized to reproduce and distribute reprints for government purposes not withstanding any copyright notation that may appear hereon.

LAWRENCE LIVERMORE LABORATORY
University of California • Livermore, California • 94550

Available from: National Technical Information Service • U.S. Department of Commerce
5285 Port Royal Road • Springfield, VA 22161 • \$5.00 per copy • (Microfiche \$3.50)

ORLIB: A Computer Code that Produces One-Energy Group, Time- and Spatially-Averaged Neutron Cross Sections

Abstract

Calculation of neutron activation of proposed fusion reactors requires a library of neutron-activation cross sections. One such library is ACTL,¹ which is being updated and expanded by Howerton.² If the energy-dependent neutron flux is also known as a function of location and time, the buildup and decay of activation products can be calculated. In practice, hand calculation is impractical without energy-averaged cross sections because of the large number of energy groups. A widely used activation computer code, ORIGEN2 (see Ref. 3), also requires energy-averaged cross sections. Accordingly, we wrote the ORLIB code to collapse the ACTL library, using the flux as a weighting function. The ORLIB code runs on the LLNL Cray computer network. We have also modified ORIGEN2 to accept the expanded activation libraries produced by ORLIB. The modified ORIGEN2 code, named FORIG, is described in Ref. 4.

The Model

Buildup of a daughter species can be found from

$$\frac{dN_2}{dt} = N_1 \sigma \phi \quad (1)$$

where dN_2 is the production rate of the daughter, N_1 is the parent population, σ is the cross section, and ϕ is the total flux (n/cm²/s). The cross section is

$$\sigma = \frac{\int_E \sigma(E) \phi(E) dE}{\int_E \phi(E) dE} = \frac{\int_E \sigma(E) \phi(E) dE}{\phi} \quad (2)$$

The energy-dependent flux is obtained from the TART neutronics code⁵ as a set of neutron-path-lengths-per-source-neutron in 175 energy bins. Then

$$\phi(E) = S \frac{L_i}{V_i} \quad (3)$$

where S is the number of source neutrons per unit time, L_i is the total neutron path length in the

zone and energy bin, V is the zone volume, and E_i is the width of the energy bin. The flux is assumed to be constant at all energies within the energy bin, i . Spatial variation of the parent density and the flux can also be included in the average cross section. In this case,

$$\phi(E) = S \frac{\sum_{\text{zones}} \frac{N_{1i}}{N_{\text{ref}}} \frac{L_i}{E_i}}{\sum_{\text{zones}} \frac{N_{1i}}{N_{\text{ref}}} V_i} \quad (4)$$

where N_{1i} is the parent population in zone i , N_1 in Eq. (1) is replaced by N_{ref} , and $N_{\text{ref}} = \sum_i N_{1i}$.

There are two limitations of this procedure: First, the flux must remain constant during the timeframe of the calculation. If the composition, and hence flux spectrum, changes enough to alter the energy-averaged cross sections, the cross sections must be periodically revised. The ORIGEN2 code includes such revisions in its various sets of fission-reactor cross-section libraries. In fusion-reactor structure, flux variation is not expected to require frequent recalculation of cross sections.

The second limitation is due to the spatial-averaging procedure. If activation of daughters is to be considered, the region of the problem must have a constant flux and density, i.e., no spatial averaging is permitted. This is because Eq. (4) must replace N_{ij} by N_{2j} , the parent of the grand-daughter, N_{3j} . However, the spatial distribution of N_{2j} is unknown during the cross-section collapse. Thus, grand-daughter production will use spatial-weighting factors that are appropriate only

for daughter production. One method of circumventing this problem is to run separate calculations for each zone. Alternatively, a scoping calculation can be used with spatial averaging if the ACTL input is restricted to the original parent nuclides. The reduced input will eliminate most daughter activations. The result can then be compared to a calculation with the full ACTL library. If there is little change, activation of daughters is probably insignificant.

The Code

The ORLIB code includes parts of the OMEGA code⁶ and an undocumented TART postprocessor code. TART is run using sentinel 11 set as the desired name of the TART output data file (which is then produced in addition to the high speed file). The TART tally type must be 2 (path length) for all zones that will be used to collapse the cross sections.

ORLIB requires an input file that specifies the TART data file name, the TART zone and tally times, any density-weighting factors, the source strength, and the nuclides of interest. The input file is described in detail in the next section. ORLIB also requires an ACTL library file.

ORLIB begins by reading the TART output data file and the input file. The density-weighting factors and the energy bin widths are applied to the path-length output, and the quantities $(\phi(E)/S)$, (ϕ/S) , (ΣV_j) are computed. The energy-dependent fluxes are in the form of a histogram. Because duplicate energy coordinates will be eliminated later, the histogram is skewed slightly, as shown in Fig. 1.

Figure 1. The histogram is shifted slightly to eliminate duplicate energy points. The shift, $\delta(E)$, is the energy coordinate divided by 10^6 .

For each reaction of each specified nuclide, the ACTL cross-section data are read (Table 1). These data are in the form of (E, σ) points with intermediate values set by linear interpolation. The energy points of the flux and cross sections are merged, and duplicates are eliminated. The flux and cross section is computed at each point by linear interpolation. The numerator of Eq. (2) is then

$$\sum_{i=1}^N \int_{E_i}^{E_{i+1}} \sigma(E)\phi(E)dE \quad (5)$$

where the E range of the integral is between the two energy points defining bin i , and N is the number of bins in the merged energy array.

Table 1. OMEGA reactions.

12 (n,2n)	29 (n,2np) α
13 (n,3n)	30 (n, γ n) α
14 (n,4n)	31 (n,2npa) α
15 (n,f)	37 (n,2 α) α
20 (n,np)	38 (n, 3 He α) α
21 (n,pn)	39 (n,tp) α
22 (n, α d)	40 (n,p)
23 (n,n α) α	41 (n,d)
24 (n,nt)	42 (n,t)
25 (n,n 3 He)	43 (n,t α) α
26 (n,n α)	44 (n, 3 He)
27 (n,n2 α) α	45 (n, α)
28 (n,n α) α	46 (n, γ)

OMEGA and ORLIB use the method of Ref. 7 to compute the integral in Eq. (5).

$$\int_a^b \sigma(E)\phi(E)dE = \left[(\phi_b + \phi_a)(\sigma_b + \sigma_a) + \frac{1}{3}(\phi_b - \phi_a)(\sigma_b - \sigma_a) \right] \frac{(E_b - E_a)}{4} \quad (6)$$

ORLIB Input

The ORLIB execution line is

ORLIB INPT AC820312 0 / t v

where INPT is the input file name and AC820312 is the ACTL library file. At LLNL the controller may be obtained from J. Blink's take directory.

XPORT

.RD .080975:ORIGEN2:ORLIB

(XPORT is an LLNL file-transport routine.) The ACTL library file name is AC820312 where 820312 is the creation date. To determine the latest library, consult R. Howerton's take directory.

XPORT

.LST .415600:CRACKT811

Select the latest AC date file (AC820312 at the time of this report).

.RD .415600:CRACKT811:AC820312

Readers outside LLNL are invited to contact the author for a copy of the code listing and the ACTL library.

The ORLIB input file has five line types:

Line 1: Format 1x,I6,1x,I6,1x,I2

```
1 2 3 4 5 6 7 8 ( 1 ) 2 3 4 5 6 7
Z Z A A A      Z Z A A A  N L
```

The two ZZAAA numbers are the range of atomic number and mass (ZA) over which the available Table 1 reactions in ACTL will be computed. All nuclides between the two bounds will be processed. If NL ≥ 0, other ZA ranges will be specified in line-type-5 lines at the end of the file. If NL < 0, this is the only ZA range of interest, and no type 5 lines will be in the file.

Line 2: Format A8,1x,I3,1x,I3,1x,E11.4

```
1 2 3 4 5 6 7 8 (1) 2 3 4 5 6 7 8 (2) 2 3 4 5 6 7 8
NAME LIB NZN      SRCSTR
```

NAME is the TART tape name, LIB is a three-digit number of the output library (≥700 if the output is to be used in FORIG), NZN is the number of zones and times to be averaged, and SRCSTR is the neutron source strength in neutrons/second.

Line 3: Format 1x,I3,1x,I3,1x,E11.4

```
1 2 3 4 5 6 7 8 ( 1 ) 2 3 4 5 6 7 8 ( 2
T I M   Z O N                               F R A C
```

TIM is the TART edit time number (1, 2, 3, etc.). ZON is the TART zone number. FRAC is the spatial-weighting factor.

$$FRAC = \frac{\rho}{\rho_{ref}} \frac{mtl}{ref\ vf} \quad (7)$$

where ρ_{ref} and ref vf are the atom density and volume fraction of the reference material. For example, if the reference material is full density graphite occupying 90 vol% of a zone, and if a particular zone has 50% density graphite occupying 80 vol% of the zone, then

$$FRAC = \left(\frac{1}{2}\right) \frac{0.8}{0.9} \quad (8)$$

and the mass of graphite used in Eq. (1) will be

$$N_i = \sum_{j=1}^{zones} V_j (vf_j) \rho_j \quad (9)$$

There is one Line 3 for each zone and time of interest; i.e., NZN lines; NZN ≤ 20.

Line 4: Format 9A8

A message up to 72 characters long will be printed on the output.

Line 5: Format—same as Line 1

It contains additional ZA ranges to be processed. The last Line 5 will have NL less than zero.

ORLIB Output

ORLIB produces four files: OLEVEL, OACT, OODD, and OGEORGE.

File OLEVEL prints the parent, daughter, and energy level of all reactions involving nuclides not in the ground state. ORLIB nuclide identification is the same as ACTL except the isomer number is added.

ACTL	ORLIB
ZZAAA	ZZAAAI

The isomer number, I , is 0 for the ground state, 1 for the first excited state, etc. Since the ORLIB code does not check the level, all excited isomers have $I = 1$. The OLEVEL file provides the data needed to manually correct the other output files if there are two or more excited states for a given nuclide. The ACTL library AC820312 had no nuclides in this category. Parenthetically, we note that the FORIG and ORIGEN2 codes cannot handle isomer numbers > 1 .

File OACT lists the nuclide identification and 11 reaction cross sections.

ZZAAAI (n,2n) (n,2n)exc (n,3n) (n,np) (n,n α) (n,p) (n,d) (n,t) (n, α) (n, γ) (n, γ)exc

where "exc" means the daughter is in an excited state. It also prints the source strength, total flux,

total zone volume, and material volume. The parent population, N_i , in Eqs. (1) and (9) is the material volume multiplied by the product of ρ_{ref} and v_{ref}

File OODD lists all other reactions.

Parent	Daughter	Cross	OMEGA
ZZAAAI	ZZAAAI	Section	Reaction
			Code

Files OACT and OODD are renamed TAPE8 and TAPE3, respectively, when they are used as FORIG input.

File OGEORGE is a modification of Files OACT and OODD requested by G. P. Lasche for hand calculations.⁸ It contains the 11 standard reactions, the odd reactions, and the total cross section. Each cross section has been multiplied by a conversion factor

$$C = \phi (1 \times 10^{-24}) \quad (10)$$

where ϕ is specified by Eqs. (2) to (4). Thus, these cross sections have units of probability per second. For hand calculations, the "OGEORGE" cross sections are multiplied by the reference parent population, N_i , in Eq. (9) to obtain the production rates of the daughters in units of atoms/s.

Summary

A computer code, ORLIB, has been written to average ACTL cross sections in energy and space using a TART calculated space and energy dependent flux and the material composition as weighting factors. The output is suitable for either

hand calculations, or input to the FORIG code. If activation of daughters is significant, the code must be run for each individual zone since spatial averaging prior to buildup of the daughters is not appropriate.

Acknowledgments

The authors are grateful for helpful discussions with J. Hovingh, R. Howerton, G. Lasche, W. Meier, and E. Plechaty, of LLNL; and A. Croff of ORNL.

References

1. M. A. Gardner and R. J. Howerton, *ACTL: Evaluated Neutron Activation Cross Section Library-Evaluation Techniques and Reaction Index*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-50400, Vol. 18 (Oct. 17, 1978).
2. R. J. Howerton, Lawrence Livermore National Laboratory, private communication (Aug. 1981).
3. A. G. Croff, *A User's Manual for the ORIGEN2 Computer Code*, Oak Ridge National Laboratory, Oak Ridge, TN, ORNL/TM-7175 (July 1980). Also published as Radiation Shielding Information Center Report CCC-371.
4. J. A. Blink, *FORIG: A Modification of the ORIGEN2 Isotope Generation and Depletion Code for Fusion Problems*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-53263 (Dec. 1981).
5. E. F. Plechaty and J. R. Kimlinger, *TARTNP: A Coupled Neutron-Photon Monte Carlo Transport Code*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-50400, Vol. 14 (July 4, 1976).
6. R. J. Howerton, R. J. Doyas, T. C. Michels, and S. T. Perkins, *An Integrated System for Production of Neutronics and Photonics Calculational Constants*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-50400, Vol. 4 (April 15, 1971).
7. R. E. Von Holdt and R. J. Howerton, "The Definite Integral of the Product of Linear Functions," *Math. Comp.* 17, 419 (1963).
8. G. P. Lasche, *Upper-Bounded Estimates of Neutron-Induced Radionuclide Populations*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-87255 (1982).