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SPOTS4

Group data library and computer code,
preparing ENDF/B-4 data for input to LEOPARD

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Abstract: The magnetic tape SPOTS4 contains in file 1 a data library to be used as input to the SPOTS4 program which is contained in file 2. The data library is based on ENDF/B-4 and consists of two parts in TEMPEST format (246 groups) and MUFT format (54 groups) respectively. From this library the SPOTS4 program produces a 172 + 54 group library for LEOPARD input. A copy of the magnetic tape is available from the IAEA Nuclear Data Section.

September 1981

SPOTS4

Tape received at NDS August 1981 from Jung-Do Kim, Korea Advanced Energy Research Institute, P.O. Box 7, Cheong Ryang, Seoul, Korea.

Content of tape

File 1: SPOTS4 input:

TEMPEST (246 group) data
MUFT (54 group) format library

File 2: SPOTS4 program:

SPOTS4 output (TAPE 1)
is 172 + 54 group library for LEOPARD

The following pages of this document contain two papers:

- Description of SPOTS4 input data (TEMPEST 246 + MUFT 54 Group Data
- Jung-Do Kim and Jong Tai Lee: Benchmark Test and Adjustment of an Updated Library from ENDF/B-4. (Note: This paper is a draft not to be quoted without consultation of the author. It was submitted for publication in the Journal of Korean Nuclear Society.)

DESCRIPTION OF SPOTS4 INPUT DATA
(TEMPEST 246 + NUFT 54 Group Data)

1.0 General

The input data to the SPOTS4 code which generates the library data tape (TAPE 1) for the LEOPARD code are in two groups: one for the thermal neutron group the other for the fast group. The description of SPOTS4 input data including the card data formats follows.

2.0 Thermal Group Data

2.1 Input Data Format

The thermal group input data follow a "THERMAL LIBRARY FOR LEOPARD" card on which the word THERMAL is punched in columns 3 through 9. This card is only for identifying the SPOTS4 input data deck. The last card of the thermal group input data must contain the word X-LAST punched in columns 1 through 6. This card signals the end of the thermal group data. For each element, the following input data and formats are required:

1. First Card Format(8A10)

   Description Card
   = THERMAL LIBRARY FOR LEOPARD

2. Second Card Format(A6, 3X, i3, 57X, i3)
   a. Columns 1 through 6 contain the element name.
   b. Columns 10, 11, and 12 contain the element identification number (hundreds, tens, and units in columns 10, 11, and 12, respectively).

c. Columns 70, 71, and 72 contain the number of tabulated entries in the library (hundreds, tens and units in columns 70, 71, and 72, respectively).

3. Third Card Format (5E10)

R_{i0} , R_{i1} , R_{i2} , R_{i3} , R_{i4} are the terms for the power series which is used to compute cross-sections from 0(0.0001) 0.0009 ev, when the cross-sections are tabulated (see 5 below). For example:

$$\sqrt{E}\,\sigma_i(E) = \sum_{j=0}^{4} R_{ij} E^{j/2}$$

where $\sigma_i(E)$ = microscopic cross section (absorption, fission, or transport) for element i for neutron energy E ev, barns. It is set to zero in the code when E = 0.

4. Fourth Card Format (5E10)

η_i, γ_i , K_i, E_i, and ν_i are the terms for the Breit-Wigner resonance formula and a spare variable. For example,

$$\sqrt{E}\,\sigma_i(E) = \frac{K_i \gamma_i}{(\gamma_i + \eta_i\sqrt{E})^2 + 4(E-E_i)^2}$$

5. Fifth and Subsequent Card Format (7E10)

If it is necessary to tabulate cross-sections as a function of energy (e. g. non-1/v or non-constant cross-sections), it is done here. The cross-sections are tabulated at 246 energy points (E_{max}= 2.0 ev).

2.2 Type of Thermal Group Cross Sections

There are three sets of cross-section data which are necessary for each element, these are denoted by Set I, II, III. Although Set IV is provided in the current SPOTS4 input, it is not required, and hence it can be eliminated.

Set I contains the tables or associated power series for $\sqrt{E}\ \sigma_a(E)$. In this set the element identification numbers must be between 0 and 99. If σ_a is a 1/v absorber, then $\sqrt{E}\ \sigma_a(E)$ is a constant and is entered as R_{i0} (see 3rd card format); otherwise $\sqrt{E}\ \sigma_a(E)$ must be tabulated. If resonance parameters are entered, then any tabulated values will be added to the resonance contributions. Likewise, a 1/v absorber with a resonance must have R_{i0} and the resonance parameters specified. ν_i is not used.

Set II contains the tables or associated power series for $\sqrt{E}\ \sigma_f(E)$. In this set the element identification numbers must be between 100 and 199. Remarks concerning resonance parameters, 1/v absorbers, and tabulated cross sections are analogous to those given for Set I. ν_i must be set equal to the number of neutrons per fission.

Set III contains the tables or associated power series for $(1-\mu)\sigma_s$.

In this set the element identification numbers must be between 200 and 299. For elements with constant σ_s and constant $(1-\mu)$, σ_s must be entered as R_{i0} and $(1-\mu)$ must be entered as ν_i. If $(1-\mu)\ \sigma_s$ is not constant, then this quantity must be tabulated and the power series entered. Also, ν_i must be set equal to 1.0.

The element identification numbers allowed in the SPOTS4 input data are preset as shown in Table 1, and these must not be changed when

the cross sections are modified. Note that these are for the thermal group only.

TABLE 1

ELEMENT IDENTIFICATION NUMBERS ALLOWED

IN THE SPOTS4 THERMAL GROUP INPUT DATA

Element Name	Identification Number		
	Set I	Set II	Set III
H	91		291
O	2		202
Zr - 2	3		203
C	4		204
Fe	6		206
Ni	7		207
Al	9		209
Cr	11		211
Mn	15		215
U - 233	50	150	250
U - 234	52		252
U - 235	34	134	234
U - 236	19		219
U - 238	20		220
Pu - 239	79	179	279
Pu - 240	81	181	281
Pu - 241	80	180	280
Pu - 242	82		282
Th - 232	62		262
Pa - 233	65		265
Xe - 135	27		227
Sm - 149	26		226
B - 10	29		229
D	38		238

3.0 Fast Group Data

3.1 Input Data Format

All the floating point numbers (numbers with a decimal point) for the SPOTS4 fast group input data must be given in the so-called floating decimal form. To transcribe an ordinaly decimal number to this from, write it in scientific notation as a decimal fraction $0.1 \leq f < 1$ multiplied by the proper power of ten. This power of ten increased by 50 is written as a two-digit number to the left of at most five digits of the fraction to form the floating point representation. The sign of the floating point number is the sign of the decimal converted. For example,

1/3 =	+5033333	
30 =	+523 =	+5230000
- 0.0055=	-4855=	-4855000
0 =	+000 =	+0000000

It should be noted that every floating point number including zero is composed of at least two decimal digits for the exponent and at least one but not more than five decimal digits for the fraction. Hence every floating point number is composed of at least three and at most seven decimal digits.

1. First Card Format (8A10)

   Description Card
   = FAST LIBRARY FOR LEOPARD

2. Second Card Format (6X, i2)

   NI is the total number of elements in the fast group, Other data in the card are irrelevant.

3. Third Card Format (8X, 16I4)

(NRAW(I), I = 1, NI). Element identification numbers for the fast group data. Since NI is 25 (dummy F.P. data included) for SPOTS4, there must be two cards of this type. See Table 2 for the description of the element identific identification numbers.

4. Fourth Card Format (8X, 8F8.5)

(DELTA(I), I = 1,54). Lethargy width for each of the 54 fine fast groups. See Table 3 for the energy breakdown of the fast group, which is expected by the SPOTS4 code. Seven cards of this type are required.

5. Fifth Card Format (8X, 8F8.5) ("+3" type cards)"

(SSC(J,M), SIGCAP (J, M), SIGI (J, M), SIGX(J, M), AN(J,M), SI(J,M), GMU(J,M),SD(J,M), M = 1,54) where J is the element index, M the group index. There are exactly 54 cards for each element, and the data must be given for each element in the order as shown on the third cards or in Table 2. The numbers in columns 1 through 8 of each card indicate card type, element identification, and fine group index, and are merely for the input data card identification. The SPOTS4 code does not require these number; hence, columns 1 through 8 can be left blank, if the cards are ordered correctly.

The "+3" type input data are defined below.

SSC = symmetric scattering cross section ($\bar{\sigma}_c^s$)

TABLE 2

DESCRIPTION OF THE ELEMENT IDENTIFICATION NUMBER
FOR THE SPOTS4 FAST GROUP INPUT DATA

Element	ID Number	Element	ID Number
H	+ 001	U - 238	- 120
O	- 002	Pu - 239	- 221
Zr - 2	- 103	Pu - 240	- 222
C	- 004	Pu - 241	- 223
Fe	- 106	Pu - 242	- 124
Ni	- 107	Th - 232	- 162
Al	- 009	Pa - 233	- 165
Cr	- 111	Xe - 135	- 027
Mn	- 115	Sm - 149	- 126
U - 233	- 250	B - 10	- 029
U - 234	- 151	D	+ 038
U - 235	- 218	F.P.**	+ 028
U - 236	- 119		

* a. If $0 < |ID| \leq 100$, no resonance data input("+3"type cards only - 54 cards)

b. If $100 < |ID| \leq 200$, resonance absorption parameters input ("+3" type cards - 54 cards, "+4" type cards - 60 cards)

c. If $200 < |ID|$, fission-to-absorption ratio in resonance data ("+3" type cards - 54 cards, "+4" type cards - 90 cards)

d. If ID negative, inelastic scattering matrix input also ("+5" type cards, in addition to above)

** e. Fission product cross sections are dummy.

TABLE 3

FAST ENERGY GROUP STRUCTURE USED IN THE SPOTS4 CODE

Group Number	Energy (ev)	Lethargy	Lethargy Width
0	10×10^6	0	
1	7.79	0.25	0.25
2	6.07	0.50	
3	4.72	0.75	
4	3.68	1.00	
5	2.86	1.25	
6	2.23	1.50	
7	1.74	1.75	
8	1.35	2.00	
9	1.05	2.25	
10	821×10^3	2.50	
11	639	2.75	
12	498	3.00	
13	387	3.25	
14	302	3.50	
15	235	3.75	
16	183	4.00	
17	143	4.25	
18	111	4.50	
19	86.5	4.75	
20	67.4	5.00	0.25
21	40.9	5.50	0.50
22	24.8	6.00	
23	15.0	6.50	
24	9.12	7.00	
25	5.53	7.50	
26	3.35	8.00	
27	2.03	8.50	0.50

(Continued)

TABLE 3 (continued)

Group Number	Energy (ev)	Lethargy	Lethargy Width
28	1.23	9.00	0.50
29	750x10^{3}	9.50	
30	454	10.00	
31	275	10.50	
32	167	11.00	0.50
33	130	11.25	0.25
34	101	11.50	
35	78.7	11.75	
36	61.3	12.00	
37	47.8	12.25	
38	37.2	12.50	
39	29.0	17.75	
40	22.6	13.00	
41	17.6	13.25	
42	13.7	13.50	
43	10.7	13.75	
44	8.32	14.00	
45	6.50	14.25	
46	5.10	14.50	
47	3.97	14.75	
48	3.06	15.00	
49	2.38	15.25	
50	1.855	15.50	0.25
51	1.440	15.7538	0.2538
52	1.125	16.00	0.2462
53	0.835	16.30	0.3000
54	0.625	16.5884	0.2884

SIGCAP = smooth capture cross section ($\bar{\sigma}_c^s$)

SIGI = total inelastic scattering cross section ($\bar{\sigma}_{in}$)

SIGX = fission cross section (σ_f)

AN = age number ($\bar{\tau}_u$; Or λ_n in Equation (9) of the MUFT-4 Manual (WAPD-TM-72)

SI = $\bar{\mu}_o \bar{\sigma}_o^s$

GNU = mumber of neutrons per fission ($\bar{\nu}$)

SD = microscopic slowing down power ($\xi \bar{\sigma}_o^s$)

6. Sixth Card Format(6X, 12, 8F8.5)("+4" type cards)

a. Cards of this type are not required for an element whose absolute value of the identification number, |ID| , is less than or equal to 100.

b. Sixty dummy or blank cards are required by an element when $100 < |ID| \leq 200$ and no resonance data are available (NR = 0)

c. Ninety dummy or blank cards are required by an element when $200 < |ID|$ and no resonance data are available (NR = 0)

d. For elements when $100 < |ID| \leq 200$ and resonance data are available, 30 pairs of the following cards (total of 60 cards) are required: N, (A(N), = 1, 8)/ N, (B(N), N = 1, 8), where N = number of parameters on the card.

$A(N) = r_n = \sigma_{on} \Gamma_{an} / \Gamma_n$

$B(N) = m_n = \sigma_{on} \Gamma_{an} / E_{on}$

σ_{on} = total cross section at the peak (occurring at energy E_{on}) of the n-th resonance having absorption width Γ_{an} and total width Γ_n)

e. If 200<|ID| , additional 30 cards of the following form are required: NQ, (C(N), N = 1, 8), where NQ = number of parameters on the card

C(N) = α_n = fission-to-absorption ratio (σ_f / σ_a) for each of the resonances given in d.

The numbers in columns 1 through 6 of each card for the "+4" type cards are irrelevant, but the cards must be arranged in the order of elements as given on the Third Cards. The current version of SPOTS4 has 17 fixed elements with resonance data and a maximum of 30 resonances per element.

7. Seventh Card Format(8X, 8F8.5) ("+5" type cards)

Cards of this type (total of 55 cards) are required only to provide inelastic scattering matrix for an element with the negative element identification number as shown in Table 2. For each element with index N;

a. (SI(N,J), J = 1,54), Inelastic scattering cross section for each of the 54 groups (7 cards).

b. $a_{m,n}$. Probability of scattering from m-th group to n-th group where m = 1,2, n-1 starting from n = 2. Use as many cards as needed to finish a given m, and start a new card when n changes.

The current version of SPOTS4 allows only 22 elements with inelastic scattering matrix as shown in Table 2.

8. Eighth Card Format (8X, 8F8.5) ("+6" type cards) (X(I), I = 1, 54). Fraction of U-235 fission on neutrons born in each of the 54 groups (total of 7 cards).

3.2 Change of Element Identification

The SPOTS4 code is written consistent with the element identification number which are shown in Table 2. Therefore, any attempt to change these numbers in the SPOTS4 fast group input data will cause difficulties in obtaining correct results.

Benchmark Test and Adjustment of an Updated Library from ENDF/B-IV

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Benchmark Test and Adjustment of an Updated Library from ENDF/B-IV

Abstract

A LEOPARD library was updated from the ENDF/B-IV evaluated data using ETOT-3 — ETOG-3 code system.

The applicability of the library was assessed through benchmark tests for many light water-moderated critical assemblies, and adjustment techniques were applied to group constants to fit critical experiments.

It is confirmed that the library from ENDF/B-IV, coupled with the use of LEOPARD code, leads to reasonable results for light water-moderated UO_2 fueled cores with the above adjustments.

요 약

ETOT-3 — ETOG-3 전산체계와 ENDF/B-IV 평가 핵자료를 이용하여 LEOPARD 코드용 핵자료 라이브러리를 생산하였다.

그리고 생산된 라이브러리의 신뢰성을 입증하기 위하여 선정된 많은 실험자료에 대한 임계계산을 수행하였다. 이 결과를 토대로 경수형 UO_2 핵연료계에 대한 수정, 평가계산을 수행하여 조정된 라이브러리가 유용함을 확인하였다.

1. Introduction

The LEOPARD[1] code developed by the Westinghouse Co. in 1963 may be regarded as one of the basic computer codes for core physics calculations of light water-moderated reactors.

This code has been frequently applied to calculations of few group constants, the neutron multiplication factor or fuel depletion effects for PWR core analysis.

The extensive developement of nuclear power calls for a highly accurate knowledge of nuclear constants of fissile and structural materials of the core.

One of the principal advantages of the LEOPARD is to have its own built-in data library, but the library is relatively old and recent nuclear data evaluations are not taken into account. In addition, the number of nuclides in the library is not much enough to be desirable or necessary for PWR core analysis. Consequently, there has arisen a need to update these library from recent and more accurate evaluated nuclear data.

The data in the LEOPARD library with 172 + 54 group structures was generated from ENDF/B-IV evaluated data using the ETOT-3 — ETOG-3 processing code system.

And then, an applicability of the updated library was assessed through benchmark tests for many light water-moderated critical assemblies. Adjustment techniques were also applied to group constants to fit critical experiments.

2. Update of LEOPARD Library

2.1. Description of Old Library

The built-in library data in the released LEOPARD were original MUFT[2] and SOFOCATE library[3] data.

The MUFT library was mainly based on tape 0 in report WAPD-TM-224 (1960), while the SOFOCATE library was based on report WAPD-TM-67 (1957) with subsequent modifications.

Therefore, almost all of the original LEOPARD library data were those in the 1950s, and raw data unavailable were replaced to those of similar nuclide. For instance, thermal transport cross sections of U-233, U-236 and U-238, and those of Pu-239 and Pu-241 were same, that is, 9.972 barns and 10.9692 barns, respectively.

In fast regions, all elastic scatterings of Pu-240, Pu-241 and Pu-242 were replaced to those of U-235. And all inelastic scatterings of Pu-240, Pu-241 and Pu-242 were also replaced to those of Pu-239.

In addition, some of bias factors to compensate the differences between calculated mean k_{eff} and experimental values were considered in this library. Namely, the bias factor of 1.0036[4] was applied to the LEOPARD calculation by uniformly adjusting ν values (neutrons per fission) of all fissile nuclides. Especially the bias factor of U-235 in fast groups was 0.9914.

2.2. —Procedure of Library Generation

The ETOT-3[5] — ETOG-3[6] system has been established to process data from ENDF/B-IV to TEMPEST[7] and MUFT[8] format.

The ETOT-3 code was used to generate thermal cross sections of TEMPEST 246 group format and the ETOG-3 code fast data of MUFT 54 group format.

In ETOT-3 calculations, fine group cross sections were not group averaged values but point values. In calculations of the resolved resonance region, single or multi-level Breit-Wigner formula was used to calculate microscopic cross sections.

In ETOG-3 calculations, group data were generated using a "1/E + U-235 fission spectrum" weighting function. The fission spectrum joined 1/E at 67.4 KeV (lower boundary of 20th group). Similarly, single or multi-level Breit-Wigner parameters were used to generate resonance data.

54 group fission-spectra of U-235 and Pu-239 were also generated as sources in MUFT calculation, respectively.

Thermal 246 group data and fast 54 group data obtained from ETOT-3 — ETOG-3 system can not be directly used as a LEOPARD input. Since the LEOPARD uses very large blocks of library data, a separate library-producing precursor code, SPOTS, has been provided to make up the library.

In this updating procedure, the SPOTS4 code [9] (an extension of the SPOTS) was used in the library generation.

As the result, an updated ENDF/B-IV LEOPARD library was prepared for all materals available at present in the code and other nuclides which may be considered to be disirable additions.

3. Benchmark Test

In order to estimate the applicability of the updated library for the design analysis of light water-moderated reactor, benchmark calculations have been performed for 59 critical experiments.

There are at least two aproaches that one can take to determine the adequacy of cross section data for reactor. The first approach involves detailed calculations for a few critical experiments. Comparison between experiments and calculations are made for such parameter as the multipilication factor, thermal flux disadvantage factor, various cadmium ratios and quantities pertinent to the fast fission and resonance absorption effects. If adequate agreement is found for all this parameters, it is assumed that all important reaction rates are being caluclated satisfactorily and cross section data used in the calculation are adequate.

The second approach is to calculate a single parameter such as the multiplication factor for a large number of experiments which include a wide range of variables. Although errors in several reaction rates could cancel to give adequate agreement in k_{eff} for some cases, it is

extremely unlikely that the errors would cancel over a wide range of variables. Consequently if the agreement in k_{eff} is good, it can be assumed that the important reaction rates are being calculated properly.

This second approach has been adopted in this paper to check the adequacy of the updated library.

Fig. 1 shows the flow diagram for production and benchmark test of LEOPARD library from ENDF/B-IV.

Fig. 1

3.1. Description of Critical Assemblies

Experimental data for a large number of critical assemblies using UO_2 and PuO_2-UO_2 fuels have been collected from available literatures.[16)~20)] Most of the cases were limited to assemblies for which experimental bucklings have been reported.

Using the experimental buckling to represent leakage, the effective multiplication factor can be calculated in a "point model", without performing any diffusion calculations.

Of the 59 assemblies studied, 44 cases are UO_2 cores and 15 cases PuO_2-UO_2.

U-235 enrichments of UO_2 fuels vary from 1.328 to 5.809 % ; moderator-to-fuel volume ratios (H_2O : U) vary from approximately 2.06 to 18.37. Pellet diameters from 0.7544 to 1.5265 cm are used ; both stainless steel and aluminum clad for UO_2 fuels and zircalloy-2 clad for PuO_2-UO_2 fuels are studied as much as both square and hexagonal lattice arrays.

The data for all the collected assemblies are given in Table 1 and Table 2, seperately for UO_2 and PuO_2-UO_2 fuels.

Table 1 and Table 2

As shown in the above Tables, it is felt that the wide variation in parameters provides a severe test for the updated cross section library.

3.2. Criticality Calculation

For all cases, effective multiplication factors were calculated using the reported experimental buckling, geometry and compositions by the LEOPARD code with the updated library. The results are given in the form of the ratio of calculated to experimental value (C/E) for each critical assembly.

On discussing the results, it is very difficult to grasp the trends of the results for the specific integral quantities from the individual C/E values.

Therefore, we used the statistical average, the standard deviation and the average of absolute difference from unity to extract the characteristics of the library data.

3.3. Result and Discussion

Results of k_{eff} calculations for 59 critical assemblies are given in Table 3 and Table 4. Statistical values are also shown in the above Tables. In k_{eff} calculations for mixed-oxide (PuO_2-UO_2) cores, fission spectrum of U-235 or Pu-239 was used as source data.

Table 3 and Table 4

From Table 3 of 44 UO_2 cases, statistical values give the average k_{eff} (C/E) of 0.9954, the standard deviation of 1.52 % and the average deviation from unity of 0.0123.

This result shows the updated library data underpridict k_{eff} by $\sim$ 0.5 % for UO_2 cores. And the standard deviation of 1.52 % or the average diviation from unity of 0.0123 shows that calculated data are scattered.

In general, Aerojet General Corporation (AGC) and JAERI data (Table 1) give a large discrepancy from unity. According to the discussion of reference 13, experimental buckling uncertainties of AGC measurements are larger than normal. And critical bucklings of JAERI data were inferred from critical loadings. In addition to buckling uncertainties, other effects that increase the standard deviation of the calculated results include impurities in the fuel, clad and moderator (impurities were neglected in the calculations) and uncertainties in physical parameters such as dimensions, densities and enrichments. Actually, disregarding cases 36 through 44 gives the standard deviation of 0.86 %.

In calculations for mixed-oxide cores, coupled with the use of U-235 source spectrum, the average k_{eff} and the standard deviation become 1.0045 $\pm$ 0.0113 and the average deviation from unity becomes 0.0103.

In fact, fissile plutonium quantity in the selected mixed-oxide fuels is 3 times more than fissile uranium.

From this consideration, in calculations of mixed-oxide cores coupled with the use of Pu-239 source spectrum, the result gives the average k_{eff} of 0.9988 and the average deviation from unity of 0.0075. This represents an improvement.

The Cross Section Evaluation Working Group (CSEWG) evaluations[21] of the ENDF/B-IV concluded that the experimental k_{eff} is generally overpredicted by 1 to 2 % for plutonium nitrate systems and underpredicted by ~ 0.5 % for high moderator-to-fuel ratios to ~1.5 % for low moderator-to-fuel ratios in light water-moderated uranium lattices. These biases have been confirmed by Kang & Hansen[22] or McCrosson[23] through benchmark analysis.

About 0.5 ~ 0.7 % underprediction of k_{eff} for the UO_2 system is very nearly the same as those of the CSEWG conclusion and the results of PuO_2-UO_2 system also show the same trend.

From the above results, a conclusion might be drawn that any bias remains in the library from ENDF/B-IV and the source spectrum greatly affects in the calculation of mixed-oxide system.

In determining whether a bias factor should be applied to the calculated value of k_{eff}, careful judgement is required.

4. Adjustment of Cross Section Data for UO_2 System

From the result of a previous discussion, 35 cases of UO_2 system (Case No. 1 through 35) were selected for data adjustment. The average k_{eff} and the standard deviation for these are 0.9929 ± 0.0086. Therefore, it will be assumed that calculated k_{eff} is always less than unity by more than 0.7 % for UO_2 fueled system.

In LEOPARD calculation, all resonance self-shielding is neglected except that in U-238. In MUFT routine for fast region, the self-shielding factor also includes the Doppler effect, since the cross section library of MUFT format contains no temperature dependence. The calculation of the resonance absorption is made in three steps: First the U-238 resonance escape probability is calculated for the lattice, then a self-shielding factor is obtained for U-238, finally the self-shielding factor is used to determine the fast spectrum and few group constants.

The microscopic scatterings of U-238 in the resonance region are important in the calculation of resonance integral. And then, these data used in the original LEOPARD library were the same values of 10.7 barns in the resonance regions, but since resonance data of U-238 from ENDF/B-IV were generated from resonance parameters, there are many resonance peaks. In fact, the LEOPARD selects a value of 45th fast group scattering data in order to calculate the above mentioned factors.

In the updated U-238 scattering data, the 45th group shows resonance peak and the value is 42.164 barns. This value is larger than the old data of 10.7 barns.

A bias factor was applied in the LEOPARD calculation by adjusting a value of U-238 scattering. The 45th group scattering cross section was adjusted from 42.164 barns to 26.667.

Table 5

The adjusted results are given in left side of Table 5. The average k_{eff} and the standard deviation are 0.9999 ± 0.0073 and the average deviation from unity is 0.0056. These values are greatly improved comparing with the values of 0.9929 ± 0.0086 in Table 3.

However, there are still some scattered values from unity. In order to reduce the scattered trend, another adjustment was tested.

In the fast region calculation of LEOPARD, the resolved resonance absorption has explicit resonance treatment, but the resolved resonance scattering is not handled explicitly. In old library, resonance scatterings of a large number of nuclides were actually treated with constant values. By an input option of ETOG-3, it can be taken to be equal to the value in the first group above the resonance region.

With this treatment, all resonance scatterings of U-238 are determined as 12.067 barns. If resonance scattering data of U-238 in the updated library are substituted to 12.067 barns and the thermal ν of U-235 are reduced by 0.8 %, calculated results for UO_2 systems are also improved as shown in right side of Table 5.

The average k_{eff} and the standard deviation are 0.9992 ± 0.0061 and the average deviation from unity is 0.0046. As the results of this adjustment, the scattered trend from unity of k_{eff} is greatly improved.

5. Conclusion

1) An updated ENDF/B-IV LEOPARD library was provided for all materials in the code which is currently available at the National Energy Software Center (U.S.A.) and other nuclides which may be considered to be desirable additions.

2) The applicability of the updated library was assessed through benchmark tests for many light water-moderated critical assemblies.

The statistical values for the ratios of the calculated k_{eff}'s to the measured are 0.9954 ± 0.0152 for 44 UO_2-fueled cores, and 0.9988 ± 0.0093 for 15 mixed-oxide (PuO_2-UO_2) plutonium-fueled cores.

In case of mixed-oxide system, it will be disirable to use mixed source spectrum of fissile materials.

3) In order to determine library bias from the result of benchmark tests, adjustment works were carried out by testing the statistical effect of k_{eff}'s on 35 UO_2-fueled system.

Changing the epithermal peak scattering of U-238 from 42.164 barns to 26.667, the average k_{eff} and the standard deviation are 0.9999 ± 0.0073.

To reduce the scattered trend from unity, another adjustment was tested. Neglecting resonance scattering effects of U-238 and reducing ν of 0.8 % in the thermal region, the standard deviation and the average deviation from unity are improved to 0.61 % and 0.0046, respectively.

Thus, it is confirmed that the library from ENDF/B-IV, coupled with the use of LEOPARD code, leads to reasonable results for light water-moderated UO_2 fueled cores with the above adjustments.

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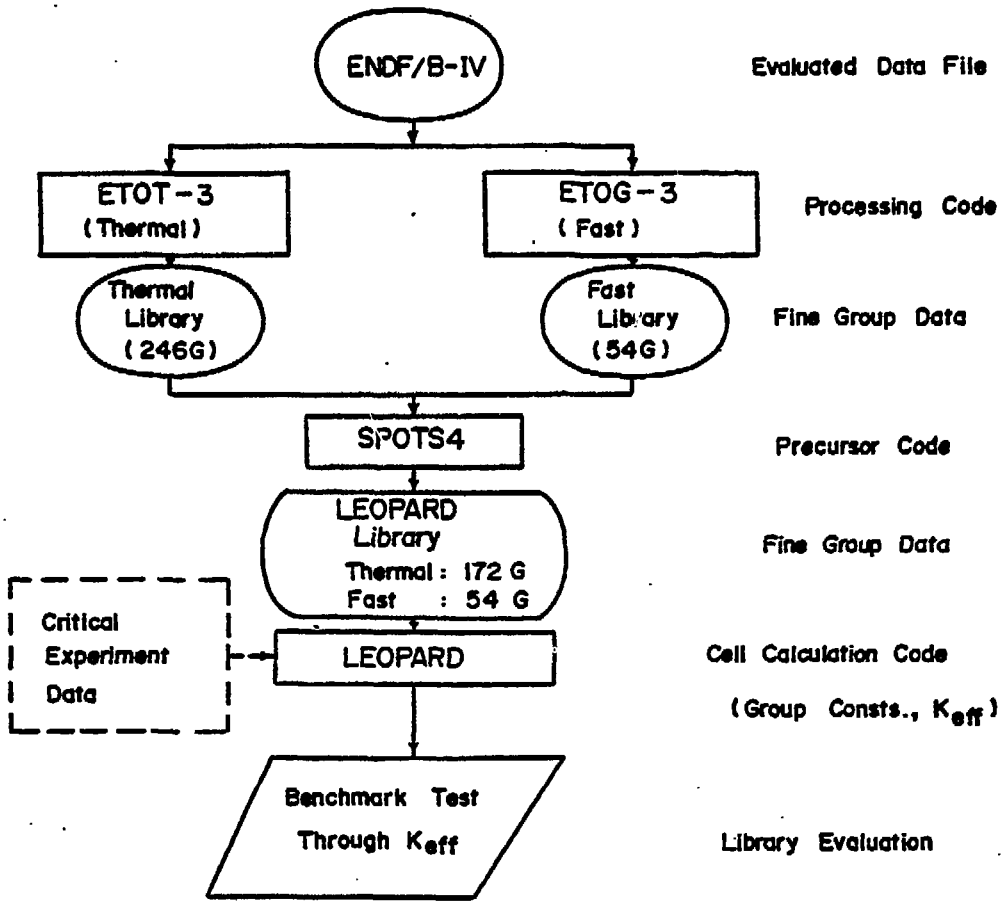

Fig. 1. Flow Diagram for Production and Benchmark Test of LEOPARD Library from ENDF/B-IV.

Table 1. Data for UO_2 Critical Experiments

Case No.	Enrich. at.%	H_2O:U Vol. Ratio	Fuel Den., g/cm^3	Pellet Dia. cm	Clad Mat.	Clad O.D. cm	Clad Thick. cm	Latt. Pitch cm	B-10 Conc. ppm	Crit. Buck. m^{-2}	Reference
1	2.734	2.18	10.18	.7620	SS 304	.8954	.04085	1.0287	0	40.75	10
2	2.734	2.93	10.18	.7620	SS 304	.8954	.04085	1.1049	0	53.23	10
3	2.734	3.86	10.18	.7620	SS 304	.8954	.04085	1.1938	0	63.26	10
4	2.734	7.02	10.18	.7620	SS 304	.8954	.04085	1.4554	0	65.64	11
5	2.734	8.49	10.18	.7620	SS 304	.8954	.04085	1.5621	0	60.07	11
6	2.734	10.38	10.18	.7620	SS 304	.8954	.04085	1.6891	0	52.92	11
7	2.734	2.50	10.18	.7620	SS 304	.8954	.04085	1.0617	0	47.50	12
8	2.734	4.51	10.18	.7620	SS 304	.8954	.04085	1.2522	0	68.80	12
9	3.745	2.50	10.37	.7544	SS 304	.8600	.04060	1.0617	0	68.30	12
10	3.745	4.51	10.37	.7544	SS 304	.8600	.04060	1.2522	0	95.10	12
11	3.745	4.51	10.37	.7544	SS 304	.8600	.04060	1.2522	0	95.38 +	13
12	3.745	4.51	10.37	.7544	SS 304	.8600	.04060	1.2522	456	74.64 +	13
13	3.745	4.51	10.37	.7544	SS 304	.8600	.04060	1.2522	709	63.66 +	13
14	3.745	4.51	10.37	.7544	SS 304	.8600	.04060	1.2522	1260	40.99 +	13
15	3.745	4.51	10.37	.7544	SS 304	.8600	.04060	1.2522	1334	38.39 +	13
16	3.745	4.51	10.37	.7544	SS 304	.8600	.04060	1.2522	1477	33.38 +	13
17	5.809	3.13	10.19	.9068	SS 304	.9931	.03810	1.3208	0	117.60	14
18	4.069	2.55	9.46	1.1278	SS 304	1.2090	.04060	1.5113	0	88.00	15
19	4.069	2.55	9.46	1.1278	SS 304	1.2090	.04060	1.5113	3392	17.20	15
20	4.069	2.14	9.46	1.1278	SS 304	1.2090	.04060	1.4500	0	79.00	15
21	3.037	2.64	9.28	1.1268	SS 304	1.2701	.07163	1.5550	0	50.75	16
22	3.037	8.16	9.28	1.1268	SS 304	1.2701	.07163	2.1980	0	68.81	16
23	4.069	2.59	9.45	1.1268	SS 304	1.2701	.07163	1.5550	0	69.25	16
24	4.069	3.53	9.45	1.1268	SS 304	1.2701	.07163	1.6840	0	85.52	16
25	4.069	8.02	9.45	1.1268	SS 304	1.2701	.07163	2.1980	0	92.84	16
26	4.069	9.90	9.45	1.1269	SS304	1.2701	.07163	2.3810	0	91.79	16
27	1.328	3.02	7.53	1.5265	Al	1.6916	.07110	2.2050	0	28.37	17
28	1.328	3.95	7.53	1.5265	Al	1.6916	.07110	2.3590	0	30.17	17
29	1.328	4.95	7.53	1.5265	Al	1.6916	.07110	2.5120	0	29.06	17
30	1.328	3.93	7.52	.9855	Al	1.1506	.07110	1.5580	0	25.28	17
31	1.328	4.89	7.52	.9855	Al	1.1506	.07110	1.6520	0	25.21	17
32	1.328	2.88	10.53	.9728	Al	1.1506	.07110	1.5580	0	32.59	17
33	1.328	3.58	10.53	.9728	Al	1.1506	.07110	1.6520	0	35.47	17
34	1.328	4.83	10.53	.9728	Al	1.1506	.07110	1.8060	0	34.22	17
35	2.490	2.84	10.24	1.0297	Al	1.2060	.08130	1.5113	1675	20.20	15

(continued)

36	2.096	2.06	10.38	1.5240	Al	1.6916	.07112	2.1737	0	58.00	18
37	2.096	2.06	10.38	1.5240	Al	1.6916	.07112	2.4052	0	80.60	18
38	2.096	4.12	10.38	1.5240	Al	1.6916	.07112	2.6162	0	85.70	18
39	2.096	6.14	10.38	1.5240	Al	1.6916	.07112	2.9891	0	77.00	18
40	2.096	8.20	10.38	1.5240	Al	1.6916	.07112	3.3255	0	61.60	18
41	2.628	1.50	10.40	1.2500	Al	1.4170	.07600	1.8490	0	83.30+	19
42	2.628	1.83	10.40	1.2500	Al	1.4170	.07600	1.9560	0	94.30+	19
43	2.628	2.48	10.40	1.2500	Al	1.4170	.07600	2.1500	0	98.30+	19
44	2.628	3.00	10.40	1.2500	Al	1.4170	.07600	2.2930	0	95.20+	19

* Hexagonal Lattice : All others are square.

\+ These bucklings were not measured directly but were inferred from critical loadings.

Table 2. Data for PuO_2-UO_2 Critical Experiments

Case No.	PuO_2 /Pu^{-240} w/o	H_2O:F Vol. Ratio	Fuel Den. g/cm^3	Pellet Dia. cm	Clad Mat.	Clad C.D. cm	Clad Thick. cm	Latt. Pitch cm	B-10 Conc. ppm	Crit. Buck. m^{-2}	Reference
45	2.0/ 7.65	2.51	9.54	1.283	Zr-2	1.443	0.076	1.753	0	69.1	20
46	2.0/ 7.65	18.37	9.54	1.283	Zr-2	1.443	0.076	3.505	0	50.3	20
47	2.0/ 7.65	9.70	9.54	1.283	Zr-2	1.443	0.076	2.694	0	95.4	20
48	2.0/ 7.65	7.76	9.54	1.283	Zr-2	1.443	0.076	2.479	0	105.9	20
49	2.0/ 7.65	7.76	9.54	1.283	Zr-2	1.443	0.076	2.479	261	83.7	20
50	2.0/ 7.65	7.76	9.54	1.283	Zr-2	1.443	0.076	2.479	526	63.1	20
51	2.0/ 7.65	2.48	9.54	1.283	Zr-2	1.443	0.076	1.753	526	58.3	20
52	2.0/ 7.65	2.48	9.54	1.283	Zr-2	1.443	0.076	1.753	261	62.6	20
53	2.0/ 7.65	3.43	9.54	1.283	Zr-2	1.443	0.076	1.905	0	90.0	20
54	2.0/23.5	7.80	9.54	1.283	Zr-2	1.443	0.076	2.479	0	79.5	20
55	2.0/23.5	9.72	9.54	1.283	Zr-2	1.443	0.076	2.694	0	73.3	20
56	3.01/22.02	2.42	6.056	1.065	Zr-2	1.223	0.070	1.825	0	80.8+	19
57	3.01/22.02	2.98	6.056	1.065	Zr-2	1.223	0.070	1.956	0	82.8+	19
58	3.01/22.02	4.24	6.056	1.065	Zr-2	1.223	0.070	2.225	0	77.9+	19
59	3.01/22.02	5.55	6.056	1.065	Zr-2	1.223	0.070	2.474	0	65.1+	19

+ These bucklings were not measured directly but were inferred from critical loadings.

Table 3. Comparison of Calculated Values of K_{eff} of Experimental UO_2 Critical Assemblies

Case Number	K_{eff}	Case Number	K_{eff}
1	0.97616	23	0.99140
2	0.98980	24	0.99570
3	0.99608	25	1.01099
4	1.00764	26	0.99464
5	1.00949	27	0.98997
6	1.00443	28	0.99622
7	0.98077	29	0.99605
8	0.99350	30	0.98875
9	0.98757	31	0.99201
10	1.00424	32	0.98872
11	1.00327	33	0.99608
12	0.99601	34	0.99595
13	0.99283	35	0.99229
14	0.98860	36	1.05256
15	0.98741	37	1.00991
16	0.98543	38	0.99327
17	1.00410	39	0.97454
18	0.98961	40	0.95412
19	0.98401	41	1.01933
20	0.97781	42	1.01055
21	0.98008	43	1.01463
22	0.98212	44	1.01839

Average K_{eff} : 0.99539
Standard Deviation : 0.01517
Average $|K_{eff} - 1.0|$: 0.01232

Without Case No. 36 through 44

Average K_{eff} : 0.99285
Standard Deviation : 0.00862
Average $|K_{eff} - 1.0|$: 0.00968

Table 4. Comparison of Calculated Values of K_{eff} of Experimental PuO_2-UO_2 Critical Assemblies

Case Number \ Source Spectrum	U - 235	Pu - 239
45	0.98645	0.98392
46	0.99625	0.99168
47	1.02306	1.01508
48	1.02273	1.01455
49	1.01051	1.00414
50	1.00083	0.99627
51	0.98553	0.99627
52	0.98913	0.98380
53	0.99927	0.99412
54	1.00813	1.00211
55	1.00637	1.00052
56	1.00579	0.99796
57	1.01178	1.00365
58	1.01292	1.00510
59	1.00909	1.00237
Average K_{eff} :	1.00451	0.99883
Standard Deviation :	0.01130	0.00930
Average $\lvert K_{eff} - 1.0 \rvert$:	0.01032	0.00730

Table 5. Comparison of Calculated Values of Experimental UO_2 Critical Assemblies by Data Adjustments

Case Number \ Adj. Method	1st * Method	2nd ** Method	Case Number \ Adj. Method	1st * Method	2nd ** Method
1	0.98896	0.99596	19	0.99245	0.99510
2	0.99960	1.00245	20	0.98786	0.99039
3	1.00380	1.00331	21	0.98899	0.99132
4	1.01201	1.00769	22	0.98524	0.97998
5	1.01307	1.00826	23	1.00004	1.00146
6	1.00743	1.00218	24	1.00236	1.00041
7	0.99216	0.99700	25	1.01413	1.00800
8	1.00012	0.99813	26	0.99712	0.99069
9	0.99850	1.00197	27	0.99804	0.99940
10	1.01068	1.00742	28	1.00252	1.00164
11	1.00970	1.00641	29	1.00111	0.99892
12	1.00239	1.00005	30	0.99690	0.99770
13	0.99918	0.99734	31	0.99857	0.99763
14	0.99492	0.99404	32	0.99792	1.00063
15	0.99372	0.99295	33	1.00361	1.00100
16	0.99172	0.99115	34	1.00157	0.99986
17	1.01191	1.01007	35	1.00093	1.00378
18	0.99837	0.99868			
			Average K_{eff} :	0.99993	0.99923
			Standard Deviation :	0.00730	0.00611
			Average $\lvert K_{eff} - 1.0 \rvert$:	0.00563	0.00459

* Changing the epithermal peak scattering of U-238 from 42.164 barns to 26.667

** Neglecting resonance scattering effects of U-238 and reducing $\bar{\nu}$ of 0.8 % in the thermal region