ORNL-TM-2880 (Rev.)
(ENDF 134R)

UKE-III: A COMPUTER PROGRAM FOR TRANSLATING NEUTRON CROSS SECTION DATA FROM THE UKAEA NUCLEAR DATA LIBRARY TO THE EVALUATED NUCLEAR DATA FILE FORMAT

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OPERATED BY UNION CARBIDE CORPORATION • FOR THE U.S. ATOMIC ENERGY COMMISSION

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Neutron Physics Division

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ABSTRACT

A computer program, UKE, has been written to translate neutron cross sections on computer tape from the United Kingdom Atomic Energy Authority Nuclear Data Library to the Evaluated Nuclear Data File, ENDF/B. The code will translate UK library smooth cross section data, secondary angular distributions, and secondary energy distributions to the ENDF/B format. No resonance parameters, thermal scattering data, or photon data are considered, however. The secondary angular distributions are translated as differential scattering probabilities only, and no Legendre expansion coefficients are given.

General information is presented concerning the format of the two libraries along with a detailed description of the translation from the UK secondary energy distribution laws to those of ENDF/B. Programming details and a user's guide are also presented.

COMPUTER CODE ABSTRACT

1. NAME: UKE-III
2. COMPUTER: UKE is designed to operate on computers of the IBM 360/50/65/75/91 and CDC 6600 class. Approximately 200K bytes or 50K words of directly addressable core are required.
3. PROBLEMS SOLVED: UKE reads a card image tape of data in the UK format and translates neutron cross sections, angular distributions, and secondary energy distributions to the ENDF/B card image format.
4. RESTRICTIONS: Since the UKE program employs fixed dimensions rather than flexible dimensions, it is important to be aware of the maximum values allowed for certain key variables such as: number of cross section data points for each reaction type ≤ 4000. A list of these restrictions is given in Section III of the referenced report.
5. TYPICAL MACHINE TIME: 10 seconds per nuclide on the IBM 360/91 (CPU time).
6. STATUS: UKE is in production use on the IBM 360/91 at the ORNL Computing Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee.
7. REFERENCE: R. Q. Wright, S. N. Cramer, and D. C. Irving, "UKE-III: A Computer Program for Translating Neutron Cross Section Data from the UKAEA Nuclear Data Library to the Evaluated Nuclear Data File Format," ORNL-TM-2880, Oak Ridge National Laboratory (Rev. Sept., 1973).

8. MACHINE REQUIREMENTS: Approximately 50K words of directly addressable core storage are needed by the program. Two tapes and four scratch data sets are needed in addition to the card reader, printer, and card punch.

9. PROGRAMMING LANGUAGE USED: The program is entirely in ASA standard FORTRAN (FORTRAN IV).

10. OPERATING SYSTEM: IBM OS/360 with the FORTRAN H compiler.

11. PROGRAMMING INFORMATION: UKE consists of 14 subroutines on approximately 1200 source cards.

12. USER INFORMATION: The code and report may be obtained from the Radiation Shielding Information Center (RSIC) at Oak Ridge National Laboratory.

I. INTRODUCTION

To a large extent the available compilations of evaluated neutron cross section data exist on computer tape in one of two formats. These are that of the United Kingdom Atomic Energy Authority Nuclear Data Library[1,2] and the Evaluated Nuclear Data File, ENDF/B[3]. Data from these libraries are not, in general, interchangeable due to differences in format conventions and theoretical models. The code described in this report has been developed to translate UK library smooth cross section data, secondary angular distributions, and secondary energy distributions to the ENDF/B format. No resonance parameters, thermal scattering data, or photon data are considered. The secondary angular distributions are translated as differential scattering probabilities only, and no Legendre expansion coefficients are given.

Section II of this report gives general information concerning the format of the two libraries. A detailed description of the translation from the UK secondary energy distribution laws to those of ENDF/B is also given here. Programming details and a user's guide are presented in Section III. A FORTRAN listing of the code is available from the Radiation Shielding Information Center, Oak Ridge National Laboratory.

II. TRANSLATION OF FORMAT AND MODELS USED

A. General Information

In order to understand the details of the UKE-III code, it is essential that the user be familiar with the ENDF/B and UK formats, and such familiarity is assumed in the discussions to follow. Only general information concerning the format of the two libraries will be considered here. The major subdivision in the UK format is the data file number, DFN. This corresponds to a material in the ENDF/B library which is designated by a material number, MAT. In the UK library, all reactions occurring for a particular DFN are classified by a five-digit "reaction type number" (R.T.N.) which is subdivided into a two-digit general classification number (G.C.N.) followed by a three-digit particular classification number (P.C.N.).

At the present time, the UKE-III code translates data for the following general classification numbers (G.C.N.)

G.C.N.	TYPE OF DATA
1	neutron cross sections
2	neutron angular distributions
3	neutron secondary energy distributions
4	miscellaneous quantities for neutron (ν, η, etc.)

The correspondence of the UK G.C.N. to ENDF/B is shown in Table 1.

Table 1. UK-ENDF/B Correspondence

G.C.N.	ENDF/B File No.
1	3
2	4
3	5

The UK particular classification numbers (P.C.N.) correspond to the reaction type number (MT) in the ENDF/B library. In the following sections we give the details involved in the translation for each UK general classification number.

B. Neutron Cross Sections (G.C.N. = 1)

Energies and corresponding cross sections are given in pairs in order of ascending energy. All cross sections are in barns and energies in MeV. With a few minor exceptions, the translation from UK to ENDF/B is completely straightforward. The energy region covered in the UK data may be divided into a number of ranges. When translating to ENDF/B, these energy ranges are combined into one energy range. Temperature dependence is not considered in the present code. When more than one temperature is encountered, data for the first temperature is translated and the rest of the data is ignored. A message is also written to indicate the number of different temperatures that were encountered. The reaction "Q" value is also translated to ENDF/B.

C. Angular Distributions (G.C.N. = 2)

Incident neutron energy variation may be considered either range-wise or point-wise in the UK library. When data are given range-wise, it is forced into point-wise representation by specifying the angular distribution twice - once at each end of the range before translating to ENDF/B. In the UK format, angular distributions may be specified in three ways:

1. Differential scattering probability versus scattering angle cosine.
2. Differential cross section (barns/steradian) versus scattering angle cosine.
3. Legendre polynomial expansion form.

The present code translates only data given in the differential scattering probability format. This is the only format used in the UK library at the present time. In a few cases, data are given where more than one angular distribution is given for the same energy range. Since this format is not allowed for in ENDF/B, a new distribution is constructed. This is accomplished by multiplying the differential scattering probability times the probability of the distribution and summing over the number of distributions.

D. Secondary Energy Distributions (G.C.N. = 3)

The UK secondary energy distributions are given by ten laws as described in ref. 2. There are also ten such laws for ENDF/B data (file #5, LF = 1,2,...10); however, in only a few cases is there a one-to-one correspondence between these laws. The following sections state each UK (G.C.N. = 3) law and the ENDF/B law to which the corresponding data has been translated. These changes were made after examination of the UK data, and certain theoretical manipulations are necessary. These approximations should be acceptable for the majority of the translated data, but individual users of the code may wish to relax or strengthen these changes as they see fit.

1. Law 1. Neutrons emitted with a known discrete energy, E', independent of the incident energy.

   This law is translated directly to LF = 2 with $\theta = E'$.

2. Law 2. Neutrons emitted with energy E' by

$$E' = k(E - E_d) \tag{1}$$

   where k = constant reduction factor

   E = incident energy

   E_d = some discrete energy

   a. When k = 1, Eq. (1) is an exact center-of-mass (CM) relationship for inelastic scattering from nuclear energy levels. In this case, Law 2 is translated directly to LF = 3 with $\theta = E_d$, the discrete energy loss.

   b. If $k < 1$ ($k > 1$ is not considered), but is in the range

$$0.99 \frac{(A^2 + 1)}{(A + 1)^2} \leq k < 1.0, \tag{2}$$

   Law 2 is converted to LF = 3 under the assumption that Law 2 is represented in the following form. Cashwell and Everett[4] show that in the L system

$$E' = \frac{(A^2 + 1)}{(A + 1)^2} E - \left(\frac{A}{A + 1}\right)\theta + \frac{2AE\mu}{(A + 1)^2} \left[1 - \left(\frac{A + 1}{A}\right)\frac{E}{\theta}\right]^{\frac{1}{2}} \tag{3}$$

   where E = incident L energy

   E' = final L energy

   θ = inelastic scattering energy loss

A = nuclide mass

μ = cosine of the CM scattering angle

Assuming scattering to be symmetric about $\mu = 0$, the angular integrated form of Eq. (3) is desired to justify the transformation.

$$E' = \frac{(A^2 + 1)}{(A + 1)^2}\left[E - \left(\frac{A^2 + A}{A^2 + 1}\right)\theta\right] \tag{4}$$

In translating Law 2 data to LF = 3 when k obeys the condition in Eq. (2), the ENDF/B energy loss is chosen as

$$\theta = \left(\frac{A^2 + 1}{A^2 + A}\right)E_d \tag{5}$$

The factor 0.99 in Eq. (2) is included to account for any round-off errors associated with the original data.

c. If $k < 0.99(A^2 + 1)/(A + 1)^2$, Law 2 is converted to the general evaporation spectrum, LF = 5. Writing Eq. (1) as

$$\frac{E'}{E - E_d} = k, \tag{6}$$

it is assumed that

$$g(x) = \delta\left[\frac{E'}{E - E_d} - k\right] \tag{7}$$

where $x = \frac{E'}{\theta}$

and $\theta = E - E_d$

Interpolation for θ is assumed linear between $(E_1 - E_d)$ and $(E_2 - E_d)$, where E_1 and E_2 are the boundaries of the incident energy range. The delta function approximation for g(x) is given in Table 2.

Table 2. General Evaporation Spectrum

x	g(x)
0.9 k	0
k	10/k
1.1 k	0

For multiple particle reactions, (n,2n) and (n,3n), where the incident energy dependent distribution probabilities are not described with cross section data, as with the inelastic level scattering, the ENDF/B probabilities for each secondary neutron are computed by multiplying the probability of the UK law (given on Card #2 in the UK format) times the distribution probability on Card #3 divided by the number of secondary neutrons. This method applies for any law.

3. Law 3. <u>Continuous normalized spectrum independent of incident energy</u>.

   a. If Law 3 applies to a fission reaction (P.C.N. = 18), an attempt is made to translate the associated distribution to LF = 6. The fit is accomplished by comparing the average energy of the UK distribution, $\overline{E}_d$, with that of the ENDF/B equation, $\overline{E}_f$, where

$$\overline{E} = \frac{\int_0^{E_m} E\, f(E) dE}{\int_0^{E_m} f(E) dE} \tag{8}$$

The E_m in Eq. (8) is the maximum energy for which there is UK data.

The f(E) used in the calculation of $\overline{E}_f$ is

$$f(E) = \sqrt{\frac{4E}{\pi\theta^3}}\ e^{-E/\theta} \tag{9}$$

where θ = constant nuclear temperature for fission.

The maximum value of f(E) in Eq. (9) occurs when $E = \theta/2$.

The value of θ, θ_{pl}, for use in f(E) in the calculation of $\overline{E}_f$ from Eq. (8) and (9) is chosen as twice the energy of the maximum f(E) from the UK data. If this f(E) has a flat top, twice the mid-energy of this flat range is used. It is assumed that any UK distributions with more than one maximum will be rejected according to the scheme to be described.

A fit of Law 3 to LF = 6 for fission reactions is accepted if

$$0.84 \leq \frac{\overline{E}_d}{\overline{E}_f} \leq 1.16 \tag{10}$$

This acceptance interval was selected after examination of this ratio for several UK distributions. The constant in Eq. (9) for the translation of Law 3 data to LF = 6 is then chosen as

$$\theta = \frac{\bar{E}_d}{\bar{E}_f}\,\theta_{pl} \tag{11}$$

$$\text{where } \bar{E}_f = \frac{3\theta_{pl}}{2}\,(1 - Y_1) \tag{12}$$

$$Y_1 = \frac{\frac{2}{3}\,X_1^{3/2}\,e^{-X_1}}{\frac{\sqrt{\pi}}{2}\,\mathrm{erf}\,(\sqrt{X_1}) - \sqrt{X_1}\,e^{-X_1}} \tag{13}$$

$$\text{and} \quad X_1 = \frac{E_m}{\theta_{pl}} \tag{14}$$

The $\bar{E}_d$ is determined by numerical integration of the data. The distribution is first represented as

$$f(E) = \alpha_i\,E + \beta_i \tag{15}$$

where $E_i \leq E \leq E_{i+1}$ $\quad i = 1, \ldots m-1$

and m is the number of data points.

The α_i and β_i are

$$\alpha_i = \frac{f_{i+1} - f_i}{E_{i+1} - E_i} \tag{16}$$

$$\beta_i = \frac{f_i\,E_{i+1} - f_{i+1}\,E_i}{E_{i+1} - E_i} \tag{17}$$

Combining Eqs. (8), (15), (16), and (17) yields

$$\bar{E}_d = \frac{\sum_{i=1}^{m} C_i\ E_i^3 + 3(f_1 E_1^2 - f_m\ E_m^2)}{\sum_{i=1}^{m} C_i\ E_i^2 + 6(f_1 E_1 - f_m\ E_m)} \tag{18}$$

where $C_i = \alpha_{i-1} - \alpha_i$ (19)

and $\alpha_0 = \alpha_m = 0$ (20)

If the condition in Eq. (10) is not satisfied, fit Law 3 to LF = 4 with $g(x) = f(E')$ and $\theta = 1$.

b. When Law 3 refers to a non-fission distribution, translate to LF = 1 where

$$g(E' \leftarrow E_1) = f(E')$$

and $g(E' \leftarrow E_2) = f(E')$.

4. Laws 4, 5, and 6. <u>Neutrons of incident energy E and final energy E' distributed by the general form</u>

$$f(E'/E^q)$$

<u>where q may have values 0, 1/2, or 1.</u>

An attempt is made to fit these distributions to an evaporation model

$$f(E) = \frac{E}{\theta^2}\ e^{-E/\theta} \tag{21}$$

This fit is identical in procedure to that for the Maxwellian model for Law 3. The maximum value of Eq. (21) occurs when $E = \theta$. The θ_{p2} used in the calculation of $\bar{E}_f$ from Eq. (8) and (21) is the energy of the maximum value of the distribution obeying Law 4, 5, or 6. In this case

$$\bar{E}_f = 2\theta_{p2}\, Y_2 \tag{22}$$

where $$Y_2 = 1 - \frac{X_2^2}{2}\, \frac{e^{-X_2}}{1 - e^{-X_2} - X_2\, e^{-X_2}} \tag{23}$$

and $$X_2 = \frac{E_m}{\theta_{p2}} \tag{24}$$

The $\bar{E}_d$ for the Law 4, 5, and 6 data is calculated exactly the same as that for the Law 3 fission data. The fit of $f(E'/E^q)$ to the evaporation model is considered successful if

$$0.94 \le \frac{\bar{E}_d}{\bar{E}_f} \le 1.06 \tag{25}$$

In this situation Law 4 is converted to LF = 8 and Laws 5 and 6 to LF = 9. Table 3 gives the forms of the evaporation model to be used.

Table 3. Nuclear Temperatures

UK Law	ENDF/B LF #	$\theta(E)$	$\theta(E)$ Interpolation
4	8	θ_{p2}	Constant
5	9	$\theta_{p2}\sqrt{E}$	Log-log
6	9	$\theta_{p2}\, E$	Linear

If the distributions for Laws 4, 5, or 6 do not satisfy Eq. (25), these laws are translated as:

Law 4 - treat as Law 3 (non-fission)

Law 5 - treat as Law 3 (non-fission)

Law 6 - treat as Law 3 (non-fission)

5. Laws 7, 8, and 9 are omitted.

6. Law 10. Neutrons emitted with secondary energy distribution

$$f(E') = \frac{E'}{T^2} e^{-E'/T} \tag{26}$$

where $T = \sqrt{E/A}$

This law is translated directly to LF = 9 with $\theta(E) = \sqrt{E/A}$ and log-log interpolation between $\theta(E_1)$ and $\theta(E_2)$ where E_1 and E_2 are the energy boundaries of the distribution.

Table 4 summarizes the translation of the UK secondary energy distributions to ENDF/B.

Table 4. Secondary Energy Distributions

UK Law	ENDF/B LF #
1	2
2	3, 5
3	1, 4, 6
4	1, 8
5	1, 9
6	1, 9
7, 8, 9	not translated
10	9

E. Miscellaneous Quantities for Neutrons (G.C.N. = 4)

The quantity $\nu(E)$ is the only UK miscellaneous quantity processed by the UKE-III code. These data are translated directly to ENDF/B file 1, MT = 452. Log-log interpolation is used for the $\nu(E)$ tabulation.

III. PROGRAM DESCRIPTION

The UKE-III program reads a card image tape of data in the UK format and translates neutron cross sections, angular distributions, and secondary energy distributions to the ENDF/B card image format. It consists of a main program and 13 subroutines. All ENDF/B data cards are written on tape and an option is provided to list the tape at the end of the run.

Data is given on the UK tape in order of the reaction type number, e.g., 1015, 2015, 3015. 1015 data will be translated to ENDF/B file 3, reaction type 91; 2015 data will be translated to ENDF/B file 4, reaction type 91; 3015 data will be translated to ENDF/B file 5, reaction type 91. Because of this ordering of the data on the UK tape, scratch tapes are used for the file 4 and file 5 data. The neutron angular distribution data is written on scratch tape ITP1 and the secondary energy distribution data is written on scratch tape ITP2. After all data for a given UK data file has been processed, the data on the scratch tapes is read back and ENDF/B files 4 and 5 are constructed. The ENDF/B data for the material can then be written on the ENDF/B tape. Any number of materials can be processed in a single run by stacking the data cards (see input description).

A. Input Description

The input data for the UKE-III program is described below.

CARD NO. 1 (2I5,16A4,A2)

ITEM	COLS.	NAME	DESCRIPTION
1	1-5	LABEL	ENDF TAPE LABEL
2	6-10	LISTIT	1, LIST ENDF/B TAPE 0, DO NOT LIST
3	11-76	B(N)	ENDF/B TPID RECØRD

CARD NO. 2 (3I5,E10.0,5A4,2E10.0)

1	1-5	IDFN	UK DATA FILE NUMBER
2	6-10	*LFI	0, material is non-fissile 1, material is fissile
3	11-15	MAT	ENDF/B material number
4	16-25	ZA	(Z,A) designation
5	26-45	H(N)	material identification
6	46-55	SPI	nuclear spin
7	56-65	AP	scattering radius

Repeat card 2 for each additional material desired. These cards should have the same order as the data file numbers on the UK tape.

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*LFI=1 if reaction type 4018 is given on the UK tape and 0 otherwise.

B. List of Subroutines

1. MAIN - read input data, control flow of the program, write out ENDF/B data cards.
2. SEARCH - search UK tape for desired data file number.
3. GCN1 - read neutron cross sections.
4. GCN2 - read angular distribution data.
5. GCN3 - read energy distributions of secondary neutrons.
6. GCN4 - read GCN4 data.
7. HEAD - write an ENDF/B HEAD record.
8. HOLL - write hollerith information for ENDF/B file 1.
9. WTAB1 - write an ENDF/B TAB1 record.
10. CONT - write an ENDF/B CONT record.
11. TERPO - interpolation routine.
12. GETMT - determine ENDF/B MT number from the UK particular classification number (P.C.N.).
13. NTAPE - read scratch files and construct the final ENDF/B tape.
14. SØRT - sort the ENDF/B file 1 index into order of increasing MT number.

C. UKE-III I/Ø Units

DESIGNATION	LOGICAL NO.	PURPOSE
ITP1	1	SCRATCH DEVICE
ITP2	2	SCRATCH DEVICE
INTAPE	4	UK TAPE
	5	CARD READER
	6	PRINTER
ITP8	8	SCRATCH DEVICE
ITP9	9	SCRATCH DEVICE
NDFB	10	ENDF/B TAPE

D. Limitations

The following is a tabulation of the dimensional limitations in UKE-III:

1. maximum number of cross section data points for each reaction type - 4000.
2. maximum number of reaction types on UK tape - 80 per material.
3. maximum number of interpolation regions for ENDF/B data - 10.
4. maximum number of UK reaction types which have angular distribution data (GCN=2) - 50 per material.
5. maximum number of UK reaction types which have secondary energy distribution data (GCN=3) - 50 per material.

APPENDIX

The Radiation Shielding Information Center (RSIC) at Oak Ridge National Laboratory was asked by the National Neutron Cross Section Center (NNCSC) at Brookhaven National Laboratory to sponsor the translation of the UKNDL Version 3 library into ENDF format. The library was received on 5 tapes (805 - 809) from NNCSC and was translated into ENDF format using UKE-III.

The original and translated libraries are available to ORNL users via RSIC. Other prospective users should request the data from NNCSC.

Table A-1 gives the contents of the translated library; the UKNDL data file number (DFN), the ENDF material number (MAT), and the number of BCD records are given for each material.

Information about older versions of the UKNDL library is given in refs. 5-7. A numerical abstract of the files in version 3 of the UKNDL library is presented in ref. 8 which gives for each data file thermal values, resonance integrals, fission-spectrum averages, and the energy range spanned by every partial cross-section. A more extensive summary is in process of reproduction as AEEW-M1208.

Table A-1. Contents of the Translated Library

Tape	DFN	Material	MAT	Records	Tape	DFN	Material	MAT	Records
805	923	H	8101	343	807	79	Nb-93	8132	5669
	905	D in D_2O	8102	1111		81	Mo	8133	1457
	252	T	8103	676		973	Ag-107	8134	1286
	220	He-3	8104	243		974	Ag-109	8135	1369
	221	He-4	8105	290		70	Cd	8136	2323
	914	Li-6	8106	1510		71	Cd-113	8137	1199
	215	Li-7	8107	902		4	Xe-135	8138	103
	967	Be-9	8108	603		921	Eu-151	8139	4007
	90	B-10	8109	608		922	Eu-153	8140	4750
	49	B-11	8110	821		328	Ta	8141	2204
	902	C	8111	1544		213	W	8142	378
	259	N	8112	3664					
	933	O	8113	1371					
	23	F-19	8114	398	808	222	Au-197	8143	968
	182	Na-23	8115	1762		26	Pb	8144	533
	35	Al-27	8116	1306		930	Th-232	8145	1055
	25	Si	8117	399		86	Pa-233	8146	981
	141	Cl	8118	563		87	U-233	8147	1876
	84	K	8119	2804		953	U-234	8148	944
	138	Ca	8120	362		159	U-235	8149	4317
	190	Ti	8121	1150		954	U-236	8150	870
	952	V	8122	935		160	U-238	8151	5868
	45	Cr	8123	1085		276	U-239	8152	1068
						277	U-240	8153	1049
						274	Pu-238	8154	634
806	906	Fe	8124	7720					
	908	Fe	8125	8164					
	907	Ni	8126	3757	809	161	Pu-239	8155	3575
	73	Cu	8127	3274		404	Pu-239	8156	4591
	250	Cu-63	8128	84		402	Pu-240	8157	2822
	251	Cu-65	8129	88		77	Pu-240	8158	1180
	105	Ga	8130	366		403	Pu-241	8159	1792
	82	Zr	8131	1958		60	Pu-241	8160	1982
						975	Pu-242	8161	1541
						956	Am-241	8162	1305
						957	Am-243	8163	666
						976	Cm-244	8164	2077

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