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Coupled Neutron and Photon Cross Sections for Transport Calculations

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COUPLED NEUTRON AND PHOTON CROSS SECTIONS
FOR TRANSPORT CALCULATIONS

by

R. J. Barrett and R. E. MacFarlane

ABSTRACT

A compact set of multigroup cross sections and transfer tables for use in neutron and photon transport calculations has been prepared from ENDF/B-IV using the NJOY processing system. The library includes prompt and steady-state coupled sets for neutrons and photons in FIDO format, prompt and steady-state fission spectra (χ vectors) for the fissionable isotopes, and a table of useful response functions including heating and gas production. These multigroup constants should be useful for a wide variety of problems where self-shielding is not important.

I. INTRODUCTION

Multigroup methods of solving the Boltzmann equation for neutron transport have been implemented in a number of computer codes, including ONETRAN.[1] Cross section input for these codes is traditionally in the form of group-to-group transfer tables (Fig. 1) accompanied by an absorption cross section ($\sigma_{a,g}$) a fission neutron production cross ($\nu\sigma_{f,g}$) and a total cross section ($\sigma_{t,g}$) for each group (g). A useful variation of this format, known as the coupled set, allows the simultaneous transport of neutrons and photons by treating the photon energy groups as if they were the lowest energy neutron groups. For example, a 42 group coupled set might have 30 neutron groups followed by 12 photon groups. This scheme makes sense physically, because neutrons can "downscatter" into the photon groups (photon production) but photons do not (appreciably) "upscatter" into the neutron groups (see Fig. 2).

Coupled sets for a number of important materials have been produced by LaBauve[2] and Seamon[3] using data from ENDF/B-III and IV.[4] The present work is intended as a replacement for those data sets, and represents a marked improvement insofar as there are many more materials and a much more complete set of response functions.

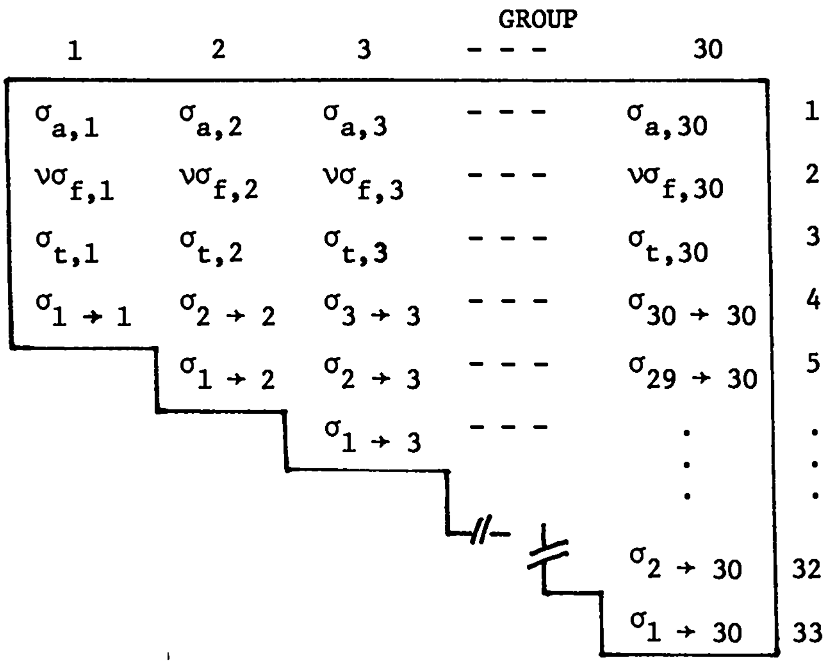

Fig. 1.
Arrangement of cross sections in a transfer table.

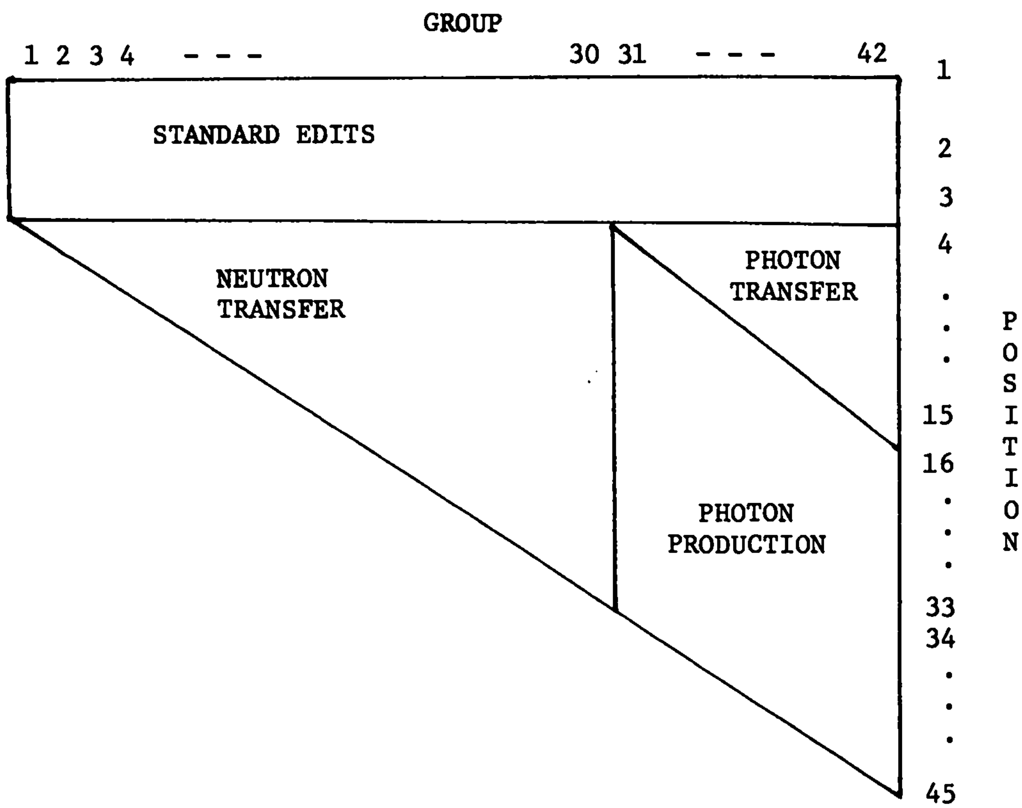

Fig. 2.
Arrangement of data in a coupled set.

II. GENERAL FEATURES

Basic evaluated data from ENDF/B-IV were used for all materials in the library except Li-6A, Be-9A and C-12A, which were based on local LASL evaluations.[5,6,7] The NJOY[8] code system was used to process the cross sections. The point cross section linearization and resonance reconstruction tolerance was 0.5%, and all cross sections were Doppler broadened to 300 K. Cross sections were averaged over 30-neutron and 12-photon energy groups (Table I) using the Bondarenko flux approximation[9] with a fusion-fission-1/E-thermal weight function. Neutron-transport, photon-production and photon-transport data in five Legendre orders were all stored on the same computer file in MATXS format. The final processing step involved several runs with the TRANSX[10] code, which translates MATXS files into the formats used in Sn codes.

The library described here consists of several computer files, as detailed below.

TABLE I

GROUP BOUNDARIES IN ELECTRON VOLTS

Group	Maximum Energy	Group	Maximum Energy
1	1.70000E+07	1	2.00000E+07
2	1.50000E+07	2	9.00000E+06
3	1.35000E+07	3	8.00000E+06
4	1.20000E+07	4	7.00000E+06
5	1.00000E+07	5	6.00000E+06
6	7.79000E+06	6	5.00000E+06
7	6.07000E+06	7	4.00000E+06
8	3.68000E+06	8	3.00000E+06
9	2.86500E+06	9	2.00000E+06
10	2.23200E+06	10	1.00000E+06
11	1.73800E+06	11	5.00000E+05
12	1.35300E+06	12	1.00000E+05
13	8.23000E+05		
14	5.00000E+05	EMIN	1.00000E+04
15	3.03000E+05		
16	1.84000E+05		
17	6.76000E+04		
18	2.48000E+04		
19	9.12000E+03		
20	3.35000E+03		
21	1.23500E+03		
22	4.54000E+02		
23	1.67000E+02		
24	6.14000E+01		
25	2.26000E+01		
26	8.32000E+00		
27	3.06000E+00		
28	1.13000E+00		
29	4.14000E-01		
30	1.52000E-01		
EMIN	1.39000E-04		

III. TRANSFER TABLES

Coupled sets of P_3 transfer tables were transport-corrected with the "inflow" approximation, in which the P_0 total cross section ($\sigma_{t,g}$) and the inscatter term for each Legendre order are corrected for the P_4 component of all scattering into the group, according to the equations

$$\sigma_{t,g} \rightarrow \sigma_{t,g} - \sum_{g'} \sigma_{4,g' \rightarrow g}\, \phi_{g'}/\phi_g \quad ,$$

$$\sigma_{n,g \rightarrow g} \rightarrow \sigma_{n,g \rightarrow g} - \sum_{g'} \sigma_{4,g' \rightarrow g}\, \phi_{g'}/\phi_g \quad ,$$

where the suffix (n) refers to Legendre order and ϕ_g is the P_0 weighted group-average flux weight function. The $\nu\sigma_f$ vector was calculated by summation of the full rectangular fission matrix

$$\nu\sigma_{f,g} = \sum_{g'} \sigma_{f,g \rightarrow g'} \quad .$$

The absorption cross section ($\sigma_{a,g}$) is simply a neutron balance, calculated from the total cross section and the P_0 transfer matrix according to the equation,

$$\sigma_{a,g} = \sigma_{t,g} - \sum_{g'} \sigma_{0,g \rightarrow g'} \quad .$$

For the more important fissile nuclides, the partial fission reactions, (n,f), (n,n'f), (n,2nf) and (n,3nf) are given in ENDF/B-IV in addition to the fission total. Because the neutrons emitted prior to fission have a quite different energy distribution from those emitted during fission, we have separated them from the $\nu\sigma_f$ and χ vectors and added them to the transfer matrix.

Separate files are given for prompt and steady-state data (see below). Both files are in FIDO format. The $2\ell + 1$ factor is not included, and a header card is included for each table.

A. Prompt Transfer Tables

The reference set of transfer tables consists of 73 isotopes, elements and mixtures as specified in Tables II and III. In this set, only the prompt secondary neutrons from fission are included in $\nu\sigma_f$, and only prompt photon production is included in the transfer matrix. Photon production data are not available in ENDF for all isotopes, and the photon production portion of the transfer matrix is non-zero only for those materials specified in Table II. Photon interaction data for Pu were used in the tables for all isotopes of Americium, Curium and Californium.

TABLE II

Material	γ-Production	Material	γ-Production	Material	γ-Production
H-1	X	V	X	U-235	X
H-2	X	Cr	X	U-236	
H-3		Mn-55	X	U-237	X
He-3		Fe	X	U-238	X
He-4		Co-59	X	U-239	X
Li-6	X	Ni	X	Np-237	
Li-6A	X	Cu	X	Pu-238	
Li-7	X	Zirc2		Pu-239	X
Be-9	X	Nb-93	X	Pu-240	X
Be-9A	X	Mo	X	Pu-241	
B-10	X	Rh-103		Pu-242	
B-11		Ag-107		Am-241	
C-12	X	Ag-109		Am-243	
C-12A	X	Cd		Cm-244	
N-14	X	Ta-181	X	Cm-245	X
O-16	X	W	X	Cm-246	X
F-19	X	Re-185		Cm-247	X
Na-23	X	Re-187		Cm-248	X
Mg	X	Au-197		Cf-249	X
Aℓ-27	X	Pb	X	Cf-250	X
Si	X	Th-232		Cf-251	X
Cℓ	X	Pa-233		Cf-252	X
K	X	U-233		STANLS	X
Ca	X	U-234		CONCRT	X
Ti	X				

TABLE III

COMPOSITIONS OF MIXED MATERIALS IN THE PROMPT TRANSFER TABLES

Material	Constituents	Concentration (%)
W	W-182	26.3
	W-183	14.3
	W-184	30.8
	W-186	28.6
STANLS	Fe	67.2
	Ni	7.8
	Cr	21.0
	Mn-55	2.0
	Si	2.0
CONCRT	H-1	8.5
	O-16	60.4
	Na-23	0.9
	Mg	0.3
	Aℓ	2.5
	Si	24.2
	K	0.7
	Ca	2.0
	Fe	0.5

B. Steady State Tables

For several isotopes (Table IV), there is information available concerning the yield and energy distribution of delayed neutrons from fission and delayed photon from fission and other reactions. A separate set of coupled group-to-group transfer tables, which include the delayed contribution, has been generated for use in steady state neutronics calculations.

Because the delayed neutron contribution has always been considered important for reactor calculations, the capability exists to add it to $\nu\sigma_f$ in an automatic way within the MATXS-TRANSX framework. Furthermore, most of the delayed neutrons are emitted within a few seconds of the original interaction, and there is no ambiguity over which neutrons should be included or excluded for a particular application.

However, because the delayed photon contribution has not traditionally been included in steady state transfer tables, the capability for handling it automatically does not yet exist, and the numbers had to be added to the matrix through an ad-hoc modification of the TRANSX code.

Delayed photon yields and spectra from the fission reaction have been calculated, as a function of cooling time, by CINDER[11] and related codes,[12] for inclusion in the ENDF system. Using the FITPULS[13] program, we have calculated photon-group-averaged constants (α and λ) which fit the time dependence of the photon yields with a summation of the type

$$f_g(t) = \sum_{i=1}^{n} \alpha_{i,g} e^{-\lambda_{i,g} t} ,$$

where g is the photon group index. By including all delayed photons emitted out to infinite cooling times, we were able to simplify the calculation of delayed photon yields for a given photon group to the summation

$$Y_g = \sum_{i=1}^{n} \frac{\alpha_{i,g}}{\lambda_{i,g}} ,$$

TABLE IV

MATERIALS INCLUDED IN THE STEADY-STATE TRANSFER TABLES

Material	Material
Be-9	Mo
Be-9A	Th-232
B-11	U-233
Na-23	U-235
Cr	U-238
Fe	Pu-239
Ni	Pu-240
Cu	Pu-241
Nb-93	STANLS
	CONCRT

Because the yield of photons falls off rapidly with time, the error introduced by our choice of infinite cooling time is small compared with the uncertainties present in both the prompt and delayed photon yields.

The dependence of yield on incident neutron energy is weak, and the yields have been assumed to be independent of neutron energy for all isotopes except U-235 and U-238, where a separate set of yields was used for neutron energies above 10 MeV.

For reactions other than fission, a select group of discrete photons (Table V) were included. Selection of these photons from among the hundreds of potential candidates was based on a combination of half-life, photon energy and the importance of the isotope.

TABLE V

DISCRETE DELAYED PHOTONS INCLUDED IN STEADY STATE TABLES

Evaluation	Reaction	Photon Energy (MeV)	Photon Group
Be-9	(n,p)	2.43	8
Be-9A	(n,p)	2.43	8
B-11	(n,γ)	7.66	3
	(n,p)	2.14	8
		5.86	5
		6.81	4
		7.97	3
Na-23	(n,γ)	1.37	9
		2.75	8
	(n,p)	0.44	11
	(n,α)	1.63	9
Cu	(n,p)	1.00	9
Fe	(n,p)	0.85	10
		1.81	9
		2.11	8
Ni	(n,2n)	1.37	9
		1.89	9
	(n,np)	SEVERAL	11
	(n,p)	0.81	10
		0.87	10
Cu	(n,p)	SEVERAL	9
	(n,α)	SEVERAL	9
Nb-93	(n,2n)	0.93	10
		0.90	10
Mo	(n,3n)	SEVERAL	11
Th-232	(n,γ)	SEVERAL	11
U-238	(n,2n)	SEVERAL	11
	(n,γ)	SEVERAL	11

IV. RESPONSE FUNCTIONS

It is difficult to anticipate what response functions the general user would want to have available for editing with calculated fluxes. Experience with past requests for data and discussions with several potential users has led us to settle on the 15 response functions described below. The response function file contains all materials for which prompt transfer tables are available (Table II).

The response functions in their order of appearance are as follows.

A. PHEAT

Prompt local heat deposition (in Joule-barns) for both neutrons and photons was calculated by the energy balance method; i.e., by subtracting the average secondary neutron and photon energies from the total available energy (incident kinetic energy plus reaction energy). Inconsistencies in some evaluations between the neutron and photon secondary yields, has resulted in inaccurate (and even negative) heating numbers in some cases.

B. THEAT

The total heat deposition is defined as the sum of the prompt heat described above and the delayed heating from β-decay. For the fission reaction, the average delayed heat was taken from Sher, Fiarman and Beck.[14] Other reactions were included only for materials of significant importance in a wide variety of calculations (Table VI). Furthermore, only those β-decays with half-lives of less than 10 days were included. This latter criterion was based on Abdou's[15] observation that longer-lived decays tend to have significantly less β energy.

C-G. HPROD, DPROD, TPROD, BPROD, APROD

All possible reactions involved in the production of ^{1}H, Deuterium, Tritium, ^{3}He, and ^{4}He respectively have been summed with proper weighting to produce these five response functions. For example, the APROD edit includes the $(n,n')3\alpha$ reaction with a weight of 3.0.

H. PARAB

Parasitic absorption includes all reactions in which the incident particle is not reemitted. For neutrons, this includes (n,γ), (n,p), $(n,t\alpha)$ .... For photons, it is the photoelectric cross section.

I. DEPLET

This edit, defined as the probability that a target neucleus will be transformed to another species, is simply the sum of all cross sections except elastic and inelastic.

J. N2N

The $(n,2n)$ reaction edit includes the $(n,2n)2\alpha$ for some materials.

K. N3N

The $(n,3n)$ reaction is included as well as the $(n,4n)$ with a multiplication of 1.5.

L. NGAM

The radiative capture (n,γ) reaction is tabulated.

TABLE VI

ACTIVATION REACTIONS INCLUDED IN TOTAL HEATING (THEAT) EDIT

Evaluation	Reaction	Heating (MeV)
Li-6 and Li-6A	(n,p)	1.56
Li-7	(n,d)	1.56
	(n,γ)	9.16*
Be-9 and Be-9A	(n,p)	7.84
	(n,α)	1.56
	(n,d)	9.16*
B-11	(n,γ)	6.59
	(n,p)	4.85
	(n,α)	9.16*
O-16	(n,p)	2.69
Na-23	(n,γ)	0.55
	(n,p)	1.92
	(n,α)	2.48
Cr	(n,p)	1.07
Fe	(n,p)	0.82
Ni	(n,2n)	0.18
Cu	(n,2n)	0.96
Cu	(n,γ)	0.42
Cu	(n,^{3}He)	0.86
Cu	(n,nα)	0.16
Cu	(n,p)	0.19
Cu	(n,α)	0.47
Nb-93	(n,γ)	0.22
	(n,α)	0.93
Mo	(n,γ)	0.24
	(n,2n)	0.25
Pb	(n,γ)	0.09
Th-232	(n,2n)	0.07
	(n,γ)	0.34
U-238	(n,2n)	0.06
	(n,γ)	0.16

M. FISSN

The fission cross section (σ_f), not $\nu\sigma_f$, is given.

N. NUSIGF

Same as $\nu\sigma_f$ in the transport tables.

O. TOTAL

Same as σ_t in the transport tables.

For ease in editing, the response functions are given in 6E12.5 format. The table for each material starts with a title card (for example, "AL-27 EDITS"). Seven cards follow for each response function, for a total of 106 cards per material.

V. FISSION SPECTRA

Both prompt and steady-state (prompt plus delayed) fission neutron spectra (χ-vectors) are available in 6E12.5 format for the 26 materials listed in Table VII. The prompt spectra were generated from the fission transfer matrix according to the formula

$$\chi_g = \sum_{g'} \sigma_{f,\, g' \rightarrow g} \times \phi_{g'} \Big/ \sum_{g} \sum_{g'} \sigma_{f,g' \rightarrow g} \times \phi_{g'} \quad ,$$

where ϕ_g is the group-averaged, P_0 weighted flux for group (g).

The steady state spectra were obtained by factoring in the delayed neutron yield (ν_d) and spectrum (χ_d)

$$\chi_{ss,g} = \sum_{g'} \phi_{g'} \left[\sigma_{f,g' \rightarrow g} + \nu_d \times \sigma_{f,g'} \chi_{d,g}\right] \Big/ \text{NUME} \quad ,$$

where NUME is the summation over (g) of the quantity in the denominator

$$\text{NUME} = \sum_{g} \sum_{g'} \phi_{g'} \left[\sigma_{f,g' \rightarrow g} + \nu_d \sigma_{f,g'} \chi_{d,g}\right] \quad .$$

TABLE VII

MATERIALS FOR WHICH FISSION NEUTRON (χ) VECTORS ARE GIVEN

Th-232*	Pu-241*
Pa-233	Am-242
U-233*	Am-241
U-234	Am-243
U-235*	Cm-244
U-236	Cm-245
U-237	Cm-246
U-238*	Cm-247
U-239	Cm-248
Np-237	Cf-249
Pu-238	Cf-250
Pu-239*	Cf-251
Pu-240*	Cf-252

*Denotes isotopes for which steady state spectra are given.

The χ vectors are given in 6E12.5 format. The data for each isotope is preceded with a title card (for example, "U-235 EDITS"), and followed by seven cards of data. Photon groups contain zeroes.

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