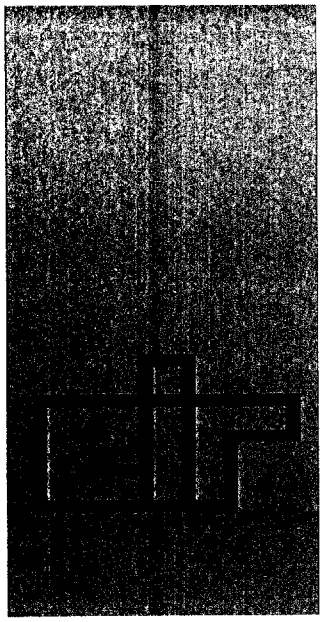
JEF REPORT 10
EIR-Bericht Nr. 636
Dezember 1987



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JEF/EFF Based Nuclear Data Libraries

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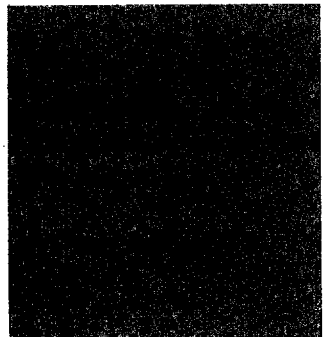
A report on work done in the frame of JEF activity under the leadership of OECD NEA DATA BANK (BANQUE DE DONNEES DE L'AEN OCDE)



Eidgenössisches Institut für Reaktorforschung
Institut Fédéral de Recherches en Matière de Réacteurs
Swiss Federal Institute for Reactor Research

CH-5303 Würenlingen Tel. 056 99 21 11 Telex 82 7417 eir ch

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JEF REPORT 10

JEF/EFF Based Nuclear Data Libraries

by

P. Vontobel S. Pelloni
Paul Scherrer Institute
CH-5303 Würenlingen

A report on work done in the frame of JEF activity under the leadership of OECD NEA DATA BANK (BANQUE DE DONNEES DE L'AEN OCDE)

December 1987

Abstract

Using the NJOY nuclear data processing system, four multigroup neutron data libraries were generated based on the European data files JEF-1 and EFF-1. These cross section libraries can be read into various transport codes such as WIMS, ONEDANT, TWODANT etc., or into the integral transport theory code MICROX-2.

For the neutron analysis of gas-cooled or water moderated thermal reactor systems (including high converter PWR's) a 70-group WIMS-BOXER and a 193-group GA-MICROX structured library were generated. Moreover a general purpose fine group library in 308 groups is provided for the analysis of thermal as well as fast reactor systems. Finally a coupled 175 neutron- 42 photon-group library in Vitamin-J structure was created for the analysis of shielding problems and fusion blanket design.

The content and the parameters taken into account for each of those libraries are given in this report.

Zusammenfassung

Die in europäischer Zusammenarbeit entstandenen Datenbasen evaluierter Neutronendaten JEF-1 und EFF-1 wurden mit dem Datengenerierungssystem NJOY zur Erzeugung von vier Multigruppenbibliotheken verwendet. Diese können von diversen Computercodes zur Lösung der Neutronentransportgleichung wie WIMS, ONEDANT, TWODANT etc., sowie dem Integral-Transport-Theorie Code MICROX-2 gelesen werden.

Für die Untersuchung thermischer Reaktorsysteme - seien sie gas- oder wassergekühlt (inklusive Hochkonverter Druckwasserreaktoren) - wurden eine 70 Gruppenbibliothek in WIMS-BOXER Struktur, sowie eine 193 Gruppenbibliothek in GA-MICROX Struktur gebildet. Ergänzend wird eine 308 Feingruppenbibliothek für die Analyse sowohl von thermischen als auch schnellen Reaktorsystemen zur Verfügung gestellt. Schliesslich bildet eine gekoppelte 175 Neutronen-, 42 Photonen-Gruppen Bibliothek in Vitamin-J Struktur die Datenbasis für Abschirmungsrechnungen und die Untersuchung von Strukturen in Kernfusionsmaschinen.

Dieser Bericht dokumentiert die Parameter und den Umfang der vier Multigruppenbibliotheken, sowie einige Erfahrungen, die bei der Generierung mit NJOY gemacht wurden.

Contents

1 Introduction

Power reactors provide at the present time a significant fraction of the electric power needs. Therefore, questions of safety and economics in the fuel cycle are of great importance. This involves performing neutronic calculations of different reactor types for which there are no benchmark data. In order to provide improved tools for the analysis of such problems, the best unadjusted available nuclear data are required.

The Joint European File (JEF) is a computer-readable repository of (mainly) neutron and photon data in the energy range up to 20 MeV. Together with the recently evaluated fusion file (EFF) it is rapidly becoming the standard European data source for thermal reactor, fast reactor, fusion, shielding and controlled-thermonuclear analysis. JEF is administered by the Nuclear Energy Agency (NEA Data bank). The file has evolved through several updates, the current one being called JEF-1.

Discrete-ordinates transport codes that solve the Boltzmann equation for the distribution of neutrons and photons in nuclear systems have reached a high level of development. However, many of the users of such codes have the same complaint: it is hard to get good, up-to-date, documented cross-section data and prepare them for input into these codes. The problems are multiplied if there is anything unusual about the problem, such as fine groups, self-shielding, or sophisticated response edits (e.g. damage or gas production).

Therefore new multigroup nuclear data libraries on the basis JEF/EFF were generated for general applications. For this purpose the NJOY nuclear data processing system (see Ref. [1]), which is the latest product in the evolution of neutron and photon cross-section processing codes, was utilized. NJOY includes sophisticated methods of correct reconstruction using multi-level Breit-Wigner resonance parameters, Doppler broadening by the accurate point-kernel method, group-to-group thermal scattering matrices, flux-weighted fission-fraction vectors, and a weighting flux produced by a pointwise solution of the slowing-down problem that accurately accounts for broad and intermediate resonance effects in the epithermal region.

The aim of this report is to document the new data libraries and to list their contents (i.e. isotope names, temperatures, degrees of anisotropy, background cross sections, weighting spectra, and so on) and sources of evaluation. Special care is given to the explanation of the processing scheme to provide deep understanding into the physics involved,

and to allow the user to analyse his results.

Section 2 describes the preparation mechanism of groupwise cross sections on the NJOY basis. Separate lists of available groupwise isotopic files in four different group structures (i.e. WIMS-BOXER, GA-MICROX, EIR/HRB, VITAMIN-J) are given. Section 3 reports on the working libraries based on these group structures related to different transport codes (i.e. ONEDANT, MICROX-2, WIMS-D, etc.). Section 4 finally gives some recommendations on the practical use of each library.

2 Generation of Groupwise Files (GENDF)

2.1 Methodology and Processing

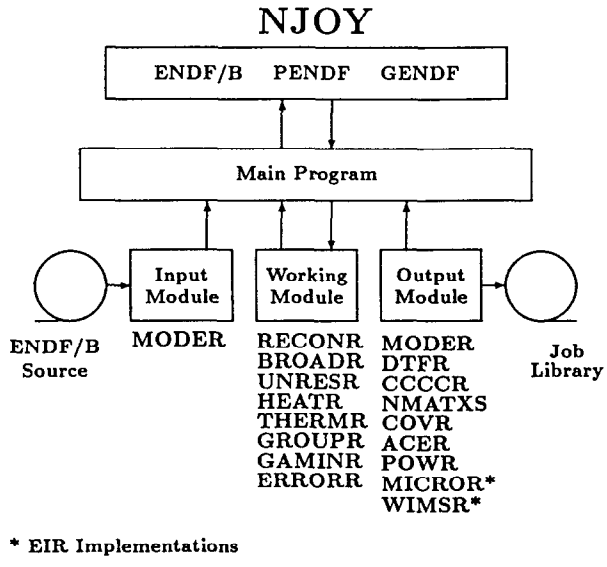

Figure 1: Basic structure of the NJOY code (overlay configuration)

All relevant files were generated using the Los Alamos NJOY system (Version 6/83, see Ref. [1]),which is illustrated in Fig.1. First, pointwise PENDF cross section files (see Ref. [2]) were processed in ENDF/B similar format using NJOY modules RECONR, BROADR, UNRESR, HEATR and THERMR. The RECONR module reconstructs pointwise (energy-dependent) cross sections from ENDF/B resonance parameters and interpolation schemes. Resonance cross sections are calculated with an extended version of the methods of RESEND (see Ref. [3]). BROADR Doppler-broadens and thins pointwise cross sections using the method of SIGMA modified for better behaviour at high temperatures and low energies (see Ref. [4]). UNRESR computes effective self-shielded pointwise cross sections in the unresolved-resonance region using the methods of ETOX (see Ref. [5]). HEATR generates pointwise heat production cross sections (kerma factors) and radiation-damage-energy production cross sections. THERMR produces incoherent

inelastic energy-to-energy matrices for free or bound scatterers, coherent elastic cross sections for hexagonal materials, and incoherent elastic cross sections.

The PENDF files were mainly produced using the JEF-1, the recently reviewed JEF-1.1, and the fusion oriented EFF-1 basic evaluations (see Refs [6,7,8]). These PENDF files include pointwise cross sections for almost all available isotopes (about 300) and temperatures up to 3000 K. The thermal region was treated according to the free gas model. For particular isotopes such as H in H_2O coherent and incoherent thermal $S(\alpha, \beta)$ matrices were included based on the recent JEF-1 German evaluation (see Ref. [9]). Second, GENDF multigroup cross section files were constructed using the GROUPR module (see Ref. [10]). GROUPR generates self-shielded groupwise vector cross sections, group-to-group neutron scattering matrices, and photon production matrices from pointwise ENDF and PENDF data. The cross sections are written onto groupwise cross section files GENDF in ENDF/B like format (see Ref. [11]). Vectors for all reaction types, matrices for reactions producing neutrons, including fission together with mixed data pertaining to fission yields of prompt and delayed neutrons can be calculated for different degrees of anisotropy at different temperatures and background cross sections.

The Bondarenko model was employed for light isotopes. Shielded multigroup cross sections of heavier resonance nuclides were estimated using the method of the flux calculator assuming a single fuel element in an infinite moderating region. Using this approach, the narrow approximation applies for the moderator but not for the absorbing nucleus, for which the Bondarenko model holds above the resolved energy range. The version 6/83 of the GROUPR module was slightly updated in order to allow

1. the automatic processing of all available ENDF and PENDF reactions.

2. The correct determination of the potential cross section from the ENDF value, and the incorporation onto record 3 of the GENDF file.

3. The estimate of the break between resolved and unresolved resonance range from the PENDF value.

4. The extension of the flux calculation based on the slowing down equation to the maximum number of points according to the PENDF value.

5. The implementation of additional worldwide broadly used group structures and weighting spectra to avoid the use of tabulators within the input stream.

This was intended to save time and to eliminate possible error sources and deficiencies in preparing large and rather complex isotope dependent GROUPR input files.

2.2 70-Group WIMS-BOXER GENDF Library

The energy structure of the WIMS-BOXER library consisting of the standard 69 WIMS structure and one additional group from 10 MeV to 14.918 MeV is shown in Appendix A.

This library (see Table 1) contains P_1 neutron data pertaining to 100 JEF-1 nuclides and 19 JEF-1.1 nuclides (i.e.^{2}H, ^{14}N, ^{16}O, ^{23}Na, ^{103}Ru, ^{135}Cs, ^{154}Gd, Gd(nat), Hf(nat), ^{233}U, ^{234}U, ^{236}U, ^{237}U, ^{237}Np, ^{241}Pu, ^{241}Am, ^{242M}Am, ^{246}Cm, ^{247}Cm).

The logarithmic energy decrement ξ (MT=252 in the ENDF terminology) is included. 42 thermal energy groups below 4.6 eV with upscatter are considered. All data available on the GENDF library are tabulated for maximum 4 temperatures (i.e. 296, 600, 900, 1200 K). Most reaction cross sections (see GROUPR description in Ref. [10]) were calculated for different background cross sections σ_0, i.e. either 10^{10}, 10^4, 10^3, 500, 200, 100, 50, 20, 10, 1 barns (10 values) for actinides, or 10^{10}, 10^4, 10^3, 100, 10, 1 barns (6 values) for structural materials, or respectively 10^{10} barns (infinite dilute case, 1 value) for light nuclides with Z values less than 12 (see Table 1). The flux calculator option was selected for isotopes with Z values larger than 11. Dry and wet WIMS-D input spectra (see Ref. [12] and Fig.2) were utilized for collapsing PENDF data into multigroup cross sections. The wet spectrum was just used for hydrogen, deuterium and oxygen. In Fig.2 a multigroup version (in the 308 neutron group structure) of the WIMS-D spectra is depicted. The list of isotopes is displayed in Table 1 .

Isotope	Temperatures Kelvin	No. of σ_0	Thermal Scattering Treatment
^{1}H	293.6 473.6 623.6	1	H in H_2O,free gas
^{2}H	293.6 473.6 573.6	1	D in D_2O,free gas
^{4}He	a	1	free gas
^{6}Li	a	1	free gas
^{7}Li	a	1	free gas
^{9}Be	296 600 1000	1	el.Be, in.Be, el.BeO, in.BeO, free gas
^{10}B	a	1	free gas
^{11}B	a	1	free gas
C(nat)	293.6 500 800 1200	1	coh, inch Graphite, free gas
^{14}N	a	1	free gas
^{16}O	296 600 1200	1	free gas
^{19}F	a	1	free gas
^{23}Na	a	1	free gas
^{27}Al	a	6	free gas
Si(nat)	b	6	free gas
Cr(nat)	a	6	free gas
^{55}Mn	a	6	free gas
Fe(nat)	a	6	free gas
^{59}Co	a	6	free gas
Ni(nat)	a	6	free gas
Cu(nat)	a	6	free gas
^{83}Kr	296	6	-
Zr(nat)	a	6	free gas
Mo(nat)	a	6	free gas
^{95}Mo	296	6	free gas
^{99}Tc	296	6	free gas
^{101}Ru	296	6	-
^{103}Ru	296	6	free gas
^{103}Rh	296	6	-
^{105}Pd	296	6	-
^{107}Pd	296	6	-
^{108}Pd	296	6	-
^{107}Ag	296	6	-

Table 1: WIMS-BOXER Structure 70 Group P_1 Neutron-Library, List of Isotopes
a:= 296, 600, 900, b:= 296, 600, 900, 1200 K

Isotope	Temperatures Kelvin	No. of σ_0	Thermal Scattering Treatment
^{109}Ag	296	6	-
Cd(nat)	a	6	free gas
^{113}In	296	6	-
^{115}In	296	6	-
^{127}I	296	6	-
^{131}I	296	6	-
^{135}I	296	6	-
^{124}Xe	b	6	-
^{126}Xe	b	6	-
^{128}Xe	b	6	-
^{129}Xe	b	6	-
^{130}Xe	b	6	-
^{131}Xe	b	6	-
^{132}Xe	b	6	-
^{133}Xe	b	6	-
^{134}Xe	b	6	-
^{135}Xe	b	6	-
^{136}Xe	b	6	-
^{133}Cs	296	6	free gas
^{135}Cs	296	6	-
^{139}La	296	6	-
^{142}Nd	296	6	-
^{143}Nd	296	6	-
^{144}Nd	296	6	-
^{145}Nd	296 900	6	free gas
^{146}Nd	296	6	-
^{148}Nd	296	6	free gas
^{150}Nd	296	6	-
^{147}Pm	296	6	-
^{148}Pm	296	6	-
^{148M}Pm	296	6	-
^{147}Sm	296	6	-
^{148}Sm	296	6	-

Table 1: WIMS-BOXER Structure 70 Group P_1 Neutron-Library, a:= 296, 600, 900, b:= 296, 600, 900, 1200 K

Isotope	Temperatures Kelvin	No. of σ_0	Thermal Scattering Treatment
^{149}Sm	b	6	-
^{150}Sm	296	6	-
^{151}Sm	b	6	-
^{152}Sm	b	6	-
^{153}Sm	b	6	-
^{154}Sm	b	6	-
^{153}Eu	296 900	6	-
^{154}Eu	296 900	6	-
^{155}Eu	a	6	free gas
^{154}Gd	b	6	free gas
^{155}Gd	b	6	free gas
^{156}Gd	b	6	free gas
^{157}Gd	b	6	free gas
^{158}Gd	b	6	free gas
^{160}Gd	b	6	free gas
^{176}Lu	296	6	-
Hf(nat)	a	6	free gas
^{174}Hf	b	6	free gas
^{176}Hf	b	6	free gas
^{177}Hf	b	6	free gas
^{178}Hf	b	6	free gas
^{179}Hf	b	6	free gas
^{180}Hf	b	6	free gas
^{181}Ta	b	6	free gas
^{182}Ta	b	6	free gas
^{197}Au	b	6	free gas
Pb(nat)	a	6	free gas
^{231}Pa	b	10	free gas
^{233}Pa	b	10	free gas
^{232}Th	b	10	free gas
^{232}U	299	10	-
^{233}U	b	10	free gas
^{234}U	b	10	free gas

Table 1: WIMS-BOXER Structure 70 Group P_1 Neutron-Library, a:= 296, 600, 900, b:= 296, 600, 900, 1200 K

Isotope	Temperatures Kelvin	No. of σ_0	Thermal Scattering Treatment
^{235}U	b	10	free gas
^{236}U	b	10	free gas
^{237}U	b	10	free gas
^{238}U	b	10	free gas
^{237}Np	b	10	free gas
^{238}Pu	b	10	free gas
^{239}Pu	b	10	free gas
^{240}Pu	b	10	free gas
^{241}Pu	b	10	free gas
^{242}Pu	b	10	free gas
^{241}Am	b	10	free gas
^{242}Am	296	10	free gas
^{242M}Am	296	10	-
^{243}Am	b	10	free gas
^{241}Cm	296	10	-
^{242}Cm	a	10	free gas
^{244}Cm	a	10	free gas
^{245}Cm	a	10	-
^{246}Cm	296 600 1800 3000	-	-
^{247}Cm	a	10	-

Table 1: WIMS-BOXER Structure 70 Group P_1 Neutron-Library, a:= 296, 600, 900, b:= 296, 600, 900, 1200 K

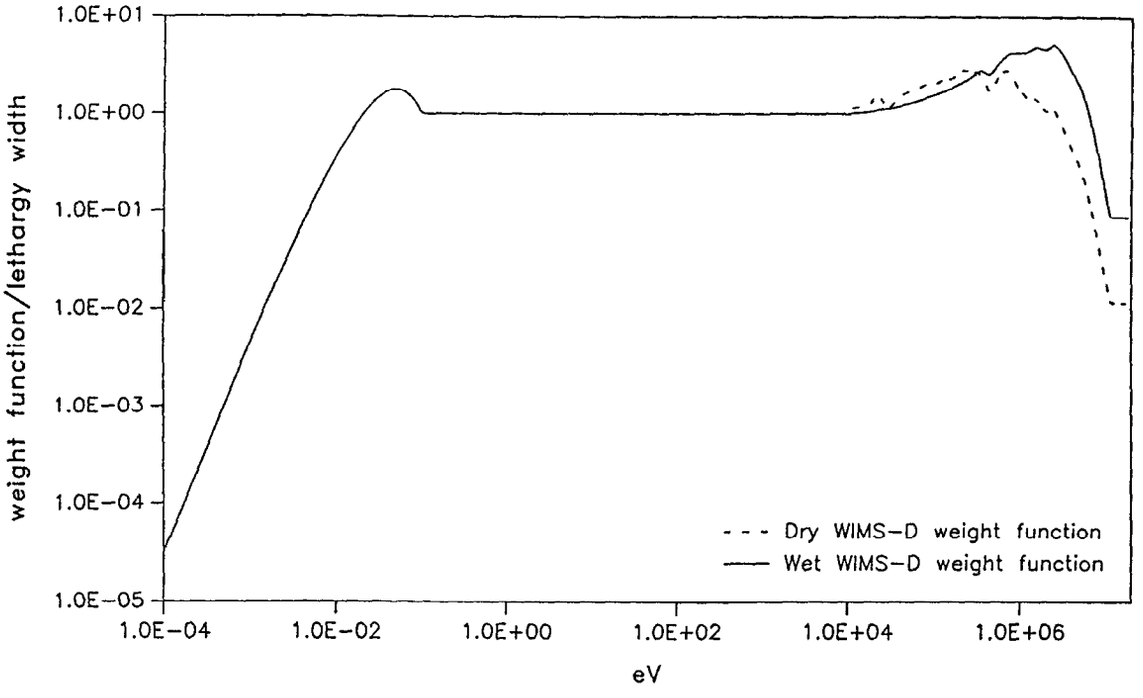

Figure 2: WIMS-D dry and wet weight functions

2.3 193-GROUP GA-MICROX GENDF Library

This library (see Table 2) contains P_3 neutron data at 296 K pertaining to 20 JEF-1 nuclides and 10 JEF-1.1 nuclides (i.e. ^{2}H, ^{14}N, ^{16}O, ^{23}Na, Hf(nat), ^{233}U, ^{234}U, ^{236}U, ^{241}Pu, ^{241}Am). 103 thermal energy groups below 4.6 eV with upscatter are considered. The boundaries of the first 93 fast energy groups are taken from the GAM-II energy structure, whereas in the thermal range below 2.33 eV the boundaries coincide with the energy points of the MICROX code (see Appendix A).

All data available on the GENDF library are given either at 7 different background cross sections σ_0, i.e. 10^{10}, 10^4, 10^3, 100, 50, 10, 1 barns for actinides and structural materials, or at infinite dilution for light isotopes with Z values less than 12.

The flux calculator option was selected for isotopes with Z values larger than 11. Dry and wet WIMS-D input spectra (see Ref. [12] and Fig.2) were utilized for collapsing PENDF data into multigroup cross sections. The wet spectrum was just used for hydrogen, deuterium and oxygen. The list of isotopes is displayed in Table 2.

Isotope	Temperatures Kelvin	No. of σ_0	Thermal Scattering Treatment
^{1}H	293.6	1	H in H_2O, free gas
^{2}H	293.6	1	D in D_2O, free gas
^{4}He	296	1	free gas
^{10}B	296	1	free gas
^{11}B	296	1	free gas
C(nat)	293.6	1	coh, inch Graphite, free gas
^{14}N	296	1	free gas
^{16}O	296	1	free gas
^{23}Na	296	1	free gas
^{27}Al	296	7	free gas
Si(nat)	296	7	free gas
Cr(nat)	296	7	free gas
^{55}Mn	296	7	free gas
Fe(nat)	296	7	free gas
^{59}Co	296	7	free gas
Ni(nat)	296	7	free gas
Cu(nat)	296	7	free gas
Mo(nat)	296	7	free gas
Hf(nat)	296	7	free gas
^{233}U	296	7	free gas
^{234}U	296	7	free gas
^{235}U	296	7	free gas
^{236}U	296	7	free gas
^{238}U	296	7	free gas
^{238}Pu	296	7	free gas
^{239}Pu	296	7	free gas
^{240}Pu	296	7	free gas
^{241}Pu	296	7	free gas
^{242}Pu	296	7	free gas
^{241}Am	296	7	free gas

Table 2: GA-MICROX structure 193 group neutron-library, list of isotopes

2.4 308 Group EIR-HRB Structure GENDF Library

The energy structure (see appendix A) of this general purpose fine group library was defined to satisfy the needs of both thermal and fast reactor analysis. Group boundaries were therefore taken in the fast energy range from the Vitamin-J structure defined in Ref. [13] (first 125 groups) and in the thermal range below 2.38 eV from the MICROX structure (101 thermal energy points) of Section 2.3. In the epithermal energy range (2.5eV - 17keV) some group boundaries from the LANL-187(MATXS8) group-structure [14] were added to the Vitamin-J energy boundaries and one at 2.5045 eV to represent better hafnium and plutonium resonances.

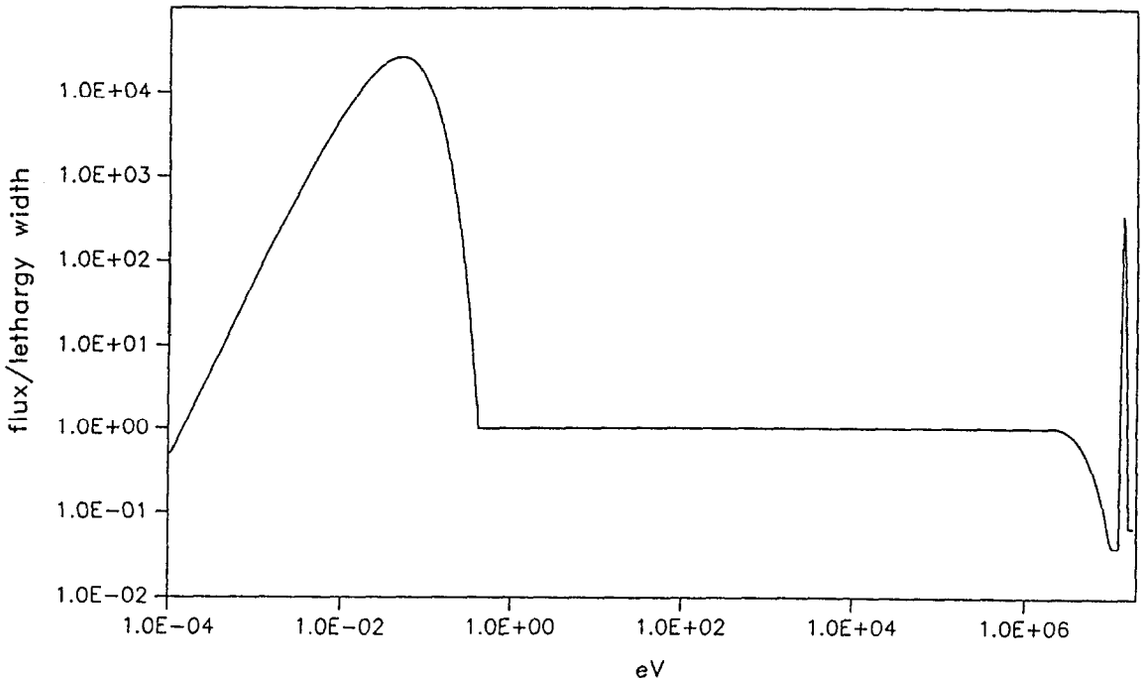

Figure 3: Vitamin-E Input Weighting Spectrum

Using the Vitamin-E input weighting spectrum [15] shown in Fig.3 for T=296 K all PENDF data for the 48 isotopes listed in Tab.3 were processed into GENDF form by considering 108 thermal energy groups below 4.6eV, P_4 Legendre order of scattering and background cross sections σ_0 with: 10^{10}, 10^4, 10^3, 100, 10 and 1 barns. The flux

calculator was used for isotopes with $Z \geq 13$. Scattering matrices in the thermal energy range were generated for all isotopes using the free gas scattering approximation. For hydrogen and graphite coherent and incoherent thermal scattering of neutrons in H_2O and graphite were additionally calculated starting from the special $S(\alpha, \beta)$ scattering laws available on the JEF-1 files (see Ref. [9]).

The data for the following isotopes were taken from the updated JEF-1.1 ENDF file : Hf(nat), ^{233}U, ^{234}U, ^{236}U, ^{237}Np, ^{241}Pu, ^{241}Am.

Isotope	Temperatures Kelvin	No. of σ_0	Thermal Scattering Treatment
^{1}H	293.6 473.6 623.6	1	incl H in H_2O
^{2}H	293.6 473.6 573.6	1	incl D in D_2O
^{4}He	a	1	free gas
^{6}Li	a	1	free gas
^{10}B	a	1	free gas
^{11}B	296 500 600	1	free gas
C(nat)	293.6 500 800 1200	1	coh, inch graphite
^{14}N	a	1	free gas
^{16}O	296 600 1200	1	free gas
^{23}Na	a	1	free gas
^{27}Al	a	6	free gas
Si(nat)	b	6	free gas
Cr(nat)	a	6	free gas
V(nat)	a	6	free gas
^{55}Mn	a	6	free gas
Fe(nat)	a	6	free gas
^{59}Co	a	6	free gas
Ni(nat)	a	6	free gas
Cu(nat)	a	6	free gas
Zr(nat)	296 600 900 3000	6	free gas
Mo(nat)	a	6	free gas
Gd(nat)	c	6	free gas
^{154}Gd	c	6	free gas
^{155}Gd	c	6	free gas
^{156}Gd	c	6	free gas
^{157}Gd	c	6	free gas
^{158}Gd	296 600 900 1200 3000	6	free gas
^{160}Gd	296 600 900 1200 3000	6	free gas
Hf(nat)	c	6	free gas
^{174}Hf	c	6	free gas
^{176}Hf	c	6	free gas

Table 3: 308 Group Structure P_4 Neutron-Library List of Isotopes
a:= 296, 600, 900, b:= 296, 600, 900, 1200, c:= 296, 600, 900, 1200, 1500, 3000 K

Isotope	Temperatures Kelvin	No. of σ_0	Thermal Scattering Treatment
^{177}Hf	c	6	free gas
^{178}Hf	c	6	free gas
^{179}Hf	c	6	free gas
^{180}Hf	c	6	free gas
^{232}Th	e	6	free gas
^{233}U	c	6	free gas
^{234}U	c	6	free gas
^{235}U	d	6	free gas
^{236}U	c	6	free gas
^{238}U	d	6	free gas
^{237}Np	e	6	free gas
^{238}Pu	d	6	free gas
^{239}Pu	d	6	free gas
^{240}Pu	d	6	free gas
^{241}Pu	296 600 900 1200 1800	6	free gas
^{242}Pu	d	6	free gas
^{241}Am	c	6	free gas

Table 3: (Continued)
a:= 296, 600, 900, b:= 296, 600, 900, 1200, c:= 296, 600, 900, 1200, 1500, 3000 K
d:= 296, 600, 900, 1200 1800, 2400, 3000, e:= 296, 600, 900, 1200, 1500, 1800, 2400, and 3000 K

2.5 Vitamin-J Structure Coupled 175 Neutron 42 Photon Group Library

The energy structure of this coupled neutron-photon multigroup library was chosen to give a fine representation of the fast and epithermal neutron energy range important for fusion blanket and shielding analysis. The Vitamin-J 175 neutron energy group structure [13] has the same boundaries as the 174 group Vitamin-E structure [15] but with an additional group boundary taken from the VITAMIN-C structure [28] at 12.84 MeV.

The 42 photon energy group structure contains the energy boundaries of the 38 group

Vitamin-E photon energy structure [15] and the following additional break points : 50, 30, 1.34 MeV, and 1keV (see Tab.4). Thus two additional fast photon energy groups above 20 MeV and one slow energy group below 10 keV were defined. The break point at 1.34 MeV was set to give a good representation of the important ^{60}Co γ-emission.

The neutron ENDF data for most isotopes were taken from JEF-1. Hf(nat), ^{233}U, ^{234}U, ^{236}U, ^{241}Pu, ^{241}Am are from JEF-1.1. Evaluations for ^{7}Li, ^{9}Be, ^{27}Al, ^{28}Si, and lead were taken from the European Fusion File EFF-1 [8] and added as well as the ENDF/B-4 evaluations of ^{238}U and ^{239}Pu because of missing photon production data in JEF-1.

The original EFF-1 lead file was written in ENDF/B-VI and contains double-differential scattering data (MF=6 in the ENDF terminology). Since the actual version of the GROUPR module is not able to process MF=6, double-differential cross-sections were translated at ECN-Petten into uncoupled angular- and energy-dependent data (i.e. MF=4, 5 in the ENDF terminology). Therefore lead groupwise data which are referred to EFF-1 do not include all features of the evaluated scattering laws. It is foreseen to adapt and to utilize the new Dutch module GROUPXS [27] to update lead multigroup scattering cross-sections and to benchmark them.

The Vitamin-E input weighting spectrum (see Fig.3) was used to process all neutron PENDF data for 83 isotopes of 43 chemical elements into GENDF form (see Tab.5). Special quantities such as the average cosine of the scattering angle $\bar{\mu}$, the average logarithmic energy decrement for elastic scattering ξ and γ , the average of the square of the logarithmic energy decrement for elastic scattering, divided by twice the average logarithmic decrement for elastic scattering, were added to the reactions available from the PENDF file. In the 11 energy groups below 4.6eV thermal scattering of neutrons was calculated using the free gas scattering approximation for most isotopes except the fission products. The special coherent and incoherent scattering laws for hydrogen (H in H_2O), Be (coherent and incoherent scattering in Be and BeO), graphite (coherent and incoherent scattering), and oxygen in UO_2 were added to the free gas approximation by taking the available S(α, β) matrices from JEF-1 [9].

All reactions were processed at the basic temperature, whereas at higher temperatures all vector cross sections (MF=3) but only the elastic and thermal matrix cross sections : MF=6, MT=2, 221, 222, 228, 229, 230, 231, 232, 233 and 234 were generated. The

42, 38 and 12 Photon Energy Group-Structures

Upper Boundary	42	38	12	Upper Boundary	42	38	12
50.0 MeV	1			1.33 MeV	23	20	
30.0	2			1.00	24	21	10
20.0	3	1	1	0.80	25	22	
14.0	4	2		0.70	26	23	
12.0	5	3		0.60	27	24	
10.0	6	4	2'	0.512	28	25	
8.0	7	5	3	0.510	29	26	11'
7.5	8	6		0.45	30	27	
7.0	9	7	4	0.40	31	28	
6.5	10	8		0.30	32	29	
6.0	11	9	5	0.20	33	30	
5.5	12	10		0.15	34	31	
5.0	13	11	6	0.10 MeV	35	32	12
4.5	14	12		75 keV	36	33	
4.0	15	13	7	70	37	34	
3.5	16	14		60	38	35	
3.0	17	15	8	45	39	36	
2.5	18	16		30	40	37	
2.0	19	17	2	20	41	38	
1.66	20	18		10	42	$E_{\min}$	$E_{\min}$
1.50	21	19		1 keV	E_{min}		
1.34 MeV	22						

Table 4: 42:=Vitamin-J(EIR), 38:=Vitamin-E, 12:=LANL-12(MATXS5)

background cross sections considered were taken at 10^{10}, 10^4, 10^3, 100, 10 and 1 barns.

The ENDF/B-V photon interaction data were taken from the DLC-99/HUGO photon file [16] (available from the Radiation Shielding Information Center RSIC), reconstructed with the NJOY RECONR module and put into multigroup form using the NJOY GAMINR module. The reconstruction tolerances in RECONR had to be chosen carefully in order to avoid inconsistencies while calculating coherent scattering matrices (MF=26, MT=502) in GAMINR (see appendix B).

The 42 group photon cross sections were generated using a constant input weighting spectrum and P_6 Legendre order of scattering. The GAMINR module automatically generated cross sections for total, coherent, incoherent, pair production and photoelectric reactions. A total heating cross section (MT=621) was created by adding the contributions from each reaction.

Isotope	Temperatures Kelvin	No. of σ_0	Thermal Scattering Treatment	Photon Prod.
^{1}H	293.6 473.6 623.6	1	incl H in H_2O	yes
^{2}H	293.6 473.6 573.6	1	incl D in D_2O	yes
^{3}H	a	1	free gas	no
^{3}He	a	1	free gas	no
^{4}He	a	1	free gas	no
^{6}Li	a	1	free gas	yes
^{7}Li	a	1	free gas	yes
^{7}Li(EFF)	a	1	free gas	yes
^{9}Be	296 600 1000	1	incl coh, inch Be and BeO	yes
^{9}Be(EFF)	a	1	free gas	yes
^{10}B	a	1	free gas	yes
^{11}B	a	1	free gas	no
C(nat)	293.6 500 800 1200	1	incl coh, inch graphite	yes
^{14}N	a	1	free gas	yes
^{16}O	296 600 1200	1	incl O in UO_2	yes
^{19}F	a	1	free gas	yes
^{23}Na	a	1	free gas	no
Mg(nat)	a	1	free gas	yes
^{27}Al	a	6	free gas	yes
^{27}Al(EFF)	a	6	free gas	yes
Si(nat)	a	6	free gas	yes
Si(nat)(EFF)	a	6	free gas	yes
Cl(nat)	a	6	free gas	yes
K(nat)	a	6	free gas	yes
Ca(nat)	a	6	free gas	yes
Ti(nat)	a	6	free gas	yes
V(nat)	a	6	free gas	yes
Cr(nat)	a	6	free gas	yes
^{55}Mn	a	6	free gas	yes
Fe(nat)	a	7	free gas	yes
^{59}Co	a	6	free gas	yes
Ni(nat)	a	6	free gas	yes
Cu(nat)	a	6	free gas	yes

Table 5: Vitamin-J Coupled 175 Neutron ,42 Photon-Group Library
List of Isotopes ; a:= 296, 600 and 900 K

Isotope	Temperatures Kelvin	No. of σ_0	Thermal Scattering Treatment	Photon Prod.
Zr(nat)	a	6	free gas	yes
^{93}Nb	a	6	free gas	yes
Mo(nat)	a	6	free gas	yes
^{107}Ag	296	6	no free gas	no
^{109}Ag	296	6	no free gas	no
Cd(nat)	a	6	free gas	no
^{114}Sn	296	6	no free gas	no
^{115}Sn	296	6	no free gas	no
^{116}Sn	296	6	no free gas	no
^{117}Sn	296	6	no free gas	no
^{118}Sn	296	6	no free gas	no
^{119}Sn	296	6	no free gas	no
^{120}Sn	296	6	no free gas	no
^{122}Sn	296	6	no free gas	no
^{124}Sn	296	6	no free gas	no
^{133}Cs	296	6	free gas	no
^{134}Ba	296	6	no free gas	no
^{135}Ba	296	6	no free gas	no
^{136}Ba	296	6	no free gas	no
^{137}Ba	296	6	no free gas	no
^{138}Ba	296	6	no free gas	no
^{145}Nd	296 900	6	free gas	no
^{147}Sm	296	6	no free gas	no
^{148}Sm	296	6	no free gas	no
^{149}Sm	a	6	free gas	no
^{150}Sm	296	6	no free gas	no
^{151}Sm	b	6	no free gas	no
^{152}Sm	296	6	no free gas	no
^{154}Sm	296	6	no free gas	no
^{154}Gd	a	6	free gas	no
^{155}Gd	a	6	free gas	no
^{156}Gd	a	6	free gas	no
^{157}Gd	a	6	free gas	no

Table 5: (Continued)a:= 296, 600, 900, b:= 296, 600, 900, 1200 K

Isotope	Temperatures Kelvin	No. of σ_0	Thermal Scattering Treatment	Photon Prod.
^{158}Gd	a	6	free gas	no
^{160}Gd	a	6	free gas	no
Hf(nat)	a	6	free gas	no
^{181}Ta	a	6	free gas	yes
^{182}W	296	6	no free gas	yes
^{183}W	296	6	no free gas	yes
^{184}W	296	6	no free gas	yes
^{186}W	296	6	no free gas	yes
Pb(nat)	a	6	free gas	yes
Pb(EFF)	a	6	free gas	yes
^{232}Th	b	6	free gas	no
^{233}U	b	6	free gas	no
^{234}U	b	6	free gas	no
^{235}U	b	6	free gas	yes
^{235}U	b	6	free gas	yes
^{236}U	b	6	free gas	no
^{238}U	b	6	free gas	no
^{238}U(B4)	b	6	free gas	yes
^{238}Pu	b	6	free gas	no
^{239}Pu	b	6	free gas	no
^{239}Pu(B4)	b	6	free gas	yes
^{240}Pu	b	6	free gas	no
^{241}Pu	b	6	free gas	no
^{242}Pu	b	6	free gas	no
^{241}Am	b	6	free gas	no

Table 5: (Continued)a:= 296, 600, 900, b:= 296, 600, 900, 1200 K

3 Working Libraries

The groupwise ENDF files presented above apply each to a broad class of problems and can be used to generate data libraries for different cross section processing and transport codes. Because the data format of the input neutron (or photon) data library looks different for the processing codes TRAMIX [17] and TRANSX-CTR [14] or the transport codes WIMS [20] and MICROX-2 [18], the GENDF files had to be reformatted to get the working libraries.

3.1 MATXS Libraries

The GENDF's of the four different neutron energy structures i.e. 70, 175, 193, and 308 groups and the 42 photon energy structure have been put into the so called MATXS format suitable for further processing with the TRANSX-CTR [14] or TRAMIX [17] code. These are codes which read nuclear data from a MATXS [14] library and produce problem specific transport tables compatible with many discrete-ordinates (S_N) and diffusion codes. Tables can be produced for neutron, photon, or coupled neutron-photon transport. Options include adjoint tables, mixtures, energy-self-shielding, group collapse, homogenization, thermal upscatter, prompt or steady-state fission, transport corrections, elastic removal corrections, and flexible response function edits.

The NJOY modules ECOMBR [11] and NMATXS [1] have been used to combine the individual isotope GENDF's for all materials and to reformat the resulting GENDF file into MATXS format. Figure 4 shows the processing steps leading to problem specific data libraries based on a MATXS file.

The MATXS file is a generalized cross section library in a flexible format similar to the CCCC standard cross section file ISOTXS [14]. Its format was designed to generalize and simplify the existing CCCC cross section files ISOTXS, BRKOXS or GRUPXS [26]. These standard CCCC cross section files have a number of shortcomings that make them difficult to use. ISOTXS is limited to a particular set of reactions that is inadequate at higher energies and does not include heating and damage energy cross sections. BRKOXS does not provide for self-shielded group-to-group scattering cross sections. In the MATXS format neutron data and photon data are treated in the same way and coupled neutron-photon data sets are produced easily. Finally each data type is divided into materials and

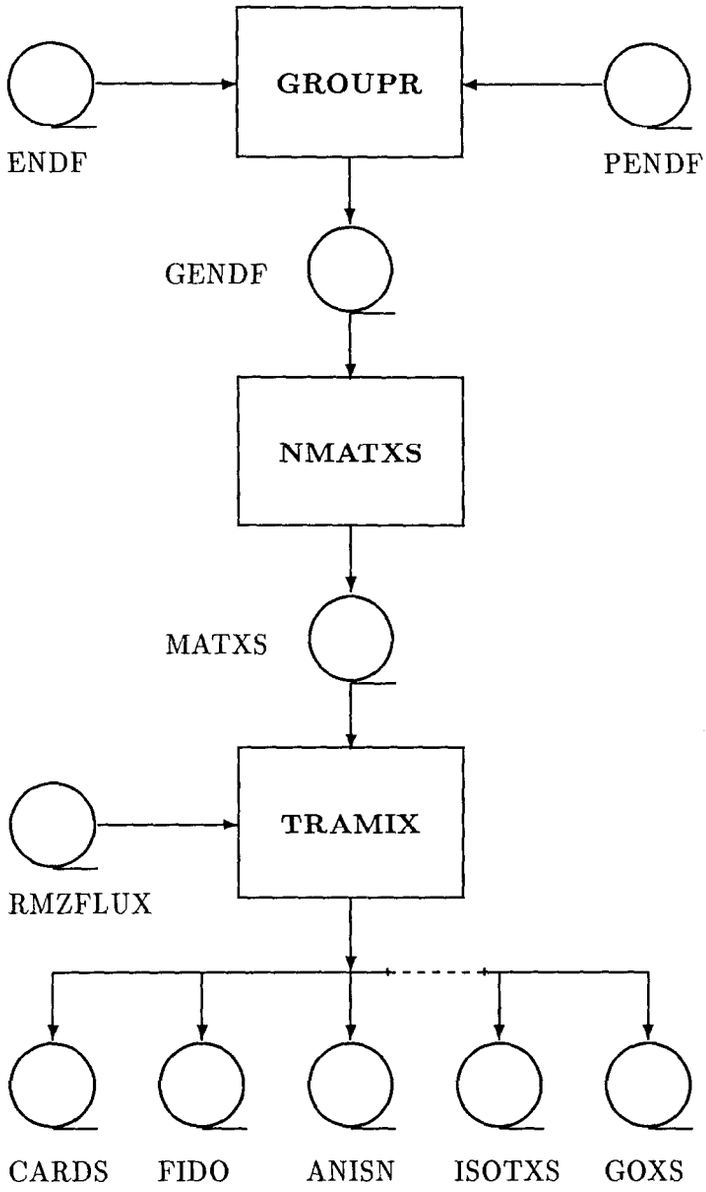

Figure 4: Generation of MATXS based problem dependent libraries

submaterials. A material might be a particular isotope or mixture. Each submaterial could then represent a temperature or σ_o background cross section in a basic library. In addition to the standard file structure described in Ref. [14] or the input description of NMATXS, the value of the potential cross section σ_p was put at the end of the material control record of the MATXS file. This value is read by the TRAMIX code, when calculating energy dependent Goldstein-Cohen λ-factors. For a detailed description of the MATXS file please refer to Ref. [14] or the input description of the NJOY NMATXS module.

Together with the MATXS library file an index is provided by the NMATXS module, showing all particle (i.e. neutron and/or photon) and reaction types as well as the temperatures and background cross section values included for each material (see appendix C for sample index).

In general all isotopes mentioned in Tables 1-3 and Table 5 together with the specified temperature, σ_0 values and special thermal scattering treatment are included in the MATXS libraries generated in the 70, 193, 308 and coupled 175/42 group structures. For the coupled 175 neutron 42 photon energy group library two versions of the MATXS working library were created. The first one contains all isotopes mentioned in Table 5, whereas the second version contains only isotopes important for fusion blanket analysis.

The isotopes on the MATXS file are called by name and not by material number. The naming convention used is that of TRANSX-CTR [14] i.e. the isotope name is given by its symbol of element followed by its number of nucleons e.g.: PU239 for ^{239}Pu. For natural mixtures of stable isotopes the number of nucleons is replaced by the three letters NAT e.g.: FENAT for natural iron. Natural materials are indicated on the GENDF lists of isotopes (Tables 1-3 and Table 5). Photon interaction data for a specific isotope of the coupled neutron-photon library is simply asked for by the symbol of element only, because photon interactions are atomic in nature; e.g. Pu for ^{239}Pu.

Processing the GENDF files with the NMATXS module of NJOY(6/83) the following options were selected : The blocking option for matrices IFOPT was set to 1 (matrices not blocked) and the subblocking parameter NSBLK was set to the number of energy groups (i.e.70, 193, 308, 175 or 42). Because of difficulties encountered when creating MATXS files containing isotopes with multiple temperatures, the subdividing of a block into partials had to be avoided (see appendix B).

In the case of the 70, 193 and 308 neutron energy group MATXS libraries only the

data types NSCAT (providing neutron vector and matrix cross sections) and NTHERM (providing thermal scattering data in the free gas approximation or any other special thermal scattering treatment) were included on the MATXS files. Besides these two data types the coupled 175/42 neutron-photon library contains also photon production data (data type NGAMA) and photon interaction data GSCAT. Although photon production data is given on the 175 group GENDF files for different σ_0 values, it was requested in data type NGAMA at infinite-dilution (NSIGZ=1) only. The subsequent processing of this data type with TRANSX-CTR or TRAMIX uses shielding factors for the corresponding neutron reaction (e.g. capture MT=102 , fission MT=18 etc) to shield each photon production matrix.

Special care had to be given to the data type NTHERM (thermal neutron scattering data) in the coupled 175/42 neutron-photon library, because of the rather small number of 11 thermal energy groups below 4.6eV. A small change of a tolerance parameter, set internally in subroutine VECIN, helped to overcome this nuisance (see appendix B).

3.2 MICROX-2 Libraries

MICROX-2 is an integral transport theory spectrum code which solves the neutron slowing down and thermalisation equations on a detailed energy grid for a two region lattice cell. The fluxes in the two regions are coupled by collision probabilities computed using the flat flux approximation. MICROX-2 accounts for overlap and interference between resonance levels (see Ref. [18]).

GENDF and PENDF data files can be edited into the input FDTAPE, GGTAPE and GARTAPE for MICROX-2 using the EIR-NJOY coupling module MICROR (see Ref. [19]). FDTAPE contains fine group dilution- and temperature- dependent cross sections for the fast energy range. The GGTAPE consists of two sections which contain infinite dilute P_1 cross sections for the fast and thermal energy ranges respectively. MICROX-2 uses only the thermal section of the GGTAPE, which includes thermal cross sections with upscatter estimated using the free gas model or the available coherent and incoherent scattering $S(\alpha, \beta)$ matrices (see [9]). The GARTAPE contains pointwise Doppler-broadened resonance cross sections in the resolved resonance range. Fine energy points up to the keV range can be considered in order to achieve an accurate solution of the slowing down equations in two zones (self-shielding of resolved resonance range). The description of the formats

of the FDTAPE, GGTAPE and GARTAPE can be found in Refs. [19,11].

Starting from the GENDF data files described in 2.2 and 2.3 two libraries for the code MICROX-2 were generated. These libraries (consisting of FDTAPE, GGTAPE, and GARTAPE) contain data at room temperature for all 30 isotopes listed in Table 2, being aimed exclusively for benchmark calculations and data testing.

The FDTAPE related to the WIMS-BOXER energy boundaries includes P_1 data in 31 groups, whereas the 99 neutron group fast library from the GA-MICROX structure contains cross sections up to P_3 (see Ref. [18]).

Because of the limitation to a maximum number of isotopes, most FDTAPE data are taken at infinite dilution. However for some actinides and structural materials background cross sections are considered (see Table 6). These isotopes have important resonances at energies above 8 keV (resolved resonances in the case of structural materials, and unresolved for actinides) so that a satisfactory resonance shielding based on the GAR file alone cannot be achieved. The selected dilution cross sections are representative for light water reactor applications. The WIMS-BOXER structured fast libraries (FD- und GG-files) contain fission spectra data for ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{235}U, ^{238}U. The GA-MICROX structured fast libraries include sequentially fission spectra data for ^{238}U, ^{235}U, ^{239}Pu, ^{240}Pu,^{238}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{233}U, ^{232}Th, ^{234}U and ^{236}U respectively. These were calculated within MICROR according to the formulas displayed in Ref. [14] by using the GENDF library flux (i.e. the WIMS-D dry weight function).

The thermal part of the GGTAPE includes upscatter cross sections for just hydrogen, deuterium, carbon and oxygen (KERN=1 in the MICROX terminology). The GA-MICROX library includes 101 thermal energy groups below 2.38 eV, whereas the WIMS-BOXER library has 40 thermal groups below 2.6 eV.

The GARTAPE, (one file for both group structures), contains pointwise Doppler-broadened resonance cross sections in the resolved resonance range. 14457 energy points between 0.414 eV and 8.0072 keV are included.

The identification number of each GAR nuclide is equivalent to the sum of the ENDF material number (see Refs. [6,7,8]) multiplied by 1000000, and the isotope temperature times 100 increased by one (i.e.4928029601 for ^{238}U). GG and FD nuclides can be identified in both libraries by multiplying the ENDF isotope number by 10000, by adding 301 and dividing the result by 100000. (i.e. 492.80301 for ^{238}U). If self-shielding factors appear,

Isotope Name	FDTAPE from the WIMS-BOXER structure (31 neutron groups)	FDTAPE from the GA-MICROX structure (99 neutron groups)
	Dilution cross sections (barns)	
Cr(nat)	10^{10} 1000 1	10^{10}
Ni(nat)	10^{10} 1000 1	10^{10}
Fe(nat)	10^{10} 10^4 100 1	10^{10} 100
^{235}U	10^{10} 10^4 1000	10^{10}
^{238}U	all as in Table 1	10^{10} 1000 10
^{238}Pu	10^{10} 10^4	10^{10}
^{239}Pu	10^{10} 10^4 1000 100 1	10^{10} 100
^{240}Pu	10^{10} 10^4	10^{10}
^{241}Pu	10^{10} 10^4	10^{10}
^{242}Pu	10^{10} 10^4	10^{10}
^{241}Am	10^{10} 10^4	10^{10}

Table 6: Dilution cross sections included in the fast data libraries FDTAPE for the code MICROX-2

the i-th set is characterized by adding 301+(i-1)10 instead of 301 (i.e. 492.80311 for the FDTAPE nuclide ^{238}U taken at 10^4 barns background cross section).

3.3 WIMS-D Data Library

The WIMS-D is a comprehensive code for reactor lattice cell calculations including burn-up calculations in a wide variety of reactor types (see Ref. [20]). The geometry can be either fuel rods or plates, in regular arrays or clusters. WIMS-D contains tabulations of temperature dependent resonance integrals accurately evaluated for homogeneous mixtures of moderator and absorber at 120000 energy points. Equivalence theorems (λ-method) are used to obtain few-group effective cross sections in heterogeneous problems. After that a calculation in 69 energy groups and 3 spatial regions (fuel, can, moderator) coupled to

collision probabilities is performed.

Starting from the basic 70 neutron group WIMS-BOXER library (see 2.2) a 69 neutron group library for the code WIMS-D was generated (see Refs. [21,22]). The 69 group WIMS structure is equivalent to the WIMS-BOXER structure without the first (highest energetic) group. Here the NJOY module WIMSR was applied to transform the GENDF cross-sections into a form suitable as input to the WIMS library management programme, WILMA (see Refs. [21,22]).

The overall data processing scheme is depicted in simplified form in Fig.5. In the processing with WIMSR and WILMA, the relevant data were calculated by considering all explicitely represented reaction types on the GENDF files. These data pertain to the isotopes listed in Table 7 and are primarily aimed to the analysis of LWHCR fresh lattices (see Refs. [23,24]). For this reason no burnup data and no fission products were considered at the present time. Individual fission energy spectra available from the fission matrices on the GENDF library (see Ref. [14]) were not used. Instead a global fission spectrum, based primarily on data for ^{235}U was taken over from the WIMS-81 library (see Ref. [25]).

The version of the WIMSR module currently used was a specially updated one (see Refs. [23,24]). This allowed a transport correction for the self-scattering cross-section, the selection of a given dilution for evaluating scattering data and a generalized "inflow" correction for the transport cross-section. Further, it was made possible that the standard interface CCCC formatted file, RMFLUX (see Ref.[14]), be used for computing the "inflow" correction with an alternative problem-oriented weighting current. WIMSR was also modified in such a way that the slowing down power (MT=252,see 2.2) is evaluated at infinite dilution and that the identification number of each nuclide can be specified in the input. This was necessary because the nuclides hydrogen, deuterium, oxygen and carbon need to be identified by material numbers ending in 001, 002, 016 and 012, respectively. An important modification to WIMSR was related to the resonance tabulations, whereby the original background cross-section grid was shifted in each energy group by the product of the potential scattering cross section and the Goldstein-Cohen λ-factor for the resonance absorber. This considers the fact that the total background cross-section in WIMS-D consists of the contributions from all isotopes including the tabulated resonance absorber.

The WIMS-D library consists as usually of transport corrected P_0 data. The "inflow"

transport correction is computed for all nuclides using a representative standard weighting current (see Refs. [24] and Fig. 6). For light isotopes such as hydrogen, deuterium, oxygen and carbon, P_1 cross-sections are available and no transport correction is performed. The same temperatures as specified in Table 1 are included. All λ-factors are taken over from Ref. [20]. For some important isotopes, additional data sets with energy dependent λ-values are added. (see Tables 7, 8 and Ref. [21]). In this way the treatment of the resolved resonance range could be improved.

Scattering data of ^{238}U are given for different dilution cross sections (i.e. 10^{10}, 100 and 1 barns) to allow a correct analysis of a broader class of reactor cores (see Ref. [24]). The format is explained in detail in Ref. [20] . Tables 7, 8 summarize the contents of the WIMS-D library.

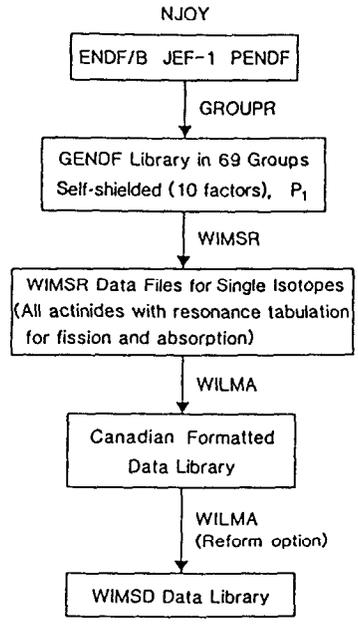

Figure 5: Calculational scheme for producing a WIMS-D formatted data library

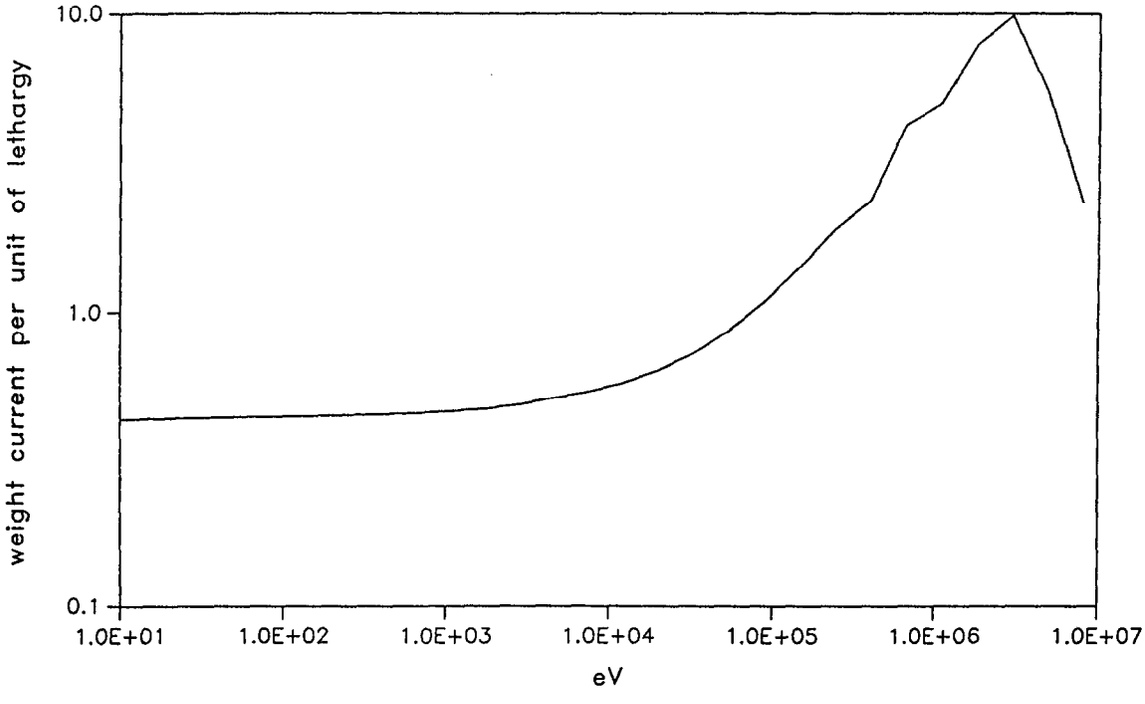

Figure 6: Weight current for transport correction in WIMS-D library

Isotope Number	Isotope Name	Resonance Tables Absorption	Resonance Tables Fission
1001	^{1}H	no	no
1002	^{2}H	no	no
12	^{12}C	no	no
14	^{14}N	no	no
7016	^{16}OL (*)	no	no
16	^{16}O	no	no
27	^{27}Al	no	no
28	Si	no	no
52	Cr	no	no
55	^{55}Mn	no	no
56	Fe	no	no
7056	FeL (*)	no	no
59	^{59}Co	no	no
58	Ni	no	no
64	Cu	no	no
91	Zr	no	no
7091	ZrL (*)	no	no
93	^{93}Nb	no	no
95	Mo	no	no
232	^{232}Th	no	no
233	^{233}U	no	no
4925	^{235}U	yes	yes
7925	^{235}UL (*)	yes	yes
4928	^{238}UFS(**)	yes	yes
5928	^{238}UID(***)	yes	yes
6928	^{238}US (****)	yes	yes
7928	^{238}UL (*) (**)	yes	yes
4948	^{238}Pu	yes	yes
4949	^{239}Pu	yes	yes
7949	^{239}PuL(*)	yes	yes
4940	^{240}Pu	yes	yes
4941	^{241}Pu	yes	yes
4942	^{242}Pu	yes	yes
4951	^{241}Am	yes	yes

(*) Energy dependent λ-vector

(**) Fully shielded scattering matrix (taken at 1 barn dilution cross section)

(***) Infinite dilute scattering matrix

(****) Scattering matrix taken at 100 barns dilution cross section

Table 7: List of isotopes pertaining to WIMS-D data library

WIMS Group	Energy dependent λ-values			
	Oxygen	Iron	Zirconium	Uranium and Plutonium Isotopes
15	0.9822	0.9857	0.9853	0.99
16	0.9930	0.9914	0.9879	0.98
17	0.9938	0.9851	0.9830	0.97
18	1.0040	0.9898	0.9803	0.96
19	0.9908	0.9862	0.9671	0.95
20	1.0007	0.9875	0.9737	0.71
21	0.9831	0.9309	0.8796	0.71
22	0.9805	0.9038	0.8158	0.33
23	0.9978	0.8391	0.6833	0.28
24	1.0247	0.5480	0.3386	0.07
25	1.0448	0.5414	0.3309	0.13
26	1.4852	0.7717	0.6686	0.63
27	0.9103	0.2398	0.1188	0.11

Table 8: Energy dependent λ-vectors included in the WIMS-D data library

4 Practical Use of MATXS Libraries

In this section some recommendations are given with respect to the practical use of MATXS libraries. First, the user should consult the index of the MATXS library to be informed about its content (i.e. data types, reactions, temperatures, shielding factors, etc.). Second, the MATXS file has to be preprocessed with the help of TRAMIX, TRANSX-CTR, or some other interface programme (e.g. JOYFOR [33]) able to read the MATXS format (see Fig. 4). In this way, a problem specific nuclear data library suitable for the available neutronics codes is generated.

This can be done independently or within the DANDE (applied nuclear DAta, Core Neutronics DEpletion) code system Ref. [29], developed at Los Alamos National Labora-

tory, and adapted at EIR. DANDE is a flexible code package which allows applications to a broad class of reactors. It consists of data processing, core neutronics and depletion modules operating in the standard CCCC file environment.

All cross sections are read into the coupling and reformatting programme TRAMIX, an EIR update of TRANSX-CTR, [17] which shields resonance data and produces neutron, photon, or coupled neutron-photon tables suitable to most transport and diffusion codes. Special features are available, such as the capability to compute accurately fission spectra from the fission matrices, to shield the data in the whole energy range (especially important in the case of the 2.7eV thermal resonance of ^{242}Pu, which is unshielded in most standard libraries of today), to generate material damage and kerma factors, to correct scattering matrices for accurate leakage calculations, and to produce a variety of library formats for neutron, photon, or coupled neutron-photon spectrum calculations.

These kinds of analyses can be achieved in DANDE or in an independent environment, when TRAMIX (or TRANSX-CTR) and a post-processor transport code such as ONEDANT are available. Furtheremore the neutron flux from the transport calculation can be coupled to burn-up or to activation calculations using some specific and detailed vector cross section data libraries associated with the DANDE system (via CINDER-3 and REAC2 modules).

Therefore only the main fuel, moderator and basic structure isotopes with full scattering matrices (characterized by high atomic number densities at the beginning or end of life) are really needed on the MATXS libraries (compare with Table 3).

Currently the data processing module of DANDE consists of the TRANSX-CTR and TRAMIX codes which process MATXS formatted cross sections. The neutronics modules include specifically different transport programmes such as the one dimensional and two dimensional discrete-ordinates transport codes ONEDANT and TWODANT, and the two dimensional finite element code TRISM, etc. The CINDER-3 code Ref. [30] is the only code used to date for the DANDE depletition module. This code does summation calculations over the various fission-product and actinide chains and provides updated nuclear densities for the principal nuclides. After each depletition step CINDER-3 collapses all involved nuclides in two categories, i.e. fission products and actinides. In this way, all computed atomic number densities are coupled with two reference scattering matrices from the MATXS library used in the next step flux calculation. Material activation pa-

rameters are carried out from the detailed density files and from the activation library. CINDER-3 was updated at EIR to account for a larger number of reactions and for a general number of energy groups, and to accept expanded chain libraries. Moreover the original 151 neutron group ENDF/B-V based Los Alamos cross section library was modified using JEF-1 data for more than 40 fission products and all actinides (see Ref. [31]). The library consists at the present time of 228 fission products and 41 actinides. The 70 neutron group MATXS library can be utilized within the DANDE system for beginning of life and burn-up calculations of thermal fission reactors, such as light water (LWR), light water high converter (LWHCR), and high temperature gas cooled reactors (HTGR) (data processing and neutronics part). The 308 neutron group library is thought for general purpose, and is adequate for fission reactor as well as fusion blanket analysis. The CINDER-3 detailed library provides all vector cross sections inclusive fission products required for burn-up analysis (depletition part). Therefore at EIR it was not necessary to accomplish the WIMS-D and MICROX-2 data libraries with a complete list of nuclides and fission products. These files are rather aimed to data testing and benchmarking of fresh cores.

The VITAMIN-J MATXS library is thought for fusion and shielding related applications within the DANDE system (data processing and neutronics part, in which the neutron and gamma spectrum distributions are determined). The group structure is a subset of the 308 groups. Therefore the VITAMIN-J library can be accomplished with shielded cross sections from a detailed 308 neutron group core calculation. In connection with the REAC2 code, this fusion library can be used for fast calculations of activation and transmutation parameters Ref. [32]. The REAC2 system consists of a pre-processor, a driver code and post-processing codes. There are libraries for vector cross sections, fluxes, decay and material data. The present cross section data are based on ENDF/B-V, ACTL and HEDL evaluated files and on systematics calculations. At the present time, the elements up to Z=84 are included.

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APPENDIX

A Energy Structure of 308, 193, 175 and 70 Neutron Group Libraries

The energy group boundaries of the libraries described in this report are given in a synoptic view in the following table. The numbers at the top of the table refer to the 308 EIR-HRB structure, to the 193 GA-MICROX structure, to the Vitamin-J 175 group structure and to the WIMS-BOXER 70 group structure. The standard 69 group WIMS structure is not a subset of the 308 group structure. Therefore some energy boundaries characterized by a ' in the last column are not identical to the first column. For the exact values of the WIMS energy boundaries please refer to Ref. [12].

Energy Structure of 308 193 175 and 70 Group Libraries

Upper Boundary	308	193	175	70	Upper Boundary	308	193	175	70
19.640 MeV	1		1		1.7377 MeV	53		53	
17.332	2				1.6530	54	23		
16.905	3				1.5724	55			
16.487	4				1.4957	56	24		
15.683	5				1.4227	57			
14.918	6	1		1	1.3533	58	25		6
14.550	7				1.2873	59			
14.191	8				1.2246	60	26		
13.840	9				1.1648	61			
13.499	10	2			1.1080	62	27		
12.840	11				1.0026 MeV	63	28		
12.523	12				961.67 keV	64			
12.214	13	3			907.18	65	29		
11.618	14				862.94	66			
11.052	15	4			820.85	67	30		7
10.513	16				780.82	68			
10.000	17	5		2	742.74	69	31		
9.5123	18				706.51	70			
9.0484	19	6			672.05	71	32		
8.6071	20				639.28	72			
8.1873	21	7			608.10	73	33		
7.7880	22				578.44	74			
7.4082	23	8			550.23	75	34		
7.0469	24				523.40	76			
6.7032	25	9			497.87	77	35		8'
6.5924	26				450.49	78	36		
6.3763	27				407.62	79	37		
6.0653	28	10		3	387.74	80			
5.7695	29				368.83	81	38		
5.4881	30	11			333.73	82	39		
5.2205	31				301.97	83	40		9
4.9658	32	12			298.49	84			
4.7237	33				297.18	85			
4.4933	34	13			294.52	86			
4.0657	35	14			287.25	87			
3.6788	36	15		4	273.24	88	41		
3.3287	37	16			247.23	89	42		
3.1664	38				235.18	90			
3.0119	39	17			223.71	91	43		
2.8650	40				212.80	92			
2.7253	41	18			202.42	93	44		
2.5924	42				192.55	94			
2.4660	43	19			183.16	95	45		10
2.3851	44				174.22	96			
2.3653	45				165.73	97	46		
2.3457	46				157.64	98			
2.3068	47				149.96	99	47		
2.2313	48	20		5	142.64	100			
2.1225	49				135.69	101	48		
2.0190	50	21			129.07	102			
1.9205	51				122.77	103	49		
1.8268 MeV	52	22	52		116.79 keV	104		104	

Energy Structure of 308 193 175 and 70 Group Libraries

Upper Boundary	308	193	175	70	Upper Boundary	308	193	175	70
111.09 keV	105	50	105	11	454.00 eV	157	72	146	
98.037	106				400.65	158			
86.517	107	51			353.57	159	73	147	22'
82.503	108				312.03	160			
79.499	109				275.36	161	74	148	
71.998	110				243.01	162			
67.379	111	52		12	214.45	163	75	149	
56.562	112				189.25	164			
52.475	113	53			167.02	165	76	150	
46.309	114				147.39	166			23'
40.868	115	54		13'	130.07	167	77	151	
34.307	116				114.79	168			
31.828	117	55			101.30	169	78	152	
28.501	118				89.398	170			
27.000	119				78.893	171	79	153	24'
26.058	120				69.623	172			
24.787	121	56		14	61.442	173	80	154	
24.175	122				54.222	174			
23.579	123				47.851	175	81	155	25'
21.875	124				42.228	176			
19.304	125	57	125		37.266	177	82	156	
17.036	126				32.888	178			
15.034	127	58	126	15	29.023	179	83	157	26'
13.268	128				25.613	180			
11.709	129	59	127		22.603	181	84	158	
10.595	130		128		19.947	182			
9.1188	131	60	129	16	17.603	183	85	159	
8.0473	132				15.535	184			27'
7.1017	133	61	130		13.710	185	86	160	
6.2673	134				12.099	186			
5.5308	135	62	131	17'	10.677	187	87	161	
4.8809	136				9.6610	188			28'
4.3074	137	63	132		9.1898	189			
3.7074	138		133		8.7416	190			
3.3546	139	64	134	18'	8.3153	191	88	162	
3.0354	140		135		7.9097	192			
2.7465	141		136		7.5240	193			
2.6126	142	65	137		7.1570	194			
2.4852	143		138		6.8080	195			
2.2487	144		139	19'	6.4759	196	89	163	
2.0347	145	66	140		6.3161	197			
1.7956	146				6.1601	198			
1.5846	147	67	141		5.5739	199			
1.3984	148			20'	5.0435	200	90	164	
1.2341	149	68	142		4.4508	201			
1.0891 keV	150				3.9279	202	91	165	29'
961.12 eV	151	69	143	21'	3.4663	203			30'
848.18	152				3.0590	204	92	166	
748.52	153	70	144		2.6996	205			
660.56	154				2.5045	206			31'
582.95	155	71	145		2.3824	207	93	167	
514.45 eV	156				2.3300 eV	208	94		

Energy Structure of 308 193 175 and 70 Group Libraries

Upper Boundary	308	193	175	70	Upper Boundary	308	193	175	70
2.2900 eV	209	95			470.00 meV	259	145		
2.2000	210	96			460.00	260	146		
2.1000	211	97		32	450.00	261	147		
2.0000	212	98			430.00	262	148		
1.9000	213	99			420.00	263	149		
1.8554	214	100	168		413.99	264	150	174	49'
1.7800	215	101			380.00	265	151		
1.7000	216	102			360.00	266	152		
1.6000	217	103			350.00	267	153		50
1.5000	218	104		33	340.00	268	154		
1.4450	219	105	169		330.00	269	155		
1.3500	220	106			320.00	270	156		51
1.3000	221	107		34	310.00	271	157		
1.2500	222	108			300.00	272	158		52
1.2000	223	109			290.00	273	159		
1.1500	224	110		35	280.00	274	160		53
1.1300	225	111			270.00	275	161		
1.1254	226	112	170	36'	260.00	276	162		
1.1100	227	113			250.00	277	163		54
1.0900	228	114		37'	240.00	278	164		
1.0800	229	115			230.00	279	165		
1.0700	230	116		38'	220.00	280	166		55
1.0600	231	117			200.00	281	167		
1.0500	232	118		39'	180.00	282	168		56
1.0250	233	119		40'	160.00	283	169		
1.0000 eV	234	120			140.00	284	170		57
990.00 meV	235	121		41'	120.00	285	171		
980.00	236	122			100.00	286	172	175	58
970.00	237	123		42'	95.000	287	173		
950.00	238	124		43'	90.000	288	174		
930.00	239	125			85.000	289	175		
910.00	240	126		44	80.000	290	176		59
890.00	241	127			75.0	291	177		
876.43	242	128	171		70.0	292	178		
850.00	243	129		45	65.0	293	179		60'
800.00	244	130		46'	60.0	294	180		61'
750.00	245	131			50.0	295	181		62
700.00	246	132			40.0	296	182		63'
682.56	247	133	172		30.0	297	183		65
650.00	248	134			25.3	298	184		66
625.06	249	135		47'	20.0	299	185		67
600.00	250	136			15.0	300	186		68
590.00	251	137			10.0	301	187		69
575.00	252	138			8.0	302	188		
550.00	253	139			7.0	303	189		
531.58	254	140	173		5.0	304	190		70
500.00	255	141		48	4.0	305	191		
490.00	256	142			2.0	306	192		
480.00	257	143			1.0	307	193		
475.00 meV	258	144			0.2	308			
					0.01 meV	E_{min}	E_{min}	E_{min}	E'_{min}

B NJOY Processing Peculiarities

Generation of Photon Multigroup Files with RECONR and GAMINR

While processing ENDF/B-V photon interaction data from DLC-99/HUGO with the NJOY RECONR module special care was given to the reconstruction tolerances in order to avoid inconsistencies in GAMINR when generating coherent scattering matrices (MF=26, MT=502) in the 42 photon energy structure. The following NJOY output shows the reconstruction tolerances of RECONR which allowed GAMINR to provide consistent coherent scattering matrices (i.e. P_0 value of MF=26, MT=502 identical to value of MF=23, MT=502) and to add correctly the total photon heating cross section MF=23, MT=621.

The coherent scattering matrix (MF=26,MT=502) was found to be wrong in the first low energy groups of the 42 group structure. This was due to an error occurring in subroutine GPANEL of the GAMINR module. The statement at line GPANEL.795 (NJOY(6/83)) did not work as it was assumed :

```
IF (EN .EQ. ENEXT .AND. IDISCF .GT. IDISC) IDISC=IDISCF
```

Here the energy EN (provided by GTFF from the array EGG(IP), containing the energy group boundaries) is compared to ENEXT (provided by GETSIG from the PENDF file). Choosing the reconstruction tolerances as in the example of the GAMINR description (Vol.III of NJOY Manual), PENDF energy values are created in the critical low energy range (1keV-60keV), which coincide almost with the energy boundary values of the 42 photon energy group-structure. Because ENEXT is not identical to EN the above mentioned statement fails. Changing the reconstruction tolerances in RECONR as shown below avoided this problem, because the fewer energy points added to the PENDF file resulted in an energy-grid, which contained exactly the energy values of the group-boundaries. (Note : This problem only existed for ENDF/B-V but not for ENDF/B-IV photon data for reasons not yet clarified)

```
RECONR...RECONSTRUCT POINTWISE CROSS SECTIONS IN PENDF FORMAT

UNIT FOR ENDF/B TAPE .................        -20
UNIT FOR PENDF TAPE ..................        -22
```

```
LABEL FOR PENDF TAPE
------------------------------------
PENDF FOR HYDROGEN FROM DLC-99 HUGO

TAPE LABEL
------------------------------------
JULY 1983 DATA FOR DLC-99/HUGO.

MATERIAL TO BE PROCESSED .............          1
RECONSTRUCTION TOLERANCE .............      0.001
RECONSTRUCTION TEMPERATURE ...........        0.K
NO. SIGNIFICANT FIGURES ..............          5
RESONANCE-INTEGRAL-CHECK TOLERANCE ...      0.001
MAX RESONANCE-INTEGRAL ERROR .........  1.000E-05

DESCRIPTIVE CARDS FOR PENDF TAPE
------------------------------------
1-HYDROGEN

PROCESSING MAT      1
------------------------------------
1-H      NBS,MPC,IPTEVAL-OCT80 J.H. HUBBELL,H.A. GIMM,I. OVERBO
```

GROUPR Input for Vitamin-J GENDF

The following sample GROUPR input (NJOY version (6/83)) shows the strategy used for the generation of the coupled Vitamin-J multigroup library :

```
*GROUPR*
20 -21 0 -29
4260 16 10 -12 6 3 7 0/
*FE-0 VITAMIN J STRUCTURE JEF-1 */
296. 600. 1200. /
1E+10 1E+4 1E+3 1E+2 10 1 0.1/
/
3/
3 251 *LAB MUBAR*/
```

```
3 -253 *ENERGY DECREMENT*/
3 221 *FREE GAS*/
6/
6 221 *FREE GAS MATRIX*/
16/
0/
3/
3 251 *LAB MUBAR*/
3 -253 *ENERGY DECREMENT*/
3 221 *FREE GAS*/
6   2 *ELASTIC MATRIX* /
6 221 *FREE GAS MATRIX*/
16/
0/
3/
3 251 *LAB MUBAR*/
3 -253 *ENERGY DECREMENT*/
3 221 *FREE GAS*/
6   2 *ELASTIC MATRIX*/
6 221 *FREE GAS MATRIX*/
16/
0/
0/
*STOP*
```

The slash on card 8A, where the flux calculator parameters have to be specified, triggered the default values for EHI (break between computed and Bondarenko flux) to be taken as the PENDF value of the energy boundary between resolved and unresolved resonance range as well as SIGPOT (estimate of potential scattering cross section) to be calculated from the ENDF value of the potential scattering radius AP read from MF=2, MT=151.

NMATXS Updates

Because of difficulties encountered when creating MATXS files containing isotopes with multiple temperatures, the NPPB parameter specified internally in subroutine VECOUT of NMATXS was set to a value which avoided the subdividing of a block. The following UPDATE directives were applied for this purpose :

```
*IDENT NMATVECO
*/ SET NPPB TO A VALUE WHICH AVOIDS SUBDIVDING OF A BLOCK.
*/ GIVES NBLK .LE. 1 OR WARNING MESSAGE.
*/ (NEEDED ONLY IF NTEMP.GT. 1 ON ANY CARD 14)
*/ CHANGE MADE BY P.VONTOBEL APRIL-14-1987
*D NMATXS.1835
      NPPB=15000/NING    (OR 26200/NING FOR 308 ENERGY GROUPS)
*I NMATXS.1836
      IF (NBLK.GT.1) WRITE(NSYSO,50)
*I NMATXS.1911
   50 FORMAT (/36H ---MESSAGE FROM VECOUT---NBLK.GT.1 )
*D NMATXS.1822
      COMMON/MAINIO/NSYSI,NSYSO,NSHORT
```

Special care had to be given to the data type NTHERM (thermal neutron scattering data) in the coupled 175/42 neutron-photon library, because of the rather small number of 11 thermal energy groups below 4.6eV. In order to get correct free gas scattering matrices at higher temperatures (i.e. different from the basic temperature) the parameter STOL of SUBROUTINE VECIN had to be decreased from 0.001 to 10^{-4} for MT=221 only. The following UPDATES were applied to NMATXS :

```
*IDENT NMATVECI
*/ ENSURES CORRECT TREATMENT OF MT=221 AT HIGHER TEMPERATURES
*/ FOR VITAMIN-J 175 GROUP STRUCTURE.
```

```
*/ DECREASES STOL TO 0.0001 FOR MT=221 ONLY.
*/ CHANGE MADE BY P.VONTOBEL JUNE-17-1987
*I NMATXS.1786
      IF(MT.EQ.221) GO TO 315
*I NMATXS.1788
  315 CONTINUE
      IF(ABS(A(LOUT)).LT.1.E-04*A(LIN)) A(LOUT)=0.
      GO TO 115
```

C Sample MATXS Index

The index listing output of the NMATXS module gives the user a detailed description of the content of the MATXS library-file. For each data type all materials (i.e. isotopes) are given with their library name, temperatures and background σ_0 values as well as the complete list of reaction types included. The convention used for naming most reactions is clear from the example given below (e.g. NG, NA, or N2N). The symbols NWT0, NWT1, NTOT0 and NTOT1 refer to the flux- and current-weighted components of the library weight function and the total cross section. Discrete-inelastic scattering in ENDF is denoted by the level plus 50; thus 51 is (n,n') first. On the MATXS library, this is given as N51. If the level decays by particle emission, the particle identifiers are tacked on after the number (e.g. N52AAA for (n,n'3α). NHEAT and NDAME are the local heat production and damage energy production cross sections. In the thermal data type, reaction names identify the binding condition; FREE for free gas, H2O for light water, etc. The coherent part is distinguished from the incoherent part by a $ sign on the end of the name. All reactions can be called by TRANSX-CTR or TRAMIX with the names listed in the index for reaction rate editing purposes.

INDEX OF MATXS FILE

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**************************************
*** FILE  MATXS         ***************
*** USER  VITJ-EIR      ***************
*** VERS    0           ***************
**************************************
```

FILE DESCRIPTION

175-GROUP VITAMIN-J STRUCTURE P6 LIBRARY
NEUTRON DATA FROM JEF-1
PHOTON DATA FROM DLC99-HUGO

DATA TYPES ON FILE

	NAME	LOCT
1	NSCAT	0
2	NGAMA	2566
3	NTHERM	2611
4	GSCAT	2776

```
**************************************
*** DATA TYPE  1 ****** NSCAT  ********
**************************************
```

MATERIALS ON FILE FOR THIS DATA TYPE

	NAME	NSUB	LOCA
1	CNAT	4	0

SUBMATERIALS FOR THESE MATERIALS

SUBMATERIAL	MATERIAL	TEMP	SIGZ
1	1	2.94E+02	1.00E+10
2	1	5.00E+02	1.00E+10
3	1	8.00E+02	1.00E+10
4	1	1.20E+03	1.00E+10

VECTOR REACTION TYPES ON FILE BY SUBMATERIAL

	1	2	3	4
1	NWTO	NWTO	NWTO	NWTO
2	NTOTO	NTOTO	NTOTO	NTOTO
3	NELAS	NELAS	NELAS	NELAS
4	NINEL	NG	NG	NG
5	N51	NHEAT	NHEAT	NHEAT
6	N52AAA	MT 401	MT 401	MT 401
7	N53AAA	NDAME	NDAME	NDAME
8	N54AAA	MT 447	MT 447	MT 447
9	N55AAA	XI	XI	XI
10	N56AAA	GAMMA	GAMMA	GAMMA
11	N57AAA			
12	N58AAA			
13	N59AAA			
14	N60AAA			
15	N61AAA			
16	N62AAA			
17	N63AAA			
18	N64AAA			
19	N65AAA			
20	N66AAA			
21	N67AAA			
22	N68AAA			
23	NCNAAA			
24	NG			
25	NP			
26	ND			
27	NA			
28	NHEAT			
29	MT 401			
30	NDAME			
31	MT 447			
32	MUBAR			
33	XI			
34	GAMMA			

MATRIX REACTION TYPES ON FILE BY SUBMATERIAL

	1	2	3	4
1	NELAS	NELAS	NELAS	NELAS
2	N51			
3	N52AAA			
4	N53AAA			
5	N54AAA			
6	N55AAA			
7	N56AAA			
8	N57AAA			
9	N58AAA			
10	N59AAA			
11	N60AAA			
12	N61AAA			
13	N62AAA			
14	N63AAA			
15	N64AAA			
16	N65AAA			
17	N66AAA			
18	N67AAA			
19	N68AAA			
20	NCNAAA			

****
*** DATA TYPE 2 ****** NGAMA ********
****

MATERIALS ON FILE FOR THIS DATA TYPE

	NAME	NSUB	LOCA
1	CNAT	4	0

SUBMATERIALS FOR THESE MATERIALS

SUBMATERIAL	MATERIAL	TEMP	SIGZ
1	1	2.94E+02	1.00E+10
2	1	5.00E+02	1.00E+10
3	1	8.00E+02	1.00E+10
4	1	1.20E+03	1.00E+10

MATRIX REACTION TYPES ON FILE BY SUBMATERIAL

	1	2	3	4
1	NG	NG	NG	NG
2	N51	N51	N51	N51

****
*** DATA TYPE 3 ****** NTHERM ********
****

MATERIALS ON FILE FOR THIS DATA TYPE

	NAME	NSUB	LOCA
1	CNAT	4	0

SUBMATERIALS FOR THESE MATERIALS

SUBMATERIAL	MATERIAL	TEMP	SIGZ
1	1	2.94E+02	1.00E+10
2	1	5.00E+02	1.00E+10
3	1	8.00E+02	1.00E+10
4	1	1.20E+03	1.00E+10

VECTOR REACTION TYPES ON FILE BY SUBMATERIAL

	1	2	3	4
1	FREE	FREE	FREE	FREE
2	GRAPH	GRAPH	GRAPH	GRAPH
3	GRAPH$	GRAPH$	GRAPH$	GRAPH$

MATRIX REACTION TYPES ON FILE BY SUBMATERIAL

	1	2	3	4
1	FREE	FREE	FREE	FREE
2	GRAPH	GRAPH	GRAPH	GRAPH
3	GRAPH$	GRAPH$	GRAPH$	GRAPH$

****
*** DATA TYPE 4 ****** GSCAT ********
****

MATERIALS ON FILE FOR THIS DATA TYPE

	NAME	NSUB	LOCA
1	C	1	0

SUBMATERIALS FOR THESE MATERIALS

SUBMATERIAL	MATERIAL	TEMP	SIGZ
1	1	0.00E+00	1.00E+10

VECTOR REACTION TYPES ON FILE BY SUBMATERIAL

	1
1	GWTO
2	GTOTO
3	GCOH
4	GINCH
5	GPAIR
6	GABS
7	GHEAT

MATRIX REACTION TYPES ON FILE BY SUBMATERIAL

	1
1	GCOH
2	GINCH
3	GPAIR

INDEX COMPLETE

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