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Vitamin-C: The CTR Processed Multigroup Cross-Section Library for Neutronics Studies

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Engineering Physics Division

Radiation Shielding Information Center

VITAMIN-C:

THE CTR PROCESSED MULTIGROUP CROSS-SECTION LIBRARY

FOR NEUTRONICS STUDIES[1]

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ABSTRACT

The program for the development, generation, validation and distribution of a general purpose Processed Multigroup Cross Section Library (PMCSL) for use in controlled thermonuclear research (CTR) neutronics studies is described. In 1974, the Radiation Shielding Information Center (RSIC) coordinated an effort to establish the CTR-PMCSL based on input requirements specified by the Energy Research and Development Administration [ERDA, now Department of Energy (DOE)] DCTR (now Office of Fusion Research) contractors. By collaborating with the ORNL Engineering Physics Division Shielding Analysis and Reactor Physics Group [which had a similar mission for the ERDA Division of Reactor Demonstration and Development (DRDD) community] it was possible to define a single 171 neutron, 36 gamma-ray group cross-section library useful for both CTR and LMFBR neutronics analysis. The master library was generated using the MINX neutron processor and the gamma-ray processor from the AMPX system. Preliminary release of the library was made to a group of ERDA contractors in AMPX and CCCC interface forms, along with appropriate retrieval and manipulation programs. Results of initial testing of the library at ORNL are described. The preliminary release was intended to stimulate implementation and testing at several installations for the purpose of improving the quality of the libraries which ultimately received general distribution under the designation DLC-41/VITAMIN-C and DLC-53/VITAMIN-4C. The successful application of VITAMIN-C as a general purpose fine-group master library has resulted in its designation by the ANS 6.1.2 Working Group on Shielding Cross Sections as an Averaged Data Set conforming to that group's "Proposed Standard on Neutron and Gamma-Ray Cross Sections for Nuclear Radiation Protection Calculations."

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1.0 Introduction

1.1 Purpose

The United States Energy Research and Development Administration (ERDA) Division of Controlled Thermonuclear Research (DCTR) began in 1974 to sponsor the Radiation Shielding Information Center (RSIC) at Oak Ridge National Laboratory (ORNL) to provide nuclear data and other information to meet the needs of ERDA-DCTR contractors. The project described in this report is the first special activity of RSIC in this role as the Nuclear Data Center for ERDA-DCTR and involves the generation, packaging, distribution, validation, and maintenance of a general-purpose multigroup cross-section library for neutronics and other radiation transport studies.

The development of the processed cross section library proceeded through the helpful cooperation of many CTR contractors. They provided valuable input in defining the specifications to ensure the relevance of the library in practical design applications and suggested procedures for the validation of the library. Several also participated in the validation program prior to the general release of the library by solving problems and comparing results to those obtained with calculations using earlier libraries and with results of experiments.

1.2 Past Role of RSIC in the DCTR Neutronics Community

During the Fusion Reactor Technology International Working Session held in Oak Ridge in 1971, an announcement was made of RSIC as a source of shielding information and data. Following the conference, we were contacted by many interested in controlled thermonuclear research (CTR) in radiation analysis. As a result, we have broadened our scope to include fusion research as we review the radiation transport literature and follow current computer code development and various programs for measuring, evaluating, and compiling cross sections. With the encouragement of several CTR government contractors, we gave support to efforts to develop data processing codes to meet unfilled needs for nuclear data (e.g. kerma factors).

A summary of services to the CTR neutronics community is presented in Ref. 1. These have been extended to include special activities as the DCTR Nuclear Data Center.

1.3 RSIC Role as the Nuclear Data Center for DCTR

RSIC began to supply the specialized cross-section requirements of the CTR neutronics community in FY 1975.

A USNDC CTR Subcommittee meeting in 1974 served as a forum in which RSIC presented plans for the establishment of an evaluated cross section library and a processed multigroup cross section library for CTR.

During discussions about the processed multigroup cross section library for use in CTR neutronics studies, various subcommittee members and other CTR contractors expressed interest in developing a processed library with more flexibility and application than that used in earlier CTR studies. It was evident that an unusual effort would be required to provide the general purpose library for DCTR contractors and the efforts of RSIC were focused on that project as the first special activity in its role as Data Center for DCTR.

1.4 Program for the Development, Generation, Validation, and Distribution of the CTR Processed Multigroup Cross Section Library (PMCSL)

The various parts of the program to produce the ERDA-DCTR Processed Library are discussed in the remainder of this report. The specifications and methods of determining them are described in Section 2.0. The computer codes used to generate the data are indicated in Section 3.0. Section 4.0 discusses the various formats for transmitting the library to other installations, and manipulation codes which will be distributed as a part of the data package are discussed in Section 5.0. The contents of the initial data library package, including the sample problems provided, are summarized in Section 6.0. A description of a limited validation program for the data library is given in Section 7.0. A discussion of the release for general distribution of the libraries and retrieval codes is given in Section 8.0. The designation of final library (VITAMIN-C) as an ANS Standard is discussed in Section 9.0.

2.0 Specifications

2.1 Survey of CTR Community Needs

2.1.1 Background

The Radiation Shielding Information Center (RSIC) prepared a draft proposal[2] titled "Nuclear Data Services for the CTR Community" which was circulated by Lester Price, an ERDA-DCTR staff member, to various interested agencies and groups. A presentation of RSIC's plans was made at the November 1974, Washington, D.C. USNDC-CTR Subcommittee meeting. The discussion at the meeting about RSIC's plans for generating multigroup data emphasized the need for further study. Don Steiner, the Subcommittee Chairman, suggested that an informal advisory committee be utilized by RSIC to try to formulate plans to better meet the current needs for CTR neutronics calculations. Following the meeting, personnel at the University of Wisconsin, Princeton Plasma Physics Laboratory, the University of Texas, Battelle Northwest, Los Alamos Scientific Laboratory, Lawrence Livermore Laboratory, General Atomic, Argonne National Laboratory, and Oak Ridge National Laboratory were contacted and their needs surveyed.

2.1.2 Results of Survey

The conversations and correspondence with the informal advisory committee resulted in a better definition of the current needs of the CTR neutronics community. In general, it was felt that the Bondarenko[2,3] formalism for self-shielding and temperature dependence effects should be utilized. Many of those contacted felt that finer energy group structure definition was needed particularly in the high energy region. The reasoning was that they would like to be able to conveniently make changes to the multigroup data which would reflect information that might be obtained from new cross section measurements for high energy reactions. Most of those contacted felt that P_3 Legendre expansion was sufficient. Some people were interested in having coupled neutron and gamma-ray cross section libraries. Others felt that gamma production and interaction data were necessary, but wanted to have the capability of doing each part of the calculation separately. It was felt desirable to have individual reaction cross sections and scattering matrices. There seemed to be consensus that energy boundaries should be related to multigroup sets that had been used previously for neutronics calculations. Finally, it was felt that within the concept of the Bondarenko formalism it was sufficient to supply means of doing a simple homogeneous interpolation and iteration for a given problem to determine the appropriate values of σ_0 and T.

A memo[4] summarizing the results of the survey and giving proposed specifications for a processed cross section library of general usefulness for CTR neutronics studies was prepared and distributed for comment. The memo identified 156 neutron groups, 23 gamma-ray groups and P_3 Legendre expansion for 44 materials. The MINX[5] neutron processor was suggested for obtaining neutron cross sections and Bondarenko factors over a wide range of temperatures and background cross sections. The output format suggested was the AMPX[6] Master Interface Format so that complete information could be made available for all reaction cross sections and transfer matrices. A weighting function was suggested which contained a Maxwellian thermal group, a "1/E" slowing down region, a fission spectrum, and a fusion peak.

Comments on these proposed specifications were then received and considered. Additional materials and energy groups were requested. It was suggested that the velocity exponential form be used to represent the fusion peak. A special weighting function for the thermal group for a few materials was suggested for more detailed study of systems in which neutron transport is dominated by Li-6. A P_5 expansion for U-238 was suggested for more detailed studies of neutron transport in that medium.

There was some feeling that the data should also be made available in CCCC[7] Interface Format. Although that format is not at the present time as flexible and comprehensive as the AMPX interface format (e.g., fewer reactions allowed, gamma-ray production treatment inadequate), it was felt that some users in the ERDA-DRRD reactor physics community might benefit by having access to the library. In addition, another project at ORNL involving the generation of multigroup cross sections, as described in Section 2.2, enhanced the prospects of providing data in both AMPX Interface and CCCC Interface formats.

2.2 Relationship to the DOE-DRRT Coupled Neutron-Gamma-Ray Libraries

As the effort to define specifications for CTR user needs was proceeding, a similar activity on behalf of the ERDA Division of Reactor Development and Demonstration (DRRD) [now DOE-RRT] was in progress within the ORNL Engineering Physics Division. The DRRT project has as its goal the generation of pseudo-composition independent fine-and broad-group neutron and gamma-ray cross section libraries as well as fine- and broad-group composition-dependent coupled libraries based on a Clinch River Breeder Reactor (CRBR) model. Since many of the materials needed for this purpose would also be requested for the CTR Library, it was felt that it would be cost effective to combine the specifications needed for both user communities and process a single master library which could serve the needs of each. This master library serves as the CTR multigroup library without further specific reduction in number of energy groups. The specifications are given in sections 2.3 and 2.4. The DRRT libraries are derived from this master and the specifications are documented in Ref. [8].

2.3 Resulting Physical Specifications

2.3.1 Materials to be Included

A list of the materials to be processed, the source of the evaluated data to be used, and values of temperatures and background cross sections for each material are given in Table 1.

The list includes materials proposed for conceptual designs of both fusion and hybrid fusion/fission systems.

2.3.2 Energy Group Structure to be Used

The energy structure selected for the 171 neutron groups contained in the CTR processed cross section library is given in Table A1 of Appendix A. Also indicated therein are the relationship of the 171 neutron group structures to those that have been commonly used in CTR neutronics work, such as the 100 group structure of DLC-2[9] and DLC-37[10] and the 52 group structure of DLC-28.[11] In addition, the relationship to the 239 group CSEWG standard[12] and to the 126 group structure of the DRRT libraries[8] are also indicated.

The energy structure selected for the 36 gamma-ray groups contained in the CTR Processed Multigroup Cross Section Library (PMCSL) is given in Table A2 of Appendix A. The relationship of this 36 group structure to other familiar gamma-ray group structure is also shown.

2.3.3 Weighting Function Used to Generate the CTR Processed Multigroup Cross Section Library

For the purpose of generating the multigroup cross sections, the neutron energy region between thermal and 17.333 MeV was divided into 6 regions and a different functional form was assumed for each region. Included are a Maxwellian thermal spectrum, a fission spectrum, and a DT

Table 1. Materials to be Included in the CTR Processed Multigroup Cross Section Library (All Data to be Generated at 300, 400, and 2100°K)

Material	MAT*	Authors	Institution	Values of σ_o(b)
H-1	1269	L. Stewart, R. LaBauve, P. Young	LASL	
H-2	1120	B. Leonard, L. Stewart	BNWL	
H-3	1269	L. Stewart	LASL	
He-4	1270	R. Nisley, G. Hale, P. Young	LASL	
Li-6	1271	G. Hale, D. Dodder, P. Young	LASL	10^3 to 1 (by decades)
Li-7	1272	R. LaBauve, L. Stewart, M. Battat	LASL	10^3 to 1
Be-9	1289	R. Howerton, S. Perkins		10^3 to 1
B-10	1273	G. Hale, R. Nisley, P. Young	LASL	10^3 to 1
B-11	1160	C. Cowan	GE	10^3 to 1
C-12	1274	F. Perey, C. Fu	ORNL	10^3 to 0.1
N-14	1275	P. Young, D. Foster, G. Hale	LASL	
O-16	1276	P. Young, D. Foster, G. Hale	LASL	10^3 to 0.1
F	1277	C. Fu, D. Larson	ORNL	10^3 to 0.1
Na-23	1156	Paik, Pitterle	WARD	10^3 to 0.1
Mg	1280	M. Drake, M. Fricke	SAI	10^3 to 0.1
Al-27	1193	P. Young, G. Foster	LASL	10^3 to 0.1
Si	1194	D. Larson, F. Perey	ORNL	10^3 to 0.1
P	7019***	R. Howerton	LLL	10^3 to 0.1
S	7020***	R. Howerton	LLL	10^3 to 0.1
K	1150	M. Drake	GGA	10^3 to 0.1
Ca	1195	C. Fu, F. Perey	ORNL	10^3 to 0.1
Ti	1286	R. Howerton, R. Haight, S. Perkins	LLL	10^3 to 0.1
V	1196	S. Penny, L. Owen	ORNL	10^3 to 0.1
Cr	1191	A. Prince	BNL	10^5 to 1
Mn-55	1197	S. Takahashi	BNL	10^3 to 0.1
Fe	1192	C. Fu, F. Perey	ORNL	10^3 to 0.1
Co-59	1199	T. Krieger (BNL), A. Smith, D. Smith	BNL, ANL	10^3 to 0.1
Ni	1190	M. Bhat	BNL	10^3 to 0.1
Cu	1295	M. Drake, M. Fricke	SAI	10^3 to 0.1
Cu-63**	1085			10^3 to 0.1
Cu-65**	1086			10^3 to 0.1
Zirc-2	1285	B. Leonard	BNWL	10^3 to 0.1
Nb-93	1189	R. Howerton (LLL), A. Smith, P. Gunther, J. Whalen	LLL, ANL	10^3 to 0.1
Mo	1287	R. Howerton	LLL	10^5 to 1
Ag-107	1138	M. Bhat, A. Prince	BNL	10^5 to 1
Ag-109	1139	M. Bhat, A. Prince	BNL	10^5 to 1
Cd	1281	S. Pearlstein	BNL	10^5 to 1
Sn	7039***	R. Howerton	LLL	10^5 to 1
Eu-151	1290	H. Takahashi	BNL	10^5 to 1

Table 1. (continued)

Material	MAT*	Authors	Institution	Values of σ_o(b)
Eu-152	1292	H. Takahashi	BNL	10^5 to 1
Eu-153	1291	H. Takahashi	BNL	10^5 to 1
Eu-154	1293	H. Takahashi	BNL	10^5 to 1
Ta-181	1285	R. Howerton, S. Perkins, M. MacGregor	LLL	10^5 to 1
W-182	1128	J. Otter, E. Ottewitte, P. Rose, P. Young (LASL)	AI, LASL	10^5 to 1
W-183	1129	J. Otter, E. Ottewitte, P. Rose, P. Young (LASL)	AI, LASL	10^5 to 1
W-184	1130	J. Otter, E. Ottewitte, P. Rose, P. Young (LASL)	AI, LASL	10^5 to 1
W-186	1131	J. Otter, E. Ottewitte, P. Rose, P. Young (LASL)	AI, LASL	10^5 to 1
Pb	1288	C. Fu, F. Perey	ORNL	10^5 to 1
Th-232	1296	W. Wittkopf, Roy, Z. Livolsi	B&W	10^5 to 1
U-233	1260	N. Steen	BAPL	10^5 to 1
U-234	1043	M. Drake, Nichols	GGA	10^5 to 1
U-235	1261	L. Stewart, H. Alter (AI), R. Hunter	LASL, AI	10^5 to 1
U-236	1163	J. McCrosson	SRL	10^5 to 1
U-238	1262	N. Paik	WARD	10^4 to 0.1
Pu-238	1050	H. Alter	AI	10^4 to 1
Pu-239	1264	B. Hutchins (GE), R. Hunter, L. Stewart	GE, LASL	10^5 to 1
Pu-240	1265	E. Pennington, H. Hummel	ANL	10^5 to 1
Pu-241	1266	H. Hummel, E. Pennington	ANL	10^5 to 1
Pu-242	1161	H. Alter, C. Dunford	AI	10^5 to 1
Am-241	1056	J. Smith, R. Grimesey	ANC	10^5 to 1

*All data generated from ENDF/B-IV unless otherwise noted (Ref. 15)
**From ENDF/B-III (Ref. 16)
***From Livermore Evaluated Data Library (Ref. 17)

Key to Laboratory Abbreviations:

AI	Atomics International
ANC	Aerojet Nuclear Company
ANL	Argonne National Laboratory
B&W	Babcock and Wilcox
BAPL	Bettis Atomic Power Laboratory
BNL	Brookhaven National Laboratory
BNWL	Battelle Northwest Laboratory
GE	General Electric
GGA	Gulf General Atomic
LASL	Los Alamos Scientific Laboratory
LLL	Lawrence Livermore Laboratory
ORNL	Oak Ridge National Laboratory
SAI	Science Applications, Inc.
SRL	Savannah River Laboratory
WARD	Westinghouse Advanced Reactor Division

fusion neutron spectrum with "1/E" slowing down regions joining these three prominent features. These are summarized in more detail in Table 2.

For the gamma-ray energy region, no energy dependence was assumed, i.e., a "flat" weighting function was used. This assumption is commonly used for producing gamma-ray multigroup cross sections.

2.3.4 Expansion Order Tolerances Used in the Neutron Cross Section Processing

The Legendre expansion order is P_3. The fractional error tolerances (percent) are set at 0.5 except for integration which is 0.1%. (The current library, used for preliminary testing, contains data processed with 0.5% tolerance for the heavy nuclides. For the light nuclides the fractional error tolerance (percent) of the current file is 1.0 for resonance reconstruction and for linearization, 0.5 for thinning, and 0.1 for integration.)

The above tolerances refer to control parameters used by the MINX program.

2.4 Resulting Format Specifications

As was mentioned earlier in Section 2.1.2, the AMPX Master Interface Format was chosen as the basic form for the CTR library because it has the generality to provide data in as much detail as is given in the basic ENDF file from which the multigroup cross sections are derived. All partial reaction cross sections and transfer matrices are present and are designated using the same identifying integers (MT numbers) as those used in ENDF.

Data are available in the form of a 171 neutron group AMPX interface, a 171 neutron, 36 gamma-ray group production AMPX interface, and a 36 group, gamma-ray interaction AMPX interface. These will give the user tremendous flexibility in having as much detailed information available as possible.

The neutron data are also available in CCCC format as ISOTXS neutron cross section and BRKOXS self-shielding factor standard interface files. In order for users of these files to have the capability of also performing coupled neutron and gamma-ray transport studies, some provisions have been made to allow the combining of these files with the AMPX gamma-ray production and interaction files to produce problem-dependent (self-shielded) coupled cross section libraries for radiation transport studies. More details of these features are provided in Section 5.2.

3.0 Codes Used for Generating the Library

3.1 MINX Computer Code for Generation of Multigroup Neutron Cross Sections with Self-Shielding Factors

For a given nuclide, MINX calculates multigroup energy-averaged microscopic neutron cross sections from evaluated cross section files in ENDF format.[18] Group constants in both the AMPX interface and CCCC interface

Table 2. Neutron Energy Weighting Function
Used for the CTR-PMCSL

Functional Form	Energy Limits
(1) Maxwellian Thermal Spectrum ($300^{o}K$) $S_1(E) = C_1 E e^{-E/kT}$	10^{-5} eV to 0.125 eV
(2) "1/E" Slowing-Down Spectrum $S_2(E) = C_2/E$	0.125 eV to 820.8 keV
(3) Fission Spectrum (Θ = 1.4 MeV) $S_3(E) = C_3 E^{1/2} e^{-E/\Theta}$	820.8 keV to 10.0 MeV
(4) "1/E" Spectrum $S_4(E) = C_4/E$	10.0 MeV to 12.57 MeV
(5) Velocity Exponential Fusion Peak (E_p = 14.07 MeV) (kT = 0.025 MeV) $S_5(E) = C_5 \exp\left[-\frac{5}{kT}\left(E^{1/2} - E_p^{1/2}\right)^2\right]$	12.57 MeV to 15.57 MeV
(6) "1/E" Spectrum $S_6(E) = C_6/E$	15.57 MeV to 17.333 MeV

formats are produced by a version of MINX which has been made operational on the IBM 360 system at ORNL and extended to allow this dual output capability. The AMPX format is more flexible than CCCC in that all partial cross section information is retained (e.g. group-to-group transfer cross sections for discrete inelastic levels, and group averaged cross sections for threshold reactions (e.g., n,n'α)). The Bondarenko method (narrow resonance approximation) is employed to create group dependent resonance self-shielding factors to account for temperature and dilution effects.

MINX was developed to calculate multigroup constants with user control over computational errors. This helps to distinguish uncertainties in the multigroup data arising from numerical approximations in the averaging procedure from those due to errors in the basic ENDF cross section data.

3.2 AMPX Modules for Gamma-Ray Production and Interaction Cross Sections Generation

The LAPHNGAS module calculates multigroup secondary gamma-ray production cross sections and/or multigroup secondary gamma-ray yields (multiplicities). To allow for self-shielded gamma-ray production matrices, LAPHNGAS was modified to place multigroup yields for all ENDF/B File 12 reactions on the LAPHNGAS output file. The ENDF/B File 13 production data is not self-shielded in the present approach.

The SMUG module calculates multigroup photon cross sections with transfer coefficients represented by a user specified Legendre approximation.

4.0 Output Formats for Distributing the Library

4.1 AMPX Interface Formats

The AMPX Master Interface Format is described in Ref. 6.

There are two forms of the format: an unformatted (binary) form which is used by modules within the AMPX system and a card image form (BCD). The BCD form will be used for distributing the library, since that form is normally not dependent on computer systems. An appropriate BCD-to-binary form conversion code will be provided so the user can transform the library into the form used in the manipulation programs.

4.2 CCCC Interface Formats

A description of the CCCC interface formats for neutron cross sections (ISOTXS) and self-shielding factors (BRKOXS) is included in Ref. 7. There are also binary and BCD forms for these files, and the BCD version, along with a conversion code will be the form used for distribution.

4.3 Working Library Formats

It is likely that special libraries will be generated from the basic master (171,36) coupled library and made available in working formats such as that used by the ANISN[19] and DTF [20] series of radiation transport computer codes. These will be generated for conditions pertinent to a particular problem and will probably not be suitable for general application.

5.0 Codes Used for Retrieving and Manipulating the Data

5.1 Retrieval and Manipulation Codes for the AMPX Interface Format.

A wide variety of user operations is available through the use of various modules of the AMPX system. The names of the codes and a brief description of their functions are given in Ref. 21.

5.2 Retrieval and Manipulation Codes for CCCC Interface Format

A similar range of user operations is available for the CCCC interface form of CTR-PMCSL. The names of the codes and a brief description of their functions are given in Appendix B. Further details, including input instructions are given in Ref. 21.

5.3 Additional Codes Used in the CTR PMCSL Sample Problems.

Some additional computer codes were utilized to allow the execution of the transport calculations by means of the ANISN program. These are described briefly in Appendix B and additional descriptions and input instructions are given in Ref. 21.

6.0 Contents of the Preliminary Data Library Package

6.1 AMPX Interface Form

The AMPX interface form of the CTR PMCSL consists of three elements: (1) AMPX BCD Master Interface Files; (2) AMPX Interface Retrieval Codes; (3) Sample Input Data and Output Results. This form of the data library is described in more detail in Appendix C. Two sample problems have been prepared and executed. The first is the calculation of the infinite medium representation of the ZPR-6/7 experiment[22] to illustrate the resonance self-shielding capabilities of the library and codes. The second is the so-called CTR standard blanket.[23]

6.2 CCCC Interface Form

The CCCC Interface form of the CTR PMCSL consists of four elements: (1) CCCC BCD Neutron Interface Files; (2) AMPX BCD Master Interface Files; (3) Appropriate CCCC Interface and AMPX Interface Retrieval Codes; (4) Sample Input Data and Output Results. This form of the Data Library is described in more detail in Appendix D.

6.3 Known Deficiencies in the Preliminary Data Package

Results of initial data testing performed on the preliminary library

During the course of library development, several MINX processing problems introduced deficiencies which influenced the usefulness of some nuclides in the preliminary library. The problems identified are listed below:

(a) Resonance Reconstruction

(1) ^{238}U has an inadequate number of points about the peaks for resonances in the 1-5 keV energy range (processing limitation in BCD ENDF/B representation employed).

(2) An IBM precision difficulty at the break points between the resonance and smooth background regions created an error in the pointwise data at the point of discontinuity.

(b) Multigroup averaging

(1) The unresolved background cross sections are not included.

(2) For materials with resonance parameters, there is a discrepancy on the order of a few percent in the group spanning the discontinuity cited in item (a.2) above.

(3) The Mo cross sections are too high in the unresolved resonance range due to the omission of the abundance in the interference term (only affects the total and elastic scattering cross sections).

(c) Inelastic scattering transfer matrix calculations

(1) There are small negative P_o matrix elements for Na (MT = 52,56), ^{55}Mn (MT = 54), ^{235}U (MT = 62,65), ^{239}Pu (MT = 75).

(2) Inelastic matrix sums do not add precisely to the group averaged cross section. Generally, the "column sums" are lower and the threshold group has the largest discrepancy.

(d) Continuum scattering transfer matrix calculation

The P_ℓ terms (where $\ell > 0$) are missing for all nuclides in the AMPX interface format.

It is emphasized that all of the above mentioned processing problems have been resolved and were eliminated from the library when those nuclides affected were reprocessed.

7.0 Validation Program

A meeting was held at ORNL in August, 1975 where several CTR contractors were invited to come and discuss procedures for validating the CTR Processed Cross Section Library. The goals of such a program were discussed, some milestones were suggested, and participation in various calculational efforts was offered by the attendees.

7.1 Goals

The goals are primarily to test the validity of the output of the neutron and gamma-ray processing codes and to determine the adequacy of the various retrieval codes that support the library. No attempt was made to separate processing approximations from nuclear data deficiencies in the basic evaluated data from which the multigroup data are derived.

7.2 Milestones

Milestones were proposed at the time of the meeting. 9/1/75: retrieval codes to be sent out; 9/26/75: library goes out; November ANS meeting: check on progress; 1/1/76: calculations completed and first round analysis done; 2/1/76: library reprocessed in final form (171 group); 3/1/76: calculations to be redone; 6/30/76: final report on validation (RSIC report). Various problems have been encountered which have caused the starting portion of the program to slip by several months. However, during the delay to release the data to participants of the validation effort, several data and programming difficulties have been discovered and corrected. The fact that these have been fixed prior to release should make the utilization that much easier for the participants.

The various calculational efforts which were tentatively offered by various installations are listed in Table 3.

7.3. Results

Participants in the voluntary validation program obtained and utilized the preliminary versions of the libraries as described in Appendices C and D. Another meeting of the group was held at ORNL in July 1977 to summarize the experience that had been gained.

Results of the validation program were very helpful in developing the versions of the cross section library and associated retrieval and manipulation codes to be released for general distribution.

The AMPX formatted version of the library was implemented at six laboratories; Argonne National Laboratory, Battelle Northwest Laboratory, Princeton Plasma Physics Laboratory, Oak Ridge National Laboratory, the University of Wisconsin, and Westinghouse Fusion Power Systems. The CCCC formatted version was implemented at Los Alamos Scientific Laboratory. Calculations at Lawrence Livermore Laboratory of the CTR Standard Blanket problem using Monte Carlo and a different library provided an independent test of the data and codes in the CTR PMCSL.

The validation effort helped debug some data sets and retrieval codes in the preliminary versions of the libraries. In addition, some participants also converted retrieval codes to UNIVAC (U. Wisconsin) and CDC (Battelle Northwest Laboratory and Westinghouse Fusion Power System) computers and made them available for general distribution through RSIC. In addition, Los Alamos Scientific Laboratory supplied improved routines for more efficient retrieval and manipulation of the CCCC formatted data.

Some results of the calculations were presented at the June 1976 American Nuclear Society Meeting[24] and at an RSIC Seminar on Multigroup Cross Sections in March 1978.[25]

8.0 General Release of the CTR-PMCSL as VITAMIN-C

8.1 Cross Section Libraries

Initial results of the validation effort indicated satisfaction with the basic form and content of the library and plans for general release were implemented. The first release of the library for general distribution was announced in the February, 1977 RSIC Newsletter. The 36 material library in AMPX format was designated VITAMIN-C (Versatile Integrated Techniques for Utilizing AMPX and MINX Cross Sections in Neutronics Calculations), and the package contained retrieval codes for AMPX formatted data as described in Appendix B.

In December 1977, the second release was announced in the RSIC Newsletter. An additional 25 materials were added to the original 36. This version, designated DLC-41B/VITAMIN-C, did not include retrieval codes. They were removed from each data library in AMPX format to ease the updating mechanism when changes were required in a retrieval code. Separate packages containing appropriate retrieval codes were planned and distributed as indicated below.

In March 1978 the VITAMIN-C library was one of the libraries featured in the Workshop portion of an RSIC Seminar-Workshop on Multigroup Methods.[25] The workshop demonstrated the utilization of the various retrieval codes for deriving problem-dependent cross sections from the basic VITAMIN-C library.

The third update, designated DLC-41C/VITAMIN-C, was announced in the July 1979 RSIC Newsletter. An additional 5 materials were added, and revisions were made to a number of the existing data sets.

The version of the library in CCCC format ('4C'), designated DLC-53/VITAMIN-4C, was announced in the June 1978 RSIC Newsletter.

8.2 Retrieval Codes

As indicated above, approximate retrieval codes which can be used to manipulate cross section libraries in AMPX and CCCC formats have been collected and packaged in RSIC.

Retrieval codes for AMPX formatted data for non-IBM hardware have been contributed by members of the validation group and other RSIC users. The RSIC package PSR-112A/MAME[26] contains CDC and PSR-112B/MAME contains UNIVAC versions, respectively, of the important retrieval codes. These were announced in the January 1978 RSIC Newsletter.

Retrieval codes for IBM hardware which can handle both AMPX and CCCC formatted data are found in PSR-117/MARS.[21] That package was originally announced in the April 1978 RSIC Newsletter and updated in May 1979. The CCCC codes came originally from LASL and WARD and were converted to IBM at ORNL. The AMPX codes come from the ORNL code system which is packaged in RSIC as PSR-63/AMPX-II.

9.0 VITAMIN-C as an ANS Standard Library

The ANS 6.1.2 Working Group on Shielding Cross Sections has prepared a proposed Standard on Neutron and Gamma-Ray Cross Sections for Nuclear Radiation Protection Calculations[27] which is currently undergoing the review and balloting procedure within the American Nuclear Society ANS-6 Radiation Protection and Shielding Standards Subcommittee. The Proposed Standard, which outlines procedures for the preparation of multigroup libraries, recommends DLC-41/VITAMIN-C as an Averaged Data Set which conforms to the Standard.

Table 3. Calculational Efforts Offered by Various Installations as Part of the CTR-PMCSL Validation Effort

OAK RIDGE NATIONAL LABORATORY

1. Standard Blanket[1]
2. TFTR
   (Compare with DLC-37)
3. Fe and C Ring Experiments
   (Compare with AMPX results)
4. Japanese Experiment[2]
5. U. Illinois Fe Sphere[3]
   (Compare with AMPX results)

WESTINGHOUSE FUSION POWER SYSTEM

1. Standard Blanket
2. TFTR Shielding
   (Compare with own library)

UNIVERSITY OF WISCONSIN

1. Standard Blanket
2. TEPR-I (ANL)[4]
3. UWMAK-III

LAWRENCE LIVERMORE LABORATORY

1. Standard Blanket
2. Pulsed Spheres[5]
3. Weale[8]
   (Compare with CLYDE, TART results)

ARGONNE NATIONAL LABORATORY

1. Standard Blanket
2. ANL-TEPR
   (Compare with DLC-37)

PRINCETON PLASMA PHYSICS LABORATORY

1. Standard Blanket
2. PRD Blanket[6]
   (Compare with DLC-28)

LOS ALAMOS SCIENTIFIC LABORATORY

1. Standard Blanket
2. RTPR Benchmark
3. Wyman Experiment[7]
4. Possibly several others

BATTELLE NORTHWEST LABORATORY

1. Standard Blanket
2. Weale Experiment
3. German Experiment
4. Japanese Experiment

References

1. ORNL-TM-4177
2. Nuclear Science and Engineering, Aug. 1975
3. Washington, D.C. Cross Section Conference, 1975
4. ANL/CTR-75-2 and ANL/CTR/TM-51
5. UCRL-74277, Rev. I (1973)
6. MATT-1050
7. Texas Symposium, 1972
8. Reactor Sci. Technol., J. Nucl. Energy, Parts A and B, 14, 91 (1961)

10.0 References

1. R. W. Roussin, D. K. Trubey, and B. F. Maskewitz, "Services to the CTR Community by the Radiation Shielding Information Center," Proceedings of the First Topical Meeting on the Technology of Controlled Nuclear Fusion, Vol. II, p. 227, CONF-740402-P2.

2. R. W. Roussin, "Nuclear Data Services for the CTR Community," presented at the 1974 Washington, D.C. USNDC-CTR Subcommittee meeting; text included in the minutes of that meeting.

3. I. I. Bondarenko, Ed., "Group Constants for Nuclear Reactor Calculations," Consultants Bureau, New York (1964).

4. R. W. Roussin, "Proposed Specifications for a Neutron and Gamma-Ray Multigroup Cross-Section Library for CTR Neutronics Calculations," ORNL Intra-Laboratory Memo, December 19, 1974.

5. C. R. Weisbin, P. D. Soran, R. E. MacFarlane, D. R. Harris, R. J. LaBauve, J. S. Hendricks, J. E. White, R. B. Kidman, "MINX: A Multigroup Interpretation of Nuclear Cross Sections from ENDF/B," LA-6486-MS (ENDF-237), September 1976. Available from the Radiation Shielding Information Center as PSR-105/MINX.

6. N. M. Greene, J. L. Luxius, L. M. Petrie, W. E. Ford, III, J. E. White, and R. Q. Wright, "AMPX: A Modular Code System for Generating Coupled Multigroup Neutron-Gamma Libraries from ENDF/B," ORNL-TM-3706 March, 1976. Available from RSIC as PSR-63/AMPX-II.

7. B. M. Carmichael, "Standard Interface Files and Procedures for Reactor Physics Codes, Version III," LA-5486-MS, February 1974.

8. C. R. Weisbin, R. W. Roussin, J. E. White, and R. Q. Wright, "Specification for Pseudo-Composition-Independent Fine-Group and Composition Dependent Fine-and Broad-Group LMFBR Neutron-Gamma Libraries at ORNL," ORNL-TM-5142 (ENDF-224), December 1975.

9. R. W. Roussin, "Abstracts of the Data Library Packages Assembled by the Radiation Shielding Information Center," ORNL-RSIC-30, Vol. I (1972).

10. D. M. Plaster, R. T. Santoro, and W. E. Ford, III, "Coupled 100-Group Neutron and 21-Group Gamma-Ray Cross Sections for EPR Calculations," ORNL-TM-4872, April 1975. Available from RSIC as DLC-37/EPR.

11. J. T. Kriese, "Coupled Neutron and Gamma-Ray Cross Section Sets for Fusion Reactor Calculations," ORNL-TM-4277, August 1973. Available from RSIC as DLC-28/CTR.

12. C. R. Weisbin and R. J. LaBauve, "Specification of a Generally Useful Multigroup Structure for Neutron Transport," LA-5277-MS (1973).

13. D. E. Bartine, J. R. Knight, J. V. Pace, III, and R. W. Roussin, "Production and Testing of the DNA Few-Group Coupled Neutron-Gamma Cross Section Library," ORNL/TM-4840, March 1977. Available from RSIC as DLC-31/(DPL-1/FEWG1).

14. E. A. Straker, "Suggested Energy Group Bounds for a General Purpose Photon Multigroup Cross Section Set," SAI-74-566-HU.

15. D. Garber, Compiler, "ENDF/B Summary Documentation," BNL 17451 (ENDF-201), 2nd Edition, October 1975.

16. O. Ozer and D. Garber, Assemblers, "ENDF/B Summary Documentation," BNL-17541 (ENDF-201) May 1973.

17. R. J. Howerton, "The Lawrence Livermore Laboratory Evaluated Nuclear Data Library (ENDL) Translated into ENDF/B Format," UCID-16727 (1975).

18. D. Garber, et al., "Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF," BNL-NCS-50496 (ENDF 102), October 1975.

19. W. W. Engle, Jr., "A Users' Manual for ANISN," K-1693 (1967).

20. K. D. Lathrop, "DTF-IV, A FORTRAN IV Program for Solving the Multigroup Transport Equation with Anisotropic Scattering," LA-3373, November 1965.

21. RSIC Package PSR-117/MARS, "Collection of Computer Codes for Manipulating Multigroup Cross Section Libraries in AMPX or CCCC Formats," available from RSIC.

22. "Cross Section Evaluation Working Group Benchmark Specifications," BNL 19302 (ENDF-202), November 1974, Fast Reactor Benchmark No. 12.

23. D. Steiner, "Analysis of a Bench-Mark Calculation of Tritium Breeding in a Fusion Reactor Blanket. The United States Contribution," ORNL-TM-4177, April 1973.

24. R. W. Roussin, C. R. Weisbin, J. E. White, N. M. Greene, R. Q. Wright, and J. B. Wright, "Progress on the Validation of the CTR Multigroup Data Package," Trans., Am. Nuc. Soc., 23 (14) June 1976.

25. D. K. Trubey and H. R. Hendrickson, Compilers, "A Review of Multigroup Nuclear Cross-Section Processing: Proceedings of a Seminar Workshop, Oak Ridge, Tennessee, March 14-16, 1978," ORNL/RSIC-41, October 1978.

26. RSIC Package PSR-112/MAME, "Miscellaneous AMPX-I Modules from Everywhere." Available from RSIC, January 1978.

27. "Neutron and Gamma-Ray Cross Sections for Nuclear Radiation Protection Calculations," Draft of Proposed Standard, November 1979, D. Harris, Chairman, ANS-6.1.2, Rensselaer Polytechnic Institute.

APPENDIX A

Neutron and Gamma-Ray Energy Group Boundaries for the CTR Processed Multigroup Cross Section Library

The 171-neutron and 36-gamma-ray energy group boundaries for the CTR Processed Multigroup Cross Section Library are given in Tables A1 and A2, respectively. The relationship of the group structures of this library to the group structures used in various other libraries is also indicated in the tables.

Table A1. CTR-PMCSL Neutron Energy Group Boundaries and Their Relationship to Those Used for Other Libraries

100n*	52n**	Suggested Upper Energy (eV)		Lethargy	239n***	126n***
		1	.17333E+08	-.55000E+00	7	
		2	.16487E+08	-.50000E+00	9	
		3	.15683E+08	-.45000E+00	11	
1	1	4	.14918E+08	-.40000E+00	13	1
		5	.14550E+08	-.37500E+00	14	
		6	.14191E+08	-.35000E+00	15	
		7	.13840E+08	-.32500E+00	16	
2	2	8	.13499E+08	-.30000E 00	17	
		9	.12840E+08	-.25000E+00	19	
3	3	10	.12214E+08	-.20000E+00	21	2
		11	.11618E+08	-.15000E+00	23	
4	4	12	.11052E+08	-.10000E+00	25	
		13	.10513E+08	-.50000E-01	27	
5	5	14	.10000E+08	0.	29	3
		15	.95123E+07	.50000E-01	31	
6	6	16	.90484E+07	.10000E+00	33	
		17	.86071E+07	.15000E+00	35	
7	7	18	.81873E+07	.20000E+00	37	4
		19	.77880E+07	.25000E+00	39	
8	8	20	.74082E+07	.30000E+00	41	
		21	.70469E+07	.35000E+00	43	
9	9	22	.67032E+07	.40000E+00	45	5
		23	.65924E+07	.41667E+00	47	
		24	.63763E+07	.45000E+00	49	
10	10	25	.60653E+07	.50000E+00	51	6
		26	.57695E+07	.55000E+00	53	
11	11	27	.54881E+07	.60000E+00	54	7
		28	.52205E+07	.65000E+00	55	
12	12	29	.49659E+07	.70000E+00	56	
		30	.47237E+07	.75000E+00	58	
13	13	31	.44933E+07	.80000E+00	60	8
14	14	32	.40657E+07	.90000E+00	62	
15	15	33	.36788E+07	.10000E+01	64	9
16	16	34	.33287E+07	.11000E+01	66	
		35	.31664E+07	.11500E+01	68	10
17	17	36	.30119E+07	.12000E+01	70	11
		37	.28650E+07	.12500E+01	71	12
18	18	38	.27253E+07	.13000E+01	72	13
		39	.25924E+07	.13500E+01	73	14
19	19	40	.24660E+07	.14000E+01	74	15
		41	.23852E+07	.14333E+01	76	16
		42	.23653E+07	.14417E+01	77	17
		43	.23457E+07	.14500E+01	78	
		44	.23069E+07	.14667E+01	79	18

Table A1 (continued)

100n*	52n**	Suggested Upper Energy (eV)		Lethargy	239n***	126n****
20	20	45	.22313E+07	.15000E+01	81	19
		46	.21225E+07	.15500E+01	82	20
21	21	47	.20190E+07	.16000E+01	83	21
		48	.19205E+07	.16500E+01	85	22
22	22	49	.18268E+07	.17000E+01	87	23
		50	.17377E+07	.17500E+01	88	24
23	23	51	.16530E+07	.18000E+01	89	25
		52	.15724E+07	.18500E+01	91	26
24	24	53	.14957E+07	.19000E+01	93	27
		54	.14227E+07	.19500E+01	94	28
25	25	55	.13534E+07	.20000E+01	95	29
		56	.12873E+07	.20500E+01	96	30
26	26	57	.12246E+07	.21000E+01	97	31
		58	.11648E+07	.21500E+01	99	32
27	27	59	.11080E+07	.22000E+01	100	33
28	28	60	.10026E+07	.23000E+01	102	34
		61	.96164E+06	.23417E+01	104	35
29	29	62	.90718E+06	.24000E+01	106	36
		63	.86294E+06	.24500E+01	107	37
30	30	64	.82085E+06	.25000E+01	108	38
		65	.78082E+06	.25500E+01	109	39
31	31	66	.74274E+06	.26000E+01	110	40
		67	.70651E+06	.26500E+01	111	41
32	32	68	.67206E+06	.27000E+01	112	42
		69	.63928E+06	.27500E+01	113	43
33	33	70	.60810E+06	.28000E+01	114	44
		71	.57844E+06	.28500E+01	115	45
34	34	72	.55023E+06	.29000E+01	116	46
		73	.52340E+06	.29500E+01	118	47
35	35	74	.49787E+06	.30000E+01	120	48
36	36	75	.45049E+06	.31000E+01	122	49
37		76	.40762E+06	.32000E+01	124	50
		77	.38774E+06	.32500E+01	125	
38		78	.36883E+06	.33000E+01	126	51
39		79	.33373E+06	.34000E+01	128	52
40	37	80	.30197E+06	.35000E+01	131	53
		81	.29850E+06	.35116E+01		54
		82	.29720E+06	.35159E+01		55
		83	.29452E+06	.35250E+01	132	56
		84	.28725E+06	.35500E+01	133	57
41		85	.27324E+06	.36000E+01	135	58
42		86	.24724E+06	.37000E+01	137	59
		87	.23518E+06	.37500E+01	138	
43		88	.22371E+06	.38000E+01	139	60
		89	.21280E+06	.38500E+01	140	61
44	38	90	.20242E+06	.39000E+01	141	62
		91	.19255E+06	.39500E+01	142	63
45		92	.18316E+06	.40000E+01	143	64
		93	.17422E+06	.40500E+01	144	65

Table A1 (continued)

100n*	52n**	Suggested Upper Energy (eV)		Lethargy	239n***	126n****
46		94	.16573E+06	.41000E+01	146	66
		95	.15764E+06	.41500E+01	148	67
47		96	.14996E+06	.42000E+01	149	68
		97	.14264E+06	.42500E+01	150	69
48	39	98	.13569E+06	.43000E+01	151	70
		99	.12907E+06	.43500E+01	152	71
49		100	.12277E+06	.44000E+01	153	72
		101	.11679E+06	.44500E+01	154	73
50		102	.11109E+06	.45000E+01	155	74
		103	.98037E+05	.46250E+01	156	75
51		104	.86517E+05	.47500E+01	157	76
		105	.82500E+05	.47975E+01		77
		106	.79500E+05	.48346E+01		78
		107	.72000E+05	.49337E+01		79
52	40	108	.67379E+05	.50000E+01	159	80
		109	.56562E+05	.51750E+01	162	81
53		110	.52475E+05	.52500E+01	163	82
		111	.46309E+05	.53750E+01	164	83
54		112	.40868E+05	.55000E+01	165	84
		113	.34307E+05	.56750E+01	168	85
55		114	.31828E+05	.57500E+01	169	86
		115	.28500E+05	.58604E+01		87
		116	.27000E+05	.59145E+01		88
		117	.26058E+05	.59500E+01	171	89
56	41	118	.24788E+05	.60000E+01	172	90
		119	.24176E+05	.60250E+01	173	
		120	.23579E+05	.60500E+01	174	91
		121	.21875E+05	.61250E+01	175	92
57		122	.19305E+05	.62500E+01	177	93
58		123	.15034E+05	.65000E+01	179	94
59		124	.11709E+05	.67500E+01	181	95
60	42	125	.91188E+04	.70000E+01	183	96
61		126	.71017E+04	.72500E+01	185	97
62		127	.55308E+04	.75000E+01	187	98
63		128	.43074E+04	.77500E+01	190	99
		129	.37074E+04	.79000E+01	192	100
64	43	130	.33546E+04	.80000E+01	193	101
		131	.30354E+04	.81000E+01	194	102
		132	.27465E+04	.82000E+01	196	103
65		133	.26126E+04	.82500E+01	197	104
		134	.24852E+04	.83000E+01	198	105
		135	.22487E+04	.84000E+01	199	106
66		136	.20347E+04	.85000E+01	200	107
67		137	.15846E+04	.87500E+01	203	108
68	44	138	.12341E+04	.90000E+01	206	109
69		139	.96112E+03	.92500E+01	207	110
70		140	.74852E+03	.95000E+01	208	111
71		141	.58295E+03	.97500E+01	209	

Table A1 (continued)

100n*	52n**	Suggested	Upper Energy (eV)	Lethargy	239n***	126n****
72		142	.45400E+03	.10000E+02	210	112
73		143	.35358E+03	.10250E+02	211	
74		144	.27536E+03	.10500E+02	212	113
75		145	.21445E+03	.10750E+02	213	114
76	46	146	.16702E+03	.11000E+02	214	115
77		147	.13007E+03	.11250E+02	215	
78		148	.10130E+03	.11500E+02	216	116
79		149	.78893E+02	.11750E+02	217	
80	47	150	.61442E+02	.12000E+02	218	117
81		151	.47851E+02	.12250E+02	219	118
82		152	.37267E+02	.12500E+02	220	119
83		153	.29023E+02	.12750E+02	221	
84	48	154	.22603E+02	.13000E+02	222	120
85		155	.17603E+02	.13250E+02	223	
86		156	.13710E+02	.13500E+02	224	
87		157	.10677E+02	.13750E+02	225	121
88	49	158	.83153E+01	.14000E+02	226	
89		159	.64760E+01	.14250E+02	227	
90		160	.50435E+01	.14500E+02	228	122
91		161	.39279E+01	.14750E+02	229	
92	50	162	.30590E+01	.15000E+02	230	
93		163	.23824E+01	.15250E+02	231	123
94		164	.18554E+01	.15500E+02	232	
95		165	.14450E+01	.15750E+02	233	
96	51	166	.11254E+01	.16000E+02	234	124
97		167	.87642E+00	.16250E+02	235	
98		168	.68256E+00	.16500E+02	237	
99		169	.53156E+00	.16750E+02	239	
100	52	170	.41399E+00	.17000E+02		125
		171	.10000E-00			126
		172	.10000E-04			

*100 GAM Group Structure of DLC-2 and DLC-37 (Refs. 9 and 10)
**52 Group Structure of Kriese DLC-28 (Ref. 11)
***239 Group CSEWG Standard of Weisbin and La Bauve (Ref. 12)
****126 Group of the DRRD LMFBR Neutron-Gamma Library (Ref. 8)

Table A2. CTR-PMCSL Gamma-Ray Energy Group Boundaries and Their Relationship to Those Used for Other Libraries

Group Number	Energy (MeV)	21γ*	Bartine**	Straker***
1	14.0	1	1	1
2	12.0	2		
3	10.0	3	2	2
4	8.0	4	3	3
5	7.5	5		
6	7.0	6	4	4
7	6.5	7		
8	6.0	8	5	5
9	5.5	9		
10	5.0	10	6	6
11	4.5	11		
12	4.0	12	7	7
13	3.5	13		8
14	3.0	14	8	9
15	2.5	15	9	10
16	2.0	16	10	11
17	1.66			12
18	1.50	17	11	
19	1.33			13
20	1.0	18	12	14
21	0.80			15
22	0.70		13	
23	0.60			16
24	0.512			
25	0.510			
26	0.45		14	17
27	0.40	19		
28	0.30		15	18
29	0.20	20		
30	0.15		16	19
31	0.10	21	17	20
32	0.075			
33	0.060			21
34	0.045		19	
35	0.030		20	22
36	0.020		21	
	0.010			

*21 Group structure of DLC-28 and DLC-37 (Refs. 11 and 10).
**D. Bartine 21 group structure of DLC-31/(DPL-1/FEWG1) (Ref. 13).
***E. Straker suggested few group version of CSEWG standard (Ref. 14).

APPENDIX B

Codes Used for Retrieving and Manipulating the Data in the CTR Processed Multigroup Cross Section Library and for Running the Packaged Sample Problems.

B.1 Retrieval and Manipulation Codes for the AMPX Interface Form

B.1.1 AIM: AMPX Module for BCD-Binary Conversion

The primary use would be to translate the library from the BCD form distributed by RSIC to the binary form used by the other AMPX modules.

B.1.2 COLGATE: AMPX Module to Copy Selected Portions of AMPX Master Interface

The primary use would be to prepare a subset of the Master by selecting only the nuclides needed for a given problem.

B.1.3 BONAMI: AMPX Module to Perform Bondarenko Resonance Self-Shielding

The primary use would be to access the Bondarenko factor data in the AMPX neutron master interface and perform self-shielding based on the homogeneous option.

B.1.4 CHOX: AMPX Module for Cross Section Interface Manipulation.

CHOX is mainly intended to take a neutron interface, the gamma-ray production interface, and a gamma-ray interaction interface and prepare a coupled neutron, gamma-ray interface.

B.1.5 MALOCS: AMPX Module to Collapse Neutron, Gamma-ray Interaction and Coupled Neutron, Gamma-ray Interfaces

The primary use would be in collapsing the 171 neutron (171,36) coupled, or 36 gamma-ray groups to a smaller number of groups prior to making actual transport calculations.

B.1.6 NITAWL: AMPX Module for Resonance Self-Shielding and Working Library Production

The only function intended for using NITAWL on the CTR library is to convert from the master interface format to a working format for either the XSDRNPM or ANISN radiation transport codes. The form of the data on the CTR library does not allow the utilization of the resonance treatments in NITAWL.

B.1.7 XSDRNPM: AMPX Module with One-Dimensional S_n Capability for Spatial Weighting

The primary use is to perform one-dimensional discrete ordinates calculations, using as input a cross section library in AMPX Working Format

produced by NITAWL. The code has many advantages such as ease of input preparation, calculation of reaction rates, and efficient storage of data which make it an attractive code for performing 1D S_n calculations.

B.1.8 RADE: AMPX Module to Check AMPX Master Cross Section Libraries

The program can be used to check the neutron, gamma-ray production, gamma-ray interaction or coupled interfaces at any stage of the data manipulation procedures.

B.1.9 DIAL: AMPX Module to Produce Selected Edits from AMPX Interfaces

This provides a very flexible capability to produce complete or selected edits of data in as much detail as desired.

B.2 Retrieval and Manipulation Codes for CCC Interface Format

B.2.1 BINX: BCD Interpretation of Neutron Cross Sections

The BINX code is utilized to translate data libraries from BCD to binary or vice versa. The translations are performed on the ISOTXS and BRKOXS files of the CCCC interface system. A selective edit option is available.

B.2.2 LINX: Library interpretation of Neutron Cross Sections

The LINX code is used to merge either two binary ISOTXS files or two binary BRKOXS files into a combined new binary library.

B.2.3 CINX: Collapsed Interpretation of Neutron Cross Sections

CINX will collapse the cross sections on CCCC-III ISOTXS and BRKOXS files to a subset group structure using fine-group fluxes specified by the user. If the user's flux is the same as the flux used to generate the original fine-group library, the collapse will be exact in the sense that the resulting broad group cross sections will be the same as those obtained by running MINX from scratch. The current version is limited to a maximum of 240 groups and a maximum Legendre order of P_3. For output, the user can choose either the CCCC-III ISOTXS and BRKOXS files or the 1DX format.

B.2.4 SPHINX: The object of the SPHINX code is to produce space and energy collapsed neutron cross sections for a given reactor size and composition. This is achieved by interpolation on a Bondarenko type cross section representation for temperature, size, and composition in the reactor. Self-shielding factors are used to account for flux depression in the vicinity of large resonances. For each energy group of each isotope, self-shielding factors are given for fission, capture, total, and elastic scattering. Cross section data in Bondarenko format is given as resonance self-shielding factors from the Bondarenko interface and scattering matrices and infinite dilution cross sections from the ISOTXS interface. The Bondarenko and ISOTXS interface files are generated by the MINX code. SPHINX also has a one-dimensional diffusion theory option which may be used to do an eigenvalue

calculation and collapse cross sections.

B.2.5 CHOXM: The function of CHOXM is to take the self-shielding factors generated by SPHINX, an infinite dilution neutron AMPX interface produced by MINX, and generate a self-shielded neutron AMPX interface for the specific problem of interest which was described in the SPHINX calculation. CHOXM can also combine the neutron interface, a gamma interface, and a photon production interface to produce a neutron-gamma coupled interface. The NITAWL module can then be used to convert from AMPX interface format to the ANISN format.

B.3 Other Programs Used in DCTR Library Sample Problems

B.3.1 AXMIX, GIP: Programs for Cross Section Mixing and Library Arrangement (RSIC Code Package PSR-75). The primary use here is to convert an ANISN format library into group-independent form to reduce the core requirements in a subsequent ANISN run.

B.3.2 ANISN: A One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering

This is one of the most widely used 1-D S_n codes and was used in one of the sample cases that were provided for the CTR cross section library.

APPENDIX C

Contents of the AMPX Interface Form of the CTR-PMCSL

The initial version of the CTR-PMCSL is available to participants in the validation effort.

Distribution of this initial version was delayed due to problems encountered in obtaining working versions of various retrieval programs and in processing some materials necessary to calculate several of the models or experiments which were designated at the validation meeting. In addition, we have tried to be sure that the sample problems accompanying the library and retrieval codes could be run in the same manner as prospective users would run them. In so doing, several problems have been encountered and corrected. Hopefully, this experience will result in making the user's task of implementing the PMCSL somewhat easier.

The materials initially available in the CTR-PMCSL are listed in Table C1.

During the validation phase, the designation PDS-41/CTR(A) was used to define the AMPX interface form of the data package. The contents of PDS-41 are summarized in Table C2.

Table C1. Materials Available in the CTR-PMCSL

Nuclide	Comments
H-1	
H-2	No Gamma-Ray Production Data (See Footnote a)
Li-6	
Li-7	
Be-9	
B-10	
B-11	No Gamma-Ray Production Data (See Footnote a)
C-12	
O-16	
N-14	
F	No Gamma-Ray Production Data (See Footnote b)
Na-23	
Mg	
Al-27	
Si	
K	
Ca	No Neutron Data (See Footnote c)
V	No Gamma-Ray Production Data (See Footnote b)
Cr	
Mn-55	
Fe	
Ni	
Cu	No Gamma-Ray Production Data (See Footnote b)
Nb-93	
Mo	
Pb	
U-234	No Gamma-Ray Production Data See Footnote a)
U-235	
U-236	No Gamma-Ray Production Data (See Footnote a)
U-238	
Pu-238	No Gamma-Ray Production Data (See Footnote a)
Pu-239	
Pu-240	
Pu-241	No Gamma-Ray Production Data (See Footnote a)
Pu-242	No Gamma-Ray Production Data (See Footnote a)
Am-241	No Gamma-Ray Production Data (See Footnote a)

a. Gamma-Ray Production Data Not Available on ENDF/B-IV.
b. Gamma-Ray Production Data Available on ENDF/B-IV, but not yet in Data Package.
c. Neutron Data Processing Awaiting MINX Update.

Table C2. Contents of PDS-41/CTR(A): The AMPX Interface Version of the CTR-PMCSL

Library Elements	Records
171 Neutron Group AMPX Interface for 35 Nuclides	227,818
171 Neutron, 36 Gamma-Ray Group Production AMPX Interface for 25 Nuclides	13,899
36 Gamma-Ray Group AMPX Interface for 38 Nuclides	15,934
AMPX Modules for Retrieving and Manipulating the Library	
AIM (BCD to Binary Conversion)	2,057
COLGATE (Selective Retrieving)	964
BONAMI (Self-Shielding Factor Interpolation)	1,971
NITAWL (Working Library Production)	5,113
CHOX (Neutron and Gamma-Ray Coupling)	1,525
RADE (Consistency Checking)	2,003
DIAL (Selective Editing)	1,131
MALOCS (Group Collapsing)	1,717
XSDRNPM (Transport Calculation)	6,953
ALOCAT (for XSDRNPM Standard Blanket Run)	5
Other Codes for Use With the Library	
GIP (ANISN Group Independent Tape Creation)	1,672
AXMIX (ANISN Library Tape Creation)	2,564
LOC (Assembly Language for AXMIX)	7
IDATE (Assembly Language for AXMIX)	16
ANISN (Transport Calculation)	4,026
CDC Versions of AMPX Modules	
NITAWL	4,094
XSDRNPM	6,720
JCL and Card Input for Sample Problems	723
Printed Output from Sample Problems	24,294

APPENDIX D

Contents of the CCCC-AMPX Interface Form of the CTR-PMCSL

Participants in the validation effort may also obtain the CCCC-AMPX form of the CTR-PMCSL.

The CCCC-AMPX interface form of the data packages was designated as PDS-42/CTR(4CA). At the time of the general release, the designations will be changed to the DLC type. The contents of PDS-42 are summarized in Table D1. It should be noted that the SPHINX code may be used for performing the interpolation on self-shielding factors and performing diffusion theory calculations and group-collapsing. The version of SPHINX included in this package does not perform a transport theory calculation. SPHINX does produce a CCCC ISOTXS file as its output which could be used as input to a transport code cross section processor which would convert the ISOTXS file into a working library. However, this approach has not been tested locally. In this package, the linking with a transport code is accomplished in a slightly different manner by using problem-dependent self-shielding factors from SPHINX. By combining these with the AMPX interfaces and utilizing the CHOX-M and NITAWL programs, the user can obtain self-shielded neutron or coupled neutron, gamma-ray cross sections which can then be used in a transport theory calculation via ANISN.

At the present time a sample problem using the CCCC-AMPX form is being prepared for distribution.

Table D1. Contents of PDS-42/CTR(4CA): The CCCC-AMPX Interface Version of the CTR-PMCSL

Library Element	Records
171 Neutron Group ISOTXS Interface for 35 Nuclides	244,000
(4 tapes)	243,600
	243,600
	53,193
171 Neutron Group BRKOXS Interface for 35 Nuclides	81,808
171 Neutron Group AMPX Interface for 35 Nuclides	227,818
171 Neutron 36 Gamma-Ray Group Production AMPX Interface for 25 Nuclides	13,899
36 Gamma-Ray Group AMPX Interface for 38 Nuclides	15,623
CCCC Codes for Retrieving and Manipulating the Library	
BINX (BCD to Binary Conversion)	731
LINX (Library Merging)	548
CINX (Group Collapsing)	1,418
SPHINX (Self-Shielding Factor Interpolation)	15,934
DEFILE (Assembly Language for SPHINX)	156
Other Codes for Use with the Library	
CHOX/M (Coupling SPHINX with AMPX Interfaces)	599
NITAWL (From RSIC Package PSR-63)*	5,159
AXMIX (ANISN Library Tape Creation)	2,564
LOC (Assembly Language for AXMIX)	7
IDATE (Assembly Language for AXMIX)	16
GIP (ANISN Group Independent Tape Creation)	1,672
ANISN (Transport Calculation)	4,026
CDC Versions of AMPX Modules	
NITAWL	4,094
XSDRNPM	6,720
JCL and Card Input for Sample Problem	(Not ready)
Printed Output from Sample Problem	(Not ready)

*This version of NITAWL uses a slightly different method of normalization between transfer matrices and smooth cross sections.

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