DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

UCRL--50400-Vol.25

DE04 007014

Omega Documentation

**R. J. Howerton, R. E. Dye, P. C. Giles,
J. R. Kimlinger, S. T. Perkins, and E. F. Plechaty**

Manuscript date: August 1983

LAWRENCE LIVERMORE NATIONAL LABORATORY
University of California • Livermore, California • 94550

Available from: National Technical Information Service • U.S. Department of Commerce
5285 Port Royal Road • Springfield, VA 22161 • \$16.00 per copy • (Microfiche \$4.50)

Foreword

The UCRL-50400 series, *An Integrated System for Production of Neutronics and Photonics Calculational Constants*, describes an integrated, computer-oriented system for the production and application of neutronics and photonics calculational constants.

The system supplies reliable, up-to-date data, selects specific types of data on request, provides output in a variety of forms (ultimately in the form of input to other computer codes), and functions rapidly and efficiently.

The UCRL-50400 series comprises the following volumes:

- Vol. 1, Part A, Rev. 3, *ECSIL: A System for Storage, Retrieval, and Display of Experimental Neutron Data*, September 1976.
- Vol. 1, Part B, *Program ECSX4 (Version 78-1): Conversion of Experimentally Measured Cross-Section Data from the Four-Center-Exchange (X-4) Format to the Livermore ECSIL Format*, December 1978.
- Vol. 2, Rev. 2, *A Bibliography of the Experimental Data of Neutron-Induced Interactions*, July 1976.
- Vol. 3, Rev. 2, *An Index of the Experimental Data of Neutron-Induced Interactions*, July 1976.
- Vol. 4, Rev. 1, *Evaluated Nuclear Data Library*, September 1981.
- Vol. 4, Rev. 1, Appendix C, *The Neutron Library (ENDL82) in the Transmittal Format*, June 1982.
- Vol. 5, Part A, Rev. 1, *CLYDE: A Code for the Production of Calculational Constants from Nuclear Data*, September 1975.
- Vol. 5, Part B, Rev. 1, *Relativistic Transformations between Center-of-Mass and Laboratory Systems for Two-Body Nuclear Reactions*, April 1978.
- Vol. 6, Rev. 2, *Tables and Graphs of Photon-Interaction Cross Sections from 1 keV to 100 MeV*, December 1978.
- Vol. 7, Part A, Rev. 1, *Major Neutron-Induced Interactions ($Z \leq 55$): Graphical, Experimental Data*, July 1976.
- Vol. 7, Part B, Rev. 1, *Major Neutron-Induced Interactions ($Z > 55$): Graphical, Experimental Data*, July 1976.
- Vol. 8, Part A, Rev. 1, *Supplemental Neutron-Induced Interactions ($Z \leq 35$): Graphical, Experimental Data*, July 1976.
- Vol. 8, Part B, Rev. 1, *Supplemental Neutron-Induced Interactions ($Z > 35$): Graphical, Experimental Data*, July 1976.
- Vol. 9, *Thresholds of Nuclear Reactions Induced by Neutrons, Photons, Deuterons, Tritons, and Alpha Particles*, September 1970.
- Vol. 10, Rev. 1, *Tabulated Experimental Data for Neutron-Induced Interactions*, July 1976.
- Vol. 11, *Experimental Data, Indexes, and Techniques of Obtaining a Selected Set of Neutron Resonance Parameters*, May 1972.
- Vol. 12, *An Atlas of Resolved Neutron Resonance Parameters*, July 1972.
- Vol. 13, *An Atlas of Unresolved Neutron Resonance Parameters*, September 1972.
- Vol. 14, *TARTNP: A Coupled Neutron-Photon Monte Carlo Transport Code*, February 1976.
- Vol. 15, Part A, *The LLL Evaluated-Nuclear-Data Library (ENDL): Evaluation Techniques, Reaction Index, and Descriptions of Individual Evaluations*, September 1975.
- Vol. 15, Part B, Rev. 1, *The LLL Evaluated-Nuclear-Data Library (ENDL): Graphs of Cross Sections from the Library*, October 1978.
- Vol. 15, Part C, *The LLL Evaluated-Nuclear-Data Library (ENDL): Translation of ENDL Neutron-Induced Interaction Data into the ENDF/B Format*, April 1976.
- Vol. 15, Part D, Rev. 1, *The LLL Evaluated-Nuclear-Data Library (ENDL): Descriptions of Individual Evaluations for $Z = 0-98$* , May 1978.
- Vol. 15, Part E, *Data Testing Results for the LLL Nuclear Data Library (ENDL-78)*, August 1979.
- Vol. 15, Part F, *Experimental and Evaluated Elastic Nuclear Plus Interference Cross Sections for Light Charged Particles*, July 1980.
- Vol. 16, Rev. 2, *Tabular and Graphical Presentation of 175 Neutron-Group Constants Derived from the LLL Evaluated-Nuclear-Data Library (ENDL)*, October 1978.
- Vol. 17, Part A, Rev. 2, *Program LINEAR (Version 79-1): Linearize Data in the Evaluated-Nuclear-Data File/Version B (ENDF/B) Format*, October 1979.

- Vol. 17, Part B, Rev. 2, Program SIGMA_L (Version 79-1): Doppler Broadened Evaluated Cross Sections in the Evaluated-Nuclear-Data File (Version B (ENDF/B) Format, October 1979.
- Vol. 17, Part C, Program RECENT: Reconstruction of Energy-Dependent Cross Sections from Resonance Parameters in the ENDF/B Format, October 1979.
- Vol. 17, Part D, Program GROUPIE: Calculation of Self-Shielded Cross Sections and Multiband Parameters from Evaluated Data in the ENDF/B Format, 1980.
- Vol. 17, Part E, Program EVALPLOT: Plot Data in the Evaluated-Nuclear-Data File (Version B (ENDF/B) Format, February 1979.
- Vol. 17, Part F, DOWNER (Version 79-1): Group Collapse Cross Section and Transfer Matrices, January 1979.
- Vol. 18, ACTL: Evaluated Neutron Activation Cross-Section Library, October 1978.
- Vol. 19, Neutron-Induced Angular and Energy Distributions: Graphical Experimental Data, April 1977.
- Vol. 20, Bondarenko Self-Shielded Cross Sections and Multiband Parameters Derived from the LLL Evaluated-Nuclear-Data Library (ENDL), July 1978.
- Vol. 21, Part A, Maxwell-Averaged Reactions Rates (σv) for Selected Reactions between Ions with Atomic Mass ≤ 11 , February 1979.
- Vol. 21, Part C, Program SIGMA_L (Version 79-1): Doppler-Broadened Evaluated Cross Sections in the Livermore-Evaluated Nuclear Data Library (ENDL) Format, March 1979.
- Vol. 22, Rev. 1, GAMIDEN: A Program to Aid in the Identification of Unknown Materials by Gamma-Ray Spectroscopy, June 1982.
- Vol. 23, ENSL and CDRL: Evaluated Nuclear Structure Libraries, February 1981.
- Vol. 23, Addendum, ENSL82 and CDRL82: The 1982 Version of Evaluated Nuclear Structure Libraries, January 1983.
- Vol. 24, Thresholds and Q Values of Nuclear Reactions Induced by Neutrons, Protons, Deuterons, Tritons, ^3He Ions, Alpha Particles, and Photons, March 1981.
- Vol. 25, Omega Documentation, August 1983.

Contents

I.	Introduction	I-1
	Appendix I - A.	I-7
	A. Encoding Methods	I-7
	B. Alternate Format for Update	I-13
II.	Update	II-1
	A. Introduction	II-3
	B. Retrieval of Data	II-4
	C. Deletion of Data	II-4
	D. Insertion of Data	II-8
	E. Making a New Library <i>ab initio</i>	II-9
	F. Output	II-9
III.	ENDEP	III-1
	A. Introduction	III-3
	B. $\bar{E}$ and Residual Models	III-4
	C. $\bar{E}$ Model Descriptions	III-7
	$\bar{E}$ Model A - Discrete two-body	III-7
	$\bar{E}$ Model B - Continuum two-body	III-8
	$\bar{E}$ Model C - Discrete two-body, continuum decay	III-9
	$\bar{E}$ Model D - General continuum	III-9
	$\bar{E}$ Model E - Fission	III-9
	$\bar{E}$ Model F - $C = 12, S = 8$ or $10, 11$ for y_i	III-9
	$\bar{E}$ Model G - Production cross sections	III-9
	Submodel G1	III-9
	Submodel G2	III-9
	$\bar{E}$ Type H - Gamma ray interaction cross sections	III-10
	Submodel H1	III-10
	Submodel H2	III-10
	Submodel H3	III-10
	Submodel H4	III-10
	D. Residual Models	III-10
	Residual Model 1 - Discrete two-body	III-10
	Residual Model 2 - Continuum two-body	III-11
	Submodel 2a	III-11
	Residual Model 3 - Continuum two-body, continuum decay	III-12
	Submodel 3a	III-13
	Residual Model 4 - Fission	III-13
	Residual Model 5 - Discrete two-body, continuum decay	III-13
	Residual Model 6 - Radiative capture	III-14
	Residual Model 7 - Gamma ray induced reactions	III-15
	Submodel 7a	III-15
	Submodel 7b	III-15
	Submodel 7c	III-15
	E. Input, Operation, and Output	III-15
	Appendix III - A. Two Body Kinematics	III-17
	Appendix III - B. Decay Kinematics	III-21
	Appendix III - C. Radiative Capture Kinematics	III-23
	References	III-24
IV.	GAMCHK	IV-1
	A. Introduction	IV-3
	B. Technique	IV-3
	C. Input, Operation, and Output	IV-4

V.	Utility	V-1
	A. Introduction	V-3
	B. Preparation of Input	V-3
VI.	CLYDE	VI-1
	A. Introduction	VI-3
	B. Special Features and Restrictions	VI-4
	C. CLYDE Equations	VI-5
	Transfer Matrix Definition	VI-5
	Transport Correction Terms	VI-6
	Average Group Flux and Inverse Speed	VI-10
	Reaction Group Average Cross Sections	VI-11
	Transfer Probability from Angular Distribution ($I = 1$) Data	VI-12
	General Relations	VI-12
	The Inner Integral	VI-15
	The Outer Integral	VI-18
	Transfer Probability from Tabular Energy Distribution ($I = 4$) Data	VI-19
	Basic Data	VI-19
	Unit Base Transformation	VI-19
	The Inner Integral	VI-21
	The Outer Integral	VI-29
	Energy Production and Deposition	VI-30
	Isotope Production	VI-31
	D. CLYDE Input Format and Instructions	VI-31
	E. CLYDE Output Format and Instructions	VI-37
	Appendix VI - A. Linear Integration Routines	VI-41
	Appendix VI - B. Numerical Integration	VI-43
	Appendix VI - C. Constants Used in Integration	VI-45
	References	VI-49
VII.	NDFL	VII-1
	A. Introduction	VII-3
	B. File Description and Usage	VII-3
	C. Input, Operation, and Output	VII-4
	Create an NDFY _i File	VII-4
	Update an NDFY _i File	VII-5
	Edit an NDFY _i File	VII-6
	Appendix VII - A. Physical Layout of a Binary NDFY _i File	VII-11
	A. Global Section	VII-11
	B. Individual Materials - Directory and Descriptor Blocks (ISODEF)	VII-12
	C. Individual Materials Data Block	VII-15
	Appendix VII - B. Physical Layout of the BDFLS ASCII File	VII-17
	Appendix VII - C. Group Collapse of the NDFY _i Files	VII-19
VIII.	CTART	VIII-1
	A. Introduction	VIII-3
	B. Preparation of Input	VIII-4
	C. Methods	VIII-5
	D. Output	VIII-6
IX.	TRTL	IX-1
	A. Introduction	IX-3
	Appendix IX - A.	IX-5
X.	MCPOINT	X-1
	A. Introduction	X-3
	B. Conversion of Data of MCNP Format	X-4

**CHAPTER I:
INTRODUCTION**

L. INTRODUCTION

OMEGA is a CRAY I computer program that controls nine codes used by the LLNL Physical Data Group for:

1. Updating the libraries of evaluated data maintained by the group (UPDATE).
2. Calculating average values of energy deposited in secondary particles and residual nuclei (ENDEP).
3. Checking the libraries for internal consistency, especially for energy conservation (GAMCHK).
4. Producing listings, indexes and plots of the library data (UTILITY).
5. Producing calculational constants such as group averaged cross sections and transfer matrices for diffusion and Sn transport codes (CLYDE).
6. Producing and updating standard files of the calculational constants used by LLNL Sn and diffusion transport codes (NDFL).
7. Producing calculational constants for Monte Carlo transport codes that use group-averaged cross sections and continuous energy for particles (CTART).
8. Producing and updating standard files used by the LLNL Monte Carlo transport codes (TRTL).
9. Producing standard files used by the LANL pointwise Monte Carlo transport code MCNP (MCPOINT).

The first four of these functions and codes deal with the libraries of evaluated data and the last five with various aspects of producing calculational constants for use by transport codes. In 1970 a series, called PD memos, of internal and informal memoranda was begun. These were intended to be circulated among the group for comment and then to provide documentation for later reference whenever questions arose about the subject matter of the memos. They have served this purpose and now will be drawn upon as source material for this more comprehensive report that deals with most of the matters covered in those memos. In addition to the PD memos, several other of the volumes of this series (UCRL 50400) deal with many of the subjects dealt with in this volume. For the convenience of the reader some developments will be repeated in part or whole. The criterion of how much technical discussion will be included is: whatever is needed to understand what the various codes do and why they do it. Since the nine codes have quite different functions, this results in significantly varied quantities of discussion for each code. The basic rule is that when in doubt, as to whether discussion of some aspect of what a code does is needed, include it.

Throughout this volume reference is made to certain quantities using their short or jargon names. This eliminates repetition of relatively long descriptive names and thus makes the discussions flow more smoothly. Each of these quantities is described in the following list:

Short Name	Definition
ZA	Designation of a nucleus by charge and mass ($1000 \times Z + A$). For elements having mixtures of isotopes A is taken to be 0. Thus, natural chlorine has ZA = 17000.
Yi	Incident particle in a reaction. For definition of values see Appendix A.
Yo	Secondary particle from a reaction. For definition of values see Appendix A.
C	Reaction descriptor numerical equivalent. e.g., C=12 signifies a reaction resulting in two secondary neutrons. For definition of values see Appendix A.
I	Reaction property numerical equivalent. e.g., I=0 signifies the cross section. For definition of values see Appendix A.
S	Reaction Modifier numerical equivalent. e.g., S=1 signifies that the reaction proceeds through a level in an intermediate nucleus. For definition of values see Appendix A.
Xi	Numerical values ($i=1,4$) required to complete definition of non-zero S-values. e.g., for S=1 (see above) the energy of the level is entered in the X1 field. For definition of the values to be entered in the Xi fields for each S-value see Appendix A.

The calling sequence for any of the codes controlled by OMEGA is:

OMEGA (code) (input file) (box no.) (hsp option) (library name) 0
(output file name) (output file size) / T V

All of the quantities enclosed in parentheses are defined below. Note that the parentheses only indicate a problem dependent value. The parentheses do not appear in the calling sequence. An example of using OMEGA to run UPDATE using file INUP with a library called ND821201 is:

omega update inup t64 fr80 nd\$21201 0 nd\$21202 20 / .9 .999

The various quantities in parentheses have the following significance:

code	This is the name of the code (one of the nine listed above) that is being run under OMEGA's control.
input file	the file required by "code" for input
box no.	user's box number
hsp option	Each "code" produces output that is descriptive and/or diagnostic for the problem. This output may be directed to the FR80 (use "fr80" for option), the high speed printer (use "hsp" for option), or kept for inspection (use "debug" for option) and/or output to RJET or other medium using ALLOUT.
library name	the library file that is being used for updating or other purposes. If a new library is being made ab initio, the word "none" is entered here (see chapter II). For the TRTL code a standard file, DT041773, is used if a totally new file is being made (see chapter IX).
0	The zero in this position indicates that the library exists as a file. The zero must be included in the calling sequence.
output file name	the name of the file to be created as output
output file size	the size of the output file to be created in units of 100000 words. In the example above, the output file will be created as 2000000 words. When the code is finished it will shrink the file to the size needed.

In that which follows, the calling sequence for each code will be described in more detail, including specifications for the form and significance of the input file that is specific to the code being run under OMEGA's control.

There are four generic libraries of evaluated data on which the codes controlled by OMEGA operate. They are:

ENDL Evaluated Neutron Data Library that contains the data associated with neutron induced reactions, including cross sections, angular distributions, energy distributions, particle multiplicities, and average energy deposits. All evaluations contained in ENDL are complete in the sense of containing data for all energetically possible reactions for incident neutron energies from 10^{-10} to 20. MeV, if the reaction cross section is judged to rise to, at least, 10 millibarns somewhere in that neutron energy range.

ACTL Neutron Activation Cross Section Library that contains cross section data for activation of specific nuclides by neutron interaction. The cross section data are for those reactions for which interest has been identified by a user of the data. Thus, the ACTL file is, by design, incomplete but infinitely hospitable to addition of new reactions as interest is identified.

ECPL Evaluated Charged Particle Library that contains the data associated with charged particle induced nuclear reactions, including cross sections, angular and energy distributions of secondary particles, particle multiplicities, average energy deposits, in-flight cross sections for hot targets, and maxwell-averaged data for hot media.

EGDL Evaluated Gamma-Ray Interaction Data Library that contains data for coherent scattering, incoherent scattering, photo-electric and pair-production processes for gamma-ray energies from .0001 to 100. MeV. This library contains no photo-nuclear reaction data. Thus, it is appropriate to the interaction of photons with the elements as cold targets and as atoms. Targets are included from $Z=1$ to $Z=100$.

APPENDIX I-A

A. ENCODING METHODS

A common practice throughout this volume is to refer to the characteristics of nuclear reactions using a shorthand or symbolic representation. This eliminates repetition of relatively long descriptive names that can become tedious for the reader. The quantities for which such representation is made are:

Short Name	Definition
ZA	Designation of a nucleus by charge and mass ($1000 \cdot Z + A$). For elements having mixtures of isotopes, A is taken to be 0. Thus natural chlorine has a ZA of 17000.
Yi	Incident particle in a reaction. For definition of values see Table 1.
Yo	Secondary particle from a reaction. For definition of values see Table 1.
C	Reaction descriptor numerical equivalent. e.g., C=12 signifies a reaction resulting in two secondary neutrons. For definition of values see Table 2.
I	Reaction property numerical equivalent. e.g., I=0 signifies the cross section. For definition of values see Table 3.
S	Reaction Modifier numerical equivalent. e.g., S=1 signifies that the reaction proceeds through a level in an intermediate nucleus. For definition of values see Table 4.
Xi	Numerical values ($i=1,4$) required to complete definition of non-zero S-values. e.g., for S=1 (see above) the energy of the level is entered in the X1 field. For definition of the values to be entered in the Xi fields for each S-value see Table 4.

TABLE I-A.1. Particle Designator, y .^a

y	Particle
0	Not applicable ^b or none
1	n
2	p
3	d
4	t
5	³ He
6	α
7	γ
8	β^+
9	β^-
10	EC
11	Neutron as residual nucleus
12	Proton as residual nucleus
13	Deuteron as residual nucleus
14	Triton as residual nucleus
15	³ He as residual nucleus
16	α as residual nucleus

^a Used to identify both the incident particle, y_i , and the outgoing particle, y_o , to which any distribution data (e.g., energy, angle) pertain: $y_i = 0 - 7$ only; $y_o = 0 - 16$.

^b If no property (e.g., energy distribution) is given the y_o is zero or left blank in input. If y_i is zero or blank, the data which follow are nuclear structure data.

TABLE I-A.2. Reaction Identifier C, for I-values of 0 through 96.

Kind of Data	C	Reaction type
Miscellaneous	1	Total ^a
	2-7	Unassigned
	8	Large angle coulomb scattering
	9	Nuclear elastic plus interference
	10	Elastic
Neutrons + gammas only	11	$(y, n\gamma)$
	12	$(y, 2n\gamma)$
	13	$(y, 3n\gamma)$
	14	$(y, 4n\gamma)$
	15	(y, Xf) total fission
	16-19	Unassigned
Neutrons + charged particles + gammas	20	$(y, n'p\gamma)$
	21	$(y, pn'\gamma)$
	22	$(y, n'd\gamma)$
	23	$[y, n'dd(\alpha)]$
	24	$(y, n't\gamma)$
	25	$(y, n'^3\text{He}\gamma)$
	26	$(y, n'\alpha\gamma)$
	27	$[y, n'2\alpha(\alpha)]$
	28	$[y, n't\alpha(\alpha)]$
	29	$(y, 2np)$
	30	$(y, \gamma n\alpha)$
	31	$[y, 2n\alpha(\alpha)]$
	32	$[y, 2nd(\alpha)]$
	33-36	Unassigned
Charged particle and/or gamma formation	37	$[y, 2\alpha(\alpha)]$
	38	$[y, ^3\text{He}\alpha(\alpha)]$
	39	$[y, pt(\alpha)]$
	40	$(y, p\gamma)$
	41	$(y, d\gamma)$
	42	$(y, t\gamma)$

TABLE I-A.2. Continued

Kind of Data	C	Reaction type
Particle or gamma production	43	$(y_p, \alpha d)$
	44	$(y_p, {}^3\text{He}\gamma)$
	45	$(y_p, \alpha\gamma)$
	46	(y_p, γ)
	47-49	Unassigned
	50	(y_p, Xp)
	51	(y_p, Xd)
	53	$(y_p, X {}^3\text{He})$
	54	$(y_p, X\alpha)$
	55	$(y_p, X\gamma)$
	56	(y_p, Xn)
	57	$(y_p, X\beta^-)$
	58-64	Unassigned
Photon interaction with cold material	65	Activation (undefined reaction)
	66-69	Unassigned
	70	Total ^a
	71	Coherent scattering
	72	Incoherent scattering
	73	Photoelectric
	74	Pair production
	75-79	Unassigned
	80-98	Unassigned

^a Not stored in the system, but obtained for output display and transmission format by combining other data.

TABLE I-A.1. Reaction property designator, I.*

I	Reaction Property	Definition
0	Integrated cross sections (b)	$\sigma(E)$
1	Angular distributions, normalized probabilities (per unit cosine)	$P(L, \mu)$
3	Energy-angle distributions, normalized probabilities.*	$P(E + \mu, E')$
4	Energy-angle distributions, normalized Legendre coefficients. $\pi^L(E + E') = p(E + E')$, the usual normalized energy probability (per MeV)	$\pi^L(E + E')$
7	Average number of neutrons per fission (prompt or delayed)	$\bar{\nu}(E)$
8	Histogram form of energy distribution	$\int P(E, E') dE'$
9	Photon or particle multiplicity	$M(E)$
10	Average energy of a secondary particle (MeV)	$E'(y_0, E)$
11	Average energy of a residual nucleus (MeV)	$E'(R, E)$
80	Maxwell average reaction rates (b-cm/sh)	$\sigma v(kT)$
81	In-flight (Doppler-broadened) cross sections (b)	$\sigma(kT, E)$
84	Maxwell-averaged energy distributions (per MeV)	$P(kT, E')$
89	Maxwell-averaged photon or particle multiplicity	$M(kT)$
90	Maxwell-averaged total average energy of secondary particle (MeV)	$E'(y_0, kT)$
91	Maxwell-averaged average energy of residual nucleus (MeV)	$E'(R, kT)$
92	Maxwell-averaged total average energy of reacting particles (MeV)	$E(y_i, kT)$

a We illustrate the use of these designations by constructing a reaction code for the energy distribution of protons from the $^{58}\text{Ni}(n, n'p)^{57}\text{Co}$ reaction:

Incident particle:	$y_i = 01$ (neutron)
Reaction property:	$I = 04$ (energy dist.)
Reaction type:	$C = 20$ ($n, n'p$)
Outgoing particle whose property is recorded:	$y_0 = 02$ (proton)
Reaction modifier:	$S = 00$ (no x-field data)
Q_0 of reaction:	$Q_0 = -8.02$

This gives for the reaction code

y_i	I	C	y_0	S	Q_0	x_1
01	04	20	02	00	-8.02	0.0

b Angular data are expressed in the center-of-mass (cm) system for all two-body breakups. Multibody breakups are, of course, in the Laboratory system.

* $l=1$ data must be present when $l=3$ data are given for a reaction with identical incident energy and cosine meshes. While the inclusion of $l=1$ data with $l=3$ data for a reaction is not a necessary condition for representing energy-angle correlated data, we have chosen this mode of representation for convenience of changing the data and for consistency.

TABLE I-A-4. Reaction Modifier, S.

S	Reaction Parameter	X field definition
00 or blank	No X-field data	---
01^a	Level excitation	$W_i(\text{MeV})$
02	Pre-equilibrium and unresolved direct interaction processes	None
03	Gamma ray production	$E_\gamma(\text{MeV})$
05^b	Activation	$(ZA)_2, W_2(\text{MeV}),$ half-life (s)
07	Delayed group half-lives	$\tau_{1/2}(\text{s})$
08	Time sequential cluster model	$W_1(\text{MeV})$
10	Wide level excitation	$W_1(\text{MeV}), \Gamma_1(\text{MeV})$
11	Second particle from wide level time-sequential reaction	$W_2(\text{MeV}), \Gamma_2(\text{MeV})$
15	Density and Temperature Dependence	$\rho, T(\text{keV})$

^a X_1 corresponds to the initial nucleus, X_2 to the second nucleus in a sequence of deexcitations, etc.

^b $(ZA)_2 = 1000 \cdot Z_2 + A_2$ of product nucleus.

B. ALTERNATE FORMAT FOR UPDATE

Because no other existing format makes provision for all the properties that are part of the LLNL data files, a transmittal format has been developed that is simple and can be used as an input format for the UPDATE code described in Chapter I. The record layout for the first two records of each set of data is given in Table I-A.5. These first two records are called the header records. The records that follow the header records are appropriately called the data records, and the layout used for the data records is a function of the reaction property ("I-value") described in the second of the two header records. Only four types of layouts, or organizations, are required to handle the data for the 16 I-values defined in Table I-A.3.

TABLE I-A.5. Field definitions for header records.

	Columns	Format	Name	Description
Record 1	1-6	I6	ZA	1000Z + A.
	8-9	I2	y_1^a	Incident particle descriptor.
	11-12	I2	Y_0^a	Outgoing particle descriptor.
	14-24	E11.4	A	Atomic mass for this ZA (amu).
	26-31	I6	DATE	Date last changed.
	34	I1	Flag	Enter a "4" to indicate type of format to follow.
	36-46	E11.4		Level energy of the target (MeV).
	48-58	E11.4		Half-life of the target(s).
Record 2	1-2	I2	C^a	Reaction number.
	3-5	I3	I^a	Reaction property designator.
	6-8	I3	S^a	Reaction modifier flag.
	10-20	E11.4	Q_0^a	Mass difference Q for the reaction.
	22-32	E11.4	X_1^a	Value depends on the value of S.
	34-44	E11.4	X_2^a	Value depends on the value of S.
	46-56	E11.4	X_3^a	Value depends on the value of S.

^a A more complete definition of these fields can be found in Tables I-A.1 to I-A.4.

All numbers in the data records are in floating-point format, in particular, E11.4 format. Following the data records is an end-of-data record that is blank except for a 1 in column 72. This facilitates skipping unneeded data, if it is desirable to do so, by reading over a set of data until the end-of-data record is encountered. Each read-command following the two header records may be done with a 6E11.4, 5x, 11 format.

For $l = 0, 7, 9, 10, 11, 80, 89, 90, 91$, and 92 , the first data record gives the number of pairs of independent/dependent variables to follow. The significance of the independent and dependent variables is given in Table II-2 for each l -value.

For $l = 1, 8, 81$, and 84 , the first record gives the number of values of the factorable parameter (incident particle energy for $l = 1, 8$; kT for $l = 81, 84$). The following data records are given in sets, with the number of sets equal to the value given in the first-record described above. Each set has a first record that gives the value of the parameter (E or kT), followed by the number of pairs of independent/dependent variables, which are defined in Table II-2 for each l -value.

For $l = 3$ there are two factorable parameters (incident particle energy and cosine of the angle of emission in the laboratory system). The first data record gives the number of incident particle energies for which $l = 3$ data are given. The second data record gives the value of the first energy and the number of cosines for the first energy. The third data record has the first cosine for the first energy and the number of cosine-secondary energy pairs to follow for the incident particle energy given in data record 2 and this cosine. Data records 4 et seq. contain the cosine-secondary energy data for the first energy-first cosine. Data records 3 through 4 (et seq.) are repeated for the number of cosines given in data record 2. This procedure is repeated for the number of incident particle energies given in the first data record.

For $l = 4$ there are two parameters (l and E). The first data record gives the number of l -values (sets of Legendre polynomial coefficients) that follow. For each set of coefficients, the first record gives the order of l , followed by the number of incident-particle energies for which secondary-energy/coefficient pairs are given. For each incident-particle energy there is a record that gives the incident-particle energy and the number of pairs of secondary-energy/coefficient pairs that follow. The remaining data for that subset are the secondary-energy/coefficient values for that order of Legendre polynomials and that incident-particle energy.

Tables I-A.6, I-A.7, I-A.8, and I-A.9 give a schematic for the four I-value-dependent layouts.

TABLE I-A.6. Field definitions for I = 0, 7, 9, 10, 11, 80, 89, 90, 91 and 92.

Record	
1	First header record, see Table I-A.5.
2	Second header record, see Table I-A.5.
3	Number of pairs of independent/dependent variables, e.g., energy/cross section (E11.4).
4 et seq.	Three pairs per record (6E11.4) of independent/dependent variables.
Last	End-of-data record (1 in column 72).

TABLE I-A.7. Field definitions for I = 1, 8, 81, 84.

Record	
1	First header record, see Table I-A.5.
2	Second header record, see Table I-A.5.
3	Number of values of the factorable parameter (NF) (E11.4). (E for I = 1, 8, kT = for I = 81, 84).
4 ^a	Value of the factorable parameter, number of pairs of independent/dependent variables that follows (2E11.4).
5 et seq. ^a	Three pairs per record (6E11.4) of independent/dependent variables [e.g., for I = 1, μ , P(E, μ)].
Last	End-of-data record (1 in column 72).

^a Repeated NF times.

TABLE I-A.8. Field definitions for I = 3.

Record	
1	First header record, see Table I-A.5.
2	Second header record, see Table I-A.5.
3	Number of incident particle energies NE, (E11.4).
4 ^a	First incident particle energy, number of cosines for this energy (2E11.4), NC.
5 ^b	Value of the first cosine, number of cosine-secondary energy pairs to follow (2E11.4).
6 et seq. ^a	Three pairs per record of secondary energies and probabilities.
Last	End-of-data record (1 in column 72).

^a Repeated NE times.

^b Repeated NC times.

TABLE I-A.9. Field definitions for I = 4.

Record	
1	First header record, see Table I-A.5.
2	Second header record, see Table I-A.5.
3	Number of values of ℓ (E11.4), NL.
4 ^a	Value of ℓ , number of incident energies for this ℓ , NE, (2E11.4).
5 ^b	Incident energy; number of secondary energy coefficients to follow (2E11.4).
6 et seq. ^a	Three pairs per record of secondary energies and coefficients (6E11.4).
Last	End-of-data record (1 in column 72).

^a Repeated NL times.

^b Repeated NE times.

**CHAPTER II:
UPDATE**

II - 1 / II - 2

II. UPDATE

A. INTRODUCTION

UPDATE is a code that retrieves data, deletes data or inserts data into any one of the evaluated libraries maintained by the Physical Data Group. The calling sequence for running **UPDATE** is:

**OMEGA UPDATE (input file) (box no.) (hsp option) (library name)
0 (output file name) (output file size) / TV**

The parentheses denote problem dependent quantities and do not appear in the calling sequence. An example of running **UPDATE** using an input file **INUP** with a library called **ND821201** to make a library **ND821202** is:

omega update inup t64 fr80 nd821201 0 nd821202 20 / .9 .999

The various quantities in parentheses have the following significance:

input file	the file required by UPDATE for input
box no.	user's box number
hsp option	UPDATE produces output that is descriptive and/or diagnostic for the problem. This output may be directed to the FR80 (use "fr80" for option), the high speed printer (use "hsp" for option), or kept for inspection (use "debug" for option) and/or output to RJET or other medium using ALLOUT .
library name	the library file that is being used for updating or other purposes. If a new library is being made ab initio, the word "none" is entered here. See below.
0	The zero in this position indicates that the library exists as a file. The zero must be included in the calling sequence.
output file name	the name of the file to be created as output. This may be a file of retrieved data or a new library.
output file size	the size of the output file to be created in units of 100000 words. In the example above, the output file will be created as 2000000 words. When the code is finished it will shrink the file to the size needed.

B. RETRIEVAL OF DATA

To retrieve data from any of the evaluated libraries, an input file is required with two sets of three records for each retrieval. Any number of retrievals may be done but for each retrieval there must be retrieval criteria specified. The first record of each set (target record) specifies the limits of the range of isotopes or elements, the incident and secondary particles of interest, and a value of 3 or 5 in column 34 that specifies the output mode of the retrieval. A value of 3 indicates that the output of the retrieval is to be in a format having one entry per record for the retrieved data. A value of 5 indicates that the output is to be in a format (transmission format) with multiple entries per record and common values factored out of the data. The second record of each set (reaction record) specifies the limits of the range of reaction descriptors and the third record of each set (data record) gives the limits of the energy range of the independent variables for which the retrieval is to be made. The specifications of the fields of the first two records can be found in Table II.1. For the third record the formats and specifications of the retrieved data are found in Table II.2, if the value of the flag in column 34 of the first record is 3. For a value of 5 in column 34 of the first record, the formats and specifications of the retrieved data are given in Tables I-A.6, I-A.7, I-A.8, and I-A.9 of Appendix I-A.

C. DELETION OF DATA

To delete data from any of the evaluated libraries, an input file is required with two sets of three records for each deletion. Any number of deletions may be done but for each deletion there must be deletion criteria specified. The first record of each set (target record) specifies the limits of the range of isotopes or elements, the incident and secondary particles of interest, and a value of 1 in column 34. The second record of each set (reaction record) specifies the limits of the range of reaction descriptors and the third record of each set (data record) gives the limits of the energy range of the independent variables for which the deletion is to be made. The specifications of the fields of the first two records can be found in Table II.1. For the third record, the formats and specifications are found in Table II.2. Both deletions and insertions of new data can be done during the same run of the code.

TABLE II.1. Record layout for retrieve, delete, or insert.

Columns	Format	Name	Description
<u>Record 1</u>			
1-6	I6	ZA	1000 Z + A.
8-9	I2	Y_i^a	Incident particle descriptor
11-12	I2	Y_o^a	Outgoing particle descriptor
14-24	E11.4	A^b	Atomic mass for this ZA (amu)
26-31	I6	DATE ^b	Current date. (YYMMDD)
33-34	I2	FLAG	Designates the type of operation: 1 = delete, 2 = insert, 3 = retrieve, 4 = insert (using transmission format), 5 = retrieval (in transmission format).
36-46	E11.4		Level energy of the target (MeV)
48-58	E11.4		Half-life of the target ^b (sec)
<u>Record 2</u>			
1-2	I2	C ^a	Reaction number
3-5	I3	I ^a	Reaction property designator
6-8	I3	S ^a	Reaction modifier flag
10-20	E11.4	Q0 ^a	Mass difference Q for the reaction (MeV)
22-32	E11.4	X ₁ ^a	Value depends upon the value of S
34-44	E11.4	X ₂ ^a	Value depends upon the value of S
46-56	E11.4	X ₃ ^a	Value depends upon the value of S

^a A more complete definition of these fields can be found in Tables I-A.1 to I-A.4 of Appendix I-A.

^b Does not need to be specified for retrieval or delete. Half-life of the target must be specified only when the material is entered for the first time.

TABLE II.2. Field definitions for input data (4E11.4 format with one set of data per record).^a

Reaction Property	I	Data stored in field:			
		1	2	3	4
Integrated cross sections	0	E	$\sigma(E)$	-	-
Angular distributions	1	E	μ	$P(E, \mu)$	-
Energy-angle correlated data	3	E	μ	E'	$P(E, \mu, E')$
Energy-angle Legendre coefficients	4	E	E'	l	$\pi^l(E \rightarrow E')$
Nu-bar	7	E	$\nu(E)$	-	-
Histogram energy distribution	8	E	E'_1	$\int_{E'_1}^{E'_2} P(E') dE'$	-
Gamma-ray multiplicity	9	E	$M(E)$	-	-
Total average energy of particle	10	E	$E'(y_0, E)$	-	-
Average energy of residual	11	E	$E'(R, E)$	-	-
Maxwell-averaged reaction rates	80	kT	$\sigma v(kT)$	-	-
In-flight cross sections	81	kT	E	$\sigma(kT, E)$	-
Maxwell-averaged energy distributions	84	kT	E'	$P(kT, E')$	-

TABLE II.2. Continued

Reaction Property	I	Data stored in field:			
		1	2	3	4
Maxwell-averaged photon as particle multiplicity	89	kT	M(kT)	-	-
Maxwell-averaged total average energy of secondary particle	90	kT	$\bar{E}(y_0, kT)$	-	-
Maxwell-averaged average energy of residual nucleus	91	kT	$\bar{E}(R, kT)$	-	-
Maxwell-averaged total average energy of reacting particles	92	kT	$\bar{E}(v_i, kT)$	-	-

^aFor certain applications it is desirable to combine all reactions leading to a specific residual nucleus. Provision for such "activation" cross sections is made. For example, the (n,n'd) and (n,t) reactions both lead to the same residual nucleus, and the sum of the cross sections for these reactions may be entered as with the following example:
⁷⁰Zn(n,n'd + n,t)⁶⁸Cu to the ground state with a half-life of 32 sec.

Incident particle: $y_i = 01$ (neutron)
 Reaction property: $I = 00$ (integrated cross section)
 Reaction type: $C = 65$ (activation)
 Outgoing particle whose
 property is recorded: $y_o = 00$ (not applicable since no property of a secondary
 particle is given)
 Reaction modifier: $S = 05$ (activation)
 Z_2A_2 : $Z_2A_2 = 29068$. (x_1 field)
 w_2 : $w_2 = 0$. (x_2 field)
 τ_2 : $\tau_2 = 32$. (x_3 field)

This gives for the reaction code

y_i	1	C	y_o	S	Q_0	x_1	x_2	x_3
01	00	(65)	(00)	05	29068.	0.	32.	

There are several special types of deletes:

- 1. To delete an entire isotope or element (ZA), set $C_{min} = 1$, $C_{max} = 99$. All other fields of the reaction record and data record may be left blank.**
- 2. To delete a particular reaction (C) or a range of reactions, set:**
 C_{min} = minimum C to be deleted,
 C_{max} = maximum C to be deleted,
 $I_{min} = 0$,
 $I_{max} = 99$.

All other fields must be set to the minimum-maximum range desired.

- 3. To delete all of a particular reaction property designator (I), leave both data records blank. All other fields must be set to the minimum-maximum range desired.**

If the limits specified by the delete request cannot be satisfied, a comment is printed and the code continues. The data sets representing deletes and inserts may be in any order in the input file. The code sorts the sets, performs the delete operations and then inserts new data one target at a time.

D. INSERTION OF DATA

If data are to be inserted into the library, the first two records (the target and reaction records) must be as described in Table II.1. These records determine the point in the library at which insertions are to be made. The third and following records are data records containing the data to be inserted. They are specified with respect to the format and content described in Table II.2 if the flag in column 34 of the first record is "2". If the flag in column 34 of the first record is "4", the format and content of the data records are as specified in Tables I-A.6, I-A.7 and I-A.8 of Appendix I-A. Following the last record of each data set to be inserted is a record with the number 1 in column 72. There is no limit to the number of data records, but angular distributions may have no more than 201 entries for each incident energy. Whenever appropriate, data are merged with existing data, but if equal points are encountered in the merge, they are printed out with the original data left in the library. The code then proceeds. If a match cannot be made between the specifications stated on the first two records of a set to be inserted and those found on the evaluated library, a new isotope (ZA), a new reaction (C), a new reaction modifier (S), any of the X_i fields, or a new reaction property designator (I) is created to fulfill the required specifications. Insert requests are read by the code until it senses an end of file, which signals the code to begin processing the requests.

There is no limit to the number of delete and insert requests that can be present.

An entry is made for the outgoing particle on the first record of a data set if and only if the data being described pertain to the outgoing particle. For example, the cross section for an (n,np) reaction would be entered without specification of an outgoing particle, while an energy distribution of the resulting neutrons would require an entry of 1 for the y_0 (outgoing particle), and energy distributions for the resulting protons would require a 2 for the y_0 . With this feature it is possible to specify completely all aspects of reactions having more than one type of emergent particle.

E. MAKING A NEW LIBRARY ab initio

In the special case of making an entirely new library file, the entry in the calling sequence for (library name) should be "none". In such a case the file used for input requires a first record with the following information:

<u>Columns</u>	<u>Significance</u>
1-6	Date (YYMMDD)
7-8	Institution (1 for LLNL, 2 for AWRE, 3 for ENDF/B)
9-10	Year
11-12	Edition of the library
13-14	Version of the edition entered in columns 11-12
15	Type of library: <ul style="list-style-type: none"> 1 = neutron interaction 2 = photon interaction with cold atoms 3 = photon interaction with hot media 4 = charged particle interaction 5 = neutron-induced activation

Making such a new library rather than updating an existing library is a rare occasion.

F. OUTPUT

There are several different forms of printout from the code which tell the user what has been done. This, of course, is in addition to any files that have been made. The order of the output is as follows:

1. The evaluated library identification word from the input library is decoded and printed with appropriate labels describing the meaning of each quantity. This is followed by the date for this library.
2. The delete and insert requests or the retrieve requests are printed as they were read from the input cards.
3. A printout is made showing the computer time used to process this update.

CHAPTER III
ENDEP AND AUTODEP

III. ENDEP AND AUTODEP

A. INTRODUCTION

Average energies are entered for each reaction in the evaluated neutron library (ENDL), the evaluated charged particle library (ECPL), and the evaluated gamma ray interaction library (EGPL). These quantities are defined by the two reaction property designators, I, as

I = 10 the total average energy in each outgoing particle field, $1 \leq y_0 \leq 16$,

I = 11 the average energy of the residual nucleus.

See Appendix I-A for the definitions of reactions and reaction property designators.

Gamma ray spectra may or may not be present in the evaluated library for a given nuclear reaction. If the spectral data are not present, then the gamma rays from the reaction are included within the gamma ray production ($C = 55$) data. In either case, the I = 10 data for the resultant gamma field are calculated by the code. Additionally, all nuclear reactions have a residual or final state nucleus. If this nucleus is either a neutron or a light charged particle, it is tagged by an outgoing particle designator, $11 \leq y_0 \leq 16$ and only I = 10 data are calculated. If the residual's $ZA > 2004$, then I = 11 data are also calculated.

ENDEP calculates the required average energies from the existing data, e.g., secondary particle spectra and multiplicities. The latter may be implicit in the reaction as with the n, 2n reaction where the implied neutron multiplicity is 2 or explicit as for gamma-rays from capture where energy dependent multiplicities are given in the library. If I = 3 double differential data are present for the reaction, no ENDEP calculation is performed and the existing I = 10 and 11 data are utilized. AUTODEP is the automatic version of ENDEP. When any changes are made in the evaluated library for a given reaction pertaining to energy deposition, e.g., changes to I=1, 4, 7-9 data, AUTODEP is initialized by the UPDATE code for the isotope in question. The new energy deposition terms are then automatically included in the update of the library. It is assumed that the target nucleus is at rest. Specifically as a function of reaction designator, C, the following energy deposits are calculated:

$8 \leq C \leq 49$ I = 10 and 11 data unless, as above, the residual nucleus has $ZA \leq 2004$. In the latter case only I = 10 data are calculated. The particle multiplicity is included in the I = 10 data.

50<C<57 **I = 10 data only. The multiplicity is accounted for in these data by being included in the production cross section.**

71<C<74 **I = 10 data only. The multiplicity is included in the I = 10 data.**

In addition to calculating the required energy deposition terms, the code insures that the multiplicity of capture gamma rays in the evaluated library is consistent with energy conservation. Any time the gamma-ray spectral data is updated for capture ($C=46$, $I=4$, $y_0=7$ data), the $I=9$ multiplicity data is recalculated. This is carried out by the use of Eq. (III.C-1) of Appendix III.C, in conjunction with Eq. (III.2). The energy deposition terms are then calculated as described in this chapter.

Two general classes of models are used to calculate the required average energies for a given reaction. These are the $\bar{E}$ models and the residual models. The method of calculating the average energy in an outgoing particle or gamma-ray field is based on the type of data in the file for the particle in question, e.g., two-body center of mass angular distribution, particle spectra, etc. This is specified by the $\bar{E}$ model. The average energy into the gamma ray field and the average energy of the residual nucleus is determined both by the $\bar{E}$ model and by the reaction C number. These specify the residual model.

Both the $\bar{E}$ models and the residual models will be defined in the next section in terms of the specific kinds of information that are characteristic of the evaluated data libraries. This will be followed by specific descriptors for each $\bar{E}$ model and then for each residual model. Finally, the required code input, operation, and output will be given.

Several comments should be made at this time regarding energy conservation and balance. If the average energy or the gamma ray field ($I = 10$, $y_0=7$) is calculated to be negative when no explicit photon spectra are entered for that reaction, it is set to zero and the calculation then continues, with an error message printed in the output. An overall reaction energy balance is conserved by this approach. If the calculated average energy of the residual nucleus ($I = 11$ data) is also negative, it is set to zero and energy is no longer conserved. Again, an error message is printed. The basic evaluated data must be revised in these cases since too much energy has been put into the evaluated secondary particle spectra. The resultant iterative procedure, when the conservation criteria are satisfied, yields an improved set of data.

B. $\bar{E}$ AND RESIDUAL MODELS

The reaction type designator, C, reaction modifier, S, and the reaction property designator, I, determine the $\bar{E}$ model for a given outgoing particle, and the model to be

used for the average energy of the residual. For incident particles, $1 \leq y_i \leq 6$, and for $8 \leq C \leq 49$, these models are given in Table III.1. For these reactions both $l = 10$, $y_0 = 7$ and $l = 11$ data are calculated. Overrides to Table III.1 based on whether the residual is a neutron or a light charged particle ($l = 11$ data then not calculated) or if $y_0 = 7$ data are present in the file are given in Table III.2. In the latter case, the $l = 10$, $y_0 = 7$ data come directly from the $y_0 = 7$ spectral and multiplicity data. In Table III.3 are overrides for special reaction modifiers, S. In these cases, the $l = 10$, $y_0 = 1$ results are not readily obtainable from the file information and are obtained from energy conservation. These models have been used for the ${}^2_1\text{H}$ and ${}^9_4\text{Be}$ (n,2n) reaction.

TABLE III.1. $\bar{E}$ and residual models for $1 \leq y_i \leq 6$, and no $y_0 > 10$ (no residual nucleus being either a neutron or a charged particle), or $y_0 = 7$ (no secondary gamma ray data) present.

C	S	l^c	$\bar{E}$ model	Residual model
8-10	0	1	A	1
11	1	1	A	1
11	0	4	D	2
12	0	4	D	3a or 2a ^b
13-14	0	4	D	2a
15	0	Many	E	4
20-22,24-26	0	4	D	3
20-22,24-26	1	1 & 4 ^a	C	5
40-42,44,45	1	1	A	1
40-42,44,45	0	4	D	2

^a $l = 1$ is for the first particle (a neutron in all cases but $C = 21$); $l = 4$ is for the second particle.

^b Both models are programmed into the code, reaction type 2a is currently being used.

^c $l = 1$ and 4 may also be given. This is an uncorrelated energy-angle reaction and only the $l = 4$ data are used.

TABLE III.2. Overrides to Table I when either $y_0 > 10$ or $y_0 = 7$ data is present.

<u>Residual model override based on y_0</u>		
Is $y_0 > 10$ present	Is $y_0 = 7$ present	Residual model
Yes	Immaterial	None ^a
No	Yes	g ^b
<u>E model override (pertains to both cases above)</u>		
y_0	1	E model
= 7	4 & 9 ^c	D ^c
≠ 7	1	A
≠ 7	4 & 9	D ^d

^a This includes C = 23, 27-29, 31, 37-39, and 43.

^b This includes C = 30 and 46.

^c If $y_0 = 9$ data are also given here, it is calculated by E model type D.

^d If the multiplicity is implied by the reactor (e.g., C = 12 implies a neutron multiplicity of 2) I = 9 data are not given.

^e I = 1 data may also be given. This is an uncorrelated energy-angle reaction and the I = 1 data are not used here.

TABLE III.3. Overrides to Table I when special reaction modifiers, S, are present for a given C.

S	y_1	C	$\bar{E}$ model	Residual model
8	1	12	F	None
10,11	1	12	F	None

The $\bar{E}$ and residual models for production cross sections are given in Table III.4. The only values calculated for these reactions are the I = 10 data for the secondary particles. These results are used in the GAMCHK code (see Chapter IV) that compares the $\sigma \cdot \bar{E}$ values (barn MeV) for the gamma ray and electron production cross sections versus the sum of the $\sigma \cdot \bar{E}$ values for I = 10, $y_0 = 7$ and 9 data for the particle interaction reactions, $11 \leq C \leq 49$. In principle, these results should be the same; in practice they often are not, and changes to one or the other types of information has to be made.

TABLE III.4. $\bar{E}$ and residual models for production cross sections, $59 \leq C \leq 57$.

C	S	I	$\bar{E}$ model	Residual model
59-57	0	4	G1	None
59-57	3	1	G2	None

Finally, the $\bar{E}$ and residual models for gamma ray induced reactions, $y_i = 7$, are shown in Table III.5. The basic assumption is that all energy is deposited locally, i.e., there are only 1 = 10 data calculated for $y_0 = 7$ and hence no residual values are calculated.

TABLE III.5. $\bar{E}$ and residual models for $y_i = 7$; $71 \leq C \leq 74$, gamma ray induced reactions.

C	I ^a	$\bar{E}$ model	Residual model
71	0	H1	7a
72	4	H2	7b
73	0	H3	7c
74	4 and 9	H4	7b

^a Ignore all other $l = 0$ data present for the reaction.

C. $\bar{E}$ MODEL DESCRIPTIONS

The specifications for each E type designater are as follows:

$\bar{E}$ Model A-Discrete two-body

Consider particle 1 interacting with target 2 yielding particle x and the residual y. We obtain the average energy for particle x, $\bar{E}_x(E_1)$, from Eq. (III-A.12) of Appendix III-A.

$$\bar{E}_x(E_1) = a_{1x}E_1 + a_{2y}(E_1 - E_{1\alpha}) + 2[a_{1x}a_{2y}E_1(E_1 - E_{1\alpha})]^{1/2}g_{x1}(E_1), \quad (\text{III.1})$$

The coefficient g_{x1} is the average collision cosine in the center of mass system and is calculated by ENDEP. It is linearly interpolable between the incident energies for which the corresponding $I = 1$ data had entries in the files. However, the $\bar{E}_x$ results have to be calculated using a fine energy mesh and then thinned to a specified criterion (usually .005) since Eq. (III.1) is not linear. If the residual is also a charged particle with $ZA \leq 2004$, the procedure is repeated for it.

$\bar{E}$ Model B - Continuum two-body

The average energy of all outgoing particles of type x , $\bar{E}_x$, is

$$\bar{E}_x(E_1) = m_x(E_1) \int_{E_{x\min}}^{E_{x\max}} E_x \pi_0(E_1 \rightarrow E_x) dE_x, \quad (\text{III.2})$$

where $\pi_0(E_1 \rightarrow E_x)$ are the $I = 4$ data ($l = 0$ only) and m_x is the particle multiplicity. Eq. (III.2) is integrated analytically since $\pi_0(E_1 \rightarrow E_x)$ are linearly interpolable in E_x . $\bar{E}_x$ is calculated at the merged energies in the $I = 4$ data and the multiplicity sets.

The multiplicities are unity except for those noted in Table III.6, and for the following cases for which m_x is energy dependent. For $C = 15$ and 46, m_x for $y_0 = 7$ is given by $I = 9$ (multiplicity) data. For $C = 15$, m_x for $y_0 = 1$ is given by $I = 7$ ($\bar{v}$) data.

TABLE III.6. Constant values for particle multiplicity greater than unity for specific C numbers and y_0 .

C	y_0	m_x
12	1	2
13	1	3
14	1	4
27	6	2
29	1	2
32	1	2
37	6	2

E Model C - Discrete 2-body, continuum decay

In this case, $I = 1$ data are given for $y_0 = 1$ and $I = 4$ data are given for all other y_0 's. ENDEP uses E model A for $y_0 = 1$ and E model B for the other y_0 's.

E Model D - General continuum

$I = 4$ and 9 data are given so that ENDEP uses E model B. Note that both $y_0 = 7$ and $y_0 = 9$ output can come from radiative capture.

If the $I = 4$ and 9 data for $y_0 = 7$ or 9 do not extend to the maximum energy (currently set at 20 MeV), the missing data have been preprocessed and are included in the particle production information ($C = 55$ and 57). We therefore must provide information for $I = 10$ at 20 MeV from Eq. (III.C.6) of Appendix III C for $y_0 = 7$,

$$\overline{E}_x(E_1) = \frac{M_2}{M_1 + M_2} E_1 + Q, \quad (\text{III.3})$$

where Q is the reaction Q value, M_2 is the target mass, and M_1 is the mass of the incident particle. If $y_0 = 9$ data are also present, we set $\overline{E}_x(E_1) = 0$, for $y_0 = 9$ and $E_1 = 20$ MeV.

E Model E - Fission

For $y_0 = 1$, $I = 4$ and 7 data are given and E model B is used. Similarly for $y_0 = 7$, $I = 4$ and 9 data are given and E model B is used.

E Model F - $C = 12$, $S = 8$ or $10, 11$ for $y_1 = 1$

In either case, for all $y_0 \neq 1$, E model B is used. For $y_0 = 1$, $\overline{E}_x$ cannot be easily determined from the data so energy conservation is used. This results in, for $y_0 = 1$,

$$\overline{E}_x = E_1 + Q - \sum_{y_0 \neq 1} \overline{E}_{y_0}, \quad (\text{III.4})$$

where Q = the mass difference Q_0 value for the multibody breakup to the final end products. For $ZA = 1002$, $Q = -2.23$ MeV and for $ZA = 4009$, $Q = -1.573$ MeV.

E Model G - Production cross sections

Submodel G1. For the given y_0 , E model D is used with multiplicity, $m_x = 1$.

Submodel G2. The incident energies come from the $I = 0$ data. Then for $y_0 = 7$, $\overline{E}_{y_0} = X1$, the value entered in the X1 field.

E Model H - Gamma ray interaction cross sections

Submodel H1. For $y_0 = 7$, the $l = 10$ data are given by

$$\bar{E}_{y_0} = E, \quad (\text{III.5})$$

where E is the incident particle energy.

Submodel H2. For $y_0 = 7$, $\bar{E}$ model B is used with the multiplicity, $m_x = 1$.

Submodel H3. No $l = 10$ data are calculated for the reaction.

Submodel H4. For $y_0 = 7$, $\bar{E}$ model B is used with a multiplicity, $m_x = 2$.

D. RESIDUAL MODELS

The description of each model used to calculate the average energy of residuals will now be given. For convenience, the nomenclature used here will be different from that used previously in this chapter. Let y = particle, A = nucleus, Q_0 = the mass difference Q value, $\bar{E}_Y$ = the $l = 10$, $y_0 = 7$ value, and $\bar{E}_R$ = the $l = 11$ data. Subscripts 0 refer to the projectile and target, 1 to the two products from the two body reaction, and 2, etc., to resultant pairs of products from subsequent decay events. Two-body kinematics are discussed in Appendix III-A and decay kinematics in Appendix III-B, with those results being used here as needed.

Residual Model 1 - Discrete two-body

Given: M_{y0} , M_{A0} , M_{y1} , $Q_{0,1}$ (reaction Q_0), W_{A1}^* (X1 field), E_{y0} , $\bar{E}_{y1}$. Calculate:
(See Appendix III-A)

$$\bar{E}_Y = W_{A1}^*, \quad (\text{III.6})$$

$$Q_{0,1} = Q_{0,1} - W_{A1}^*, \quad (\text{III.7})$$

$$\bar{E}_R = \bar{E}_{A1} = E_{y0} + Q_{0,1} - \bar{E}_{y1}. \quad (\text{III.8})$$

Residual Model 2 - Continuum two-body

Given: M_{y_0} , M_{A_0} , M_{y_1} , $Q_{0,1}$ (reaction Q_0), E_{y_0} , $\bar{E}_{y_1}$.
 Calculate: (see Appendix III-A)

$$M_{A_1} = M_{y_0} + M_{A_0} - M_{A_1}, \quad (\text{III.9})$$

$$\bar{W}_{A_1}^* = Q_{0,1} + \frac{(M_{y_0} M_{y_1} + M_{A_0} M_{A_1})}{M_{A_1} (M_{y_0} + M_{A_0})} E_{y_0} - \frac{M_{y_0} + M_{A_0}}{M_A} \bar{E}_{y_1}, \quad (\text{III.10})$$

$$\bar{E}_Y = \bar{W}_{A_1}^*, \quad (\text{III.11})$$

$$Q_{0,1} = Q_{0,1} - \bar{W}_{A_1}^*, \quad (\text{III.12})$$

$$\bar{E}_R = \bar{E}_{A_1} = E_{y_0} + Q_{0,1} - \bar{E}_{y_1}. \quad (\text{III.13})$$

Submodel 2a

Let m = multiplicity of y_1 ($m = 2$, $C = 12$; $m = 3$, $C = 13$; $m = 4$, $C = 14$). Then let

$$M_{y_1} = m M(y_1), \quad (\text{III.14})$$

$$\bar{E}_{y_1} = \bar{E}_{mn}. \quad (\text{III.15})$$

where $\bar{E}_{mn}$ is the $I = 10$ value calculated from the ENDL (or ECPL) $I = 4$ data as defined by $\bar{E}$ model B. Repeat Eqs. (III.9) - (III.13) above using the results of Eqs. (III.14) and (III.15).

Residual Model 3 - Continuum two-body, continuum decay

Note that this reaction is very similar to residual model 5.

Given: $M_{y_0}, M_{A_0}, M_{y_1}, M_{y_2}, Q_{0,2}$ (reaction Q_0), $E_{y_0}, \bar{E}_{y_1}, \bar{E}_{y_2}$.
 Calculate: (see Appendices III-A and III-B)

$$ZA(A_1) = ZA(y_0) + ZA(A_0) - ZA(y_1), \quad (\text{III.16})$$

$$\text{Obtain } M_{A_1} \text{ from mass tables } M_{A_1} = M(ZA(A_1)) \quad (\text{III.17})$$

$$Q_{0,1} = [(M_{y_0} + M_{A_0}) - (M_{y_1} + M_{A_1})] c^2, \quad (\text{III.18})$$

$$\text{Redefine } M_{A_1} \text{ as per Eq. (III.9),} \quad (\text{III.19})$$

$$\bar{W}_{A_1}^* \text{ from Eq. (III.10),} \quad (\text{III.20})$$

$$Q_{0,1} \text{ from Eq. (III.12),} \quad (\text{III.21})$$

$$\bar{E}_{A_1} = E_{y_0} + Q_{0,1} - \bar{E}_{y_1}, \quad (\text{III.22})$$

$$M_{A_2} = M_{A_1} - M_{y_2}, \quad (\text{III.23})$$

$$Q_{0,2} = Q_{0,1} - Q_{0,2}, \quad (\text{III.24})$$

$$\bar{W}_{A_2}^* = Q_{0,1,2} + \bar{W}_{A_1}^* + \frac{M_{y_2}}{M_{A_2}} \bar{E}_{A_1} - \frac{M_{A_1}}{M_{A_2}} \bar{E}_{y_2}, \quad (\text{III.25})$$

$$\bar{E}_Y = \bar{W}_{A_2}^{\bullet} , \quad (\text{III.26})$$

$$\bar{E}_R = \bar{E}_{A_2} = E_{y_0} + Q_{0,2} - \bar{E}_{y_1} - \bar{E}_{y_2} - \bar{E}_Y . \quad (\text{III.27})$$

Submodel 3a -

$$y_1 = y_2 \quad (\text{III.28})$$

$$\bar{E}_{y_1} = \bar{E}_{y_2} = \frac{\bar{E}_{2n}}{2} \quad (\text{III.29})$$

where $\bar{E}_{2n}$ is the $i = 10$ value calculated from the ENDL (or ECPL) $i = 4$ data as defined by $\bar{E}$ model B. Repeat Eqs. (III.20) - (III.27) above using the result of Eq. (III.29).

Residual Model 4 - Fission

Given: M_{y_0} , M_{A_0} , Q_0 (reaction Q_0 value), $\bar{E}_{y_1}$, $\bar{E}_Y$.

Calculate:

$$\bar{E}_R = \bar{E}_{2FP} = E_{y_0} + Q_0 - \bar{E}_{y_1} - \bar{E}_Y . \quad (\text{III.30})$$

Residual Model 5 - Discrete two-body, continuum decay

Note that this reaction is very similar to residual model 3.

Given: M_{y_0} , M_{A_0} , M_{y_1} , M_{y_2} , $Q_{0,2}$ (reaction Q_0), $W_{A_1}^*$ (XI field), E_{y_0} , $\bar{E}_{y_1}$, $\bar{E}_{y_2}$. Calculate: (See Appendices III-A and III-B)

$$ZA(A_1) \text{ from Eq. (III.16) ,} \quad (\text{III.31})$$

$$M_{A_1} \text{ from Eq. (III.17) ,} \quad (\text{III.32})$$

$$Q_{0,1} \text{ from Eq. (III.18) ,} \quad (\text{III.33})$$

$$Q_{0,i} \text{ from Eq. (III.7) ,} \quad (\text{III.34})$$

$$\bar{E}_{A_1} \text{ from Eq. (III.8) ,} \quad (\text{III.35})$$

$$M_{A_2} \text{ from Eq. (III.23) ,} \quad (\text{III.36})$$

$$Q_{0,1,2} \text{ from Eq. (III.24) ,} \quad (\text{III.37})$$

$$\bar{W}_{A_2}^* \text{ from Eq. (III.25) ,} \quad (\text{III.38})$$

$$\bar{E}_Y \text{ from Eq. (III.26) ,} \quad (\text{III.39})$$

$$\bar{E}_R = E_{A_2} \text{ from Eq. (III.27) ,} \quad (\text{III.40})$$

Residual Model 6 - Radiative capture

Given: M_{y_0} , M_{A_0} , $Q_{0,1}$, (reaction Q_0), E_{y_0} , $\bar{E}_Y$.

Calculate: (See Appendix IIIC)

$$\bar{E}_R = \bar{E}_\gamma = E_{\gamma_0} + Q_{0,1} - \sum_{\gamma_0=1}^{16} \bar{E}_{\gamma_0} \quad (\text{HL-41})$$

Residual Model 7 - Gamma ray induced reactions

Submodel 7a. No $l = 11$ data are calculated.

Submodel 7b. $\bar{E}_R = E - \bar{E}_\gamma$, (HL-42)
where E is the incident energy.

Submodel 7c. $\bar{E}_R = E$. (HL-43)

E. INPUT, OPERATION, AND OUTPUT

The input file for ENDEP contains the following information:

<u>Columns</u>	<u>Format</u>	<u>Remarks</u>
1	i1	γ_1 - incident particle designator.
2-5	F4.3	EPCK - fractional error for energy check printout. Only when the calculated energy discrepancy > EPCK will a comment be printed on output.
6-11	i6	NNZAB - Beginning target ZA number.
12-17	i6	NNZAE - Ending target ZA number.
18-20	i3	NRCTB - Beginning reaction C number.
21-23	i3	NRCTE - Ending reaction C number.
24-26	i3	NDELOP = 0, make necessary $l = 10$ and 11 delete cards for update in the output file. $=1$, no delete cards will be made.
27-29	i3	NPNTOP - If > 0, increasing amounts of debug output are given as NPNTOP increases from 1 to 5.

The calling sequence for ENDEP is:

omega endep (input file) (box no.) (hsp option) (library name)
0 (output file name) (output file size) / TV

The parentheses denote problem dependent quantities and do not appear in the calling sequence. The various quantities in parentheses have the following significance:

input file	the file required by ENDEP for input
box no.	user's box number
hsp option	ENDEP produces output that is descriptive and/or diagnostic for the problem. This output may be directed to the F800 (use "f800" for option), the high speed printer (use "hsp" for option), or kept for inspection (use "debug" for option) and/or output to RJET or other medium using ALLOUT.
library name	The library file of evaluated data used by the code.
0	The zero in this position indicates that the library exists as a file. The zero must be included in the calling sequence.
output file name	The name of the file to be created as output. This file contains the I = 10 and 11 data.
output file size	If equal or less than 99, it is the size of the file to be created in units of 100000. If greater than 99, it is the actual file size to be created. When the code finishes it will shrink the file to the size needed.

An example of running ENDEP using an input file DEPIN with a library called ND821201 to make an output file (with the I = 10 and 11 data) called DEPOUT is

omega endep depin T61 debug nd821201 0 depout 10 / .9 .999

The HSP output consists of the following information:

1. The y_i , C, S, Q_0 , and X_1 fields for all reactions.
2. If $\bar{E}_Y$ is calculated to be negative, the code prints out $EBARG(i) = \text{_____}$, where i is the counter for the I = 10, $y_0 = 7$ data.
3. If $\bar{E}_R$ is calculated to be negative, the code prints out $EBARA1(i) = \text{_____}$, where i is the counter for the I = 11 data.
4. The available energy for a reaction is $E + Q$. The Out (output) energy is $\sum_{\text{all}} y_0$ (I = 10) + (I = 11). Then if $| \text{Available} - \text{Out} | / \text{Available} > \text{EPCK}$, write out ENERGY DISCREPANCY = Available - Out, = $| \text{Available} - \text{Out} | * 100 / \text{Available} \%$.

APPENDIX III-A - TWO BODY KINEMATICS

In this appendix, two-body kinematics as required for energy deposition calculations will be briefly given. The starting point is the discrete reaction in which the final state is either two particles, or a particle and a residual nucleus ($ZA > 2000$), the latter being either in the ground or an excited state. The analysis is then extended to the case where the final state is in the continuum.

In the discrete two-body reaction, one has projectile 1, energy E_1 , interacting with a stationary target 2 yielding reaction products x and y with energies E_x and E_y , respectively. Conservation of energy in the laboratory (L) frame yields

$$E_1 + Q = E_x + E_y \quad (III-A.1)$$

where the reaction Q value is given by (note that W_1^* is usually zero):

$$Q = Q_0 + (W_1^* + W_2^*) - (W_x^* + W_y^*) \quad (III-A.2)$$

and

$$Q_0 = [(M_1 + M_2) - (M_x + M_y)] c^2 \quad (III-A.3)$$

In these expressions, W refers to level excitation energy and M to mass. The next step is to transform to the center of mass (CM) system, use energy and momentum conservation, and transform back to the L system to obtain for the kinetic energy of particle x,^{1,2}

$$E_x = a_{1x} E_1 + a_{2y} (E_1 - E_{1\alpha}) + 2[a_{1x} a_{2y} E_1 (E_1 - E_{1\alpha})]^{1/2} \eta_x \quad (III-A.4)$$

where η_x is the collision cosine of particle x in the CM system. The other terms in Eq. (III-A.4) are defined by

$$a_{1x} = \frac{M_1 M_x}{(M_1 + M_2)(M_x + M_y)} \quad (III-A.5)$$

$$a_{2y} = \frac{M_2 M_y}{(M_1 + M_2)(M_x + M_y)} \quad (III-A.6)$$

and

$$E_{1c} = - \frac{M_1 + M_2}{M_2} Q. \quad (\text{III-A.7})$$

The term of interest for the discrete reaction is the average final particle energy, $\bar{E}_x$, where (the multiplicity of particle x is unity in this case)

$$\bar{E}_x = \int_{E_{x\min}}^{E_{x\max}} E_x v_0(E_1 \rightarrow E_x) dE_x. \quad (\text{III-A.8})$$

Since $v_0(E_1 \rightarrow E_x) dE_x = g_x(E_1, \eta_x) d\eta_x$, where $g_x(E_1, \eta_x)$ is the CM normalized (over η_x) angular distribution, Eq. (III-A.8) becomes

$$\bar{E}_x = \int_{-1}^{+1} E_x(E_1, \eta_x) g_x(E_1, \eta_x) d\eta_x, \quad (\text{III-A.9})$$

where $E_x(E_1, \eta_x)$ is given by Eq. (III-A.4). Expanding the angular distribution in Legendre polynomials,

$$g_x(E_1, \eta_x) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} g_{x\ell}(E_1) P_{\ell}(\eta_x), \quad (\text{III-A.10})$$

where

$$g_{x\ell}(E_1) = \int_{-1}^{+1} g_x(E_1, \eta_x) P_{\ell}(\eta_x) d\eta_x. \quad (\text{III-A.11})$$

Substituting Eq. (III-A.10) into Eq. (III-A.9) and carrying out the integration with the use of the orthogonality relation yields

$$\bar{E}_x = a_{1x} E_1 + a_{2y} (E_1 - E_{1\alpha}) + 2[a_{1x} a_{2y} E_1 (E_1 - E_{1\alpha})]^{1/2} g_{x1}(E_1). \quad (\text{III-A.12})$$

Since $g_{x1}(E_1) = \overline{\eta_x(E_1)}$, comparing to Eq. (III-A.4), it is seen that $\bar{E}_x = E_x[E_1, \overline{\eta_x(E_1)}]$. The average energy of the other reaction product, $\bar{E}_y$, may either be obtained from Eq.

(III-A.12) by interchanging x and y or from conservation of energy, Eq. (III-A.1). Finally, it should be noted that if, for example, particle x is the residual nucleus in an excited state and the reaction is truly two-body, i.e., not the first step of a time sequential process, then the total average ray energy $\bar{E}_y$ is

$$\bar{E}_y = W_x^* . \quad (\text{III-A.13})$$

Let us now assume that reaction product y is a particle with known average energy, $\bar{E}_y$, and that the residual nucleus x has excitation energy, $\bar{W}_x^*$, in the continuum. For the residual nucleus, one assumes an isotropic CM angular distribution and using Eq. (III-A.12) and solving for Q (an average value since the transition is to the continuum),

$$\bar{Q} = \left(\frac{M_1 + M_2}{M_y} \right) \bar{E}_x - \left[\frac{M_1 M_x + M_2 M_y}{M_y (M_1 + M_2)} \right] E_1 . \quad (\text{III-A.14})$$

This equation has two unknowns, $\bar{Q}$ and $\bar{E}_x$. For the other equation, one uses conservation of average energy from Eq. (III-A.1),

$$E_1 + \bar{Q} = \bar{E}_x + \bar{E}_y , \quad (\text{III-A.15})$$

along with the definition of $\bar{Q}$ from Eq. (III-A.2),

$$\bar{Q} = Q_0 + W_2^* - \bar{W}_x^* . \quad (\text{III-A.16})$$

Solving these relations

$$\bar{W}_x^* = Q_0 + W_2^* + \frac{(M_1 M_y + M_2 M_x)}{M_x (M_1 + M_2)} E_1 - \frac{(M_1 + M_2)}{M_x} \bar{E}_y , \quad (\text{III-A.17})$$

and

$$\bar{E}_x = \frac{M_1 (M_x - M_y)}{M_x (M_1 + M_2)} E_1 + \frac{M_y}{M_x} \bar{E}_y . \quad (\text{III-A.18})$$

If this is the final end point of the reaction, i.e., no subsequent decay processes, then the total average gamma ray energy is

$$\bar{E}_y = \bar{W}_x^* . \quad (\text{III-A.19})$$

APPENDIX III-B: DECAY KINEMATICS

Decay kinematics are briefly described in this Appendix. First, the discrete reaction in which the final state is either two particles, or a particle and a residual nucleus ($ZA > 2004$), the latter in either the ground or an excited state, is investigated. The analysis is then extended to the case where the excitation energy of the residual nucleus is in the continuum. It should be noted that decay reactions may be preceded by either discrete or continuum reactions (two-body or other decays).

The discrete decay reaction is defined here as a recoil nucleus, energy E_1 , decaying into two reaction products x and y with energies E_x and E_y , respectively. Conservation of energy in the laboratory (L) frame yields

$$E_1 + Q = E_x + E_y \quad (\text{III-B.1})$$

where the reaction Q value is defined by Eqs. (III-A.2) and (III-A.3) of Appendix III-A with $W_2^* = M_2 = 0$. To obtain the pertinent energy of particle x , E_x , one transforms to the center of mass (CM) system, utilizes energy and momentum conservation, and transforms back to the L frame to obtain

$$E_x = \frac{M_x}{M_1} E_1 + \frac{M_y}{M_1} Q + \frac{2}{M_1} (M_x M_y E_1 Q)^{1/2} \eta_x \quad (\text{III-B.2})$$

where η_x is the decay cosine of particle x in the CM frame. It has been assumed in Eq. (III-B.2) that $M_1 = M_x + M_y$ which neglects Q/c^2 , the nonrelativistic approximation.

The average final particle energy, $\bar{E}_x$, can be obtained analogous to the results of Eqs. (III-A.8) - (III-A.12) of Appendix III-A. Simply quoting the results, one obtains

$$\bar{E}_x = \frac{M_x}{M_1} E_1 + \frac{M_y}{M_1} Q + \frac{2}{M_1} (M_x M_y E_1 Q)^{1/2} g_{x1}(E_1), \quad (\text{III-B.3})$$

where $g_{x1}(E_1)$ is given by Eq. (III-A.11) of Appendix III-A. In general the angular distribution of the decay products is not known and the valid assumption is made that the decay is isotropic, i.e., $g_{x1}(E_1) = 0$. Equation (III-B.3) then reduces to

$$\bar{E}_x = \frac{M_x}{M_1} E_1 + \frac{M_y}{M_1} Q. \quad (\text{III-B.4})$$

Now, assume that reaction product y is a particle with known average energy, $\bar{E}_y$, and that the residual nucleus has an average excitation energy, $\bar{W}_x^*$, in the continuum. From Eq. (III-B.4),

$$\bar{E}_x = \frac{M_x}{M_1} E_1 + \frac{M_y}{M_1} \bar{Q}, \quad (\text{III-B.5})$$

where the Q value is an average since the transition is to the continuum. Analogous to the results leading up to Eq. (III-A.17), one now employs conservation of average energy using Eq. (III-B.1) and the definition of the Q value,

$$\bar{Q} = Q_0 + W_1^* - \bar{W}_x^*, \quad (\text{III-B.6})$$

and solving these expressions

$$\bar{W}_x^* = Q_0 + W_1^* + \frac{M_y}{M_x} E_1 - \frac{M_1}{M_x} \bar{E}_y, \quad (\text{III-B.7})$$

and

$$\bar{E}_x = \left(\frac{M_x - M_y}{M_x} \right) E_1 + \frac{M_y}{M_x} \bar{E}_y. \quad (\text{III-B.8})$$

If this stage is the final stage of the reaction, then the total average gamma ray energy is

$$\bar{E}_Y = \bar{W}_x^*. \quad (\text{III-B.9})$$

APPENDIX III-C RADIATIVE CAPTURE KINEMATICS

Radiative capture is considered as a two-body process (See Appendix III-A) with the gamma ray momentum being given by E_γ/c , c being the speed of light. One considers particle 1, hitting a stationary target 2, giving off a gamma ray and a residual nucleus with energies E_γ and E_x , respectively. Proceeding with energy and momentum conservation and assuming center of mass (CM) isotropy of the reaction products, as with the analysis leading to Eq. (III-A.12) of Appendix III-A, gives

$$E_\gamma = M_x c^2 [(1+z)^{1/2} - 1] , \quad (\text{III-C.1})$$

where

$$z = \frac{2}{M_x c^2} \left(\frac{M_2}{M_1 + M_2} E_1 + Q \right) , \quad (\text{III-C.2})$$

$$Q = Q_0 + (W_1^* - W_x^*) , \quad (\text{III-C.3})$$

and

$$Q_0 = (M_1 + M_2 - M_x) c^2 . \quad (\text{III-C.4})$$

Now, for $z \ll 1$, as is always the case,

$$(1+z)^{1/2} = 1 + \frac{z}{2} . \quad (\text{III-C.4})$$

Equation (III-C.1) then becomes

$$\bar{E}_\gamma = \frac{M_2}{M_1 + M_2} E_1 + Q , \quad (\text{III-C.5})$$

and additionally,

$$\bar{E}_x = \frac{M_1}{M_1 + M_2} E_1 . \quad (\text{III-C.6})$$

In the above analysis, a single gamma ray had been assumed. If one assumes a cascade of gamma-rays and the same assumptions as used previously, then the same results hold and the total average gamma-ray energy is also given by Eq. (III.2).

REFERENCES

1. E. Amaldi, "Neutrons and Related Gamma Ray Problems," Encyclopedia of Physics, Vol. 36/2, p. 98, S. Flügge, Ed. (Springer-Verlag, Berlin, 1959).
2. S. T. Perkins, Nucl. Sci. Eng. 80, 130 (1982).

CHAPTER IV:
GAMCHK

IV. GAMCHK

A. INTRODUCTION

The CLYDE processing code (see Chapter VI) calculates multigroup gamma ray production, (y_p, Xy) , transfer matrices using both the available reaction data ($11 \leq C \leq 46$) and the available production data ($C = 55$). Photons produced by specific reactions are included wherever these data can be identified with the reaction. In most cases, however, and especially at incident particle energies above the threshold of inelastic scattering reactions, such identification cannot be made, so that photon production is lumped into a total photon production cross section and associated spectra. The reaction information includes cross sections ($I = 0$), energy spectra ($I = 4, y_0 = 7$), multiplicities ($I = 9, y_0 = 7$), and possibly angular distributions ($I = 1, y_0 = 7$). These latter data are treated as uncorrelated with the energy spectra. Reactions may be considered as either continuum ($S = 0$) or discrete level excitation ($S = 1$). The production information $C = 55$ contains the same types of data, excluding the multiplicity which is included within the production cross section. Production data are also considered as either continuum ($S = 0$), or discrete gamma production ($S = 3$).

As noted above, for most reactions there is no secondary photon ($y_0 = 7$) evaluated information given in the file. Whenever this information is not included in the reaction data, it is included in the production data. Thus, when CLYDE uses both components, it expects to obtain the whole. The one type of data common to both reaction and production is the total average energy into the γ and β^- fields ($I = 10, y_0 = 7$ and 9). This information is calculated by the ENDEP code (see Section III). Using these data, one can calculate the rate coefficients, $\overline{E}_Y \sigma_R$, summed over all reactions for which there are no specific evaluated (y_p, Xy) data given for $y_0 = 7$, and compare it to the equivalent sum over all γ and β^- production components. This is what the GAMCHK code does. For energy conservation, the two sums should be equal, with any difference indicating how badly conservation is violated.

B. TECHNIQUE

Define $\overline{E}_Y(E)$ and $\overline{E}_\beta(E)$ as the $I = 10, y_0 = 7$ and $I = 10, y_0 = 9$ data respectively for a given reaction. Furthermore, define $\sigma_c(E)$ as the corresponding reaction cross section. The same definitions apply to γ ray production, $C = 55$, and electron production, $C = 57$. A merged set of incident particle energies is obtained for all reaction and production data. All cross sections and $I = 10$ data are obtained at this merged set of energies by linear interpolation. Note that $\overline{E}(E)\sigma(E)$ is no longer linear interpolable but is quadratically interpolable.

For the reaction data, obtain the sum,

$$[\bar{E}(E)\alpha(E)]_R = \sum_{e=11}^{49} [\bar{E}_\gamma(E)\sigma_e(E) + \bar{E}_\beta(E)\sigma_e(E)] , \quad (IV.1)$$

where reactions only appear in the sum if there are no evaluated gamma or electron production data given for the reaction at the incident energy in question.

For the production data, obtain the sum,

$$[\bar{E}(E)\alpha(E)]_P = \sum_{\text{all } 55} \bar{E}_\gamma(E)\sigma_{55}(E) + \sum_{\text{all } 57} \bar{E}_\beta(E)\sigma_{57}(E) . \quad (IV.2)$$

Then calculate the difference

$$\Delta(E) = [\bar{E}(E)\alpha(E)]_R - [\bar{E}(E)\alpha(E)]_P , \quad (IV.3)$$

and the % difference

$$\% \Delta(E) = \frac{\Delta(E) \times 100}{[\bar{E}(E)\alpha(E)]_R} . \quad (IV.4)$$

INPUT, OPERATION, AND OUTPUT

The input file for GAMCHK contains the following information:

<u>Columns</u>	<u>Format</u>	<u>Remarks</u>
1-3	F3.0	EPIA—A percentage error for printout.
4-15	E11.4	BARDIN—An energy error for printout (MeV).
16-21	i6	NNZAB—Beginning target ZA number.
22-27	i6	NNZAE—Ending target ZA number.
28-30	i3	NPNTOP—If > 0, increasing amounts of debug output are given.

The calling sequence for GAMCHK is:

omega gamchk (input file) (box no.) (hsp option) (library name) 0 / TV

The parentheses denote problem dependent quantities and do not appear in the calling sequence. The various quantities in parentheses have the following significance:

input file	the file required by GAMCHK for input
box no.	user's box number
hap option	GAMCHK produces output that is descriptive and/or diagnostic for the problem. This output may be directed to the FRSU (use "frsu" for option), the high speed printer (use "hap" for option), or kept for inspection (use "debug" for option) and/or output to RJET or other medium using ALLOUT.
library name	the library file of evaluated data used by GAMCHK.
0	The zero in this position indicates that the library exists as a file. The zero must be included in the calling sequence.

An example of running GAMCHK using an input file GAMIN with a library called ND821201 would be

```
omega gamchk gamin T61 debug nd821201 0 / .9 .999
```

The output consists of lines for each isotope containing:

- 1) incident particle energy
- 2) $C < 55$ - Eq. (IV.1)
- 3) $C = 55, 57$ - Eq. (IV.2)
- 4) difference - Eq. (IV.3)
- 5) % - Eq. (IV.4)

If the difference is negative, % will be followed by ***. If the incident energy is one of those in the production component ($C = 55, 57$), % is followed by (). It should be noted that only when Eq. (IV.3) > BARDIN and then also Eq. (IV.4) > EPIA is there printout.

**CHAPTER V:
UTILITY**

v-1 / v-2

V. UTILITY

A. INTRODUCTION

UTILITY is a code that produces indexes, plots and lists of data included in any of the libraries maintained by the Physical Data Group. The calling sequence of **UTILITY** is:

OMEGA UTILITY (input file) (box no.) (output option) (library name) 0

The parentheses denote problem dependent quantities and do not appear in the calling sequence. The various quantities in parentheses have the following significance:

input file	the file required by UTILITY for input
box no.	user's box number
output option	UTILITY produces indexes, plots or lists of data as requested by the input file. This output may be directed to the FR80 (use "fr80" for option), the high speed printer (use "hsp" for option), or kept for inspection (use "debug" for option) and/or output to RJET or other medium using ALLOUT .
library name	the library file that is being used
0	The zero in this position indicates that the library exists as a file. The zero must be included in the calling sequence.

An example of running **UTILITY** using an input file **INUT** with a library called **ND821201** is:

omega utility inut t64 fr80 nd821201 0 / .9 .999

B. PREPARATION OF INPUT

The format of the input file that must be used with **UTILITY** is:

i2,2i6,2(1x,e11.4).

Any number of lists or indexes may be run at one time by including separate requests in the input file. Problems that produce plots must be run separately but any number of plot requests may be included in an input file for plot runs. The significance of the fields of the records in the input file is:

Columns	Values	Significance
1-2	1	Listing of the data as they appear on the binary form of the library.
	2	Reaction index in an encoded form.
	4	Plots of the data with hardcopy output.
	24	Plots of the data with micro-fiche output.
	5	Labeled listings of all the data. Total and non-elastic cross sections are included where appropriate.
	25	Same as 5 except that only cross sections are listed.
	6	Listing of cross sections and energy deposits for each reaction. Note that these quantities are also included with the rest of the data under a value of 5.
	8	Index with the various reaction numbers (Yi,Yo,C,I,S,Xi) translated from their numerical values to English equivalents.
3-8	ZA-Min	Minimum Value of ZA.
9-14	ZA-Max	Maximum Value of ZA.
16-26	Min-E	Minimum value of the level energy of a target nucleus to be considered.
28-38	Max-E	Maximum value of the level energy of a target nucleus to be considered.

CHAPTER VI:
CLYDE

VI-1 / VI-2

VI. CLYDE

A. INTRODUCTION

The CLYDE code has been developed to handle a broad range of cross section processing requirements for many types of user codes. The present version processes interaction and production data for neutrons, gamma rays, and light charged particles $ZA \leq 2004$. The code operates on the CRAY-1 computer and processes data for user codes that calculate particle transport using a deterministic theory, usually diffusion or S_n . Data for codes using Monte Carlo transport are processed by CTART, described in Chapter VIII.

The evaluated nuclear data that are used by CLYDE must be in the form of a disk file in the binary mode of one of the Evaluated Nuclear Data Libraries (ENDL, ECPL, or EGDL). The user must specify group boundaries, weighting fluxes, and the target isotopes for which processed data are required. Certain sets of group boundaries and weighting fluxes are standard and can be used by specifying them in the ASCII file, BDFLS (see Appendix VII.B).

The code calculates flux-averaged group cross-sections, transfer matrices, total average energies associated with each outgoing particle field, isotope production multiplicities, and appropriate group averages of collateral quantities such as the average number of neutrons per fission.

CLYDE has the following general characteristics:

1. For all practical purposes, it is unlimited in the amount of data and the number of groups it can handle. It has a practical limit (approximately 10), to the order of transfer matrices that it should be used to generate.
2. The appropriate data for any material can be calculated for a standard group structure and scattering order in a reasonable amount of computer time.
3. It does not have any particular model or parameters built in.
4. Redundant forms of input information that are allowed in the evaluated library are not processed by CLYDE.
5. Since both the input data and evaluated library are arranged in increasing energy, the code operates from low to high energy. The transport code calculations, on the other hand, usually compute from the greatest energy group to the least. Therefore, the code inverts all output arrays so that numbering and listing of groups and cross section begins with the greatest energy group. With each code run, a printout is produced that includes all pertinent information in a convenient form.
6. Units are cross sections in barns, energies in MeV, and speeds in cm/shake (1 shake = 10^{-8} seconds).

A. SPECIAL FEATURES AND RESTRICTIONS

Special features and restrictions of CLYDE are the following:

1. The technique used to calculate the transfer matrices depends on the type of data found in the evaluated file for the outgoing particle of interest (see Appendix L.A). If $l=1$ data are present, it is assumed that the reaction is two-body and the calculation proceeds through the LEGXFR subroutine. If $l=4$ data are present, the reaction is assumed to be a continuum process and the code uses the TABXFR subroutine. If both $l=1$ and $l=4$, $l=0$ only, data are present, the reaction is assumed to be uncorrelated in energy and angle and the angular distribution is assumed to be in the laboratory (L) system. The $l=4$ data for $l>0$ are then calculated from the relation¹

$$\pi_2(E \rightarrow E') = \pi_0(E \rightarrow E') f^l(E) . \quad (VI.1)$$

Here, $f^l(E)$ is the l^{th} Legendre coefficient of the $l=1$ data in the L system, e.g., $f^1(E) = \overline{\mu(E)}$, the average collision cosine.

2. All one dimensional arrays, e.g., $\alpha(E)$, are linearly interpolable in incident energy. $l=1$ data are linearly interpolable in cosine and also incident energy. $l=4$ data are linearly interpolable in final particle energy and also in scaled incident energy after making the unit base transformation (see Sec. VI-C). This latter case preserves linearity in interpolated areas.

3. The $l=0$ particle interaction matrices for each reaction are renormalized

$$\sigma_{o \rightarrow h} = \sigma_{o \rightarrow h} \left(\frac{m_g \sigma_g}{\sum_h \sigma_{o \rightarrow h}} \right) , \quad (VI.2)$$

where m_g is the reaction multiplicity and σ_g is the reaction cross section.

4. The l^{th} moment of the angular flux expansion, $\phi^l(E)$, is used to weight all l^{th} order terms. If the input spectrum do not extend up to the order required, i.e., $l_{\text{max}}+1$, CLYDE will use the highest order available to calculate the remaining terms up to the order required.

5. Evaluated data and weighting spectrum must span the group bounds of the incident particle.

6. The group bounds on the outgoing particle are arbitrary. Transfer below the lower bound of the lowest outgoing energy group is put into the lowest group. Transfer above the upper bound of the highest outgoing energy group is put into the highest group. Particles are therefore conserved.

7. The lower bound on the lowest groups should be greater than zero. If it is input as zero, it will be set to $1.0E-10$ MeV.

C. CLYDE EQUATIONS

Consider an incident particle of energy E in group g , $1 \leq g \leq G$. The incident particle undergoes a reaction, releasing an outgoing particle of energy E' in group h , $1 \leq h \leq H$. Group 1 in either of these group structures is that of highest energy. We now proceed with the various multigroup relations used in CLYDE.

Transfer Matrix Definition.

CLYDE, upon input option, can calculate several different types of transfer matrices. Consider the numerator of the multigroup transfer matrix element for a specific reaction (given $l=1$ or $l=4$ data)

$$J_{g \rightarrow h}^l = \int_g dE \varphi^l(E) m(E) \sigma(E) Z_h^l(E). \quad (VI.3)$$

The inner integral, $Z_h^l(E)$, is written in a general form as

$$Z_h^l(E) = \int_h \pi_l(E \rightarrow E') [(1-W) + WE'] dE', \quad (VI.4)$$

where W is a selection parameter. Setting $W=0$ leads to a particle conserving matrices. Energy conserving matrices are obtained by setting $W=1$. The input index, IECFLG, specifies the type of matrix calculated and its final deposition:

1. IECFLG=0. The selection parameter, W , is set equal to zero and the particle conserving matrices are calculated for all l ,

$$\sigma_{g \rightarrow h}^l = \frac{\int_g dE \varphi^l(E) \sigma(E) \int_h \pi_l(E \rightarrow E') dE'}{\int_g dE \varphi^l(E)}. \quad (VI.5)$$

2. IECFLG = 1. W is set equal to one and the energy production conservation matrix, as has been used in gamma-ray production, is calculated for $l=0$,

$$\sigma_{g \rightarrow h} = \frac{\int_{E_g} dE \varphi^0(E) \alpha(E) \int_h \tau_0(E+E') E' dE'}{\bar{E}_h \int_{E_g} dE \varphi^0(E)} \quad (VL6)$$

where

$$\bar{E}_h = \frac{1}{2}(E_{h+1} + E_h) \quad (VL7)$$

and E_h , etc., are the group boundaries.

3. IECFLG=2. W becomes 1 and the energy conserving matrix is calculated for $l=0$,

$$\langle E \sigma \rangle_{o_{g \rightarrow h}} = \frac{\int_{E_g} dE \varphi^0(E) \alpha(E) \int_h \tau_0(E+E') E' dE'}{\int_{E_g} dE \varphi^0(E)} \quad (VL8)$$

3. IECFLG=3. Group-split matrices, conserving both particles and energy, as used in charged particle production and transport.² Initially, the particle conserving matrices, IECFLG=0, are calculated for all l . Then W is set to one and the energy conserving matrix, IECFLG=2, is calculated for $l=0$. The average energy of the outgoing particles in group h (for a given incident group g) is then

$$\langle E \rangle_h = \frac{\langle E \sigma \rangle_{o_{g \rightarrow h}}}{\sigma_{o_{g \rightarrow h}}} \quad (VI.9)$$

However, under group splitting, the energy of all particles in a group is the arithmetic average, $\bar{E}_h$, given by Eq. (VL7). Defining

$$\tilde{\sigma}_{o_{g \rightarrow h}}$$

as being a matrix element after splitting, number and energy conservation for groups h and $h+1$ yield

$$\sigma_{o_{g \rightarrow h}} = \tilde{\sigma}_{o_{g \rightarrow h}} + \tilde{\sigma}_{o_{g \rightarrow h+1}} \quad (VI.10)$$

$$\langle E \rangle_h \sigma_{o_{g \rightarrow h}} = \bar{E}_h \tilde{\sigma}_{o_{g \rightarrow h}} + \bar{E}_{h+1} \tilde{\sigma}_{o_{g \rightarrow h+1}} \quad (VI.11)$$

Solving these two expressions for the matrix elements after splitting

$$\tilde{\sigma}_{o_{g \rightarrow h}} = f_h \sigma_{o_{g \rightarrow h}} \quad (VL12)$$

$$\tilde{\sigma}_{o_{g \rightarrow h+1}} = (1 - f_h) \sigma_{o_{g \rightarrow h}} \quad (VL13)$$

where

$$f_h = \frac{\langle E \rangle_h - \bar{E}_{h+1}}{\bar{E}_h - \bar{E}_{h+1}} \quad (VL14)$$

These relations are only valid for $\langle E \rangle_h \leq \bar{E}_h$, since one must have $0 \leq f_h \leq 1$ for the elements after splitting to be non-negative. Similarly, for groups h and h-1, one obtains

$$\tilde{\sigma}_{o_{g \rightarrow h}} = f_h \sigma_{o_{g \rightarrow h}} \quad (VL15)$$

$$\tilde{\sigma}_{o_{g \rightarrow h-1}} = (1 - f_h) \sigma_{o_{g \rightarrow h}} \quad (VL16)$$

where here,

$$f_h = \frac{\bar{E}_{h-1} - \langle E \rangle_h}{\bar{E}_{h-1} - \bar{E}_h} \quad (VL17)$$

which is valid for $\langle E \rangle_h \geq \bar{E}_h$. After splitting for all H groups (for a given incident group g), group h may have received components from itself and from the two adjacent groups. Thus, group splitting repartitions the transfer matrix in order to insure both energy and particle conservation. The average energy into the particle field in question after splitting is simply

$$\langle E \tilde{\sigma} \rangle_g = \sum_h \langle E \tilde{\sigma} \rangle_{o_{g \rightarrow h}} = \sum_h \bar{E}_h \tilde{\sigma}_{o_{g \rightarrow h}} \quad (VL18)$$

There are, however, two cases in which splitting cannot be done, or one would be splitting out of the existing group structure. In these cases

$$\tilde{\sigma}_{o_{g \rightarrow h}} = \sigma_{o_{g \rightarrow h}} \quad (VL19)$$

These occur for $h=1$ with $\langle E \rangle_1 > \bar{E}_1$, and also for $h=H$ with $\langle E \rangle_H < \bar{E}_H$. In the former case, i.e., (VI.18) is still assumed to be valid and the excess energy, i.e.,

$$\langle E \sigma \rangle_{0, g \rightarrow h} - \langle E \sigma \rangle_{0, g \rightarrow h}^{\sim},$$

will be deposited locally. On the other hand, when $h=H$, Eq. (VI.18) cannot be used since it would imply too much energy into the outgoing particle field and therefore too little local deposition. One therefore uses

$$\langle E \sigma \rangle_{0, g \rightarrow h}^{\sim} = \langle E \sigma \rangle_{0, g \rightarrow h}.$$

Including these two cases, the average energy into the particle field after splitting, Eq. (VI.18), is generalized to

$$\langle E \sigma \rangle_g^{\sim} = \sum_h \bar{E}_h \sigma_{0, g \rightarrow h} \quad \text{if } \langle E \rangle_H \geq \bar{E}_H, \quad (\text{VI.20})$$

$$= \sum_h \bar{E}_h \tilde{\sigma}_{0, g \rightarrow h} - [\bar{E}_H \tilde{\sigma}_{0, g \rightarrow H} - \langle E \sigma \rangle_{0, g \rightarrow H}] \quad \text{if } \langle E \rangle_H < \bar{E}_H. \quad (\text{VI.21})$$

Transport Correction Terms.

Transport corrections are used to take into account higher Legendre moments of both the angular flux and the transfer matrices which are truncated during the actual calculation.³ They cause modifications to both the group total cross section as well as the ingroup transfer matrix elements. These corrections, as used in CLYDE, consist of two parts.

Transport theory codes typically admit only one total cross section to be entered. The first correction accounts for the inexactness of weighting the total cross sections with an $\ell=0$ flux spectrum by supplying all higher orders of weighting up to L , where L is the order above which the transfer matrices are truncated. Consider the azimuthally symmetric transport equation for simplicity. The removal term on the left hand side of this equation is $\Sigma_t(E) f(E, \mu)$, Σ_t being the total cross section and f being the angular flux. The removal term is moved to the right hand side of the equation and incorporated into the Legendre expansion of the collision integral. The expression is then integrated over energy to obtain the multigroup form. Now define

$$\sigma_{t_g}(l) = \frac{\int \sigma_{t_g}(E) \phi^l(E) dE}{\int \phi^l(E) dE} \quad (VI.22)$$

one now adds

$$I_{t_g}(0) - I_{t_g}(l)$$

to both sides of the transport equation. The microscopic total cross section then is

$$\sigma_{t_g} = \sigma_{t_g}(0) \quad (VI.23)$$

and the corrected transfer matrices, $0 \leq l \leq L$, are

$$\sigma_{l_{g \rightarrow g'}}^{(corr)} = \sigma_{l_{g \rightarrow g'}} + [\sigma_{t_g}(0) - \sigma_{t_g}(l)] \delta_{g'g} \quad (VI.24)$$

The second (and more familiar) transport correcting term arises from the truncation of the transfer matrices at some order L . This leads to the so called extended transport approximation. Consider again the azimuthally symmetric multigroup transport equation and subtract

$$\Sigma_{L+1_g} f_g(\mu)$$

from both sides of this expression where this cross section term is yet undefined. On the right hand side, incorporate this term into the Legendre moment expansion of the collision integral and break this resulting sum into the ranges of $0 \leq l \leq L$ and $L+1 \leq l \leq \infty$. In this latter sum, all l^{th} moment transfer rates are assumed to be the same as for $l=L+1$, and requiring that this summation identically vanish, yields for the microscopic $L+1$ transport correcting cross section,

$$\sigma_{tr\ corr_g} = \sigma_{L+1_g} = \frac{\sum_{g'} \sigma_{L+1_{g \rightarrow g'}} \phi_{g'}^{L+1}}{\phi_g^{L+1}} \quad (VI.25)$$

The group cross section, σ_g , then becomes

$$\sigma_g = \sigma_{t_g} - \sigma_{tr\ corr_g} \quad (VI.26)$$

and the transfer matrix elements, $0 \leq l \leq L$, are

$$\sigma_{t_{g'g}}^{(corr)} = \sigma_{t_{g'g}} - \sigma_{tr\ corr_g} \delta_{g'g} \quad (VI.27)$$

In CLYDE, Eq. (VI.25) is referred to as the exact transport correcting cross section. This form, however, has caused numerical difficulties in some codes when it becomes so large so as to drive the group cross section, Eq. (VI.26) negative. Large transport corrections can arise from two conditions: (1) a very rapidly ascending assumed flux weighting spectrum (which may be inappropriate to the material in question); (2) too low an order of Legendre expansion (in many cases this will be a code limitation) in the case of a highly anisotropic scatterer. A negative diagonal transfer term can arise even in the absence of these conditions, if the group g is sufficiently small that the self-scatterer term is less than the in-scatterers.

To help alleviate this problem, it is assumed in Eq. (VI.25) that the rate of transfer into group g for order $L+1$ is equal to the rate of transfer out, which yields in this case

$$\sigma_{tr\ corr_g} = \sum_{g'} \sigma_{L+1_{g \rightarrow g'}} \quad (VI.28)$$

This expression is referred to in the code as the approximate transport correcting cross section and is the more commonly used version, since it assumes no knowledge of the $L+1$ group fluxes. Excluding the conditions of high particle multiplicity and large forward scattering, the approximate form cannot lead to a negative group cross section, although it can lead to a negative ingroup transfer matrix element.

CLYDE has the additional option of letting the code choose the appropriate form for the transport correcting term. In this case, one starts with Eq. (VI.25) and if for any group Eq. (VI.26) becomes negative, then for that group Eq. (VI.28) is employed for the transport correcting cross section. One can also choose to omit the transport correction altogether.

Average Group Flux and Inverse Speed

The group flux is calculated from

$$\phi_g^L \equiv \int_{E_{g-1}}^{E_g} dE \phi^L(E), \quad (VI.29)$$

for each order L from 0 to $L+1$. Here, $\phi^L(E)$ is the weighting spectrum used in generating the calculational constants from the evaluated data.

The flux-weighted average of the inverse speed of the incident particles (y_i) within each group is to be used as $1/v$ coefficients for time-dependent equations and in a/v terms for converting time-dependent problems to stationary ones. This average is expressed as

$$\frac{1}{v_g} = \frac{\int_{E_{g-1}}^{E_g} dE \frac{\phi^0(E)}{v(E)}}{\int_{E_{g-1}}^{E_g} \phi^0(E) dE} . \quad (VI.30)$$

The analytic solution to this equation for linearly interpolable ϕ^0 in segment i is

$$\begin{aligned} \frac{1}{v_g} = & \frac{M^{1/2}}{13.8915 \phi_g^0} \left[\sum_{i=g-1}^i \left(\frac{2}{3} (\phi_{i+1}^0 - \phi_i^0) (E_{i+1} + \sqrt{E_{i+1} E_i} + E_i) \right. \right. \\ & \left. \left. + \frac{2(E_{i+1} \phi_i^0 - E_i \phi_{i+1}^0)}{\sqrt{E_{i+1}} + \sqrt{E_i}} \right) \right] . \end{aligned} \quad (VI.31)$$

Here the i 's denote elements in the merged table of group bounds and flux energies from the input flux table. The numerical factor converts the speed to the units of cm/shake, where 1 shake = 10^{-8} sec; also M is the atomic mass (amu) of the incident particle.

Reaction Group Average Cross Sections

The group averages of the linearly interpolable integrated cross sections are weighted with appropriate fluxes over the group structure. The averages are expressed by

$$\sigma_{x_g}^l = \frac{\int_{E_{g-1}}^{E_g} dE \sigma_x(E) \phi^l(E)}{\int_{E_{g-1}}^{E_g} dE \phi^l(E)} . \quad (VI.32)$$

These quantities are generated for each l , $0 \leq l \leq L+1$. The values obtained for $l > 0$ are used in making the Legendre flux expansion correction to the total cross section, as discussed in the section on the transport correction.

The above integrals, being comprised only of products of linear functions, are analytic [see UNINT, DIINT, TRIINT subroutine descriptions in Appendix (VI.A)].

Transfer Matrices from Angular Distribution (G-1) Data:

General Relations. The subroutine LEU.XFK calculates the transfer matrices for the general two-body interaction-arbitrary (non zero) particle masses and reaction Q value.⁴ It therefore plays a role for two-body reactions as well as sequential multi-daughter interactions where the first product particle is from a virtual two-body process. One again considers an incident particle 1, energy E in group g undergoing a reaction with target 2, which is at rest. The reaction yields the particle of interest x, energy E' in group h and a residual (nucleus or particle) y. Define further η as being the center of mass (CM) collision cosine of particle x and u as being its laboratory (L) system collision cosine. The normalized CM angular probability, $g(E', \eta)$, is assumed to be a piecewise linear function. Under these conditions, the inner integral for the transfer matrix can be evaluated analytically.⁵

The integrals of interest for the transfer matrix has been expressed by Eq. (VL.3) and (VL.4). For the general two-body reaction, the Legendre moments of the transference probability are given by

$$\pi_L(E \rightarrow E') = \left[\frac{d}{dE'} \eta(E, E') \right] P_L[\mu(E, E')] g[E, \eta(E, E')] , \quad (VL.33)$$

where $P_L(\mu)$ is the Legendre coefficient of order L.

The kinematic relations between the incident particle energy E, the L and CM collision cosines of particle x, and its final energy E' are given in Refs. 4 and 5. One has

$$\eta = \alpha [\mu \pm r(\mu)]^2 - \gamma , \quad (VL.34)$$

and

$$E' = a_{1x} E [\mu \pm r(\mu)]^2 , \quad (VL.35)$$

$$\text{where } \alpha = \frac{a_{1x} E}{2[a_{1x} a_{2y} E(E - E_{1\alpha})]^{1/2}} , \quad (VL.36a)$$

$$r(\mu) = (\beta^2 + \mu^2)^{1/2} , \quad (VL.36b)$$

$$\beta^2 = \frac{a_{2y} (E - E_{1\alpha})}{a_{1x} E} - 1 , \quad (VL.36c)$$

$$\gamma = \frac{a_{1x} E + a_{2y} (E - E_{1\alpha})}{2a_{1x} a_{2y} E (E - E_{1\alpha})^{1/2}} \quad (VL34)$$

$$a_{1x} = \frac{M_1 M_x}{(M_1 + M_2)(M_x + M_y)} \quad (VL35)$$

$$a_{2y} = \frac{M_2 M_y}{(M_1 + M_2)(M_x + M_y)} \quad (VL36)$$

and

$$E_{1\alpha} = - \left(\frac{M_1 + M_2}{M_2} \right) Q \quad (VL36g)$$

M denotes particle mass, and Q is the usual reaction Q value. In Eq. (VL34) and (VL35) and what follows, the (+) sign is used, unless (β^2) is less than zero. In that case the minimum L collision cosine is

$$\mu_{\min} = (-\beta^2)^{1/2} = \left[1 - \frac{a_{2y} (E - E_{1\alpha})}{a_{1x} E} \right]^{1/2} \quad (VL37)$$

and the corresponding CM collision cosine is

$$\eta(\mu_{\min}) = - \left[\frac{a_{2y} (E_1 - E_{1\alpha})}{a_{1x} E} \right]^{1/2} \quad (VL38)$$

This implies that the (+) sign in Eqs. (VL34) and (VL35) is to be used down to the energy

$$E(\mu_{\min}) = a_{1x} E - a_{2y} (E - E_{1\alpha}) \quad (VL39)$$

and the (-) sign then used at all lower energies.

Finally, from Eq. (VL34),

$$\frac{d\eta}{d\mu} = \pm \frac{2\alpha}{r(\mu)} [\mu \pm r(\mu)]^2 \quad (VL40)$$

with the sign convention as described above. A special case arises when considering the recoil nucleus of elastic scattering, or when the emergent particles from elastic scattering are identical. In that case, [referring to Eqs. (IV.36)], $a_{1x} = a_{2y}$ and $E_{1\alpha} = 0$, and

(b)(7)(D)

(VL-42)

(VL-40)

(VL40)

of the various parameters are shown in Fig. 1. More detail is given in Ref. 4.

FIG. 1. Collision domain in the E' , E plane.

By combining Eqs. (VL.34) and (VL.35) and setting η to ± 1 ,

$$E'_{\max}(\omega) = a_{1x} L \left(\frac{\omega-1}{\omega} \right) = \{ (a_{1x} \omega)^{1/2} + (a_{2y} (\omega - \omega_{12}))^{1/2} \}^2, \quad (\text{VL.45})$$

$$E'_{\min}(\omega) = a_{1x} L \left(\frac{\omega+1}{\omega} \right) = \{ (a_{1x} \omega)^{1/2} - (a_{2y} (\omega - \omega_{12}))^{1/2} \}^2, \quad (\text{VL.46})$$

and from Eqs. (VL.35) and (VL.37),

$$E'(\omega_{\min}) = a_{1x} \mu_{\min}^2 = a_{2y} L \alpha - (a_{2y} - a_{1x}) E. \quad (\text{VL.47})$$

The Inner Integral. The inner integral is expressed by Eq. (VL.4) in conjunction with Eq. (VL.33). One now changes the integration variable from final particle energy, E' , to its L system collision cosine, μ ,

$$Z_h^L(E) = \int P_L(\omega) g(E, \omega) \frac{d\eta}{d\mu} [(1-W) + W E'(\omega)] d\mu. \quad (\text{VL.48})$$

The CM angular probability data are given in the form for a given E_i ,

$$-1, g(E_i, -1), \dots, \eta_{ij} g(E_i, \eta_j), \dots, 1, g(E_i, 1),$$

which are linearly interpolable both in incident energy and in CM cosine. The functional form of the $g(E, \eta)$ data is $g = a_j(E) + b_j(E)\eta$. The $g(E, \eta)$ data are found by interpolating in (E) the linear data in η at the surrounding data sets at (E_i) and (E_{i+1}) . The sets of breakpoints in η at E_i and E_{i+1} may not be identical, so a new set of η breakpoints at E is constructed by melding those for E_i and E_{i+1} . By inverting Eq. (VL.34) we calculate a corresponding set of breakpoints in (ω) . In addition, a breakpoint at $\mu_{\min}$ is included, if appropriate. Finally, by inverting Eq. (VL.35), we include two breakpoints corresponding to (E'_h) and (E'_{h+1}) , and two for $E'_{\min}(E)$ and $E'_{\max}(E)$, providing they fall within the range $(-1 < \eta < +1)$ and $(-1 < \mu < +1)$.

Equation (IV.48) is expressed now as

$$Z_h^L(E) = \sum_{k=k_{\min}}^{k(\mu_{\min})-1} Z_{-k}^L(E) + \sum_{k=k(\mu_{\min})}^{k_{\max}} Z_{+k}^L(E), \quad (\text{VL.49})$$

and

$$Z_{\pm k}^L(\omega) = \int_{\mu_k}^{\mu_{k+1}} d\mu P_L(\mu) (\mu_k + b_k [a(\omega\mu)^2 - \gamma]) (a \frac{\mu}{r} (\omega\mu)^2) (1 - \omega) W A_{1x} (\omega\mu)^2). \quad (VL.50)$$

where the subscript k includes all breakpoints. Proceeding with the exact integration of Eq. (VL.50) we rewrite it as

$$Z_{\pm k}^L(\omega) = (a_k - b_k \gamma) (1 - \omega) [{}^0 Z_{\pm k}^L(\omega) + (a_k - b_k \gamma) W A_{1x} \omega + b_k \alpha (1 - \omega)] [{}^2 Z_{\pm k}^L(\omega)] + (b_k \alpha W A_{1x} \omega) [{}^4 Z_{\pm k}^L(\omega)], \quad (VL.51)$$

$$\text{where } {}^0 Z_{\pm k}^L = \pm 2\alpha \int_{\mu_k}^{\mu_{k+1}} d\mu P_L(\mu) \left[\frac{2\mu^2 + \beta^2}{r} \pm 2\mu \right], \quad (VL.52a)$$

$${}^2 Z_{\pm k}^L = \pm 2\alpha \int_{\mu_k}^{\mu_{k+1}} d\mu P_L(\mu) \left[\frac{8\mu^4 + 8\beta^2 \mu^2 + \beta^4}{r} \pm (8\mu^3 + 4\beta^2 \mu) \right], \quad (VL.52b)$$

$$\text{and } {}^4 Z_{\pm k}^L = \pm 2\alpha \int_{\mu_k}^{\mu_{k+1}} d\mu P_L(\mu) \left[\frac{32\mu^6 + 48\beta^2 \mu^4 + 18\beta^4 \mu^2 + \beta^6}{r} \pm (32\mu^5 + 32\beta^2 \mu^3 + 6\beta^4 \mu) \right], \quad (VL.52c)$$

where $r = (\mu^2 + \beta^2)^{1/2}$.

Further, $P_L(\mu)$ may be expressed as a finite series

$$P_L(\mu) = \sum_{m=l, -2}^0 \frac{C_{mL}}{d_L} \mu^m. \quad (VL.53)$$

Equations (VL.52) then become:

$${}^0 Z_{\pm k}^L = \pm 2\alpha \sum_{m=l, -2}^0 \frac{C_{mL}}{d_L} (2\Delta H_{m+2} + \beta^2 \Delta H_m \pm 2\Delta F_{m+1}), \quad (VL.54a)$$

$${}^2 Z_{\pm k}^L = \pm 2\alpha \sum_{m=l, -2}^0 \frac{C_{mL}}{d_L} [8\Delta H_{m+4} + 8\beta^2 \Delta H_{m+2} + \beta^4 \Delta H_m \pm (8\Delta F_{m+3} + 4\beta^2 \Delta F_{m+1})], \quad (VL.54b)$$

$$\Delta H_n = \frac{1}{2} \sum_{m=0}^n \left\{ \frac{C}{r} [32M_{m+3}^2 + 32M_{m+2}^2 + 64M_{m+1}^2 + 32M_{m+2}^2 + 32M_{m+1}^2] \right\} \quad (VI.54c)$$

$$\text{where } \Delta H_n = \int_{\mu_k}^{\mu_{k+1}} \frac{\mu^n}{r} d\mu \quad , \quad (VI.55a)$$

$$\text{and } \Delta F_n = F_n(\mu_{k+1}) - F_n(\mu_k) = \frac{\mu_{k+1}^{n+1}}{n+1} - \frac{\mu_k^{n+1}}{n+1} \quad . \quad (VI.55b)$$

The integration of (VI.55a) proceeds as follows: The function $G_n = \mu^n r d\mu$ is integrated in two ways: First by making use of the functional form of r :

$$\Delta G_n = \int \frac{\mu^n}{r} (\mu^2 + \beta^2) d\mu = \Delta H_{n+2} + \beta^2 \Delta H_n \quad , \quad (VI.56a)$$

and secondly by integrating by parts:

$$\begin{aligned} \Delta G_n &= \Delta(\mu^{n+1} r) - \int (\mu^n r + \frac{\mu^{n+2}}{r}) d\mu \quad , \\ &= \Delta(\mu^{n+1} r) - n(\Delta H_{n+2} + \beta^2 \Delta H_n) - \Delta H_{n+2} \quad . \end{aligned} \quad (VI.56b)$$

Equating the two forms of the integral brings us to an iterative expression for ΔH_{n+2} :

$$\Delta H_{n+2} = \frac{n+1}{n+2} [\Delta(F_n r) - \beta^2 \Delta H_n] \quad . \quad (VI.57)$$

The two base integrals, ΔH_0 and ΔH_1 are, from standard tables,

$$\Delta H_0 = \ln \frac{\mu_{k+1} + r_{k+1}}{\mu_k + r_k} \quad , \quad (VI.58a)$$

$$\text{and } \Delta H_1 = r_{k+1} - r_k \quad . \quad (VI.58b)$$

In the special case of elastic scattering ($\beta^2 = 0$), it is clear from inspecting Eq. (VI.55) that

$$\Delta H_n = \Delta F_{n-1} \quad .$$

We can then proceed by the use of Eqs. (VL57) and (VL58) to calculate ΔH_n for any order n . However, when $\beta^2 > 0$, errors grow, and these equations are unstable. In this case, one resorts to backward recurrence, details of which are given in Ref. 5.

It is important, especially when calculating iteratively on a finite bit machine, to factor out difference quantities wherever possible.

A case in point is the factor $\Delta u_k = u_{k+1} - u_k$, which is woven into the expressions for Δu_n , ΔF_n , and $\Delta(F_n r)$. It may be factored directly out of the Δu_n , $\Delta(F_n r)$ and the odd-subscripted ΔH_n :

$$\Delta F_n = \frac{\Delta u}{(n+1)} (u_{k+1}^n + u_{k+1}^{n-1} u_k + \dots + u_{k+1}^{n-1} u_k^{n-1} + u_k^n), \quad (\text{VL59a})$$

$$\Delta H_1 = \Delta u_k \frac{u_{k+1} + u_k}{r_{k+1} + r_k}, \text{ etc.}, \quad (\text{VL59b})$$

$$\Delta(F_n r) = \frac{(\gamma_{k+1}^{n+2} + u_k^{n+2}) \Delta F_{n+2} + \beta^2 (u_{k+1}^{n+1} + u_k^{n+1}) \Delta F_{n+1}}{(r_{k+1}^{n+2} + r_{k+1}^{n+2} r_k + r_k^{n+2} r_k)} \quad (\text{VL59c})$$

The even ordered ΔH_n are not so easily factored; however, ΔH_0 may be calculated by referring to its expression using center of mass cosines:

$$\Delta H_0 = \ell n \frac{u_{k+1} + r_{k+1}}{u_k + r_k} = \pm \frac{1}{2} \ell n \frac{\gamma + \eta_{k+1}}{\gamma + \eta_k}, \quad (\text{VL60})$$

where the sign is plus if η_k and η_{k+1} are both greater than or less than $\eta_1(\mu_{\min})$. Where

$$\Delta \eta \ll (\gamma + \bar{\eta}),$$

the first few terms of the logarithmic expansion may be used.

The Outer Integral. The outer integral is given by Eq. (VL3). The evaluations of the outer integrals are done simultaneously for all ℓ . These integrals are subdivided; the intervals being the same for all ℓ . The bounds are determined at these various energies:

1. all the breakpoints for any ℓ in the flux $[\Phi^\ell(E)]$ data;
2. the breakpoints in the cross-section $[\sigma(E_i)]$ data;
3. the breakpoints in the angular distribution $[g(E_i, \eta)]$ data;
4. the singular points at $E_{1\alpha}$ and $E_{1\gamma}$;

3. the crossings of $E'_{\text{max}}(E)$ and $E'_{\text{min}}(E)$ with E'_{ij} and $E'_{i+1,j}$; and
4. in the case of elastic scattering of identical particles, the energy, corresponding to the angle in the angular distribution beyond which the scattering probability remains zero, becomes also a sub-boundary.

These integrals are evaluated numerically, by a modified Gaussian technique, described in Appendix (VL8). This numerical integration is done iteratively, each cycle requiring two additional evaluation points, until the integral evaluation differences for all i fall below an acceptable amount. As the iteration process begins, if it appears that any of the functions (E) being integrated are highly peaked in E at one boundary or the other, the peaked end is broken off and treated as another subinterval.

The final operation in computing the transfer matrix elements is to divide the outer integral by the group flux, Eq. (VL29).

Transfer Probability from Tabular Energy Distribution (I=4) Data*

Basic Data. The tabular energy distribution data ($I = 4$) consist of a series of incident energies E_i , at each of which is given a set of emission energies E'_{ij} and their corresponding probabilities $\pi_{ij}^l(E_i \rightarrow E'_{ij})$. These points are assumed to be linearly interpolable in emission energy. Interpolation in incident energy, however, is not straightforward. There is a set of these data for each l th Legendre coefficient of the expansion of the correlated energy-angle distribution data. The integrals to be evaluated are again given by Eqs. (VL3) and (VL4), the analysis being done in the TABXFR subroutine.

Unit Base Transformation. Simple linear interpolation in incident energy to obtain a distribution at an intermediate energy, E , would, in general, lead to an intermediate distribution that would have finite probabilities of transfer to energies above E , which in turn would lead to transfer probabilities that do not conserve energy. A scheme that avoids this would be to use linear interpolation in incident energy, E , of the end points, and to connect the break points of the line segment distributions based on their relative proportion of the energy span of the distribution, with a resulting distribution constructed by linearly connecting (in E) the interpolated (in E') probabilities. This process, however, does not result in the integral of the distribution at an intermediate energy being linearly interpolable, as would be desirable. If linear interpolation is used to connect two right trapezoids on parallel planes, the intermediate areas so constructed are not linear in the

* $I = 3$ data are transformed to $I = 4$ data for processing by CLYDE.

separation variable - - unless the two bases are equal. Therefore, a transformation to equal (unit) basis is used in TANKF8, so that linearly interpolable areas result from linear interpolation of the transfer probabilities in the transformed coordinate system.^{6,7}

The transformation is indicated by a tilde and is specified by:

$$\tilde{E} = \frac{E - E'_{\min}(E)}{E'_{\max}(E) - E'_{\min}(E)} \quad (VL61)$$

Conservation of probability under the transformation leads to:

$$\pi^L(E \rightarrow \tilde{E}) = \pi^L(E \rightarrow E') (E'_{\max}(E) - E'_{\min}(E)) \quad (VL62)$$

The data are available in the form

$$E_i, E'_{ij\min}, \pi^L(E_i \rightarrow E'_{ij\min}), \dots, E'_{ij},$$

$$\pi^L(E_i \rightarrow E'_{ij}), \dots, E'_{ij\max}, \pi^L(E_i, E'_{i\max})$$

At E_i Eqs. (VL61) and (VL62) are

$$\tilde{E}_{ij} = \frac{E'_{ij} - E'_{ij\min}}{E'_{ij\max} - E'_{ij\min}}, \quad (VL63)$$

and

$$\pi^L(E_i \rightarrow \tilde{E}_{ij}) = \pi^L(E_i \rightarrow E'_{ij}) (E'_{ij\max} - E'_{ij\min}), \quad (VL64)$$

respectively. At all other energies (E) the distributions in $\tilde{E}$ are determined by the following procedure:

1. The two E_i table entries which span the desired incident energy E are determined (E_i, E_{i+1}), and their corresponding E', π^L tables are transformed according to Eqs. (VL63) and (VL64).
2. The break points and their corresponding π^L 's on each of the transformed distributions are listed.
3. The two lists of break points are merged into an $\tilde{E}_k$ list.

4. Missing π^L values of the merged list for each distribution are found by linear interpolation in $\tilde{E}$:

$$\pi^L(E_i, \tilde{E}_k) = \pi^L(E_i, \tilde{E}_j) + \frac{\pi^L(E_{i+1}, \tilde{E}_{j+1}) - \pi^L(E_i, \tilde{E}_j)}{\tilde{E}_{j+1} - \tilde{E}_j} (\tilde{E}_k - \tilde{E}_j) . \quad (\text{VL65})$$

5. The form for the distribution is established at a general energy (E) by a linear interpolation in energy between the foregoing quantities:

$$\pi^L(E, \tilde{E}_k) = \pi^L(E_i, \tilde{E}_k) + \frac{\pi^L(E_{i+1}, \tilde{E}_k) - \pi^L(E_i, \tilde{E}_k)}{E_{i+1} - E_i} (E - E_i) . \quad (\text{VL66})$$

6. At $\tilde{E}$'s between the $\tilde{E}_k$'s, this distribution is linearly interpolable:

$$\pi^L(E, \tilde{E}) = \pi^L(E, \tilde{E}_k) + \frac{\pi^L(E, \tilde{E}_{k+1}) - \pi^L(E, \tilde{E}_k)}{\tilde{E}_{k+1} - \tilde{E}_k} (\tilde{E} - \tilde{E}_k) ; \quad (\text{VL67})$$

this is the general form needed for the inner integral, Eq. (VI.4). An example of the unit base transformation is shown in Fig. 2.

The Inner Integral. The inner integral, Eq. (VI.4), is restated after transforming to unit base coordinates:

$$Z_h^L(E) = \int_{\tilde{E}_h}^{\tilde{E}_{h+1}} d\tilde{E} \pi^L(E, \tilde{E}) [(1 - W) + WE'] . \quad (\text{VL68})$$

Equation (VL68) is first subdivided into intervals in $\tilde{E}$, each bounded either by an $\tilde{E}_k$, or $\tilde{E}_h$ or $\tilde{E}_{h+1}$:

$$Z_h^L(E) = \sum_{m=m_{\min}}^{m_{\max}-1} \int_{\tilde{E}_m}^{\tilde{E}_{m+1}} d\tilde{E} \pi^L(E, \tilde{E}) [(1 - W) + WE'] . \quad (\text{VL69})$$

The indices ($m_{\min}$) and ($m_{\max}$) are such that:

$$1. \quad \tilde{E}_{m_{\min}} = \tilde{E}_h \text{ and}$$

$$2. \quad \tilde{E}_{m_{\max}} = \tilde{E}_{h+1} ;$$

the other indices (m) are the indices (k) wherein

$$\tilde{E}_{m \min} < \tilde{E}_k < \tilde{E}_{m \max}.$$

E' may be expressed as a function of $\tilde{E}$ by inverting Eq. (VL.61)

$$E' = A_1(E) + A_2(E) \tilde{E}, \quad (\text{VL.70})$$

where

$$A_1(E) = E'_{\min}(E) \quad (\text{VL.71a})$$

and

$$A_2(E) = E'_{\max}(E) - E'_{\min}(E). \quad (\text{VL.71b})$$

Similarly from Eq. (VL.67), the transformed probability may be expressed as:

$$\pi^k(E \rightarrow \tilde{E}) = A_3(E) + A_4(E) \tilde{E}, \quad (\text{VL.72})$$

where

$$A_4(E) = \frac{\pi^k(E \rightarrow \tilde{E}_{k+1}) - \pi^k(E \rightarrow \tilde{E}_k)}{\tilde{E}_{k+1} - \tilde{E}_k} \quad (\text{VL.73a})$$

and

$$A_3(E) = \pi^k(E \rightarrow \tilde{E}_k) - A_4(E) \tilde{E}_k. \quad (\text{VL.73b})$$

The components of Eq. (VL.69) are integrated analytically:

$$\begin{aligned} Z_{h \min}^k(E) &= \int_{\tilde{E}_m}^{\tilde{E}_{m+1}} d\tilde{E} [A_5(E) + A_6(E) \tilde{E} + A_7(E) \tilde{E}^2] \\ &= D_m(E) [A_5(E) + A_6(E) \overline{\tilde{E}_m}(E) + A_7(E) \overline{\tilde{E}_m^2}(E)], \end{aligned} \quad (\text{VL.74})$$

where

$$A_5(E) = [(1 - W) + W A_1(E)] A_3(E), \quad (\text{VL.75a})$$

$$A_6(E) = [(1 - W) + W A_1(E)] A_4(E) + W A_2(E) A_3(E), \quad (\text{VL.75b})$$

$$A_1(E) = w A_2(E) A_3(E) \quad (\text{VL75c})$$

$$U_m(E) = \bar{E}_{m+1} - \bar{E}_m, \quad (\text{VL75d})$$

$$\bar{E}_m(E) = .5 (\bar{E}_{m+1} + \bar{E}_m), \quad (\text{VL75e})$$

and

$$\bar{E}^2(E) = \frac{1}{3} [(\bar{E}_{m+1})^2 + \bar{E}_{m+1}\bar{E}_m + (\bar{E}_m)^2]. \quad (\text{VL75f})$$

Equation (VL75) expresses analytically the inner integration over the m^{th} interval in $\bar{E}$. All the component factors, Eqs. (VL75), must be stated explicitly as functions of E , in anticipation of the outer integration operation. $E'_{\min}(E)$ and $E'_{\max}(E)$ are evaluated by linearly interpolating between their respective

$$E'_{\min}(E_i) \text{ and } E'_{\min}(E_{i+1}):$$

$$E'_{\min}(E) = b_3 + b_4 E \quad (\text{VL76a})$$

and

$$E'_{\max}(E) = b_1 + b_2 E; \quad (\text{VL76b})$$

where

$$b_2 = \frac{E'_{\max}(E_{i+1}) - E'_{\max}(E_i)}{E_{i+1} - E_i}, \quad (\text{VL77a})$$

$$b_1 = E'_{\max}(E_i) - b_2 E_i, \quad (\text{VL77b})$$

$$b_4 = \frac{E'_{\min}(E_{i+1}) - E'_{\min}(E_i)}{E_{i+1} - E_i}, \quad (\text{VL77c})$$

and

$$b_j = E_{\min}^j(E_j) - b_j E_j .$$

(VL.77d)

There are four distinct cases, according to the nature of the upper and lower limits of integration ($\tilde{E}_{m+1}$ and $\tilde{E}_m$, respectively):

$$\text{Case 0: } \tilde{E}_m > \tilde{E}_h(E) ; \text{ and } \tilde{E}_{m+1} < \tilde{E}_{h+1}(E)$$

$$\text{Case L: } \tilde{E}_m = \tilde{E}_h(E) ; \text{ and } \tilde{E}_{m+1} < \tilde{E}_{h+1}(E)$$

$$\text{Case R: } \tilde{E}_m > \tilde{E}_h(E) ; \text{ and } \tilde{E}_{m+1} = \tilde{E}_{h+1}(E)$$

$$\text{Case RL: } \tilde{E}_m = \tilde{E}_h(E) ; \text{ and } \tilde{E}_{m+1} = \tilde{E}_{h+1}(E)$$

Equations (VL.75d, e, f) take the following form, depending on the case type:

<u>Case 0</u>	<u>Case $\neq 0$</u>	
$D_m(E) : \tilde{E}_{m+1} - \tilde{E}_m$	$\frac{b_{15} + b_{16} E}{b_8 + b_9 E}$	(VL.78a)

$\tilde{E}_m(E) : .5 (\tilde{E}_{m+1} + \tilde{E}_m)$	$\frac{b_{10} + b_{11} E}{b_8 + b_9 E}$	(VL.78b)
---	---	----------

$\tilde{E}_m^2(E) : \frac{1}{3} [(\tilde{E}_{m+1})^2 + E_{m+1} \tilde{E}_m + (\tilde{E}_m)^2]$	$\frac{b_{12} + b_{13} E + b_{14} E^2}{(b_8 + b_9 E)^2}$	(VL.78c)
--	--	----------

b_8 through b_{16} may be evaluated numerically for the various non-zero cases by using Eq. (VL.61) and all of Eqs. (VL.77):

$$b_8 = b_1 - b_3 \quad \text{(all non-zero cases)} \quad \text{(VL.79a)}$$

$$b_9 = b_2 - b_4 \quad \text{(VL.79b)}$$

TABLE VI.1. Constants for the various cases.

Constants	Values
-----------	--------

Case L

$$b_{10} : \frac{1}{2}(\tilde{E}_{m+1} b_8 + E'_h - b_3)$$

$$b_{11} : \frac{1}{2}(\tilde{E}_{m+1} b_9 - b_4)$$

$$b_{12} : \frac{1}{3}[\tilde{E}_{m+1}^2 b_8^2 + \tilde{E}_{m+1} b_8 (E'_h - b_3) + (E'_h - b_3)^2]$$

$$b_{13} : \frac{1}{3}[2\tilde{E}_{m+1}^2 b_8 b_9 + \tilde{E}_{m+1} [(E'_h - b_3) b_9 - b_4 b_8] - 2b_4 (E'_h - b_3)]$$

$$b_{14} : \frac{1}{3}(\tilde{E}_{m+1}^2 b_9^2 - \tilde{E}_{m+1} b_4 b_9 + b_4^2)$$

$$b_{15} : \tilde{E}_{m+1} b_8 - (E'_h - b_3)$$

$$b_{16} : \tilde{E}_{m+1} b_9 + b_4$$

Case R

$$b_{10} : \frac{1}{2}(E'_{h+1} - b_3 + \tilde{E}_m b_8)$$

$$b_{11} : \frac{1}{2}(-b_4 + \tilde{E}_m b_9)$$

$$b_{12} : \frac{1}{3}[(E'_{h+1} - b_3)^2 + \tilde{E}_m b_8 (E'_{h+1} - b_3) + \tilde{E}_m^2 b_8^2]$$

TABLE VI.1. Continued.

Constants	Values
$b_{13}:$	$\frac{1}{3} [- 2(E'_{h+1} - b_3) b_4 + \bar{E}_m [(E'_{h+1} - b_3) b_9 - b_4 b_8] + 2\bar{E}_m^2 b_8 b_9]$
$b_{14}:$	$\frac{1}{3} (b_4^2 - \bar{E}_m b_4 b_9 + \bar{E}_m^2 b_9^2)$
$b_{15}:$	$(E'_{h+1} - b_3) - \bar{E}_m b_8$
$b_{16}:$	$- b_4 - \bar{E}_m b_9$
<u>Case RL:</u>	
$b_{10}:$	$\frac{1}{2} (E'_h + E'_{h+1} - 2b_3)$
$b_{11}:$	$- b_4$
$b_{12}:$	$\frac{1}{3} [(E'_{h+1} - b_3)^2 + (E'_{h+1} - b_3)(E'_h - b_3) + (E'_h - b_3)^2]$
$b_{13}:$	$\frac{1}{3} [- 2(E'_{h+1} - b_3) b_4 - b_4 (E'_{h+1} + E'_h - 2b_3) - 2(E'_h - b_3) b_4]$
$b_{14}:$	b_4^2
$b_{15}:$	$(E'_{h+1} - E'_h)$
$b_{16}:$	0

The functions A_3 and A_4 depend on the functions $\pi^L(E + \tilde{E}_m)$, which in turn are interpolations of the unit - transformed tabular entries $\pi^L(E_i + \tilde{E}_m)$. Specifically:

$$\pi^L(E + \tilde{E}_m) = p + qE, \text{ and} \quad (\text{VL.80a})$$

$$\pi^L(E + \tilde{E}_{m+1}) = r + sE, \text{ where} \quad (\text{VL.80b})$$

$$q = \frac{\pi^L(E_{i+1} + \tilde{E}_m) - \pi^L(E_i + \tilde{E}_m)}{E_{i+1} - E_i}, \quad (\text{VL.81a})$$

$$p = \pi^L(E_i + \tilde{E}_m) - qE_i, \quad (\text{VL.81b})$$

$$s = \frac{\pi^L(E_{i+1} + \tilde{E}_{m+1}) - \pi^L(E_i + \tilde{E}_{m+1})}{E_{i+1} - E_i}, \text{ and} \quad (\text{VL.81c})$$

$$r = \pi^L(E_i + \tilde{E}_{m+1}) - sE_i. \quad (\text{VL.81d})$$

Equations (VL.80a, b and VL.81a, b) lead to

$$A_4(E) = b_{19} + b_{20}E, \text{ and} \quad (\text{VL.82a})$$

$$A_3(E) = b_{21} + b_{22}E, \text{ where} \quad (\text{VL.82b})$$

$$b_{19} = \frac{r - p}{\tilde{E}_{m+1} - \tilde{E}_m}, \quad (\text{VL.82c})$$

$$b_{20} = \frac{s - q}{\tilde{E}_{m+1} - \tilde{E}_m}, \quad (\text{VL.82d})$$

$$b_{21} = p - b_{19} \tilde{E}_m, \text{ and} \quad (\text{VL.82e})$$

$$b_{22} = q - b_{20} \tilde{E}_m. \quad (\text{VL.82f})$$

The components of the inner integral, Eq. (VL.74) are then equal to

$$\mathcal{L}_{g+h}^L(E) = \frac{(c_1 + c_2 E + c_3 E^2 + c_4 E^3 + c_5 E^4)_m}{(b_8 + b_9 E)_m^2} \quad (\text{VL.83})$$

where the constants (c_i) are defined in Appendix VI-C.

The Outer Integral. For the outer integral, Eq. (VL.3), we define

$$\alpha(E) = 1 + uE, \quad (\text{VL.84a})$$

$$\phi^L(E) = v + wE, \quad (\text{VL.84b})$$

$$m(E) = g + hE. \quad (\text{VL.84c})$$

The outer integral, over a given inner subintegral m , using Eqs. (VL.3), (VL.83), and (VL.84) becomes

$$J_{g+h}^L(m) = \int dE \frac{(1+uE)(v+wE)(g+hE)(c_1 + c_2 E + c_3 E^2 + c_4 E^3 + c_5 E^4)_m}{(b_8 + b_9 E)_m^2} \quad (\text{VL.85})$$

A word about the outer integration limits: As with the inner integral, it must be subdivided at breakpoints determined by the data entry locations of $\alpha(E)$, $\phi^L(E)$, or $m(E)$, and $\pi^L(E+E')$. In addition, there are breakpoints in the outer integral where the case type of the inner integral changes. That is, whenever $\tilde{E}_h$ crosses $E_{m\min}$ or whenever $\tilde{E}_{h+1}$ crosses $E_{m\max}$. The outer integral is thus a double sum of subintegrals in E and $\tilde{E}$:

$$J_{g+h}^L = \sum_{n_{\min}}^{n_{\max}-1} \sum_{m_{\min}}^{m_{\max}-1} J_{g+h}^{(m,n)}, \quad (\text{VL.86})$$

where each $J_{g+h}^{(m,n)}$ has the form Eq. (VL.85)

$$J_{g+h}^{(m,n)} = \int_{E_n}^{E_{n+1}} dE \sum_{i=1}^{i_{\max}} \frac{d_i E^{i-1}}{(b_8 + b_9 E)^2}. \quad (\text{VL.87})$$

The constants (d_i) are defined in Appendix VI-C. $i_{\max}$ is six if the selection parameter (W) and the case type are both zero. It is seven if only one criterion is zero, and it is eight if both are non-zero.

In the event that (b_g) is zero (as happens with case type zero, or when the ranges of the $x^i(E_i - E_{i-1})$ distributions spanning the n^{th} subinterval in E are equal, Eq. (VL87) takes its simplest form:

$$J(m,n)_{g \rightarrow h} = \frac{1}{D} \sum_{i=1}^{i_{\max}} \frac{d_i (E_{n+1}^i - E_n^i)}{1} \quad (\text{VL88})$$

(D) is one for case 0, and (b_g^2) for case $\neq 0$. Otherwise, the general solution of Eq. (VL87) is

$$J(m,n)_{g \rightarrow h} = \frac{1}{2} \ln \left(\frac{B + E_{n+1}}{B + E_n} \right) + f_1 \frac{E_{n+1} - E_n}{(B + E_{n+1})(B + E_n)} + \sum_{i=3}^{i_{\max}} f_i (E_{n+1}^{i-2} - E_n^{i-2}) \quad (\text{VL89})$$

B is the ratio b_g/b_0 , and the f_i are defined in Appendix VI-C.

It is important to note that in order to minimize computing roundoff error in a finite bit machine, close attention must be paid to factoring out difference terms where possible. ($E_{n+1} - E_n$) is an obvious example. Using this philosophy, TABXFR requires only single precision to obtain results with negligible error.

Energy Production and Deposition

For each target isotope under consideration, CLYDE obtains various rate coefficients which pertain to energy conservation. Specifically, these items are total available energy, energy production, and the energy in the outgoing particle field. These data allow a user to calculate, within his transport code, the energy production as well as the local energy deposition which is specific to the choice of particles being transported.²

When CLYDE is used to calculate multigroup constants for identical incident and outgoing particles, e.g., $y_0 = y_1$, it computes an average energy of the incident particle y_1 entering into the reaction

$$\langle E\sigma \rangle_g = \sum_r \frac{\int_g E \sigma_r(E) \varphi^0(E) dE}{\int_g \varphi^0(E) dE} \quad (\text{VI.90})$$

where subscript r pertains to reaction. Under these same conditions an average energy production term is also calculated,

$$\langle Q \rangle_g = \sum_r C_r \frac{\int \sigma_r(E) \phi^0(E) dE}{\int \phi^0(E) dE} = \sum_r \sigma_r \phi_{r,g} \quad (VI.91)$$

From these last two relations, the total available energy is obtained

$$\langle E \rangle_{\text{tot avail}_g} = \langle E \rangle_g + \langle Q \rangle_g \quad (VI.92)$$

For all CLYDE calculations (independent of whether or not $v_0 = v_i$), the code computes the total average energy in the outgoing particle field for the specified v_0 .

$$\langle E \rangle_g = \sum_r \frac{\int \bar{E}_r(E) \sigma_r(E) \phi^0(E) dE}{\int \phi^0(E) dE} \quad (VI.93)$$

In Eq. (VI.93), $\bar{E}_r(E)$ is the total average energy to the y_0 particle field induced by reaction r . This term is precalculated by ENDEP (see Chapter III) and stored in the evaluated library for each reaction and outgoing particle as I=10 type data.

With the above rate coefficients, the local energy deposition may be programmed, at transport code time, to be the total available energy less the sum only of the total average energy in the outgoing particle field of those particles to be specifically transported.²

Isotope Production

CLYDE lists, with each reaction, a set of data pairs, which list all secondary particles, including residual nuclei, and their multiplicities. There are two exceptions: neutrons resulting from fission reactions are listed with "zero" multiplicity, and gamma ray secondaries are not listed at all. The multiplicities in these two situations depend on the initial particle energies, and are consequently made implicit in the respective transfer matrices for these particles.

D. INPUT, OPERATION, AND OUTPUT

The format of the ASCII input file for CLYDE is described in Table VI.2.

TABLE VII. CLYDE Input File Specifications.

Columns	Format	Remarks
<u>Record Type 1</u>		
<u>Record 1-1</u>		
1-6	i6	NNZA (1000 * Z + A of the material to be processed) - if left blank then record type 1-2 must follow immediately.
7	i1	<p>NSUP - Normally 0 - If more than one target material is present in the library with the same ZA but different states (e.g., ground state and .271 MeV), then the range of levels may be specified by record type 1.3. Similarly, with more than one temperature available, a range of temperatures may be specified by record type 1.4.</p> <p>NSUP = 0 - Process all levels and temperatures in the library for this (these) material(s).</p> <p>= 1 - A range of levels is specified.</p> <p>= 2 - A range of temperatures is specified.</p> <p>= 3 - Ranges of both levels and temperatures are specified.</p>
8-9	i2	<p>IYI - Incident particle designator. Particle types are:</p> <p>1 = neutron</p> <p>2 = proton</p> <p>3 = deuteron</p> <p>4 = triton</p> <p>5 = ³He</p> <p>6 = ⁴He</p> <p>7 = gamma</p>
11-12	i2	IYO - Outgoing particle designator. In addition to particle identifiers described above, the library recognizes 11 through 16 as residuals (IYO+10). If IYO+10 data are found, they are processed with the IYO data.
14-15	i2	<p>NGPI - Incident particle group structure designator - If NGPI = 0, group bounds must be supplied by using record type 2. If NGPI > 0, a standard group structure from the BDFLS file (see Appendix VIII.B) will be used. Consult with the Physical Data Group regarding available standard group structures. If NGPI = - 1, the group structure used in processing the previous record type 1 will be used.</p>

TABLE VI.2. Continued.

Columns	Format	Remarks
17-18	i2	NFLX - Specification of weighting flux denominator. If NFLX = 0, flux spectra must be specified by using record type 3. If NFLX > 0, standard weighting fluxes from the BDFLS file (see Appendix VII-B) will be used. For these weighting spectra consult with the Physical Data Group. If NFLX = -1, the weighting flux used for the previous problem will be used. If no weighting flux of order L is specified, the highest order that is specified will be used for order L.
21	i1	IECFLG - Controls the energy/particle conservation method to be used by CLYDE. = 0 - particle conservation = 1 - energy production conservation = 2 - energy conservation = 3 - group splitting. Regardless of input, if the outgoing particle is a neutron, IECFLG is set to 0. It should also be 0 for gamma in - gamma out, otherwise 1 for gamma out. It should be 3 for outgoing charged particles.
29-30	i2	NPNTOP - controls the amount of hsp output and is normally 0. If NPNTOP = 2, energy deposits and transfer matrix contributions will be output to hsp as they are calculated for each reaction. Values of NPNTOP less than 0, or greater than 2, are used only for debug purposes, and result in much output.
33	i1	NOUTOP - If NOUTOP = 0, only hsp output will result. If NOUTOP = 1, output will go in an appropriate format to the output file specified on the execute line.
36	i1	NOUT - If NOUT = 0, NPNTOP is set to 2, and all reactions defined for a material in the library will be processed, but no total transfer matrix or fission matrix will be output. If NOUT = 1, the appropriate reactions will be processed for a transport/diffusion code. Fission is output as a fission matrix separate from the transfer matrix, but is also added into the total transfer matrix.
38-45	E8.1	EPIA - Specifies the relative order of accuracy desired in doing numerical integrations. EPIA = .0001 produces good results without using excessive machine time.
47-48	i2	LLMAX - specifies the maximum order of transfer matrices, L, to be calculated. The code calculates (LLMAX + 1) matrices and uses the <u>LLMAX + 1st</u> matrix to form a transport correction. If <u>LLMAX = -1</u> , then the code calculates only group cross-sections and energy deposits.

TABLE VI.2. Continued.

Columns	Format	Remarks
51	i1	<p>NSPFLG - specifies how the fission reaction is to be processed.</p> <p>= 0 - Process prompt neutron data only</p> <p>= 1 - Process prompt and delayed neutron data, summing the results into one matrix</p> <p>= 2 - Process prompt and delayed neutron into two separate matrices.</p>
68	i1	<p>NSPFLG - If NSPFLG = 0, output group bounds are the same as input group bounds. If NSPFLG = 3, output group bounds are not the same as input group bounds, see record 1-5 for specification of output group bounds. If NSPFLG = 6, Use output group bounds from previous problem.</p>
69	i1	<p>NTCFLG specifies the transport correction to be used. If $0 < \text{NTCFLG} < 3$, the transport correction term is included in the total transfer matrix. If $4 < \text{NTCFLG} < 7$, all transport correction terms up through order $\text{LLMAX}+1$ are included in a separate array. This latter form is the required input for NDPL (see Chapter VII). If NTCFLG = 0 or 4, the code decides. If NTCFLG = 1 or 5, an approximate correction will be used. If NTCFLG = 2 or 6, the exact correction will be used. If NTCFLG = 3 or 7, no correction will be used.</p>
71	i1	<p>IVFLG multiplies $\sigma_x(E)$ by velocity $V(E)$, so that CLYDE produces $(\sigma_x v)_g$ rather than σ_{xg}.</p>
72	i1	<p>NLAST is the last problem flag. If NLAST = 0, another problem is to follow. If NLAST = 1, no more problems follow.</p>
76-80	i5	<p>IWALT is a selective output sentinel. It allows suppression of output to the output ASCII file but not to the hsp file. Since IWALT may be changed internally during the calculation, this sentinel should not be used without consulting the Physical Data Group. Each type of output has associated with it an ID. To get all output leave IWALT blank, but to get selected output calculate IWALT as follows:</p>

ID	Output Item	$2^{\text{ID}-1}$
1	Group bounds	1
2	Speed	2
3	Group flux	4
4	Group cross section	8
5	Energy available	16
6	Energy production	32

TABLE VII. Continued.

Columns	Format	Remarks
	7	Energy to Y0 46
	8	Isotope production 128
	9	Transport correction 216
	10	Total cross section 512
	11	Transfer matrix 1024
	12	number sigma fission 2048
	13	Fission matrix 4096
The sum of the $(2^{10-1})_k$ is entered as IWALT.		
Record 1-2	Range of materials (Needed only if NNZA of record 1 is blank)	
1-6	i6	NNZAB beginning material = 1000 * Z + A for the first material
7-10	i6	NNZAE ending material = 1000 * Z + A for the last material
Record 1-3	Needed only if NSUP = 1 or 3	
1-12	E12.5	ELVB least energy of a level in a target material.
13-24	E12.5	ELVE greatest energy of a level in a target material.
Record 1-4	Needed only if NSUP = 2 or 3	
1-12	E12.5	TEMPB least material temperature.
13-24	E12.5	TEMPE greatest material temperature.
Record 1-5	Needed only if NSPFLG = 3	
1-3	i3	NGPO - Outgoing particle group structure designator. If NGPO = 0, the user supplies the group structure using record type 2. If NGPO > 0, a standard group structure from the BDFLS file (see Appendix VII-B) will be used. Consult with the Physical Data Group for information about standard group structures.
Record Type 2		
Record 2-1	Needed only if NGPI or NGPO is 0	
1-4	i4	NEBI or NEBO - number of energy boundaries to be read from record 2-2. Number of bounds = number of groups + 1.

TABLE VII. Continued.

Columns	Format	Remarks
<u>Record 2-2</u>		
1-12	6E12.5	EBOUND or EBOUND0 - Energy boundaries in increasing energy. If the first energy is 0, it will be set to 1.0E-10
.		
.		
.		
61-72		
Record type 2 for input bounds must precede record type 2 for output bounds if both are being supplied.		
<u>Record Type 3</u>		
Needed only if NFLX = 0		
<u>Record 3-1</u>		
1-4	i4	LFLUX is the highest order, L, for which fluxes are supplied.
<u>Record 3-2</u>		
LFLUX + 1 records are required; one for each L		
1-4	i4	NFLUX(L) number of entries to be read from record 3-3 for L=0 (i.e., 2 times number of E, ϕ pairs)
.		
.		
.		NFLUX for all orders of L must precede records 3-3.
<u>Record 3-3</u>		
E, ϕ pairs - start new record for each L order		
1-12	6E12.5	EFLUX - Energy flux pairs in increasing energy. Energies must span the group bounds used for the problem. If the problem is to be run to a higher Legendre expansion order than that for which fluxes are provided, the highest order fluxes available are used for all higher orders.
.		
.		
.		
Records 3-3 are supplied as sets for each L-order.		

The calling sequence for CLYDE is the following:

```

      omega clyde (input file) (box no.) (hsp option)
      (library name) 0 (output file name) (output file size) / T V
  
```

The parentheses denote problem dependent quantities and do not appear in the calling sequence. The various quantities in parentheses have the following significance.

input file	the file required by CLYDE for input (see Table VI.2).
box no.	user's box number
hsp option	CLYDE produces output that is descriptive and/or diagnostic for the problem. The descriptive information is dependent on the type of output called for and is contained in the family of files HSHMM000, HSHMM001, . . . , HSHMM00X. The diagnostic information contains the input calling sequence and the run description, and is in the file PRT/HMM. The numbers HMM are the three right hand numbers of the machine generated time (24 hour scale) e.g., if the time the problem was generated was 0431 or 1431, then HMM = 431. This output may be directed to the PR80 (use "fr80" for option), the high speed printer (use "hsp" for option), or kept for inspection (use "debug" for option) and/or output to RJET or other medium using ALLOUT.
library name	the evaluated nuclear data file, e.g., ENDL file.
0	The zero in this position indicates that the library exists as a file. The zero must be included in the calling sequence.
output file name	the name of the CLYDE ASCII file to be created as output.
output file size	If equal or less than 99, it is the size of the file to be created in units of 100000. If greater than 99, it is the actual file size to be created. When the code finishes it will shrink the file to the size needed.

E. CLYDE OUTPUT FORMAT AND INSTRUCTIONS

The format of the ASCII output file for CLYDE is described in Table VI.3.

TABLE VI.3. CLYDE Output (Code Usable ASCII File).

Data Type	Record Type	Remarks
<u>A</u>		Two records identify the CLYDE run
	1	Date of CLYDE run and library identification Format (2X, I6, 30X, "ID Word^--^", I12)
	2	Date of last change to library Format (12X, "Date of last change to Lib used^--^", 4X, I6)

TABLE VI.1. Continued.

Data Type	Record Type	Remarks
Subsequent Data types relate to material data. For each material there are one or two records to identify the material and the processing parameters.		
<u>B</u>		Material ZA, maximum order of Legendre expansion, fission sentinel, type calculation done, number of output groups, number of input groups, transport correction type, number of reactions, number of particles produced, input group structure ID No., flux spectrum ID No., conservation sentinel, and output group structure ID No. Format (I6, 15I3, 20X, "nn")
<u>C</u>		Conditional - If the transport correction flag is more than 3, then output incident and outgoing particle identifiers, material excitation level, material temperature, atomic mass, and date of last change. Format (2I2, 3E11.4, 1X, I6)
<u>D</u>		Conditional - If the incident and outgoing particles are the same, then output a list of the reaction identifiers for all reactions processed. Format (24I3)
<u>E</u>		May be selectively suppressed by user or by code. The following data consist of two or more records, the first of which identifies the type of data following, and has a format of the form (I4, I4, 1X, A8). The second variable is sometimes unused.
<u>E, ID = 1 CP BDS</u>	1	Data type ID, Group structure ID, and data type. Format ("^^^1", I4, 1X, "GP^BDS^^")
	2*	Group boundaries. (NEBI values, 6E12.5)**
<u>E, ID = 2 Speed</u>	1	Data type ID and data type. Format ("^^^2^^^0 speed^^")
	2*	Group speeds. (NEGI values, 6E12.5)***
<u>E, ID = 3 GP FLUX</u>	1	Data type ID, Flux structure ID, and data type. Format ("^^^3", I4, 1X, "GP^Flux^^")
	2*	Group fluxes. (NEGI values, 6E12.5)
<u>E, ID = 4 GP X-Sect</u>	1	Data type ID and data type. Format ("^^^4^^^0^GP^X^sec")

TABLE VI.1. Continued.

Data Type	Record Type	Remarks
	2A Reaction ID and name. Format (I4, 5X, 3A8)	
	2B X, Q, X1, X2, X3, and effective Q. Format (I3, 5E11.4)	
	2C* Reaction cross-sections. (NEGI values, 6E12.5)	
	3 The number of particle types produced. Format (I2)	
	4 (Particle ZA, multiplicity) pairs. Format (15F6)	
<u>E, ID=5 Energy Available</u>	If incident particle is the same as outgoing particle, then output the energy available by group.	
	1 Data type ID and data type. Format ("~~~5~~~0~en~avail")	
	2* Energy available. (NEGI values, 6E12.5)	
<u>E, ID = 6 EN PROD</u>	If incident particle is the same as outgoing particle, then output the energy produced by group.	
	1 Data type ID and data type. Format ("~~~6~~~0~~prod~~~")	
	2* Energy available. (NEGI values, 6E12.5)	
<u>E, ID = 7 EN DEP TO YO</u>	1 Data type ID, outgoing particle type, and data type. Format ("~~~7", I4, IX, "ENDEPTOYO")	
	2* Energy deposited to outgoing particle. (NEGI values, 6E12.5)	
<u>E, ID = 9 Trans Corr</u>	If transport correction flag is more than 3 for each expansion order thru LMAX:	
	1 Data Type ID, Legendre order, and data type. Format ("~~~9", I4, IX, "TR~CORR~")	
	2 The group transport correction (NEGI values, 6E12.5).	
<u>E, ID = 10 Sigt Trans</u>	1 Data type ID and data type. Format ("~~10~~~0~SIGT~TR~")	

TABLE VI.1. Continued.

Data Type	Record Type	Description
	2	Transfer corrected total cross-section. (NEGI values, 6E12.5)
<u>E, ID = 11 Trans Mat</u>	1	Data type ID, Legendre order, and data type. Format ("..11", I4, 1X, "XFER-MAT")
	2*	Total transfer matrix. (NEGI * NEGO values, 6E12.5)***
If number of transfer matrices calculated is less than the number requested, output zeros for the other matrices		
<u>E, ID = 12 Nubar Sigf</u>	1	Data type ID, 0(for prompt), and data type. Format ("..12....0-NUBRSIGF")
	2*	Prompt Nubar Sigma Fission (NEGI values, 6E12.5)
If delayed Nubar was requested:		
	1	Data type ID, 1(for delayed), and data type. Format ("..12....1-NUBRSIGF")
	2*	Delayed Nubar Sigma Fission (NEGI values, 6E12.5)
<u>E, ID = 13 Fiss Mat</u>	1	Data type ID, 0(for prompt), and data type. Format ("..13....0-FISS-MAT")
	2*	Fission transfer matrix (NEGI * NEGO values, 6E12.5)
<u>F</u>		Material End Sentinel Format ("99")
<u>G</u>		Run End Sentinel Format ("999999")

Note: The symbol . in the table signifies a blank.

* As many repetitions of the record as required

** NEBI -- Number of energy bounds = NEGI + 1 III

*** NEGI -- Number of incident groups

**** NEGO -- Number of emission groups

APPENDIX VI-A LINEAR INTEGRATION ROUTINES

UNIINT integrates a piecewise, continuous linear function. The function list is input at all breakpoints of the function and the integration limits in nondecreasing order, and contains the values of the integrand at those points. The operation performed is⁸

$$\int_{x(K_1)}^{x(K_2)} dx F = \sum_{K=K_1}^{K_2-1} \frac{1}{2} [x(K+1) - x(K)] [F(K+1) + F(K)] ,$$

where K_1, K_2 define the limits of integration over the variable x and function F .

DIINT

DIINT integrates the product of two piecewise, continuous linear functions.⁸ The variable of integration is listed at the integration limits and at the breakpoints of both functions; the two function lists contain the values of the functions at these entries of the variable list:

$$\int_{x(K_1)}^{x(K_2)} dx F \cdot G = \frac{1}{6} \sum_{K=K_1}^{K_2-1} [x(K+1) - x(K)] \{ [F(K+1) + F(K)] \cdot [G(K+1) + G(K)] + F(K) \cdot G(K) + F(K+1) G(K+1) \} ,$$

where F, G are the functions and K_1, K_2 the integration limits.

TRIINT

TRIINT integrates the product of three piecewise continuous linear functions,⁸ of the same form as in **DIINT**, above. The equation is

$$\int_{x(K_1)}^{x(K_2)} dx F \cdot G \cdot H = \frac{1}{12} \sum_{K=K_1}^{K_2-1} [x(K+1) - x(K)] \cdot \{ [2F(K) \cdot G(K) \cdot H(K) + F(K+1) \cdot G(K+1) \cdot H(K+1) + [F(K) + F(K+1)] [G(K) + G(K+1)] [H(K) + H(K+1)] \} .$$

APPENDIX VI-B NUMERICAL INTEGRATION

The numerical integration of the outer integral in LEGXFR uses a modified Gaussian integration scheme devised by Giles.⁹ This procedure is more economical than the classic Gauss Scheme, at least in an iterative environment, and is more accurate than Simpson's rule. Strictly speaking, Simpson's rule is only 3rd order accurate, with the magnitude of the 4th order term diminishing as $\sim -\frac{84}{15} (M-1)^{-4}$. [(M) is the number of measurements, or subroutine entries, made in the interval of integration, as it is subranged.] Gauss integration, on the other hand, is accurate to order $2M-1$ of an expansion in Legendre polynomials. The Modified Gauss scheme is accurate to order M of a power series expansion.

When iterating, however, the Gaussian integration, so as to advance to the next higher order, requires a complete new set of arguments. A figure of merit, the ratio of order of accuracy, to the cumulative number of arguments required to arrive at that accuracy is:

$$S \approx \frac{2(2I+1)}{(I+1)^2 + 1}$$

where I is the iteration number. It is clear that as more iterations are required the "cost effectiveness" goes down. The Modified Gauss system uses only two new arguments with each iteration, so that its figure of merit is always one independent of (I).

In the modified Gauss system, the function being integrated is represented by a power series in the interval (-1,1):

$$F = \sum_{m=0}^{\infty} a_m r^m ; \quad (\text{VI-B.1})$$

$$\text{its integral is } J = \int_{-1}^1 F dr = 2 \sum_{m=0}^{\infty} \frac{a_{2m}}{2m+1} . \quad (\text{VI-B.2})$$

Consider a pair of measurements at arguments ($\pm r_i$); their sum is

$$F_i = F(r_i) + F(-r_i) = 2 \sum_{m=0}^{\infty} a_{2m} r_i^{2m}$$

The i^{th} estimate of the integral J is a linear combination of the set of P_i , where $0 \leq i \leq k$

$$J_i = \sum_{j=0}^I \alpha_{i,j} P_j = 2 \sum_{j=0}^I \alpha_{i,j} \sum_{m=0}^I a_{2m} r_i^{2m} \quad (\text{VI-B.3})$$

(J_i) will approximate the integral (J) to order of accuracy $(2I+1)$, if

$$J = J_i$$

$$2 \sum_{m=0}^I \frac{a_{2m}}{2m+1} = 2 \sum_{m=0}^I a_{2m} \sum_{i=0}^I \alpha_{i,j} r_i^{2m} ;$$

leading to a set of $(I+1)$ equations of the form

$$\frac{1}{2m+1} = \sum_{i=0}^I \alpha_{i,j} r_i^{2m} \quad 0 \leq m \leq I \quad (\text{VI-B.4})$$

The first two argument sets, used in the Modified Gauss scheme are legislated to be $r_0^2 = 0$ and $r_1^2 = 1$, so as to be able to test early in the iterative process for an empty interval or for a highly peaked function. Subsequent values of r_i^2 are chosen from the interval $(0,1)$. Starting then, with $i = 2$, the Eqs. (VI-B.4) are solved by machine, using trial r_i 's, for the corresponding set of $\alpha_{i,j}$'s. That r_i is chosen for which its value of

$$\sum_{i=0}^I (\alpha_{i,j})^2$$

is minimized. This criterion is used so as to reduce round-off error in computing Eq. (VI-B.3) as much as possible. As each (r_i) is chosen, a choice is again made for an (r_{i+1}) and the process is repeated. In this way a set of (R_i) and their attendant coefficients $(\alpha_{i,j})$ are precalculated, and stored as program constants in LEGXFR.

When LEGXFR attempts an integration iteratively, two new functions are calculated at arguments r_i and $-r_i$ by subroutine entry. These new functions, along with the previously determined set at $\pm r_{i-1}$ are linearly combined, using the coefficients $\alpha_{i,j}$, to give a new estimate of the integral J_i . When J_i is satisfactorily close to J_{i-1} , the integration is said to have converged, and the process is terminated. The convergence criterion is an input parameter.

APPENDIX VI-C

To recapitulate, the inner integral is expressed by Eq. (VL74):

$$Z_{n_m}^L = D_m(E) [A_5(E) + A_6(E) \bar{E}_m(E) + A_7(E) \bar{E}_m^2(E)] , \quad (\text{VL74})$$

where

$$A_5(E) = [(1 - W) + WA_1(E)] A_3(E) , \quad (\text{VL75a})$$

$$A_6(E) = [(1 - W) + WA_1(E)] A_4(E) + WA_2(E) A_3(E) , \quad (\text{VL75b})$$

$$\text{and } A_7(E) = WA_2(E) A_4(E) . \quad (\text{VL75c})$$

Furthermore $A_1(E) = b_3 + b_4 E$, from Eqs. (VL71a) and (VL76a), $A_2(E) = b_8 + b_9 E$, from Eqs. (VL71b), (VL76a), and (VL76b); also,

$$A_3(E) = b_{21} + b_{22} E , \quad (\text{VL82b})$$

$$\text{and } A_4(E) = b_{19} + b_{20} E , \quad (\text{VL82a})$$

and finally,

<u>Case 0</u>	<u>Case $\neq 0$</u>	
$D_m(E) = b_{15}$	$\frac{b_{15} + b_{16} E}{A_2(E)}$	(VL78a)

$\bar{E}_m(E) = b_{10}$	$\frac{b_{10} + b_{11} E}{A_2(E)}$	(VL78b)
-------------------------	------------------------------------	---------

$\bar{E}_m^2(E) = b_{12}$	$\frac{b_{12} + b_{13} E + b_{14} E^2}{A_2^2(E)}$	(VL78c)
---------------------------	---	---------

Distinguishing between case 0 and case $\neq 0$, we express Eq. (VL74) in terms of the numerical constants b and powers of E :

Case 0

$$\begin{aligned} Z_{hm}^2 = & b_{15} \{ [(1-W+Wb_3)+Wb_4E] (b_{21}+b_{22}E) + [(1-W+Wb_3)+Wb_4E] (b_{19}+b_{20}E) b_{10} \\ & + Wb_8(b_{21}+b_{22}E) b_{10} + Wb_8(b_{19}+b_{20}E) b_{12} \} \end{aligned} \quad (VI-C.1)$$

Case #0

$$\begin{aligned} J_{hm}^2 = & \frac{b_{15} + b_{16}E}{(b_8 + b_9E)^2} \{ [(1-W + Wb_3) + Wb_4E] (b_{21} + b_{22}E) (b_8 + b_9E) \\ & + [(1-W+Wb_3) + (Wb_4E) (b_{19}+b_{20}E) (b_{10}+b_{11}E) + W(b_8+b_9E) (b_{21}+b_{22}E)(b_{10}+b_{11}E) \\ & + W(b_{19}+b_{20}E) (b_{12}+b_{13}E + b_{14}E^2) \} \end{aligned} \quad (VI-C.2)$$

The evolution of the succeeding constants into the constants c_1 through c_5 follows the programming in the subroutine EINTG. For Case 0:

$$CI_2 = b_{15}(b_{21} + b_{19}b_{10}) \quad (VI-C.3a)$$

$$CI_3 = b_{15}(b_{22} + b_{20}b_{10}) \quad (VI-C.3b)$$

$$\text{and } CI_1 = CI_4 = CI_5 = CI_6 = 0. \quad (VI-C.3c)$$

In the event the selection parameter W is zero, the constants CC are all zero. Otherwise,

$$CC_2 = b_8(b_{21}b_{10} + b_{19}b_{12}) \quad (VI-C.4a)$$

$$CC_3 = b_8(b_{22}b_{10} + b_{20}b_{12}). \quad (VI-C.4b)$$

For Case #0:

$$C_7 = b_8b_{21} + b_{10}b_{19} \quad (VI-C.5a)$$

$$C_8 = b_9b_{21} + b_{10}b_{20} + b_8b_{22} + b_{11}b_{19} \quad (VI-C.5b)$$

$$C_9 = b_9b_{22} + b_{11}b_{20} \quad (VI-C.5c)$$

$$CI_2 = b_{15}C_7 \quad (VI-C.8a)$$

$$CI_3 = b_{16}C_7 + b_{15}C_8 \quad (VI-C.8b)$$

$$CI_4 = b_{16}C_8 + b_{15}C_9 \quad (VI-C.8c)$$

$$CI_5 = b_{16}C_9 \quad (VI-C.8d)$$

Again, if the selection parameter (W) is zero, all constants (CC) are zero. Otherwise

$$C_{10} = b_8b_{22} + b_9b_{21} \quad (VI-C.7a)$$

$$C_{11} = b_{12}b_{20} + b_{13}b_{19} \quad (VI-C.7b)$$

$$C_{12} = b_{14}b_{19} + b_{13}b_{20} \quad (VI-C.7c)$$

$$CC_2 = b_8b_{10}b_{21} + b_{12}b_{19} \quad (VI-C.7d)$$

$$CC_3 = b_{10}b_{11}C_{10} + b_{11}b_8b_{21} + C_{11} \quad (VI-C.7e)$$

$$CC_4 = b_{11}C_{10} + b_{10}b_9b_{22} + C_{12} \quad (VI-C.7f)$$

Finally, for all cases, if the selection parameter W is zero:

$$c_i = CI_{i+1} \quad (VI-C.8)$$

If it is not, then

$$c_1 = b_3 * CI_2 + b_{15} * CC_2 \quad (VI-C.9a)$$

$$c_2 = b_3 * CI_3 + b_4 * CI_2 + b_{15} * CC_3 + b_{16} * CC_2 \quad (VI-C.9b)$$

$$c_3 = b_3 * CI_4 + b_4 * CI_3 + b_{15} * CC_4 + b_{16} * CC_3 \quad (VI-C.9c)$$

$$c_4 = b_3 * CI_5 + b_4 * CI_4 + b_{15} * CC_5 + b_{16} * CC_4 \quad (VI-C.9d)$$

$$c_5 = b_4 * CI_5 + b_{16} * CC_5 \quad (VI-C.9e)$$

These are constants in Eq. (VI.83).

The subroutine TABHLUP calculates the numerical constants (e_j) involving $t, u, v, w, g,$ and h referred to in Eq. (VI.85):

$$ee_1 = vg \quad (VI-C.10a)$$

$$ee_2 = vh + wg \quad (VI-C.10b)$$

$$ee_3 = wh \quad (VI-C.10c)$$

$$e_4 = u * ee_3 \quad (VI-C.10d)$$

$$e_3 = t * ee_3 + u * ee_2 \quad (VI-C.10e)$$

$$e_2 = t * ee_2 + u * ee_1 \quad (VI-C.10f)$$

$$e_1 = t * ee_1 \quad (VI-C.10g)$$

Subroutine EINTG calculates the (d_j) simply as:

$$d_j = \sum_{i=1}^5 c_i e_{j+1-i} \quad (VI-C.11)$$

where it is taken that any (e) with subscript outside the range (1-4) is zero.

The integration of Eq. (VI.87) in the general case uses the strategy of factoring ($b_8/b_9 + E$) successively from the numerator to create a series of integrals of the form $\int dE f_i E^{i-2}$. Equation (VI.87) is modified:

$$J(m,n)_{g \rightarrow h} = \frac{1}{b_9^2} \int_{E_n}^{E_{n+1}} dE \sum_{i=1}^{i_{\max}} \frac{d_i E^{i-1}}{(B + E)^2}, \text{ where } B = \frac{b_8}{b_9} \quad (VI-C.12)$$

EINTG calculates the f_i in Eq. (VI.89) as follows:

$$D_1 = d_1 - B [d_{i+1} - B (d_{i+2} - \dots - B d_{i_{\max}}) \dots] \quad (VI-C.13)$$

and from this,

$$f_1 = D_1$$

$$\text{and } f_{i \neq 1} = D_1 - B [D_{i+1} - B (D_{i+2} - \dots - B D_{i_{\max}}) \dots]. \quad (VI-C.14)$$

REFERENCES

1. S. T. Perkins, Nucl. Sci. Eng. 31, 156 (1968).
2. S. T. Perkins and R. J. Howerton, Multigroup Transfer Matrices for Charged Particle and Neutron Induced Reactions, Part III, Energy Conservation and Local Deposition, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-89228 (1983), accepted for publication in Nucl. Sci. Eng.
3. G. L. Bell, G. E. Hansen, and H. A. Sandmeier, Nucl. Sci. Eng. 28, 376 (1967).
4. S. T. Perkins, Nucl. Sci. Eng. 80, 130 (1982).
5. S. T. Perkins and P. C. Giles, Nucl. Sci. Eng. 80, 579 (1982).
6. R. J. Doyas and S. T. Perkins, Interpolation Transformations for Two-Dimensional Tabular Data, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-51290 (1982).
7. R. J. Doyas and S. T. Perkins, Nucl. Sci. Eng. 50, 390 (1973).
8. R. E. von Holt and R. J. Howerton, Math. Comp. 17, 84 (1963).
9. P. C. Giles, Lawrence Livermore National Laboratory, Livermore, CA, unpublished (1982).

CHAPTER VII:
NDFL

VII. NDFL

A. INTRODUCTION

In analyzing complex systems, the simultaneous transport of different particle species, i.e., neutrons, light charged particles, and gamma rays must be calculated. In the multigroup sense, these particle fields are coupled through the various particle production matrices. Furthermore, the energy deposition to the thermal ions and electrons and the depletion and accretion of the thermal ion constituents due to nuclear reactions must be taken into account. The same comments apply to the more restrictive fields of reactor neutronics, reactor shielding, and reactor blanket analysis except that charged particle transport is of less importance when dealing with reactor concepts.

The NDFY_i files have been designed to be the nuclear data base for coupled particle multigroup transport analysis. The suffix Y_i refers to the incident particle designator (see Table I-A.1, of Appendix I-A, e.g., NDF2 is the file for which the incident particle is the proton). All information within these files is in binary mode and is generated by the CLYDE code (see Chapter VI.) The function of the NDFL code is multipurpose. It creates the NDFY_i files, updates these files, and produces various edits of the files.

In the next section, the organization of the files and their use by the transport codes at problem generation time will be discussed. This will be followed by a description of the input, operation, and output for the various NDFL functions.

B. FILE DESCRIPTION AND USAGE

Each NDFY_i file contains multigroup data to be used in transport analysis for a specific light particle species. Each target material within a file is designated by its ZA value (1000*Z+A), level excitation energy, and thermal ion temperature. For each material, the following types of data are given: 1. cross sections; 2. types of reaction products for each reaction; 3. rate coefficient for available energy, energy production, and energy to the various outgoing particle fields; 4. particle interaction transfer matrices (higher Legendre moments may be present); and 5. particle production matrices (only $\ell=0$ matrices are present). The layout of the binary NDFY_i file is given in Appendix VII-A.

For codes that do transport calculations, the NDFY_i files are usually read at problem generation or restart times. The transport code reading the file may collapse the data to fewer groups than are given in the NDFY_i file. Standard collapse fluxes, group bounds, and atomic weights are contained in the file, BDFLS, whose layout is given

in Appendix VII-B. BDFLS is also used by various other components of OMEGA, e.g., CLYDE. The collapse procedure is described in Appendix VII-C. Group collapse may also be done by NDFL by using the proper editing option (see Section VII-C.3).

C. INPUT, OPERATION, AND OUTPUT

NDFL has the following three functions: (a) to create an NDFY_i file, (b) to update an NDFY_i file as needed, and (c) to edit an NDFY_i file. The procedures used to:

Create an NDFY_i file.

The input file is a CLYDE output file (in ASCII) with the transport correction indicator, NTCFLG, set for the CLYDE run $4 \leq \text{NTCFLG} \leq 7$ (see Chapter VI). Several runs of NDFL must be made to create the final file, the first for the particle interaction properties followed by one for each of the particles that can be produced by the various interactions. The order in which this is done is: The initial run is for the outgoing particle designator, y_o , equal to the incident particle designator, y_i (see Table I-A.1). All subsequent runs are for the other possible secondary particles (y_o 's), starting with the least value of y_o and going to the greatest.

The calling sequence for NDFL in this case is:

```
omega ndfl (input file) (box no.) (hsp option)
(library name) 0 (output file name) (output file size) / T V
```

The parentheses denote problem dependent quantities and do not appear in the calling sequence. The various quantities in parentheses have the following significance.

input file	the file required by NDFL for input, i.e., the CLYDE output.
box no.	user's box number
hsp option	NDFL produces output that is descriptive and/or diagnostic for the problem. The descriptive information is dependent on the type of output called for and is contained in the family of files HSHMM000, HSHMM001, . . . , HSHMM00X. The diagnostic information contains the input calling sequence and the run description, and is in the file PRT/HMM. The numbers HMM are the three right hand numbers of the machine generated time (24 hour scale) e.g., if the time the problem was generated was 0431 or 1431, then HMM = 431. This output may be directed to the FR80 (use "fr80" for option), the high speed printer (use "hsp" for option), or kept for inspection (use "debug" for option) and/or output to RJET or other medium using ALLOUT.

library name the NDFY_i file that is being updated. If a new library is being made ab initio, the word "none" is entered here. See below.

0 The zero in this position indicates that the library exists as a file. The zero must be included in the calling sequence.

output file name the name of the NDFY_i file to be created as output.

output file size If equal or less than 99, it is the size of the file to be created in units of 100000. If greater than 99, it is the actual file size to be created. When the code finishes it will shrink the file to the size needed.

Update an NDFY_i File.

NDFL will delete or insert data for the NDFY_i files on a per material basis only. This is because a change in a single evaluated cross section may change not only the cross sections in the file but also transfer matrices for the outgoing particles and the various energy rate coefficients. Data for a material must be deleted before new data for the material can be inserted so that updating a file requires multiple runs of NDFL.

The input file required to delete the data for a material is in the following format:

TABLE VII.1. Input file required to delete the data for a material.

Columns	Format	Remarks
(Record 1)	i6	Date
(Record 2)		This card is blank.
(Record 3)		
1-6	i6	Negative of the ZA value for the material to be deleted
(Record 4)		
1-11	E11.4	Level energy (MeV) of the material to be deleted
12-22	E11.4	Material temperature (MeV) of the material to be deleted
NOTE: Repeat records 3 and 4 for all materials to be deleted.		
(Last record)		
1-6	i6	999999 (end of data flag)

The calling sequence to make deletions with NDFL is identical to that used in creating the file (see Section VII-C.1).

To insert replacement data after a deletion, follow the procedure for creating a file (see Section VII-C.1).

EDIT on NDFY₁ FILE

Three edits of an NDFY₁ file can be made using NDPL. One (short edit) is a table of contents for the file and gives one a quick overview of the information that is present. The second (long edit) lists all numerical values in the file. The third is an ASCII file that is similar in form to the CLYDE ASCII output. The latter can be group collapsed by NDPL and can be used as a data file for computer programs that do not collapse data at generation time.

The input file required to produce one of these three files contains the following information:

TABLE VII.2. Input file required to produce edit output.

Columns	Format	Remarks
<u>Record Type 1</u>		
<u>Record 1-1</u>		
3-4	i2	NEDIT - specifies type of edit output desired 1 - reserved for debug use only 2 - short edit 3 - long edit, similar to CLYDE hsp output 4 - ASCII file in the same form as a CLYDE output file
5-10	i6	NNZAB - beginning isotope ZA number
11-16	i6	NNZAE - ending isotope ZA number NOTE: NNZAB and NNZAE are specified only when NEDIT = 3. If NNZAB and NNZAE are both blank, then all isotopes are included in the edit.
NOTE: This is the only input record required for $1 \leq \text{NEDIT} \leq 3$.		
<u>Record Type 2</u>		
<u>Record 2-1</u>		
8-9	i2	IYI - incident particle designator
11-12	i2	IYO - outgoing particle designator (<10)
14-15	i2	NGPI - incident particle group structure designator from the BDFLS file (see Appendix VII.B). If NGPI = 0, then read in incident particle group bounds on Record Type 5.
17-18	i2	NFLX - Multigroup weighting flux designator from the BDFLS file (see Appendix VII.B). If NFLX = 0, then read in multigroup fluxes on Record Type 7.
30	i1	NPNTOP controls the amount of HSP output and is normally 0. If NPNTOP = 6, a large amount of debug output is given.

TABLE VII.2. Continued.

Columns	Format	Remarks
47-48	i2	LLMAX - the maximum order of the transfer matrices. Must not be specified larger than the order of the corresponding data in the NDFY _i file.
68	i1	NSPFLG - outgoing particle group structure flag. 0 - incident and outgoing particle bounds are the same. 3 - outgoing particle group structure designator is given on Record Type 4.
69	i1	NTCFLG specifies the transport correction to be used. If NTCFLG=4, the code decides. If NTCFLG=5, an approximate correction will be used. If NTCFLG=6, the exact correction will be used. If NTCFLG=7, no correction will be used.
72	i1	NLAST - Last problem flag. 0 - more problems follow 1 - this is the last problem.
76-80	i5	IWALT is a selective output sentinel. It allows suppression of output to the output card image file but not to the hsp file. Since IWALT may be changed internally during the calculation, this option should not be used without contacting the Physical Data Group. Each type of output has associated with it an ID. To get all output leave IWALT blank, but to get selected output calculate IWALT as follows:

ID	Output Item	2^{ID-1}
1	Group bounds	1
2	Speed	2
3	Group flux	4
4	Group cross section	8
5	Energy available	16
6	Energy production	32
7	Energy to y_0	64
8	Isotope production	128
9	Transport correction	256
10	Total cross section	512
11	Transfer matrix	1024
12	Nubar sigma fission	2048
13	Fission matrix	4096

The sum of the (2^{ID-1}) 's is entered as IWALT.

TABLE VII.2. Continued.

Columns	Format	Remarks
<u>Record Type 3</u>		
<u>Record 3-1</u>		
1-6	i6	NNZAB - Beginning isotope ZA number
7-12	i6	NNZAE - Ending isotope ZA number
<u>Record Type 4 (only specify if NSPFLG = 3)</u>		
<u>Record 4-1</u>		
2-3	i3	NGPO - outgoing particle group structure designator from the BDPLS file (see Appendix VII.B). If NGPO = 0, then read in final particle group bounds on Record Type 6.
<u>Record Type 5 (only read in if NGPI = 0)</u>		
<u>Record 5-1</u>		
1-4	i4	NEBI - specifies the number of incident particle group bounds to be found on the following records.
<u>Record 5-2</u>		
1-11 etc.	6E12.5	EBOUND - group bounds in order of increasing energy (MeV).
<u>Record 5-3, etc.</u>		
1-11 etc.	6E12.5	continuation; up through all NEBI values.
NOTE: These bounds must be a subset of the corresponding bounds in the NDFY _i file.		
<u>Record Type 6 (only read in if NGPO = 0)</u>		
<u>Record 6-1</u>		
1-4	i4	NEBO - specifies the number of outgoing particle group bounds to be found on the following records.
<u>Record 6-2</u>		
1-11, etc.	6E12.5	EBOUND0 - group bounds in order of increasing energy (MeV).
<u>Record 6-3, etc.</u>		
1-11, etc.	6E12.5	continuation; up through all NEBO values.
NOTE: These bounds must be a subset of the corresponding bounds in the NDFY _i file.		
<u>Record Type 7 (only read in if NFLX = 0)</u>		
<u>Record 7-1</u>		
1-2	i2	LFLUX - the highest Legendre order of weighting flux spectrum to be read (<u>></u> 0 and also consistent with LLMAX).

TABLE VII.2. Continued.

Columns	Format	Remarks
<u>Record 7-2</u>		
1-5	i5	NFLUX - Twice the number of energy-flux pairs for the lowest order l .
<u>Record 7-3</u>		
1-11, etc.	6E12.5	Energy-flux (in that order) pairs, for $l=0$ in order of increasing energy (energy in MeV, flux in MeV ⁻¹).
<u>Record 7-4 etc.</u>		
1-11, etc.	6E12.5	continuation; up through all NFLUX/2 pairs.

Repeat records 7-3 for all higher order values of l through LFLUX.

NOTE: The energies for each l must span the energies of the incident particle group structure. Furthermore, for any required l^{th} mode weighting flux that is >LFLUX, the values given for LFLUX will be used.

The calling sequence for NDFL in the edit mode is:

omega ndfl (input file) (box no.) (hsp option) (library name) 0 / TV

The parentheses denote problem dependent quantities and do not appear in the calling sequence. The various quantities in parentheses have the following significance:

input file	the file required by NDFL for input
box no.	user's box number
hsp option	NDFL produces output that is descriptive and/or diagnostic for the problem. The descriptive information is dependent on the type of output called for and is contained in the family of files HSHMM000, HSHMM001, . . . , HSHMM00X. The diagnostic information contains the input calling sequence and the run description, and is in the file PRT/HMM. The numbers HMM are the three right hand numbers of the machine generated time (24 hour scale) e.g., if the time the problem was generated was 0431 or 1431, then HMM = 431. This output may be directed to the FR80 (use "fr80" for option), the high speed printer (use "hsp" for option), or kept for inspection (use "debug" for option) and/or output to RJET or other medium using ALLOUT.

library name use NDFY_i file that is being used.

0 The zero in this position indicates that the library exists as a file. The zero must be included in the calling sequence.

An example of running NDFL using an input file NDFLIN with an NDFY_i library called NDF1 would be

omega ndf1 ndflin T61 debug ndf1 0 /.9 .999

The type of output edit depends on the value of the input value NEDIT. The short edit (NEDIT=2) contains the following information:

- o ZA numbers of the materials in the library;
- o incident particle, maximum L^{th} order of interaction transfer matrices, and number of incident groups;
- o incident groups bounds, speeds, and group fluxes;
- o types of outgoing particles, number of groups, and type of transfer matrix present in the file, e.g., particle conserving;
- o first word address and data length of each material; and
- o particle types and multiplicities produced from each reaction.

The long edit (NEDIT=3) is similar to the CLYDE hsp output but is larger since it includes data for all outgoing particles. It contains all of the information of the short edit (NEDIT=2) plus the following additional information for each material:

- o reaction group cross sections;
- o available energy, energy production, and energy transfer to each outgoing particle field;
- o group transport correcting cross section up through LMAX+1;
- o group total cross section;
- o interaction transfer matrices up through LMAX;
- o particle production matrices for each outgoing particle field; and
- o fission matrix if the material is fissionable.

The ASCII output (NEDIT=4) is contained in the output file NDFOUT. The format of NDFOUT is identical to that of the CLYDE ASCII output (see Chapter VI). The advantage of doing this form of NDFY_i edit rather than doing a series of CLYDE calculations is that group collapse, both incident and outgoing particle, can be done directly using multigroup data of the input NDFY_i file. Note that standard fluxes that may be used for group collapse are contained in the ASCII file, BDFLS (see Appendix VII-B).

APPENDIX VI-A. PHYSICAL LAYOUT OF A BINARY NDFY₁ FILE

Each NDFY₁ file consists, first, of a global section containing directories and data that apply to all materials, and then sections for individual materials that contain a directory, descriptive data and finally the group cross sections and matrices.

A. GLOBAL SECTION

a. Directory - (DIRTAB) - Starts at word 1 of NDF Library

1. Incident particle designator	(iyil)
2. Length of global section	(ldir)
3. Date library was made	(libdayt)
4. Maximum size of array needed for individual material directory and definition	(mxdef)
5. Maximum size of array needed for material data	(mxdat)
6. Input group structure ID	(idgps)
7. Number of groups	(ngps)
8. FWA of group boundary table	(igpfwa)
9. FWA of group speed table	(ispfwa)
10. Number of collapse weighting fluxes	(newf)
11. Length of collapse weighting flux table	(lenfl)
12. FWA of collapse weighting flux table	(iflflwa)
13. Number of particle designators in library	(npp)
14. Length of particle designator table	(lenpp)
15. FWA of particle designator table	(ippfwa)
16. Number of target materials in library	(matnum)
17. Length of target material designator table	(leniso)
18. FWA of target material designator table	(isofwa)
19. Number of supplemental data blocks	(nsupp)
20. Length of supplemental data block array	(lensup)
21. FWA of supplemental data block array	(isupfwa)

b. Group Boundary Table - (GPTAB) - ngps + 1 values.

(Directory pointers from Aa; 7, 8).

e. Group Speed Table - (SPDTAB) - agps values.

(Directory pointers from Aa; 7,9).

d. Collapse Weighting Flux Table - (PLTAB) - (agps + 1) *acwf values.

Flux designator and weighting flux.

Repeat for all weighting fluxes.

(Directory pointers from Aa; 7, 10, 11, 12).

e. Particle Designator Table - (PPTAB) - 7* npp values.

y No., Z, A, corresponding material ZA No., and E_{level} if applicable. Also, nego, the number of groups in the particle production matrices, and iecflg, which indicates conservation type.

0 = conserves particles

1 = conserves energy production

2 = conserves energy

3 = conserves particles and energy (group splitting)

Repeat for all particles.

(Directory pointers from Aa; 13, 14, 15).

f. Target Material Designator Table - (ISOTAB) - matnum *5 values.

ZA No., E_{level} , kT, FWA and length of individual material directory and descriptor blocks (ISODEF).

Repeat for all materials.

(Directory pointers from Aa; 16, 17, 18).

g. Supplemental Data Blocks - (SUPTAB) - c (length of each data block) values.

Designator and length of data block followed by data.

Repeat for all designators.

(Directory pointers from Aa; 19, 20, 21).

B. INDIVIDUAL MATERIALS - DIRECTORY AND DESCRIPTOR BLOCKS (ISODEF)

a. Directory

Locations within ISODEF array with respect to first location in the array for each material. The Directory, Ba, is 50 locations long. The Reaction Descriptor Block, Bb, starts in location 51.

<u>Index</u>	<u>Description</u>	<u>Index Name</u>	<u>Variable Name</u>
1.	Material ZA (1000*Z+A)	(loemat)	(maza)
2.	Material level excitation energy	(loeel)	(eliv)
3.	Material temperature	(loet)	(tmp)
4.	Length of directory and descriptor blocks	(loedl)	
5.	Length of material data record	(loeil)	
6.	Maximum expansion order for total transfer matrix	(locord)	(lmax)
7.	Date of latest evaluation	(locday)	(libdate)
8.	Atomic weight	(locat)	(atw)
9.	Number of reactions	(loenrs)	(nrs)
10.	Number of outgoing particle production matrices	(loenp)	(np)
11.	Number of supplemental parameters	(loesun)	(nsup)
15.	Length of reaction descriptors	(loecd1)	
16.	Length of transport correction descriptors	(locetd1)	
17.	Length of total transfer matrix descriptors	(locttd1)	
18.	Length of particle production descriptors	(loepd1)	
19.	Length of outgoing particle average energy descriptors	(loeced1)	
20.	Length of supplementary parameter descriptors	(loesud1)	
24.	Length in data record of total transfer matrix	(loctt1)	
25.	Length in data record of nubar fission	(locnul)	
29.	FWA of material data record	(locifw)	
30.	FWA of reaction descriptors	(loecdf)	
31.	FWA of transport correction descriptors	(locetdf)	
32.	FWA in total transfer matrix descriptors	(locttdf)	
33.	FWA of particle production descriptors	(loepdf)	
34.	FWA of outgoing particle average energy descriptors	(loecedf)	
35.	FWA of supplementary parameter descriptors	(loesudf)	
39.	FWA in data record of total cross section	(loctxf)	
40.	FWA in data record of transport correction terms	(locttf)	
41.	FWA in data record of total transfer matrix	(locttf)	

<u>Index</u>	<u>Description</u>	<u>Index Name</u>	<u>Variable Name</u>
42.	FWA in data record of nuclear fission	(locnrf)	
43.	FWA in data record of maximum available energy	(locemxf)	
44.	FWA in data record of energy production	(locexpf)	
45.	FWA of fission matrix	(locfis)	
46.	FWA in data record of supplementary parameters	(locsuf)	

b. Reaction Descriptor Block

$9 * nrs + 2 * nrs$ npp (nrs) values

C, S, Q, X1, X2, X3, Q_{eff} , and FWA of the reaction c/s data. This is followed by the number of pairs, (npp(c)), of (ZA, multiplicity) being produced from this reaction and the corresponding values of these pairs. By definition, a multiplicity of zero designates a value that is group dependent, e.g., v_g for neutrons. Repeat for all reactions.

Data pointers from Ba; 9, 15, 30.

c. Outgoing Particle Average Energy Descriptor Block

$2 * np$ values

Y_o , and FWA of outgoing particle average energy data. Repeat for all values of y_o .

Data pointers from Ba; 10, 19, 34.

d. Transport Correction Descriptor Block

$2 * (lmax + 1)$ values

Value of l and FWA of transport correcting term data. Repeat for all values of l through $lmax + 1$.

Data pointers from Ba; 6, 16, 31.

e. Total Transfer Matrix Descriptor Block

$(5 + 2 * ngps) * (lmax + 1)$ values

Value of l , g_{min} , g_{max} , and FWA and length of $\sigma(g \rightarrow g')$ c/s data. This is followed by a table of $g'_{min}(g)$ and $g'_{max}(g)$ for $g_{min} \leq g \leq g_{max}$. Repeat for all values of l through $lmax$.

Data pointers from Ba; 6, 17, 32.

f. Outgoing Particle Production Descriptor Block

$(6 + 2 * ngps) * np$ values

y_o , $idogs$, g_{min} , g_{max} , and FWA and length of $\sigma(g \rightarrow g')$ c/s data. This is followed by a table of $g'_{min}(g)$ and $g'_{max}(g)$ for $g_{min} \leq g \leq g_{max}$. Repeat for all values of y_o . $idogs$ is in the output group structure ID.

Data pointers from Ba; 10,18,33.

g. Supplemental Parameters Descriptor Block

Data pointers from Ba; 20, 35.

C. INDIVIDUAL MATERIALS DATA BLOCK

a. Total cross section

$ngps$ values

Data pointers from Ba; 39

b. Reaction cross sections

$\sum_{nrs} g_{max}(C)$ values

Data pointers from Bb

c. Transport correcting cross sections

$(lmax + 1) * ngps$ values

Data pointers from Ba; 40, Bd

d. Total transfer matrix ($y_i \rightarrow y_i$)

$(lmax + 1) * \sum_{g_{min}}^{g_{max}} (g'_{max}(g) - g'_{min}(g) + 1)$ values

Data pointers from Ba; 24, 41; Be

e. Outgoing particle production matrix ($y_i \rightarrow y_o$)

$$ng \sum_{E_{min}}^{E_{max}} (E'_{max}(E) - E'_{min}(E) + 1) \text{ values}$$

Data pointers from Bf

f. Supplemental parameters data

$$\sum_{nsup} (\text{size of each data})$$

Data pointers from Ba; 11, 46; Bg

g. Sigma*nubar fission data

ngps values

Data pointers from Ba; 25, 42

h. Maximum available energy data

ngps values

Data pointers from Ba; 43

i. Energy production data

ngps values

Data pointers from Ba; 44

j. Outgoing particle average energy data

ngps*np values

Data pointers from Bc

k. Fission matrix

ngps**2 values

Data pointers from Ba; 45

APPENDIX VII-B. PHYSICAL LAYOUT OF THE BDFLS ASCII FILE

The file, BDFLS, contains sets of group bounds, weighting fluxes, and atomic weights. These data are used throughout OMEGA, e.g., CLYDE (see Chapter VI) to produce multigroup constants, and by programs other than OMEGA, e.g., to collapse the cross sections at generation time.

BDFLS contains group boundaries corresponding to each incident particle (y_i). For each incident particle, there is one master set, i.e., the set with which the corresponding NDFY_i file was generated. There are also several additional group structures for the same incident particle. Each of the additional sets is a subset of the master set and is used for group collapse. The weighting fluxes are given as pointwise data, linear-linear interpolable in energy. These fluxes are used both for group collapse and to generate the multigroup data with CLYDE.

The format of the BDFLS file is as follows:

TABLE VII-B.1. BDFLS file format.

Columns	Format	Remarks
GROUP BOUNDS CARDS - Record Type 1		
<u>Record 1-1</u>		
1-4	i4	Group bounds ID number.
5-44	5A8	Alphanumeric information.
<u>Record 1-2</u>		
1-4	i4	Number of group bounds.
<u>Record 1-3</u>		
1-11,etc.	6E12.5	Group bounds in order of increasing energy (MeV).
<u>Record 1-4</u>		
1-11,etc.	6E12.5	continuation of record 1-3; up through all group bounds.
NOTE: Continue through all sets of group bounds in the file. Follow the last set with a card which is blank except for a 1 in column 73.		
GROUP FLUX CARDS - Record Type 2		
<u>Record 2-1</u>		
1-4	i4	Group flux ID number.
5-44	5A8	Alphanumeric information.

TABLE VII-B.1. BDFL file format.

Columns	Format	Remarks
<u>Record 2-2</u>		
1-4	i4	LMAX, the highest ℓ order for the Legendre moments of the weighting flux. LMAX+1 subsets of weighting fluxes are given (LMAX>0).
<u>Record 2-3</u>		
1-4	i4	Number of entries, i.e., twice the number of energy-flux pairs for $\ell=0$.
<u>Record 2-4</u>		
1-4	i4	Repeat record 2-3 for all ℓ 's up through LMAX.
<u>Record 2-5</u>		
1-11,etc.	6E12.5	Energy flux (in that order) pairs, for $\ell=0$ in order of increasing energy (energy in MeV, flux in MeV^{-1}).
<u>Record 2-6</u>		
1-11,etc.	6E12.5	Continuation of record 2-5 up through all entries for $\ell=0$.
<u>Record 2-7</u>		
1-11,etc.	6E12.5	Repeat records 2-5 and 2-6 for all ℓ 's up through LMAX.
NOTE: Continue through all sets of group weighting fluxes in the file. Follow the last set with a card which is blank except for a 1 in column 73.		
ATOMIC WEIGHT CARDS - Record Type 3		
<u>Record 3-1</u>		
5-10	i6	ZA number, i.e., 1000Z + A.
11-22	E12.5	Atomic weight (amu).
NOTE: Continue through all ZA-atomic weight pairs in the file. Follow the last set with a card which is blank except for a 1 in column 73.		
FILE END CARD		
5-10	i6	999999.

APPENDIX VII-C. GROUP COLLAPSE OF THE NDFY₁ FILES

Consider an NDFY₁ file for a given incident particle whose group structure is designated as j . Within the file are group cross sections, particle interaction transfer matrices, etc., which are based on this group structure. Also in the file are particle production matrices with group structures in general not the same as each other and not the same as the incident particle group structure. Designate one of the outgoing particle group structures as j' . To collapse these group constants to a subset of the original, define the following group structures:

incident particle groups

j (uncollapsed) $1 \leq j \leq J$,

g (collapsed) $1 \leq g \leq G$;

final particle groups

j' (uncollapsed) $1 \leq j' \leq J'$,

g' (collapsed) $1 \leq g' \leq G'$.

Group 1 in any of the group structures is that of highest energy. To determine the limits for the summations, define for a given group g ,

$$j_{\min} = \text{minimum } j \text{ in } g, \quad (\text{VII-C.1})$$

$$j_{\max} = \text{maximum } j \text{ in } g. \quad (\text{VII-C.2})$$

and for a given group g' ,

$$\begin{aligned} j'_{\min} &= \text{minimum } j' \text{ in } g' \text{ for } g' \neq 1 \\ &= 1 \text{ for } g' = 1 \end{aligned} \quad (\text{VII-C.3})$$

$$\begin{aligned} j'_{\max} &= \text{maximum } j' \text{ in } g' \text{ for } g' \neq G' \\ &= J' \text{ for } g' = G'. \end{aligned} \quad (\text{VII-C.4})$$

These latter bounds on j' insure particle conservation. Note further that the group boundaries for the group structure g are a subset of the boundaries for the group structure j . This also applies for the group structures g' and j' . In the NDFY₁ files, transfer matrices are given up through order $l_{\max}$. Transport correcting cross sections are given up through $l_{\max} + 1$. At transport calculation generation time, particle interaction transfer matrices are required up through order L and transport correcting cross sections only for order $L+1$, where $L \leq l_{\max}$.

The group weighting fluxes, ϕ_j^0 , are obtained by integrating the pointwise data over the relevant uncollapsed group, exactly as calculated by CLYDE (see Chapter VII). Since the group speeds in the NDFY₁ file, as calculated by CLYDE, are inverse averaged, this procedure must be repeated at collapse time,

$$v_g = \frac{\sum_j \phi_j^0}{\sum_j \frac{1}{v_j}} \quad (\text{VII-C.5})$$

The group cross sections are collapsed by the relation

$$\sigma_g = \frac{\sum_j \sigma_j \phi_j^0}{\sum_j \phi_j^0} \quad (\text{VII-C.6})$$

With one exception, the energy rate coefficients, i.e., available energy, energy production, and energy to particle field y_0 , are collapsed analogous to the group cross sections, Eq. (VII-C.6). This exception occurs when group splitting is used in CLYDE, i.e., the parameter IECFLG=3 (see Chapter VI), and will be discussed below.

Transfer matrix collapse depends on which IECFLG option was used by CLYDE to generate the data. This will be discussed below.

IECFLG = 0 (conserves particles)

For all l , one has

$$\sigma_{l_{g \rightarrow g'}}^l = \frac{\sum_j \sum_{j'} \sigma_{l_{j \rightarrow j'}}^l \phi_j^l}{\sum_j \phi_j^l} \quad (\text{VII-C.7})$$

IECFLG = 1 (conserves energy production)

In this case,

$$\sigma_{0_{g \rightarrow g'}}^0 = \frac{\sum_j \sum_{j'} \sigma_{0_{j \rightarrow j'}}^0 \phi_j^0 \bar{E}_{j'}}{\bar{E}_{g'} \sum_j \phi_j^0} \quad (\text{VII-C.8})$$

where

$$E_{j'} = (E_{j'+1} + E_j) / 2 \quad (\text{VII-C.9})$$

$$E_{g'} = (E_{g'+1} + E_g) / 2 \quad (\text{VII-C.10})$$

and E_j , $E_{g'}$, etc., are the group boundaries.

IECFLG = 2 (conserves energy)

$$\langle E \rangle_{g \rightarrow g'}^0 = \frac{\sum_j \sum_{j'} \langle E \rangle_{j \rightarrow j'}^0 \phi_j^0}{\sum_j \phi_j^0} \quad (\text{VII-C.11})$$

IECFLG = 3 (conserves particles and energy, i.e., group splitting)

Group splitting is done only for the $l=0$ transfer matrices. For all l , calculate $\sigma_{l, g \rightarrow g'}$ from Eq. (VII-C.7). Since the average energy of the outgoing particles in group j' is equal to $E_{j'}$ [see Eq. (VII-C.9) and Chapter VI], the average energy of the outgoing particles in group g' (for a given group g also) is,

$$\langle E \rangle_{g'}^0 = \frac{\sum_j \phi_j^0 \sum_{j'} \sigma_{0, j \rightarrow j'}^0 E_{j'}}{\sum_{j'} \sigma_{0, g \rightarrow g'}^0 \sum_j \phi_j^0} \quad (\text{VII-C.12})$$

Define $\tilde{\sigma}_{0, g \rightarrow g'}$ as the $l=0$ transfer matrix after group splitting. Then, proceeding exactly as with the method used in CLYDE (see Chapter VI) with the definition of the arithmetic averaged group energy, $E_{g'}$, given by Eq. (VII-C.10) leads to

for $\langle E \rangle_{g'} < E_{g'}$ (splitting to lower energy) :

$$f_{g'} = \frac{\langle E \rangle_{g'} - \bar{E}_{g'+1}}{\bar{E}_{g'} - \bar{E}_{g'+1}}, \quad (\text{VII-C.13})$$

$$\tilde{\sigma}_{0, g \rightarrow g'} = f_{g'} \sigma_{0, g \rightarrow g'}, \quad (\text{VII-C.14})$$

$$\bar{\sigma}_{0_{g \rightarrow g'+1}} = (1 - f_{g'}) \sigma_{0_{g \rightarrow g'}} \quad (\text{VII-C.15})$$

For $E_{g'} \leq \langle E \rangle_{g'}$ (splitting to higher energy):

$$f_{g'} = \frac{\bar{E}_{g'-1} - \langle E \rangle_{g'}}{\bar{E}_{g'-1} - \bar{E}_{g'}} \quad (\text{VII-C.16})$$

$$\bar{\sigma}_{0_{g \rightarrow g'}} = f_{g'} \sigma_{0_{g \rightarrow g'}} \quad (\text{VII-C.17})$$

$$\bar{\sigma}_{0_{g \rightarrow g'-1}} = (1 - f_{g'}) \sigma_{0_{g \rightarrow g'}} \quad (\text{VII-C.18})$$

Note that the group split matrix element, $\bar{\sigma}_{0_{g \rightarrow g'}}$, may receive contributions from groups $g'-1$, g' , and $g'+1$. There are two cases in which no splitting is done, i.e.,

$$\bar{\sigma}_{0_{g \rightarrow g'}} = \sigma_{0_{g \rightarrow g'}} \quad (\text{VII-C.19})$$

These occur when

$$g' = G' \quad \text{with } \langle E \rangle_{g'} < E_{g'} \quad (\text{VII-C.20})$$

$$g' = 1 \quad \text{with } E_{g'} < \langle E \rangle_{g'} \quad (\text{VII-C.21})$$

Thus particles cannot be split out of the collapsed group structure. Group splitting to a final group structure, when done directly by CLYDE, does not, in general, result in the same final transfer matrix as when done by the group collapse method. Both particles and energy however, are conserved in both cases. As was noted above, the energy rate coefficient for deposition to particle field y_0 is different under group splitting than when group splitting is not done. For group splitting and including the two special cases described above,

$$\langle E \sigma \rangle_g^{y_0} = \sum_{g'} \bar{E}_{g'} \bar{\sigma}_{0_{g \rightarrow g'}} \quad \text{for } \langle E \rangle_{G'} \geq \bar{E}_{G'} \quad (\text{VII-C.22})$$

$$= \sum_{g'} \bar{E}_{g'} \bar{\sigma}_{0_{g \rightarrow g'}} + [\bar{E}_{G'} \sigma_{0_{g \rightarrow G'}} - \langle E \rangle_{G'} \sigma_{0_{g \rightarrow G'}}] \quad \text{for } \langle E \rangle_{G'} < \bar{E}_{G'} \quad (\text{VII-C.23})$$

with $\bar{E}_g$ given by Eq. (VI-C.18).

Finally, the local energy deposition rate coefficient for any of the MCFLG options is given at transport calculation time by the relation

$$\langle E \rangle_g^{loc} = \langle E \rangle_g^{tot avail} - \sum_{y_0} \langle E \rangle_g^{y_0} \quad (VII-C-24)$$

where the first term on the right hand side of this expression is the available-energy rate coefficient and the second term is the sum of the energy rate coefficients to particle y_0 . The summation over y_0 includes only those particles that will be followed in the transport calculations.

CLYDE can calculate the transport correcting cross section by three different methods (see Section C.2 of Chapter VI). These are designated as "exact," "approximate," or "the code chooses." The same technique will be used for the NDFL edit output option. The files will be made utilizing the approximate form of the transport correcting cross sections, which from Eq. (VI.28) is

$$\sigma_{tr corr_j}^{(l)} = \sum_{j'} \sigma_{l_{j \rightarrow j'}}^{(l)}$$

$$\text{for } 1 \leq l \leq l_{max} + 1. \quad (VII.C-25)$$

Then on edit request, NDFL calculates analogous to CLYDE results, for $l \leq L+1$,

1. exact

$$\sigma_{tr corr_g}^{(l)} = \frac{\sum_{g'} \sigma_{l_{g' \rightarrow g}}^{(l)} \phi_{g'}^{(l)}}{\phi_g^{(l)}}, \quad (VII.C-26)$$

and 2. approximate

$$\sigma_{tr corr_g}^{(l)} = \frac{\sum_j \sigma_{tr corr_j}^{(l)} \phi_j^{(l)}}{\sum_j \phi_j^{(l)}}, \quad (VII.C-27)$$

this latter form using directly the uncollapsed results. It should also be noted that if the uncollapsed transport correcting cross section had been generated by CLYDE in the

"enact" form [see Eq. (VL26)], Eq. (VILC-27) could not be put into the correct form, Eq. (VILC-28), unless the CLYDE weighting spectra and the collapse weighting spectra were the same. This points out the unusefulness of the "enact" approximation for use in the files if group collapse is to be later done. One finally has the option,

3. The code change. Here one defines a transport corrected group cross section as

$$\sigma_g(l) = \sigma_{t_g} - \sigma_{tr\ corr_g}(l) \quad (VILC-28)$$

where σ_{t_g} is the collapsed total group cross section. The transport correcting cross section is first used from Eq. (VILC-26). If Eq. (VILC-28) then becomes negative, Eq.

- (VILC-28) is used for the transport correcting cross section.

For $L+1 > l_{max}$, the "approximate" form will be used. This is the only possible option here since the transfer matrix for $l_{max}+1$ is not in the files.

CHAPTER VIII:
CTART

VIII. CTART

A. INTRODUCTION

CTART is a code that processes data from an **ENDL** library into the for: and format required by the **TRTL** code to make files of either neutron interaction or photon production data required by the **TARTNP** and other **LLNL** codes that use the Monte Carlo package developed for the **TARTNP** code. The calling sequence for running **CTART** is:

**OMEGA CTART (input file) (box no.) (hsp option) (library name)
0 (output file name) (output file size) / T V.**

The parentheses denote problem dependent quantities and do not appear in the calling sequence. The various quantities in parentheses have the following significance:

input file	the file required by CTART for input
box no.	user's box number
hsp option	CTART produces output that is descriptive and/or diagnostic for the problem. This output may be directed to the FR80 (use "fr80" for option), the high speed printer (use "hsp" for option), or kept for inspection (use "debug" for option) and/or output to RJET or other medium using ALLOUT.
library name	the library that is being used for the calculation.
0	The zero in this position indicates that the library exists as a file. The zero must be included in the calling sequence.
output file name	the name of the file to be created as a data file for use by the TRTL code to make a TARTND or TARTPPD data file.
output file size	the size of the output file to be created in units of 100000 words. In the example below, the output file will be created as 2000000 words. When the code is finished it will shrink the file to the size needed.

An example of running **CTART** using an input file **CTIN** with a library called **ND821201** to make a data file **CTOUT** that can be used with the **TARTNP** code is:

omega ctart ctin t64 fr80 nd821201 0 ctout 20 / .9 .999

II. PREPARATION OF INPUT

The input file used by CTART requires either one or two records depending upon whether one or more materials (isotopes or elements) is to be processed. If only one material is to be processed, only one record is required. The format of the records is 18,443 for the first record and 216 for the second record. The field definitions are:

Column	Value	Significance
First Record		
1-6	ZA	ZA value of element or isotope if only one is to be processed.
	0	Flag that indicates a range of ZA values is to be processed. The range will be given on the second record.
7-9	Yi	The numerical equivalent of the incident particle. See Table IA-1 of Appendix IA.
10-12	Yo	The numerical equivalent of the secondary particle type for which this run is being made. See Table IA-1 of Appendix IA.
13-15	6	Number associated with the energy mesh for which mean value cross sections etc. are to be calculated. For the standard TARTNP data file the entry is 6. For other meshes special arrangements must be made. See R.J. Howerton or R.E. Dye.
16-18	1	Signifies that a flat flux is to be used in averaging the quantities for which mean values will be calculated.
Second Record (if needed)		
1-6	ZA1	Least ZA value to be processed.
7-12	ZA2	Greatest ZA value to be processed.

C. METHODS

In general, energy dependent integral quantities such as cross sections, multiplicities, and energy deposits are handled in the libraries with incident-particle energy meshes such that linear interpolation between successive entries will yield values of the energy dependent quantities that are accurate to the knowledge we have of their values. The TARTNP code follows the particles in a continuous energy mode but assumes that the cross sections are histograms within a preselected energy mesh. Currently the code uses 175 energy groups between 10^{-10} and 20 Mev for neutrons. These groups were selected to be more dense in important energy regimes and less dense in less important energy regimes. The importance of an energy regime has been determined, for example, by determining whether important reactions have their thresholds in that range of energies. The histogram values are obtained in CTART by calculating the integral mean value of the quantity in question within the boundaries of each group. Thus, in the usual parlance of group neutronics or photonics theory, the cross sections are flat-weighted group cross sections. For those reactions that threshold within a group, the group cross section is for the entire group so that it has a non-zero value below the threshold. This is clearly an unacceptable situation that is corrected by the TARTNP code by checking for the threshold and rejecting the reaction type if the particle energy is less than the threshold energy.

In the TARTNP code total and local energy deposits are used for each incident particle energy group for each isotope or element. The total energy deposit is the cross section weighted sum of the average secondary particle energies and residual nucleus energy for all particles except the particle being followed in the problem. The local energy deposit is a similar cross section weighted sum but the average gamma-ray energy is excluded. CTART first calculates the sum of the average secondary energies for all particles other than the particle being followed and adds to that the average energy of the residual nucleus, if any, for each reaction to obtain the total energy deposit for the reaction. A similar sum is calculated excluding the average photon energy and this is the local energy deposit for the reaction. These two sums are then cross section weighted and averaged over the energy groups to form the group total and local energy deposits for the isotope or element.

Angular and energy distributions of secondary particles of the type being followed in the TARTNP code are transformed from their differential form, as they are represented in the libraries, to an integral form for the TARTNP code. More explicitly, each angular

or energy distribution is represented by a set of cosines or secondary energies that form equally probable intervals in the appropriate range, i.e., from -1. to +1. for cosines and from 0 to E_{max} for secondary energies. As currently implemented the number of intervals is 32 for angular distributions, 32 for secondary energy distributions other than for fission, and 256 for secondary fission neutrons. The number of intervals required was determined to be optimum by running TARTNP problems with the number of intervals varied to test the results.

D. OUTPUT

The output from the CTART code is a file that can be used by the TRTL code to either create or update a data file that can be used by the TARTNP code. In addition to the file that will be used by the TRTL code, there are two other output files that are created by CTART. One describes the input and output of the problem and the other gives any diagnostics that the code might write. Depending upon the option used for the "hsp option" in the calling sequence of the code, these two files will either be sent for printing or will be kept in the case of using the "debug" option. If the latter is used the first of the two files will be labeled in the form "HSTTT000" and the latter "PRT/TTT". The "TTT" in each file is the hour and minute that the problem was run with the convention that the hour is designated by one digit so that at 10:00 AM the number in the first place is 0 etc. If there is more output than can be contained in a single file the "HSTTT000" file will be closed and a new file "HSTTT001" will be opened. This procedure of creating new files will continue until no more are needed. The amount of output that is generated for the "PRT/TTT" file is relatively small so that only one file is needed.

The layout of the data files produced by CTART is given in Appendix VIII-A.

CHAPTER IX:
TRTI.

IX. TRTL

A. INTRODUCTION

TRTL is a code that either updates or produces an entirely new file of nuclear data in the form required by the TARTNP code and other LLNL codes that use the Monte Carlo package developed for TARTNP. The calling sequence for running TRTL is:

OMEGA TRTL (input file) (box no.) (hsp option) (old file name)
0 (output file name) (output file size) / T V.

The parentheses denote problem dependent quantities and do not appear in the calling sequence. The various quantities in parentheses have the following significance:

input	the file required by TRTL for input. This file will be an output file from the CTART code.
box no.	user's box number
hsp option	TRTL produces output that is descriptive and/or diagnostic for the problem. This output may be directed to the FR80 (use "fr80" for option), the high speed printer (use "hsp" for option), or kept for inspection (use "debug" for option) and/or output to RJET or other medium using ALLOUT.
old file name	the name of the existing data file that is to be updated. If an entirely new file is to be made a file called DT041773 must be used. The latter may be obtained by using XPORT with the command rd .415600:dvt:dt041773.
0	The zero in this position indicates that the library exists as a file. The zero must be included in the calling sequence.
output file name	the name of the file to be created as a data file for use by the TARTNP code.
output file size	the size of the output file to be created in units of 100000 words. In the example below, the output file will be created as 2000000 words. When the code is finished it will shrink the file to the size needed.

An example of running TRTL using an input file CTOUT with a data file called t1821201 to make a data file called t1821202 is:

omega trtl ctout t64 fr80 t1821201 0 t1821202 20 / .9 .999

An example of creating an entirely new data file called t1821202 from the output of a CTART run called CTARTOUT is

omega trtl ctartout t64 fr00 dt041773 0 t1821202 20 / .9 .999

The layout of the data files that are used by the TARTNP and other LLNL codes for neutron and gamma-ray interaction are give in Appendix IX-A.

APPENDIX IX-A

Disk layout of neutron and gamma ray production data files.

First Word Address	Length	Contents
0	1	0
1	1	NM Number of Materials (isotopes or elements) in the file if NM is greater than 100. If the number of materials is $\leq$ 100, NM = 100 (see Note 1).
2	NM	ZA(M) where ZA(m) is $1000 \cdot Z + A$ for material M, e.g., for M=7 the material is ${}^6\text{Li}$ so ZA(7) = 3006, for M=18 the material is elemental Mg so ZA(18) = 12000.
2+NM	NM	FWA(M) The first word address of the data in the file for the material (M).
2+2*NM	NM	L(M) The number of words in the data file for the material (M).
2+3*NM	NM	AW(M) Atomic weight of material (M) in amu.
2+4*NM	JMAX	EGV(J) Energy group limit in speed units (cm/sh) for group limit J.
2+4*NM+JMAX	JMAX	EGM(J) Energy group limits in energy units (MeV) for group limit J.
III=2+4*NM+2*JMAX		
III	INDX	T(1) First* table to be used to find the group index (J) based on neutron speed.
III+INDX	INDX	T(2) Second table to be used to find the group index (J) based on neutron speed.
III+2*INDX	INDX	T(3) Third table to be used to find the group index (J) based on neutron speed.
III+3*INDX	INDX	T(4) Fourth table to be used to find the group index (J) based on neutron speed.
III+4*INDX	INDX	T(5) Fifth table to be used to find the group index (J) based on neutron speed.
II2=FWA(1)-5		Where FWA(1) is the contents of location 2+NM (the first word address of the data for the first material).

First Word Address	Length	Contents
II2	1	LN Library name in ASCII.
II2+1	1	DVT Name of the file that contains the EGV(J), EGM(J), T(I) values stored above. Only used when making a new file.
II2+2	1	JMAX The number of energy group limits
II2+3	1	INDX The number of equally probable secondary energy intervals used for all reactions other than fission in this file (usually 32). For fission the number is 256.
II2+4	1	NEQ The number of equally probable angular distribution intervals used for all anisotropic reactions in this file (usually 32).
FWA(1)	L(1)	Number of words required for the first material.

* The tables T(L), L=1,5 represent five subdivisions of the neutron speed (energy) regime such that multiplying a neutron speed that lies within T(L) by a value characteristic of the table [MU(L)] will give a value that has as its integer part the location within T(L) that contains the index of the energy group in which the neutron belongs.

TABLE IX-A.1. Layout of the disk file for any material.

First word addresses	Contents
IWG(1)	Number of words in control table.
IWG(2)	The date of the last complete or partial evaluation in ASCII (yyymmdd).
IWG(3)	ZA for the material (1000*Z+A).
AWG(4)	Atomic number Z (floating point). Last six octal digits is the FWA (IWW22) for the depletion-accretion tables (see Note 2).

TABLE IX-A.1. Continued.

First word addresses	Contents
AWG(8)	Atomic weight (A) in amu (floating point).
IWG(8)	Number of kinematic methods and merge lists (see Note 3).
IWG(7)	Number of reactions for this material (NR). If fission is present then IWG(7) is the number of reactions plus one (NR+1). This is to include ν_f in the same group structure as the cross sections. For each reaction there will be the cross sections followed by appropriate energy deposit tables. For ν_f, no energy deposit tables follow because they follow the cross section for the fission reaction.
IWG(8)	Number of words after last energy deposit list of the first reaction used to describe energy and/or angular distributions of secondary neutrons for the specific reaction.
•	
•	
•	
IWG(8+N-1)	Number of words after energy deposit tables of the Nth reaction used to describe energy and/or angular distributions of secondary neutrons.
•	
•	
•	
IWG(8+IWG(7)-1)	Number of words after reaction IWG(7) used to describe energy and/or angular distributions of the secondary neutrons.
•	
•	
•	
IWW=8+IWG(7)	
IWG(IWW)	Kinematics method sentinel for the first reaction in the first merge list. This sentinel is used to specify the type of kinematics to be used in the collision routine.
•	
•	
•	
IWG(IWW+IWG(7)-1)	Kinematics method sentinel for the last reaction in the first merge list.
IWG(IWW+IWG(7))	First merge number of first merge list. The reactions with the same merge number are added. This control is mainly used for neutron absorption reactions (see Note 3).
•	
•	
•	

TABLE IX-A.1. Continued.

First word addresses	Contents
IWG(IWW+2*IWG(7)) . . .	Kinematic method sentinel for the first reaction in the second merge list.
IWG(IWW+2*IWG(8*IWG(7)-1))	Last merge number in last merge list.
IWW1=(IWW+2*IWG(8*IWG(7)) IWG(IWW1)	Minimum energy index for the first reaction (group number).
IWG(IWW1+1) . . .	Maximum energy index (group number) for the first reaction.
IWG(IWW1+2*IWG(7)-1)	Maximum energy index for the last reaction.
IWW2=IWW1+2*IWG(7)	
AWG(IWW2)	The reaction Q-value (MeV).
IWG(IWW2+1)	C (reaction type).
IWG(IWW2+2)	I (reaction property).
IWG(IWW2+3) . . .	S (reaction modifier).
IWG(IWW2+4*IWG(7)-1) ****	The reaction modifier (S) for the last reaction. END HEADING AND CONTROL INFORMATION for an isotope.
Note: IWW2 is recalculated after processing each reaction.	
IWG(IWW2+4*IWG(7))	The number of different types of energy deposit sets (controlled by data available in the evaluated library), for the first reaction. For example, one set can be all energy deposited except the energy of the emitted neutrons; or all energy deposited except the energy of the emitted neutrons and gamma rays, and/or others.
IWW3=IWW2+4*IWG(7)+1	
AWG(IWW3) . . .	First cross section for the first reaction.

TABLE IX-A.1. Continued.

First word addresses	Contents
$AWG(IWW3-(IWG(IWW3-1)+1))$ $(IWG(IWW1+1)-IWG(IWW1)+1)-1$	Last energy deposit of the first reaction.
$IWW4-IWW3-(IWG(IWW3-1)+1)*(IWG(IWW1+1)-IWG(IWW1)+1)-1$	
$AWG(IWW4+1)$ or $IWG(IWW4+1)$	First additional descriptor required for the first reaction. $IWG(8+N-1)$ is zero only when the neutron induced reaction is fission or capture for reaction neutronics; fission or absorption for emission neutronics. The fission spectrum data follow the ν_f list. The collision type is found in $IWG(IWW+N-1)$ for the Nth reaction. The meaning of the contents of $AWG(IWW4+1)$ or $IWG(IWW4+1)$ is collision type dependent (see below).

The description of the data required for each collision type follows, these data are used by the subroutine GEN 2.

TABLE IX-A.2. Description of the data required for each collision type.

First word addresses	Contents
<u>Collision Type 1 - Anisotropic Elastic Scattering in the COM System</u>	
$IWG(IWW4+1)$	Number of angular distributions specified for this reaction, i.e., the number of energies at which the angular distributions are specified.
$IWG(IWW4+2)$	Number of cosines used to define equally probable intervals in the integral for an anisotropic distribution (usually 33).
$IWG(IWW4+3)$	Energy group index for the least neutron energy at which an anisotropic distribution is given.
$IWG(IWW4+4)$	Sentinel which describes whether the set of angular distributions are for a standard energy mesh (each element has its angular distribution at the same energy) or a non-standard energy mesh (the angular distributions are only at the energies that are in the evaluated library). Standard = 0, non-standard = 1. All current data are in the non-standard mode.

TABLE IX-A.2. Continued.

First word addresses	Contents
IWW5-IWW4+4	
<u>Non-standard mesh</u>	
AWG(IWW5+1) . . .	First energy at which an angular distribution is specified.
AWG(IWW5+IWG(IWW4+1))	Last energy at which an angular distribution is specified.
IWW6-IWW5+IWG(IWW4+1) AWG(IWW6+1) . . .	First word of the first angular distribution corresponding to the first energy AWG(IWW5+1)
AWG(IWW6+IWG(IWW4+1))* IWG(IWW4+2)	Last word of the angular distribution data corresponding to the last energy AWG(IWW5+IWG(IWW4+1))
<u>Standard mesh</u>	
AWG(IWW5+1)	First word of the first angular distribution corresponding to the first energy of the standard energy mesh.
AWG(IWW5+IWG(IWW4+1))* IWG(IWW4+2)	Last word of the last angular distribution corresponding to the last energy of the standard energy mesh.
<u>Collision Type 2 - Absorption (i.e., no secondary neutrons from the reaction)</u>	
No additional information is needed.	
<u>Collision Type 3 - Level Scattering, Isotropic in the Center of Mass System</u>	
AWG(IWW4+1)	Energy of the excited level.
<u>Collision Type 4 - Level Scattering Anisotropic in the Center of Mass System</u>	
IWG(IWW4+1)	Number of angular distributions for this reaction.
IWG(IWW4+2)	Number of entries in an angular distribution (usually 33).
AWG(IWW4+3)	Energy of the excited level (MeV).

TABLE IX-A.2. Continued.

First word addresses	Contents
IWW5-IWW4+3	
AWG(IWW5+1)	First neutron speed at which an angular distribution is specified.
•	
•	
AWG(IWW5+IWG(IWW4+1))	Last neutron speed at which an angular distribution is specified.
IWW6-IWW5+IWG(IWW4+1)	
AWG(IWW6+1)	First entry of the first angular distribution.
•	
•	
AWG(IWW6+IWG(IWW4+1)* IWG(IWW4+2))	Last entry of the last angular distribution.
<u>Collision Type 5, 7 - Temperature Model Isotropic in the Center of Mass System (Not used)</u>	
IWG(IWW4+1)	Number of temperatures for statistical model.
AWG(IWW4+2)	Laboratory threshold for this reaction (in MeV).
AWG(IWW4+3)	First temperature (in MeV).
•	
•	
AWG(IWW4+2+IWG(IWW4+1))	Last temperature.
AWG(IWW4+3+IWG(IWW4+1))	First incident neutron energy at which the temperature model applies.
•	
•	
AWG(IWW4+2+2*IWG(IWW4+1))	Last incident neutron energy at which the temperature model applies.
<u>Collision Type 6,8 - Combined Anisotropic Wide Level and Tabular Method</u>	
IWG(IWW4+1)	Number of angular distributions for this reaction.
IWG(IWW4+2)	Number of entries in an angular distribution (usually 33).
AWG(IWW4+3)	Energy of the excited level (W) (in MeV).

TABLE IX-A.2. Continued.

First word addresses	Contents
IWW5-IWW4+3	
AWG(IWW5+1) : : :	First neutron speed at which an angular distribution is specified.
AWG(IWW5+IWG(IWW4+1))	Last neutron speed at which an angular distribution is specified.
IWW6-IWW5+IWG(IWW4+1)	
AWG(IWW6+1) : : :	First entry of the first angular distribution.
AWG(IWW6+IWG(IWW4+1))* IWG(IWW4+2)	Last entry of the last angular distribution.
IWW77=IWW6+IWG(IWW4+1)*(IWW4+2)+1	
IWG(IWW77)	Number of neutron energy groups for which the cross section is non-zero.
IWG(IWW77+1)	Energy index of first non-zero group cross section for wide level reaction.
AWG(IWW77+2)	Width of level in MeV(Γ).
AWG(IWW77+3)	$\text{TAN}^{-1} \left(\frac{2}{\Gamma} (- W) \right)$, where W = is the energy of the level in MeV.
AWG(IWW77+4) : : :	$\text{TAN}^{-1} \left(\frac{2}{\Gamma} \left(\frac{AE(IWG(IWW77+1))}{A+1} - W \right) \right)$, where A is the atomic mass in amu and E is the lower bound of the least energy group for which the cross section is non-zero.
AWG(IWW77+IWG(IWW77)+3)	$\text{TAN}^{-1} \left(\frac{2}{\Gamma} \left(\frac{AE(IWG(IWW77+IWG(IWW77)))}{A+1} - W \right) \right)$, where A is the atomic mass in amu, and E is the upper bound of the greatest energy group for which the cross section is non-zero.

TABLE IX-A.2. Continued.

First word addresses	Contents
It is assumed that the spectra and angular distributions are given at the same energies.	
$IWW7 = IWW77 + IWG(IWW77) + 4$	
$IWG(IWW7+1)$	Number of entries in each spectrum table of emitted neutrons (usually 33).
$IWG(IWW7+2)$	Number of spectra tables, i.e., number of incident neutron energies at which a spectrum is given.
$IWG(IWW7+3)$	Number of entries in an anisotropic distribution (usually 33).
$IWG(IWW7+4)$	Blank.
$AWG(IWW7+5)$. . .	Least neutron speed at which a secondary neutron spectrum is given.
$AWG(IWW7+4 + IWG(IWW7+2))$	Greatest neutron speed at which a secondary neutron spectrum is given.
$IWW8 = IWW7 + 4 + IWG(IWW7+2)$	
$AWG(IWW8+1)$. . .	First entry in the first angular distribution table.
$AWG(IWW8 + IWG(IWW7+2) * IWG(IWW7+3))$	Last entry in the last angular distribution table.
$IWW9 = IWW8 + IWG(IWW7+2) * IWG(IWW7+3)$	
$AWG(IWW9+1)$. . .	First neutron speed in the first secondary neutron emission spectrum.
$AWG(IWW9 + IWG(IWW7+1) * IWG(IWW7+2))$	Last neutron speed in the last secondary neutron emission spectrum.

TABLE IX-A.2. Continued.

First word addresses	Contents
<u>Collision Type 9, 10 - Tabular Method, Isotropic in the Laboratory System</u>	
IWG(IWW4+1)	Number of entries in each spectrum table of emitted neutrons (usually 33, except usually 237 for fission spectrum, see Collision Type 19, 20).
IWG(IWW4+2)	Number of spectra tables.
AWG(IWW4+3)	First neutron speed at which a spectrum is given.
.	
.	
.	
AWG(IWW4+2+IWG(IWW4+2))	Last neutron speed at which a spectrum is given.
IWW5=IWW4+2+IWG(IWW4+2)	
AWG(IWW5+1)	First neutron speed in the first spectrum.
.	
.	
.	
AWG(IWW5+IWG(IWW4+1))	
*IWG(IWW4+2))	Last neutron speed in the last spectrum.

Collision Type 11, 12 - Cluster Model, Isotropic in the Center of Mass System
Level constant in center of mass system is the Q of the reaction (see AWG(IWW2)).

Collision Type 13, 14, 15 - Tabular Method,
Energy and Angle Uncorrelated in Laboratory System

It is assumed that the spectra and angular distributions are given at the same energies.

IWG(IWW4+1)	Number of entries in each spectrum table of emitted neutrons (usually 33).
IWG(IWW4+2)	Number of spectra tables, i.e., the number of incident neutron energies at which a spectrum is given.
IWG(IWW4+3)	Number of entries in an anisotropic distribution (usually 33).
IWG(IWW4+4)	Blank.
AWG(IWW4+5)	First neutron speed at which a spectrum is given.
.	
.	
.	

TABLE IX-A.2. Continued.

First word addresses	Contents
AWG(IWW4+4+IWG(IWW4+2))	Last neutron speed at which a spectrum is given.
IWW5=IWW4+4+IWG(IWW4+2)	
AWG(IWW5+1)	First entry in the first angular distribution table.
•	
•	
•	
AWG(IWW5+IWG(IWW4+2) *IWG(IWW4+3))	Last entry in the last angular distribution table.
IWW6=IWW5+IWG(IWW4+2)*IWG(IWW4+3)	
AWG(IWW6+1)	First neutron speed in the first emission spectrum.
•	
•	
•	
AWG(IWW6+IWG(IWW4+1) *IWG(IWW4+2))	Last neutron speed in the last emission spectrum.
<u>Collision Type 16, 17, - Combined Anisotropic Tabular and Level Method</u>	
IWG(IWW4+1)	Number of angular distributions for this reaction.
IWG(IWW4+2)	Number of entries in an angular distribution (usually 33).
AWG(IWW4+3)	Energy of excited level.
IWW5=IWW4+3	
AWG(IWW5+1)	First neutron speed at which an angular distribution is specified.
•	
•	
•	
AWG(IWW5+IWG(IWW4+1))	Last neutron speed at which an angular distribution is specified.
IWW6=IWW5+IWG(IWW4+1)	
AWG(IWW6+1)	First entry of first angular distribution.
•	
•	
•	

TABLE IX-A.2. Continued.

First word addresses	Contents
AWG(IWW6+IWG(IWW4+1) *IWG(IWW4+2))	Last entry of the last angular distribution.
It is assumed that the spectra and angular distributions are given at the same energies.	
IWW7=IWW6+IWG(IWW4+1)*IWG(IWW4+2)	
IWG(IWW7+1)	Number of entries in each spectrum table of emitted neutrons (usually 33).
IWG(IWW7+2)	Number of spectra tables, i.e., the number of incident neutron energies at which the spectrum is given.
IWG(IWW7+3)	Number of entries in an anisotropic distribution (usually 33).
IWG(IWW7+4)	Blank.
AWG(IWW7+5)	First neutron speed at which a spectrum is given.
.	
.	
.	
AWG(IWW7+4+IWG(IWW7+2))	Last neutron speed at which a spectrum is given.
IWW8=IWW7+4+IWG(IWW7+2)	
AWG(IWW8+1)	First entry in the first angular distribution table.
.	
.	
.	
AWG(IWW8+IWG(IWW7+2) *IWG(IWW7+3))	Last entry in the last angular distribution table.
IWW9=IWW8+IWG(IWW7+2)*IWG(IWW7+3)	
AWG(IWW9+1)	First neutron speed in the first emission spectrum.
.	
.	
.	
AWG(IWW9+IWG(IWW7+1) *IWG(IWW7+2))	Last neutron speed in the last emission spectrum.

TABLE IX-A.2. Continued.

First word addresses

Contents

Collision Type 19, 20, 24 - Multiple Fission Spectra Method,

Isotropic in Laboratory System

Both σ_f and ν_f are given as a function of energy; σ_f is treated as any other reaction cross section, ν_f has multiple spectra using models 9, 10, following it (see the description of models 9 and 10).

Collision Type 21, 22, 23 - Fission Spectra Method,

Isotropic in Laboratory System (Not used)

σ_f is treated as any other reaction, ν_f has no energy deposits and only one spectrum (energy independent).

IWG(IWW4+1) Number of entries in fission spectrum.

AWG(IWW4+2) First neutron speed in fission spectrum.

•
•
•

AWG(IWW4+IWG(IWW4+1)) Last neutron speed in the fission spectrum.
Same as 9, 10.

Accretion/Depletion Data for the Material

IAD(IWW22) Number of accretion/depletion lists to follow.

IAD(IWW22+1) Number of reactions considered in the first list.

IAD(IWW22+2) C-value for the first reaction of the first list.

IAD(IWW22+3) Number of products from the first reaction of the first list.

IAD(IWW22+4) First product from the first reaction of the first list.

•
•
•

END OF DATA FOR THE MATERIAL

GAMMA RAY PRODUCTION DISK FILE

The layout of the gamma ray production data is an exact duplicate of the neutron file. The data required for the calculation of the photon production line and spectra follows.

TABLE IX-A.3. Data required for calculation of photo production line and spectra.

First word addresses	Contents
<u>Line Source Isotropic in Laboratory System</u>	
AWG(IWW4+1)	Energy of the line (MeV).
<u>Line Source Anisotropic in Laboratory System</u>	
IWG(IWW4+1)	Number of angular distributions.
IWG(IWW4+2)	Number of entries in an anisotropic distribution (usually 33).
AWG(IWW4+3)	Energy of the line (MeV).
IWW5=IWW4+3	
AWG(IWW5+1)	First neutron speed at which an angular distribution is specified.
.	
.	
.	
AWG(IWW5+IWG(IWW4+1))	Last neutron speed at which an angular distribution is specified.
IWW6=IWW5+IWG(IWW4+1)	
AWG(IWW6+1)	First entry in the first photon angular distribution.
.	
.	
.	
AWG(IWW6+IWG(IWW4+1)	
*IWG(IWW4+2))	Last entry in the last photon angular distribution.
<u>Tabular Spectra Isotropic in Laboratory System</u>	
IWG(IWW4+1)	Number of entries in each spectrum table of emitted photons (usually 33).
IWG(IWW4+2)	The number of neutron speeds at which spectra are given.
AWG(IWW4+3)	First neutron speed at which a spectrum is given.
.	
.	
.	
AWG(IWW4+2+IWG(IWW4+2))	Last neutron speed at which a spectrum is given.
IWW5=IWW4+2+IWG(IWW4+2)	

TABLE IX-A.1. Continued.

First word addresses	Contents
AWG(IWW5+1) . . .	First energy in the first spectrum.
AWG(IWW5+IWG(IWW4+1) *IWG(IWW4+2))	Last energy in the last spectrum.
<u>Tabular Spectra - Anisotropic in Laboratory System</u>	
IWG(IWW4+1)	Number of energies in each spectrum table of emitted photons (usually 33).
IWG(IWW4+2)	Number of spectra tables, i.e., the number of incident neutron energies at which the spectra are given.
IWG(IWW4+3)	Number of entries in an anisotropic angular distribution (usually 33).
IWG(IWW4+4)	Blank.
AWG(IWW4+5) . . .	First neutron speed at which a photon spectrum is given.
AWG(IWW1+4+IWG(IWW4+2))	Last neutron speed at which a photon spectrum is given.
IWW5=IWW4+4+IWG(IWW4+2)	
AWG(IWW5+1) . . .	First entry in the first table of photon angular distributions.
AWG(IWW5+IWG(IWW4+2) *IWG(IWW4+3))	Last entry in the last table of photon angular distributions.
IWW6=IWW5+IWG(IWW4+2)*IWG(IWW4+3)	
AWG(IWW6+1) . . .	First photon energy in the first photon spectrum.
AWG(IWW6+IWG(IWW4+1) *IWG(IWW4+2))	Last photon energy in the last photon spectrum.

Note 1:

The layout of this file was done before the advent of the large memory computers. The value NM was assumed at that time to be 100 and dimensioning was done accordingly in the routines that use these data. The current number of materials is 97 so it is likely that the value of 100 will be surpassed at some time. The routines of the TART code have been modified to be dimensioned according to the value NM when it is greater than 100. Other codes that use this data file have not yet been modified to accept more than 100 materials, and they need not be until NM reaches 101. Since their programmers have more pressing duties, they will not be asked to change their routines until such changes are necessary.

Note 2:

One of the codes that uses this data file has need for depletion/accretion data. They are stored at the end of the data for each material. Since this is a special use that will not interfere with other uses of the file and since the Z value cannot exceed three decimal digits, the address of the depletion/accretion data is stored in the last six octal digits of this word. This is the only case of packing a word in the file.

Note 3:

Frequent reference is made to kinematics methods, merge lists, and collision types. Kinematics methods and collision types are synonymous in the sense that a particular type of collision implies the use of a kinematic method for determining the energy and angular distributions of secondary particles (i.e., neutrons or photons). Merge lists are lists of the reactions for the material that indicates whether or not certain reactions are to be combined depending on the mode in which the code that uses the data is to be run. There are two modes, reaction neutronics and emission neutronics. In the former, each nuclear reaction is dealt with separately so no combination of reactions is done. For emission neutronics, all neutron producing reactions are dealt with individually, but all reactions that do not produce neutrons are combined into a single absorption reaction. In the terminology of the ENDL encoding system, all reactions with $C \leq 31$ are treated individually and all reactions with $32 \leq C \leq 49$ are lumped together. For definitions of the "C" values for the reactions, see UCRL 50400, Vol. 4, Rev. 1, pp. 8 and 9. The lumping together of the absorption reactions is done by the subroutine that prepares the data from this file for use by the code that will be using the data (i.e., the combining of reactions, if any, takes place at generation time for the problem to be run).

In addition to the two merge lists for reaction and emission neutronics, there is a third list that lies between the other two, conceptually. The third merge list treats neutron emitting reactions as with the other two lists but deals with the non-neutron emitting reactions according to whether they emit certain charged particles. Those reactions that produce the designated charged particles are dealt with individually and the remainder of the reactions are lumped together.

This method of handling neutron emitting reactions and non-neutron emitting reactions differently provides some economy in the number of words of computer memory required to describe the data for a material. This economy of memory was of much greater importance a decade ago than it is now because of the much smaller memory capacity of computers that existed at that time. Given the current memory size of the computers on which codes that use this file run, it is likely that if the file were to be designed now, no distinction would be made between neutron producing and non-neutron producing reactions and all problems would be run in the reaction neutronics mode. To revise the codes that use this file, such that they would run only in the reaction neutronics mode, would not be cost-effective.

CHAPTER X:
MCPOINT

X-1 / X-2

X. MCPOINT

A. INTRODUCTION

MCPOINT is a code that processes the data in one of the **ENDL** libraries into the form and format required by the **LANL MCNP** code. The calling sequence for running **MCPOINT** is:

OMEGA MCPOINT (input file) (box n.n.) (hsp option) (library name)
0 (output file name) (output file size) / T V.

The parentheses denote problem dependent quantities and do not appear in the calling sequence. The various quantities in parentheses have the following significance:

input file	the file required by MCPOINT for input
box no.	user's box number
hsp option	MCPOINT produces output that is descriptive and/or diagnostic for the problem. This output may be directed to the FR80 (use "fr80" for option), the high speed printer (use "hsp" for option), or kept for inspection (use "debug" for option) and/or output to RJET or other medium using ALLOUT .
library name	the ENDL library that is being used to produce the file for the MCNP code.
0	The zero in this position indicates that the library exists as a file. The zero must be included in the calling sequence.
output file name	the name of the file to be created as a data file for use by the MCNP code.
output file size	the size of the output file to be created in units of 100000 words. In the example above, the output file will be created as 2000000 words. When the code is finished it will shrink the file to the size needed.

An example of running **MCPOINT** using an input file **MCIN** with a library called **ND821201** to make a data file **MCN POUT** that can be used with the **MCNP** code is:

omega mepoint mein t64 fr80 nd821201 0 menpout 20 / .9 .999

B. CONVERSION OF DATA TO MCNP FORMAT

The specifications of the output format from the MCFOUNT code were provided by Pat Seran of LANL. In general, for cross sections the data are merely read from the ENDL library and changed in format. Since both the MCNP code and the ENDL library represent cross sections as being linearly interpolable, this simple operation is all that is required for cross section information with the added step that MCNP requires an energy mesh that is identical for all reactions and ENDL allows each interaction cross section to be represented with an energy mesh that is independent of all other meshes. For angular distributions, data are stored in ENDL in differential form and MCNP requires cosines for 32 equally probable intervals. For energy distributions MCNP makes provision for several possible laws associated with secondary particles. One of these coincides with the method used in ENDL, namely, all secondary energy distributions in ENDL are given explicitly at a mesh of incident energies such that linear interpolation between successive entries (on a unit base basis) will yield a distribution for an intermediate energy. The conversion that is required is to change from the differential form used by ENDL to 32 equally probable entries of secondary energies used by MCNP.