

**ETOE,
A PROGRAM FOR ENDF/B TO MC^2
DATA CONVERSION**

D. M. Green

T. A. Pitterle

United States Atomic Energy Commission
Contract No. AT(11-1)-865
Project Agreement No. 18

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Approved



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Project Engineer
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ETOE CODE ABSTRACT

1. NAME OF CODE: ETOE--ENDF/B to MC**2 Data Conversion
2. COMPUTER FOR WHICH CODE WAS WRITTEN: Originally, a limited version of ETOE was written for the IBM 7094. It has since been converted to the CDC 3600.
3. NATURE OF PROBLEM SOLVED: ETOE accepts cross section data from a mode 2 ENDF/B tape (Reference 2) and prepares the binary cross section and Legendre polynomial tape for the MC**2 code written by Argonne National Laboratory.
4. METHOD OF SOLUTION: The method of solution is discussed in the ETOE report (Reference 4)
5. RESTRICTIONS OR COMPLEXITY: The restrictions as to storage limitations and options are basically those imposed by the 1966 ENDF/B restrictions and the MC**2 program.
6. TYPICAL RUNNING TIME: The average running time varies from three to six minutes on the CDC 3600 per material processed dependent on resonance scattering calculations and Legendre polynomial calculations.
7. UNUSUAL FEATURES: The ETOE program is made up of six overlays.
8. RELATED PROGRAMS: ETOE prepares input to the MC**2 program (Reference 1) using a mode 2 ENDF/B tape. The DAMMET program (Reference 3) may be used to create the mode 2 binary tape.
9. STATUS: The present version of the program has been checked out using ENDF/B tapes available February 1968.
10. REFERENCES:
 1. Toppel, B. J., Rago, A. L., O'Shea, D. M., "MC², A Code to Calculate Multigroup Cross Section," ANL-7318, June 1967.
 2. Honeck, H. C., "ENDF/B Specifications for an Evaluated Nuclear Data File for Reactor Applications," BNL 50066(T-467), ENDF-102 (May 1966, revised July 1967).

3. Honeck, H. C., Filberbaum, J., "DAMMET, A Program to Delete, Alter Mode, and Merge ENDF/B Tapes," ENDF-110 (1967).
4. Green, D. M., and Pitterle, T. A., "ETOE, A Program for ENDF/B to MC² Data Conversion," APDA-219 (ENDF/B-120) (1968).

11. MACHINE REQUIREMENTS: A 65K word memory is required.
12. PROGRAMMING LANGUAGE: ASA Standard FORTRAN(FORTRAN-IV) eliminating incompatibilities between computers where possible.
13. OPERATING SYSTEM: The CDC 3600 version uses 6.2b scope.
14. OTHER PROGRAMMING INFORMATION: ETOE requires a minimum of seven magnetic tapes; standard input, standard output, ENDF/B, MC**2, two scratch tapes, and an overlay tape.
15. MATERIAL AVAILABLE: FORTRAN deck (approximately 3,500 cards), sample case (approximately 300 cards), and the ETOE report, Reference 4.

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I. INTRODUCTION

ETOE (ENDF/B to E = MC²) is a FORTRAN-IV code for preparing an MC² cross section library tape¹ from an ENDF/B tape.² The code accepts as input a Mode 2 (segmented, binary tape arranged by file, material, reaction type) ENDF/B tape. A Mode 2 ENDF/B tape can be converted from either a Mode 1 or Mode 3 (binary or BCD card images arranged by material, file, reaction) ENDF/B tape by use of the DAMMET³ program. ETOE output is a complete cross section data tape for MC² including the W-table and Legendre polynomial expansions of the elastic scattering cross section.

Certain sections of the ENDF/B data require only alterations of formats and ordering of the data for compatibility with MC². This category includes the resonance parameters (ENDF/B File 2), the smooth cross sections (ENDF/B File 3), and the secondary energy distributions (ENDF/B File 5). Other ENDF/B data can require considerable processing by ETOE for MC² input. ENDF/B formats include an option specifying that the scattering cross section be calculated from resolved and/or unresolved resonance parameters. In this case, File 3 includes only a smooth background scattering cross section. Since MC² requires that the smooth scattering cross section be the total scattering cross section and does not calculate resonance scattering, the ETOE code will calculate the resonance scattering cross section and add the calculated values to the smooth File 3 cross section before writing the MC² tape.

Another area requiring the significant processing by ETOE is the angular dependence of elastic scattering. MC² requires angular expansions given for specific energy points (2041 energies) as a product of the elastic scattering cross section and the Legendre polynomial expansion coefficients in the center of mass system. ENDF/B permits either Legendre expansion coefficients at arbitrary energy points or tabulations of cross section and angle. When tabulations are given, ETOE will fit a Legendre expansion to the given distribution. Necessary normalization of the Legendre expansions, multiplication by the scattering cross section, and ordering of the angular data for MC² are carried out by ETOE.

The ENDF/B data permits more generality in types of cross sections and secondary energy distributions than allowed for MC² data. As a result, not all of the ENDF/B materials can be used with MC². The user of ETOE must examine the ENDF/B data for MC² compatibility before selecting materials for the MC² tape. ETOE does include some checks on ENDF/B to MC² compatibility as discussed in this report.

ETOE is written completely in FORTRAN-IV and has been run on the CDC 3600 with about 50K of memory available for the code and associated storage. For use on a machine with smaller memories, the maximum array sizes for data must be reduced below that allowed in MC². The code uses overlays to reduce required storage. A separate overlay is used for each ENDF/B file along with an additional overlay called FILE6 for Legendre data manipulation.

Chapter II of this report describes each of the routines or subroutines included in ETOE and Chapter III describes the input, output, and use of the program.

II. PROGRAM DESCRIPTION

The ETOE program consists of a main program or control routine, several utility subprograms common to the entire program, and six overlays or subsections. Overlays 1 through 5 are made up of various subprograms and process the data from Files 1 through 5 of the ENDF/B tape. The sixth overlay rearranges the Legendre polynomial expansion data to the required MC² format. These routines are described in detail in the following sections. Each section covers an ENDF/B file.

The data required by MC² for each file is given in Table I.

TABLE I - ENDF/B CROSS SECTION DATA USED
IN PREPARING MC² TAPE

File 1

MT = 451 Heading Information and Table of Reactions
MT = 452, $\nu(E)$ Coefficients or Tabulation

File 2

LRU = 1, LRF = 1 or 2, Resolved Parameters, Type 1
LRU = 2, LRF = 1, Unresolved Parameters, Type 1

File 3

MT = 2, Elastic Scattering
MT = 4, Inelastic Scattering
MT = 16, (n, 2n) Scattering
MT = 18, Fission
MT = 102, (n, γ)
MT = 103, (n,p)
MT = 104, (n,d) } Used only as specified by input option LF₃
MT = 105, (n,t)
MT = 106, (n,He³)
MT = 107, (n, α)
MT = 251, $\bar{\mu}_L$

File 4

MT = 2, Legendre Coefficients or tabulated distributions

File 5

MT = 4, NK or NK-1 Inelastic Distributions LF = 3
MT = 4, 0 or 1 Inelastic Distribution LF = 8 or 9
MT = 16, One (n, 2n) Distribution LF = 8 or 9
MT = 18, Fission Distribution LF = 6 and/or 8

A. CONTROL ROUTINE AND UTILITY SUBPROGRAMS

This section describes the ETOE control routine (main program) and various utility subprograms. The utility subprograms are routines of a general nature, which are common to the entire ETOE program. Some of these routines were distributed generally to the Cross Section Evaluation Working Group (CSEWG), the group responsible for preparation of ENDF/B data and associated processing codes, and are denoted by an asterisk (*). These routines report error conditions via the ERROR subroutine as error numbers rather than comments on the output tape. A list of these error numbers is given in Table II.

TABLE II - ERROR NUMBERS REPORTED BY ERROR

<u>Error Number</u>	<u>Calling Routine</u>	<u>Description</u>
1	TERP	The value of the interpolation code is less than one (linear-linear is used).
2	TERP	The value of the interpolation code is greater than five (linear-linear is used).
3	--	General non-fatal error. The error condition is printed on the output tape.
4	--	General fatal error. The error condition is printed on the output tape.
110	ECSI	The interpolation code is less than one or greater than five.

1. Control Routine - ETOE

The control routine, Figure 1, reads the material data cards and controls the flow of the calculations. Also, any parameters which may vary between computers are, in general, assigned in the control routine. An example is that all tapes used by ETOE have variable tape numbers which are assigned in the control routine and carried in COMMON.

The input supplied by the user is described in detail in Chapter III. Briefly, it consists of a header card followed by one card per material required for the MC² tape. These cards may be in any order, since the data is sorted by the control routine on increasing ENDF/B material number. Thus the order of the MC² tape will also be by increasing ENDF/B number.

2. KLOCK

The KLOCK subroutine is used to print the time required to process each ENDF/B file. If the argument to the subroutine is zero, the routine will read the value of the timer. If the argument is non-zero, the routine reads the timer, subtracts the value of the argument, and prints the result. The present version reads the timer $T = \text{TIMEF}(1)$ in milliseconds and prints the elapsed time in minutes and seconds.

3. ERROR

The ERROR routine is used to terminate the execution of a run and flag any error conditions that cannot be processed by ETOE. There is, however, a distinction made between types of errors as to fatal and nonfatal. Fatal errors are those which alter the logical flow of the program, necessitating termination of the run; nonfatal errors are those conditions that cannot be processed by ETOE but will not alter the logical flow, i. e., the MC² tape created will be usable although the validity of the data which caused the error is questionable. While all fatal errors will cause termination of a run, nonfatal errors may or may not cause termination, depending on an input option (Chapter III).

A call to ERROR produces a comment on the output tape consisting of the error number and an error count. A list of the error numbers and a description of the errors is found in Table II. Only errors numbered 4 are fatal.

4. READE

The READE subroutine reads energies and, where appropriate, interpolation parameters from the input tape. One input set consists of a header card, interpolation parameters (if necessary), and the energy points. The header card contains the ENDF/B material number, a flag indicating the type of data, the number of interpolation regions (zero if no interpolation scheme), and the number of points. The material number and flag supplied in the CALL statement are compared with those given in the data as a check to see that the input type is correct. If they do not agree with those from the calling program, a fatal error is reported. The flag and input format are explained in Chapter III.

5. RTAB1

The RTAB1 subroutine is used to read a TAB1² record from a binary tape. The subroutine returns the parameters in the TAB1 record via the calling sequence.

6. SKPMF, SKPMAT, SKPMT

The SKPMF, SKPMAT, SKPMT subroutines are used to bypass remaining data in a file, material, or section, respectively, that is not required for MC² conversion. The routines read through each record, as a CONT record, testing for a FEND, MEND, or SEND record.

7. TERP*

The TERP subroutine is the interpolation routine distributed to the CSEWG.² The routine has been modified so that if the desired point lies outside the range specified by the curve, the routine will extrapolate using the two nearest end points and the associated interpolation scheme. The indicator L is still used to indicate whether extrapolation has occurred.

8. TERP1

The interpolation parameters as given in the ENDF/B format differ from those required by TERP. Rather than an interpolation code for each region, TERP requires that each point have an associated interpolation code. TERP1 converts the parameters from ENDF/B to TERP format. The original ENDF/B values are not destroyed.

9. AVET

The AVET subroutine is similar to TERP with the exception that instead of interpolating a curve to a given value, AVET averages the curve over a given interval. This routine does not extrapolate, in that if any of the interval lies outside the range specified by the curve, that part will not be included in the average. The same L parameter used in TERP is used in AVET.

AVET uses the ECSI subroutine.

10. ECSI*

Given the end points of a line, an integration interval, and interpolation code ECSI² will compute the integral over the given interval. The end points of the interval may be equal or they may lie outside the end points of the curve.

11. COMBN1

The COMBN1 subroutine is used to add two curves (A and B) that are specified in ENDF/B format. The resulting curve is also in ENDF/B format.

In the range (abscissa) where curves A and B coincide, the curves are summed at every point on both curves. The interpolation region boundaries coincide with the region boundaries of curves A and B, and the interpolation code for a region is taken as the maximum (largest number) interpolation code of the two curves. That is, if one curve specifies log-log interpolation (INT = 5) and the other linear-linear (INT = 2), the resulting curve uses log-log.

If curve A covers a lower range than curve B, the resulting curve uses the same points and interpolation scheme of curve A to the point of overlap. At this point, a double valued point (discontinuity) is set up. The first point has the value of curve A evaluated at the first point of curve B. The second point of the double value is the sum of curve A and curve B at the first point of curve B. If the first point of curve B is zero, no double valued point is set up. The remaining portions of curves A and B that coincide are combined as described above.

In the case where curve A covers a higher range than curve B, the lower range of the curve is formed as described above. A double valued point is set up at the point of overlap, last point of curve B. The first point of the double value is the sum of curves A and B at that point. The second point is the value of curve A only. The interpolation region of the resulting curve includes the second point of the double value. If the last point on curve B is zero, no double value is set up. The remainder of the curve consists of the remaining points and interpolation codes of curve A.

If the point of overlap of the two curves occurs at a double valued point on one of the curves, curve A for example, the resulting curve will also have a double value. The first point of the double value is the same as the first point of the double value on curve A. The second point will be the sum of the second point of the double value on curve A and the end point of curve B. Also, if both input curves have double valued points that coincide, the first point of the double value on the resulting curve will be the sum of the first points of the double value on the input curves, and the second point of the double value will be the sum of the second points on the input curves.

Curves A and B may be interchanged with no effect on the resulting curve.

12. COMBN2

The COMBN2 subroutine is similar to the COMBN1 subroutine with the exception that COMBN2 multiplies, rather than adds, two curves. The resulting curve is evaluated at every point of both input curves, but only in the range where the two input curves overlap. The interpolation region boundaries of the new curve coincide with the regions of the input curves, and the interpolation code for a region is taken as the maximum (largest

number) interpolation code of the two input curves. That is, if one curve specified log-log interpolation (INT = 5) and the other linear-linear (INT = 2), the resulting curve would use log-log. A further test is made to ensure that the resulting curve is not zero in a region of either log-log (INT = 5) or log y - linear x (INT = 4) interpolation. If this condition occurs, the interpolation code for the region is set to linear-linear (INT = 2).

13. CNGINT

The CNGINT subroutine is used to change the interpolation parameters from ENDF/B format to MC² format. The conversion is performed immediately prior to writing the MC² tape. Thus the routines in ETOE which use the interpolation data all use the ENDF/B format. The original ENDF/B interpolation parameters (NBT and INT) are replaced by the MC² parameters.

The following is a list of the differences between the ENDF/B and MC² interpolation parameters that are processed by CNGINT.

- a. The interpolation codes, given in Table III, differ; that is, an interpolation code of 1 in the ENDF/B is constant interpolation, while in MC² format 1 is log-log.
- b. In addition, MC² does not allow a constant or log y versus linear x interpolation. The constant code is set by CNGINT to a linear MC² code, and the log y versus linear x is set to log-log.
- c. MC² requires that the NBT for a region be the point number of the last point in the region. MC² requires NBT to be the number of points in a region. CNGINT calculates the NBT for MC² as the difference of adjacent ENDF/B NBT's.

TABLE III - ENDF/B AND MC² INTERPOLATION CODES

<u>ENDF/B Code</u>	<u>Description</u>	<u>Changed to MC² Type</u>
1	Constant	3*
2	Linear x versus linear y	3
3	Log x versus linear y	2
4	Linear x versus log y	1*
5	Log x versus log y	1

* MC² does not allow constant or linear x versus log y.

- d. MC² does not allow double valued points, i. e., discontinuities, in the data. CNGINT eliminates the discontinuities by multiplying one abscissa by 1.00001.
- e. In addition, the routine checks for nonpositive y values when log y interpolation is used. If nonpositive y values occur, they are set to 10⁻⁴.

B. FILE1 - GENERAL INFORMATION

The FILE1 routine shown in Figure 2 processes the material description and the ν data. In addition, this routine also copies the W-table to the MC² tape and creates the ENDF/B tape if the sample problem is used (see Chapter III. B). The material description and a list of the reactions given in each file, if present, is read from the ENDF/B tape and printed out. The first 66 characters of the material description are saved and used as a heading in the printout for each material in the remaining files.

Since MC² requires $\bar{\nu}$ to be given as a third order polynomial and ENDF/B will allow either a polynomial or tabular representation, provisions are included to "fit" the tabular data or reduce a higher order polynomial to third order. A least-squares fitting procedure is used to obtain a polynomial approximation to a tabulated distribution. The distribution tabulated in the ENDF/B file may not include sufficient energy points to permit an adequate fit to the data. Therefore, additional interpolated values of ν , besides the tabular points, are included in the fit at energies of 0.1, 0.25, 0.5, 0.75, 1.0, 1.25, 1.5, 1.75, 2.0, 2.5, 3.0, 3.5, 4.0, 5.0, 6.5, 9.0, 10.0, 12.0, and 15.0 Mev. The GNUFT subroutine fits the tabulated data, GNUFT1 reduces an nth order polynomial to third order, and both routines use the SMEQ routine to solve the resulting simultaneous linear equations. The W-table,¹ which is used by MC² to obtain values of $\psi(x, \xi)$, is also prepared in the FILE1 routine. The W-table may be read either from a binary tape, possibly an old MC² tape, or as input (both methods are described in Chapter III); however, in either case the data must consist of two sets of 3,844 (62 x 62) values in exactly the same order as required by MC².

C. FILE2 - RESONANCE DATA

The FILE2 routine, Figure 3, processes the resolved and unresolved resonance parameters. This file includes two main routines, FILE2 and XILE2, which were separated to limit the program size of a routine.

Unlike ENDF/B, MC² requires some resonance information for every material. A minimum is the potential scattering cross section which must be supplied by the user if the ENDF/B material does not have resonance data.

The resonance information on the ENDF/B tape is ordered by isotope, with present format restrictions limiting the resolved and unresolved data to one energy range each for an isotope. This restriction is included in ETOE. The MC² program requires that the number of resonance data records (NRREC) be written on the MC² tape at the beginning of the resonance data, followed by unresolved data for all isotopes, and then by resolved resonance data. As the ENDF/B order differs from this MC² order, all resonance data for a material must be read from the ENDF/B tape before writing the MC² tape.

The number of records is calculated from the following formula:

$$NRREC = LRUR + 2 + LRUU * \sum_{NIS} \left\{ 1 + \sum_{NLS} [1+2*NJS] \right\}$$

where

LRUR = 0 there is no resolved data for this material
 = 1 there is resolved data for this material

LRUU = 0 there is no unresolved data for this material
 = 1 there is unresolved data for this material

NIS = the number of isotopes with unresolved data

NLS = the number of ℓ states for each isotope

NJS = the number of J states for each ℓ state

Several quantities required by MC² and not given directly on the ENDF/B tape are calculated as the resolved data is read in. These quantities are:

1. Statistical factor

$$g = \frac{2J+1}{2(2I+1)}$$

2. MC requires that only Γ (total width), Γ_γ , and Γ_f be given. The value of Γ given on the ENDF/B tape is ignored and the total for each resonance is calculated as the sum of Γ_γ , Γ_n , and Γ_f .

$$\Gamma = \Gamma_\gamma + \Gamma_n + \Gamma_f$$

3. Peak resonance cross section

$$\sigma_0 = \frac{2.6036E6}{|E_r|} \left(\frac{A+1}{A} \right)^2 g \frac{\Gamma_n}{\Gamma}$$

$$4. \quad \xi = \Gamma \left(\frac{3.44672E4 |E_r|}{A} \right)^{-1/2}$$

5. A coefficient in the term for interference between resonance and potential scattering. For resolved resonances with total angular momentum $l > 0$, AFAC is set equal to zero.

$$\text{AFAC} = \left[\sigma_o \ g \ \sigma_p \ \frac{\Gamma_n}{\Gamma} \right]^{1/2}$$

6. Potential scattering cross section where R is obtained from

$$C = R / (\bar{\lambda}_o \sqrt{E}).$$

$$\sigma_p = 4\pi R^2 = 2.6036E6 \left(\frac{A+1}{A} \right)^2 C^2$$

If there is no resolved data for a material, SIGP is obtained from C given in the unresolved data. If C is not given, the spin-independent radius AM is used for the SIGP calculation.

MC² requires that energies be specified for unresolved resonance calculations; ETOE provides the user three options for obtaining these energies. If the fission widths are given, the energy points at which the widths are tabulated may be used. The points may also be taken at equal lethargy increments over the specified energy range, or the user may specify the points as input. If no fission widths are given in ENDF/B and the energies are not specified by the user, the points will be taken at 15 equal lethargy increments over the range. The energy points are checked so that all points are within the specified energy range. In addition, there must be a point within ± 5 per cent of the end points of the range. The fission widths are then interpolated, if necessary, to the new energy points and written on the MC² tape.

MC² permits the use of energy-dependent, average-reduced neutron widths and fission widths in the unresolved resonance data, while ENDF/B formats permit only fission widths to be energy dependent. ETOE includes an option for specifying energy-dependent neutron widths as input data.

ENDF/B includes an option (LIS) specifying that the resonance scattering cross section must be calculated from the resolved and/or unresolved resonance parameters and added to the smooth background cross section of FILE3. The subroutines RESCAT and UNSCAT, described below, calculate the scattering cross sections. For the resolved energy range, the user may specify the energy points for the calculation or calculate the energy points by the subroutine EPT. Energies for the unresolved resonance calculation are taken to be the same as specified for the MC² tape. A total of 4,000 and

100 (25 per isotope) energy points for the respective resolved and unresolved resonance calculations are permitted. The user should ensure that the sum of the energy points from the resonance scattering calculation plus the total points of the smooth data (MT = 2, FILE3) do not exceed the 5,000 points allowed in MC². If there is more than one isotope requiring unresolved calculations, the energy points for the isotopes are sorted (subroutine SORT) to form a single energy array. Within the appropriate energy range for each isotope, the isotopic contributions are then interpolated to the sorted energy array and added. The unresolved resonance energy array is then joined with the resolved resonance energy array by interpolating the unresolved data to the resolved data points if the arrays overlap. Finally the combined array for the resolved and unresolved data is written on tape (LTPS1) for later combination with the FILE3 smooth data. A log-log interpolation scheme is assumed for the scattering data.

1. RESCAT

Subroutine RESCAT performs the calculation of the resolved resonance scattering cross section for the Mth ETOE material which has NIS isotopes, NRES resonances. NSE, the number of energy points used for the calculation, is determined in EPT by a call from RESCAT or is read from input cards. Calculated energy points span the maximum energy range formed by combining the ENDF/B specified ranges for all isotopes in the material. However, a particular isotope in a material is calculated only over its specified energy range.

NROPT specifies the resonance formulae to be used in the calculation. For the resolved resonance formulae of the ENDF/B format specifications,² NROPT=2 if LRU=1, LRF=1 and the input variable TEMP=0; NROPT=3 if LRU=1, LRF=2 and TEMP=0 or NROPT=3 if TEMP<0; and NROPT=1 if TEMP>0. For these options, the scattering cross section is calculated as follows:

NROPT=1

This option represents a Doppler-broadened form of the ENDF/B specifications² for LRU=1, LRF=1.

$$\sigma_s(E) = \sum (2\ell+1) 4\pi \lambda^2 \sin^2 \varphi_\ell$$

$$+ 4\pi \lambda^2 \sum_{r(\ell, J)} g_J \frac{\Gamma_{nr}(E)}{\Gamma_r} \left[\left(\frac{\Gamma_{nr}(E)}{\Gamma_r} - 2 \sin^2 \varphi_\ell \right) \psi(x_r, \xi_r) + \chi(x_r, \xi_r) \sin 2\varphi_\ell \right]$$

$$\lambda^2 = \frac{2.6036 \times 10^6}{E} \left(\frac{A+1}{A} \right)^2$$

$$\Gamma_{nr}(E) = \Gamma_{nr} \left(\frac{E}{E_r} \right)^{1/2}$$

$$\Gamma_r = \Gamma_{nr} + \Gamma_r + \Gamma_{fr}$$

$$x_r = \frac{E-E_r}{\Gamma_r/2}$$

$$\xi_r = \frac{\Gamma_r}{\Delta_r} = \Gamma_r \left(\frac{E_r \cdot 3.44672 \times 10^4}{A} \right)^{-1/2}$$

$$\Psi(x_r, \xi_r) = \frac{\xi_r}{2\sqrt{\pi}} \int_{-\infty}^{\infty} dy \frac{\exp\left[-\frac{\xi_r^2}{4} (x_r-y)^2\right]}{1+y^2}$$

$$\chi(x_r, \xi_r) = \frac{\xi_r}{2\sqrt{\pi}} \int_{-\infty}^{\infty} dy y \frac{\exp\left[-\frac{\xi_r^2}{4} (x_r-y)^2\right]}{1+y^2}$$

$$\rho = \frac{R}{\lambda}$$

$$\varphi_\ell = \text{phase shift} \left(\varphi_0 = \rho, \varphi_1 = \rho - \tan^{-1} \rho \right)$$

In these equations, the total width, Γ_ν , is taken as independent of energy for consistency with the Doppler broadened approximation. The subscript r indicates the rth resonance with its associated ℓ and J values.

NROPT=2

This option represents the single-level Breit-Wigner approximation (LRU=1, LRF=1) for zero temperature.

$$\sigma_s(E) = \sum_{\ell} (2\ell+1) 4\pi\lambda^2 \sin^2 \varphi_\ell$$

$$+ 4\pi\lambda^2 \sum_{r(\ell, J)} \frac{\xi_J \Gamma_{nr}(E)}{(1+x_r^2)^2 \Gamma_r(E)} \left(\frac{\Gamma_{nr}(E)}{\Gamma_r(E)} - 2 \sin^2 \varphi_\ell + x_r^2 \sin 2\varphi_\ell \right)$$

$$x_r^2 = \frac{(E-E_r^2)}{\Gamma_r(E)/2}$$

$$\Gamma_{nr}(E) = \frac{P_\ell(E) \Gamma_{nr}(|E_r|)}{P_\ell(|E_r|)}$$

$$\Gamma_r(E) = \Gamma_{nr}(E) + \Gamma_{\gamma r} + \Gamma_{fr}$$

$$E'_r = E_r + \left(\frac{S_\ell(|E_r|) - S_\ell(E)}{2 P_\ell(|E_r|)} \right) \Gamma_{nr}(|E_r|)$$

$$S_\ell = \text{shift factor} \left(S_0 = 0; -S_1 = \frac{1}{1 + \rho^2} \right)$$

$$P_\ell = \text{penetration factor} \left(P_0 = \rho; P_1 = \frac{\rho^3}{1 + \rho^2} \right)$$

NROPT=3

For this option, a multilevel scattering term (LRU=1, LRF=2) for resonance-resonance interference is calculated as a correction to the calculation for NROPT=2. This term is given by

$$4\pi\lambda^2 \sum_{r=2}^{N_r(\ell, J)} g_J \frac{2\Gamma_{nr}(E)}{\Gamma_r(E)(1+x_r'^2)} \sum_{s=1}^{r-1} \frac{\Gamma_{ns}(E)(x_r'x_s'+1)}{\Gamma_s(E)(1+x_s'^2)}$$

and is calculated only for resonances of the same isotope ℓ and J values.

For NROPT=1, the Doppler broadening functions, $\psi(x, \xi)$ and $X(x, \xi)$ are calculated by the subroutine CROSS. For resonances such that $|x_r|$ minimum $(\xi_r, 1) > \text{XOPT}$, the scattering cross section is taken to be constant and equal to the potential scattering cross section. XOPT is set to 400 as the first executable statement of the RESCAT routine and can be easily modified by the user. Small values of XOPT materially shorten the calculation time with corresponding decrease in accuracy.

For options 1 and 2 or finite XOPT for option 3, it is possible to calculate a negative scattering cross section due to the interference between resonance and potential scattering. If a negative scattering cross section is calculated, the value is reset to 0.001 barns in RESCAT.

2. EPT

Subroutine EPT calculates the energy point grid between a minimum and maximum energy. The method used is based on the UNICORN code.⁴

The routine initially sets up an energy array (up to 200 points per resonance) in the variable x to describe a resonance. An optimized point spacing for pointwise representation of $(1+x^2)^{-1}$ and logarithmic interpolation is used. The criterion used is that between any two points the magnitude of the difference between the exact integral of $(1+x^2)^{-1}$ and the

integral assuming logarithmic interpolation be within 1% of a constant. This constant is determined by the number of points selected to represent an isolated resonance. Additional details of this calculation are given in Reference 4.

Using the optimized x array, EPT steps through the resolved resonance energies in the problem to set up an array of absolute energies. In this calculation, the maximum of the Doppler width or natural width of the resonance is used in defining the x variable to approximately distribute the energy points over the Doppler-broadened shape of the resonance. The energy grid is determined by using the x values calculated from the closest resonance (in x value) so that the entire set of x values is normally not used for any resonance. All resonance energies, the midpoint (in x) between resonances, and the minimum and maximum energies of the problem are included in the energy array.

EPT calculates the total energy points in the final energy array which may be considerably less than the product of the number of points per resonance (NPR) and the number of resonances (NRES). Before the EPT routine is executed, RESCAT adjusts NPR to $4400/NRES$ if the input $NPR * NRES > 4400$, thus allowing for a 10% reduction in forming the energy array.

3. CROSS, GAMINC

Subroutine CROSS calculates the $\Psi(x, \xi)$ and $X(x, \xi)$ functions for the resolved resonance calculation. GAMINC is called by CROSS for calculation of the incomplete gamma function. These routines are taken from the FASDOP program;⁵ the methods are described in detail in Reference 5. Briefly, CROSS uses convergent or asymptotic series expansions depending on the values of x and ξ .

4. UNSCAT

Subroutine UNSCAT calculates the scattering cross section from unresolved resonance parameters from all energy points and (J, ξ) states or resonance sequences. The following variations are calculated: NUOPT=1 if the input variables TEMP and SIGPEN are both greater than zero; NUOPT=2 if TEMP=0 and SIGPEN=0; and NUOPT=3 if TEMP = 0 or SIGPEN=0. For options 1 and 2, the cross section is self-shielded to a constant value (SIGPEN) of the nonresonant cross section per atom of the resonance material. Option 3 represents an infinite dilution calculation. The method of calculation is based on the narrow resonance approximation for an isolated resonance. The asymmetric interference between resonance and potential scattering is ignored as the first order contribution of this term vanishes due to the antisymmetric behavior of the X(x, E) function.

In the isolated narrow-resonance approximation for isotope i with abundance I^i , the general formula for the scattering cross section at energy E_0 can be written

$$\tilde{\sigma}_s^i = \sum_{\ell} I_i^{(2\ell+1)} 4\pi\lambda_o^2 \sin^2\varphi_{\ell} + I_i^{\langle\sigma_{sr}^i\rangle}$$

$$\langle\sigma_{sr}^i\rangle = \sum_{(\ell,J)^i} \frac{\int_{\Delta E} dE \sigma_{sr}^i(E)/\sigma_t(E)}{\int_{\Delta E} dE 1/\sigma_t(E)}$$

The integral over ΔE can be transformed through an average over k resonances to a statistical average

$$\int_{\Delta E} dE f(E) \rightarrow \sum_k \int_{\Delta E} dE f_k(E) \rightarrow \sum_k \int_{-\infty}^{\infty} dx \frac{\Gamma_k}{2} f_k(x) \rightarrow n \langle \frac{\Gamma}{2} f \rangle$$

$$\Delta E \rightarrow n \langle D \rangle$$

where n indicates the number of resonance with average spacing $\langle D \rangle$ in ΔE . Then ($\sigma_n = \text{SIGPIN}$)

$$\sigma_s^i(E) = \sigma_{ot} \left(\frac{\Gamma}{\Gamma} - 2 \sin^2\varphi_{\ell} \right) \Psi(x, \xi)$$

$$\sigma_t^i(E) = \sigma_n + I_i^{\langle\sigma_{ot}\rangle} \cos 2\varphi_{\ell} \Psi(x, \xi)$$

$$\sigma_{ot} = 4\pi\lambda^2 g \frac{\Gamma}{\Gamma}$$

$$\frac{1}{\sigma_t} = \frac{1}{\sigma_n} \left(1 - \frac{I_i^{\langle\sigma_{ot}\rangle} \cos 2\varphi_{\ell} \Psi(x, \xi)}{\sigma_t(E)} \right)$$

the resonance scattering contribution becomes

$$\langle\sigma_{sr}^i\rangle = \frac{\left\langle \frac{1}{I_i \cos 2\varphi_{\ell}} \int_0^{\infty} dx \frac{\Gamma_n \Psi - 2 \sin^2 \varphi_{\ell} \Gamma \Psi}{\frac{\sigma_n}{I_i \sigma_{ot} \cos 2\varphi_{\ell}} + \Psi} \right\rangle}{\frac{1}{\sigma_n} \left(\langle D \rangle - \left\langle \int_0^{\infty} dx \frac{\Gamma \Psi}{\frac{\sigma_n}{I_i \sigma_{ot} \cos 2\varphi_{\ell}} + \Psi} \right\rangle \right)}$$

$$= \frac{\sigma_n}{I_i (\cos 2\varphi_{\ell}) \langle D \rangle} \left(\frac{\langle \Gamma_n J \rangle - 2 \sin^2 \varphi_{\ell} \langle \Gamma J \rangle}{1 - \langle \Gamma J \rangle / \langle D \rangle} \right)$$

$$J(\beta, \xi) = \int_0^{\infty} dx \frac{\Psi(x, \xi)}{\beta + \Psi(x, \xi)}$$

$$\beta = \frac{\sigma_n}{I^i(\cos 2\varphi_l) \sigma_{ot}}$$

Then the equation solved for the scattering cross section is

$$\begin{aligned} \tilde{\sigma}_s^i &= \sum_l I^i(2l+1) 4\pi\lambda^2 \sin^2\varphi_l \\ &+ \sum_{(l,J)}^i \frac{\sigma_n}{\cos 2\varphi_l \langle D \rangle} \frac{\langle \Gamma_n J \rangle - 2 \sin^2\varphi_l \langle \Gamma J \rangle}{1 - \langle \Gamma J \rangle / \langle D \rangle} \end{aligned}$$

This equation reduces to the various options by the following selection of the J function

NUOPT = 1 J obtained numerically by JFUNC subroutine
as a function of β and ξ

NUOPT = 2 $J = \frac{\pi}{2\sqrt{\beta(1+\beta)}}$

NUOPT = 3 $J = \frac{\pi}{2\beta}$

This rather cursory derivation of the unresolved resonance scattering cross section given above is presented to demonstrate the treatment of the terms involving $\sin^2\varphi_l$ and $\cos 2\varphi_l$. More detailed derivations can be obtained from such references as the MC² report.¹ In general, the method is correct for overlap effects between resonance sequences when second order effects can be neglected and neglects self-overlap effects between resonances of the same spin state. The averages over statistical distributions of the neutron and fission widths indicated by brackets in the equation are calculated by the methods used in MC².

5. JFUNC

Subroutine JFUNC calculates $J(\beta, \xi)$ for each point of the statistical averaging over neutron and fission width distributions in UNSCAT. The method used is a semi-empirical approximation accurate to about 2% over the range of ξ, β of interest in reactor calculations. This routine is taken from IDIOT code⁸ and details of the method and accuracy are given in Reference 8.

6. SORTE

The SORTIE subroutine transfers an energy array E to a second array E2 and sorts E2 by increasing energy while eliminating

equal energies from the E2 array. This routine is used to sort the unresolved resonance energies when more than one isotope in a material requires the unresolved resonance scattering calculation.

D. FILE3 - SMOOTH CROSS SECTION DATA

The smooth data is processed by the FILE3 routine, Figure 4. The smooth data consists of a series of tabulations for various reaction types (MT numbers) and the associated interpolation parameters. The reactions required by MC² are given in Table I. Due to the relative order of the data as given on ENDF/B and required by MC², all data for a material must be processed before being written on the MC² tape. This limits the number of points that can be handled by ETOE to a total of 12,000 points for MC² data in this file. MC² allows an upper limit of 5,000 points for each reaction type.

The smooth scattering cross section (MT=2) is combined with the resonance scattering array calculated in the FILE2 overlay before writing the MC² tape. For this combination of data, the COMBN1 routine discussed in Section A is utilized.

ETOE recognizes only the cross section types given in Table I. Other reaction types are not allowed in MC² and are not processed by ETOE. MC² does not include reaction types MT=104-106 as normal input cross sections; however, a provision has been included in ETOE to combine these reactions with MT=103 or 107 and write the combined data as (n,p) or (n,α) data on the MC² tape. To utilize this option, the user must provide an energy array and interpolation parameters (in ENDF/B format) as input data. ETOE will then interpolate each of the reaction types to the input energies and add the respective contributions to form the combined data.

If an ENDF/B material includes important reaction types other than those given in Table I, the user must modify the ENDF/B data to incorporate the data into the MT numbers of Table I before ETOE processing.

As will be discussed in the following sections, some of the smooth data is needed for processing in other files. The elastic data needed for the Legendre data in FILE4 and the inelastic data needed in FILE5 are written on an intermediate tape, LTPS. In addition, there is an indicator for (n,2n) data and the threshold energy for the (n,2n) reaction carried in COMMON for use in FILE5. The threshold energy is taken as the first energy point of the (n,2n) distribution if the first probability is nonzero, or as the energy preceding the first nonzero probability if the first probability is zero.

As explained in Section A, the interpolation codes of MC² and ENDF/B differ. The data is changed to the MC² format immediately before being written on the MC² tape.

E. FILE4 - LEGENDRE DATA

The Legendre polynomial coefficients are obtained from elastic secondary angular distributions given in file four using the FILE4 routine, Figure 5. There is an input option whereby the user may specify which materials are to have Legendre polynomial data on the MC² tape. In addition, if the input specifies Legendre data and there is no File 4 elastic data given on ENDF/B for a material, no Legendre data is given and an error comment occurs. The error is not reported through the ERROR routine.

The details of the structure of the Legendre coefficient data required by MC² are given in Reference 1. The coefficients must be given in the center of mass system and are defined as $\beta_\ell = \sigma_s f_\ell (2\ell + 1)/4\pi$. The energy structure is currently fixed by MC² to an upper limit of 10 Mev (lethargy 0). The lower energy limit corresponds to a lethargy of 17 and the data is tabulated in decreasing energy at lethargy increments of 1/120, resulting in 2041 energy points (the blocks overlap by one energy point) for each material. In addition, the transformation matrix ($\ell = 1$ only) for converting the β_ℓ 's from the center of mass to the laboratory system must be given for each material. The energy points are divided into 33 blocks. The first block consists of the Legendre polynomial coefficients for the given energies and the MC² material identification number for each material. In addition, the first block contains the transformation matrix for each material.

If the angular data is given as tabulated distributions of cross section and angle, ETOE will calculate the Legendre expansion for the tabulated distribution using the LEGEND subroutine. The order of the Legendre expansion is specified as input data or the order of the transformation matrix if given in the ENDF/B data will be used. If the order is not specified by the input data and the transformation matrix is not given, a 19th order expansion is used to fit the tabulated distributions.

After the Legendre coefficients are obtained in the center of mass system, ETOE reads the elastic scattering cross sections from the intermediate tape written in FILE3. At each energy point of the MC² Legendre data, the cross sections are averaged over the lethargy width associated with each energy point; that is, half the lethargy width to the next highest and to the next lowest energy points. The Legendre coefficients are interpolated to the MC² energy points. Then the β_ℓ products of cross section and coefficients are formed and written on another intermediate tape, LTPS1. Tape LTPS1 is ordered by material and is processed by the FILE6 overlay described in Section G.

1. LEGEND, LGCK

Subroutine LEGEND⁶ computes the Legendre coefficients of the differential scattering cross section given at a set of cosines of the scatter-

ing angle. The necessary integrals are computed analytically assuming linear interpolation between data points.

Subroutine LGCK checks the tabulated angular data to ensure that data points are given at scattering cosines of -1.0 and 1.0 . If these data points are not included in the given data, an extrapolation based on the nearest two data points and interpolation scheme is used for the -1.0 and 1.0 values.

2. MATRIX, CLEB, BLOCK

The subroutine package MATRIX⁶ computes either the transformation matrix for transforming Legendre scattering coefficients from the center of mass system into the laboratory system or the inverse matrix for transformations from the laboratory into the center of mass system. MATRIX calculates the transformation matrices while CLEB calculates Clebch-Gordon coefficients and is called by MATRIX. BLOCK stores from 0 to 100 factorial in argument and exponent form for use by MATRIX and CLEB.

F. FILE5 - SECONDARY ENERGY DISTRIBUTIONS

Secondary energy distributions for inelastic scattering ($n, 2n$) and fission are processed by the FILE5 routine. A later modification of the ENDF/B specifications adopted since the publication of Reference 2 allows the FILE5 data to be given in either the center of mass or the laboratory system. ETOE assumes that all data is given in the laboratory system ($LFE=0$). If the data is given in the center of mass system ($LFE=1$), an error comment is given and processing continues as though the data were in the laboratory system. ETOE processes only the distributions permitted in MC² (see Table I) for the respective reaction types. Since any missing reaction types cause non-fatal errors and processing may continue, and since much of the MC² data processed in this file depends on the smooth data, the flow chart for this routine (Figure 6) is more detailed than those for the other routines.

For inelastic scattering (MT=4 only) MC² allows only the discrete energy loss distribution ($LF=3$) for resolved levels and the Maxwellian distribution ($LF=8$ or 9) for statistical scattering. Only one statistical distribution is permitted and the number of resolved levels is limited by ETOE to 37. Also ETOE limits the total number of points in the inelastic cross section data (resolved levels and statistical distributions) to 9,000. For statistical scattering, the nuclear temperatures are changed to Mev as required by MC² and the threshold energy is taken as the first energy point of the distribution immediately preceding the first nonzero probability.

For each distribution in File 5 of the ENDF/B data, the cross section is given as a probability of the total cross section given in File 3. ETOE obtains the absolute cross section for each level by multiplying the probability times the File 3 cross section using the COMBN2 subroutine (see Section A).

For (n,2n) data, MC² allows only a single statistical distribution (LF=8 or 9). If an LF=8 or 9 distribution is given as one of a set of distributions, ETOE will use this distribution for the MC² tape and assume a nonfatal error. If an LF=8 or 9 distribution is not given, ETOE assumes a nonfatal error and performs an order of magnitude calculation for the nuclear temperature as

$$\theta = \frac{2}{3} \frac{E}{a}^{1/2} \text{ Mev}$$

$$a = 0.1 A$$

where A is the atomic mass and the energy range is given as the threshold energy (FILE3) to 15 Mev with linear interpolation. This formula is based on the assumptions that the (n,2n) nuclear temperature is about 2/3 (Reference 7) the elastic scattering temperature approximated by (E/a)^{1/2}. Inclusion of this calculation in ETOE is intended to permit the preparation of a complete MC² tape when the (n,2n) reaction may not be important for reactor calculations.

For fission spectrum data, MC² permits a linear combination of the ENDF/B LF=6 and LF=8 distributions. Any other distributions are ignored by ETOE. The ENDF/B material number is used as the MC² source number.

MC² requires that if inelastic (MT=4) cross sections are given as smooth data, secondary energy distributions must be given, while ENDF/B formats do not specifically require the secondary energy distributions. If the ENDF/B data does not include the secondary energy distributions, ETOE assumes a nonfatal error. While the MC² tape is usable, the user should exercise caution in using this material in MC² calculations.

For (n,2n) reactions, the above mentioned approximate calculation of the nuclear temperature will permit preparation of a useful MC² tape.

G. LEGENDRE POLYNOMIAL DATA SORT

The Legendre data as written on scratch tape LTPS1 in the FILE4 routine (Section E of this chapter) is in the required MC² format except that the tape is ordered by energy blocks within each material. The FILE6 routine (overlay 6, not to be confused with ENDF/B File 6) sorts the data by energy block as required by MC².

FILE6 consists of two sections. The first section reads through tape LTPS1 and simultaneously copies the information on scratch tape LTPS, prints the Legendre data (if required by the print option), and writes the data for the first block on the MC² tape. The second section reads through either tape LTPS or LTPS1 for each energy block (blocks 2 through 33 in the

present MC² format) and writes the information for the block on the MC² tape for each material. Tapes LTPS and LTPS1 are used so that as the program is reading one tape, the other is being rewound.

III. CODE OPERATION

This chapter describes the user-supplied input to ETOE and the printed output. In section B, a special routine for checkout of the code is described. A brief description of the compatibility of the code with machines other than a CDC 3600 with 65K memory is discussed in section C.

A. INPUT DESCRIPTION AND OUTPUT

The user-supplied input to ETOE is described in Table IV. In general, only one data card for each material is required as ETOE input. Other input may be optionally included following the material descriptions, such as W-table, energies, and resonance data.

TABLE IV - ETOE INPUT DESCRIPTION

Header Card			
<u>Columns</u>	<u>Format</u>	<u>Variable</u>	<u>Description</u>
1-6	16	NMAT	Number of materials for MC ² tape
7-12	16	LERR	= 0 - All errors will terminate the run = 1 - Nonfatal errors continue processing
13-18	16	LWTBL	= 0 - No W-table written on MC ² tape = 1 - W-table read from cards >1 - Read W-table from binary tape #LWTBL sample problem option (section III. B)
19-24	16	LMERGE	= 1 - Read in sample problem = 0 - Do not read sample problem
25-30	16	LNEU	Unresolved resonance energy option = 0 - Use energies tabulated for fission widths = 1 - Read energies (FLAG=2) >1 - Calculate energies using LNEU equal-lethargy increments

Note: If LNEU=0 for a nonfissionable material with unresolved data, 15 equal-lethargy increments are used to obtain the energies.

TABLE IV - ETOE INPUT DESCRIPTION (Continued)

<u>Columns</u>	<u>Format</u>	<u>Variable</u>	<u>Description</u>
31-36	16	LNER	Resolved resonance energy option for calculation of scattering cross section. Required only when ENDF/B resolved resonance data specifies the scattering cross section to be calculated (LIS=0). = 0 - Calculate energies using 51 energy points per resonance = 1 - Read energies (FLAG=1) >1 - Calculate energies using LNER energy points per resonance
37-48	E12.4	SIGPIN	When the ENDF/B data for this material does not include resonance parameters, SIGPIN = potential scattering cross section for this material. When the ENDF/B data for this material includes resonance parameters and the scattering cross section is to be calculated (LIS=0), SIGPIN is the nonresonant scattering per atom cross section for self-shielding of the calculated scattering cross section with the following option. This LIS=0 option applies only for unresolved resonances. = 0 - Use 10^5 barns/atom - ∞ dilution >0 - Barns/atom cross section

Material Cards (One card per material)

<u>Columns</u>	<u>Format</u>	<u>Variable</u>	<u>Description</u>
1-6	A6	MATM	MC ² material ID
7-12	16	MATE	ENDF/B material number
13-18	16	MATL	= 0 - Do not write Legendre polynomials on MC ² tape = 1 - Write Legendre polynomials on MC ² tape >1 - If the elastic scattering angular data in ENDF/B is given as a tabulated distribution rather than as Legendre

TABLE IV - ETOE INPUT DESCRIPTION (Continued)

<u>Columns</u>	<u>Format</u>	<u>Variable</u>	<u>Description</u>
			expansions, MATL = order of Legendre expansion to be used in fitting the distribution.
19-24	16	LPRNT	Print Option = 0 - Print only material headings = 1 - Print only resonance data = 2 - Print only smooth data = 3 - Print resonance and smooth data = 4 - Not used = 5 - Print everything
49-60	E12.4	TEMP	Temperature T for resonance scattering cross section calculation (LIS=0 only). >0 - NROPT and NUOPT = 1 = 0 - NROPT and NUOPT = 2 <0 - NROPT and NUOPT = 3
61-66	16	LGNO	Reduced neutron width option required only if this material has unresolved resonance data. = 0 - Use constant ENDF/B Γ_n^o for all energy points. = 1 - Read energies and Γ_n^o for each energy and each spin state. Interpolate ENDF/B fission widths. = 2 - Read energies and Γ_n, Γ_f pairs for each energy and each spin state.
			<u>Note:</u> When LGNO > 0, this option replaces the LNEU option.
67-72	16	LF3	Required only if this material has ENDF/B reaction types MT=104, 105, or 106. = 0 - Ignore these reactions for MC ² tape = 1 - Read energies and interpolation scheme (FLAG=3) and write combined data in (n,p) reaction type of MC ² tape. For this option, the ENDF/B reaction types MT=103, 104, 105, and 106 are interpolated to the input energies, summed, and written as (n,p) data on the MC ² tape.

TABLE IV - ETOE INPUT DESCRIPTION (Continued)

<u>Columns</u>	<u>Format</u>	<u>Variable</u>	<u>Description</u>
			= 2 - As for LF3=1 but reaction types MT=104, 105, 106, and 107 are combined as (n, α) data on the MC ² tape.

LWTBL = 1 Only

Card 1

Format, enclosed in parentheses, for reading in W-table. Read in with an 18A4 format. Example: (6E12.4).

Card Set 2

W-table read in as two 62 x 62 arrays in the same order as required by MC² (Reference 1).

Additional input cards required by input options LNEU, LNER, or LGNO. When required, these cards are to be given in the following order for each material and then arranged for all materials in order of increasing ENDF/B number.

FLAG=1, LNER=1 Only

<u>Column</u>	<u>Format</u>	<u>Description</u>
<u>Card 1</u>		
1-12	I12	ENDF/B material number
13-24	I12	FLAG=1
25-36	I12	Must be 0 or blank
37-48	I12	NP = number of energy points. These energy points should cover the energy range specified in the ENDF/B data for the resolved energy range. If more than one isotope for this material, the energy range should span the broadest energy range formed by combining the energy ranges of all isotopes.

Card Set 2

1-72	(6E12.4)	NP energy points in order of increasing energy.
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TABLE IV - ETOE INPUT DESCRIPTION (Continued)

FLAG=2, LNEU=1 or LGNO >0 Only

This set of cards is required for each isotope of the material which has unresolved resonance parameters. They are to be arranged with the isotopes in the same order as given on the ENDF/B tape.

<u>Column</u>	<u>Format</u>	<u>Description</u>
<u>Card 1</u>		
1-12	I12	ENDF/B Material number
13-24	I12	FLAG=2
25-36	I12	Must be 0 or blank
37-48	I12	NP = number of energy points. These energy points should cover the energy range specified for the unresolved resonance calculation for this isotope in ENDF/B.
<u>Card Set 2</u>		
1-72	(6E12.4)	NP energy points in order of increasing energy.

If LGNO=1, the above cards are to be followed by one set of cards giving NP Γ_n in a (6E12.4) format for each sequence or spin state of the unresolved resonance calculation. The cards for each sequence are to be arranged in the same order as the sequences are given for the ENDF/B data.

If LGNO=2, NP pairs of (Γ_n^o , Γ_f) in a (6E12.4) format are required for each sequence with the sequences arranged as given in the ENDF/B data.

After the above data is given for all required materials, the following data, arranged by increasing ENDF/B material number, is required only for materials with LF3 > 0.

TABLE IV - ETOE INPUT DESCRIPTION (Continued)

<u>Column</u>	<u>Format</u>	<u>Description</u>
<u>Card 1</u>		
1-12	I12	ENDF/B Material number
13-24	I12	FLAG=3
25-36	I12	NR = Number of interpolation ranges for the combined data.
37-48	I12	NP = Number of energy points.
<u>Card Set 2</u>		
1-72	(6I12)	NR pairs (NBT(I), INT(I), I=1, NR) where NBT is the number of the last energy point in the interpolation scheme with INT as the interpolation code (ENDF/B interpolation code).
<u>Card Set 3</u>		
1-72	(6E12.4)	NP energies for combined array.

The header card is required for all problems. NMAT specifies the number of materials to be transferred from the ENDF/B tape to the MC² tape. The error option has been discussed in Section A of Chapter II. Normally an error indicates that the ENDF/B data for a particular material is not compatible with MC². Many errors or incompatibilities of this type do not necessitate termination of the code although the MC² tape generated should be used with caution. This option is included primarily to permit a continued search through the ENDF/B to determine whether incompatibilities exist for the selected materials.

The MC² data tape requires that the first file of the tape be the W-table, which gives the real and imaginary parts of W(x, y) as two 62 x 62 arrays.¹ ETOE permits the W-table to be read from input cards, transferred from another binary tape, or to be neglected in writing the MC² tape. In the latter case, the user must perform the necessary tape transfer to obtain the W-table on the MC² tape.

On the material cards, the MC² material identification can be chosen to be different from the ENDF/B material number and can be any six alphanumeric characters. Not all materials in the MC² library are required to have Legendre polynomial expansions. ETOE includes an option, MATL, for writing Legendre data on the MC² tape. For materials which have the

elastic scattering angular data given as tabulations of angle and cross section, MATL specifies the order of the Legendre expansion to be used in fitting the data. If MATL=1 for a tabulated distribution, the order of the ENDF/B transformation matrix, if given, will be used for the expansion or a 19th order expansion is used if the order is not specified. For unresolved resonances, MC² requires that the energies for the calculations be given as a part of the resonance data. The LNEU option provides for these energies and is required only if the ENDF/B material has unresolved resonance data.

ENDF/B formats include an option (LIS=0) specifying that the scattering cross section is to be calculated from the resolved and/or unresolved resonance parameters. As MC² does not include this calculation, the calculations if required are made in ETOE. For unresolved resonances, the energy points used for the MC² data are used. For resolved resonances, the energy points are specified by the LNER option. The temperature, TEMP, must be specified when the scattering cross section is to be calculated. Also SIGPIN specifies the constant nonresonant cross section to be used for self-shielding of the calculated unresolved resonance scattering cross section. When no resonance data is given for an ENDF/B material, SIGPIN must be given as the microscopic potential scattering cross section for the MC² data.

MC² permits the average reduced neutron widths to be specified at each point of the unresolved resonance calculation while ENDF/B data gives a constant value. The LGNO option allows the user to overwrite the ENDF/B data to utilize this feature of MC².

For neutron capture reactions, MC² includes provisions only for (n, γ), (n, p), and (n, α) reactions. ETOE includes the LF3 option to combine ENDF/B reaction types MT=104, 105, 106 with the (n, p) or (n, α) cross section for the MC² data tape. When this option is used, the energy points and interpolation scheme for the combined data must be supplied as input data. The specified reaction types are interpolated to the input energies and added together to form the combined data array. ETOE will override the input choice of the (n, p) or (n, α) reaction for the combined array if no ENDF/B data is given for one of these reactions.

If specified by input options on the material cards, additional energy cards are required. These cards must be given in the order specified in Table II; that is, FLAG=1 and 2 cards are given as required for each material and arranged in order of increasing ENDF/B material number. After these cards, the required FLAG=3 cards arranged by increasing ENDF/B material number, are given.

The ETOE output is, in general, printed at the same time the MC² tape is being prepared, so that the order of the printed output corresponds to the order of the MC² tape. There is an input option included which will suppress printing of the output for any file or material. However, the in-

formation for FILE1 along with the headings for each file and material and any error comments will always be printed.

The amount of output per material for each file is given below:

FILE1	1 to 2 pages. The print option is not used in this file.
FILE2	1 to 20 pages depending on the data and the number of isotopes.
FILE3	5 to 20 pages.
FILE4	1 to 2 pages. The print option is not used in this file.
FILE5	2 to 10 pages. The same option controls both files 3 and 5 printout.
Legendre Sort	30 to 70 pages depending on the number of coefficients and energy range.

B. SAMPLE PROBLEM

A meaningful sample problem for ETOE is complicated by the many options and decisions available, the changing nature of the ENDF/B tape, and the volume of input required for a problem. However, there is a test case distributed with ETOE, the results of which are easily verified by hand. It is based on the ABSURD program distributed by R. A. Danels of Westinghouse using the material absurdium. There is an option available which allows the ENDF/B input to be read from the input tape and written in binary on a simulated ENDF/B Mode 2 tape. The option LMERGE is entered in I-format in columns 19 to 24 of the header card. A zero in this field indicates that the ENDF/B data is on a normal Mode 2 tape. A 1 indicates that the data is to be read from the input tape immediately following the material data cards.

The input and conversion to binary tape is performed by the subroutines MERGE (modification of ABSURD), HOLL, CONT, LIST, TAB1, and TAB2 which are part of overlay 1. These routines do not use variable tape numbers. The input tape is 5, the output tape is 6, and the ENDF/B tape is 4. These routines may be removed from the ETOE program by removing the first call to overlay 1 in the ETOE main program (card ETOE0430) and the call to MERGE in the FILE1 routine (cards FIL10090 through FIL10110).

C. PROGRAMMING DETAILS

This section briefly describes the changes that may have to be made if ETOE is run on a machine other than the CDC 3600. Also a list of the

routines and the approximate size (amount of core storage required in decimal) of each routine, based on the CDC 3600, is given in Table V.

TABLE V - ETOE SUBROUTINES¹

<u>General (7048)</u>		<u>FILE1 (11556)²</u>		<u>FILE3 (30654)</u>	
/MATERL/	2343	COMMON	10000	COMMON	29444
/TAPE/	10	FILE1	737	FILE3	1210
ETOE	465	GNUFT	276		
KLOCK	101	GNUFT1	211		
ERROR	143	SMEQ	332	<u>FILE4 (32667)</u>	
READE	190	MERGE	312 ³	COMMON	29432
RTAB1	133	HOLL	134 ³	FILE4	1253
SKPMF	65	CONT	85 ³	LGCK	238
SKPMAT	92	LIST	120 ³	LEGEND	663
SKPMT	92	TAB1	177 ³	MATRIX	675
TERP1	77	TAB2	130 ³	CLEB	204
TERP	275			BLOCK	000 ⁴
AVET	268			/FACTRL/	202
ECSI	441	<u>FILE2 (27305)</u>			
COMBN1	1578	COMMON	22044		
COMBN2	573	FILE2	1101	<u>FILE5 (30151)</u>	
CNGINT	202	XILE2	1531	COMMON	28340
		RESCAT	679	FILE5	1811
		UNSCAT	512		
		EPT	662		
		SORTE	131	<u>Legendre SORT (3125)</u>	
		JFUNC	164	COMMON	2473
		CROSS	393	FILE6	652
		GAMINC	88		

1. The size of these routines is based on the CDC 3600 version as of June 1968 and is intended only as an approximation of the relative sizes of each routine. They will differ with each computer installation and each modification of the ETOE code. The COMMON is common only within an overlay and not between overlays.
2. Total does not include MERGE, HOLL, CONT, LIST, TAB1 or TAB2.
3. These routines are needed for sample problems only and may be removed (Sec. III. B).
4. Defines COMMON BLOCK /FACTRL/.

1. Tape Numbers

ETOE (with the exception of the routines needed for the sample problem, Section B) uses variable tape numbers which are defined in the ETOE main program and carried in COMMON labeled /TAPE/. At present they are input-5, output-6, ENDF/B-8, MC²-9, and two scratch tapes-18 and 19. The overlay tape 23 is not variable and is defined by the control cards and also in the CALL OVERLAY call statements in the ETOE main program.

2. Hollerith Formats

The Hollerith formats in ETOE are used to print the material descriptions. These material descriptions are obtained from the ENDF/B tape which is in binary (Mode 2); therefore the formats in ETOE must be exactly the same as the formats used to read the data originally from cards. Since the DAMMET³ program was most likely used to create the Mode 2 tape, ETOE uses the same format (17 words per card, with a 16A4,A2 format). If this format is to be changed, the changes to the ETOE program would be as follows:

- a. Change the dimension of H in COMMON /MATERL/.
- b. Change the number of words per card, NWD, in the ETOE main program.
- c. Change formats 1604 and 1605 in FILE1.
- d. Change format 1601 in the FILE2, FILE3, FILE4, FILE5, and FILE6 routines.

The MC² material identification number is also read with a Hollerith format. This must correspond to the format used in MC². It is currently A6.

3. DATA Statement

The form of the DATA statement differs between the CDC 3600 and other computers. These must be changed when changing computers. The routines that use DATA statements are FILE1, UNSCAT, JFUNC, and BLOCK.

4. Overlay Feature

The overlay feature for the CDC 3600 differs from that used by other computers. Rather than each overlay consisting of only subroutines, with overlays separated only by control cards, the CDC 3600 assumes that

every overlay consists of a main program with associated subroutines. The call to an overlay is of the form CALL OVERLAY (...) rather than a call to a subroutine within the overlay. The changes necessary for other machines are: change the call statements in the ETOE main program and change the FILE1, FILE2, FILE3, FILE4, FILE5, and FILE6 routines to subroutines (described in the next section).

5. PROGRAM Cards

The CDC computers require that each main program begin with a PROGRAM card similar to the SUBROUTINE card that begins each subroutine. Currently the main programs in ETOE are ETOE, FILE1, FILE2, FILE3, FILE4, FILE5, and FILE6. When changing computers, the PROGRAM ETOE card is removed. As discussed in the section above on overlays, the other programs are changed to subroutines by replacing the PROGRAM cards with SUBROUTINE cards.

6. Control Cards

Since the control cards will most likely change between installations, no attempt is made here to completely describe the necessary changes in control cards. The deck as distributed is set up to compile, create an overlay tape, and execute the sample problem. The EQUIP cards define the tape label on the ENDF/B and MC² tapes, and also equivalence tapes 5 and 6 to 60 and 61 (the standard input and output tapes). The FILE, OVERLAY, and FILE END cards define the overlays and the FTN and SCOPE cards define the source deck as Fortran and return the control from the compiler back to the monitor, respectively. For more information on the control cards as distributed with ETOE, refer to either a Control Data Fortran or Scope (CDC Monitor) manual.

When changing computers, all control cards (cards that are not sequenced) may be replaced. This includes the cards discussed above plus the MAIN, BANK, LOAD, and RUN cards.

7. KLOCK Subroutine

The KLOCK subroutine may have to be modified for use at various installations, depending on how the computer clock is called. The version of KLOCK distributed with ETOE calls the TIMEF(1) function which returns the time in milliseconds.

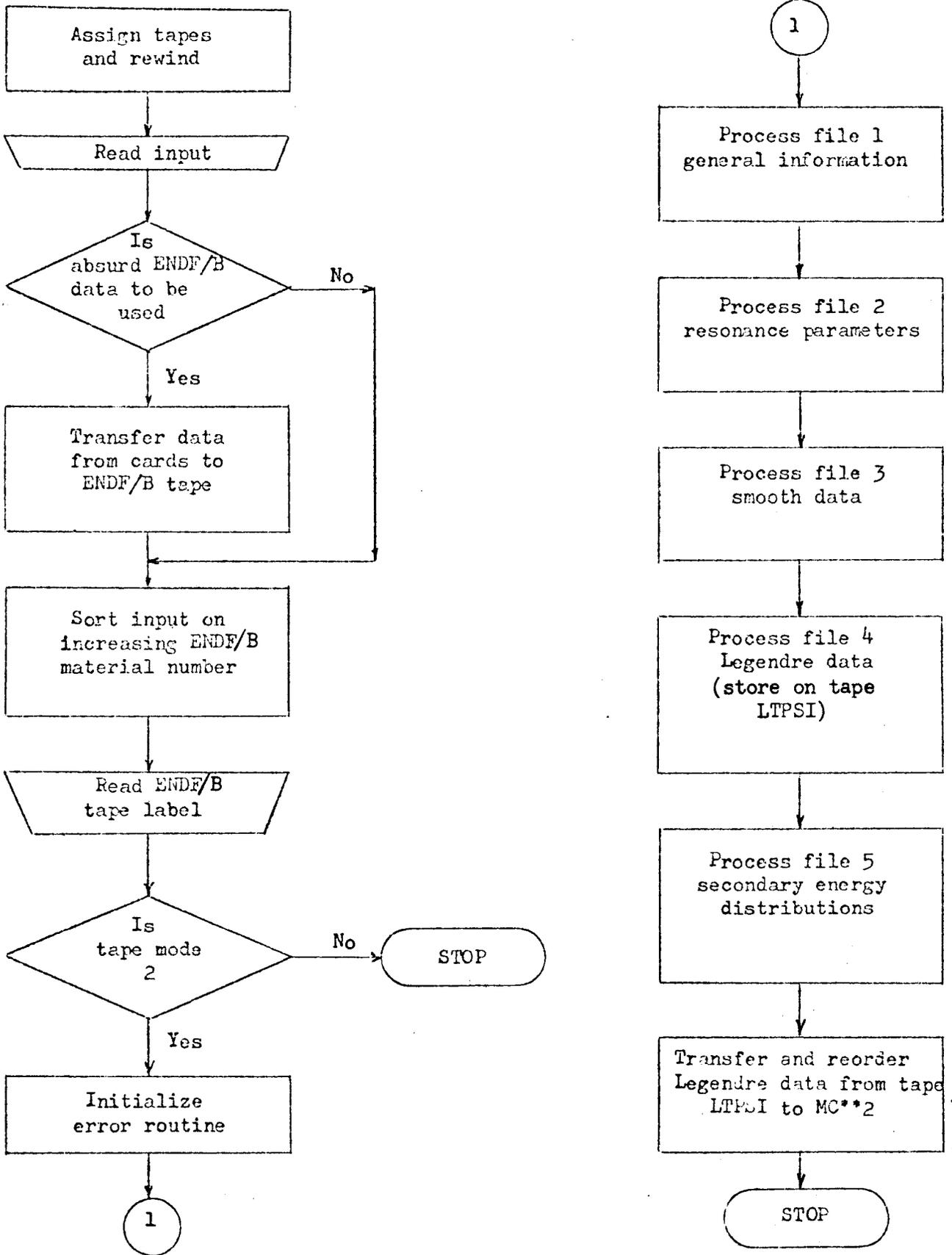


FIGURE 1 - ETOE CONTROL ROUTINE

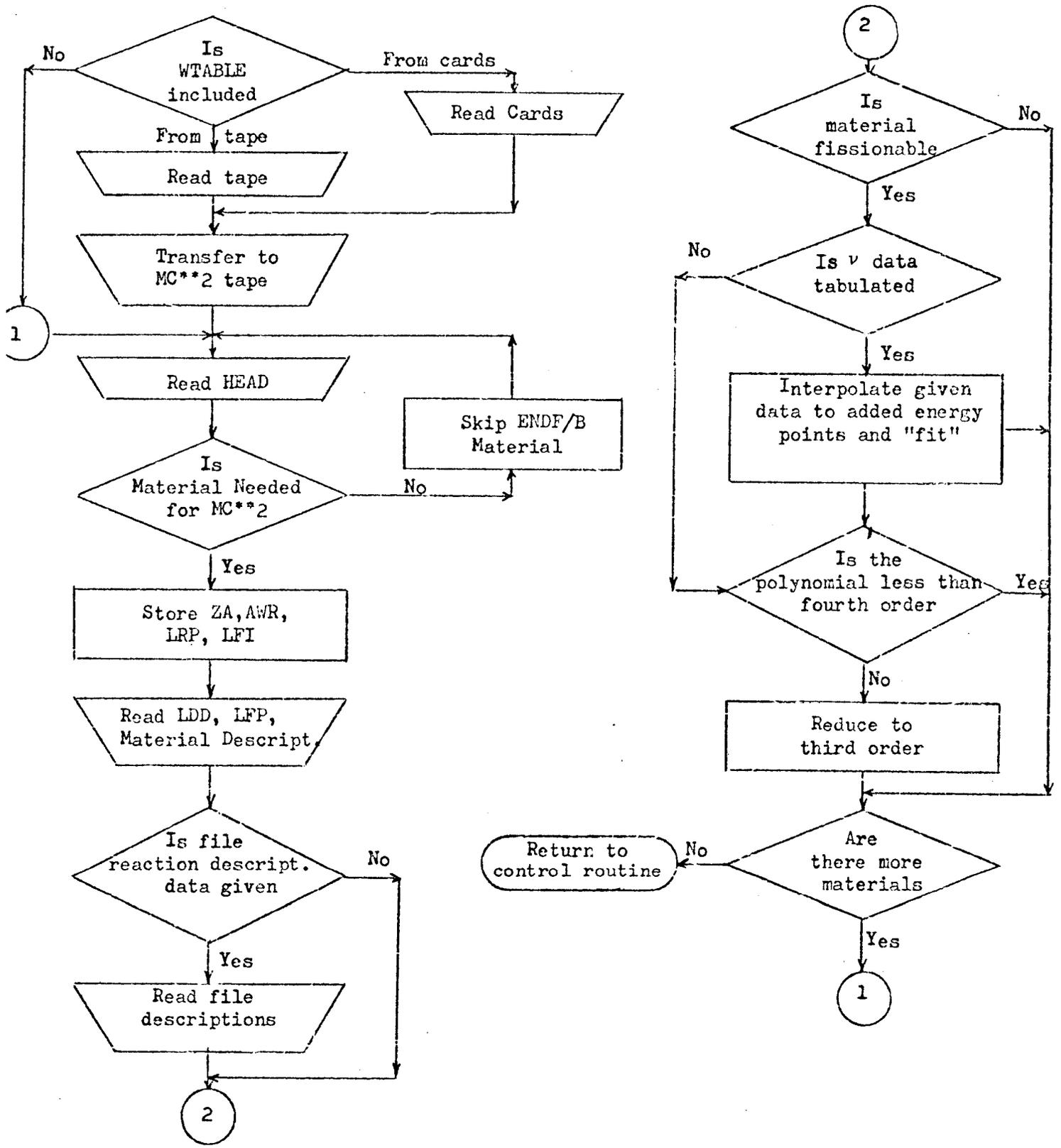


FIGURE 2 - GENERAL INFORMATION (FILE1)

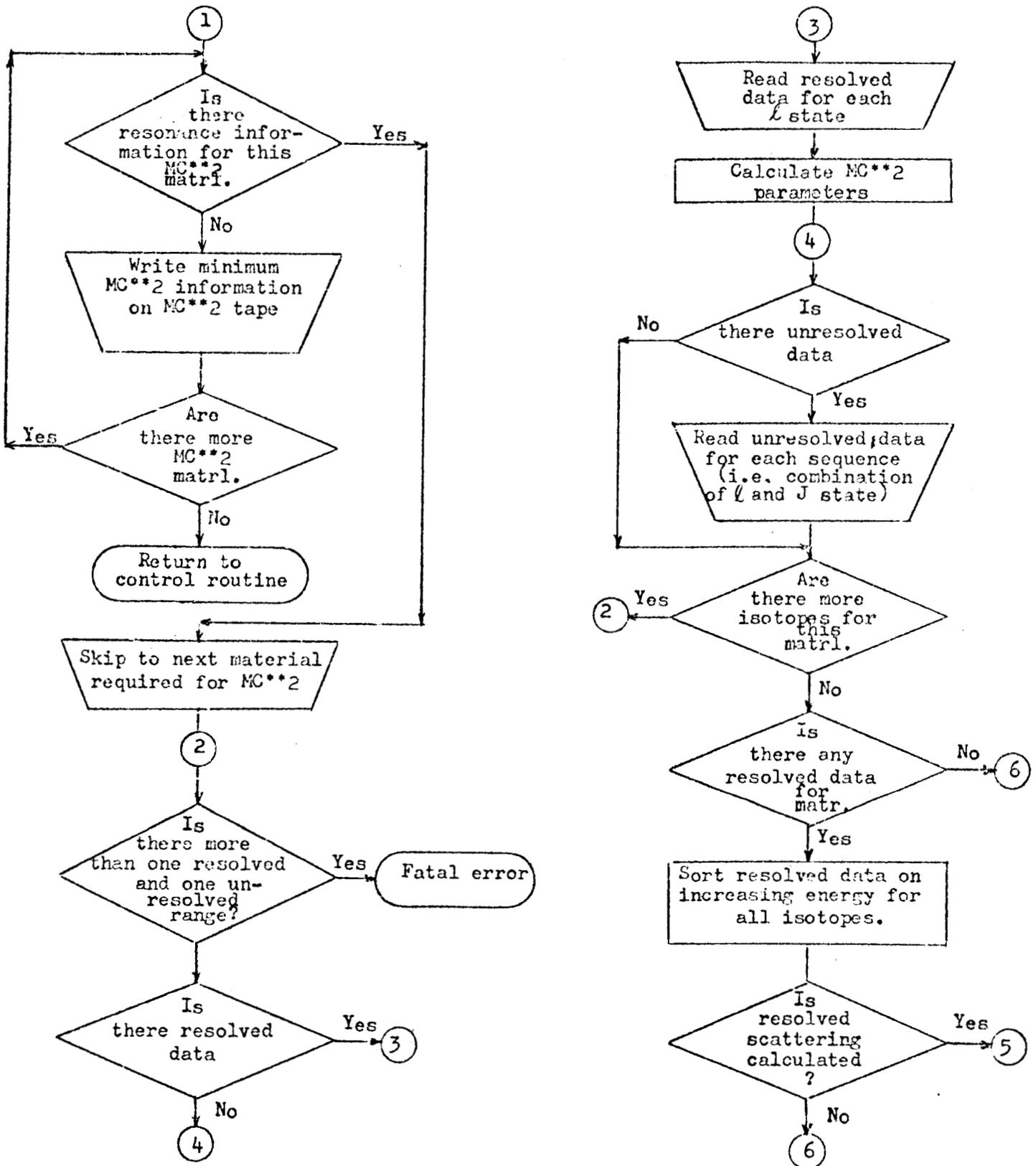


FIGURE 3 - RESONANCE PARAMETERS (FILE2)

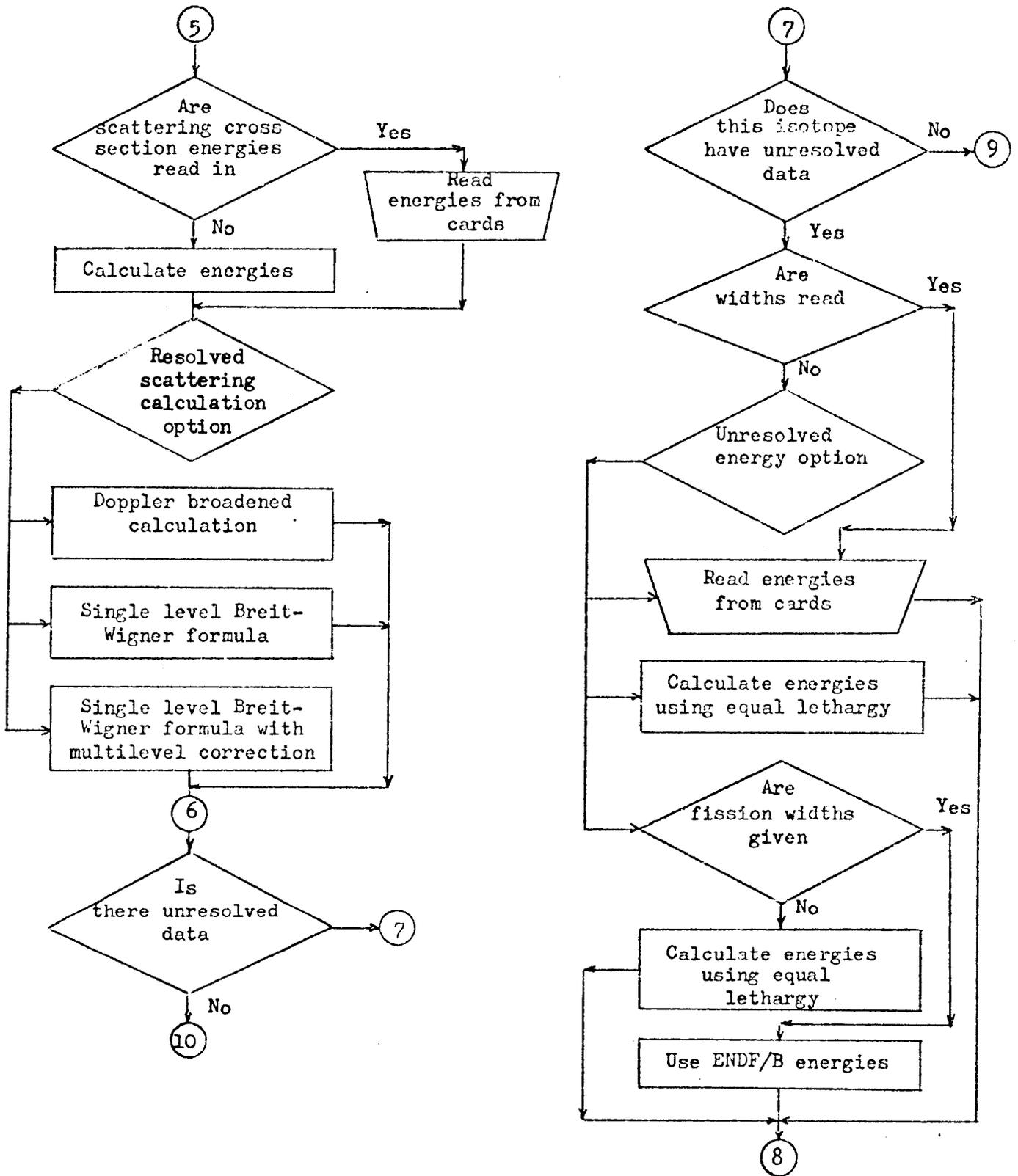


FIGURE 3 - (Continued)

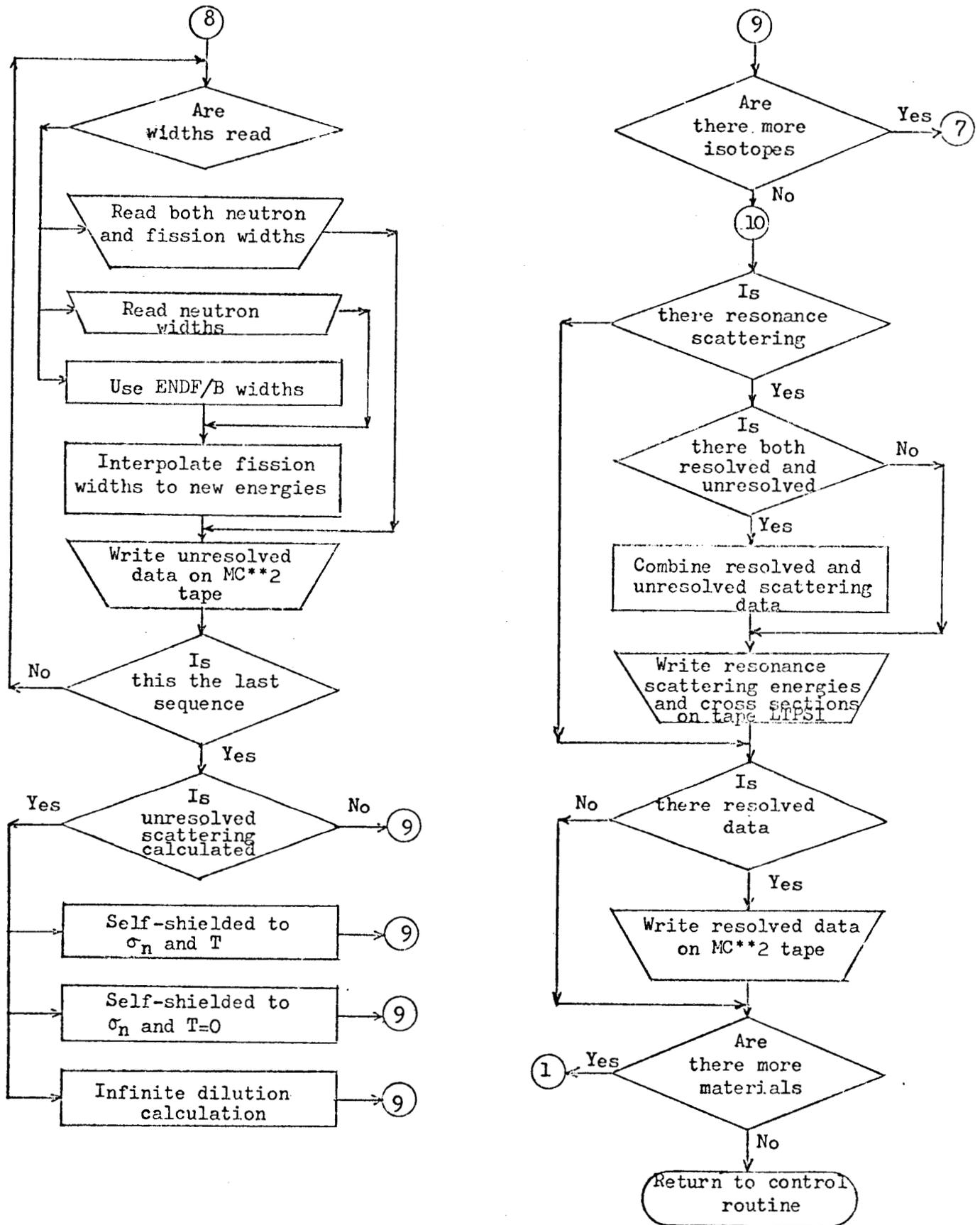


FIGURE 3 (Cont'd)

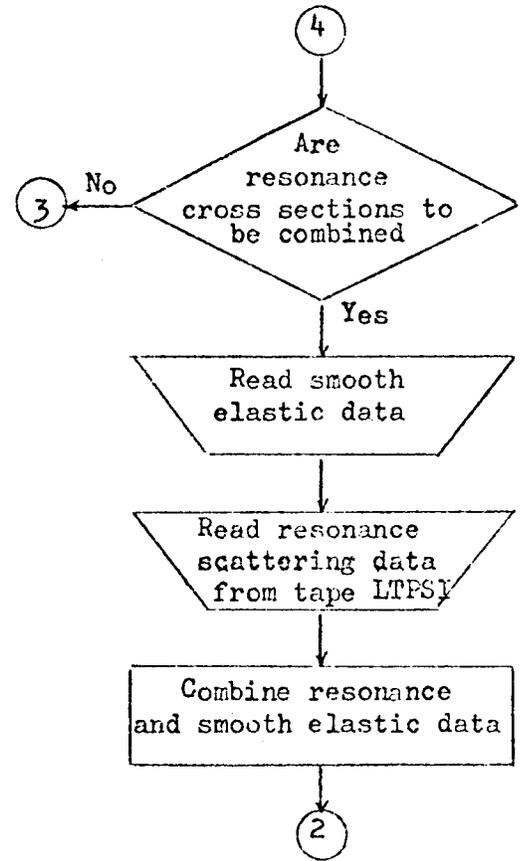
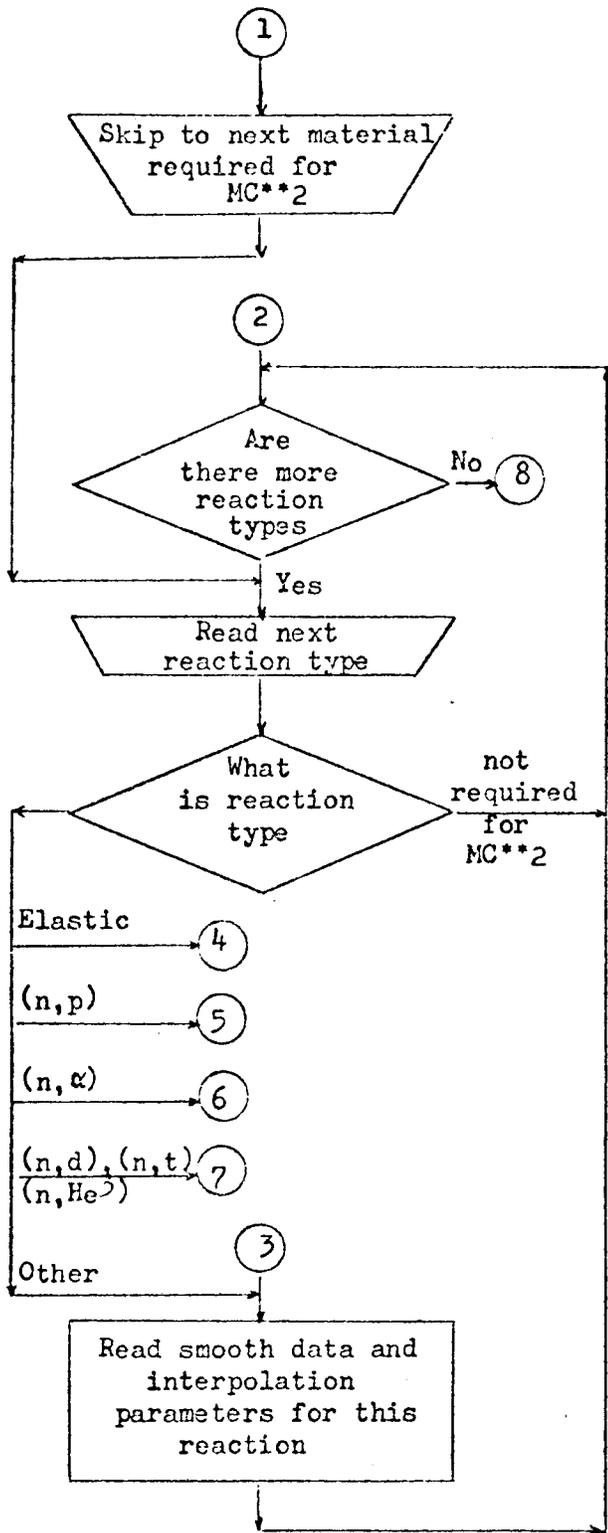


FIGURE 4 - SMOOTH DATA (FILE3)

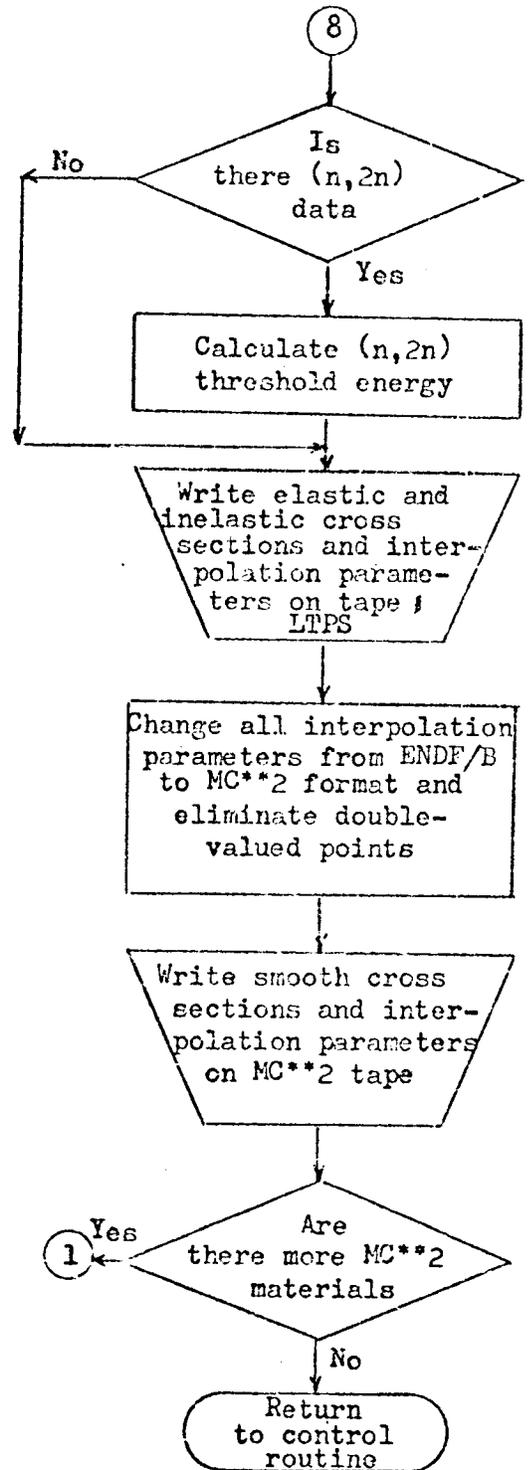
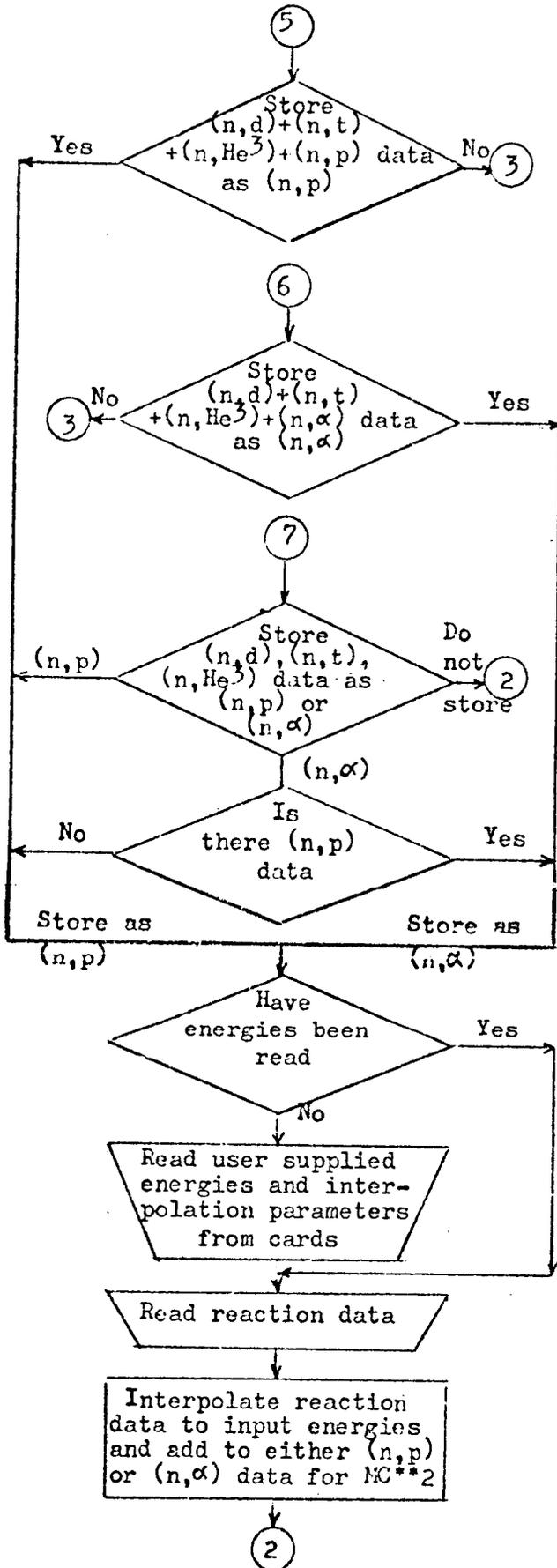


FIGURE 4 - (Continued)

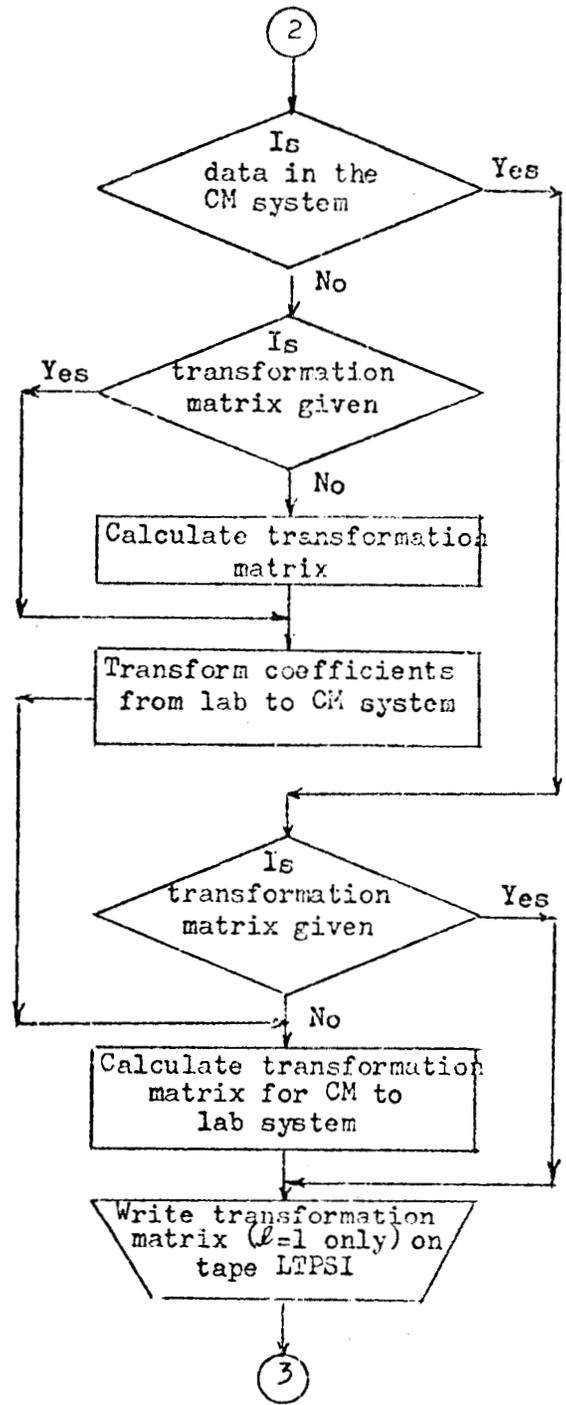
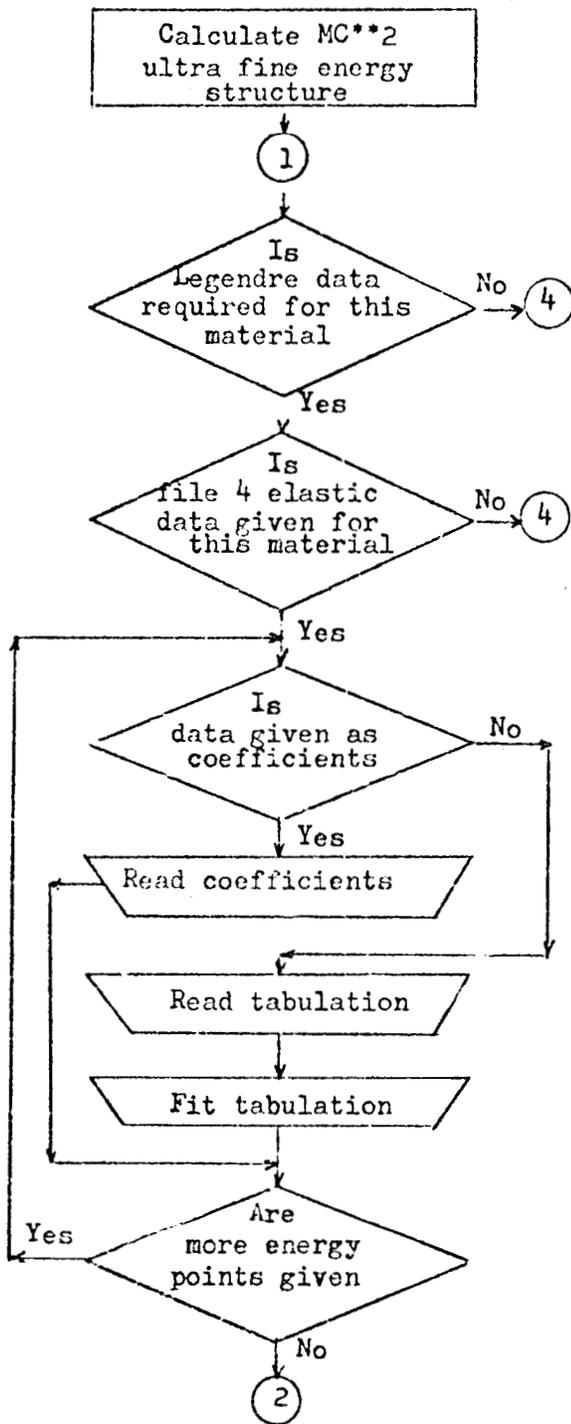


FIGURE 5 - LEGENDRE POLYNOMIAL DATA (FILE4)

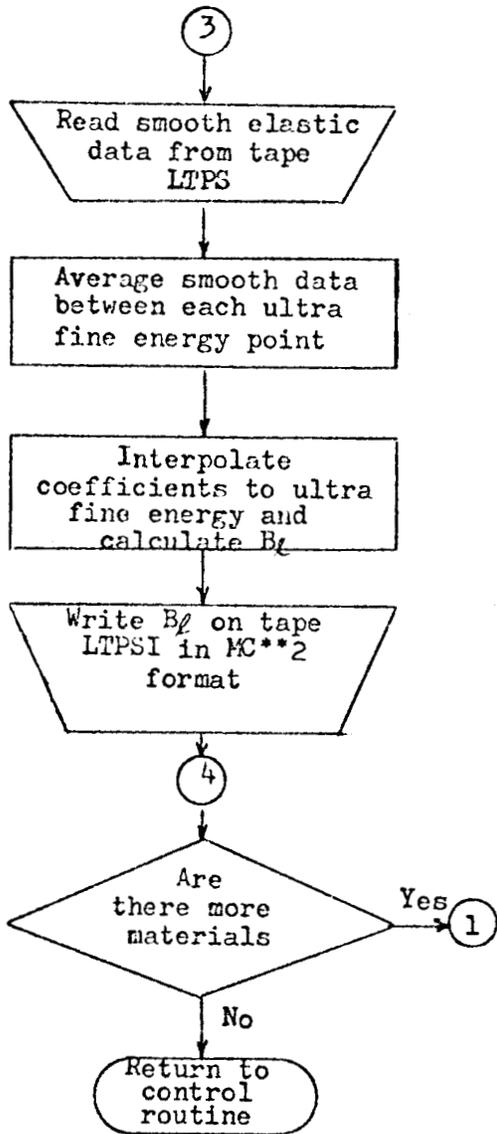


FIGURE 5 - (Continued)

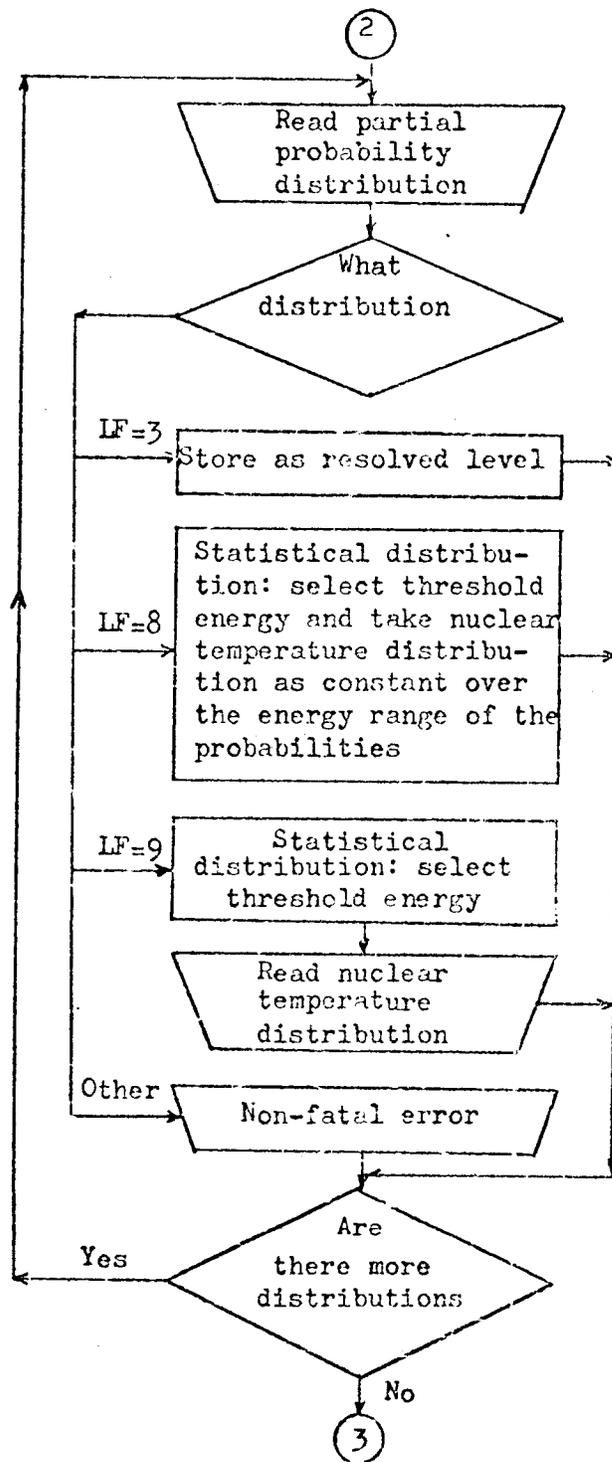
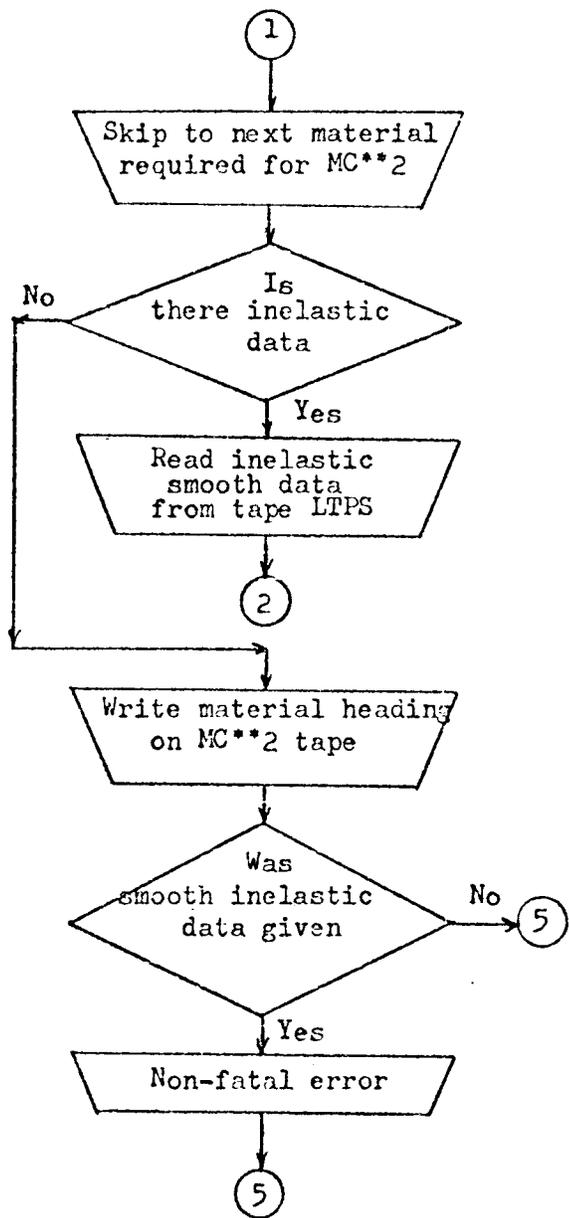


FIGURE 6 - SECONDARY ENERGY DISTRIBUTIONS (FILE5)

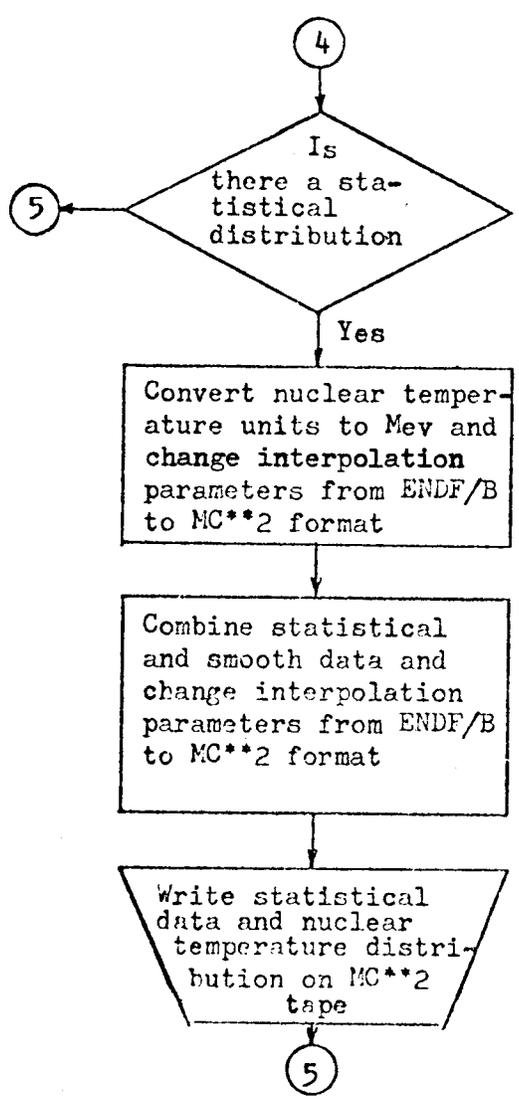
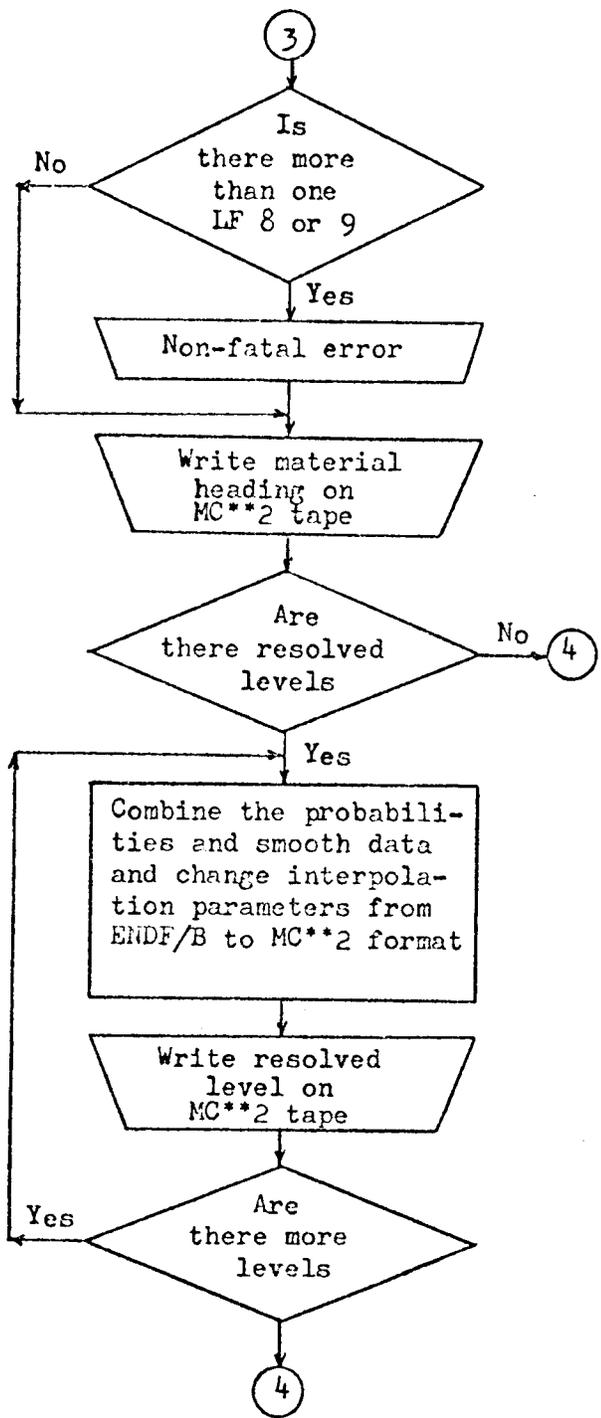


FIGURE 6 - (Continued)

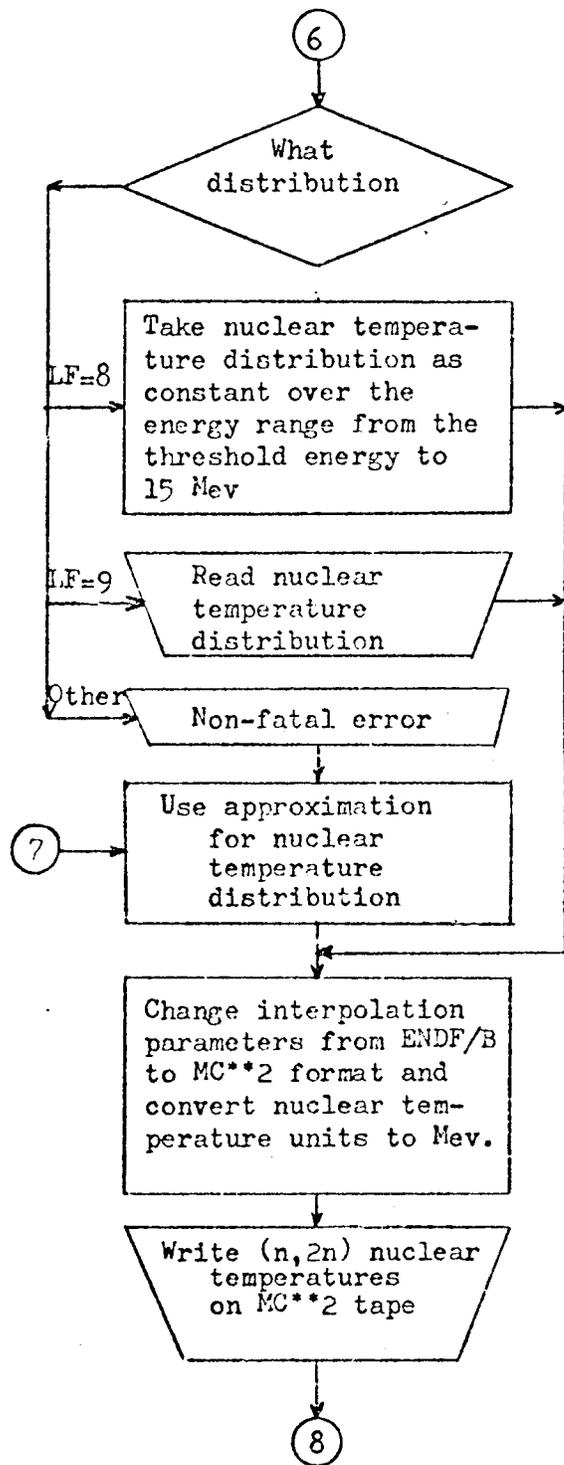
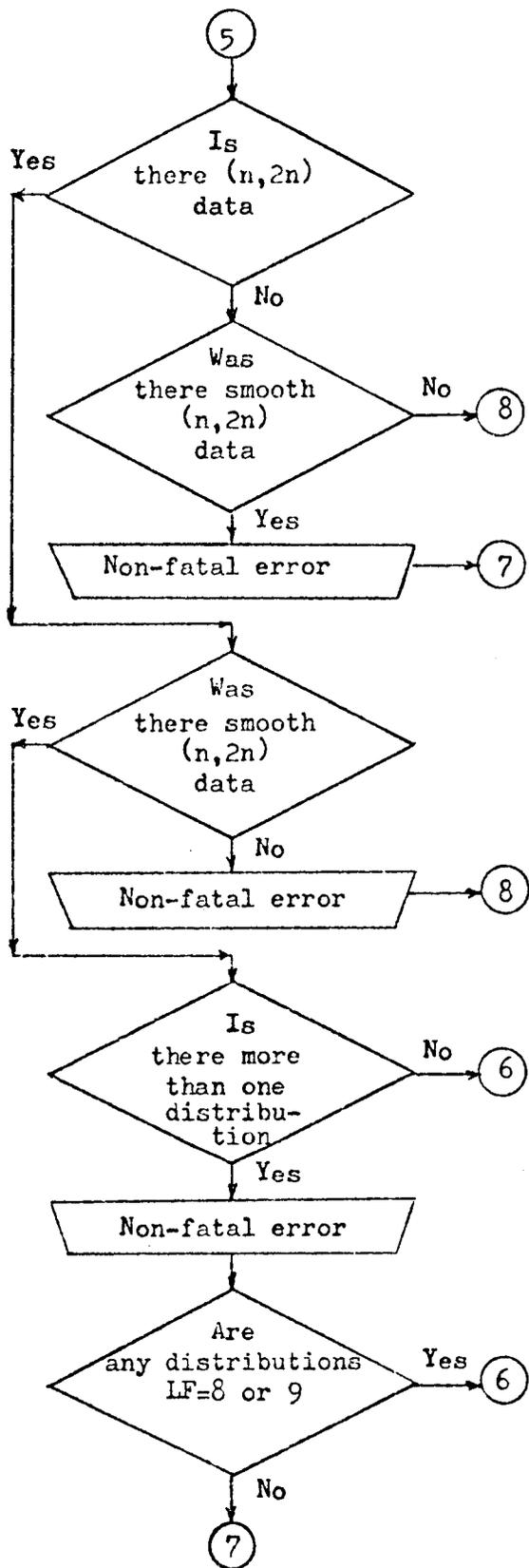


FIGURE 6 - (Continued)

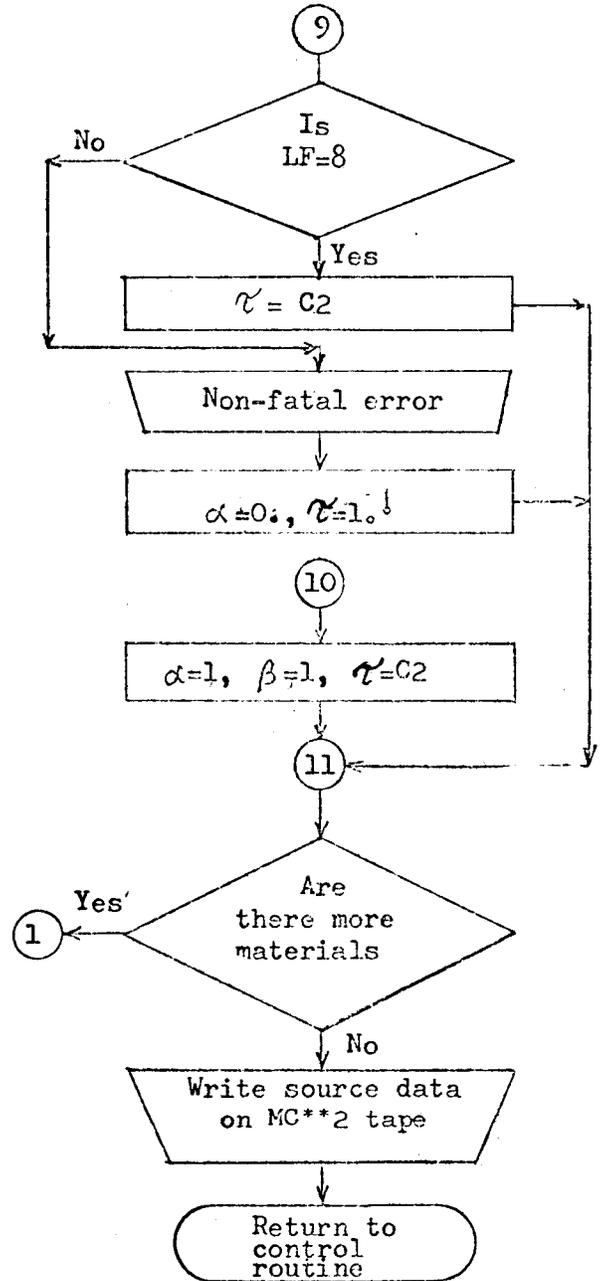
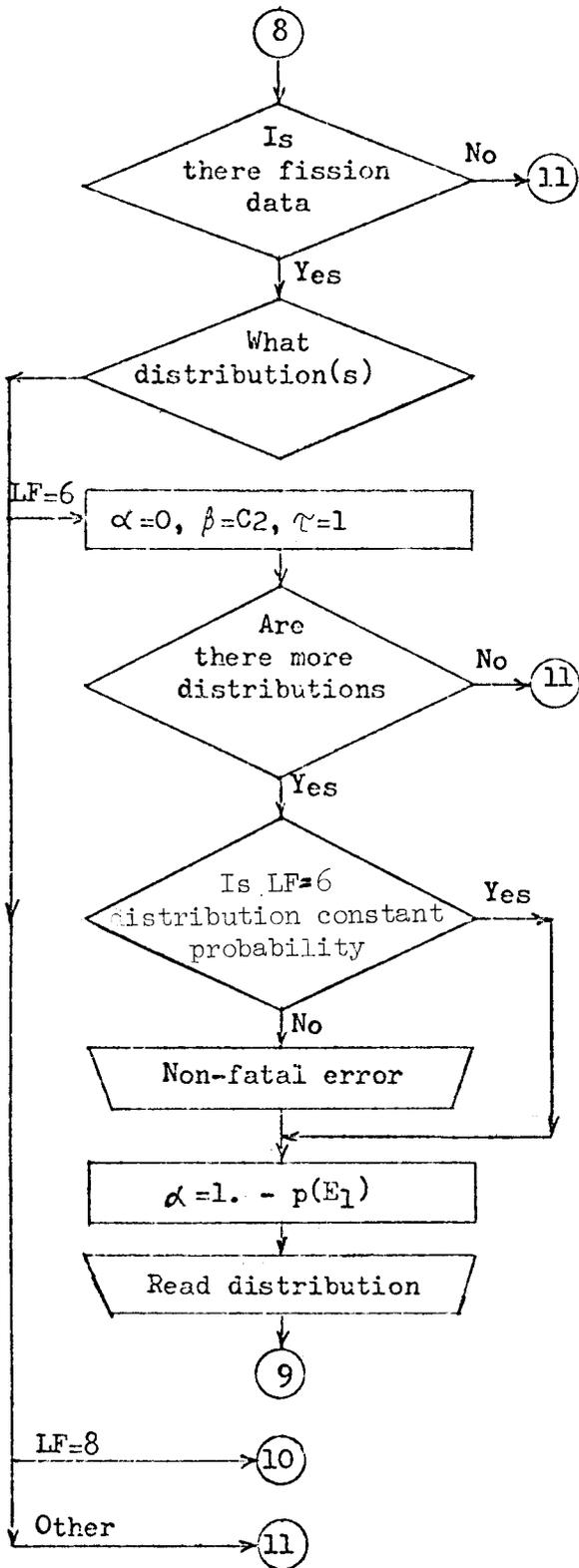


FIGURE 6 - (Continued)

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