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MC^2-2: A Code to Calculate Fast Neutron Spectra and Multigroup Cross Sections

by

H. Henryson II, B. J. Toppel,
and C. G. Stenberg

BASE TECHNOLOGY

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Applied Physics Division

June 1976

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MC^2-2: A CODE TO CALCULATE FAST NEUTRON SPECTRA AND MULTIGROUP CROSS SECTIONS

CODE ABSTRACT

1. Program Identification: MC^2-2

2. Computer for which program is designed and others on which it is operable: IBM 370/195, any IBM OS system with 600K core, CDC 7600.

3. Description of Function: MC^2-2 solves the neutron slowing down equations to determine spectra for use in generating multigroup neutron cross sections.

4. Method of Solution: The extended transport P_1, B_1, consistent P_1, and consistent B_1 fundamental mode ultra-fine-group equations are solved using continuous slowing down theory and multigroup methods. Fast and accurate resonance integral methods are used in the narrow resonance resolved and unresolved resonance treatments. Multigroup neutron cross sections are generated for arbitrary group structures. A hyper-fine-group integral transport slowing down calculation is available on option to treat the low energy spectrum where the narrow resonance approximation is not valid.

5. Restrictions: Variable dimensioning is used throughout the program so that computer core requirements depend on a variety of problem parameters. Space requirements range from 400K bytes to 800K bytes on IBM equipment depending on the complexity of the problem.

6. Running Time: An 1740 group consistent P_1 homogeneous twelve isotope problem with 27 broad groups requires about 4.2 min. CPU and 6 min. PP time on an IBM 370/195. The same problem requires approximately 30% less CPU time on the CDC 7600.

7. Unusual Features of the Program: Extreme flexibility is provided in specifying the rigor of a calculation including a choice of four distinct slowing down treatments: multigroup, improved and standard Greuling-Goertzel continuous slowing down, and integral transport theory. All binary data transfers are localized in standard subroutines REED/RITE. Broad group cross section files may be generated in the ARC System XS.ISO[1] and/or CCCC ISOTXS[2] formats.

8. Related and Auxiliary Programs: Input data files required by MC^2-2 may be generated from ENDF/B data[3] by the code ETOE-2[4]. The hyper-fine-group integral transport theory module of MC^2-2, RABANL, is an improved version of the RABBLE[5]/RABID[6] codes. Many of the MC^2-2 modules are used in the SDX[7] code.

9. Status:

10. References: H. Henryson II, B. J. Toppel, C. G. Stenberg, "MC^2-2: A Code to Calculate Fast Neutron Spectra and Multigroup Cross Sections," Argonne National Laboratory, ANL-8144 (1976).

11. Machine Requirements: A large amount of fast peripheral storage is required. Core requirements depend on problem complexity but virtually any reasonable problem may be executed on IBM equipment with 800K bytes or CDC equipment with 50,000 words of SCM and 100,000 words of directly addressable LCM.

12. Programming Language Used: FORTRAN IV. Both IBM and CDC versions of MC^2-2 contain a few Assembler language routines.

13. Operating System or Monitor under which Program is Executed: The IBM version of MC^2-2 may be executed under OS or VS operating systems and compiled using the Fortran H or program product compilers with the highest level of optimization. The CDC 7600 version of MC^2-2 has been implemented on both the LRL Berkeley and Brookhaven National Laboratory computers with their special COKE/SCOPE operating systems. The SEGMENTATION LOADER is required and directly addressable LCM is used. The code was compiled using the FORTRAN Extended Compiler under OPT=1 optimization.

14. Any Other Programming or Operating Information or Restrictions:

15. Name and Establishment of Authors:

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B. J. Toppel
C. G. Stenberg
Applied Physics Division
Argonne National Laboratory
Argonne, Illinois 60439

16. Material Available: Separate tapes are available for the IBM and CDC versions of MC^2-2. The MC^2-2 package includes:

i) Source decks
ii) Test problem input decks
iii) Test problem output
iv) Eight binary library files processed from ENDF/B-IV
v) Source code and BCD library files to generate binary libraries
vi) Reference report

17. Category: B
Keywords: cross sections, group constants, spectra, multigroup, resonance, B_L method, P_L method, slowing down, infinite media, homogeneous, heterogeneous, ENDF/B, cell calculation

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ABSTRACT

MC^2-2 is a program to solve the neutron slowing down problem using basic neutron data derived from the ENDF/B data files. The spectrum calculated by MC^2-2 is used to collapse the basic data to multigroup cross sections for use in standard reactor neutronics codes. Four different slowing down formulations are used by MC^2-2: multigroup, continuous slowing down using the Goertzel-Greuling or Improved Goertzel-Greuling moderating parameters, and a hyper-fine-group integral transport calculation. Resolved and unresolved resonance cross sections are calculated accounting for self-shielding, broadening and overlap effects. This document provides a description of the MC^2-2 program. The physics and mathematics of the neutron slowing down problem are derived and detailed information is provided to aid the MC^2-2 user in preparing input for the program and implementation of the program on IBM 370 or CDC 7600 computers.

I. INTRODUCTION

MC^2-2 is a program for solving the neutron slowing down problem to determine a detailed spectrum for use in deriving multigroup cross sections. The code has been developed to satisfy the need for a rigorous and computationally efficient capability which can serve as a standard for fast reactor calculations. Recent advances in neutron slowing down theory, resonance theory, and numerical methods have been incorporated into the MC^2-2 calculation. A large number of options are available which permit great flexibility in specifying the rigor of a calculation.

The MC^2-2 code was developed at Argonne National Laboratory in the ARC System[1] environment. The programming was performed with strict adherence to the standards established by the Committee on Computer Code Coordination[2]. As a consequence the modifications required to develop standalone versions of the code for alternative computer configurations are minor. Both IBM and CDC standalone versions of the code have been implemented. The program is structured in eight principal modules (overlays):

1) Input Processor (CSI010)

2) Unresolved Resonance Calculation (CSC004)

3) Resolved Resonance Calculation (CSC005)

4) Resolved-Unresolved Resonance Interaction (CSC006)

5) Macroscopic Data Processing (CSC007)

6) Ultra-Fine-Group Spectrum Calculation and Broad-Group Cross Section Collapse (CSC008)

7) Hyper-Fine-Group Integral Transport Spectrum Calculation - RABANL (CSC009)

8) Broad-Group Spectrum Calculation (CSC010)

Figure 1 indicates the program flow through these modules. The basic data required by MC^2-2 are structured in eight data files. The file formats are provided in Appendix C. These data files may be created from the ENDF/B data[3] by the program ETOE-2[4]. Multigroup cross sections generated by MC^2-2 are processed in the ARC System XS.ISO[1] and/or the CCCC ISOTXS[2] formats. These structures are included in Appendix C for the sake of completeness.

The major features of MC^2-2 include:

1. the ability to specify the rigor of a calculation through input options,

2. P_1, B_1, consistent P_1 and consistent B_1 extended transport theory algorithms,

3. multigroup, improved or standard Greuling-Goertzel continuous slowing down theory solutions,

4. hyper-fine-group integral transport theory solutions,

5. flexible broad group structures in a choice of formats,

6. consistent treatment of all ENDF/B Version III and Version IV data formats,

7. fast and accurate resonance integral treatment of Breit-Wigner and Adler-Adler resolved resonances,

8. fast and accurate treatment of unresolved resonances including interference scattering and same-sequence overlap effects,

9. isotope dependent fission spectra,

10. inhomogeneous source calculation,

11. buckling search or group dependent buckling calculations,

12. flexible output options.

This report is organized into seven chapters which are intended to provide the physics, mathematics and code user documentation for the program MC^2-2. Chapter II contains the theoretical development of all the methods and approximations used in the ultra-fine-group fundamental mode spectrum calculation of MC^2-2. Chapter III contains the information relevant to the calculation of resonance integrals from resolved resonance parameters and Chapter IV is concerned with the calculation of cross sections and resonance integrals from average parameters in the unresolved resonance energy regions. Chapter V describes the RABANL module of the code MC^2-2. The RABANL calculation is a hyper-fine-group integral transport slowing down calculation which treats resolved resonance absorption rigorously. The module is modeled after the resonance absorption codes RABBLE[5] and RABID.[6] Chapter VI provides a guide for user application and Chapter VII contains information relevant to the programming of MC^2-2.

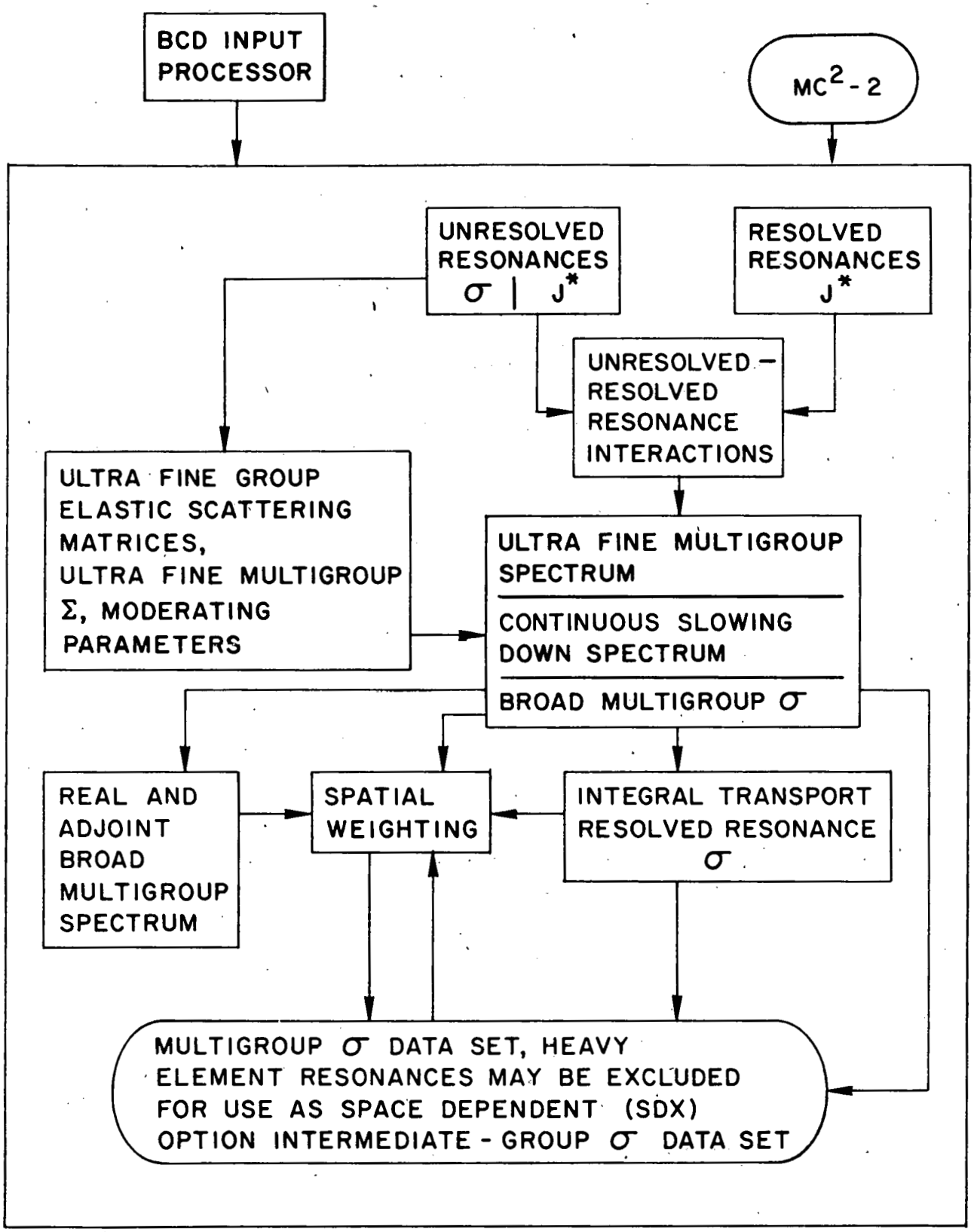

Fig. 1. MC^2-2 Program Flow

II. FUNDAMENTAL MODE SPECTRUM CALCULATION

A. P_1 and B_1 Extended Transport Equations

The time independent transport equation is written

$$\nabla \cdot \underline{\Omega}\,\psi + \Sigma_t\,\psi(\underline{r},\, u,\, \underline{\Omega}) = \iiint du'\, d\Omega'\, \psi(\underline{r},\, u',\, \underline{\Omega}') \cdot$$

$$\Sigma_s\,(u' \to u,\, \underline{\Omega} \cdot \underline{\Omega}') + S(\underline{r},\, u)/4\pi \qquad \text{(II.1)*}$$

where ψ is the flux defined such that $\psi dV du d\Omega$ is the flux in the volume dV about $\underline{r}$, in the element of solid angle $d\Omega$ about $\underline{\Omega}$, in the lethargy range du about u. The lethargy u is defined as $\ell n(E_o/E)$. Similarly S is the isotropic source density in the same element of phase space and includes contributions due to fission and/or sources independent of the flux ψ. The macroscopic total cross section is denoted by Σ_t and the macroscopic scattering transfer cross section by Σ_s. If one assumes a homogeneous mixture so that the above quantities are not space dependent and makes use of the fundamental mode ansatz

$$\psi(\underline{r},\, u,\, \underline{\Omega}) \equiv \psi(u,\, \underline{\Omega}) e^{i\underline{B}\cdot\underline{r}};\quad S(\underline{r},\, u) \equiv S(u) e^{i\underline{B}\cdot\underline{r}} \qquad \text{(II.2)}$$

then Eq. II.1 may be written,

$$(\Sigma_t + i\underline{B} \cdot \underline{\Omega})\,\psi(u,\, \underline{\Omega}) = \iiint du'\, d\Omega'\, \psi(u',\, \underline{\Omega}')\, \Sigma_s(u' \to u,\, \mu_o)$$

$$+ S(u)/4\pi \qquad \text{(II.3)}$$

where $\mu_o \equiv \underline{\Omega} \cdot \underline{\Omega}'$. In order to simplify the notation, consider only plane geometry. Expanding the flux and scattering transfer cross section in spherical harmonics,

$$2\pi\,\psi(u,\, \underline{\Omega}) = \psi(u,\, \mu) = \sum_{\ell=0}^{\infty} \frac{2\ell + 1}{2}\, \phi_\ell(u)\, P_\ell(\mu)$$

$$\Sigma_s(u' \to u,\, \mu_o) = \sum_{\ell=0}^{\infty} \frac{2\ell + 1}{2}\, \Sigma_s^\ell(u' \to u)\, P_\ell(\mu_o) \qquad \text{(II.4)}$$

where $P_\ell(\mu)$ is the ℓ^{th} order Legendre polynomial, substituting into Eq. II.3 and making use of the addition theorem for Legendre polynomials yields

---

*Equation numbering convention of the form N.n is used where N is the chapter number and n is the equation number in Chapter N.

$$iB\mu\ \psi(u,\ \mu) + \Sigma_t\ \psi(u,\ \mu) = \sum_{\ell=0}^{\infty} \frac{2\ell + 1}{2} \iint du'\ d\mu\ \Sigma_s^{\ell}(u' \to u)\ \phi_{\ell}(u')\ P_{\ell}(\mu) + \frac{S(u)}{2} \qquad \text{(II.5)}$$

Multiplying by $P_{\ell}(\mu)$, integrating over the range of μ, and using the recursion relation gives

$$\frac{\ell + 1}{2\ell + 1}\ iB\phi_{\ell+1}(u) + \frac{\ell}{2\ell + 1}\ iB\phi_{\ell-1}(u) + \Sigma_t\phi_{\ell}(u) = S(u)\ \delta_{\ell}^{o} + \int dE'\ \Sigma_s^{\ell}(u' \to u)\ \phi_{\ell}(u') \qquad \ell = 0,\ 1,\ \ldots,\ \infty$$

$$\phi_{-1}(u) = 0\ . \qquad \text{(II.6)}$$

Two well known approximations to this infinite set of coupled equations are the P_N and B_N methods[8]. The P_N approximation assumes

$$\phi_{N+1} = 0, \qquad \text{(II.7a)}$$

and the B_N approximation assumes

$$\int du'\ \Sigma_s^{\ell}(u' \to u)\ \phi_{\ell}(u') = 0 \qquad \ell > N$$

which is equivalent to taking

$$\phi_{N+1} = \phi_N \frac{Q_{N+1}\ (-\ \Sigma_t/iB)}{Q_N(-\ \Sigma_t/iB)} \qquad \text{(II.7b)}$$

where $Q_{\ell}(x)$ is a Legendre function of the second kind. Using Eq.II.7a or II.7b, Eqs. II.6 may be written

$$\frac{\ell + 1}{2\ell + 1}\ iB\phi_{\ell+1} + \frac{\ell}{2\ell + 1}\ iB\phi_{\ell-1} + \Sigma_t\phi_{\ell} = S(u)\ \delta_{\ell}^{o} + \int du'\ \Sigma_s^{\ell}(u' \to u)\ \phi_{\ell}(u') \qquad \ell = 0,\ 1,\ \ldots,\ N - 1$$

$$\frac{N}{2N + 1}\ iB\phi_{N-1} + \gamma\Sigma_t\phi_N = \int du'\ \Sigma_s^{N}(u' \to u)\ \phi_N(u')$$

$$\phi_{-1} = 0$$

$$\gamma = \begin{cases} 1 & P_N \\ 1 + \dfrac{N + 1}{2N + 1}\ \dfrac{iB}{\Sigma_t}\ \dfrac{Q_{N+1}\ (-\ \Sigma_t/iB)}{Q_N\ (-\ \Sigma_t/iB)} & , \quad B_N \end{cases} \qquad \text{(II.8)}$$

The set of Eqs. II.8 may be further simplified by use of the extended transport approximation[9] which assumes that anisotropic scattering takes place without a change in lethargy so that

$$\int du' \, \Sigma_s^{\ell}(u' \to u) \, \phi_{\ell}(u') = \Sigma_s^{\ell}(u) \, \phi_{\ell}(u) \qquad \ell = 2, \ldots, N \tag{II.9}$$

where

$$\Sigma_s^{\ell}(u) \equiv \int du' \, \Sigma_s^{\ell}(u \to u').$$

Using Eq.II.9 in Eqs.II.8 one obtains the consistent P_1 and B_1 order N extended transport equations.

$$iB\phi_1(u) + \Sigma_t\phi_0(u) = \varepsilon(u) + \int du' \, \Sigma_s^0(u' \to u) \, \psi_0(u')$$

$$\frac{iB}{3} \phi_0(u) + A_1(B, u, N) \, \phi_1(u) = \int du' \, \Sigma_s^1(u' \to u) \, \phi_1(u') \tag{II.10}$$

$$\phi_{\ell}(u) = - \frac{\ell}{2\ell + 1} \, iB \, \phi_{\ell-1}(u)/A_{\ell}(B, u, N) \qquad \ell = 2, \ldots, N$$

where

$$A_{\ell}(B, u, N) = b_{\ell-1} + \frac{a_{\ell}}{b_{\ell}+} \, \frac{a_{\ell+1}}{b_{\ell+1}+} \cdots \frac{a_{N-1}}{b_{N-1}}$$

$$a_{\ell} = \frac{\ell + 1}{2\ell + 1} \, \frac{\ell + 1}{2(\ell + 1) + 1} \, B^2 \qquad 1 \leq \ell \leq N - 1 \tag{II.11}$$

$$b_0 = \begin{cases} \Sigma_t(u), & P_1 \\ \Sigma_t(u), & B_1, \; N > 1 \\ \gamma\Sigma_t(u) = \dfrac{B \tan^{-1} B/\Sigma}{3(1 - \frac{\Sigma}{B} \tan^{-1} \frac{B}{\Sigma})}, & B_1, \; N = 1 \end{cases}$$

$$b_{\ell} = \begin{cases} \Sigma_t(u) - \Sigma_s^{\ell+1}, & P_1 \\ & \ell = 1, 2, \ldots, N - 1 \\ \Sigma_t(u) - \Sigma_s^{\ell+1}(u) + \dfrac{N + 1}{2N + 1} \, iB \, \dfrac{Q_{N+1}(-\Sigma_t/iB)}{Q_N(-\Sigma_t/iB)} \, \delta_{\ell}^{N-1}, & B_1 \end{cases}$$

The consistent P_1 and B_1 Eqs.II.10 with the continued fraction definitions of Eqs.II.11 reduce to the standard forms programmed in the MC^2[10] and GAM[11] co if one takes the order of the extended transport approximation, N, as unity.

The inconsistent P_1 and B_1 equations are obtained by assuming that Eq. II.9 is applicable for $\ell = 1$. In this case the P_1 integral of Eqs. II.10 disappears and the coefficient b_0 of the continued fraction is modified,

$$b_\ell = \begin{cases} \Sigma_t(u) - \Sigma_s^{\ell+1}(u), & P_1 \\ & \ell = 0, 1, \ldots, N-1 \\ \Sigma_t(u) - \Sigma_s^{\ell+1}(u) + \dfrac{N+1}{2N+1} iB \dfrac{Q_{N+1}(-\Sigma_t/iB)}{Q_N(-\Sigma_t/iB)} \delta_\ell^{N-1}, & B_1 \end{cases} \qquad \text{(II.12)}$$

The sets of Eqs. II.10, II.11 and II.12 define the four spectrum options, consistent and inconsistent P_1 and B_1 extended transport approximations, which are available in the ultra-fine-group spectrum calculations of the MC^2-2 code. The following sub-sections will discuss the methods by which these equations are solved.

B. Source Term

The source term of Eqs. II.10, $S(u)$, describes neutron sources due to fission and inhomogeneous sources independent of the flux. The source is assumed to be isotropic in the laboratory system. In MC^2-2 scattering sources due to inelastic and (n,2n) scattering are also assumed isotropic and it is convenient to include these scattering sources as components of $S(u)$. With this convention the equations of Section II.A above are applicable if $\Sigma_s^\ell(u' \to u)$ is taken to be the elastic scattering transfer cross section and $S(u)$ is defined

$$S(u) = \frac{1}{k} S_f(u) + S_{ne}(u) + S_{fix}(u) \qquad \text{(II.13)}$$

$S_f(u) \equiv$ fission source

$S_{ne}(u) \equiv$ non-elastic scattering source

$S_{fix}(u) \equiv$ inhomogeneous source

The fission source has the form

$$S_f(u) = \sum_i \chi_i(u) N_i \int du' \, \nu_i(u') \sigma_{f_i}(u') \phi(u') \qquad \text{(II.14)}$$

where the sum is over all isotopes in the mixture, N_i is the atom density of isotope i, $\chi_i(u)$ is the fraction of fission neutrons emitted in the lethargy range du about u for isotope i, $\nu_i(u)$ is the number of neutrons emitted per fission for isotope i, $\sigma_{f_i}(u)$ is the microscopic fission cross section for isotope i. The fission spectrum distribution $\chi_i(u)$ may actually depend upon the fission lethargy, but such a possibility is not permitted by the MC^2-2 code. An option is available in the code to assign library fission

spectra to problem isotopes thus permitting a single fission spectrum distribution for all fissionable isotopes. The scalar k of Eq.II.13 has the value unity if $S_{fix}(u) \neq 0$. If $S_{fix}(u) = 0$, then Eqs.II.10 have a solution only if k is the eigenvalue of the system of equations.

C. Continuous Slowing Down Theory

Two sets of algorithms for the solution of Eqs.II.10 are available in the MC^2-2 code, multigroup and continuous slowing down theory. In this section the form of the continuous slowing down equations treated by MC^2-2 is derived. The algorithms are based on the work of Stacey[12] and are included in this report to provide a self-contained presentation for the convenience of the reader. A general review of continuous slowing down theory has been prepared by Stacey[13].

The ℓ-th order angular component of the elastic slowing down density is defined

$$\bar{q}_\ell(u) \equiv \sum_i \int_{u-\ell n^1/\alpha_i}^{u} du' \int_{u}^{u'+\ell n^1/\alpha_i} du'' \, \Sigma_{s_i}^{\ell}(u' \to u'') \, \phi_\ell(u') \qquad \text{(II.15)}$$

where

$$\alpha_i = \left(\frac{A_i - 1}{A_i + 1} \right)^2$$

A_i = mass of isotope i/neutron mass

$\Sigma_{s_i}^{\ell}(u' \to u) \equiv$ macroscopic elastic scattering transfer cross section for isotope i

The scattering transfer cross sections of Eqs.II.4 and II.10 are given by

$$\Sigma_s^{\ell}(u' \to u) = \sum_i \Sigma_{s_i}^{\ell}(u' \to u)$$

as a consequence of the conventions assumed in Section II.B. It is convenient to define an elastic transfer kernel $P_i^{\ell}(u' \to u)$ and a slowing down kernel $K_i^{\ell}(u' \to u)$ in the following manner,

$$\Sigma_{s_i}^{\ell}(u' \to u) = \Sigma_{s_i}(u') \, P_i^{\ell}(u' \to u) \qquad \text{(II.16)}$$

$$K_i^{\ell}(u' \to u) = \int_{u}^{u'+\ell n^1/\alpha_i} du'' \, P_i^{\ell}(u' \to u''). \qquad \text{(II.17)}$$

Differentiation of Eq. II.15 gives

$$\frac{d\bar{q}_\ell(u)}{du} = \Sigma_s^{\ell}(u) \, \phi_\ell(u) - \sum_i \int_{u-\ell n^1/\alpha_i}^{u} du' \, \Sigma_{s_i}(u') \, P_i^{\ell}(u' \to u) \, \phi_\ell(u') \, . \qquad \text{(II.18)}$$

A continuous slowing down approximation results from assuming

$$F_i^{\ell}(u') \equiv g_i(u')\ \phi_{\ell}(u') = F_i^{\ell}(u) + (u' - u)\ \frac{d}{du}\ F_i^{\ell}(u) \qquad \text{(II.19)}$$

$$u \geq u' \geq u - \ell n(1/\alpha)$$

where $g_i(u')$ is taken to be either the isotopic scattering cross section, $\Sigma_{s_i}(u')$, or the macroscopic total cross section $\Sigma_t(u')$. The validity of either approximation depends upon the mixture and the lethargy range in question. Since the total collision density is likely to be a more slowly varying quantity than each of the isotopic scattering collision densities, the latter choice of $g_i(u')$ has a greater range of validity. As the scattering band for Hydrogen ($A_H \tilde{\simeq} 1$) is infinite, the two term expansion of Eq.II.19 is not valid in this case for either choice of $g_i(u)$. Hydrogen is therefore treated separately and the slowing down density is represented as

$$\bar{q}_{\ell}(u) = q_{\ell}(u) + \eta_{\ell}(u)$$

where $\eta_{\ell}(u)$ is the Hydrogen slowing down density and $q_{\ell}(u)$ is given by Eq.II.15 with the sum excluding Hydrogen. Substitution of Eq.II.19 into Eqs.II.15 and II.18 gives

$$q_{\ell}(u) = \sum_{i \neq H} [\xi_i^{\ell}(u)\ F_i^{\ell}(u) + a_i^{\ell}(u)\ \frac{d}{du}\ F_i^{\ell}(u)] \qquad \text{(II.20)}$$

$$\frac{dq_{\ell}(u)}{du} = \sum_{i \neq H} [c_i^{\ell} F_i^{\ell}(u) - e_i^{\ell}(u)\ \frac{d}{du}\ F_i^{\ell}(u)] \qquad \text{(II.21)}$$

with the moderating parameters given by

$$\xi_i^{\ell}(u) = \int_{u-\ell n 1/\alpha_i}^{u} du'\ \frac{\Sigma_{s_i}(u')}{g_i(u')}\ K_i^{\ell}(u' \to u)$$

$$a_i^{\ell}(u) = \int_{u-\ell n 1/\alpha_i}^{u} du'\ (u' - u)\ \frac{\Sigma_{s_i}(u')}{g_i(u')}\ K_i^{\ell}(u' \to u) \qquad \text{(II.22)}$$

$$c_i^{\ell}(u) = \frac{\Sigma_{s_i}^{\ell}(u)}{g_i(u)} - \int_{u-\ell n 1/\alpha_i}^{u} du'\ \frac{\Sigma_{s_i}(u')}{g_i(u')}\ P_i^{\ell}(u' \to u)$$

$$e_i^{\ell}(u) = \int_{u-\ell n^1/\alpha_i}^{u} du' \, (u' - u) \, \frac{\Sigma_{s_i}(u')}{g_i(u')} \, P_i^{\ell}(u' \to u)$$

If consideration is limited to the case, $g_i(u') = \Sigma_t(u)$, then composite moderating parameters may be defined

$$\xi_{\ell}(u) = \sum_{i \neq H} \xi_i^{\ell}(u), \quad a_{\ell}(u) = \sum_{i \neq H} a_i^{\ell}(u),$$

$$c_{\ell}(u) = \sum_{i \neq H} c_i^{\ell}(u), \quad e_{\ell}(u) = \sum_{i \neq H} e_i^{\ell}(u) \tag{II.23}$$

and Eqs. II.20 and II.21 may be combined to give

$$\frac{dq_{\ell}(u)}{du} = \varepsilon_{\ell}(u) \, \hat{\xi}_{\ell}(u) \, F_{\ell}(u) - \varepsilon_{\ell}(u) \, q_{\ell}(u) \tag{II.24}$$

where

$$\varepsilon_{\ell}(u) = \frac{1}{\gamma_{\ell}(u)} = \frac{e_{\ell}(u)}{a_{\ell}(u)} \tag{II.25}$$

$$\hat{\xi}_{\ell}(u) = \xi_{\ell}(u) + \gamma_{\ell}(u) \, c_{\ell}(u) \tag{II.26}$$

and

$$F_{\ell}(u) = \Sigma_t(u) \, \phi_{\ell}(u).$$

If one considers the case $g_i(u') = \Sigma_{s_i}(u')$, and defines the composite moderating parameters

$$\xi_{\ell}(u) = -e_{\ell}(u) = \sum_{i \neq H} \frac{\Sigma_{s_i}(u) \, \xi_i^{\ell}}{\Sigma_t(u)}$$

$$a_{\ell}(u) = \sum_{i \neq H} \frac{\Sigma_{s_i}(u) \, a_i^{\ell}}{\Sigma_t(u)} \tag{II.27}$$

$$c_{\ell}(u) = 0$$

then combination of Eqs. II.20 and II.21 gives Eq. II.24 with the parameter $\hat{\xi}_{\ell}$ defined

$$\hat{\xi}_{\ell}(u) = \xi_{\ell}(u) \left[1 - \frac{d\gamma_{\ell}(u)}{du} \right] . \tag{II.28}$$

A result formally similar to Eq. II.24 was obtained by Goertzel and Greuling.[14] They obtained their results by replacing the slowing down kernel $K_i(u' \to u)$ by a synthetic kernel and preserving moments. The standard Goertzel-Greuling approximation corresponds to Eqs. II.24, II.25, II.27 and II.28 with $\frac{d\gamma_{\ell}}{du} = 0$.

The set of Eqs. II.23, II.24, II.25 and II.26 defines the "Improved Goertzel-Greuling Approximation" derived by Stacey.[12] The microscopic moderating parameters for both approximations are given by Eqs.II.22 with

$$g_i(u) = \begin{cases} \Sigma_{s_i}(u) & \text{Goertzel-Greuling} \\ \Sigma_t(u) & \text{Improved Goertzel-Greuling} \end{cases}$$

In Section II.D of this report explicit definitions of the moderating parameters will be given.

The slowing down Eq.II.24 may be combined with the P_1/B_1 balance Eqs.II.10 to obtain solutions for the flux and slowing down density. For the inconsistent P_1/B_1 approximations, one sets

$$\frac{dq_1(u)}{du} = 0$$

which is equivalent to Eq.II.9 for $\ell = 1$. Equation II.10 may then be written

$$\Sigma_{ne}(u)\ \phi_o(u) = S(u) - \frac{d\bar{q}_o}{du} \tag{II.29}$$

where the non-elastic cross section has been defined

$$\Sigma_{ne}(u) \equiv \Sigma_t(u) + \frac{B^2}{3A_1\ (B,\ u,\ N)} - \Sigma_s(u). \tag{II.30}$$

Equations II.24 and II.29 are combined to obtain:

Inconsistent P_1/B_1 Approximation

$$\frac{dq_o(u)}{du} = \frac{[-\ (\Sigma_{ne}(u) + \Sigma_{s_H}(u))\ q_o(u) + \hat{\xi}_o(u)\ \Sigma_t(u)\ (S(u) + \eta_o(u))]}{M(u)} \tag{II.31}$$

$$\phi_o(u) = \frac{q_o(u) + \gamma_o(u)\ [S(u) + \eta_o(u)]}{M(u)} \tag{II.32}$$

$$M(u) = \hat{\xi}_o(u)\ \Sigma_t(u) + \gamma_o(u)\ [\Sigma_{ne}(u) + \Sigma_{s_H}(u)]\ . \tag{II.33}$$

Equation II.31 may be integrated directly

$$q_o(u) = \exp\left[-\int_o^u du' \frac{[\Sigma_{ne}(u') + \Sigma_{s_H}(u')]}{M(u')}\right] \cdot \left\{q_o(0) + \right. \tag{II.34}$$

$$\left. \int_o^u du' \frac{\hat{\xi}_o(u')\,\Sigma_t(u')\,(S(u') + \eta_o(u'))}{M(u')} \exp\left[\int_o^{u'} du'' \frac{[\Sigma_{ne}(u'') + \Sigma_{s_H}(u'')]}{M(u'')}\right]\right\}.$$

Equations II.31-II.34 have been written for the general situation which includes Hydrogen in the mixture. If there were no Hydrogen, the above equations are applicable with $\Sigma_{s_H}(u) = 0$, $\eta_o(u) = 0$.

If one retains both the $\ell = 0, 1$ terms of Eqs.II.10 and II.24, the consistent P_1/B_1 coupled equations are obtained,

Consistent P_1/B_1 Approximation

$$\frac{1}{\Delta(u)} \left\{\left[[\Sigma_t - \Sigma_s + \Sigma_{s_H}]\,(A_1 - \Sigma_s^1 + \frac{2}{3}\Sigma_{s_H} + \epsilon_1\hat{\xi}_1\Sigma_t) + \frac{1}{3}B^2\right].\right.$$

$$\left.[\epsilon_o q_o + S + \eta_o] + iB\epsilon_o\hat{\xi}_o\Sigma_t\,[\epsilon_1 q_1 + \frac{3}{2}\eta_1]\right\}$$

$$+ \frac{dq_o}{du} = S(u) + \eta_o(u)$$

$$\frac{1}{\Delta(u)} \left\{\left[[(A_1 - \Sigma_s^1 + \frac{2}{3}\Sigma_{s_H})(\Sigma_t - \Sigma_s + \Sigma_{s_H} + \epsilon_o\hat{\xi}_o\Sigma_t) + \frac{B^2}{3}\right].\right.$$

$$\left.[\epsilon_1 q_1 + \frac{3}{2}\eta_1] + \frac{iB}{3}\epsilon_1\hat{\xi}_1\Sigma_t\,[\epsilon_o q_o + S + \eta_o]\right\}$$

$$+ \frac{dq_1}{du} = \frac{3}{2}\eta_1(u) \tag{II.35}$$

$$\Delta(u) = (A_1 - \Sigma_s^1 + \frac{2}{3}\Sigma_{s_H} + \epsilon_1\hat{\xi}_1\Sigma_t)(\Sigma_t - \Sigma_s + \Sigma_{s_H} + \epsilon_o\hat{\xi}_o\Sigma_t) + \frac{1}{3}B^2$$

and

$$\phi_o(u) = \frac{1}{\Delta(u)}\left[(A_1 - \Sigma_s^1 + \frac{2}{3}\Sigma_{s_H} + \epsilon_1\hat{\xi}_1\Sigma_t)(\epsilon_o q_o + S_o + \eta_o)\right.$$

$$\left. - iB\,(\epsilon_1 q_1 + \frac{3}{2}\eta_1)\right] \tag{II.36}$$

$$\phi_1(u) = \frac{1}{\Delta(u)}\left[(\Sigma - \Sigma_s + \Sigma_{s_H} + \epsilon_o\hat{\xi}_o\Sigma_t)(\epsilon_1 q_1 + \frac{3}{2}\eta_1)\right.$$

$$\left. - \frac{iB}{3}\,(\epsilon_o q_o + S + \eta_o)\right].$$

In writing Eqs.II.35 and II.35 Hydrogen elastic scattering has been assumed isotropic in the center of mass system so that

$$\Sigma^1_{s_H}(u) = \frac{2}{3}\Sigma_{s_H}(u)$$

$$\eta_o(u) = \int_o^u du' \, \Sigma_{s_H}(u') \, \phi_o(u') \, e^{-(u-u')} \tag{II.37}$$

$$\eta_1(u) = \frac{2}{3}\int_o^u du' \, \Sigma_{s_H}(u') \, \phi_1(u') \, e^{-\frac{3}{2}(u-u')}.$$

The difference equations used by MC^2-2 in the solution of Eqs.II.32-II.36 will be discussed in Section F.

D. Continuous Slowing Down Moderating Parameters

It is well known that the microscopic Legendre moments of the elastic scattering transfer cross section defined in Eq.II.14 may be represented in the form,[15]

$$\sigma_s^{\ell}(u' \to u) = \frac{\sigma_s(u') \, P_\ell[\mu_o(u' \to u)] \, e^{-(u-u')}}{1-\alpha} \sum_{n=0}^{N} (2n+1) \, f_n(u') \cdot$$

$$P_n[\mu_c(u' \to u)] \tag{II.38}$$

where

$f_n(u')$ = nth Legendre expansion coefficient at lethargy u' in the center of mass system. $f_o(u') = 1$

The MC^2-2 code permits all $N \leq 20$.

μ_c = cosine of scattering angle in the center of of mass system.

$$\mu_c = \frac{(A+1)^2 \, e^{-(u-u')} - (A^2+1)}{2A} = \frac{1}{1-\alpha}\left[2e^{-(u-u')} - (1+\alpha)\right] \tag{II.39}$$

μ_o = cosine of scattering angle in the laboratory system $(\underline{\Omega} \cdot \underline{\Omega}')$

$$\mu_o = \frac{(A+1) \, e^{-\frac{(u-u')}{2}} - (A-1) \, e^{\frac{(u-u')}{2}}}{2} \tag{II.40}$$

and all other terms have been defined previously. To simplify the notation, the isotope index i has been dropped. Equation II.38 along with Eqs.II.16, II.17 may be used to obtain explicit forms for the isotopic moderating parameters of Equations II.22.

1. Goertzel-Greuling Moderating Parameters

Setting $g_i(u') = \Sigma_{s_i}(u')$ and dropping the isotope index i,

Eqs. II.22 may be written,

$$\xi^{\ell} = -e^{\ell} = \frac{1}{1-\alpha} \sum_{n=0}^{N} (2n+1) \int_{u-\ell n^1/\alpha}^{u} du' \int_{u}^{u'+\ell n^1/\alpha} du'' \, f_n(u') \, e^{-(u''-u')} \cdot$$

$$P_{\ell}[\mu_o(u' \to u'')] \, P_n[\mu_c(u' \to u'')]$$

$$a^{\ell} = \frac{1}{1-\alpha} \sum_{n=0}^{N} (2n+1) \int_{u-\ell n^1/\alpha}^{u} du' \, (u'-u) \int_{u}^{u'+\ell n^1/\alpha} du'' \, f_n(u') \, e^{-(u''-u')} \cdot$$

$$P_{\ell}(\mu_o) \, P_n(\mu_c)$$

$$c^{\ell} = 0.$$

Transforming variables to $U = u'' - u'$ and switching orders of integration gives

$$\xi^{\ell} = \sum_{n=0}^{N} \frac{(2n+1)}{2} \int_{o}^{\ell n^1/\alpha} dU \, P_n[\mu_c(U)] \, P_{\ell}[\mu_o(U)] \left(-\frac{d\mu_c}{dU}\right) \int_{u-U}^{u} du' \, f_n(u')$$

$$a^{\ell} = \sum_{n=0}^{N} \frac{(2n+1)}{2} \int_{o}^{\ell n^1/\alpha} dU \, P_n(\mu_c) \, P_{\ell}(\mu_o) \left(-\frac{d\mu_c}{dU}\right) \int_{u-U}^{u} du' \, (u'-u) \, f_n(u')$$

If the scattering coefficients $f_n(u)$ are assumed constant in the scattering band $[u - \ell n(1/\alpha), u]$, the Goertzel-Greuling moderating parameters may be written

$$\xi_i^{\ell}(u) = -e_i^{\ell}(u) = -\sum_{n=0}^{N} f_n(u) \, T_{\ell n}^{1}(\alpha_i)$$

$$a_i^{\ell}(u) = -\sum_{n=0}^{N} f_n(u) \, T_{\ell n}^{2}(\alpha_i) \qquad \text{(II.41)}$$

$$c_i^{\ell}(u) = 0$$

where

$$T_{\ell n}^{m}(\alpha_i) \equiv \frac{(-)^m}{m!} \frac{(2n+1)}{2} \int_{o}^{\ell n^1/\alpha_i} dU \, U^m \, P_{\ell}(\mu_o(U)) \, P_n(\mu_c(U)) \cdot$$

$$\left(-\frac{d\mu_c(U)}{dU}\right) \cdot \qquad \text{(II.4}$$

The quantities $T^m_{\ell n}$ relate Legendre moments of the scattering cross sections in the center of mass and laboratory systems and have been studied in detail.[16-18] Precalculated values of $T^m_{\ell n}$ are provided in the MC^2-2 library (MCC2F8 of Appendix C) for each isotope. Numerical experience has shown that six terms in the sums of Eqs.II.41 suffice to calculate the parameters accurately. This is a consequence of the fact that $T^m_{\ell n}(\alpha)$ approaches zero at least as fast as the faster of A^{-m} and $A^{-|\ell-n|}$.(6)

2. Improved Goertzel-Greuling Moderating Parameters

Setting $g_i(u') = \Sigma_t(u')$ Eqs. II.22 may be written

$$\xi_i^\ell(u) = \frac{1}{1-\alpha_i} \sum_{n=0}^{N} (2n+1) \int_{u-\ell n 1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} f_{n_i}(u') \cdot \int_u^{u'+\ell n 1/\alpha_i} du'' \, e^{-(u''-u')} P_\ell(\mu_o) P_n(\mu_c)$$

$$a_i^\ell(u) = \frac{1}{1-\alpha_i} \sum_{n=0}^{N} (2n+1) \int_{u-\ell n 1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} (u'-u) f_{n_i}(u') \cdot \int_u^{u'+\ell n 1/\alpha_i} du'' \, e^{-(u''-u')} P_\ell(\mu_o) P_n(\mu_c) \qquad \text{(II.43)}$$

$$e_i^\ell(u) = \frac{1}{1-\alpha_i} \sum_{n=0}^{N} (2n+1) \int_{u-\ell n 1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} (u'-u) f_{n_i}(u') \cdot e^{-(u-u')} P_\ell(\mu_o) P_n(\mu_c)$$

$$c_i^\ell(u) = \frac{\Sigma_{s_i}^\ell(u)}{\Sigma_t(u)} - \frac{1}{1-\alpha_i} \sum_{n=0}^{N} (2n+1) \int_{u-\ell n 1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} f_{n_i}(u') \cdot e^{-(u-u')} P_\ell(\mu_o) P_n(\mu_c) .$$

For heavy isotopes which have a small scattering band width, it is reasonable to assume

$$\frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} f_{n_i}(u') \approx \left\langle \frac{\Sigma_{s_i} f_{n_i}}{\Sigma_t} \right\rangle_u \qquad u - \ell n 1/\alpha_i \le u' \le u$$

where $\langle\ \rangle_u$ denotes an average over the lethargy band. With this approximation the same operations which led to Eqs.II.41 give

$$\xi_i^{\ell}(u) = -\, e_i^{\ell}(u) = -\sum_{n=0}^{N} \left\langle \frac{\Sigma_{s_i}}{\Sigma_t} f_{n_i} \right\rangle_u T^1_{\ell n}(\alpha_i)$$

$$a_i^{\ell}(u) = -\sum_{n=0}^{N} \left\langle \frac{\Sigma_{s_i}}{\Sigma_t} f_{n_i} \right\rangle_u T^2_{\ell n}(\alpha_i) \qquad \text{(II.44)}$$

$$c_i^{\ell}(u) = \sum_{n=0}^{N} \left[\frac{\Sigma_{s_i}(u)}{\Sigma_t(u)} f_{n_i}(u) - \left\langle \frac{\Sigma_{s_i}}{\Sigma_t} f_{n_i} \right\rangle_u \right] T^0_{\ell n}(\alpha_i) \approx 0$$

where the definition

$$\Sigma^{\ell}_{s_i}(u) = \sum_{n=0}^{N} \Sigma_{s_i}(u)\, f_{n_i}(u)\, T^0_{\ell n}(\alpha_i) \qquad \text{(II.45)}$$

has been used. The setting of $c_i^{\ell}(u)$ to zero is an approximation required in MC^2-2 to avoid numerical difficulties. In the MC^2-2 code Eqs. II.44 are used for isotopes of mass $A_i \geq 200$ $(\ell n^1/\alpha_i < .02)$ so that the averaging assumption is expected to be valid. Numerical experience has shown that four terms in the sums of Eqs. II.44, N = 3, suffice to calculate the parameters accurately for the heavy isotopes.

For lighter materials ($A_i < 200$) the Improved Goertzel-Greuling moderating parameters are derived in the following manner. Define the quantity

$$\mathcal{D}^i_{n'}(u) \equiv \sum_{n=n'-1}^{N} \frac{2n+1}{2} f_{n_i}(u)\, K^i_{nn'}(\alpha_i) \qquad \text{(II.46)}$$

where

$$K^i_{nn'}(\alpha_i) \equiv \frac{1}{2^n (n'-1)!} \left(\frac{2}{1+\alpha_i}\right)^{n'} \sum_{k=0}^{K_{max}} \frac{(-)^{n+1-k-n'}\,(2n-2k)!}{k!\,(n-k)!\,(n+1-2k-n')!} \left(\frac{1+\alpha_i}{1-\alpha_i}\right)^{n+1-2k}$$

$$K_{max} \equiv \min\left\{ [n/2],\ \left[\frac{n+1-n'}{2}\right] \right\} . \qquad \text{(II.47)}$$

Noting that the Legendre Polynomials $P_n(\mu)$ may be expanded

$$P_n(\mu) = \sum_{k=0}^{[n/2]} \frac{(-)\ (2n-2k)!}{2^n\, k!\,(n-k)!\,(n-2k)!}\, \mu^{n-2k}$$

and using Eqs.II.39 and II.40 it can be shown that the $\ell = 0, 1$ Eqs. II.43 may be written in the form

$$\xi_i^o(u) = \sum_{n'=1}^{N+1} \frac{1}{n'} \left\{ \int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \mathcal{D}_{n'}^i(u') \, e^{-n'(u-u')} \right.$$

$$\left. - \alpha_i^{n'} \int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \mathcal{D}_{n'}^i(u') \right\}$$

$$a_i^o(u) = - \sum_{n'=1}^{N+1} \frac{1}{n'} \left\{ \int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \mathcal{D}_{n'}^i(u') \, (u - u') \, e^{-n'(u-u')} \right.$$

$$\left. - \alpha_i^{n'} \int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} (u - u') \, \mathcal{D}_{n'}^i(u') \right\}$$

$$c_i^o(u) = \sum_{n'=1}^{N+1} \left\{ \frac{\Sigma_{s_i}(u)}{\Sigma_t(u)} \frac{(1 - \alpha_i^{n'})}{n'} \mathcal{D}_{n'}^i(u) - \int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \right.$$

$$\left. \mathcal{D}_{n'}^i(u') \, e^{-n'(u-u')} \right\}$$

$$= \frac{\Sigma_{s_i}(u)}{\Sigma_t(u)} - \sum_{n'=1}^{N+1} \int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \mathcal{D}_{n'}^i(u') \, e^{-n'(u-u')}$$

$$e_i^o(u) = \sum_{n'=1}^{N+1} \int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \mathcal{D}_{n'}^i(u') \, (u - u') \, e^{-n'(u-u')} \qquad \text{(II.48)}$$

$$\xi_i^1(u) = \sum_{n'=1}^{N+1} \left\{ \frac{(A_i + 1)}{2n' + 1} \left[\int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \mathcal{D}_{n'}^i(u') \, e^{-(n'+1/2)(u-u')} \right. \right.$$

$$\left. - \alpha_i^{n'+1/2} \int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \mathcal{D}_{n'}^i(u') \right]$$

$$- \frac{(A_i - 1)}{2n' - 1} \left[\int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \mathcal{D}_{n'}^i(u') \, e^{-(n'-1/2)(u-u')} \right.$$

$$\left. \left. - \alpha_i^{n'-1/2} \int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \mathcal{D}_{n'}^i(u') \right] \right\}$$

$$a_i^1(u) = -\sum_{n'=1}^{N+1} \left\{ \frac{(A_i + 1)}{2n' + 1} \left[\int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \cdot \right. \right.$$

$$\mathcal{D}_{n'}^{i}(u') \; (u - u') \; e^{-(n'+1/2) \; (u-u')}$$

$$\left. - \alpha_i^{n'+1/2} \int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \; (u - u') \; \mathcal{D}_{n'}^{i}(u') \right]$$

$$- \frac{(A_i - 1)}{2n' - 1} \left[\int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \; \mathcal{D}_{n'}^{i}(u') \cdot \right.$$

$$(u - u') \; e^{-(n'-1/2) \; (u-u')}$$

$$\left. \left. - \alpha_i^{n'-1/2} \int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \; (u - u') \; \mathcal{D}_{n'}^{i}(u') \right] \right\}$$

$$c_i^1(u) = \sum_{n'=1}^{N+1} \frac{\Sigma_{s_i}(u)}{\Sigma_t(u)} \; \mathcal{D}_{n'}^{i}(u) \left[\frac{A_i + 1}{2n' + 1} \left(1 - \alpha_i^{n'+1/2} \right) \right.$$

$$\left. - \frac{A_i - 1}{2n' - 1} \left(1 - \alpha_i^{n'-1/2} \right) \right]$$

$$- 1/2 \sum_{n'=1}^{N+1} \left\{ (A_i + 1) \int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \cdot \right.$$

$$\mathcal{D}_{n'}^{i}(u') \; e^{-(n'+1/2) \; (u-u')}$$

$$\left. - (A_i - 1) \int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \; \mathcal{D}_{n'}^{i}(u') \; e^{-(n'-1/2) \; (u-u')} \right\}$$

$$= \frac{\Sigma_{s_i}(u)}{\Sigma_t(u)} \sum_{n'=0}^{N} T^o_{ln'}(\alpha_i)\, f_{n'i}(u) - 1/2 \sum_{n'=1}^{N+1} \Bigg\{ (A_i + 1) \int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \mathcal{D}^i_{n'}(u')\, e^{-(n'+1/2)(u-u')}$$

$$- (A_i - 1) \int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \mathcal{D}^i_{n'}(u')\, e^{-(n'-1/2)(u-u')} \Bigg\}$$

$$e^1_i(u) = 1/2 \sum_{n'=1}^{N+1} \Bigg\{ (A_i + 1) \int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \mathcal{D}^i_{n'}(u')\,(u-u') \cdot$$

$$e^{-(n'+1/2)(u-u')} - (A_i - 1) \int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \mathcal{D}^i_{n'}(u')\,(u-u') \cdot$$

$$e^{-(n'-1/2)(u-u')} \Bigg\}.$$

Numerical experience has shown that only four terms need be retained in the sums of Eqs. II.48, N = 3. The mass dependent coefficients $K_{llll'}(\alpha)$ defined by Eq. II.47 are given in Table I. These coefficients are provided in the MC^2-2 library (MCC2F8 of Appendix C).

TABLE I. Coefficients $K_{nn'}(\alpha)$

n/n'	1	2	3	4	5
0	$\frac{2}{1-\alpha}$	-	-	-	-
1	$\frac{-2}{(1-\alpha)}\left(\frac{1+\alpha}{1-\alpha}\right)$	$\frac{4}{(1-\alpha)^2}$	-	-	-
2	$\frac{1}{1-\alpha}\left[3\left(\frac{1+\alpha}{1-\alpha}\right)^2 - 1\right]$	$-12\,\frac{(1+\alpha)}{(1-\alpha)^3}$	$\frac{12}{(1-\alpha)^3}$	-	-
3	$\frac{(1\ \alpha)}{(1-\alpha)^2}\left[-5\left(\frac{1+\alpha}{1-\alpha}\right)^2 + 3\right]$	$\frac{6}{(1-\alpha)^2}\left[5\left(\frac{1+\alpha}{1-\alpha}\right)^2 - 1\right]$	$-60\,\frac{(1+\alpha)}{(1-\alpha)^4}$	$\frac{40}{(1-\alpha)^4}$	-
4	$\frac{1}{4(1-\alpha)}\left[35\left(\frac{1+\alpha}{1-\alpha}\right)^4 - 30\left(\frac{1+\alpha}{1-\alpha}\right)^2 + 3\right]$	$10\,\frac{(1+\alpha)}{(1-\alpha)^3}\left[-7\left(\frac{1+\alpha}{1-\alpha}\right)^2 + 3\right]$	$\frac{30}{(1-\alpha)^3}\left[7\left(\frac{1-\alpha}{1-\alpha}\right)^2 - 1\right]$	$-280\,\frac{(1+\alpha)}{(1-\alpha)^5}$	$\frac{140}{(1-\alpha)^5}$

E. Narrow Resonance Attenuation

The formalism developed in the previous sections is directly applicable to narrow resonances provided that effective resonance cross sections could be calculated. Such a calculation is quite time consuming as evidenced by the fact that the resonance calculation of the code MC^2 [10] is about one-half of the total computing time for typical problem executions. It is, therefore, advantageous to ignore these resonances in defining the moderating parameters of Section D and then superimpose their effect by attenuating the slowing down density. This is the strategy employed by the code MC^2-2 for the treatment of narrow resolved resonances. In particular, the wide resonances of light materials are treated by the code which prepares the library for MC^2-2 from basic nuclear data, e.g. ETOE-2 [4]. MC^2-2 treats these resonance cross sections as effective smooth cross sections and includes their contribution in the calculation of moderating parameters. Similarly, effective smooth cross sections for heavy isotopes are calculated by MC^2-2 from unresolved resonance parameters according to the algorithms specified in Chapter IV and included in the calculation of the moderating parameters. An asymptotic slowing down density, $q_\ell^{asy}(u)$, is calculated using these parameters in Eqs. II.34 or II.35 and the effects of the narrow resolved resonances are superimposed on $q_\ell^{asy}(u)$ by use of attenuation factors. The form of the narrow resonance attenuation factors is derived below.

For the sake of simplicity consider the P_1/B_1 equations for a single material and assume zero buckling,

$$F(u) = \int_o^u du'\, P^o\,(u - u')\, h(u')\, F(u') + S(u) \qquad \text{(II.49)}$$

where

$$F(u) = \Sigma_t(u)\, \phi_o(u)$$

$$h(u) = \Sigma_s(u)/\Sigma_t(u)$$

and all other terms have been defined previously. If one neglects the narrow resolved resonance cross sections, Eq. II.49 has the form

$$F_{as}(u) = \int_o^u du'\, P^o\,(u - u')\, h_{as}(u')\, F_{as}(u') + S(u) \qquad \text{(II.50)}$$

where the asymptotic cross sections are defined

$$\Sigma_t^{as}(u) = \Sigma_t(u) - \Sigma_t^r(u), \quad \text{etc.}$$

and r represents the narrow resolved resonance cross sections. Subtracting Eq. II.50 from Eq. II.49,

$$F(u) = F_{as}(u) + \int_o^u du'\, P^o(u - u')\, [h(u')\, F(u') - h_{as}(u')\, F_{as}(u')]\,.$$

Following the methods used by Corngold,[19] define the Laplace transform as

$$\tilde{f}(s) \equiv L[f(u)] \equiv \int_o^\infty du\, e^{-su} f(u)$$

so that

$$\tilde{F}(s) = \tilde{F}_{as}(s) + \tilde{P}^o(s)\ [L(hf) - L(h_{as}F_{as})].$$

Define

$$h(u) = 1 - g(u)$$
$$h_{as}(u) = 1 - g_{as}(u)$$

where

$$g(u) = \frac{\Sigma_{ne}^{as} + \Sigma_{ne}^{r}}{\Sigma_t^{as} + \Sigma_t^{r}}$$

$$g_{as}(u) = \frac{\Sigma_{ne}^{as}}{\Sigma_t^{as}}$$

and

$$\tilde{F}(s) = \tilde{F}_{as}(s) - \frac{\tilde{P}^o(s)\ [L(gF) - L(g_{as}F_{as})]}{1 - \tilde{P}^o(s)} \quad . \tag{II.51}$$

Defining

$$\tilde{\psi}(s) = \frac{\tilde{P}^o(s)}{1 - \tilde{P}^o(s)}$$

Equation II.51 may be inverted to obtain

$$F(u) = F_{as}(u) - \int_o^u du'\ \psi(u - u')\ [g(u')\ F(u') - g_{as}(u')\ F_{as}(u')] \tag{II.52}$$

where the kernel ψ satisfies

$$\psi(u) = \int_o^u du'\ P^o(u - u')\ \psi(u') + P^o(u) \quad . \tag{II.53}$$

It is obvious from Eq. II.53 that $\psi(u)$ is the solution of Eq.II.49, for a delta function source in the absence of absorption. It is well known that asymptotically

$$\psi(u) \to \frac{1}{\xi} \simeq \frac{\Sigma_{ne}^{as}\ \phi^{as}}{q^{as}} \quad . \tag{II.54}$$

Using Eq.II.54 in Eq.II.52 an expression for the attenuation in the asymptotic (non-resonance) collision density is obtained,

$$F(u) \approx F_{as}(u) \prod_{\substack{r \\ u_r < u}} (1 - p_r) \tag{II.55}$$

where the product is taken over all resonances in the interval $0 \leq u_r \leq u$ and

$$p_r \equiv \left\{ \frac{\Gamma_a^r}{E_r} J^*_{a_r} - \frac{\Sigma_{ne}^{as}}{\Sigma_t^{as}} \frac{\Gamma_t^r}{E_r} J^*_{t_r} \right\} \frac{\Sigma_{ne}^{as} \phi^{as}}{q^{as}} \tag{II.56}$$

$$J^*_{x_r} = \frac{E_r}{\Gamma_x^r} \int_{-\infty}^{\infty} \frac{\Sigma_x^r}{\Sigma_t^{as} + \Sigma_t^r} du \quad . \tag{II.57}$$

The method for calculating the J* function will be discussed in Chapter III. Stacey[12] derived an attenuation factor formalism by considering the resonance as a point absorber. This leads to Eq.II.56 without the second term in the brackets, thus neglecting the competition between scattering and absorption of the resonance.

F. Ultra-Fine-Group Equations

The lethargy (energy) domain of interest is assumed to be partitioned into equal lethargy intervals of width Δu. The corresponding energy widths are denoted ΔE_g. By convention, increasing g represents increasing lethargy (decreasing energy),

$$u_{g+1} = u_g + \Delta u$$
$$E_{g+1} = E_g e^{-\Delta u}.$$

The lethargy group width is assumed to be small and, following the MC^2[10] conventions, calculations performed in this structure are called ultra-fine-group calculations. The group structure is fixed by the MC^2-2 library (Appendix C). It is usually set at $\Delta u \simeq 1/120$, corresponding to the MC^2 structure, giving 2040 groups from 10 MeV to 0.414 eV.

Figure 2 gives a schematic representation of the MC^2-2 group structure. From the maximum problem energy, E_{max}, to a user specified energy, E_{CSD}, the code uses a multigroup form of Eqs.II.10-II.12 in the spectrum calculation. From E_{CSD} to E_{min} the equations of Section II.C, Continuous Slowing Down Theory, are applicable. The user specified energy E_{CSD} must satisfy the relationship

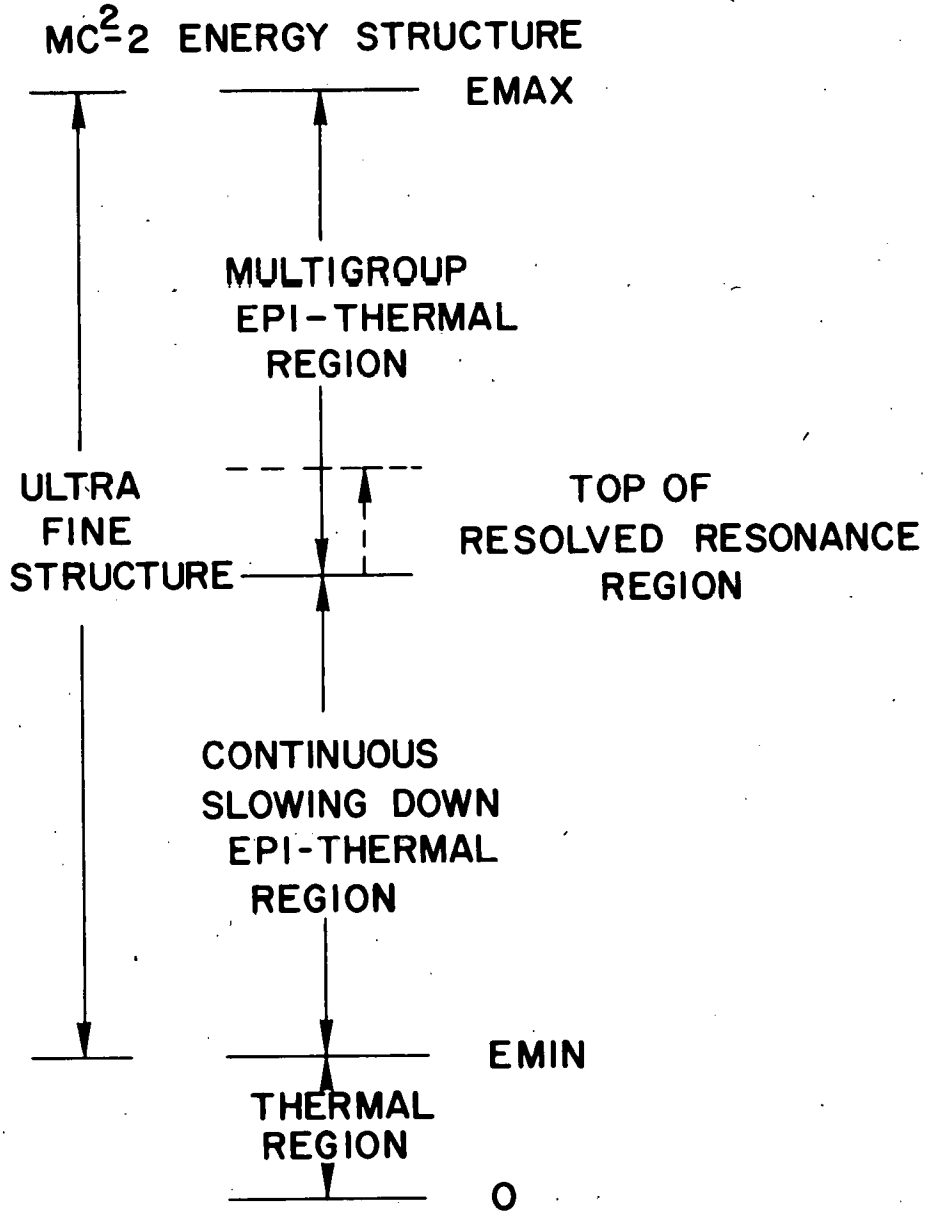

Fig. 2. MC^2-2 Energy Structure

$$E_R < E_{CSD} \leq E_{max} \tag{II.58}$$

where

E_R = energy of highest energy resolved resonance in the problem mixture

This restriction is a consequence of the use of the attenuation factor treatment of resolved resonances (c.f. Section II.E) in the continuous slowing down energy domain.

The remainder of this section presents the ultra-fine-group equations for the multigroup and continuous slowing down formulations.

1. Multigroup Equations

Integrating Eqs.II.10 and II.11 over a group one obtains

$$iB\phi_1^g + \Sigma_t^g \phi_0^g = S^g + \sum_{g' \leq g} \Sigma_s^o (g' \to g)\ \phi_o^{g'}$$

$$i\ \frac{B}{3}\ \phi_o^g + A_1^g \phi_1^g = \sum_{g' \leq g} \Sigma_s^1 (g' \to g)\ \phi_1^{g'} \tag{II.59}$$

$$\phi_\ell^g = -\ \frac{\ell}{2\ell + 1}\ iB\phi_{\ell-1}^g / A_\ell^g \qquad \ell = 2, \ \ldots\ , N$$

where

$$\phi_\ell^g = \int_{u_{g-1}}^{u_g} \phi_\ell(u)\ du \tag{II.60}$$

and

$$\Sigma_t^g = \frac{1}{\phi_o^g} \int_{u_{g-1}}^{u_g} \Sigma_t(u)\ \phi_o(u)\ du$$

$$\Sigma_s^\ell (g' \to g) = \frac{1}{\phi_\ell^{g'}} \int_{u_{g-1}}^{u_g} du \int_{u_{g'-1}}^{u_{g'}} du'\ \Sigma_s^\ell (u' \to u)\ \phi_\ell(u') \tag{II.61}$$

$$A_\ell^g = \int_{u_{g-1}}^{u_g} A_\ell(B, u, N)\ du\ .$$

Since the flux moments $\phi_\ell(u)$ are unknown a spectrum must be assumed in order to derive the ultra-fine-group cross sections defined by Eqs.II.61. This averaging is performed by the processing code which prepares the library files for MC^2-2. These ultra-fine-group data are the basic input to MC^2-2 and later sections of this report will describe how these data are processed to permit a solution of Eqs. II.59.

As noted earlier in this report, an option of the code permits group dependent buckling. In this case one is solving Eqs.II.59 with B replaced by B_g. To simplify notation, only the group independent buckling equations will be developed.

In writing Eqs.II.59 it has been assumed that a neutron cannot gain energy as a result of scattering thus precluding the use of MC^2-2 in the thermal energy domain.

Equations II.59 may be written:

Consistent P_1/B_1 Approximation

$$\phi^g = \frac{S^g + \sum_{g'<g} \left[\Sigma_s^o(g' \to g)\ \phi^{g'} - \frac{B}{\Sigma_{r_1}^g}\ \Sigma_s^1(g' \to g)\ J^{g'}\right]}{\Sigma_{r_o}^g + \frac{B^2}{3\Sigma_{r_1}^g}}$$

$$J^g = \frac{\frac{B}{3}\ \phi^g + \sum_{g'<g} \Sigma_s^1(g' \to g)\ J^{g'}}{\Sigma_{r_1}^g} \qquad \text{(II.62)}$$

$$\phi_\ell^g = -\frac{\ell}{2\ell + 1}\ iB\ \phi_{\ell-1}^g / A_\ell^g$$

$$\phi^g \equiv \phi_o^g$$

$$J^g \equiv i\phi_1^g$$

and

$$\Sigma_{r_o}^g \equiv \Sigma_t^g - \Sigma_s^o(g \to g) - \Sigma_{inel}(g \to g) - 2\Sigma_{n,2n}(g \to g)$$

$$\Sigma_{r_1}^g \equiv A_1^g - \Sigma_s^1(g \to g) \qquad \text{(II.63)}$$

$$S^g \equiv \frac{1}{k} S_f^g + S_{fix}^g + \sum_{g'<g} \left[\Sigma_{inel}(g' \to g) + 2\Sigma_{n,2n}(g' \to g)\right] \phi^{g'}$$

In Eqs. II.63 explicit account has been taken of the elastic (Σ_s^{ℓ}), inelastic (Σ_{inel}), and (n,2n), ($\Sigma_{n,2n}$) scattering sources and the source term S^g has been redefined to exclude non-elastic in-group scattering which has been incorporated in the removal cross section $\Sigma_{r_o}^g$. Equations II.62 and II.63 define the multigroup consistent P_1/B_1 approximation. The inconsistent P_1/B_1 equations are written:

Inconsistent P_1/B_1 Approximation

$$\phi^g = \frac{S^g + \sum_{g'<g} \bar{\Sigma}_s^o(g' \to g)\, \phi^{g'}}{\Sigma_{r_o}^g + \frac{B^2}{3A_1^g}} \qquad \text{(II.64)}$$

$$J^g = \frac{B}{3A_1^g}\, \phi^g$$

2. Continuous Slowing Down Equations

If one assumes

$$\int_{u_{g-1}}^{u_g} f(u)\, du \simeq [\theta f_+ + (1 - \theta)\, f_-]\, \Delta u \qquad \text{(II.65)}$$

where

$f_+ \equiv f(u_g) = f(u)$ $\quad u_g > u > u_g - \theta\Delta u$

$f_- \equiv f(u_{g-1}) = f(u)$ $\quad u_{g-1} < u < u_g - \theta\Delta u$

$\theta \equiv$ integration factor $\quad 0 \leq \theta \leq 1$

$\Delta u \equiv u_g - u_{g-1}$

then the inconsistent P_1/B_1 slowing down Eq.II.34 may be written

Inconsistent P_1/B_1 Approximation

$$q_o(u_g) = q_o(u_{g-1}) \exp\left\{ - (\Sigma^g_{ne} + \Sigma^g_{s_H}) \Delta u \left[\frac{\theta}{M^g_+} + \frac{(1-\theta)}{M^g_-} \right] \right\}$$
$$+ \frac{(S^g + \eta^g_o)}{\Delta u} \frac{\Sigma^g_t}{\Sigma^g_{ne} + \Sigma^g_{s_H}} \left\{ \hat{\xi}_o(u_{g-1}) \exp\left[- \frac{(\Sigma^g_{ne} + \Sigma^g_{s_H})}{M^g_+} \theta \Delta u \right] \cdot \right.$$
$$\left[1 - \exp\left(- \frac{(\Sigma^g_{ne} + \Sigma^g_{s_H})}{M^g_-} (1-\theta)\Delta u \right) \right] \qquad \text{(II.66)}$$
$$\left. + \hat{\xi}_o(u_g) \left[1 - \exp\left(- \frac{(\Sigma^g_{ne} + \Sigma^g_{s_H})}{M^g_+} \theta \Delta u \right) \right] \right\}$$

where

$$\Sigma^g_{ne} = \Sigma^g_t + \frac{B^2}{3A^g_1} - \Sigma^g_s$$

$$M^g_+ = \hat{\xi}_o(u_g) \Sigma^g_t + \gamma_o(u_g) \left[\Sigma^g_{ne} + \Sigma^g_{s_H} \right] \qquad \text{(II.67)}$$

$$M^g_- = \hat{\xi}_o(u_{g-1}) \Sigma^g_t + \gamma_o(u_{g-1}) \left[\Sigma^g_{ne} + \Sigma^g_{s_H} \right] .$$

The group flux ϕ^g may be derived from Eq. II.32

$$\phi^g = \left[\frac{\theta q_o(u_g)}{M^g_+} + \frac{(1-\theta)\, q_o(u_{g-1})}{M^g_-} \right] \Delta u$$
$$+ (S_g + \eta^g_o) \left[\frac{\theta \gamma_o(u_g)}{M^g_+} + \frac{(1-\theta)\, \gamma_o(u_{g-1})}{M^g_-} \right] \qquad \text{(II.68)}$$

or from the balance Eq. II.29

$$\phi^g = \frac{S^g + \eta^g_o + q_o(u_{g-1}) - q_o(u_g)}{\Sigma^g_{ne} + \Sigma^g_{s_H}} . \qquad \text{(II.69)}$$

The consistent P_1/B_1 recursion relations are derived by differencing of Eqs. II.35 and II.36 using the approximations

$$\frac{dq}{du} \approx \frac{q(u_g) - q(u_{g-1})}{\Delta u}$$

$$f(u)q(u) \approx \theta f_+ q(u_g) + (1 - \theta) f_- q(u_{g-1}).$$

Consistent P_1/B_1 Approximation

$$\begin{aligned} q_o(u_g) = \frac{1}{N^g} \Bigg\{ & \left([\theta Z_+^g + \frac{1}{\Delta u}][(1 - \theta) W_-^g - \frac{1}{\Delta u}] - \theta X_+^g (1 - \theta) Y_-^g \right) q_o(u_{g-1}) \\ & + \left([\theta Z_+^g + \frac{1}{\Delta u}][(1 - \theta) X_-^g] - \theta X_+^g [(1 - \theta) Z_-^g - \frac{1}{\Delta u}] \right) q_1(u_{g-1}) \\ & - \Big([\theta Z_+^g + \frac{1}{\Delta u}][1 - \gamma_o(u_g)\ \theta W_+^g - (1 - \theta)\ \gamma_o(u_{g-1})\ W_-^g] \\ & + \theta X_+^g [\gamma_o(u_g)\ \theta Y_+^g + \gamma_o(u_{g-1})(1 - \theta)\ Y_-^g] \Big) \left(\frac{S^g + \eta_o^g}{\Delta u} \right) \\ & + \Big([\gamma_1(u_g)\ \theta X_+^g + \gamma_1(u_{g-1})(1 - \theta)\ X_-^g][\theta Z_+^g + \frac{1}{\Delta u}] \\ & + \theta X_+^g [1 - \gamma_1(u_g)\ \theta Z_+^g - \gamma_1(u_{g-1})(1 - \theta)\ Z_-^g] \Big) \frac{3}{2} \frac{\eta_1^g}{\Delta u} \Bigg\} \end{aligned} \qquad \text{(II.70)}$$

$$\begin{aligned} q_1(u_g) = \frac{-1}{(\theta Z_+^g + \frac{1}{\Delta u})} \Bigg\{ & [(1 - \theta)\ Z_-^g - \frac{1}{\Delta u}]\ q_1(u_{g-1}) \\ & + \theta Y_+^g\ q_o(u_g) + (1 - \theta)\ Y_-^g\ q_o(u_{g-1}) \\ & + [\gamma_o(u_g)\ \theta Y_+^g + \gamma_o(u_{g-1})(1 - \theta)\ Y_-^g] \left(\frac{S^g + \eta_o^g}{\Delta u} \right) \\ & + [\gamma_1(u_g)\ \theta Z_+^g + \gamma_1(u_{g-1})(1 - \theta)\ Z_-^g]\ \frac{3}{2} \frac{\eta_1^g}{\Delta u} \Bigg\} \end{aligned} \qquad \text{(II.71)}$$

where

$$N^g \equiv (\theta Y_+^g)(\theta X_+^g) - (\theta Z_+^g + \frac{1}{\Delta u})(\theta W_+^g + \frac{1}{\Delta u})$$

$$W^g \equiv \frac{1}{\gamma_o}\left[(\Sigma_t^g - \Sigma_s^g + \Sigma_{s_H}^g)(A_1^g - \Sigma_s^{1,g} + \frac{2}{3}\Sigma_{s_H}^g + \frac{\hat{\xi}_1}{\gamma_1}\Sigma_t^g) + \frac{B^2}{3}\right]\Big/\Delta^g$$

$$X^g \equiv \frac{1}{\gamma_o\gamma_1}\hat{\xi}_o\Sigma_t^g B/\Delta^g \qquad \text{(II.72)}$$

$$Y^g \equiv -\frac{B}{3}\frac{1}{\gamma_o\gamma_1}\hat{\xi}_1\Sigma_t^g/\Delta^g$$

$$Z^g \equiv \frac{1}{\gamma}\left[(A_1^g - \Sigma_s^{1,g} + \frac{2}{3}\Sigma_{s_H}^g)(\Sigma_t^g - \Sigma_s^g + \Sigma_{s_H}^g + \frac{\hat{\xi}_o}{\gamma_o}\Sigma_t^g) + \frac{B^2}{3}\right]\Big/\Delta^g$$

$$\Delta^g \equiv (A_1^g - \Sigma_s^{1,g} + \frac{2}{3}\Sigma_{s_H}^g + \frac{\hat{\xi}_1}{\gamma_1}\Sigma_t^g)(\Sigma_t^g - \Sigma_s^g + \Sigma_{s_H}^g + \frac{\hat{\xi}_o}{\gamma_o}\Sigma_t^g) + \frac{B^2}{3}$$

Expressions for the flux and current follow directly from Eqs. 36,

$$\phi^g = \left[\theta R_+^g q_o(u_g) + (1-\theta) R_-^g q_o(u_{g-1}) - \theta T_+^g q_1(u_g)\right.$$
$$\left. - (1-\theta) T_-^g q_1(u_{g-1})\right]\Delta u + (S^g + \eta_o^g)[\gamma_o(u_g)\,\theta R_+^g + \gamma_o(u_{g-1})\,(1-\theta) R_-^g]$$
$$- \frac{3}{2}\eta_1^g\left[\gamma_1(u_g)\,\theta T_+^g + \gamma_1(u_{g-1})\,(1-\theta) T_-^g\right] \qquad \text{(II.73)}$$

$$J^g = \left[\theta V_+^g q_o(u_g) + (1-\theta) V_-^g q_o(u_{g-1}) + \theta U_+^g q_1(u_g)\right.$$
$$\left. + (1-\theta) U_-^g q_1(u_{g-1})\right]\Delta u + (S^g + \eta_o^g)\left[\gamma_o(u_g)\,\theta V_+^g + \gamma_o(u_{g-1})\,(1-\theta) V_-^g\right]$$
$$+ \frac{3}{2}\eta_1^g\left[\gamma_1(u_g)\,\theta U_+^g + \gamma_1(u_{g-1})\,(1-\theta) U_-^g\right] \qquad \text{(II.74)}$$

where

$$R^g \equiv \frac{1}{\gamma_o}\left[A_1^g - \Sigma_s^{1,g} + \frac{2}{3}\Sigma_{s_H}^g + \frac{\hat{\xi}_1}{\gamma_1}\Sigma_t^g\right]/\Delta^g$$

$$T^g \equiv \frac{B}{\gamma_1}\frac{1}{\Delta^g} \qquad \text{(II.75)}$$

$$U^g \equiv \frac{1}{\gamma_1}\left[\Sigma_t^g - \Sigma_s^g + \Sigma_{s_H}^g + \frac{\hat{\xi}_o}{\gamma_o}\Sigma_t^g\right]/\Delta^g$$

$$V^g \equiv \frac{B}{3\gamma_o}\frac{1}{\Delta^g}$$

The calculation of the moderating parameters required in Eqs. II.66-II.75 will be described in Section I. The Hydrogen slowing down density η_ℓ^g may be calculated recursively. From Eqs. II.37 it follows that

$$\eta_\ell(u_g) \approx \eta_\ell(u_{g-1})\, e^{-\frac{(2\ell+1)}{(\ell+1)}\Delta u} + \frac{(\ell+1)}{(2\ell+1)}\,\frac{\Sigma_{s_H}^{g\ell}\,\phi_\ell^g}{\Delta u}\cdot$$

$$\left[1 - e^{-\frac{(2\ell+1)}{(\ell+1)}\Delta u}\right] \qquad \ell = 0,\ 1 \qquad \text{(II.76)}$$

$$\eta_\ell^g = \int_{u_{g-1}}^{u_g} \eta_\ell(u)\, du \approx \eta_\ell(u_{g-1})\,\Delta u\ . \qquad \text{(II.77)}$$

The initial conditions for the continuous slowing down calculation are given by

$$\eta_\ell(0) = 0$$

$$q_\ell(0) = 0$$

$$q_\ell(u_{CSD}) = \sum_{i\neq H}\sum_{g=1}^{G}\sum_{g'=G+1}^{NG+1}\Sigma_{s_i}^{\ell}(g\to g')\,\phi_\ell^g \qquad G > 1 \qquad \text{(II.78)}$$

where

$$u_{CSD} \equiv u_G = \ell n\left(\frac{E_{max}}{E_{CSD}}\right)$$

$$G \equiv \frac{u_G}{\Delta u}\ ,\ NG = \frac{1}{\Delta u}\,\ell n\left(\frac{E_{max}}{E_{min}}\right)\ .$$

G. Elastic Scattering Transfer Matrix

The multigroup spectrum calculation of MC^2-2 requires ultra-fine-group elastic scattering transfer matrices. Using Eqs. II.38 and II.61, the transfer matrices are defined

$$\sigma_s^{\ell}(g' \to g) = \frac{1}{\phi_{\ell}^{g'}} \int_{u_{g-1}}^{u_g^*} du \int_{u_{g'-1}^*}^{u_{g'}} du' \frac{\sigma_s(u')}{1-\alpha} P_{\ell}[\mu_o(u' \to u)]\, e^{-(u-u')}\, \phi_{\ell}(u')$$

$$\cdot \sum_{n=0}^{N} (2n+1)\, f_n(u')\, P_n[\mu_c(u' \to u)] \quad . \qquad \text{(II.79)}$$

Noting that $\sigma_s(u')$ does not include the heavy element resolved resonance structure so that in the ultra-fine-group g', $\sigma_s(u') \approx \sigma_s^{g'}$ and assuming a constant weighting function, Eq. II.79 may be written

$$\sigma_s^{\ell}(g' \to g) = \frac{\sigma_s^{g'}}{(1-\alpha)\,\Delta u} \sum_{n=0}^{N} (2n+1) \int_{u_{g-1}}^{u_g^*} du \int_{u_{g'-1}}^{u_{g'}} du'\, f_n(u') \cdot$$

$$P_{\ell}(\mu_o)\, P_n(\mu_c)\, e^{-(u-u')}. \qquad \text{(II.80)}$$

The code evaluates $\sigma_s(g' \to g)$ in three different options depending upon the mass A of the scattering material.

1. Light Elements

For light materials other than Hydrogen which scatter more than three ultra-fine-groups

$$1 < A < \frac{e^{1.5\Delta u} + 1}{e^{1.5\Delta u} - 1}$$

an algorithm similar to that of the MC^2 code is used to evaluate the transfer matrix. Writing Eq. II.80

$$\sigma_s^{\ell}(g' \to g) = \frac{\sigma_s^{g'}}{\Delta u} \int_{u_{g'-1}^*}^{u_{g'}} du'\, P_{\ell}(u' \to g) \qquad \text{(II.81)}$$

$$P_{\ell}(u' \to g) \equiv \sum_{n=0}^{N} \frac{2n+1}{1-\alpha} \int_{u_{g-1}}^{u_g^*} du\, f_n(u')\, P_{\ell}(\mu_o)\, P_n(\mu_c)\, e^{-(u-u')} \qquad \text{(II.82)}$$

it is clear that $P_\ell(u' \to g)$ may be evaluated analytically. Considering the case $\ell = 0$, define the variable

$$r \equiv \frac{1 - e^{-(u-u')}}{1 - \alpha} \leq 1$$

so that

$$P_o(u' \to g) = \sum_{n=0}^{N} (2n + 1) \int_{r_{g-1}}^{r_g} f_n(u')\, P_n(1 - 2r)\, dr$$

$$= \sum_{n=0}^{N} (2n + 1) \int_{r_{g-1}}^{r_g} f_n(u') \sum_{m=0}^{n} (-)^m \frac{(n + m)!}{(n - m)!} \frac{r^m}{m!\, m!}\, dr$$

$$= \sum_{m=0}^{N} A_m \left(r_g^{m+1} - r_{g-1}^{m+1}\right) \qquad \text{(II.83)}$$

where

$$A_m \equiv \sum_{n=m}^{N} f_n(u') \quad \frac{(-)^m (2n + 1)\, (n + m)!}{m!\, (m + 1)!\, (n - m)!} \; .$$

Using the analytical expression, Eq.II.83, the transfer matrix of Eq.II.81 is evaluated in the following manner. Each ultra-fine-group, Δu, is subdivided into M hyper-fine-groups, as shown in Fig. 3, such that

$$M\delta u = \Delta u$$

$$u_{g_o} = u_g$$

$$u_{g_{M+1}} = u_{g+1}$$

$$u_{g_n} = u_g + n\delta u$$

The number of hyper-fine-groups per ultra-fine-group, M, is chosen so that (i) M does not exceed a user input number; (ii) M = 1 if scattering is isotropic or linearly anisotropic in the center of mass system ($N \leq 1$); (iii) M = 1 if isotope scatters at least twenty ultra-fine-groups, (iv) M is calculated to ensure that isotope scatters at least twenty hyper-fine-groups, $M = -20\, \Delta u\, \ell n\alpha$ the scattering from lethargy $u_{g'_m}$ to hyper-fine-group g_n, $P_o(u_{g'_m} \to g_n)$ is calculated using Eq. II.83 with the factorial coefficients for A_m precalculated. The transfer matrix is then obtained using a trapezoidal rule integration,

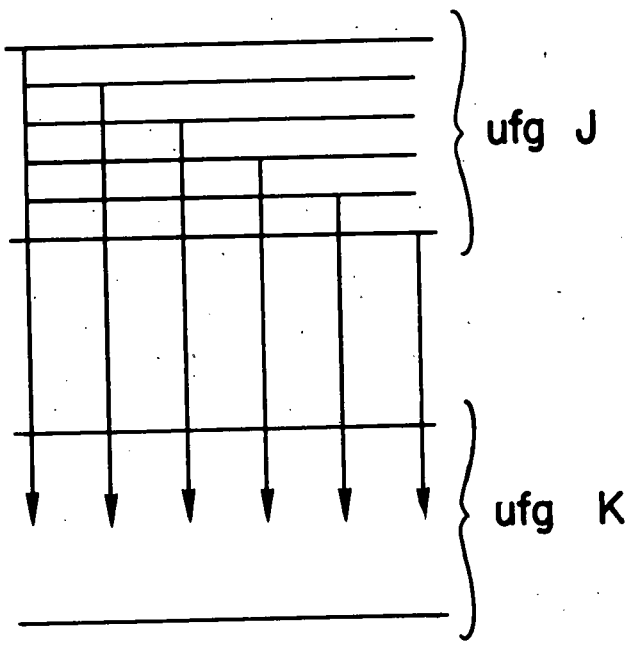

Fig. 3. Elastic Scattering Group Structure

$$P_o(u' \to g) = \sum_{g_n \epsilon g} P_o(u' \to g_n)$$

$$\sigma_s^o(g' \to g) = \frac{\sigma_s^{g'}}{2M} \left[P_o(u_{g'-1} \to g) + P_o(u_{g'} \to g) + 2 \sum_{m=1}^{M-1} P_o(u_{g'-1} + m\delta u \to g) \right] . \quad \text{(II.84)}$$

For the last group which can be reached from g', the matrix element is calculated by balance,

$$\sigma_s^o(g' \to g^*) = \sigma_s^{g'} - \sum_{g=g'}^{g^*-1} \sigma_s^o(g' \to g) \quad \text{(II.85)}$$

where

$$u_{g^*-1} < u_{g'} + \ell n \frac{1}{\alpha} \leq u_{g^*} .$$

For the consistent P_1/B_1 options of MC^2-2, the matrix elements of Equations II.81-II.82 for ℓ=1 are required. Although it is possible to derive $P_1(u' \to g)$ analytically as with Eq. II.83, this expression is time consuming and difficult to evaluate numerically. It is furthermore possible to obtain a fast and accurate evaluation of the integral by taking

$$P_1(u' \to g_n) \approx \mu_o(u' \to \bar{g}_n) \; P_o(u' \to g_n). \quad \text{(II.86)}$$

The small group size, $\delta u \leq \Delta u \approx .008$ makes this a good approximation. The code uses the energy midpoint of the hyper-fine sink group in this calculation. From Eq. II.40, μ_o is given by

$$\mu_o(u' \to \bar{g}_n) \equiv \frac{1}{2} \bar{X}_n^{-\frac{1}{2}} \left(1 + A - \frac{A - 1}{\bar{X}_n}\right) \quad \text{(II.87)}$$

$$\bar{X}_n \equiv \frac{1}{2} e^{-(n-1)\delta u} \left[1 + e^{-\delta u}\right] .$$

Equations II.86 and II.87 are used to calculate the P_1 matrix in a manner analagous to that of the P_o matrix,

$$P_1(u' \to g) = \sum_{g_n \epsilon g} \mu_o(u' \to \bar{g}_n) \; P_o(u' \to g_n)$$

$$\sigma_{s_1}^1(g' \to g) = \frac{\sigma_s^{g'}}{2M} \left[P_1(u_{g'-1} \to g) + P_1(u_{g'} \to g) + 2 \sum_{m=1}^{M-1} P_1(u_{g'-1} + m\delta u \to g) \right] \quad \text{(II.88)}$$

where $\sigma_{s_1}^{g'}$ is calculated from Eq. II.45,

$$\sigma_{s_1}^{g} = \sum_{n=0}^{N} \sigma_s^g f_n^g T_{\ell n}^o(\alpha) \tag{II.89}$$

and scattering into the last group is calculated by balance as in Eq.II.85

$$\sigma_s^1(g' \to g^*) = \sigma_{s_1}^{g'} - \sum_{g=g'}^{g^*-1} \sigma_s(g' \to g) \ . \tag{II.90}$$

The accuracy of these methods has been documented by Henryson, et al.[20]

2. Heavy Elements

For materials which scatter less than four ultra-fine-groups (A > 160 for $\Delta u = 1/120$) the method reported by Henryson[21] is used. Equation II.79 is written

$$\sigma_s^\ell(g' \to g) = \frac{\sum_{n=0}^{N} \left\langle \sigma_n(u')\ \phi_\ell(u') \right\rangle_{g'} A_n^\ell(g' \to g)}{\Delta u \left\langle \phi_\ell(u') \right\rangle_{g'}} \tag{II.91}$$

where $\langle\ \ \rangle$ designates a suitable average over the group, and

$$A_n^\ell(g' \to g) \equiv \frac{(2n+1)}{1-\alpha} \int_{g'} du' \int_g du\ P_\ell(\mu_o)\ P_n(\mu_c)\ e^{-(u-u')} \ . \tag{II.92}$$

As with the light elements, one takes the group width to be small enough to permit a constant weight function so that

$$\left\langle \sigma_n(u')\ \phi_\ell(u') \right\rangle_{g'} \tilde{\sim} 1/2\ \sigma_s^{g'}\ [f_n(u_{g'-1}) + f_n(u_{g'})].$$

As shown in Ref. 21, it is possible to change variables and switch the order to integration so as to write Eq. II.92 in terms of a function

$$\bar{T}_{\ell n}^m(\alpha,\beta) \equiv \frac{(-)^m}{m!} \frac{(2n+1)}{2} \int_0^\beta dU\ U^m\ P_\ell(\mu_o)\ P_n(\mu_c)\ (-\frac{d\mu_c}{dU}) \ . \tag{II.93}$$

It is not difficult to show that on integrating Eq.II.92 over all sink groups,

$$A_n^\ell(g') = \Delta u\ T_{\ell n}^o(\alpha) = \Delta u\ \bar{T}_{\ell n}^o(\alpha,\ \ell n \frac{1}{\alpha})$$

where the T function was defined by Equation II.42. The matrix elements $A_n^\ell(g' \to g)$ are given in Table II. These precalculated elements are given on File 8 of the MC^2-2 library (Appendix C) for each of the heavy isotopes and are used by MC^2-2 in the calculation of Equation II.91.

TABLE II. Heavy Mass Matrix Elements $A_n^{\ell}(j \to k)$

k	Group Width/Mass ($q \equiv \ell n\ 1/\alpha$)	$A_n^{\ell}(j \to k)$
	$1/3\ q \leq \Delta u < 1/2\ q$	
j		$\Delta u \bar{T}^0_{\ell n}(\alpha,\Delta u) + \bar{T}^1_{\ell n}(\alpha,\Delta u)$
j + 1		$2\Delta u[\bar{T}^0_{\ell n}(\alpha,2\Delta u) - \bar{T}^0_{\ell n}(\alpha,\Delta u)] + \bar{T}^1_{\ell n}(\alpha,2\Delta u) - 2\bar{T}^1_{\ell n}(\alpha,\Delta u)$
j + 2		$3\Delta u T^0_{\ell n}(\alpha) + T^1_{\ell n}(\alpha) - 2\bar{T}^1_{\ell n}(\alpha,2\Delta u) + \bar{T}^1_{\ell n}(\alpha,\Delta u) - \Delta u[4\bar{T}^0_{\ell n}(\alpha,2\Delta u) - \bar{T}^0_{\ell n}(\alpha,\Delta u)]$
j + 3		$-2\Delta u T^0_{\ell n}(\alpha) - T^1_{\ell n}(\alpha) + 2\Delta u \bar{T}^0_{\ell n}(\alpha,2\Delta u) + \bar{T}^1_{\ell n}(\alpha,2\Delta u)$
	$1/2\ q \leq \Delta u < q$	
j		$\Delta u \bar{T}^0_{\ell n}(\alpha,\Delta u) + \bar{T}^1_{\ell n}(\alpha,\Delta u)$
j + 1		$2\Delta u T^0_{\ell n}(\alpha) + T^1_{\ell n}(\alpha) - 2\Delta u \bar{T}^0_{\ell n}(\alpha,\Delta u) - 2\bar{T}^1_{\ell n}(\alpha,\Delta u)$
j + 2		$-T^1_{\ell n}(\alpha) - \Delta u T^0_{\ell n}(\alpha) + \Delta u \bar{T}^0_{\ell n}(\alpha,\Delta u) + \bar{T}^1_{\ell n}(\alpha,\Delta u)$
	$\Delta u \geq q$	
j		$\Delta u T^0_{\ell n}(\alpha) + T^1_{\ell n}(\alpha)$
j + 1		$-T^1_{\ell n}(\alpha)$

3. Hydrogen Elastic Scattering

It is impossible to treat Hydrogen elastic scattering in the manner outlined for the light elements above because of the computer storage problems associated with a full ultra-fine-group scattering band. Simple recursive relationships exist which are used by MC^2-2 in lieu of storing the Hydrogen matrix. These relationships are given below.

Let $S^g_{\ell_H}$ be the P_ℓ elastic scattering source into group g from all groups above g due to scattering from Hydrogen. Assuming the scattering to be isotropic in the center of mass system, and taking A=1, Eqs. II.40 and II.79 are used to give

$$S^g_{\ell_H} \equiv \int_{u_{g-1}}^{u_g} du \int_0^{u_{g-1}} du' \, \Sigma_{s_H}(u') \, \phi_\ell(u') \, e^{-(1 - \frac{\ell}{2})(u-u')} , \qquad \ell = 0, 1 . \tag{II.94}$$

Performing the integration over group g it is simple to show

$$S^g_{\ell_H} = \eta_\ell(u_{g-1}) \, [1 - e^{-(1 + \frac{\ell}{2})\Delta u}] , \qquad \ell = 0, 1 \tag{II.95}$$

where the Hydrogen slowing down density $\eta_\ell(u)$ is given by Eqs.II.37 and II.76.

H. Inelastic and (n,2n) Scattering

As noted in Section B above, non-elastic scattering (inelastic, (n,2n)) is treated as a source term in the ultra-fine-group spectrum calculation. The development of the continuous slowing down equations made use of this separation explicitely. In the multigroup formulation this separation is implicit since the code does not prepare a non-elastic ultra-fine-group scattering matrix because of the excessive storage requirements for such a matrix. Rather, the non-elastic scattering source is calculated directly on each pass through the ultra-fine-groups. This is the most time consuming part of the ultra-fine-group spectrum calculation in MC^2-2.

For both inelastic and (n,2n) scattering, the MC^2-2 code permits three descriptions of the secondary energy distributions: (i) tabulated function; (ii) evaporation spectrum; (iii) discrete levels. The remainder of this section will be concerned with the methods used to calculate the ultra-fine-group non-elastic scattering source for each of these descriptions.

1. Tabulated Function

The following data are provided on the MC^2-2 library file MCC2F6 (c.f. Appendix C),

$P_x(g \rightarrow E_{tab})$	Probability that a neutron is scattered by process x (inelastic or (n,2n)) from group g to energy point E_{tab}
E_{tab}	An array of "sink" energy points
KT	An interpolation law on the sink energies E_{tab}
$\sigma^g_{x_{tab}}$	Cross section in group g for process x multiplied by the fraction of scattering events described by the P_x law

From these definitions it is obvious that the non-elastic scattering source into group g described by the tabulated law is given by

$$S^g_{ne_{tab}} = \sum_{g'} \phi^{g'} \left\{ \sigma^{g'}_{inel_{tab}} \int_{E_{g-1}}^{E_g} dE\, P_{inel}(g' \rightarrow E) + 2\, \sigma^{g'}_{n,2n_{tab}} \int_{E_{g-1}}^{E_g} dE\, P_{n,2n}(g' \rightarrow E) \right\} . \qquad \text{(II.96)}$$

The integrals of Eq. II.96 are evaluated analytically using the interpolation law defined by the KT data.

2. Evaporation Spectrum

For both inelastic and (n,2n) scattering, the MC^2-2 library provides evaporation temperatures and fractional probabilities such that

$$S^g_{ne_{evap}} = S^g_{evap_{inel}} + 2\, S^g_{evap_{n,2n}}$$

$$S^g_{evap_x} = \sum_{g'} \sigma^{g'}_x \phi^{g'} \sum_n \frac{W^{g'}_{n,x}}{I^{g'}_{n,x}} \int_{E_{g-1}}^{E_g} dE\, P_{ev,x,n}(g' \to E) \qquad \text{(II.97)}$$

$$P_{ev,x,n}(g' \to E) = \begin{cases} 0 & E > E_{g'-1} - U_{x,n} \\ E \exp\left(-\dfrac{E}{\theta^{g'}_{x,n}}\right) & E \leq E_{g'-1} - U_{x,n} \end{cases}$$

where the subscript n is used to indicate a sum over all evaporation spectra for process x and $I^{g'}_{n,x}$ is a normalization factor,

$$I^{g'}_{n,x} = \int_0^{E_{g'-1} - U_{x,n}} dE\, P_{ev}(g' \to E) \quad .$$

For (n,2n) events the constant U is assumed to be zero.

The evaluation of Eq.II.97 requires an exponential for each ultra-fine sink group, and it is this calculation which controls the computing time of an MC^2-2 spectrum calculation. A fast exponential function[22] (Appendix A) is used by MC^2-2 to evaluate the required exponentials. Furthermore, the calculation over sink groups g is terminated once the criterion

$$\frac{\int_{E_{g-1}}^{E_g} dE\, P_{ev,x,n}(g' \to E)}{\int_{E_{g-1}}^{E_{g'-1} - U_{x,n}} dE\, P_{ev,x,n}(g' \to E)} \leq 10^{-4}$$

is met. The integrals of Eq.II.97 are calculated analytically.

3. Discrete Levels

The MC^2-2 library file MCC2F6 provides Q values and ultra-fine-group level cross sections for all inelastic and/or (n,2n) discrete scattering levels. In addition the library provides the average cosine of the scattering angle in the center of mass system for discrete inelastic scattering by level and group. These data are processed in the manner indicated below.

a. Approximate Treatment Neglecting Energy-Angle Correlation

It is well known that energy and momentum conservation give

$$E = \frac{1 + A^2}{(1 + A)^2} E' - \frac{A}{A + 1} Q_\lambda + \frac{2A}{(1 + A)^2} \mu E' \left[1 - \frac{A + 1}{A} \frac{Q_\lambda}{E'}\right]^{\frac{1}{2}} \quad \text{(II.98)}$$

where

E = lab energy after collision

E' = lab energy before collision

μ = cosine of c.m. angle of scatter

Q_λ = -Q value of reaction for level λ

A = mass of scattering isotope.

The threshold energy of the reaction is

$$E_\lambda = \frac{A + 1}{A} Q_\lambda \ , \quad \text{(II.99)}$$

A rigorous evaluation of the group to group transfer probability accounting for the energy-angle correlation of Eq.II.98 is quite complicated.[23] Two assumptions serve to simplify the situation without much loss in accuracy:

(i) angle of scattering is fixed;

(ii) $\left(1 - \frac{E_\lambda}{E'}\right)^{\frac{1}{2}} \approx 1 - 1/2 \frac{E_\lambda}{E'}$.

With these assumptions one can write

$$E = E' \left[\frac{1 + A^2 + 2A \langle\mu\rangle}{(1 + A)^2}\right] - \frac{(A + \langle\mu\rangle)}{A + 1} Q_\lambda \quad \text{(II.100)}$$

$$E' = \frac{(1 + A)^2}{1 + A^2 + 2A \langle\mu\rangle} E + \frac{(A + \langle\mu\rangle)\ (A + 1)\ Q_\lambda}{1 + A^2 + 2A \langle\mu\rangle} \ . \quad \text{(II.101)}$$

It is clear from Eq. II.100 that the probability of scattering from group j to group k for discrete level λ is identically zero unless group k lies between the energy boundaries

$$E_{j-1} \left[\frac{1 + A^2 + 2A \langle\mu\rangle}{(1 + A)^2}\right] - \frac{(A + \langle\mu\rangle)\ Q_\lambda}{1 + A} \ ,$$

$$\max(E_j, E_\lambda) \left[\frac{1 + A^2 + 2A\langle\mu\rangle}{(1 + A^2)}\right] - \frac{(A + \langle\mu\rangle)}{1 + A} Q_\lambda \qquad \text{(II.102)}$$

and it has been assumed that at least a part of group j lay above the threshold,

$$E_{j-1} > E_\lambda .$$

For those groups, k, which fall partially or totally within this range, the probability of scattering from group j to group k is given by the fractional part of group j which scatters into group k. This can be derived directly from Eq. II.101,

$$P_\lambda(j \to k) \equiv \frac{E^*_{j-1} - E^*_j}{E_{j-1} - E_j} \qquad \text{(II.103)}$$

where

$$E^*_{j-1} = \min \left[E_{j-1}, \frac{(1 + A^2)\, E_{k-1} + (A + 1)\,(A + \langle\mu\rangle)\, Q_\lambda}{1 + A^2 + 2A\langle\mu\rangle}\right]$$

$$E^*_j = \max \left[E_j, E_\lambda, \frac{(1 + A^2)\, E_k + (A + 1)\,(A + \langle\mu\rangle)\, Q_\lambda}{1 + A^2 + 2A\langle\mu\rangle}\right] . \qquad \text{(II.104)}$$

The Eqs.II.102-II.104 are used by MC^2-2 to calculate the discrete scattering source,

$$S^g_{ne,d} = \sum_{g'} \phi^{g'} \left\{ \sum_\lambda \sigma^{g'}_{inel_\lambda} P_\lambda(g' \to g) + 2 \sum_{\lambda'} \sigma^{g'}_{n,2n_{\lambda'}} P_{\lambda'}(g' \to g) \right\} .$$

The average cosine of the scattering angle is taken to be zero (isotropic in center of mass) for scattering from all (n,2n) levels. The λ,λ' sums represent sums over all discrete levels.

The complete microscopic non-elastic scattering source is given by

$$S^g_{ne} = S^g_{ne_{tab}} + S^g_{ne_{cvp}} + S^g_{ne_d} .$$

The macroscopic sources are defined by summing over all materials using the appropriate atom densities.

b. Rigorous Treatment Assuming Isotropic Scattering

The approximations made above are quite good for source energies far above threshold where the level cross sections σ^g_λ are large. The simplicity of the formulation along with its accuracy suggest that Eqs. II.102-II.104 provide the recommended procedure for evaluating the discrete inelastic source. On option the user may, however, specify a more rigorous, and correspondingly more time consuming, treatment of discrete level scattering. The option follows the work of Segev,[23] which accounts

explicitely for the fact that a neutron scattered at energy E' scatters into a band of energies defined from Eq. II.98 as

$$\left[\frac{1 \pm A\left(1 - \frac{E_\lambda}{E'}\right)^{1/2}}{1 + A}\right]^2 E' \quad . \tag{II.105}$$

This band of energies must be used instead of Eq. II.100 to define the possible sink groups. Similarly, a neutron scattered into energy E' may be scattered from a range of source energies defined by

$$\left[\frac{1 + A\left(1 + \frac{A-1}{A+1}\frac{E_\lambda}{E}\right)^{1/2}}{1 - A}\right]^2 E \tag{II.106}$$

and

$$\max\left\{E_\lambda^{(c)}, \left[\frac{1 - A\left(1 + \frac{A-1}{A+1}\frac{E_\lambda}{E}\right)^{1/2}}{1 - A}\right]^2 E\right.$$

where

$$E_\lambda^{(c)} = \frac{A^2}{A^2 - 1} E_\lambda$$

is a pseudo-threshold energy defined to avoid the need to consider the double valued nature of E' for a given E. This source group band width replaces Eq. II.101 of the approximate treatment. Accounting for the above energy bands leads to four domains of integration in evaluating the probability of scattering from group j to group k as

$$P_\lambda(j \to k) = \frac{1}{E_{j-1} - E_j} \int_{\text{group } j} dE' \int_{\text{group } k} dE$$

$$\cdot \sum_n \frac{(2n+1)}{(1-\alpha)E'} \frac{f_n(E')}{\left[1 - \frac{E_\lambda}{E'}\right]^{\frac{1}{2}}} P_n(\mu) \quad . \tag{II.107}$$

In the more rigorous option of MC^2-2, Eq. II.107 is evaluated analytically taking proper account of the four domains of integration as discussed in Ref. 23. Because of the time consuming nature of the calculation, Eq. II.107 is solved assuming isotropic scattering in the center-of-mass. For standard fast reactor configurations, it has been found that the discrete inelastic calculation using the approximate method defined by Eqs. II.103-II.104 is quite accurate and significantly faster than the algorithms discussed above which account explicitely for the energy-angle correlation of discrete level scattering as defined by Eq. II.98.

I. Ultra-Fine-Group Macroscopic Data

The macroscopic data required for solution of the spectrum equations discussed in Section F may in almost all cases be derived from the simple expression

$$\Sigma_x^g = \sum_i N_i \sigma_{x_i}^g \tag{II.108}$$

where N_i is the atom density of isotope i in the homogeneous mix and $\sigma_{x_i}^g$ is the ultra-fine-group cross section for isotope i and process x. This expression is clearly applicable to the scattering matrix data discussed in Sections G and H above. The ultra-fine-group microscopic reaction cross sections are available on the MC^2-2 library file MCC2F5 (c.f. Appendix C). These data are generally processed directly from the ENDF/B data files by the code ETOE-2 assuming a constant weighting.

The unresolved resonance cross sections are treated in the same manner as the above data. The calculation of the ultra-fine-group unresolved cross sections is discussed in Chapter IV. The remainder of this section is concerned with the calculation of macroscopic data which require more processing than that given by Eq. II.108.

1. Fission Source Data

The fission source of Eq. II.14 may be written in group form as

$$S_f^g = \sum_i \chi_i^g N_i \sum_{g'} \nu_i^{g'} \sigma_{f_i}^{g'} \phi^{g'} . \tag{II.109}$$

The number of neutrons per fission, ν_i^g, is derived from the expression

$$\nu_i^g = \frac{1}{E_{g-1} - E_g} \int_{E_g}^{E_{g-1}} \nu_i(E)\, dE$$

$$\nu_i(E) = A_o^i + A_1^i E + A_2^i E^2 + A_3^i E^3. \tag{II.110}$$

The fission spectrum distribution is given by

$$\chi_i^g = \frac{\int_{E_g}^{E_{g-1}} dE\ \chi_i(E)}{\int_{E_{min}}^{E_{max}} dE\ \chi_i(E)} = \frac{\hat{\chi}_i^g}{\sum_{g'} \hat{\chi}_i^{g'}} \tag{II.111}$$

with

$$\chi_i(E) = \alpha_i \frac{E}{\tau_i^2} e^{-E/\tau_i} + (1 - \alpha_i) \sqrt{\frac{4E}{\pi \beta_i^3}}\, e^{-E/\beta_i} .$$

This combination of a Maxwellian plus an evaporation spectrum suffices to describe all but one of the fission spectra for the most recent release of the ENDF/B data files. Integration of Eq. II.111 gives

$$\hat{\chi}_i^g = \alpha_i \left[\left(1 + \frac{E_g}{\tau_i}\right) e^{-E_g/\tau_i} - \left(1 + \frac{E_{g-1}}{\tau_i}\right) e^{-E_{g-1}/\tau_i} \right]$$

$$+ (1 - \alpha_i) \left[\operatorname{erf}\left[(E_{g-1}/\beta_i)^{\frac{1}{2}}\right] - \operatorname{erf}\left[(E_g/\beta_i)^{\frac{1}{2}}\right] \right. \qquad \text{(II.112)}$$

$$\left. - \left(\frac{4E_{g-1}}{\pi\beta_i}\right)^{\frac{1}{2}} e^{-E_{g-1}/\beta_i} + \left(\frac{4E_g}{\pi\beta_i}\right)^{\frac{1}{2}} e^{-E_g/\beta_i} \right] .$$

Equation II.112 is used by MC^2-2 to evaluate the fission spectrum distribution. It should be noted that the "temperatures" τ_i and β_i are not energy dependent in the MC^2-2 formulation although such a description is not rigorous. In practice the temperatures in the MC^2-2 library are those characteristic of the average fission energy of a typical fast reactor assembly. It is possible on user option to input the fission spectrum temperature β_i by isotope which the code will use in lieu of the library data taking α_i to be zero.

2. Ultra-Fine-Group Extended Transport Cross Section

The transport-like cross sections A_ℓ^g defined as

$$A_\ell^g = \int_{u_{g-1}}^{u_g} A_\ell(B, u, N)\, du$$

are required in solution of the ultra-fine-group spectrum equations. $A_\ell(B, u, N)$ is defined by the continued fraction expansion of Eqs.II.11 and II.12 . The MC^2-2 code does not actually perform the required integration. Rather the parameters b_ℓ are simply defined in terms of the group cross sections, so that, for example,

$$A_1^g = \frac{B \tan^{-1} B/\Sigma_t^g}{3\left(1 - \frac{\Sigma_t^g}{B} \tan^{-1} \frac{B}{\Sigma_t^g}\right)}$$

in the consistent B_1 approximation. The cross sections A_ℓ^g are clearly dependent upon the buckling B^2 which may change during the coarse of a calculation if the user specifies a buckling search option. The code does not recalculate A_ℓ^g in that case. Rather, a special user input buckling, κ^2 is used in the calculation of A_ℓ^g. This same value of κ^2 is also used

in the leakage correction to the background cross section in the resonance calculation of MC^2-2, as described in Chapters III and IV. The value of κ^2 is set by the user and may or may not equal the B^2 used in the ultra-fine group spectrum calculation.

The continued fraction coefficients depend upon the ratio of Legendre functions of the second kind which can not be calculated for all arguments using the standard forward recurrence relation without a significant loss of accuracy. The algorithms used in MC^2-2 to calculate this ratio are summarized in Appendix A.

3. Improved Goertzel-Greuling Moderating Parameters

In Section D.2 integral expressions were derived defining the isotopic moderating parameters ξ_i^ℓ, a_i^ℓ, c_i^ℓ and e_i^ℓ. The numerical evaluation of these expressions is described below.

The heavy isotope moderating parameters are given by Eq. II.44. The effective ratios are calculated by integrating over the scattering bandwidth,

$$\left\langle \frac{\Sigma_{s_i}}{\Sigma_t} f_{n_i} \right\rangle_u \approx \frac{1}{\ell n \frac{1}{\alpha_i}} \left\{ \Delta u \sum_{n=1}^{N_i} \frac{\Sigma_{s_i}(u - (n - \tfrac{1}{2})\Delta u)}{\Sigma_t(u - (n - \tfrac{1}{2})\Delta u)} f_{n_i}(u - (n-1)\Delta u) \right. \tag{II.113}$$

$$\left. + (\ell n \frac{1}{\alpha_i} - N_i \Delta u) \frac{\Sigma_{s_i}(u - (N_i + \tfrac{1}{2})\Delta u)}{\Sigma_t(u - (N_i + \tfrac{1}{2})\Delta u)} f_{n_i}(u - N_i \Delta u) \right\}$$

where N_i is the nearest whole integer to the ratio $-\frac{\ell n \alpha_i}{\Delta u}$ $\left(= \left[-\frac{\ell n \alpha_i}{\Delta u}\right]\right)$. The ratio is evaluated at ultra-fine-group boundaries and group cross sections are used so that

$$\frac{\Sigma_{s_i}(u_g - \tfrac{1}{2}\Delta u)}{\Sigma_t(u_g - \tfrac{1}{2}\Delta u)} \equiv \frac{\Sigma_{s_i}^g}{\Sigma_t^g} .$$

The evaluation of the light element moderating parameters as defined by Eqs. II.48 is somewhat more complex. The first step in the development is the definition of integrating factors which permit an accurate numerical evaluation of the integrals:

$$\int_{u-\ell n 1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \mathcal{P}_m^i(u') \approx W_{1_i} \sum_{n=1}^{N_i} \frac{\Sigma_{s_i}(u - (n - \tfrac{1}{2})\Delta u)}{\Sigma_t(u - (n - \tfrac{1}{2})\Delta u)} \mathcal{P}_m^i(u - (n - \tfrac{1}{2})$$

$$\int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \mathcal{D}_m^i(u')\ (u-u') \approx W_{2_i} \sum_{n=1}^{N_i} \frac{\Sigma_{s_i}(u-(n-\tfrac{1}{2})\Delta u)}{\Sigma_t(u-(n-\tfrac{1}{2})\Delta u)}$$

$$\mathcal{D}_m^i(u-(n-\tfrac{1}{2})\Delta u)\ (n-\tfrac{1}{2})$$

$$\int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \mathcal{D}_m^i(u')\ e^{-x(u-u')} \approx \tag{II.114}$$

$$W_{3_i}^x \sum_{n=1}^{N_i} \frac{\Sigma_{s_i}(u-(n-\tfrac{1}{2})\Delta u)}{\Sigma_t(u-(n-\tfrac{1}{2})\Delta u)} \mathcal{D}_m^i(u-(n-\tfrac{1}{2})\Delta u)\ e^{-x(n-\frac{1}{2})\Delta u}$$

$$\int_{u-\ell n^1/\alpha_i}^{u} du' \frac{\Sigma_{s_i}(u')}{\Sigma_t(u')} \mathcal{D}_m^i(u')\ (u-u')\ e^{-x(u-u')} \approx$$

$$W_{4_i}^x \sum_{n=1}^{N_i} \frac{\Sigma_{s_i}(u-(n-\tfrac{1}{2})\Delta u)}{\Sigma_t(u-(n-\tfrac{1}{2})\Delta u)} \mathcal{D}_m^i(u-(n-\tfrac{1}{2})\Delta u)\ (n-\tfrac{1}{2})\ e^{-x(n-\frac{1}{2})\Delta u}\ .$$

It is clear from the development of the improved Goertzel-Greuling slowing down theory that if

$$\frac{\Sigma_{s_i}}{\Sigma_t} f_n^i$$

is constant over a scattering band, then the IGG moderating parameters should reduce to the standard Goertzel-Greuling form. If this characteristic of the moderating parameters is retained, then it is possible to define integration factors in the following manner:

$$W_{1_i} \equiv \ell n^1/\alpha_i/N_i$$

$$W_{2_i} \equiv (\ell n^1/\alpha_i/N_i)^2$$

$$W_{3_i}^x \equiv \frac{1}{x}(1-\alpha_i^x) \Big/ \sum_{n=1}^{N_i} e^{-x(n-\frac{1}{2})\Delta u} \tag{II.115}$$

$$W_{4_i}^x \equiv \frac{1}{x^2}(1-\alpha_i^x(1+x\,\ell n^1/\alpha_i)) \Big/ \sum_{n=1}^{N_i} (n-\tfrac{1}{2})\ e^{-x(n-\frac{1}{2})\Delta u}\ .$$

The improved Goertzel-Greuling moderating parameters are then calculated by replacing the integrals of Eqs. II.48 by the numerical approximations

$$\xi_i^o(u) = \sum_{n'=1}^{N+1} \frac{1}{n'} \left[W_{3_i}^{n'} \; b_i^{n',n'}(u) - \alpha_i^{n'} \; W_{1_i} \; d_i^{n'}(u) \right]$$

$$a_i^o(u) = - \sum_{n'=1}^{N+1} \frac{1}{n'} \left[W_{4_i}^{n'} \; f_i^{n',n'} - \alpha_i^{n'} \; W_{2_i} \; g_i^{n'}(u) \right]$$

$$c_i^o(u) = \frac{\Sigma_{s_i}(u)}{\Sigma_t(u)} - \sum_{n'=1}^{N+1} W_{3_i}^{n'} \; b_i^{n',n'}(u)$$

$$c_i^o(u) = \sum_{n'=1}^{N+1} W_{4_i}^{n'} \; f_i^{n',n'} \qquad \text{(II.116)}$$

$$\xi_i^1(u) = \sum_{n'=1}^{N+1} \left\{ \frac{(A_i+1)}{2n'+1} \left[W_{3_i}^{n'+\frac{1}{2}} \; b_i^{n'+\frac{1}{2},n'}(u) - \alpha_i^{n'+\frac{1}{2}} \; W_{1_i} \; d_i^{n'}(u) \right] \right.$$

$$\left. - \frac{(A_i-1)}{2n'-1} \left[W_{3_i}^{n'-\frac{1}{2}} \; b_i^{n'-\frac{1}{2},n'}(u) - \alpha_i^{n'-\frac{1}{2}} \; W_{1_i} \; d_i^{n'}(u) \right] \right\}$$

$$a_i^1(u) = - \sum_{n'=1}^{N+1} \left\{ \frac{(A_i+1)}{2n'+1} \left[W_{4_i}^{n'+\frac{1}{2}} \; f_i^{n'+\frac{1}{2},n'}(u) - \alpha_i^{n'+\frac{1}{2}} \; W_{2_i} \; g_i^{n'}(u) \right] \right.$$

$$\left. - \frac{(A_i-1)}{2n'-1} \left[W_{4_i}^{n'-\frac{1}{2}} \; f_i^{n'-\frac{1}{2},n'}(u) - \alpha_i^{n'-\frac{1}{2}} \; W_{2_i} \; g_i^{n'}(u) \right] \right\}$$

$$c_i^1(u) = \frac{\Sigma_{s_i}(u)}{\Sigma_t(u)} \sum_{n'=0}^{N} T_{1n'}^o(\alpha_i) \; f_{n'_i}(u) - \tfrac{1}{2} \sum_{n'=1}^{N+1} (A_i + 1) \; W_{3_i}^{n'+\frac{1}{2}} \; b_i^{n'+\frac{1}{2},n'}(u)$$

$$+ \tfrac{1}{2} (A_i - 1) \sum_{n'=1}^{N+1} W_{3_i}^{n'-\frac{1}{2}} \; b_i^{n'-\frac{1}{2},n'}(u)$$

$$e_i^1(u) = \tfrac{1}{2} \sum_{n'=1}^{N+1} \left\{ (A_i + 1) \; W_{4_i}^{n'+\frac{1}{2}} \; f_i^{n'+\frac{1}{2},n'} - (A_i - 1) \; W_{4_i}^{n'-\frac{1}{2}} \; f_i^{n'-\frac{1}{2},n'}(u) \right\}$$

where

$$b_{i(u)}^{x,m} = \sum_{n=1}^{N_i} \frac{\Sigma_{s_i}(u - (n - \tfrac{1}{2}) \Delta u)}{\Sigma_t(u - (n - \tfrac{1}{2}) \Delta u)} \mathcal{D}_m^i(u - (n - \tfrac{1}{2}) \Delta u) \; e^{-x(n-\frac{1}{2})\Delta u}$$

$$d_i^m(u) = \sum_{n=1}^{N_i} \frac{\Sigma_{s_i}(u - (n - \tfrac{1}{2}) \Delta u)}{\Sigma_t(u - (n - \tfrac{1}{2}) \Delta u)} \mathcal{D}_m^i(u - (n - \tfrac{1}{2}) \Delta u) \qquad \text{(II.117)}$$

$$f_i^{x,m}(u) = \sum_{n=1}^{N_i} \frac{\Sigma_{s_i}(u - (n - \tfrac{1}{2})\,\Delta u)}{\Sigma_t(u - (n - \tfrac{1}{2})\,\Delta u)}\, \mathcal{D}_m^i(u - (n - \tfrac{1}{2})\,\Delta u)\,(n - \tfrac{1}{2})\, e^{-x(n-\frac{1}{2})\Delta u}$$

$$g_i^m(u) = \sum_{n=1}^{N_i} \frac{\Sigma_{s_i}(u - (n - \tfrac{1}{2})\,\Delta u)}{\Sigma_t(u - (n - \tfrac{1}{2})\,\Delta u)}\, \mathcal{D}_m^i(u - (n - \tfrac{1}{2})\,\Delta u)\,(n - \tfrac{1}{2}) \quad .$$

The Eqs. II.117 are used to calculate the coefficients at the lethargy U_{CSD} between the multigroup and continuous slowing down regions of the calculation. For the lethargy boundaries $u_g > U_{CSD}$ recursion relations are used:

$$b_i^{x,m}(u + \Delta u) = b_i^{x,m}(u)\, e^{-x\Delta u} + e^{-x\frac{\Delta u}{2}} \left\{ \frac{\Sigma_{s_i}(u + \frac{\Delta u}{2})}{\Sigma_t(u + \frac{\Delta u}{2})}\, \mathcal{D}_m^i(u + \frac{\Delta u}{2}) - \right.$$

$$\left. \frac{\Sigma_{s_i}(u - (N_i - \tfrac{1}{2})\,\Delta u)}{\Sigma_t(u - (N_i - \tfrac{1}{2})\,\Delta u)}\, \mathcal{D}_m^i(u - (N_i - \tfrac{1}{2})\,\Delta u)\, e^{-xN_i\Delta u} \right\}$$

$$d_i^m(u + \Delta u) = d_i^m(u) + \left\{ \frac{\Sigma_{s_i}(u + \frac{\Delta u}{2})}{\Sigma_t(u + \frac{\Delta u}{2})}\, \mathcal{D}_m^i(u + \frac{\Delta u}{2}) \right.$$

$$\left. - \frac{\Sigma_{s_i}(u - (N_i - \tfrac{1}{2})\,\Delta u)}{\Sigma_t(u - (N_i - \tfrac{1}{2})\,\Delta u)}\, \mathcal{D}_m^i(u - (N_i - \tfrac{1}{2})\,\Delta u) \right\}$$

$$f_i^{x,m}(u + \Delta u) = e^{-x\Delta u}\, f_i^{x,m}(u) + b_i^{x,m}(u + \Delta u) \qquad \text{(II.118)}$$

$$- e^{-x\Delta u/2} \left\{ \frac{1}{2}\, \frac{\Sigma_{s_i}(u + \frac{\Delta u}{2})}{\Sigma_t(u + \frac{\Delta u}{2})}\, \mathcal{D}_m^i(u + \frac{\Delta u}{2}) \right.$$

$$\left. + (N_i - \tfrac{1}{2})\, \frac{\Sigma_{s_i}(u - (N_i - \tfrac{1}{2})\,\Delta u)}{\Sigma_t(u - (N_i - \tfrac{1}{2})\,\Delta u)}\, \mathcal{D}_m^i(u - (N_i - \tfrac{1}{2})\,\Delta u)\, e^{-xN_i\Delta u} \right\}$$

$$g_i^m(u + \Delta u) = g_i^m(u) + d_i^m(u + \Delta u)$$

$$- \frac{1}{2} \frac{\Sigma_{s_i}(u + \frac{\Delta u}{2})}{\Sigma_t(u + \frac{\Delta u}{2})} \mathcal{D}_m^i(u + \frac{\Delta u}{2})$$

$$- (N_i - \tfrac{1}{2}) \frac{\Sigma_{s_i}(u - (N_i - \tfrac{1}{2})\,\Delta u)}{\Sigma_t(u - (N_i - \tfrac{1}{2})\,\Delta u)} \mathcal{D}_m^i(u - (N_i - \tfrac{1}{2})\,\Delta u) \ .$$

As noted in Section D.2, the sums over Legendre coefficients of Eqs. II.116 are limited to four terms (N = 3) within the MC^2-2 code.

J. Ultra-Fine-Group Solution Strategies

Once the resonance, transfer matrix, moderating parameter and cross section data have been processed on an ultra-fine-group mesh the solution of the spectrum equations presented in Section F must be performed. In this section the strategies involved in treating the resonance attenuation, buckling search, flux iterations and fixed source or eigenvalue problems are discussed.

1. Ultra-Fine-Group Spectrum Solution

Given an initial fission source, S_f^g, and a buckling, B^2, it is possible to solve both the multigroup equations, II.62 or II.64 and the continuous slowing down equations II.66 or II.70 and II.71 by sweeping down the energy mesh from group 1 to the last ultra-fine-group in the problem. Both the sources due to inelastic and/or (n,2n) scattering and the Hydrogen slowing down density are updated after calculating the flux (and current) for a given ultra-fine-group. In the continuous slowing down region, the equations II.66 or II.70 are used to obtain $q_o^{asy}(u_g)$ from the values $q_\ell(u_{g-1})$. The $q_o^{asy}(u_g)$ so obtained does not feel any effects of narrow resonances in the group g. The attenuation of the asymptotic slowing down density is performed in the manner outlined in Section E. One defines

$$q_o(u_g) = Q_g q_o^{asy}(u_g)$$

where the attenuation factor Q_g is defined

$$Q_g = \prod_{r \epsilon g} (1 - p_r)$$

$$p_r = \left\{ \frac{\Gamma_a^r}{E_r} J^*_{a_r} - \frac{\Sigma_{ne}^g}{\Sigma_t^g} \frac{\Gamma_t^r}{E_r} J^*_{t_r} \right\} (\Sigma_t^g + \frac{B^2}{3A_1^g}) \ (C_0 + C_1)$$

and

$$\left.\begin{aligned} C_0 &= \frac{\theta}{M_+^g} + \frac{(1-\theta)}{M_-^g} \\ C_1 &= 0 \end{aligned}\right\} \qquad \text{Inconsistent } P_1/B_1$$

$$\left.\begin{aligned} C_0 &= \theta R_+^g + (1-\theta)R_-^g \\ C_1 &= -\left[(\theta T_+^g + (1-\theta)T_-^g \frac{q_1(u_r)}{q_0(u_r)}\right] \end{aligned}\right\} . \qquad \text{Consistent } P_1/B_1$$

In the absence of resonances the slowing down density $q_\ell(u)$ is assumed to vary linearly between group boundaries,

$$q_\ell^{as}(u) = q_\ell^{as}(u_{g-1}) + \left[q_\ell^{as}(u_g) - q_\ell^{as}(u_{g-1})\right] \frac{(u - u_{g-1})}{\Delta u} .$$

The presence of a resonance r introduces a discontinuity such that

$$q_o(u_{r+}) = (1 - p_r) q_o(u_{r-}) .$$

With these conventions and the Eqs. II.32 and II.36 expressions may be derived for the ultra-fine-group flux and current as well as resonance reaction rates.

If A_x^r is the reaction rate for process x (capture, fission, total) of resonance r, then

$$A_x^r = \int \Sigma_{x_r} \phi \, du$$

which using the narrow resonance approximation can be written

$$A_x^r \approx \frac{\Gamma_x}{E_r} J_x^* \left(\Sigma_t^g + \frac{B^2}{3A_1^g}\right) \tilde{\phi}(u_r) . \qquad \text{(II.119)}$$

The flux of Eq. II.119 is obtained from Eq. II.32 or II.36 using the attenuated slowing down density $q_o(u_r)$,

$$\tilde{\phi}(u_r) = \begin{cases} \left[\frac{\theta}{M_+^g} + \frac{(1-\theta)}{M_-^g}\right] q_o(u_r) + \frac{(S_g + \eta_o^g)}{\Delta u} \left[\frac{\theta \gamma_o(u_g)}{M_+^g} + \frac{(1-\theta)\gamma_o(u_{g-1})}{M_-^g}\right] , \\ \qquad \text{Inconsistent } P_1/B_1 \\ \left[\theta R_+^g + (1-\theta)R_-^g\right] q_o(u_r) - \left[\theta T_+^g + (1-\theta)T_-^g\right] q_1(u_r) \\ \quad + \frac{(S_g + \eta_o^g)}{\Delta u} \left[\theta R_+^g \gamma_o(u_g) + (1-\theta)R_-^g \gamma_o(u_{g-1})\right] \\ \quad - \frac{1.5\,\eta_1^g}{\Delta u} \left[\theta T_+^g \gamma_1(u_g) - (1-\theta)T_-^g \gamma_1(u_{g-1})\right] , \\ \qquad \text{Consistent } P_1/B_1 . \end{cases} \qquad \text{(II.120)}$$

The group flux ϕ^g and current J^g are obtained in a similar manner,

$$\phi^g = \begin{cases} \left[\frac{\theta}{M_+^g} + \frac{(1-\theta)}{M_-^g}\right] (1-f) \int_g q_o(u)\, du \\ \quad + (S_g + \eta_o^g) \left[\frac{\theta\gamma_o(u_g)}{M_+^g} + \frac{(1-\theta)\,\gamma_o(u_{g-1})}{M_-^g}\right], & \text{Inconsistent } P_1/B_1 \\ \left[\theta R_+^g + (1-\theta)\, R_-^g\right](1-f) \int_g q_o(u)\, du \\ \quad - \left[\theta T_+^g + (1-\theta)\, T_-^g\right] \int_g q_1(u)\, du \\ \quad + (S_g + \eta_o^g) \left[\theta R_+^g \gamma_o(u_g) + (1-\theta)\, R_-^g \gamma_o(u_{g-1})\right] \\ \quad - 1.5\, \eta_1^g \left[\theta T_+^g \gamma_1(u_g) + (1-\theta)\, T_-^g \gamma_1(u_{g-1})\right], \\ & \text{Consistent } P_1/B_1 \end{cases} \tag{II.121}$$

$$J^g = \left[\theta V_+^g + (1-\theta)\, V_-^g\right] \int_g q_o(u)\, du + \left[\theta U_+^g + (1-\theta)\, U_-^g\right] \int_g q_1(u)\, du + (S^g + \eta_o^g) \left[\gamma_o(u_g)\, \theta V_+^g + \gamma_o(u_{g-1})\, (1-\theta)\, V_-^g\right] + 1.5\, \eta_1^g \left[\gamma_1(u_g)\, \theta U_+^g + \gamma_1(u_{g-1})\, (1-\theta)\, U_-^g\right] . \tag{II.122}$$

The flux depression factor (1 - f) is defined by use of the narrow resonance approximation,

$$f = \frac{1}{\int_g q_o(u)\, du} \sum_{r \in g} \frac{\Gamma_t}{E} J_t^* q_o(u_r) . \tag{II.123}$$

The thermal flux, ϕ^{th} is given by

$$\phi^{th} = \frac{(S^{th} + \eta_o(u_{NG}) + q_o(u_{NG}))}{\Sigma_a^{th} \quad \frac{B^2}{3\Sigma_t^{th}}} \quad . \tag{II.124}$$

The thermal cross sections are either provided by the user or given by the cross sections of the last ultra-fine-group of the problem (g = NG).

2. Eigenvalue Solution

By decomposing the source term S^g of the ultra-fine-group spectrum equations, it is possible to write the equations in matrix form as

$$H\Phi = \lambda M\Phi + S_{fix} . \tag{II.125}$$

If S_{fix}, the inhomogeneous source vector, is zero Eq. II.125 represents an eigenvalue problem with

$$\lambda = \frac{1}{k_{eff}} \tag{II.126}$$

From Eq.II.14 it is clear that the non-zero elements of the vector $M\Phi$ have the form

$$S_f^g = \sum_i \chi_i^g \sum_{g'} (\nu\Sigma_f^{g'})_i \phi^{g'} \tag{II.127}$$

If the fission spectrum distribution is isotope independent, then one can take

$$S_f^g = \chi^g \tag{II.128}$$

and

$$k_{eff} = \sum_{g'} \nu\Sigma_f^{g'} \phi^{g'} \tag{II.129}$$

so that no flux iterations are required in the spectrum solution. If the fission spectrum distribution is isotope dependent then one assumes a flux, calculates S_f^g from Eq. II.127, solves the spectrum equations as detailed in the previous section, and calculates a new fission source and eigenvalue k_{eff}. This process is repeated until the eigenvalue has converged. Convergence is assumed if on the first iteration

$$\max \left| \frac{S_f^{g(1)} - S_f^{g(0)}}{S_f^{g(0)}} \right| < .001 \tag{II.130}$$

or on following iterations

$$\left| \frac{k^{(n+1)} - k^{(n)}}{k^n} \right| < .0001 \quad n \geq 1 . \tag{II.131}$$

3. Inhomogeneous Source Solution

If there are no fissionable isotopes in the problem mixture then Eq. II.125 becomes

$$H\Phi = S_{fix}$$

which may be solved directly by sweeping through the ultra-fine-group equations once in precisely the same manner as that used to solve the eigenvalue equation with isotope independent fission spectra. If both fission and inhomogeneous sources are present a different solution strategy is required. Assuming an isotope independent fission spectrum distribution for the sake of simplicity, Eq. II.25 may be written

$$(I - H^{-1} M)\Phi = H^{-1} S_{fix} \tag{II.132}$$

where

$$M = \chi f^T = \begin{pmatrix} \chi^1 \\ \chi^2 \\ \vdots \\ \vdots \end{pmatrix} (\nu\Sigma_f^1, \nu\Sigma_f^2, \ldots) \; . \tag{II.133}$$

Substituting Eq. II.133 into Eq.II.132 and multiplying through by f^T it is easy to obtain

$$f^T\Phi = \frac{f^T H^{-1} S_{fix}}{I - f^T H^{-1} \chi} \tag{II.134}$$

but

$$\Phi = H^{-1} S_{fix} + H^{-1} \chi(f^T\Phi) \tag{II.135}$$

or from Eq. II.134

$$\Phi = H^{-1} S_{fix} + H^{-1} \chi \frac{f^T H^{-1} S_{fix}}{I - f^T H^{-1} \chi} \; . \tag{II.136}$$

If the eigenvalue equation is defined

$$\begin{aligned} H\Phi_o &= \chi \\ f^T\Phi_o &= \lambda_o \end{aligned} \tag{II.137}$$

then

$$\Phi = H^{-1} S_{fix} + \frac{\Phi_o}{1 - \lambda_o} f^T H^{-1} S_{fix}$$

or

$$\Phi = \Phi_1 + \frac{\lambda_1 \Phi_o}{1 - \lambda_o} \tag{II.138}$$

where

$$\begin{aligned} H\Phi_1 &= S_{fix} \\ \lambda_1 &= f^T\Phi_1 \; . \end{aligned} \tag{II.}$$

Based on these equations a three-step strategy is involved in the solution of the inhomogeneous equations:

(a) Solve the eigenvalue problem of Eqs. II.137 for Φ_o and λ_o as outlined in the previous section iterating on the flux if isotope fission spectra are in problem mixture;

(b) Solve the inhomogeneous problem of Eqs. II.139 for Φ_1 and λ_1;

(c) Construct the fission source from Eq. II.137 as $\chi f^T \Phi$ and solve Eq.II.135 for the flux Φ.

Step (c) is not strictly necessary since the flux is given by Eq.II.138 but it is required to calculate the resonance reaction rates A_x^r of Eq. II.119 which are used in the broad-group cross-section calculation.

4. Buckling Search to Critical

The spectrum and eigenvalue are clearly dependent upon the buckling B^2. For eigenvalue problems ($S_{fix} = 0$) with group independent buckling, the code MC^2-2 provides an option to search on B^2 to $k_{eff} = 1$. In order to invoke this option of the code, the user provides two starting guesses, B_1^2, B_2^2 and a convergence criterion ε_{B^2}. The code solves the slowing down problem and calculates an eigenvalue for each of these values of B^2. Later estimates of B^2 are based upon linear or parabolic fits to the best available k_{eff} vs. B^2 data. The search procedure ends if

$$\left| k_{eff}^{(n)} - 1 \right| \leq \varepsilon_{B^2} .$$

For problems with isotope dependent fission spectra data, the flux iteration discussed above is not converged until the buckling search has been completed. The algorithms invoked in choosing the points for the linear or parabolic fit are based upon those used in the ARC System neutronics search modules[4], and depend upon both the sign and magnitude of $1 - k_{eff}$. Several checks are made to insure that a search is not permitted to continue if a pathological situation arises, e.g. search to critical for a highly subcritical (blanket) composition.

K. Group Condensation

The individual material microscopic broad-group cross sections are obtained by averaging the ultra-fine-group data over the flux and current spectra obtained by solving the multigroup and continuous slowing down equations. The broad groups are user specified but must be defined such that broad-group energy boundaries fall on ultra-fine-group boundaries. The broad group data are written in the ISOTXS[2] and/or XS.ISO[1] formats as defined in Appendix C. On user option it is possible to neglect the contributions of resolved and unresolved resonances in the edited cross sections thus making it possible to use MC^2-2 for the generation of fine-group SDX libraries.[7] The broad-group averaging algorithms are defined below.

1. Broad-Group Inelastic and (n,2n) Cross Sections

The broad-group inelastic and (n,2n) transfer matrices are calculated using the algorithms defined in Section H above. In particular

$$\sigma^{m}_{x_{G'\to G}} = \frac{\sum_{g\varepsilon G}\sum_{g'\varepsilon G'}\left[S^{g'\to g}_{x_{tab}} + S^{g'\to g}_{x_{evap}} + S^{g'\to g}_{x_{d}}\right]}{\phi G'} \qquad \text{(II.140)}$$

where

x ≡ inelastic or (n,2n)

$\sum_{g\varepsilon G}$ ≡ sum over ultra-fine-groups g contained in broad-group G

$S^{g'\to g}_{x_{tab}}$ ≡ tabulated law contribution as given inside g' sum of Eq. II.96

$S^{g'\to g}_{x_{evap}}$ ≡ evaporation law contribution as given inside g' sum of Eq. II.97

$S^{g'\to g}_{x_{d}}$ ≡ discrete law contribution as given inside g' sum of equation following Eq. II.104 using either rigorous or approximate P_λ

and the broad-group flux is given by

$$\phi^{G'} \equiv \sum_{g'\varepsilon G'} \phi^{g'} \quad . \qquad \text{(II.141)}$$

The total inelastic and (n,2n) cross sections are obtained by summing over all sink groups

$$\sigma^{m}_{x_{G'}} = \sum_{G} \sigma^{m}_{x}(G' \to G) \quad . \qquad \text{(II.142)}$$

Since the microscopic ultra-fine-group data required by Eq.II.140 are not saved during the course of the MC^2-2 spectrum calculation, the data required for the broad-group condensation are calculated specifically for the cross section edits. It is this calculation which controls both the timing and space requirements of the MC^2-2 condensation calculation. As the number of broad-groups increases beyond approximately 100, I/O times become quite large because of the data management requirements for calculation of Eq.II.140.

2. Broad-Group Absorption Cross Sections

The MC^2-2 library file MCC2F5 (Appendix C) contains ultra-fine-group cross section data which are averaged over the flux spectrum as

$$\sigma^m_{x_G} = \sum_{g\epsilon G} \sigma^m_{x_g} \phi^g/\phi^G \qquad \text{(II.143)}$$

where x includes the six reactions (n,H^1), (n,H^2), (n,H^3), (n,f), (n,γ) and (n,α). The (n,α) cross section calculated from Eq.II.143 is actually a sum of (n,He^4) and (n,He^3) cross sections. This summing was performed since the ISOTXS format does not allow editing of both the partials. Since the $\sigma^m_{x_g}$ data from the file MCC2F5 do not include either resolved or unresolved resonance contributions, the fission and radiative capture cross sections of Eq.II.143 are not complete. The contributions from unresolved resonances are obtained using Eq.II.143 with the ultra-fine-group (n,γ) and (n,f) cross sections given by Eq.IV.68. The contribution of resolved resonances to the broad-group radiative capture and fission cross sections is derived from the resonance reaction rates, A^r_x, defined by Eq.II.119. Using this equation it is clear that the resolved resonance contribution to the broad group cross section is given by

$$\frac{\text{Resolved Resonance Reaction Rate in Broad-Group G}}{\text{Group G Flux}} = \frac{1}{N_m \phi^G} \sum_{\substack{r\epsilon G \\ r\epsilon m}} A^r_x \qquad \text{(II.144)}$$

where the sum is over all resolved resonances of material m which fall into group G,

$$E_g < E_r < E_{g-1} .$$

Thus the broad-group (n,γ) and (n,f) cross sections for a material with both resolved and unresolved data would be given by

$$\sigma^m_{x_G} = \left\{ \sum_{g\epsilon G} (\sigma^m_{x_g} + \bar{\sigma}^m_{x_g}) \phi^g + \frac{1}{N_m} \sum_r A^r_x \right\} \Big/ \phi^G \qquad \text{(II.145)}$$

where

$\sigma^m_{x_g}$ ≡ floor cross sections from MCC2F5

$\bar{\sigma}^m_{x_g}$ ≡ unresolved cross sections from Eq.IV.68

A^r_x ≡ resolved resonance reaction rate from Eq.II.119.

3. Elastic Scattering Cross Sections

In Section G of this chapter the calculation of ultra-fine-group elastic transfer matrices was discussed. The ultra-fine-group cross sections derived from that calculation $\sigma^f_s(g' \to g)$ include contributions from the ultra-fine-group library (MCC2F5) and the unresolved resonances from Chapter IV. The group condensation of these data are accomplished as

$$\sigma^{o^m}_{e\ell}(G' \to G) = \frac{\sum_{g'\epsilon G'} \sum_{g\epsilon G} \sigma^{o^m}_{e\ell}(g' \to g)\phi^{g'}}{\phi^{G'}} \qquad \text{(II.146)}$$

$$\sigma^{l^m}_{e\ell}(G' \to G) = \frac{\sum_{g'\epsilon G'} \sum_{g\epsilon G} \sigma^{l^m}_{e\ell}(g' \to g)J^{g'}}{J^{G'}} \; . \qquad \text{(II.147)}$$

The P_1 calculation is performed only for the consistent P_N or consistent B_N spectrum options in which case the ultra-fine-group current J^g is calculated directly using Eqs.II.62 and II.122 and the broad-group current is given by

$$J^G = \sum_{g\epsilon G} J^g \; . \qquad \text{(II.148)}$$

The contributions of resolved resonances to the elastic transfer matrix cannot be calculated by use of Eqs.II.146-II.147 since ultra-fine-group resolved resonance scattering cross sections are not available. An approximate method adapted from the work of Stacey[39] which accounts for the position of the resonance in the group and the shape of the resonance is used in lieu of requiring ultra-fine-group resonance cross sections. The method adopted assumes that resolved resonance materials can scatter only one broad-group. Since the current MC^2-2 library described in Table VIII has resolved data only for materials of mass greater than one hundred, this assumption fixes the smallest broad-group lethargy width at .04 ($\sim$5 ultra-fine-groups). Following the methods used in calculating the resolved absorption cross sections we take

$$\sigma^{o\,m}_{res}\,(G \to G') = \frac{1}{N_m \phi^G} \sum_{\substack{r\in G \\ r\in m}} A^r_s\, P(r \to G') \qquad \text{(II.149)}$$

where

A^r_s resolved resonance r elastic reaction rate

$P(r \to G')$ probability of scattering a neutron by resonance r into Group G'.

The resonance reaction rate is calculated directly from the resonance integrals discussed in Chapter III,

$$A^r_s = \frac{1}{E_r}\{\Gamma_t J^*_t - \Gamma_\gamma J^*_\gamma - \Gamma_f J^*_f\}\left(\Sigma^g_t + \frac{B^2}{3A^g_1}\right)\overset{\gamma}{\phi}(u_r) \qquad \text{(II.150)}$$

which is the scattering equivalent of Eq.II.119. The resonance integrals of Eq.II.150 take account of overlap, self-shielding, and Doppler broadening effects as described in Chapter III. The removal probability is taken as

$$P(r \to G+1) \overset{\sim}{\sim} \frac{\displaystyle\int_{\varepsilon}^{u_G} du\, K(u,u_G)\,\frac{\sigma^r_s(u)}{\Sigma_t(u)}}{\displaystyle\int_{u_{G-1}}^{u_G} du\,\frac{\sigma^r_s(u)}{\Sigma_t(u)}} \qquad \text{(II.151)}$$

where

$$K(u,u_G) \equiv \frac{e^{-(u_G-u)} - \alpha}{1-\alpha}$$

and ε is the larger of u_{G-1} and $u_G - \ell n\,\frac{1}{\alpha}$.

It is further assumed that the resonance is isolated and that natural line shapes[26] are applicable so that

$$\frac{\sigma^r_s}{\Sigma_t} \overset{\sim}{\sim} \frac{\psi + a\chi}{\beta + \psi + a\chi}$$

$$\psi(u) \overset{\sim}{\sim} \frac{1}{1 + \Delta^2[e^{u_r-u} - 1]^2} \qquad \text{(II.152)}$$

$$\chi(u) \overset{\sim}{\sim} \frac{\Delta[e^{u_r-u} - 1]}{1 + \Delta^2[e^{u_r-u} - 1]^2}$$

$$\Delta \equiv \frac{2E_r}{\Gamma}\,.$$

The terms are defined in detail in Chapter III. The above assumptions make it possible to integrate Eq.II.151 analytically. The integrals are reported in Eqs. 12, 13, 19, 20, 23 of Reference 39. It is important to note that the above approximations are used only to distribute the resolved elastic reaction rate between in-group and removal and have no impact on the ultra-fine-group spectrum or the far more general resonance integral calculations of Chapters III and IV. The in-group probability is given by

$$P(r \to G) = 1 - P(r \to G + 1)$$

so that the elastic transfer matrix may be calculated from Eqs.II.149-II.151. The P_1 transfer matrix is calculated in the consistent spectrum options as

$$\sigma^{1\,m}_{res}(G \to G') = \frac{2}{3A^m N_m J^G} \sum_r \frac{J(u_r)}{\tilde{\phi}(u_r)} A^r_s P(r \to G') \qquad \text{(II.153)}$$

where $J(u_r)$ is the current at lethargy u_r in direct analogy with Eq.II.120. The total elastic scattering matrix is given by the sums of II.146 and II.149 or for the P_1 matrix, II.147 and II.153. The elastic cross section is obtained by summing over sink groups according to Eq.II.142.

The Hydrogen elastic scattering cross sections are collapsed by assuming that scattering is isotropic in the center of mass system. With this assumption it is not difficult to show

$$\sigma^{o\,H}_{e\ell}(G \to G') = \frac{(E_{G'-1} - E_{G'})}{\phi^G} \frac{(e^{\Delta u} - 1)}{\Delta u} \sum_{g \epsilon G} \frac{\sigma^g_{s_H} \phi^g}{E_{g-1}} \qquad \text{(II.154)}$$

$$\sigma^{1\,H}_{e\ell}(G \to G') = \frac{4}{9} \frac{(E^{3/2}_{G'-1} - E^{3/2}_{G'})}{J^G} \frac{(e^{3/2\Delta u} - 1)}{\Delta u} \sum_{g \epsilon G} \frac{\sigma^g_{s_H} J^g}{E^{3/2}_{g-1}} . \qquad \text{(II.155)}$$

Eq.II.155 is used only for the consistent spectrum options. The corrections required to Eqs.II.154-II.155 to treat in-group scattering are straightforward.

4. Total Cross Section

The flux weighted total cross section is obtained by summing all of the partials discussed above,

$$\sigma^{o\,m}_{t_G} = \sigma^m_{inel_G} + \sigma^m_{n,2n_G} + \sigma^{o\,m}_{e\ell_G} + \sigma^m_{f_G} + \sigma^m_{n\gamma_G} + \sigma^m_{nH^1{}_G} + \sigma^m_{nH^2{}_G} + \sigma^m_{nH^3{}_G} + \sigma^m_{n\alpha_G}$$

(II.156

and the broad-group partial cross sections include floor, unresolved and resolved resonance contributions as discussed above. A current weighted total cross section is calculated as

$$\sigma^{l^m}_{t_G} = \frac{1}{J^G} \sum_{g\epsilon G} \gamma_g \sigma^m_{t_g} J^g + \frac{1}{N_m \phi^G} \sum_{\substack{r\epsilon G \\ r\epsilon m}} \frac{\Gamma_t}{E_r} J^*_t \left(\Sigma^g_t + \frac{B^2}{3A^g_1}\right) \tilde{\phi}\,(u_r) \qquad \text{(II.157)}$$

where

J^g ≡ ultra-fine-group current calculated from Eqs.II.62 and II.122 for consistent options and Eq.II.64 for inconsistent options.

J^G ≡ broad group current from Eq.II.148.

$\sigma^m_{t_g}$ ≡ ultra-fine-group total floor cross section from library file MCC2F5 plus ultra-fine-group total unresolved cross sections from Eq.IV.68.

γ_g ≡ spectrum coefficient

$$\begin{cases} \dfrac{\frac{B}{\Sigma^g_t} \tan^{-1} \frac{B}{\Sigma^g_t}}{3\left(1 - \frac{\Sigma^g_t}{B} \tan^{-1} \frac{B}{\Sigma^g_t}\right)} & \text{consistent } B_1 \\ 1 & P_N \text{ or } B_N \text{ with } N>1 \end{cases}$$

and the resolved resonance contribution is simply the reaction rate integral used with the flux weighted cross section of Eq.II.156.

For spectrum calculations using the extended transport approximation, higher order flux moments ϕ^g_ℓ are calculated recursively from Eq.II.62. Total cross section moments equivalent to Eq.II.157 are then calculated,

$$\sigma^{\ell^m}_{t_G} = \frac{1}{\phi^G_\ell} \sum_{g\epsilon G} \gamma_g \sigma^m_{t_g} \phi^g_\ell + \sigma^{o^m}_{t_{res_G}} \qquad \ell = 2,3,\ldots,N \qquad \text{(II.158)}$$

where

$$\gamma_g = \begin{cases} \dfrac{N+1}{2N+1} \dfrac{iB}{\Sigma^g_t} \dfrac{Q_{N+1}(-\Sigma_t/iB)}{Q_N(-\Sigma_t/iB)} \delta^N_\ell & \text{for } B_N \\ 1 & \text{for } P_N \end{cases}$$

and all other terms have been defined.

5. Transport Cross Section

In analogy with the total cross section, the MC^2-2 code calculates moments of the transport cross section if the order of the extended transport approximation is greater than unity. The transport cross section algorithms are spectrum option dependent. In all cases, however, the algorithms are defined to conserve the relation

$$\Sigma^{\ell}_{tr_G} = \frac{-\ell}{2\ell + 1} iB \frac{\phi^G_{\ell-1}}{\phi^G_{\ell}} \qquad \ell = 1,2,\ldots,N \tag{II.159}$$

or for the special case of $\ell = 1$

$$J = -\frac{B}{3\Sigma_{tr}} \phi \quad . \tag{II.159'}$$

The algorithms further conserve the relation

$$\Sigma_{tr} = \sum_i N_i \sigma_{tr_i} \quad .$$

a. Inconsistent P_1 or B_1 Spectrum

$$\sigma^{\ell^m}_{tr_g} = \sigma^{\ell^m}_{t_G} - \sigma^{\ell^m}_{e\ell_G} \qquad \ell = 1,2,\ldots,N \tag{II.160}$$

where

$\sigma^{\ell^m}_{t_G}$ = P_ℓ moment of total cross section given by Eq.II.157 or II.158.

$\sigma^{\ell}_{e\ell_G}$ = P_ℓ moment of elastic scattering cross section.

The elastic scattering cross section moments are calculated from Eq.II.45 and II.150 and it is assumed that resolved resonances do not contribute to the cross sections for moments greater than unity,

$$\sigma^{\ell^m}_{e\ell_G} = \left\{ \sum_{g\in G} \sum_n \sigma^g_{e\ell} f^g_n T^o_{\ell n}(\alpha_m)\phi_\ell + \frac{2\delta^1_\ell}{3A^m N_m} \sum_{\substack{r\in G \\ r\in m}} A^r_s \frac{J(u_r)}{\tilde{\phi}(u_r)} \right\} \Big/ \phi^G_\ell, \qquad \ell = 1,2,\ldots,N \tag{II.161}$$

b. Consistent P_1 or B_1 Spectrum

The Eqs.II.160 and II.161 are used in the consistent spectrum options as well as the inconsistent options for moments greater than unity ($\ell > 1$). The P_1 moment is however calculated directly from the elastic transfer matrices in direct analogy with Eqs.II.147 and II.153. In particular

$$\sigma_{tr_G}^{1^m} = \sigma_{t_G}^{1^m} - \frac{1}{J^G} \sum_{g\epsilon G} \sum_{g' \le g} \sigma_{e\ell}^{1^m}(g' \to g) J^{g'}$$

$$- \frac{1}{J^G} \frac{2}{3A^m N_m} \sum_r \frac{J(u_r)}{\gamma\phi(u_r)} A_s^r P(r \to G) \quad . \tag{II.162}$$

6. Average Number of Neutrons per Fission

The average number of neutrons per fission is given by

$$\nu_G^m = \frac{\left[\sum_{g\epsilon G} \nu_m^g \sigma_{f_g}^m \phi^g + \frac{1}{N_m} \sum_{\substack{r\epsilon G \\ r\epsilon m}} \nu_m^g A_f^r\right]}{\sigma_{f_G}^m \phi^G} \tag{II.163}$$

where

$\nu_m^g \equiv$ number of neutrons per fission for material m in ultra-fine-group g from Eq.II.110.

$\sigma_{f_g}^m \equiv$ floor plus unresolved ultra-fine-group fission cross section.

$\sigma_{f_G}^m \equiv$ broad-group fission cross section.

$A_f^r \equiv$ resolved resonance fission reaction rate from Eq.II.119.

7. Fission Spectrum Distribution

The isotopic fission spectrum distributions are derived by summing the ultra-fine-group vectors of Eq.II.112,

$$\chi_m^G = \sum_{g\epsilon G} \hat{\chi}_m^g \quad . \tag{II.164}$$

The MC^2-2 code edits a set-wide fission spectrum vector as well as the isotopic vectors of Eq.II.164. The set-wide vector is defined

$$\chi^G_{set} = \frac{\sum_{g\epsilon G} \sum_m \hat{\chi}^g_m S_{f_m}}{\sum_m S_{f_m}} \qquad \text{(II.165)}$$

where $\hat{\chi}^g_m$ are the ultra-fine-group vectors of Eq.II.112 and S_{f_m} are the fission sources for material m,

$$S_{f_m} = \sum_g N_m \nu^g_m \sigma^m_{f_g} \phi^g + \sum_{r\epsilon m} \nu^{g_r}_m A^r_f \quad . \qquad \text{(II.166)}$$

8. XS.ISO Cross Sections

The ARC System[1] cross section file XS.ISO (c.f. Appendix B) is less general than the CCCC file ISOTXS and contains derived cross sections in addition to the standard cross sections given above. The following conversions for XS.ISO cross sections are consistent with the MC^2 derived cross sections of Reference 10:

$$\left[\sigma^m_{tr_G}\right]_{ARC} = \sigma^{1^m}_{tr_G} \qquad \text{(II.167)}$$

$$\left[\sigma^m_{e\ell}(G \to G)\right]_{ARC} = \sigma^{1^m}_{tr_G} - \sigma^{0^m}_{t_G} + \sigma^{0^m}_{e\ell}(G \to G) \qquad \text{(III.168)}$$

$$\left[\sigma^{anis^m}_{e\ell}(G \to G)\right]_{ARC} = \sigma^{1^m}_{t_G} - \sigma^{0^m}_{t_G} + \sigma^{0^m}_{e\ell}(G \to G) \quad . \qquad \text{(III.169)}$$

Equations II.168 and II.169 are consistent with Equations 116-118 of Ref. 10.

L. Broad Group Spectrum

The microscopic broad-group cross section data calculated according to the algorithms of Section K are appropriate for use in general multigroup neutronics calculations. One such calculation, extended transport P_1 real and adjoint fundamental mode spectrum, is available in MC^2-2 at user option. The module (overlay) CSC010 solves the following broad-group flux equations

$$\Sigma_{r_o}^G \phi_o^G - B\phi_1^G = Q^G + \sum_{G'<G} \Sigma_s^o(G' \to G)\phi_o^{G'}$$

$$\frac{B}{3}\phi_o^G + \Sigma_{r_1}^G \phi_1^G + \frac{2}{3}B\phi_2^G = \sum_{G'<G} \Sigma_s^1(G' \to G)\phi_1^{G'} \qquad \text{(II.170)}$$

$$-(i)^{2\ell} \frac{\ell}{2\ell+1} B\phi_{\ell-1}^G + \Sigma_{tr_G}^{\ell} \phi_\ell^G - (i)^{2\ell} \frac{\ell+1}{2\ell+1} B\phi_{\ell+1}^G = 0 \qquad \ell = 2,\ldots,N$$

$$\phi_{N+1}^G = 0$$

where

$$\Sigma_s^o(G' \to G) = \sum_m N_m \left[\sigma_{e\ell}^{o\,m}(G' \to G) + \sigma_{ine\ell}^m(G' \to G) + 2\,\sigma_{n,2n}^m(G' \to G)\right]$$

$$\Sigma_s^1(G' \to G) = \sum_m N_m\, \sigma_{e\ell}^{1\,m}(G' \to G)$$

$$\Sigma_{tr_G}^{\ell} = \sum_m N_m\, \sigma_{tr_G}^{\ell}$$

$$\Sigma_{r_o}^G = \sum_m N_m \left[\sigma_{t_G}^{o\,m} - \sigma_{e\ell}^{o\,m}(G \to G) - \sigma_{ine\ell}^m(G \to G) - 2\sigma_{n,2n}^m(G \to G)\right]$$

$$\Sigma_{r_1}^G = \sum_m N_m \left[\sigma_{t_G}^{1\,m} - \sigma_{e\ell}^{1\,m}(G \to G)\right]$$

$$Q^G = \frac{1}{K}\chi_{set}^G \sum_m N_m \sum_{G'} \nu_{G'}^m \sigma_{f_{G'}}^m \phi_o^{G'} + \sum_{g\epsilon G} S_{fix}^g \quad .$$

The inconsistent spectrum option is defined by setting $\Sigma_s^1(G' \to G)$ to zero and taking

$$\Sigma_{r_1}^G = \Sigma_{tr_G}^1 \quad .$$

If there are no inhomogeneous sources, $S_{fix} = 0$, then Equations II.170 specify an eigenvalue problem. In this case the code will search on B^2 to K = 1 according to the procedures noted in Section J.4 and reference 4. The first buckling used will be the critical B^2 from the

ultra-fine-group calculation and the second guess increases (decreases) B^2 by 1% if the eigenvalue of the ultra-fine-group calculation is greater (less) than 1.0. The buckling search is stopped when

$$|K - 1| \leq 10^{-4} .$$

The adjoint eigenvalue problem is also solved by MC^2-2,

$$\Sigma_{r_o}^{G} \phi_o^{G^*} - B\, \phi_1^{G^*} = Q^{G^*} + \sum_{G'>G} \Sigma_s^o(G \rightarrow G')\phi_o^{G'^*}$$

$$\frac{B}{3} \phi_o^{G^*} + \Sigma_{r_1}^{G} \phi_1^{G^*} + \frac{2}{3} B\, \phi_2^{G^*} = \sum_{G'>G} \Sigma_s^1(G \rightarrow G')\phi_1^{G'^*} \qquad \text{(II.171)}$$

$$-(i)^{2\ell} \frac{\ell}{2\ell + 1} B\, \phi_{\ell-1}^{G^*} + \Sigma_{tr_G}^{\ell} \phi_\ell^{G^*} - (i)^{2\ell} \frac{\ell + 1}{2\ell + 1} B\, \phi_{\ell+1}^{G^*} = 0 \qquad \ell = 2,\ldots,N$$

$$\phi_{N+1}^{G^*} = 0$$

with

$$Q^{G^*} = \frac{1}{K} (\nu\Sigma_f)_G \sum_{G'} \chi_{set}^{G'} \phi_o^{G'^*} .$$

The solution of the tridiagonal equations II.170 and II.171 is performed using the forward elimination-backward substitution technique[41], a specialization of the standard Gauss reduction. Since the flux equations II.170 are obtained by summing the ultra-fine-group equations II.59 and using the flux weighted broad-group cross section definitions of Section K, the fluxes, currents and eigenvalue calculated by the module CSC010 should agree with those obtained from the ultra-fine-group spectrum solution. In practice the differences in resonance treatments, slowing down formulations and computational precision limit this agreement. Eigenvalue agreement tends always to be better than 0.1% and spectrum agreement is excellent down to the resolved resonance energy domain where the ultra-fine-group spectrum tends to attenuate faster than the broad group spectrum. Because flux weighting is used to collapse the cross section data, it is clear that the broad-group adjoint spectrum of Eq.II.171 is not equivalent to the adjoint of the ultra-fine-group equations.

III. CALCULATION OF RESOLVED RESONANCE INTEGRALS

A. General Formulation

The algorithms involved in the resolved resonance integral calculation developed by R. Hwang[25] assume the narrow resonance approximation and account for interference scattering and the effects of overlap with neighboring resolved resonances. Both single level Breit-Wigner and multilevel Breit-Wigner or Adler-Adler representations are accommodated including interaction of single and multilevel resonances.

The effective macroscopic capture cross section over the lethargy range u_1, u_2 of width Δu due to resonances i for an isotope having atom density N_i can be written as

$$\bar{\Sigma}_c = N_i \bar{\sigma}_c = \frac{\sum_i \int_{u_1}^{u_2} \frac{N_i \sigma_{c_i}(u)\, F(u)\, du}{\Sigma_t(u)}}{\int_{u_1}^{u_2} \frac{F(u)\, du}{\Sigma_t(u)}} \qquad \text{(III.1)}$$

where F(u) is the collision density, σ_{c_i} is the microscopic capture cross section due to resonance i, and Σ_t is the total macroscopic cross section for the mixture. If we consider the case of Breit-Wigner single level resonances, extend the range of integration to cover all lethargies, replace du by - dE/E, assume E remains constant at the resonance energy E_{o_i}, and assume a constant collision density over each resonance, we may rewrite Eq.III.1 as

$$\bar{\Sigma}_c = \frac{\sum_i F_i \int_{-\infty}^{\infty} \frac{N_i \sigma_{o_i} \frac{\Gamma_{\gamma_i}}{\Gamma_i} \psi(\theta_i, x_i) \frac{\Gamma_i}{2}\, dx_i \frac{1}{E_{o_i}}}{\Sigma_t(u)}}{\frac{\Delta u}{\Sigma_p} \cdot f}$$

$$= \sum_i F_i \frac{\Sigma_p \Gamma_{\gamma_i}}{\Delta u E_{o_i} f} \cdot \frac{1}{2} \int_{-\infty}^{\infty} \frac{N_i \sigma_{o_i} \psi_i\, dx_i}{\Sigma_t(u)}$$

$$= \sum_i F_i \frac{\Sigma_p \Gamma_{\gamma_i}}{\Delta u E_{o_i} f} \cdot \frac{1}{2} \int_{-\infty}^{\infty} \frac{\psi_i dx_i}{\beta_i + \psi_i + a_i \chi_i + \sum_{i' \neq i} (A_{i'} \psi_{i'} + B_{i'} \chi_{i'})}$$

$$= \sum_i F_i \frac{\Sigma_p \Gamma_{\gamma_i}}{\Delta u E_{o_i} f} J^{*s\ell}_{x_i}. \qquad \text{(III.2)}$$

where $\Sigma_t(u) = \Sigma_p + N_i \sigma_{o_i} \psi(\theta_i, x_i) + N_i \sigma_{o_i} a_i \chi(\theta_i, x_i) + \sum_{i' \neq i} N_{i'} \sigma_{o_{i'}} \psi(\theta_{i'}, x_{i'})$

$$+ N_{i'} \sigma_{o_{i'}} a_{i'} \chi(\theta_{i'}, x_{i'})$$

F_i is the constant collision density for resonance i
and f is the so-called flux correction factor which can be written as

$$f = \sum_i F_i - \frac{1}{\Delta u} \sum_j F_j \frac{\Gamma_{t_j}}{E_{o_j}} J^{*s\ell}_{t_j}$$

The sum in f extends over all resonances in the mixture, and $J^{*s\ell}_{t_j}$ is the total resonance integral defined later in Eq.III.24. The $s\ell$ superscript refers to single level and Eq.III.2 defines the resonance integral $J^{*s\ell}_{x_i}$.

Eq.III.2 is the starting point in defining the ultra-fine-group reaction rates and fluxes as given in Chapter II Equations II.119, II.121-II.123. The weighting functions F_i are calculated from the slowing down density attenuated by higher energy resonances.

In deriving Eq.III.2, we have used the approximation that $E = E_{o_i}$ so that

$$\sigma_{c_i} = \sigma_{o_i} \frac{\Gamma_{\gamma_i}}{\Gamma_i} \psi(\theta_i, x_i) \equiv \sigma_{o_i} \frac{\Gamma_{\gamma_i}}{\Gamma_i} \psi_i \qquad \text{(III.3)}$$

with a similar expression for σ_{f_i} where Γ_{f_i} replaces Γ_{γ_i}, and

$$\sigma_{t_i} = \sigma_{p_i} + \sigma_{o_i} \psi_i + \sigma_{o_i} a_i \chi(\theta_i, x_i) = \sigma_{p_i} + \sigma_{o_i} \psi_i + \sigma_{o_i} a_i \chi_i \qquad \text{(III.4)}$$

where

σ_{o_i} = the peak cross section of the resonance

$$= \frac{2.6039953 \times 10^6}{|E_{o_i}|} \left[\frac{A_i + 1}{A_i}\right]^2 g_{J_i} \frac{\Gamma_{n_{o_i}}}{\Gamma_i}$$

A_i = the mass number of the nucleus having resonance i

g_{J_i} = $\frac{2J + 1}{2(2I + 1)}$ where J is the total spin of the compound nucleus and I is the spin of the target nucleus

Γ_{γ_i} = the radiative capture line width

Γ_i = the total line width

$\Gamma_{n_{o_i}}$ = the neutron width evaluated at the resonance energy

$\psi(\theta_i, x_i) \equiv \psi_i$ = the Doppler broadened symmetric line shape function given in Eq. A.1 of Appendix A and calculated as described there

θ_i = the ratio of natural width to Doppler width Γ_i/Δ_i evaluated at the resonance energy

$\Delta_i = \left[\frac{4kT_iE_{o_i}}{A_i}\right]^{\frac{1}{2}}$ with Boltzmann's constant

$k = 8.6168 \times 10^{-5}$ eV/degree Kelvin

T_i = temperature of isotope having resonance i in degrees Kelvin

$x_i = 2(E - E_{o_i})/\Gamma_i$

$a_i = \left[\frac{g_{J_i}\Gamma_{n_{o_i}}\sigma_{p_{a_i}}}{\Gamma_i\sigma_{o_i}}\right]^{\frac{1}{2}}$

$\sigma_{p_{a_i}}$ = the atom potential scattering cross section

$\chi(\theta_i, x_i) \equiv \chi_i$ = the Doppler broadened antisymmetric line shape function given in Eq. A.2 of Appendix A and calculated as described there .

The summation in the denominator of Eq. III.2 is over all other resonances $i' \neq i$ in the mixture and

$$A_{i'} = \frac{N_{i'}\sigma_{o_{i'}}}{N_i\sigma_{o_i}}$$

$$B_{i'} = a_{i'}A_{i'} \qquad \text{(III.5)}$$

$$\beta_i = \frac{\Sigma_p}{N_i\sigma_{o_i}} = \frac{\sigma_p}{\sigma_{o_i}} .$$

The code computes resonance integrals for a homogeneous mixture, and for heterogeneous slab geometries or cylindrical geometries. Whether the system is homogeneous or heterogeneous, and whether slab or cylinder determines the value used for Σ_p and hence for β by use of an equivalence principle.

For homogeneous mixtures, Σ_p is given by

$$\Sigma_p = \sum_m N_m \sigma_{t_m} + \frac{\kappa^2}{3 \sum_m N_m \sigma_{t_m}} \tag{III.6}$$

where the summation is over all isotopes in the homogeneous mixture, N_m is the atom density of isotope m, σ_{t_m} is the smooth total cross section library data for the ultra fine group into which the resonance in question falls, and κ^2 is the user supplied extended-transport approximation buckling as used in the continuous slowing down calculation.

For slab geometries, for each slab k and for the material i whose resonance integral is being calculated

$$\Sigma^k_{p_i} = \sum_{m \in k} N^k_m \sigma_{t_m} + \frac{\kappa^2}{3 \sum_m N_m \sigma_{t_m}} + \Sigma^{*k}_{e_i} \tag{III.7}$$

where the first summation is over all isotopes m contained in slab region k and the second summation as in Eq. III.6 is over all isotopes in the equivalent homogeneous mixture obtained by homogenizing all slab regions. The so-called "escape" cross section (for the material i whose resonance integral is being calculated) intended to account for the heterogeneity is calculated using

$$\Sigma^{*k}_{e_i} = \Sigma^k_e \frac{a_1(1 - C^k_i)}{1 + (a_2 - 1)C^k_i} \tag{III.8}$$

where

$$\Sigma^k_e = \frac{S^k}{4V^k} \tag{III.9}$$

with S^k and V^k the surface area and volume of region k, a_1 and a_2 are user supplied with default values of 1.09, and the Dancoff factor C^k_i is given by

$$C^k_i = E_3(\tau^k_{L_i}) + E_3(\tau^k_{R_i}). \tag{III.10}$$

In Eq.III.10, E_3 is the exponential integral of order three defined in Eq.A.37 of Appendix A. The optical thicknesses to the left and right of slab region k for material i denoted by, respectively, $\tau^k_{L_i}$ and $\tau^k_{R_i}$, are computed as follows,

$$\tau_{L_i}^k = \sum_{j \neq i} \sum_{\substack{r \text{ to the} \\ \text{left of } k}} N_j^r \Delta x_r \sigma_{t_j} \tag{III.11}$$

$$\tau_{R_i}^k = \sum_{j \neq i} \sum_{\substack{r \text{ to the} \\ \text{right of } k}} N_j^r \Delta x_r \sigma_{t_j} \tag{III.12}$$

where Δx_r is the thickness of region r. The summation over r continues until a region s is found such that

$$\frac{N_i^s \Delta x_s}{N_i^k \Delta x_k} > \varepsilon_{het}. \tag{III.13}$$

The criterion ε_{het} is a user input parameter and has the default value of 0.1.

For cylindrical geometry, the resonance integrals are evaluated only for the central region. All outer regions are homogenized into a single outer region. Denoting the central region with superscript 0 and the homogenized outer region with superscript 1, we have

$$\Sigma_p^0 = \sum_{m \in 0} N_m^0 \sigma_{t_m} + \frac{\kappa^2}{3 \sum_m N_m \sigma_{t_m}} + \Sigma_e^{*0} \tag{III.14}$$

where the first summation extends over all isotopes contained in the central region and the second summation is as in Eq. III.7 over all isotopes in the equivalent homogeneous mixture of all cylindrical regions.

The escape cross section for the central region Σ_e^{*0} is calculated as

$$\Sigma_e^{*0} = \Sigma_e^0 \frac{a_1(1 - C^0)}{1 + (a_2 - 1)C^0} \tag{III.15}$$

where

$$\Sigma_e^0 = \frac{S^0}{4V^0} \tag{III.16}$$

with S^0 and V^0 the surface area and volume of the central region, a_1 and a_2 are user supplied with default values of 1.35, and the Dancoff factor C^0 is given by

$$C^0 = 1 - \gamma - \gamma^4(1 - \gamma). \tag{III.17}$$

In Eq. III.17

$$\gamma = \frac{\Sigma_t^1}{\Sigma_t^1 + \Sigma_e^1} \tag{III.18}$$

with

$$\Sigma_t^1 = \sum_{m\varepsilon 1} N_m^1 \sigma_{t_m} \tag{III.19}$$

$$\Sigma_e^1 = \frac{S^0}{4V^1} \tag{III.20}$$

and V^1 is the volume of the homogenized outer regions. The summation in Eq. III.19 extends over all isotopes contained in the outer regions, including the isotope i if it should be present.

The x on $J_{x_i}^{*s\ell}$ in Eq. III.2 refers to either capture or fission. Thus the effective macroscopic fission cross section for the interval u_1, u_2 can similarly be written as in Eq. III.2

$$\overline{\Sigma}_{f_i} = \frac{\Sigma_p \Gamma_{f_i}}{\Delta u E_{o_i} f} J_{x_i}^{*s\ell} \tag{III.21}$$

where Γ_{f_i} is the fission width for resonance i.

In the case of the total cross section, we have

$$\overline{\Sigma}_{t_i} = \frac{\Sigma_p \Gamma_{t_i}}{\Delta u E_{o_i}} \frac{1}{2} \int_{-\infty}^{\infty} \frac{(\psi_i + a_i \chi_i)\, dx_i}{\beta_i + \psi_i + a_i \chi_i + \sum_{i' \neq i} (A_{i'} \psi_{i'} + B_{i'} \chi_{i'})}$$

$$= \frac{\Sigma_p \Sigma_{t_i}}{\Delta u E_{o_i} f} J_{t_i}^{*s\ell} . \tag{III.22}$$

Now the resonance integrals can be factored [25] to display a lead term corresponding to the isolated resonance integral (the usual resonance integral as discussed, e.g. by Dresner [26]) and a term due to the overlap of other resonances in the mixture. In particular, $J_{x_i}^{*s\ell}$ can be rewritten as

$$J_{x_i}^{*s\ell} = \frac{1}{2} \int_{-\infty}^{\infty} dx_i \frac{\psi_i}{\beta_i + \psi_i + a_i \chi_i} - \frac{1}{2} \int_{-\infty}^{\infty} dx_i \frac{\psi_i}{\beta_i + \psi_i + a_i \chi_i}$$

$$\cdot \frac{\sum_{i' \neq i} (A_{i'} \psi_{i'} + B_{i'} \chi_{i'})}{\beta_i + \psi_i + a_i \chi_i + \sum_{i' \neq i} (A_{i'} \psi_{i'} + B_{i'} \chi_{i'})} = J_i^{x,s\ell} - O_{i,i',o}^{x,s\ell} \tag{III.23}$$

where the first integral denoted by $J_i^{x,s\ell}$ is the usual isolated resonance integral and the second denoted by $O_{i,i',o}^{x,s\ell}$ is the overlap integral due to other single level resonances i'. The zero indicates that resonances are all of one type, that is, all single level.

Eq. III.22 may be similarly factored with $\psi_i + a_i\chi_i$ replacing ψ_i in the numerators of each of the integrals in Eq. III.23. Therefore

$$J^{*s\ell}_{t_i} = \frac{1}{2}\int_{-\infty}^{\infty} dx_i \frac{\psi_i + a_i\chi_i}{\beta_i + \psi_i + a_i\chi_i} - \frac{1}{2}\int_{-\infty}^{\infty} dx_i \frac{\psi_i + a_i\chi_i}{\beta_i + \psi_i + a_i\chi_i} \cdot \frac{\sum_{i'\neq i}(A_{i'}\psi_{i'} + B_{i'}\chi_{i'})}{\beta_i + \psi_i + a_i\chi_i + \sum_{i'\neq i}(A_{i'}\psi_{i'} + B_{i'}\chi_{i'})} = J_i^{t,s\ell} - O^{t,s\ell}_{i,i',o} . \quad \text{(III.24)}$$

Now in the case of multilevel resonances, instead of the expressions given in Eqs. III.3 and III.4 we have

$$\sigma_{c_k} = \sigma_{o_k}\frac{G_{\gamma_k}}{|G_{t_k}|}\left[\psi_k + b_{\gamma_k}\chi_k\right] \quad \text{(III.25)}$$

$$\sigma_{f_k} = \sigma_{o_k}\frac{G_{f_k}}{|G_{t_k}|}\left[\psi_k + b_{f_k}\chi_k\right] \quad \text{(III.26)}$$

$$\sigma_{t_k} = \sigma_{o_k}\left[\frac{G_{t_k}}{|G_{t_k}|}\psi_k + a_k\chi_k\right] . \quad \text{(III.27)}$$

In Eqs. III.25-III.27 we again set $E = E_{o_k}$ and use the shorthand notation $\psi_k = \psi(\theta_k,x_k)$ and $\chi_k = \chi(\theta_k,x_k)$.

The definition of the various coefficients depends upon whether the resonance k is represented by the Adler-Adler or Breit-Wigner forms. In the following, we will assume the flux correction factor f equals 1.

Multilevel Breit-Wigner

σ_{o_k} = (single level Breit-Wigner σ_o) $\cdot |G_{t_k}|$ where the single level Breit-Wigner σ_o is defined above

G_{t_k} = Breit-Wigner multilevel parameter for the total reaction which is 1 plus the symmetric level-level interference contribution

G_{γ_k} = Breit-Wigner multilevel parameter for the radiative capture reaction

$= \Gamma_{\gamma_k}/\Gamma_{t_k}$

Γ_{t_k} = Breit-Wigner multilevel total line width

$b_{\gamma_k} = 0$

G_{f_k} = Breit-Wigner multilevel parameter for the fission reaction

$= \Gamma_{f_k}/\Gamma_{t_k}$

$b_{f_k} = 0$

a_k = (single level Breit-Wigner a) plus the antisymmetric level-level interference contribution, all divided by $\left|G_{t_k}\right|$.

$\theta_k = \Gamma_{t_k}/\Delta_k$

$x_k = 2(E - E_{o_k})/\Gamma_{t_k}$

Multilevel Adler-Adler

$$\sigma_{o_k} = \frac{2.6039953 \times 10^6}{\left|E_{o_k}\right|}\left[\frac{A_k + 1}{A_k}\right]^2 \frac{\left|G_{t_k}\right|}{2\Gamma_k^{(s)}}$$

$$G_{t_k} = \sqrt{\left|E_{o_k}\right|}\left[G_k^T \cos 2\phi_{\ell_k} + H_k^T \sin 2\phi_{\ell_k}\right]$$

G_k^T = Adler-Adler symmetric capture cross section parameter from ENDF/B

H_k^T = Adler-Adler antisymmetric capture cross section parameter from ENDF/B

ϕ_{ℓ_k} = phase shift

$\Gamma_k^{(s)}$ = S-matrix total line width for the Adler-Adler formulation

$$G_{\gamma_k} = \sqrt{\left|E_{o_k}\right|}\left[G_k^c \cos 2\phi_{\ell_k} + H_k^c \sin 2\phi_{\ell_k}\right]$$

G_k^c = Adler-Adler symmetric capture cross section parameter from ENDF/B

H_k^c = Adler-Adler antisymmetric capture cross section parameter from ENDF/B

$$b_{\gamma_k} = -0.5\left[\frac{H_k^c \cos 2\phi_{\ell_k} - G_k^c \sin 2\phi_{\ell_k}}{G_{\gamma_k}}\right]\sqrt{\left|E_{o_k}\right|}$$

$$G_{f_k} = \sqrt{|E_{o_k}|}\left[G_k^F \cos 2\phi_{\ell_k} + H_k^F \cos 2\phi_{\ell_k}\right]$$

G_k^F = Adler-Adler symmetric fission cross section parameter from ENDF/B

H_k^F = Adler-Adler antisymmetric fission cross section parameter from ENDF/B

$$b_{f_k} = -0.5\left[\frac{H_k^F \cos 2\phi_{\ell_k} - G_k^F \sin 2\phi_{\ell_k}}{G_{f_k}}\right]\sqrt{|E_{o_k}|}$$

$$a_k = -0.5\left[\frac{H_k^T \cos 2\phi_{\ell_k} - G_k^T \sin 2\phi_{\ell_k}}{|G_{t_k}|}\right]\sqrt{|E_{o_k}|}\ .$$

Using Eqs. III.25-III.27 in Eq. III-1, we have for the case of all Adler-Adler multilevel resonances in the mixture, for example

$$\overline{\Sigma}_{c_i} = \frac{\Sigma_p G_{\gamma_k} \Gamma_k^{(s)}}{\Delta u E_{o_k} |G_{t_k}|}\frac{1}{2}\int_{-\infty}^{\infty} dx_k \frac{\psi_k + b_{\gamma_k}\chi_k}{\beta_k + S_k\psi_k + a_k\chi_k + \sum_{k',\neq k}(S_{k'}A_{k'}\psi_{k'} + B_{k'}\chi_{k'})}$$

$$= \frac{\Sigma_p \Gamma_k^{(s)}}{\Delta u E_{o_k}}\frac{G_{t_k}}{|G_{t_k}|} J_{\gamma_k}^{*m\ell} = \frac{\Sigma_p \Gamma_k^{(s)}}{\Delta u E_{o_k}} S_k J_{\gamma_k}^{*m\ell} \qquad \text{(III.28)}$$

Equation III.28 may be compared with Eq. III.2 and $S_k = G_{t_k}/|G_{t_k}|$. The $m\ell$ superscript refers to multilevel. In the case of multilevel Breit-Wigner resonances, $\Gamma_k^{(s)}$ is replaced by the multilevel total line width and b_{γ_k} is zero. A_k, B_k, and β_k are defined as in Eq. III.5 with σ_{o_k} and a_k defined as appropriate to the multilevel representation involved.

In the case of fission, Eq. III.28 becomes

$$\overline{\Sigma}_f = \frac{\Sigma_p G_{f_k} \Gamma_k^{(s)}}{\Delta u E_{o_k} |G_{t_k}|} J_{f_k}^{*m\ell} \qquad \text{(III.29)}$$

where $J_{f_k}^{*m\ell}$ is given by the integral of Eq. III.28 but with b_{f_k} replacing b_{γ_k}.

For the total cross section

$$\overline{\Sigma}_{t_k} = \frac{\Sigma_p \Gamma_k^{(s)}}{\Delta u E_{o_k}} \frac{1}{2} \int_{-\infty}^{\infty} dx_k \frac{S_k\psi_k + a_k\chi_k}{\beta_k + S_k\psi_k + a_k\chi_k + \sum_{k' \neq k} (S_{k'}A_{k'}\psi_{k'} + B_{k'}\chi_{k'})}$$

$$= \frac{\Sigma_p \Gamma_k^{(s)}}{\Delta u E_{o_k}} J_{t_k}^{*m\ell} . \qquad \text{(III.30)}$$

As in the case of the single level resonances, the multilevel resonance integrals may be factored into a lead term and a term due to the overlap of other resonances in the mixture. Thus the integral in Eq. III.28 can be written as

$$J_{\gamma_k}^{*m\ell} = \frac{1}{2} \int_{-\infty}^{\infty} dx_k \frac{\psi_k + b_{\gamma_k}\chi_k}{\beta_k + S_k\psi_k + a_k\chi_k} - \frac{1}{2} \int_{-\infty}^{\infty} dx_k \frac{\psi_k + b_{\gamma_k}\chi_k}{\beta_k + S_k\psi_k + a_k\chi_k}$$

$$\cdot \frac{\sum_{k' \neq k} (S_{k'}A_{k'}\psi_{k'} + B_{k'}\chi_{k'})}{\beta_k + S_k\psi_k + a_k\chi_k + \sum_{k' \neq k} (S_{k'}A_{k'}\psi_{k'} + B_{k'}\chi_{k'})}$$

$$= J_k^{\gamma,m\ell} - O_{k,k',0}^{\gamma,m\ell} . \qquad \text{(III.31)}$$

The factored form of Eq. III.29 can, by comparison with Eq. III.31 be written

$$J_{f_k}^{*m\ell} = J_k^{f,m\ell} - O_{k,k',0}^{f,m\ell} . \qquad \text{(III.32)}$$

Also, Eq. III.30 may be factored to yield

$$J_{t_k}^{*m\ell} = \frac{1}{2} \int_{-\infty}^{\infty} dx_k \frac{S_k\psi_k + a_k\chi_k}{\beta_k + S_k\psi_k + a_k\chi_k} - \frac{1}{2} \int_{-\infty}^{\infty} dx_k \frac{S_k\psi_k + a_k\chi_k}{\beta_k + S_k\psi_k + a_k\chi_k}$$

$$\cdot \frac{\sum_{k' \neq k} (S_{k'}A_{k'}\psi_{k'} + B_{k'}\chi_{k'})}{\beta_k + S_k\psi_k + a_k\chi_k + \sum_{k' \neq k} (S_{k'}A_{k'}\psi_{k'} + B_{k'}\chi_{k'})} = J_k^{t,m\ell} - O_{k,k',0}^{t,m\ell} .$$

(III.33)

So far we have considered the case of a mixture of either all single level (Eqs. III.23-III.24) or all multilevel (Eqs. III.31-III.33) resonances. Two other situations may also arise, namely a single level resonance in the presence of other single and multilevel level resonances, or a multilevel resonance in the presence of other single and multilevel resonances. Each of these cases may be written in factored form to yield a lead integral for the isolated single level (multilevel) resonance, minus integrals resulting from overlap with other single level (multilevel) and other multilevel (single level) resonances.

Thus, for a single level resonance i we have

$$J^{*s\ell}_{x_i} = J^{x,s\ell}_{i} - O^{x,s\ell}_{i,i',o} - O^{x,s\ell}_{i,i',k} \qquad \text{(III.34)}$$

and

$$J^{*s\ell}_{t,i} = J^{t,s\ell}_{i} - O^{t,s\ell}_{i,i',o} - O^{t,s\ell}_{i,i',k} \quad . \qquad \text{(III.35)}$$

$J^{x,s\ell}_{i}$ and $O^{x,s\ell}_{i,i',o}$ are given in Eq. III.23 and $J^{t,s\ell}_{i}$ and $O^{t,s\ell}_{i,i',o}$ are given in Eq. III.29. The second overlap terms which depend upon the single level resonances i and i' and upon the multilevel resonances k can be written explicitly as

$$O^{x,s\ell}_{i,i',k} = \frac{1}{2}\int_{-\infty}^{\infty} dx_i \; \frac{\psi_i}{\beta_i + \psi_i + a_i\chi_i + \sum\limits_{i'\neq i}(A_{i'}\psi_{i'} + B_{i'}\chi_{i'})} \cdot$$

$$\int_{-\infty}^{\infty} \frac{\sum\limits_{k}(S_k A_{ki}\psi_k + B_{ki}\chi_k)}{\beta_i+\psi_i+a_i\chi_i+\sum\limits_{i'\neq i}(A_{i'}\psi_{i'}+B_{i'}\chi_{i'}) + \sum\limits_{k}(S_k A_{ki}\psi_k+B_{ki}\chi_k)} \qquad \text{(III.36)}$$

and

$$O^{t,s\ell}_{i,i',k} = \frac{1}{2}\int_{-\infty}^{\infty} dx_i \; \frac{\psi_i + a_i\chi_i}{\beta_i + \psi_i + a_i\chi_i + \sum\limits_{i'\neq i}(A_{i'}\psi_{i'} + B_{i'}\chi_{i'})} \cdot$$

$$\int_{-\infty}^{\infty} \frac{\sum\limits_{k}(S_k A_{ki}\psi_k + B_{ki}\chi_k)}{\beta_i+\psi_i+a_i\chi_i+\sum\limits_{i'\neq i}(A_{i'}\psi_{i'}+B_{i'}\chi_{i'}) + \sum\limits_{k}(S_k A_{ki}\psi_k+B_{ki}\chi_k)} \quad . \qquad \text{(III.37)}$$

In Eqs. III.36 and III.37, $A_{i'}$ and $B_{i'}$ are defined in Eq. III.5 and

$$A_{ki} = \frac{N_{o_k}\sigma_{o_k}}{N_{o_i}\sigma_{o_i}}$$

$$B_{ki} = a_k A_{ki} \quad . \qquad \text{(III.38)}$$

Similarly, for a multilevel resonance k we have

$$J^{*m\ell}_{\gamma_k} = J^{\gamma,m\ell}_{k} - O^{\gamma,m\ell}_{k,k',o} - O^{\gamma,m\ell}_{k,k',i} \qquad \text{(III.39)}$$

$$J^{*m\ell}_{f_k} = J^{f,m\ell}_{k} - O^{f,m\ell}_{k,k',o} - O^{f,m\ell}_{k,k',i} \qquad \text{(III.40)}$$

$$J^{*m\ell}_{t_k} = J^{t,m\ell}_{k} - O^{t,m\ell}_{k,k',o} - O^{t,m\ell}_{k,k',i} \quad . \qquad \text{(III.41)}$$

In Eqs. III.37-III.41 the indices k and k' refer to multilevel resonances and ind i refers to single level resonances in the mixture.

$J_k^{\gamma,m\ell}$ and $O_{k,k',o}^{\gamma,m\ell}$ are given in Eq. III.31. $J_k^{f,m\ell}$ and $O_{k,k',o}^{f,m\ell}$ are the above expressions with b_{f_k} replacing b_{γ_k}. $J_k^{t,m\ell}$ and $O_{k,k',o}^{t,m\ell}$ are given in Eq. III.33. The second overlap terms can be written explicitly as

$$O_{k,k',i}^{\gamma,m\ell} = \frac{1}{2}\int_{-\infty}^{\infty} dx_k \frac{\psi_k + b_{\gamma_k}\chi_k}{\beta_k + S_k\psi_k + a_k\chi_k + \sum_{k'\neq k}(S_{k'}A_{k'}\psi_{k'} + B_{k'}\chi_{k'})} \cdot$$

$$\int_{-\infty}^{\infty} \frac{\sum_i (A_{ik}\psi_i + B_{ik}\chi_i)}{\beta_k + S_k\psi_k + a_k\chi_k + \sum_{k'\neq k}(S_{k'}A_{k'}\psi_{k'} + B_{k'}\chi_{k'}) + \sum_i (A_{ik}\psi_i + B_{ik}\chi_i)} \quad \text{(III.42)}$$

with $O_{k,k',i}^{f,m\ell}$ as in Eq. III.42 with b_{f_k} replacing b_{γ_k}, and

$$O_{k,k',i}^{t,m\ell} = \frac{1}{2}\int_{-\infty}^{\infty} dx_k \frac{S_k\psi_k + a_k\chi_k}{\beta_k + S_k\psi_k + a_k\chi_k + \sum_{k'\neq k}(S_{k'}A_{k'}\psi_{k'} + B_{k'}\chi_{k'})} \cdot$$

$$\int_{-\infty}^{\infty} \frac{\sum_i (A_{ik}\psi_i + B_{ik}\chi_i)}{\beta_k + S_k\psi_k + a_k\chi_k + \sum_{k'\neq k}(S_{k'}A_{k'}\psi_{k'} + B_{k'}\chi_{k'}) + \sum_i (A_{ik}\psi_i + B_{ik}\chi_i)} \quad \text{(III.43)}$$

B. Calculation of Isolated Resonance Integrals

Each of the isolated resonance integrals $J_i^{x,s\ell}$, $J_i^{t,s\ell}$, $J_k^{\gamma,m\ell}$, $J_k^{f,m\ell}$, and $J_k^{t,m\ell}$ as given in Eqs. III.23, III.24, III.31, III.32 and III.33 represents a special case of the general resonance integral representation

$$J(\beta,\theta,a,b) = \frac{1}{2}\int_{-\infty}^{\infty} dx \frac{T\psi + b\chi}{\beta + S\psi + a\chi} \cdot \quad \text{(III.44)}$$

In particular for single level resonances T = S = 1, and b = 0 for capture or fission, and equals a for total. Similarly, for multilevel resonances $b = b_\gamma$, b_f, or a for capture, fission or total, T = 1 for capture and fission, and T = S for total.

Assuming that $\beta + S\psi + a\chi > o$, Equation III.44 can be factored[25]

$$J(\beta,\theta,a,b) = J(\beta,\theta,0,0) + I(\beta,\theta,a) - bM(\beta,\theta,a) \tag{III.45}$$

where

$$J(\beta,\theta,0,0) = T\int_0^\infty dx\,\frac{\psi}{\beta + S\psi} \tag{III.46}$$

$$I(\beta,\theta,a) = Ta^2\int_0^\infty dx\,\frac{\psi}{\beta + S\psi}\cdot\frac{\chi^2}{(\beta + S\psi)^2 - a^2\chi^2} \tag{III.47}$$

$$M(\beta,\theta,a) = a\int_0^\infty dx\,\frac{\chi^2}{(\beta + S\psi)^2 - a^2\chi^2}\,. \tag{III.48}$$

The quantities $J(\beta,\theta,0,0)$, $I(\beta,\theta,a)$ and $M(\beta,\theta,a)$ are calculated using the numerical methods described in Section IV of Appendix A involving fixed point Gauss-Jacobi quadrature or asymptotic expressions depending upon the size of β.

The user may specify that all resonances for a particular isotope be assigned the infinitely dilute resonance integral limiting value $\pi/(2\beta)$. In this case, none of the resonances of this isotope will be involved in the calculation of the overlap integrals for any other resonance in the mixture.

C. Calculation of Overlap Integrals

1. Selection of Overlapping Resonances

In the calculation of the various overlap integrals, only those neighboring resonances are included which satisfy the following criterion.

Two "widths" are computed for each resonance i

$$W_i^1 = \frac{\Gamma_i}{\theta_i}\sqrt{\ell n\left[2 + \frac{\psi(\theta_i,0)}{\beta_i}\right]} \tag{III.49}$$

and

$$W_i^2 = \frac{\Gamma_i}{2}\sqrt{\frac{\beta_i+1}{\beta_i}} \tag{III.50}$$

where Γ_i is the total line width (or S-matrix total line width for Adler-Adler multilevel resonances) and $\psi(\theta_i,0)$ is calculated as in Eq.A.15 of Appendix A. Denoting by L_i the larger of W_i^1 and W_i^2

$$L_i = \max\left[W_i^1, W_i^2\right], \tag{III.51}$$

we include resonance i' in the overlap integral for resonance i if

$$\left|E_{o_i} - E_{o_{i'}}\right| < 10\ L_i . \qquad \text{(III.52)}$$

Otherwise resonance i' is ignored.

The code defaults to four neighbors on each side of each resonance as candidates for inclusion in the overlap integrals, but the number of overlap candidates can be specified by the user.

2. Asymptotic Algorithms

The code first evaluates the asymptotic or "large β" approximations[25] for the various overlap integrals. The integrands of these integrals (Eqs. III.23, III.24, III.31, III.32, III.33, III.36, III.37, III.42 and III.43) consist of products of ψ and χ functions times a factor of the form

$$\frac{1}{\beta^2 + f} \qquad \text{(III.53)}$$

where f represents the energy dependent part of the denominator. If we add and subtract a quantity σ*, to be defined below, we can write

$$\begin{aligned}
\frac{1}{\beta^2 + f} &= \frac{1}{\beta^2 + \sigma^* - (\sigma^* - f)} \\
&= \frac{1}{\beta^2 + \sigma^*}\left[1 - \frac{1}{\dfrac{\sigma^* - f}{\beta^2 + \sigma^*}}\right] \\
&\approx \frac{1}{\beta^2 + \sigma^*}\left[1 + \frac{\sigma^* - f}{\beta^2 + \sigma^*} + \ldots\right] \\
&\approx \frac{1}{\beta^2 + \sigma^*} + \frac{\sigma^* - f}{(\beta^2 + \sigma^*)^2} \ . \qquad \text{(III.54)}
\end{aligned}$$

As a specific example, consider $O^{x,\delta\ell}_{i,i',o}$ as given in Eq. III.23. Using Eq. III.54 we can write

$$\begin{aligned}
O^{x,\delta\ell}_{i,i',o} &\approx \frac{1}{2}\int_{-\infty}^{\infty} dx_i \ \frac{\psi_i \sum\limits_{i'\neq i}\left(A_{i'}\psi_{i'} + B_{i'}\chi_{i'}\right)}{\beta_i^2 + \sigma^*_{i,i',0}} \\
&+ \frac{1}{2}\int_{-\infty}^{\infty} dx_i \ \frac{\left[\sigma^*_{i,i',0} - f_{i,i',0}\right]\ \psi_i \sum\limits_{i'\neq i}\left(A_{i'}\psi_{i'} + B_{i'}\chi_{i'}\right)}{\left[\beta_i^2 + \sigma^*_{i,i',0}\right]^2} \qquad \text{(III.55)}
\end{aligned}$$

where

$$f_{i,i',0} = 2\beta_i(\psi_i + a_i\chi_i) + (\psi_i + a_i\chi_i)^2 + \beta_i \sum_{i'\neq i} (A_{i'}\psi_{i'} + B_{i'}\chi_{i'})$$

$$+ (\psi_i + a_i\chi_i) \sum_{i'\neq i} (A_{i'}\psi_{i'} + B_{i'}\chi_{i'})$$

$$\approx 2\beta_i(\psi_{i'} + a_{i'}\chi_{i'}) + \beta_i \sum_{i'\neq i} (A_{i'}\psi_{i'} + B_{i'}\chi_{i'}). \qquad \text{(III.56)}$$

Now if we define

$$\sigma^{s\ell *}_{i,i',0} = \frac{\int_{-\infty}^{\infty} dx_i \, f_{i,i',0}\psi_i \sum_{i'\neq i} (A_{i'}\psi_{i'} + B_{i'}\chi_{i'})}{\int_{-\infty}^{\infty} dx_i \psi_i \sum_{i'\neq i} (A_{i'}\psi_{i'} + B_{i'}\chi_{i'})} \qquad \text{(III.57)}$$

with $f_{i,i',0}$ given by Eq. III.56, the second order term of Eq. III.55 will vanish and we are left with the approximation

$$O^{x,s\ell}_{i,i',o} \approx \frac{1}{2} \int_{-\infty}^{\infty} dx_i \, \frac{\psi_i \sum_{i'\neq i} (A_{i'}\psi_{i'} + B_{i'}\chi_{i'})}{\beta_i^2 + \sigma^{s\ell *}_{i,i',0}} \, . \qquad \text{(III.58)}$$

Similarly, the total overlap integral as given in Eq. III.24 can be written as the sum of two terms

$$O^{t,s\ell}_{i,i',o} = OV^{x,s\ell}_{1\,i,i',o} + OV^{t,s\ell}_{2\,i,i',o} \qquad \text{(III.59)}$$

where $OV^{x,s\ell}_{1\,i,i',o}$ is $O^{x,s\ell}_{i,i',o}$ as given in Eq. III.23 and approximated in Eq. III.58 and

$$OV^{t,s\ell}_{2\,i,i',o} = \frac{1}{2} \int_{-\infty}^{\infty} dx_i \, \frac{a_i\chi_i \sum_{i'\neq i} (A_{i'}\psi_{i'} + B_{i'}\chi_{i'})}{f_{i,i',o}} \qquad \text{(III.60)}$$

where $f_{i,i',o}$ is again given by Eq. III.56.

Using the same technique as above, we may approximate Eq. III.60 as

$$OV^{t,s\ell}_{2\,i,i',o} \approx \frac{1}{2} \int_{-\infty}^{\infty} dx_i \, \frac{a_i\chi_i \sum_{i'\neq i} (A_{i'}\psi_{i'} + B_{i'}\chi_{i'})}{\beta_i^2 + \sigma^{s\ell **}_{i,i',0}} \qquad \text{(III.61)}$$

with $\sigma^{**}_{i,i',o}$ defined as

$$\sigma^{s\ell**}_{i,i',o} = \frac{\int_{-\infty}^{\infty} dx_i f_{i,i',o} a_i \chi_i \sum_{i' \neq i} (A_{i'} \psi_{i'} + B_{i'} \chi_{i'})}{\int_{-\infty}^{\infty} dx_i a_i \chi_i \sum_{i' \neq i} (A_{i'} \psi_{i'} + B_{i'} \chi_{i'})} . \qquad \text{(III.62)}$$

This same technique is used to obtain asymptotic expressions for the various other overlap integrals $O^{\gamma,m\ell}_{k,k',o}$, $O^{x,s\ell}_{i,i',k}$, etc. where each requires the definition of a corresponding σ^* and σ^{**} appropriate to the specific form of the integrand involved. Note that each of the multilevel overlap integrals, and the single level overlap integral for the total cross section can be written as in Eq. III.58 as the sum of a symmetric term OV_1 and an antisymmetric term OV_2.

Once the σ^* and σ^{**} have been evaluated, as described later, the integrals remaining in these asymptotic expressions all involve infinite integrals of products of ψ and χ functions for the resonance being evaluated and for the neighboring resonances included in the overlap calculation. These may be integrated using the following identities.[27]

$$\int_{-\infty}^{\infty} dx_i \psi(\theta_i, x_i) \psi(\theta_j, x_j) = \int_{-\infty}^{\infty} dx_i \psi_i \psi_j$$

$$= \pi \frac{\Gamma_j}{\Gamma_i + \Gamma_j} \psi \left[\frac{\Gamma_i + \Gamma_j}{\sqrt{\Delta_i^2 + \Delta_j^2}} , \frac{E_{o_i} - E_{o_j}}{\frac{\Gamma_i + \Gamma_j}{2}} \right]$$

$$= \pi \frac{\Gamma_j}{\Gamma_i + \Gamma_j} \psi \left[\theta_{ij}, x_{ij} \right]$$

$$= \pi \frac{\Gamma_j}{\Gamma_i + \Gamma_j} \psi_{ij} \qquad \text{(III.63)}$$

$$\int_{-\infty}^{\infty} dx_i \chi_i \chi_j = 4\pi \frac{\Gamma_j}{\Gamma_i + \Gamma_j} \psi_{ij} \qquad \text{(III.64)}$$

$$\int_{-\infty}^{\infty} dx_i \psi_i \chi_j = \pi \frac{\Gamma_j}{\Gamma_i + \Gamma_j} \chi_{ij} \qquad \text{(III.65)}$$

where χ_{ij} implies the same notation for χ as in the case of Eq. III.63 for ψ_{ij}

$$\int_{-\infty}^{\infty} dx_i \chi_i \psi_j = -\pi \frac{\Gamma_j}{\Gamma_i+\Gamma_j} \chi_{ij} \tag{III.66}$$

$$\int_{-\infty}^{\infty} dx_i \psi_i^2 = \frac{\pi}{2} \psi(\sqrt{2}\theta_i,0) \tag{III.67}$$

$$\int_{-\infty}^{\infty} dx_i \chi_i^2 = 2\pi \psi(\sqrt{2}\theta_i,0) \quad . \tag{III.68}$$

The more compact notation identified in Eq. III.63 is used for Eqs. III.64-III.68.

Making use of Eqs. III.63-III.68 in Eqs. III.58-III.61, and in the analogous integrals for the other cases discussed above, we finally may tabulate the asymptotic overlap integrals as follows.

$$O^{x,s\ell}_{i,i',o} \approx \frac{\pi}{2} \frac{\sum_{i'\neq i} \frac{\Gamma_{i'}}{\Gamma_i+\Gamma_{i'}} (A_i,\psi_{ii'},+B_i,\chi_{ii'})}{\beta_i^2+\sigma^{s\ell *}_{i,i',o}} = OV^{x,s\ell}_{1\,i,i',o} \tag{III.69}$$

$$O^{t,s\ell}_{i,i',o} \approx OV^{x,s\ell}_{1\,i,i',o} + \frac{\pi}{2} \frac{a_i \sum_{i'\neq i} \frac{\Gamma_{i'}}{\Gamma_i+\Gamma_{i'}} (-A_i,\chi_{ii'},+4B_i,\psi_{ii'})}{\beta_i^2+\sigma^{s\ell *}_{i,i',o}}$$

$$= OV^{x,s\ell}_{1\,i,i',o} + OV^{t,s\ell}_{2\,i,i',o} \tag{III.70}$$

$$O^{\gamma,m\ell}_{k,k',o} \approx \frac{\pi}{2} \frac{\sum_{k'\neq k} \frac{\Gamma_{k'}}{\Gamma_k+\Gamma_{k'}} (S_k,A_k,\psi_{kk'},+B_k,\chi_{kk'})}{\beta_k^2+\sigma^{m\ell *}_{k,k',o}}$$

$$+ \frac{\pi}{2} \frac{b_{\gamma_k} \sum_{k'\neq k} \frac{\Gamma_{k'}}{\Gamma_k+\Gamma_{k'}} (-S_k,A_k,\chi_{kk'},+4B_k,\psi_{kk'})}{\beta_k^2+\sigma^{m\ell **}_{k,k',o}}$$

$$= OV^{x,m\ell}_{1\,k,k',o} + OV^{\gamma,m\ell}_{2\,k,k',o} \tag{III.71}$$

$$o^{f,m\ell}_{k,k',o} \approx ov^{x,m\ell}_{1_{k,k',o}} + ov^{f,m\ell}_{2_{k,k',o}} = ov^{x,m\ell}_{1_{k,k',o}} + \frac{b_{f_k}}{b_{\gamma_k}} ov^{\gamma,m\ell}_{2_{k,k',o}} \qquad \text{(III.72)}$$

$$o^{t,m\ell}_{k,k',o} \approx S_k \, ov^{x,m\ell}_{1_{k,k',o}} + ov^{t,m\ell}_{2_{k,k',o}}$$

$$= S_k \, ov^{x,m\ell}_{1_{k,k',o}} + \frac{a_k}{b_{\gamma_k}} ov^{\gamma,m\ell}_{2_{k,k',o}} \qquad \text{(III.73)}$$

$$o^{x,s\ell}_{i,i',k} \approx \frac{\pi}{2} \frac{\sum_k \frac{\Gamma_k}{\Gamma_i+\Gamma_k} (S_k A_{ki}\psi_{ik} + B_{ki}\chi_{ik})}{\beta_i^2+\sigma^{s\ell*}_{i,i',k}} = ov^{x,s\ell}_{1_{i,i',k}} \qquad \text{(III.74)}$$

$$o^{t,s\ell}_{i,i',k} = ov^{x,s\ell}_{1_{i,i',k}} + \frac{\pi}{2} \frac{a_i \sum_k \frac{\Gamma_k}{\Gamma_i+\Gamma_k} (-S_k A_{ki}\chi_{ik} + 4B_{ki}\psi_{ik})}{\beta_i^2+\sigma^{s\ell**}_{i,i',k}}$$

$$= ov^{x,s\ell}_{1_{i,i',k}} + ov^{t,s\ell}_{2_{i,i',o}} \qquad \text{(III.75)}$$

$$o^{\gamma,m\ell}_{k,k',i} \approx \frac{\pi}{2} \frac{\sum_i \frac{\Gamma_i}{\Gamma_i+\Gamma_k} (A_{ik}\psi_{ki} + B_{ik}\chi_{ki})}{\beta_k^2+\sigma^{m\ell*}_{k,k',i}}$$

$$+ \frac{\pi}{2} \frac{b_{\gamma_k} \sum_i \frac{\Gamma_i}{\Gamma_i+\Gamma_k} (-A_{ik}\chi_{ki} + 4B_{ik}\psi_{ki})}{\beta_k^2+\sigma^{m\ell**}_{k,k',i}}$$

$$= ov^{x,m\ell}_{1_{k,k',i}} + ov^{\gamma,m\ell}_{2_{k,k',o}} \qquad \text{(III.76)}$$

$$o^{f,m\ell}_{k,k',i} \approx ov^{x,m\ell}_{1_{k,k',i}} + ov^{f,m\ell}_{2_{k,k',i}} = ov^{x,m\ell}_{1_{k,k',i}} + \frac{b_{f_k}}{b_{\gamma_k}} ov^{\gamma,m\ell}_{2_{k,k',i}} \qquad \text{(III.77)}$$

$$o^{t,m\ell}_{k,k',i} \approx S_k \; ov^{x,m\ell}_{1\,k,k',i} + \frac{a_k}{b_{\gamma_k}} ov^{\gamma,m\ell}_{2\,k,k',i} \quad . \tag{III.78}$$

In the above, A_i and B_i are defined in Eq.III.5, A_{ki} and B_{ki} are defined in Eq.III.38, and ψ_{ik} and χ_{ik} are defined by Eq.III.63. Also, we use the indices i and i' to denote single level resonances and k and k' to denote multilevel resonance.

The evaluation of the σ^* and σ^{**} which appear in Eqs.III.69-III.78 involve infinite integrals of triple products of ψ and χ functions as can be seen for example by using Eq.III.56 in Eqs.III. 57 or III.62. Integrals over triple products of different indices are ignored in this process. That is, for example

$$\int_{-\infty}^{\infty} \psi_i \sum_{i' \neq i} A_{i'} \psi_{i'} \sum_{i' \neq i} B_{i'} \chi_{i'} dx_i = \int_{-\infty}^{\infty} \psi_i \sum_{i' \neq i} A_{i'} \psi_{i'} \sum_{i'' \neq i} B_{i''} \chi_{i''} dx_i$$

$$= \int_{-\infty}^{\infty} \left[\psi_i \sum_{i' \neq i} A_{i'} \psi_{i'} B_{i'} \chi_{i'} + \psi_i \sum_{i' \neq i} A_{i'} \psi_{i'} \sum_{i'' \neq i} B_{i''} \chi_{i''} \right] dx_i$$

$$\approx \int_{-\infty}^{\infty} \psi_i \sum_{i' \neq i} A_{i'} \psi_{i'} B_{i'} \chi_{i'} dx_i \quad .$$

Similarly, the integral

$$\int \psi_k \sum_{k' \neq k} S_{k'} A_{k'} \psi_{k'} \sum_i A_{ik} \psi_i dx_k$$

will be ignored since it involves the triple index k, k', i.

As a specific example, we may write out the expression for $\sigma^{s\ell*}_{i,i',o}$ in detail, with the above approximation, as follows.

$$\sigma^{s\ell*}_{i,i',o} \approx \frac{\beta_i \int_{-\infty}^{\infty} dx_i \psi_i \; S}{\int_{-\infty}^{\infty} \psi_i \sum_{i' \neq i} (A_{i'} \psi_{i'} + B_{i'} \chi_{i'}) \; dx_i} \tag{III.79}$$

where

$$S = 2\psi_i \sum_{i'\neq i} A_{i'}\psi_{i'} + 2 \sum_{i'\neq i} A_{i'}\psi_{i'}a_i\chi_i + \sum_{i'\neq i} (A_{i'}\psi_{i'})^2$$

$$+ 2 \sum_{i'\neq i} A_{i'}\psi_{i'}B_{i'}\chi_{i'} + 2\psi_i \sum_{i'\neq i} B_{i'}\chi_{i'} + 2 \sum_{i'\neq i} B_{i'}\chi_{i'}a_i\chi_i + \sum_{i'\neq i} (B_{i'}\chi_{i'})^2. \quad \text{(III.80)}$$

The denominators in Eq. III.79 and the corresponding expressions for the other σ^* and σ^{**} are evaluated using Eqs. III.63-III.68. The various integrals of triple products in the numerators are evaluated using the following expressions[25] where we use the notation of Eq.III.63. Also, we use the transformation

$$\hat{\chi}_k = \frac{1}{2}\chi_k \quad \text{(III.81)}$$

$$\int_{-\infty}^{\infty} \psi_k^2\psi_{k'}dx_k = \sqrt{\frac{\pi}{2}}\frac{\pi}{4}\theta_k \frac{2\Gamma_{k'}}{\Gamma_k+\Gamma_{k'}}(I_1 + I_2) \quad \text{(III.82)}$$

$$\int_{-\infty}^{\infty} \psi_k^2\hat{\chi}_{k'}dx_k = \sqrt{\frac{\pi}{2}}\frac{\pi}{4}\theta_k \frac{2\Gamma_{k'}}{\Gamma_k+\Gamma_{k'}}(I_3 + I_4) \quad \text{(III.83)}$$

$$\int_{-\infty}^{\infty} \hat{\chi}_k^2\psi_{k'}dx_k = \sqrt{\frac{\pi}{2}}\frac{\pi}{4}\theta_k \frac{2\Gamma_{k'}}{\Gamma_k+\Gamma_{k'}}(I_1 - I_2) \quad \text{(III.84)}$$

$$\int_{-\infty}^{\infty} \hat{\chi}_k^2\hat{\chi}_{k'}dx_k = \sqrt{\frac{\pi}{2}}\frac{\pi}{4}\theta_k \frac{2\Gamma_{k'}}{\Gamma_k+\Gamma_{k'}}(I_3 - I_4) \quad \text{(III.85)}$$

$$\int_{-\infty}^{\infty} \hat{\chi}_k\hat{\chi}_{k'}\psi_{k'}dx_k = \sqrt{\frac{\pi}{2}}\frac{\pi}{4}\theta_k \frac{2\Gamma_{k'}}{\Gamma_k+\Gamma_{k'}} I_2 \quad \text{(III.86)}$$

$$\int_{-\infty}^{\infty} \hat{\chi}_k\psi_{k'}\psi_k dx_k = -\sqrt{\frac{\pi}{2}}\frac{\pi}{4}\theta_k \frac{2\Gamma_{k'}}{\Gamma_k+\Gamma_{k'}} I_4. \quad \text{(III.87)}$$

The quantities I_1 through I_4 are given by[25]

$$I_1 = A_4\left[A_5\psi_{kk'} - A_7\frac{\partial\hat{\chi}_{kk'}}{\partial x_{kk'}} - A_8\frac{\partial^2\psi_{kk'}}{\partial x^2_{kk'}} + A_9\frac{\partial^3\hat{\chi}_{kk'}}{\partial x_{kk'}}\right] \quad \text{(III.88)}$$

$$I_2 = \frac{2}{\sqrt{\pi}}A_3\left[\frac{\partial\hat{\chi}_{kk'}}{\partial x_{kk'}} - \frac{2}{3}A_3^2\frac{\partial^2\hat{\chi}_{kk'}}{\partial x_{kk'}}\right] \quad \text{(III.}$$

$$I_3 = A_4 \left[A_5 \hat{\chi}_{kk'} + A_7 \frac{\partial \psi_{kk'}}{\partial x_{kk'}} - A_8 \frac{\partial^2 \hat{\chi}_{kk'}}{\partial x_{kk'}} - A_9 \frac{\partial^3 \psi_{kk'}}{\partial x_{kk'}} \right] \tag{III.90}$$

$$I_4 = - \frac{2}{\sqrt{\pi}} A_3 \left[\frac{\partial \psi_{kk'}}{\partial x_{kk'}} - \frac{2}{3} A_3^2 \frac{\partial^3 \psi_{kk'}}{\partial x^3_{kk'}} \right] \tag{III.91}$$

where

$$\frac{\partial \psi_{kk'}}{\partial x_{kk'}} = \frac{\theta^2_{kk'}}{2} \left[\hat{\chi}_{kk'} - x_{kk'} \psi_{kk'} \right] \tag{III.92}$$

$$\frac{\partial \hat{\chi}_{kk'}}{\partial x_{kk'}} = \frac{\theta^2_{kk'}}{2} \left[1 - x_{kk'} \hat{\chi}_{kk'} - \psi_{kk'} \right] \tag{III.93}$$

$$\frac{\partial^2 \hat{\chi}_{kk'}}{\partial x^2_{kk'}} = - \frac{\theta^2_{kk'}}{2} \left[\hat{\chi}_{kk'} + x_{kk'} \frac{\partial \hat{\chi}_{kk'}}{\partial x_{kk'}} + \frac{\partial \psi_{kk'}}{\partial x_{kk'}} \right] \tag{III.94}$$

$$\frac{\partial^2 \psi_{kk'}}{\partial x^2_{kk'}} = \frac{\theta^2_{kk'}}{2} \left[\frac{\partial \hat{\chi}_{kk'}}{\partial x^2_{kk'}} - \psi_{kk'} - x_{kk'} \frac{\partial \psi_{kk'}}{\partial x_{kk'}} \right] \tag{III.95}$$

$$\frac{\partial^3 \psi_{kk'}}{\partial x^3_{kk'}} = \frac{\theta^2_{kk'}}{2} \left[\frac{\partial^2 \hat{\chi}_{kk'}}{\partial x^2_{kk'}} - 2 \frac{\partial \psi_{kk'}}{\partial x_{kk'}} - x_{kk'} \frac{\partial^2 \psi_{kk'}}{\partial x_{kk'}} \right] \tag{III.96}$$

$$\frac{\partial^3 \hat{\chi}_{kk'}}{\partial x^3_{kk'}} = - \frac{\theta^2_{kk'}}{2} \left[2 \frac{\partial \hat{\chi}_{kk'}}{\partial x_{kk'}} + x_{kk'} \frac{\partial^2 \hat{\chi}_{kk'}}{\partial x^2_{kk'}} + \frac{\partial^2 \psi_{kk'}}{\partial x^2_{kk'}} \right] \tag{III.97}$$

and the coefficients A_3 through A_9 depend upon the size of θ_k.

For $\theta_k \leq 5.5 \sqrt{2}$

use is made of the rational approximation

$$e^{t^2} \operatorname{erfc}(t) \approx \sum_{i=1}^{3} \frac{a_i}{1 + pt}$$

with, $a_1 = 0.3480242$; $a_2 = -0.0958798$; $a_3 = 0.7478556$; $p = 0.47047$ and

$$A_3 = \frac{\frac{\Gamma_k}{\theta_k}}{\sqrt{2}\ (\Gamma_k + \Gamma_{k'})} \tag{III.98}$$

$$A_4 = \frac{1}{1 + \frac{p\theta_k}{\sqrt{2}}} \tag{III.99}$$

$$A_5 = a_1+a_2A_4+a_3A_4^2 \tag{III.100}$$

$$A_6 = pA_3$$

$$A_7 = A_4A_6(a_1+2a_2A_4+3a_3A_4^2) \tag{III.101}$$

$$A_8 = (A_4A_6)^2(a_1+3a_2A_4+6a_3A_4^2) \tag{III.102}$$

$$A_9 = (A_4A_6)^3(a_1+4a_2A_4+10a_3A_4^2). \tag{III.103}$$

For $\theta_k > 5.5\sqrt{2}$

$$A_3 = \frac{\frac{\Gamma_k}{\theta_k}}{\sqrt{2}\ (\Gamma_k+\Gamma_{k'})}, \text{ as before}$$

$$A_4 = \frac{1}{\frac{\sqrt{\pi}\ \theta_k}{\sqrt{2}}} \left\{1 - \left[1 - \frac{3\sqrt{2}}{2\theta_k}\right]/\theta_k^2\right\} \tag{III.104}$$

$$A_5 = 1 \tag{III.105}$$

$$A_6 = A_3 \tag{III.106}$$

$$A_7 = \frac{\sqrt{2}}{\theta_k} A_6 \tag{III.107}$$

$$A_8 = A_7^2 \tag{III.108}$$

$$A_9 = A_7^3. \tag{III.109}$$

Note that the expression for A_4 when $\theta_k > 5.5\sqrt{2}$ and the break point $5.5\sqrt{2}$ both differ from the values reported in Hwang's original work (c.f. Eq. B.22 of Ref. 25). The values used in the code reflect the results of numerical studies aimed at optimizing execution efficiency and minimizing errors in the calculated results.

Now in the evaluation of the quantities I_1 through I_4, the $\psi_{kk'}$ and $\hat{\chi}_{kk'}$, as in other parts of MC^2-2 are normally evaluated as described in Section III of Appendix A by a bivariate interpolation in prestored tables. However, if $\left|x_{kk'}\theta_{kk'}/2\right| > 12$ or $\theta_{kk'}/2 > 12$, where $x_{kk'}$ and $\theta_{kk'}$ are defined in Eq.III.63, then the following asymptotic expressions are used for $\psi_{kk'}$, $\hat{\chi}_{kk'}$ and their second derivatives.

$$\psi_{kk'} \approx \frac{1}{1+x_{kk'}^2}\left[1+\frac{2}{\theta_{kk'}^2}\frac{3x_{kk'}^2-1}{(1+x_{kk'}^2)^2}+\frac{12}{\theta_{kk'}^4}\frac{(1-10x_{kk'}^2+5x_{kk'}^4)}{(1+x_{kk'}^2)^4}\right] \quad \text{(III.110)}$$

$$\hat{\chi}_{kk'} \approx \frac{x_{kk'}}{1+x_{kk'}^2}\left[1+\frac{2}{\theta_{kk'}^2}\frac{x_{kk'}^2-3}{(1+x_{kk'}^2)^2}+\frac{12}{\theta_{kk'}^4}\frac{(x_{kk'}^4-10x_{kk'}^2+5)}{(1+x_{kk'}^2)^4}\right] \quad \text{(III.111)}$$

$$\frac{\partial^2\psi_{kk'}}{\partial x_{kk'}^2} \approx \frac{1}{1+x_{kk'}^2}\left[2\frac{3x_{kk'}^2-1}{(1+x_{kk'}^2)^2}+\frac{24}{\theta_{kk'}^2}\frac{(1-10x_{kk'}^2+5x_{kk'}^4)}{(1+x_{kk'}^2)^4}\right] \quad \text{(III.112)}$$

$$\frac{\partial^2\hat{\chi}_{kk'}}{\partial x_{kk'}^2} \approx \frac{x_{kk'}}{1+x_{kk'}^2}\left[2\frac{x_{kk'}^2-3}{(1+x_{kk'}^2)^2}+\frac{24}{\theta_{kk'}^2}\frac{(x_{kk'}^4-10x_{kk'}^2+5)}{(1+x_{kk'}^2)^4}\right]. \quad \text{(III.113)}$$

After computing the asymptotic approximations to the overlap integrals, Eqs.III.69-III.78, the code tests whether these results are adequate or rather if the calculations should be performed using Gauss-Jacobi quadrature and if so, how many quadrature points should be used. The logic used in these tests is shown in Fig. 4. Note that the selection criteria depend upon the ratios of β^2/σ^*, β^2/σ^{**}, and $|OV_2/OV_1|$ for the particular overlap integral being evaluated.

The Gauss-Jacobi quadrature algorithms are described below.

3. Gauss-Jacobi Quadrature Algorithms

The various overlap integrals given in Eqs.III.23, III.24, III.31, III.32, III.33, III.36, III.37, III.42, and III.43 are evaluated using 13, 33, or 61 fixed point Gauss-Jacobi quadrature determined as indicated in Fig. 4.

Since the variable of integration is x_i, other resonances such as i' have their $x_{i'}$ transformed as

$$x_{i'} = \frac{E-E_{o_{i'}}}{\frac{\Gamma_{i'}}{2}} = \frac{E-E_{o_i}+E_{o_i}-E_{o_{i'}}}{\frac{\Gamma_i}{2}\left[\frac{\Gamma_{i'}}{\Gamma_i}\right]}$$

$$= \frac{x_i}{\frac{\Gamma_{i'}}{\Gamma_i}}+\frac{E_{o_i}-E_{o_{i'}}}{\frac{\Gamma_{i'}}{2}} \quad \text{(III.114)}$$

The variable of integration is transformed as in the case of the Gauss-Jacobi quadrature for the isolated resonance integrals as described in Section IV of Appendix A. Now, however, since the integration ranges from $-\infty$ to ∞, all N Gauss-Jacobi points are used. Also, as discussed in Ref. 25, after transforming the variable of integration as in Eq.A.17 of Appendix A, a_i/β_i

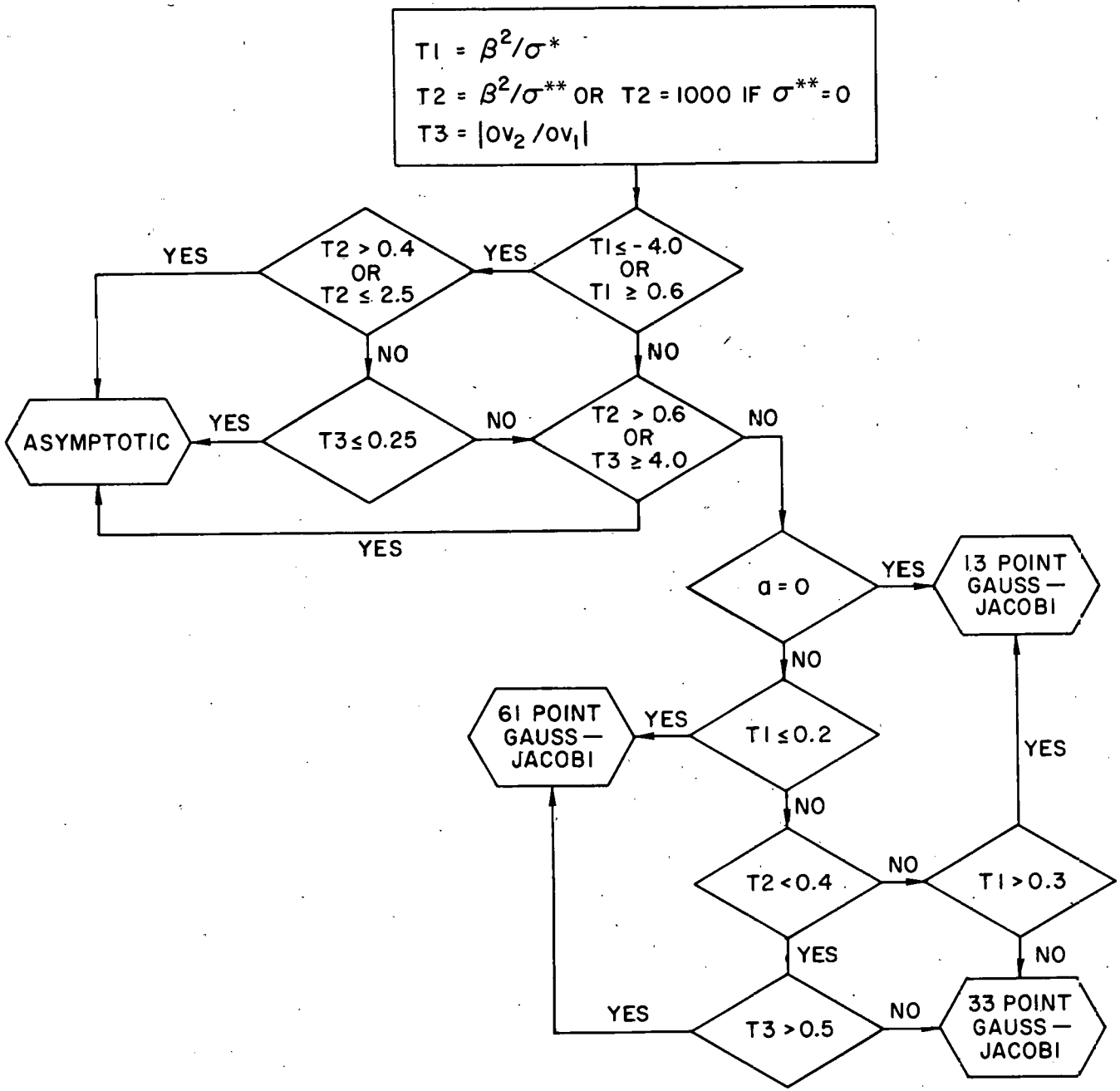

Fig. 4. Gauss-Jacobi Quadrature Point Selection

is subtracted from the result to provide a better distribution of quadrature abscissae over the distribution of the integrands involved, which are peaked to the left of the origin.

After completing the integrations as indicated above, the asymmetric parts of the multilevel resonance overlap integrals, or of the total overlap integral for single level resonances, may be recomputed depending upon the testing described below.

As a specific example, we rewrite the asymmetric part of the total overlap integral for the case of all single level resonances, Eq.III.60, as

$$O_{2_{i,i',o}}^{t,s\ell} = \frac{1}{2} \sum_{i' \neq i} \int_{-\infty}^{\infty} dx_i \, \frac{a_i \chi_i}{\beta_i + \psi_i + a_i \chi_i} \cdot \frac{A_{i'} \psi_{i'} + B_{i'} \chi_{i'}}{\beta_i + \psi_i + a_i \chi_i + \sum_{i' \neq i} (A_{i'} \psi_{i'} + B_{i'} \chi_{i'})} \, . \tag{III.115}$$

The quantity

$$\text{SEPTST} = \frac{\left| E_{o_i} - E_{o_{i'}} \right|}{L_i + L_{i'}} \tag{III.116}$$

is computed for each term of the sum in Eq.III.115, where L_i and $L_{i'}$ are obtained as indicated in Eqs. 49-51. If SEPTST $\leq$ 2.5, the value obtained for the Gauss-Jacobi integration of Eq.III.115 for that i' is used.

However, if SEPTST > 2.5, a special integration procedure described below is used to re-evaluate that term of the sum.

By algebraic manipulation, each term of Eq.III.115 can be written as the sum of two integrals

$$O_{2_{i,i',o}}^{t,s\ell} = \sum_{i' \neq i} \left[F_{i,i',o}^{t,s\ell} - S_{i,i',o}^{t,s\ell} \right] \tag{III.117}$$

where

$$F_{i,i',o}^{t,s\ell} = \frac{1}{2} \int_{-\infty}^{\infty} dx_i \, \frac{a_i \chi_i}{\beta_i} \cdot \frac{A_{i'} \psi_{i'} + B_{i'} \chi_{i'}}{\beta_i + \sum_{i' \neq i} (A_{i'} \psi_{i'} + B_{i'} \chi_{i'})} \tag{III.118}$$

and

$$S^{t,s\ell}_{i,i',o} = \frac{1}{2}\int_{-\infty}^{\infty} dx_i \frac{a_i\chi_i(\psi_i+a_i\chi_i)\ (A_{i'}\psi_{i'}+B_{i'}\chi_{i'})}{\beta_i\left[\beta_i+\psi_i+a_i\chi_i+\sum_{i'\neq i}(A_{i'}\psi_{i'}+B_{i'}\chi_{i'})\right]} \cdot$$

$$\frac{2\ \beta_i+\psi_i+a_i\chi_i+\sum_{i'\neq i}(A_{i'}\psi_{i'}+B_{i'}\chi_{i'})}{\left[\beta_i+\psi_i+a_i\chi_i\right]\left[\beta_i+\sum_{i'\neq i}(A_{i'}\psi_{i'}+B_{i'}\chi_{i'})\right]} . \qquad \text{(III.119)}$$

$S^{t,s\ell}_{i,i',o}$ is evaluated using the Gauss-Jacobi quadrature as discussed earlier. For $F^{t,s\ell}_{i,i',o}$, an asymptotic algorithm similar to that described in Section C.2 is first tried. That is, we approximate $F^{t,s\ell}_{i,i',o}$ as

$$F^{t,s\ell}_{i,i',o} \approx \frac{1}{2}\int_{-\infty}^{\infty} dx_i \frac{a_i\chi_i\left[A_{i'}\psi_{i'}+B_{i'}\chi_{i'}\right]}{\beta_i^2+\sigma^{s\ell***}_{i,i',o}} \qquad \text{(III.120)}$$

where

$$\sigma^{s\ell***}_{i,i',o} = \frac{\int_{-\infty}^{\infty} dx_i\chi_i\left[A_{i'}\psi_{i'}+B_{i'}\chi_{i'}\right]\left[\beta_{i'}+\sum_{i'\neq i}(A_{i'}\psi_{i'}+B_{i'}\chi_{i'})\right]}{\int_{-\infty}^{\infty} dx_i\chi_i\left[A_{i'}\psi_{i'}+B_{i'}\chi_{i'}\right]} . \qquad \text{(III.121)}$$

Products of triple indices are ignored in Eq.III.121 and Eq.III.120 is evaluated using Eq.III.121 and the various Eqs.III.63-III.68 and Eqs.III.82-III.108 as for the case of the earlier σ* and σ**.

A criterion T4 is then evaluated, namely

$$T4 = \frac{\beta_i^2}{\sigma^{s\ell***}_{i,i',o}} . \qquad \text{(III.122)}$$

If $T4 \geq 0.6$ or if $T \leq -3.0$ the asymptotic expression above is used for $F^{t,s\ell}_{i,i',o}$. However, if not, the criterion T5 is evaluated as

$$T5 = \frac{L_i}{L_{i'}} . \qquad \text{(III.123)}$$

If $SEPTST \leq 3.5$ and $T5 \geq 1.0$, then the code reverts to the use of the original Gauss-Jacobi quadrature of Eq.III.115. However, if not, then $F^{t,s\ell}_{i,i',o}$ is finally approximated by

$$F^{t,\delta\ell}_{i,i',o} \approx \frac{1}{2}\frac{a_i}{\beta_i}\chi\left[\theta_i, \frac{E_{o_{i'}} - E_{o_i}}{\frac{\Gamma_i}{2}}\right] \cdot \int_{-\infty}^{\infty} dx_i \frac{A_{i'}\psi_{i'}+B_{i'}\chi_{i'}}{\beta_i+A_{i'}\psi_{i'}+B_{i'}\chi_{i'}}$$

$$= \frac{1}{2}\frac{a_i}{\beta_i}\chi\left[\theta_i, \frac{E_{o_{i'}} - E_{o_i}}{\frac{\Gamma_i}{2}}\right] \cdot \frac{\Gamma_{i'}}{\Gamma_i} \int_{-\infty}^{\infty} dx_{i'} \frac{\psi_{i'}+a_{i'}\chi_{i'}}{\beta_{i'}+\psi_{i'}+a_{i'}\chi_{i'}}$$

$$= \frac{a_i}{\beta_i}\chi\left[\theta_i, \frac{E_{o_{i'}} - E_{o_i}}{\frac{\Gamma_i}{2}}\right] \cdot \frac{\Gamma_{i'}}{\Gamma_i} J(\beta_{i'},\theta_{i'},a_{i'},a_{i'}). \qquad \text{(III.124)}$$

This procedure is similarly used on all the other overlap integrals having an asymmetric part, that is a part proportional to χ.

IV. CALCULATION OF UNRESOLVED RESONANCE INTEGRALS

A. General Formulation

The algorithms involved in the unresolved resonance integral calculation developed by R. Hwang[25] assume the narrow resonance approximation and account for interference scattering, the effects of accidental overlap with resonances in other spin sequences, and the effects of self-overlap with resonances of the same spin sequence. The single level Breit-Wigner representation is used for the resonance cross sections.

The effective macroscopic capture cross section for material m within an arbitrary energy interval $E_2 - E_1$ can be written as

$$\bar{\Sigma}_c^m(E^*) = N^m \bar{\sigma}_c^m(E^*) = \frac{\frac{1}{E_2 - E_1}\int_{E_1}^{E_2} \frac{N^m \sigma_c^m(E)dE}{\Sigma_t(E)}}{\frac{1}{E_2 - E_1}\int_{E_1}^{E_2} \frac{dE}{\Sigma_t(E)}} \qquad \text{(IV.1)}$$

where E^* is an energy point within the interval $E_2 - E_1$. Eq. IV.1 is equivalent to Eq. III.1. N^m is the atom density of material m, σ_c^m is the microscopic capture cross section for material m, Σ_t is the total macroscopic cross section for the mixture, and as in the case of the resolved resonance integral calculations we assume that the narrow resonance approximation is valid. In order to satisfy the statistical criteria described below we assume no significant attenuation of flux in the energy interval E_2-E_1 and a constant collision density.

σ_c^m and Σ_t correspond to sums over contributing resonances belonging to various spin sequences, that is, resonances having a particular angular momentum and channel spin. If we separate the total cross section in Eq. IV.1 into a resonant part $\Sigma_r(E)$ and a remaining non-resonant part Σ_p, we can rewrite Eq. IV.1 as

$$\bar{\Sigma}_c^m(E^*) = \frac{\frac{1}{E_2 - E_1}\int_{E_1}^{E_2} \frac{N^m \sum_{si} \sum_{i} \sigma_i^{ms}(E)dE}{\sum_{msi} \sum_{i} \Sigma_{r_i}^{ms}(E) + \Sigma_p}}{\frac{1}{E_2 - E_1}\int_{-\infty}^{\infty} \frac{dE}{\sum_{msi} \sum_{i} \Sigma_{r_i}^{ms}(E) + \Sigma_p}} \qquad \text{(IV.2)}$$

In Eq. IV.2, s represents a particular spin sequence and i represents the resonances in that sequence. The sums in the numerator of the upper integral ranges only over those sequences belonging to material m while the other sums are over all materials.

Now the interval $E_2 - E_1$ may be replaced by the average spacing of the resonances of the particular sequence being considered, $\langle D_s \rangle$, times the number of resonances contained within the interval, N_s. Also, on the assumption that a large number of resonances i exist in the interval, we may replace $\frac{1}{N_s} \sum_i$ by an integration over the chi-squared distribution with μ degrees of freedom as indicated in Eq. A.30 of Appendix A. This latter step corresponds to providing a statistical average over the distribution functions of the resonance parameters. Thus, as an example, we may write

$$\lim_{\Delta E \to \infty} \frac{1}{\Delta E} \sum_i f(\Gamma_n^i) = \frac{1}{\langle D \rangle} \int_o^\infty P_\mu(x) f(x\overline{\Gamma_n(E^*)}) dx = \frac{1}{\langle D \rangle} \langle f \rangle_{E^*} \qquad \text{(IV.3)}$$

where x corresponds to the ratio of neutron width at energy E to mean neutron width at E*, $\overline{\Gamma_n(E^*)}$ is the mean neutron width at energy E*, and μ is the number of entrance channels for neutrons of the particular spin sequence under consideration. P_μ is the chi-squared distribution of order μ given in Eq. A.31 of Appendix A. The fission width would be similarly averaged with perhaps a different number of exit channels as appropriate to the data involved. The angular brackets $\langle\ \rangle$ will be used to designate the expectation value due to the statistical integration.

The mean neutron width at E* for neutrons of angular momentum ℓ and total channel spin J is given by

$$\overline{\Gamma_n(E^*)}_{\ell,J} = \overline{\Gamma_n^o(E^*)}_{\ell,J} \sqrt{E^*}\, V_\ell \mu_{\ell,J} \qquad \text{(IV.4)}$$

where $\overline{\Gamma_n^o(E^*)}_{\ell,J}$ is the reduced neutron width at energy E*, V_ℓ is the penetration factor for neutrons of angular momentum ℓ, and $\mu_{\ell,J}$ is the number of entrance channels for neutrons of the ℓ,J sequence.

$$\begin{aligned} V_o &= 1 \\ V_1 &= \frac{n^2}{1 + n^2} \\ V_2 &= \frac{n^4}{9 + 3n^2 + n^4} \\ n &= \frac{R}{\lambda^*} \end{aligned} \qquad \text{(IV.5)}$$

where R is the channel radius and λ^* is the reduced neutron wavelength at energy E*.

Resonances in different spin sequences are assumed to be completely uncorrelated whereas resonances in a given spin sequence are assumed to be distributed according to the Dyson two-level correlation function[25]

$$\Omega(y) = 1 - \{\xi(y)\}^2 + \frac{\partial \xi(y)}{\partial y} \; si(y) \tag{IV.6}$$

where

$$y = \frac{\pi |E_{o_k} - E_{o_{k'}}|}{\langle D \rangle} \tag{IV.7}$$

$$\xi(y) = \frac{\sin|y|}{y} \tag{IV.8}$$

$$si(y) = -\int_y^\infty \frac{\sin t}{t} \, dt \; . \tag{IV.9}$$

Eqs. III.3 and III.4 express the resolved resonance capture and total cross sections in terms of the symmetric and antisymmetric Doppler broadened line shapes ψ and χ. Eq. III.3 is still appropriate for the unresolved region but the low energy limit form of Eq. III.4 must be rewritten for use here as

$$\sigma_{t_i} = \cos 2\delta_{\ell_i} \left[\frac{\sigma_{p_i}}{\cos 2\delta_{\ell_i}} + \sigma_{o_i} \psi_i + \sigma_{o_i} a_i \chi_i \right] \tag{IV.10}$$

where δ_{ℓ_i} is the phase angle for angular momentum ℓ given by

$$\begin{aligned} \delta_o &= m \\ \delta_1 &= m - \arctan m \\ \delta_2 &= m - \arctan \left[\frac{3m}{3 - m^2} \right] \\ m &= \frac{R}{\lambda^*} \; . \end{aligned} \tag{IV.11}$$

R is the effective scattering radius and λ^* is the reduced neutron wavelength at energy E*. ψ_i and χ_i are the usual shorthand notation for $\psi(\theta_i, \chi_i)$ and $\chi(\theta_i, \chi_i)$.

In Eq. IV.10, the interference factor a_i is given by

$$a_i = \frac{1}{2} \tan(2\delta_{\ell_i}) \; . \tag{IV.12}$$

If we express Eq. IV.2 in terms of the ψ and χ functions, perform the statistical average over the distribution functions for the resonance parameters, and factor the resulting equation in a manner typified by Eq. III.23, we may finally write for the expectation value for a given spin sequence

$$\frac{\cos 2\delta_\ell}{\langle D_k \rangle} \left\langle \Gamma_{\gamma_k} J_k^* \right\rangle \simeq \left\{ \frac{1}{\langle D_k \rangle} \left\langle \Gamma_{\gamma_s} J(\beta_k, \theta_k, a_k, 0) \right\rangle - O_{\gamma_k} \right\} \cdot S + \sum_{i \neq k} r_{\gamma_{ki}} \quad . \tag{IV.13}$$

In Eq.IV.13, J is defined in Eqs.III.44-III.48 and β_k is defined as in Eq. III.5 except divided by $\cos 2\delta_\ell$. S represents the first-order correction for the accidental overlap with the uncorrelated resonances in spin sequences $i \neq k$ given by[25]

$$S = 1 - \sum_{i \neq k} \left[\frac{1}{\langle D_i \rangle} \left\langle \Gamma_{t_i} J(\beta_i, \theta_i, a_i, a_i) \right\rangle - O_{t_i} \right] . \tag{IV.14}$$

The $r_{\gamma_{ki}}$ represent the higher order corrections for the accidental overlap effect which, to second order is approximately given by[25]

$$r_{\gamma_{ki}} \simeq \frac{\langle \tau_{\gamma_k} \rangle}{\langle D_k \rangle} \frac{1}{\langle D_i \rangle} \left\langle \Gamma_{t_i} \beta_i \frac{\partial J(\beta_i, \theta_i, 0, 0)}{\partial \beta_i} \right\rangle \tag{IV.15}$$

$$\langle \tau_{\gamma_k} \rangle = \left\langle \frac{\Gamma_{\gamma_k}}{2\beta_k} \int_{-\infty}^{\infty} \frac{\psi^2(\theta_k, x_k)\, dx_k}{\beta_k + \psi(\theta_k, x_k)} \right\rangle . \tag{IV.16}$$

MC^2-2 assumes that $r_{\gamma_{ki}}$ in Eq.IV.13 is negligible.

O_{γ_k} represents the capture self-overlap term for resonances of the same spin sequence k and is approximated by

$$O_{\gamma_k} \simeq \frac{1}{\langle D_k \rangle} \left\langle \frac{\Gamma_{\gamma_k}}{2} \int_{-\infty}^{\infty} \Omega(\delta) \frac{d\delta}{\langle D_k \rangle} \cdot \int_{-\infty}^{\infty} \frac{\psi_k}{\beta_k + \psi_k} \frac{A_{k'} \psi_{k'} dx_k}{\beta_k + \psi_k + {}_{k'}\psi_{k'}} \right\rangle_{k \text{ and } k'} . \tag{IV.17}$$

In Eq.IV.17 the resonances k and k' all belong to the same spin sequence k. $\Omega(\delta)$ is the probability of finding a resonance k' at a distance $\delta = E_{o_k} - E_{o_{k'}}$ from a given resonance k as given in Eq.IV.6, ψ_k is a shorthand notation referring to $\psi(\theta_k, x_k)$, and $A_{k'}$ is defined in Eq.III.5. Note that the contribution from the asymmetric line shape function χ is ignored for the self-overlap calculation. O_{t_i} in Eq.IV.14 is given by Eq.IV.17 where Γ_{t_i} replaces Γ_{γ_k}.

In deriving Eq.IV.13, it has been explicitly assumed that products of more than two ψ or χ functions can be neglected. This is the so-called "nearest neighbor" approximation.[28] As a simple example, consider

$$\frac{\sigma_c^1}{\sigma_r^1+\sigma_r^2+\sigma_r^3+\sigma_p} = \frac{\sigma_c^2}{\sigma_r^1+\sigma_p} - \frac{\sigma_c^1}{\sigma_r^1+\sigma_p}\,\frac{\sigma_c^2+\sigma_c^3}{\sigma_r^1+\sigma_r^2+\sigma_r^3+\sigma_p}$$

$$= \frac{\sigma_c^1}{\sigma_r^1+\sigma_p} - \frac{\sigma_c^1}{\sigma_r^1+\sigma_p}\left\{\frac{\sigma_r^2}{\sigma_r^2+\sigma_p} - \frac{\sigma_r^2}{\sigma_r^2+\sigma_p}\,\frac{\sigma_r^1+\sigma_r^3}{\sigma_r^1+\sigma_r^2+\sigma_r^3+\sigma_p}\right.$$

$$\left. + \frac{\sigma_r^3}{\sigma_r^3+\sigma_p} - \frac{\sigma_r^3}{\sigma_r^3+\sigma_p}\,\frac{\sigma_r^2+\sigma_r^3}{\sigma_r^1+\sigma_r^2+\sigma_r^3+\sigma_p}\right\}$$

$$\approx \frac{\sigma_c^1}{\sigma_r^1+\sigma_p}\left\{1 - \frac{\sigma_r^2}{\sigma_r^2+\sigma_p} - \frac{\sigma_r^3}{\sigma_r^3+\sigma_p}\right\} \qquad \text{(IV.18)}$$

We shall also later use the fact that Eq.IV.18 can be approximated by

$$\frac{\sigma_c^1}{\sigma_r^1+\sigma_r^2+\sigma_r^3+\sigma_p} \approx \frac{\sigma_c^1}{\sigma_r^1+\sigma_p}\left\{1 - \frac{\sigma_r^2}{\sigma_r^2+\sigma_p}\right\}\left\{1 - \frac{\sigma_r^3}{\sigma_r^3+\sigma_p}\right\} \qquad \text{(IV.19)}$$

where again we have neglected triple products. Eq.IV.19 makes use of the general first order approximation

$$1 - \sum_i B_i \approx \prod_i (1 - B_i) \quad . \qquad \text{(IV.20)}$$

The expression corresponding to Eq.IV.13 for fission simply requires replacing Γ_{γ_k} with Γ_{f_k} so that O_{γ_k}, $r_{\gamma_{ki}}$, and $\langle\tau_{\gamma_k}\rangle$ become respectively O_{f_k}, $r_{f_{ki}}$, and $\langle\tau_{f_{k'}}\rangle$. In the case of the total reaction, Γ_{t_k} replaces Γ_{γ_k} and $J(\beta_k,\theta_k,a_k,a_k)$ is used in Eq.IV.13. Also, in this case the factor $\cos 2\delta_\ell$ does not appear in Eq.IV.13.

Since the J integrals and other related integrals can be readily evaluated as described in Section B of Chapter III with the statistical averaging accomplished as specified in Section V Appendix A, the main computational effort is related to the evaluation of the self-overlap integrals.

As in the case of the resolved resonances, Eq.IV.13 is evaluated for a homogeneous mixture, and for heterogeneous slab geometries or cylindrical geometries with the value used for Σ_p and hence for β determined as specified in Eqs.III.16-III.20.

B. Evaluation of the Self-Overlap Term

In order to evaluate Eq.IV.17, we note that

$$\int_{-\infty}^{\infty} \frac{\psi_k}{\beta_k + \psi_k} \frac{A_{k'}\psi_{k'}}{\beta_k + \psi_k + A_{k'}\psi_{k'}} dx_k =$$

$$\int_{-\infty}^{\infty} \frac{\psi_k}{\beta_k + \psi_k} \left\{ \frac{\psi_{k'}}{\beta_{k'} + \psi_{k'}} - \frac{A_k \psi_k \psi_{k'}}{(\beta_{k'} + \psi_{k'})^2} + \ldots \right\} \qquad \text{(IV.21)}$$

provided the resulting integrals are uniformly convergent. In Eq.IV.21, $A_k = 1/A_{k'}$. Substituting Eq.IV.21 into Eq.IV.17, Hwang has shown[25] that

$$O_{\gamma_k} = K_1 - K_2 + \ldots \qquad \text{(IV.22)}$$

where $K_1 >> K_2$ if the self-shielding effect is relatively weak.

$$K_1 = \frac{1}{\langle D_k \rangle^2} \left\langle \Gamma_{\gamma_k} J_k \right\rangle \left\langle \Gamma_{k'} J_{k'} \right\rangle - L_1 \qquad \text{(IV.23)}$$

$$L_1 = \frac{1}{\langle D_k \rangle} \int_{-\infty}^{\infty} W\left(\frac{\delta}{\langle D_k \rangle}\right) \frac{d\delta}{\langle D_k \rangle}$$

$$\cdot \int_{-\infty}^{\infty} \left\langle \frac{\Gamma_{\gamma_k}}{2} \frac{\psi_k}{\beta_k + \psi_k} \right\rangle_k \left\langle \frac{\psi_{k'}}{\beta_{k'} + \psi_{k'}} \right\rangle_{k'} dx_k \qquad \text{(IV.24)}$$

$$K_2 = -r_{\gamma_{kk'}} - L_2 \qquad \text{(IV.25)}$$

where $r_{\gamma_{kk'}}$ is given by Eqs.IV.15 and IV.16 and

$$L_2 = -\frac{1}{\langle D_k \rangle} \int_{-\infty}^{\infty} W\left(\frac{\delta}{\langle D_k \rangle}\right) \frac{d\delta}{\langle D_k \rangle} \int_{-\infty}^{\infty} \left\langle \frac{\Gamma_{\gamma_k}}{2} \frac{\psi_k^2}{\beta_k(\beta_k + \psi_k)} \right\rangle_k$$

$$\cdot \left\langle \beta_{k'} \frac{\partial}{\partial \beta_{k'}} \frac{\psi_{k'}}{\beta_{k'} + \psi_{k'}} \right\rangle_{k'} dx_k \cdot \qquad \text{(IV.26)}$$

In Eq.IV.24 and IV.25

$$W\left(\frac{\delta}{\langle D_k\rangle}\right) = 1 - \Omega\left(\frac{\delta}{\langle D_k\rangle}\right) \tag{IV.27}$$

and in Eq.IV.26

$$-\frac{\partial}{\partial\beta_k}\left(\frac{\psi_k}{\beta_k+\psi_k}\right) = \frac{\psi_k}{(\beta_k+\psi_k)^2} \tag{IV.28}$$

The computational effort now is centered on the evaluation of the term L_1 since L_2 can easily be obtained once L_1 is known.

1. Evaluation of L_1

Using the Fourier transform technique, Hwang has shown that Eq.IV.24 can be written in the form

$$L_1 = \frac{1}{2\langle D_k\rangle^2}\int_{-\infty}^{\infty}\sqrt{2\pi}\,\omega(\xi)\left\langle\Gamma_{\gamma_k}P_k\left(\frac{\Gamma_{t_k}}{2}\xi\right)\right\rangle_k \cdot\left\langle\frac{\Gamma_{t_{k'}}}{2}P_{k'}\left(\frac{\Gamma_{t_{k'}}}{2}\xi\right)\right\rangle_{k'}d\xi \tag{IV.29}$$

where P_k is the Fourier transform

$$P_k(\xi) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{\psi_k\exp(i\xi x_k)}{\beta_k+\psi_k}dx_k = F\left\{\frac{\psi_k}{\beta_k+\psi_k}\right\} \tag{IV.30}$$

and $\omega(\xi)$, the Fourier transform of the Dyson function, is given

$$\omega(\xi) = \frac{\langle D_k\rangle}{\sqrt{2\pi}}\left\{1-\left|\frac{\langle D_k\rangle\xi}{\pi}\right|+\left|\frac{\langle D_k\rangle\xi}{2\pi}\right|\ell n\left[1+\left|\frac{\langle D_k\rangle\xi}{\pi}\right|\right]\right\}; \quad \left|\frac{\langle D_k\rangle\xi}{2\pi}\right|\le 1$$

$$= \frac{\langle D_k\rangle}{\sqrt{2\pi}}\left\{-1+\left|\frac{\langle D_k\rangle\xi}{2\pi}\right|\ell n\left[\frac{|\langle D_k\rangle\xi/\pi|+1}{|\langle D_k\rangle\xi/\pi|-1}\right]\right\}; \quad \left|\frac{\langle D_k\rangle\xi}{2\pi}\right| > 1 \tag{IV.31}$$

As usual, in Eq.IV.29 the quantities inside the angular brackets are the statistically averaged values over the appropriate chi-squared distribution functions of the resonance parameters, and the resonances k and k' belong to the same spin sequence.

Now we make a change of variable to convert Eq.IV.29 into a form amenable to Gauss-Hermite quadrature. If we let

$$\eta = \alpha\xi$$

$$\alpha = \sqrt{\frac{\langle D_k \rangle^2}{\pi} + \frac{\Delta^2}{2} + \gamma^2} \qquad \text{(IV.32)}$$

$$\gamma = \left\langle \Gamma_{t_k} \sqrt{\frac{\beta_k + 1}{\beta_k}} \right\rangle$$

and multiplying the integral in Eq.IV.29 by $\exp(-\eta^2) \cdot \exp(\eta^2)$, Eq.IV.29 can be converted into the equivalent form

$$L_1 = \frac{1}{2\langle D_k \rangle^2} \frac{1}{\alpha} \int_{-\infty}^{\infty} e^{-\eta^2} \left\{ \sqrt{2\pi}\, \omega\left(\frac{\eta}{\alpha}\right) \left\langle \Gamma_{\gamma_k} e^{\frac{\Delta^2\eta^2}{4\alpha^2}} P_k \left(\frac{\Gamma_{t_k}\eta}{2\alpha}\right) \right\rangle_k \right.$$

$$\left. \cdot \left\langle \frac{\Gamma_{t_{k'}}}{2} e^{\frac{\Delta^2\eta^2}{4\alpha^2}} P_{k'} \left(\frac{\Gamma_{t_{k'}}\eta}{2\alpha}\right) \right\rangle_{k'} e^{\left[\frac{\langle D_k \rangle^2}{\pi^2\alpha^2} + \frac{\gamma^2}{\alpha^2}\right]\eta^2} \right\} d\eta \,. \qquad \text{(IV.33)}$$

Eq.IV.33 is of the form

$$\int_{-\infty}^{\infty} e^{-y^2} f(y)dy = \sum_{i=1}^{N} a_i f(y_i) + R_N \qquad \text{(IV.34)}$$

where a_i and y_i are the weights and zeros of the Hermite polynomial and Eq.IV.34 corresponds to the usual Gauss-Hermite quadrature with the remainder term R_N. Since P_k and ω are each symmetric, only a sum over the positive zeros y_i is required to evaluate Eq.IV.33. The code uses N = 10 for the quadrature. Specifically, with N = 10 we assume

$$L_1 = \frac{1}{2\langle D_k \rangle^2} \frac{2}{\alpha} \sum_{i=1}^{N/2} a_i \sqrt{2\pi}\, \omega\left(\frac{\eta_i}{\alpha}\right) \left\langle \Gamma_{\gamma_k} e^{\frac{\Gamma^2\eta_i^2}{4\alpha^2}} P_k \left(\frac{\Gamma_{t_k}\eta_i}{2\alpha}\right) \right\rangle_k$$

$$\cdot\left\langle \frac{\Gamma_{t_k'}}{2} \; e^{\frac{\Delta^2\eta_i^2}{4\alpha^2}} \; P_{k'}\left(\frac{\Gamma_{t_k'}\eta_i}{2\alpha}\right)\right\rangle_{k'} e^{\left[\frac{\langle D_k\rangle^2}{\pi^2\alpha^2}+\frac{\gamma^2}{\alpha^2}\right]\eta_i^2} \qquad \text{(IV.35)}$$

The evaluation of Eq.IV.35 depends upon the availability of the Fourier transforms $P_k(\Gamma_{t_k}\xi/2)$. Two algorithms are used depending upon the size of β_k relative to $\psi(\theta_k,0)$. The large β approximation or asymptotic algorithms provide significant computational economy as compared with the non-asymptotic algorithms. Since β_k is usually large compared to $\psi(\theta_k,0)$ for many of the unresolved resonances, the large β approximation is frequently invoked for realistic problems with subsequent savings in execution time.

a. Asymptotic Algorithms for L_1

If $(\beta_k + \psi(\theta_k,0))/\psi(\theta_k,0) \geq 2.5$, P_k may be approximated by[25]

$$P_k\left(\frac{\Gamma_{t_k}\xi}{2}\right) \simeq \sqrt{\frac{\pi}{2}}\exp\left[-\frac{\Delta^2}{4}\xi^2 - \frac{\Gamma_{t_k}}{2}|\xi|\right]\cdot Q_k(\xi)/(\beta_k+\rho) + \ldots \qquad \text{(IV.36)}$$

where Δ is the Doppler line width as defined below Eq.III.4 with E_{o_i} replaced by E*.

$$Q_k(\xi) = 1 + \frac{\rho - U}{\beta_k + \rho} \qquad \text{(IV.37)}$$

$$U_k = \frac{\theta_k\sqrt{\pi}}{2\sqrt{2}}\left[\exp\left(\frac{\Delta|\xi|}{2\sqrt{2}}+\frac{\theta_k}{\sqrt{2}}\right)^2 \text{Erfc}\left(\frac{\Delta|\xi|}{2\sqrt{2}}+\frac{\theta_k}{\sqrt{2}}\right)\right.$$

$$\left. + \exp\left(\frac{\Delta^2\xi^2}{8}\right) \text{Erf}\left(\frac{\Delta|\xi|}{2\sqrt{2}}\right)\right] \qquad \text{(IV.38)}$$

$$\rho = \frac{1}{2}\psi(\sqrt{2}\theta_k,0) \qquad \text{(IV.39)}$$

and Erfc and Erf are respectively the complementary error function and the error function which are evaluated as specified for Eq.A.15 of Appendix A.

The asymptotic evaluation of L_1 is then completed with the variable change of Eq.IV.32 and substitution of Eq.IV.36 into Eq.IV.35.

b. Non-Asymptotic Algorithms for L_1

When $(\beta_k + \psi(\theta_k,0))/\psi(\theta_k,0) < 2.5$, the more elaborate algorithms described below must be used to obtain the P_k for use in the solution of Eq.IV.35.

$P_k\left(\frac{\Gamma_{t_k}\xi}{2}\right)$ is the unique solution of the integral equation

$$\beta_k P_k\left(\frac{\Gamma_{t_k}\xi}{2}\right) + \frac{1}{4}\Gamma_{t_k}\int_{-\infty}^{\infty} e^{-\frac{\Delta^2}{4}(\xi-t)^2 - \frac{\Gamma_{t_k}}{2}|\xi-t|} P_k\left(\frac{\Gamma_{t_k}t}{2}\right)dt = \sqrt{\frac{\pi}{2}}\, e^{-\frac{\Delta^2\xi^2}{4} - \frac{\Gamma_{t_k}|\xi|}{2}} \quad . \tag{IV.40}$$

Making the substitutions $y = \alpha\xi$ and $x = \alpha t$ and multiplying the integral by $\exp(-x^2) \cdot \exp(x^2)$, Eq.IV.40 may be cast into the form suitable for Gauss-Hermite quadrature

$$e^{\frac{\Delta^2 y^2}{4\alpha^2}}\beta_k P_k\left(\frac{\Gamma_{t_k}y}{2\alpha}\right) + \frac{1}{4}\frac{\Gamma_{t_k}}{\alpha}\int_{-\infty}^{\infty} e^{-x^2}\cdot e^{\frac{\Delta^2 yx}{2\,\alpha\alpha} - \frac{\Delta^2}{4}\frac{x^2}{\alpha^2} - \frac{\Gamma_{t_k}}{2}\left|\frac{y-x}{\alpha}\right| + x^2} P_k\left(\frac{\Gamma_{t_k}x}{2\alpha}\right)dx = \sqrt{\frac{\pi}{2}}\, e^{-\frac{\Gamma_{t_k}}{2}\left|\frac{y}{\alpha}\right|} \quad . \tag{IV.41}$$

The integral in Eq.IV.41 can again be written as a ten point Gauss-Hermite quadrature, so that at each mesh point y_i we have

$$e^{\frac{\Delta^2 y_i^2}{4\alpha^2}}\beta_k P_k\left(\frac{\Gamma_{t_k}y_i}{2\alpha}\right) + \frac{1}{4}\frac{\Gamma_{t_k}}{\alpha}\sum_{i=1}^{10} a_j e^{\frac{\Delta^2}{2}\frac{y_i}{\alpha}\frac{x_j}{\alpha} - \frac{\Delta^2}{4}\frac{x_j^2}{\alpha^2} - \frac{\Gamma_{t_k}}{2}\left|\frac{y_i-x_j}{\alpha}\right| + x_j^2} P_k\left(\frac{\Gamma_{t_k}x_j}{2\alpha}\right) = \sqrt{\frac{\pi}{2}}\, e^{-\frac{\Gamma_{t_k}}{2}\left|\frac{y_i}{\alpha}\right|} \quad . \tag{IV.42}$$

Equation IV.42 can be looked at as a system of 10 equations in the ten unknowns

$$P_k\left(\frac{\Gamma_{t_k}y_i}{2\alpha}\right) .$$

Thus we may write the matrix equation

$$A\,P = B \tag{IV.43}$$

so that the desired P may be obtained by inversion of the A matrix

$$P = A^{-1}B. \tag{IV.44}$$

Eqs.IV.42 are normalized by dividing each row of the A matrix by the respective diagonal element, namely

$$N_i^o = e^{\frac{\Delta^2 y_i^2}{4\alpha^2}} \left\{ \beta_k + \frac{\Gamma_{t_k}}{4\alpha} a_i e^{y_i^2} \right\} . \tag{IV.45}$$

Therefore

$$B_i = \frac{\sqrt{\frac{\pi}{2}}\, e^{-\frac{\Gamma_{t_k}}{2}\left|\frac{y_i}{\alpha}\right|}}{N_i^o} \tag{IV.46}$$

$$A_{ii} = 1 \tag{IV.47}$$

$$A_{ij} = \left\{ \frac{\Gamma_{t_k} a_j}{4\alpha} e^{\frac{\Delta^2 y_i x_j}{2\alpha^2} - \frac{\Gamma_{t_k}|y_i - x_j|}{2\alpha}} \cdot e^{\frac{\Delta^2 x_j^2}{4\alpha^2}} e^{\left[\frac{\langle D_k \rangle^2}{\pi^2\alpha^2} + \frac{\gamma^2}{\alpha^2}\right] x_j^2} \right\} \Big/ N_i^o . \tag{IV.48}$$

In Eq.IV.48 we have made use of the identity

$$e^{x_j^2} = e^{\frac{\Delta^2 x_j^2}{2\alpha^2} + \frac{\langle D_k \rangle^2 x_j^2}{\pi^2\alpha^2} + \frac{\gamma^2 x_j^2}{\alpha^2}} \tag{IV.49}$$

with α and γ defined as before in Eqs.IV.32.

The inversion of the 10 x 10 matrix A can be considerably simplified and the execution time thereby significantly reduced by partitioning A into four sub-matrixes and recognizing the fact that $A_{ij} = A_{ji}$ as is obvious from Eq.IV.48. If we let D represent the inverse of A, we can write

$$AA^{-1} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix} = I \tag{IV.50}$$

where I is the 10 x 10 identity matrix and each of the submatrices is 5 x 5.

By algebraic manipulation of the equations represented by Eq.IV.50, we can easily show that

$$\begin{aligned} D_{11} &= (A_{11} - A_{12}A_{11}^{-1}A_{12})^{-1} \\ D_{12} &= -A_{11}^{-1}A_{12}D_{11} \\ D_{22} &= D_{11} \\ D_{21} &= D_{12} \end{aligned} \tag{IV.51}$$

where we have made use of the fact that $A_{11} = A_{22}$ and $A_{12} = A_{21}$.

Thus the inversion of the 10 x 10 A matrix can be accomplished by the much faster inversion of two 5 x 5 matrices as shown in Eqs.IV.51.

Finally, taking advantage of the fact that P_k is symmetric, we need be concerned only with the positive Gauss-Hermite quadrature points so that we may obtain the upper half of the P vector from $(D_{11}\ D_{12})B$.

The non-asymptotic evaluation of L_1 is then completed using the P_k obtained as above in Eq.IV.35.

2. Evaluation of L_2

Using the same technique as was used to convert Eq.IV.24 into the form of Eq.IV.29 for L_1, Hwang has converted Eq.IV.26 into the form

$$L_2 = -\frac{1}{2\langle D_k\rangle^2}\int_{-\infty}^{\infty}\sqrt{2\pi}\,\omega(\xi)\left\langle \Gamma_{\gamma_k}\left\{\sqrt{\frac{\pi}{2}}\,\frac{e^{-\frac{\Delta^2\xi^2}{4}-\frac{\Gamma_{t_k}|\xi|}{2}}}{\beta_k} - P_k\left(\frac{\Gamma_{t_k}\xi}{2}\right)\right\}\right\rangle_k$$

$$\cdot\left\langle \frac{\Gamma_{t_{k'}}}{2}\beta_{k'},\ \frac{\partial}{\partial\beta_{k'}}P_{k'},\ \left(\frac{\Gamma_{t_{k'}}\xi}{2}\right)\right\rangle_{k'} d\xi \ . \tag{IV.52}$$

Making the variable changes indicated in Eqs.IV.32 and multiplying the integral by $\exp(-\eta^2)\exp(\eta^2)$ as for the case of L_1, Eq.IV.52 can be converted to the equivalent form

$$L_2 = \frac{1}{2\,D_k^{\,2}}\,\frac{1}{\alpha}\int_{-\infty}^{\infty} e^{-\eta^2}\left\{\sqrt{2\pi}\;\omega\left(\frac{\eta}{\alpha}\right)\;\Gamma_{\gamma_k}\left[\sqrt{\frac{\pi}{2}}\,\frac{e^{-\frac{\Gamma_{t_k}|\eta|}{2\alpha}}}{\beta_k} - e^{\frac{\Delta^2\eta^2}{4\alpha^2}}\,P_k\left(\frac{\Gamma_{t_k}\eta}{2\alpha}\right)\right]_k\right.$$

$$\left.\cdot\left\langle\frac{\Gamma_{t_{k'}}}{2}\,e^{\frac{\Delta^2\eta^2}{4\alpha^2}}\,R_{k'}\left(\frac{\Gamma_{t_{k'}}\eta}{2\alpha}\right)\right\rangle_{k'} e^{\left[\frac{\langle D_k\rangle^2}{\pi^2\alpha^2}+\frac{\gamma^2}{\alpha^2}\right]}\right\}d\eta \qquad \text{(IV.53)}$$

where

$$R_k = -\beta_k\,\frac{\partial}{\partial\beta_k}\;P_k\left(\frac{\Gamma_{t_k}\xi}{2}\right)\;. \qquad \text{(IV.54)}$$

Eq.IV.53 as before can be evaluated using Gauss-Hermite quadrature. Note that after obtaining L_1 as described earlier, the only new quantity needed to obtain L_2 is R_k.

As for L_1, two algorithms are used to obtain R_k depending upon the size of β_k relative to $\psi(\theta_k,0)$.

a. Asymptotic Algorithms for L_2

As for L_1, a fast, large β approximation is used to obtain R_k if $(\beta_k + \psi(\theta_k,0))/\psi(\theta_k,0) \geq 2.5$. Specifically,

$$R_k\left(\frac{\Gamma_{t_k}\xi}{2}\right) \simeq \sqrt{\frac{\pi}{2}}\,\beta_k \exp\left[-\frac{\Delta^2\xi^2}{4} - \frac{\Gamma_{t_k}|\xi|}{2}\right]\cdot\frac{1 + 2[\rho - U_k(\xi)]/(\beta_k+\rho)}{(\beta_k+\rho)^2} \qquad \text{(IV.55)}$$

where U_k and ρ are given in Eqs.IV.38 and IV.39.

b. Non-Asymptotic Algorithms for L_2

When $(\beta_k + \psi(\theta_k,0))/\psi(\theta_k,0) < 2.5$, R_k is obtained in a manner similar to that used for obtaining P_k in the non-asymptotic case.

In order to obtain $R_{k'}$, we differentiate Eq.IV.41 with respect to β_k to obtain a new matrix equation similar to Eq.IV.43, namely

$$AR = V \qquad \text{(IV.56)}$$

where A is the matrix defined in Eqs.IV.47 and IV.48 and

$$V_i = \frac{\beta_k P_k\left(\frac{\Gamma_{t_k} y_i}{2\alpha}\right) e^{\frac{\Delta^2 y_i^2}{4\alpha^2}}}{N_i^o} \qquad \text{(IV.57)}$$

with N_i^o the previously defined normalization factor given in Eq.IV.45.

Thus we have

$$R = A^{-1}V . \tag{IV.58}$$

Since A^{-1} has already been obtained for use in computing L_1, L_2 is also available with little additional computational effort.

C. Evaluation of Unresolved Resonance Cross Sections

As stated previously, MC^2-2 neglects the higher order corrections for the accidental overlap so that, for example Eq.IV.13 becomes

$$\frac{1}{\langle D_k \rangle} \left\langle \Gamma_{\gamma_k} J_k^* \right\rangle \simeq \frac{1}{\cos 2\delta_\ell} \left\{ \frac{1}{\langle D_k \rangle} \left\langle \Gamma_{\gamma_k} J(\beta_k, \theta_k, a_k, 0) \right\rangle - O_{\gamma_k} \right\} \cdot S \tag{IV.59}$$

where S is defined by Eq.IV.14 and the evaluation of the overlap term O_{γ_k} has been discussed in Section B above.

If we define the flux correction factor f as

$$f = 1 - \sum_k \left[\frac{1}{\langle D_k \rangle} \left\langle \Gamma_{t_k} J(\beta_k, \theta_k, a_k, a_k) \right\rangle - O_{t_k} \right] \tag{IV.60}$$

where f is just Eq.IV.14 except that the sum extends over all spin sequences, we may write the effective unresolved resonance capture cross section for a given spin sequence k as

$$\bar{\sigma}_{c_k} = \frac{\sigma_p \left\langle \Gamma_{\gamma_k} J_k^* \right\rangle}{\langle D_k \rangle f} . \tag{IV.61}$$

If we accept the approximation given in Eq.IV.20, $\bar{\sigma}_{c_k}$ depends to first order only on the resonances of sequence k since all other terms cancel in the ratio S/f. Thus

$$S \simeq \prod_{i \neq k} \left\{ 1 - \left[\frac{1}{\langle D_i \rangle} \left\langle \Gamma_{t_i} J(\beta_i, \theta_i, a_i, a_i) \right\rangle - O_{t_i} \right] \right\} \tag{IV.62}$$

and

$$f \simeq \prod_{k} \left\{ 1 - \left[\frac{1}{\langle D_k \rangle} \left\langle \Gamma_{t_i} J(\beta_i, \theta_i, a_i, a_i) \right\rangle - O_{t_i} \right] \right\} \tag{IV.63}$$

so that

$$\bar{\sigma}_{c_k} \approx \frac{\sigma_P \left\{ \frac{1}{\langle D_k \rangle} \left\langle \Gamma_{\gamma_k} J(\beta_k, \theta_k, a_k, 0) \right\rangle \div 0_{\gamma_k} \right\}}{\cos 2\delta_\ell \left\{ 1 - \left[\frac{1}{\langle D_k \rangle} \left\langle \Gamma_{t_k} J(\beta_k, \theta_k, a_k, a_k) \right\rangle - 0_{t_k} \right] \right\}} \qquad \text{(IV.64)}$$

with similar expressions for the fission and total cross sections where Γ_{γ_k} is replaced by Γ_{f_k} and Γ_{t_k} respectively,

The unresolved cross sections at each library specified E* energy are finally obtained by summing the partial contributions such as given by Eq. IV.64 over all spin sequences. Thus the unresolved cross section for process x (capture, fission or total), material m at energy point E* is given by

$$\bar{\sigma}_x^m(E^*) = \sum_{k \in m} \bar{\sigma}_{x_k}(E^*) \qquad \text{(IV.65)}$$

where the sum ranges over all sequences belonging to material m.

D. Unresolved Resonance Integrals and Resolved-Unresolved Resonance Interaction

Since the E* points for which the average unresolved resonance parameters are supplied in the library vary from isotope to isotope of each material, the code generates a fixed energy grid onto which the resonance integrals as given by Eq.IV.59 are linearly interpolated. The user may specify the energy grid, or the code will generate the grid using the following algorithm.

The first grid point corresponds to the energy of the top of the highest energy broad group. For points 2 through 25, the successive mesh point energies are in the ratio exp(-0.25); for points 26 through 125 in the ratio exp(-0.05); for points 126 through 149 in the ratio exp(-0.25); and finally mesh point 150 corresponds to EMIN, the energy at the top of the thermal group. If EMIN is encountered before mesh point 150, the grid terminates with point EMIN and fewer than 150 points are in the fixed energy grid. Finally, the fixed grid is truncated so that only those points remain which fall within the unresolved E* points of any of the isotopes in the problem under investigation.

If there is more than one E* point between any of the fixed energy grid points, the unresolved resonance integrals are averaged over the several E* points so that there is a single average resonance integral at a single average energy E* between any two fixed energy grid points. These average resonance integrals as well as the flux correction factors f are then linearly interpolated onto the fixed grid.

Figure 5 schematically represents the energy structure if we denote the fixed energy grid points by ESR_i with corresponding midpoint energies E_i.

In the case where resolved and unresolved resonances are present in the same energy region, the code accounts for interaction effects in the following way.

If resolved resonances j have energies lying with energies E_i and E_{i-1} in Fig 5, then the unresolved resonance integral at mesh point ESF_i is modified to

$$\frac{1}{\langle D_k \rangle} \left\langle \Gamma_{\gamma_k} J^*_k \right\rangle \left\{ 1 - \frac{1}{E_i - E_{i-1}} \sum_j J^{*\delta\ell}_{t_i} \right\} \qquad \text{(IV.66)}$$

where the sum in Eq.IV.66 includes all resolved resonances in the energy range $E_i - E_{i-1}$ and $J^{*\delta\ell}_{t_i}$ is given by Eq.III.24. If the resolved resonances are multilevel resonances, the $J^{*\delta\ell}_{t_i}$ is replaced by the appropriate multilevel expression given by Eq.III.33. Similar corrections are made to the unresolved fission and total resonance integrals.

The resolved resonance integrals for resonances i in the energy range $E_i - E_{i-1}$ are similarly modified to

$$\frac{J^{*\delta\ell}_{x_i}}{E_{o_i}} \quad f \qquad \text{(IV.67)}$$

where f is given by Eq.IV.63 and the value corresponding to grid point ESF_i, $J^{*\delta\ell}_{x_i}$ is given by Eq.III.23, and E_{o_i} is the energy of resolved resonance i. Corresponding expressions for multilevel resolved resonance integrals are used where appropriate.

For resolved resonances falling within the end points and first corresponding midpoint energies, such as the range $ESF_1 - E_1$ for example, the f is the value corresponding to the last grid point.

E. Ultra-Fine-Group Unresolved Resonance Cross Sections

The ultra-fine-group spectrum calculation described in Chapter II and the hyper-fine-group RABANL calculation described in Chapter V make use of group averaged unresolved resonance cross sections. These cross sections are derived by assuming a constant weighting function in the ultra-fine-group so that

$$\sigma^g_{x_m} = \frac{1}{E_{g-1} - E_g} \int_{E_g}^{E_{g-1}} \bar{\sigma}^m_x(E)\,dE \qquad \text{(IV.68)}$$

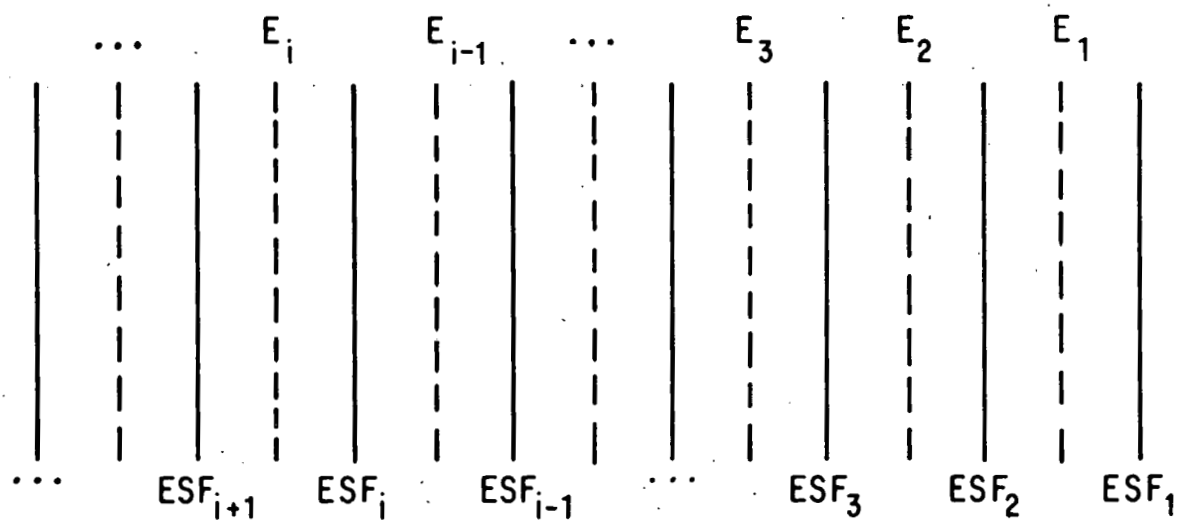

Fig. 5. Unresolved Resonance Energy Grid.

and $\bar{\sigma}_x^m(E)$ is defined by Eq.IV.65. Future releases of the ENDF/B data files will provide information to specify the functional form of $\bar{\sigma}_x^m(E)$ versus E. Since such information is not available with ENDF/B-IV, the code MC^2-2 assumes that $\ell n\ \bar{\sigma}_x^m(E)$ is linear in ℓn E,

$$\bar{\sigma}_x^m(E) = \left(\frac{E}{E_n^*}\right)^{A_n} \bar{\sigma}_x^m(E_n^*)$$

$$A_n \equiv \frac{\ell n\left(\frac{\bar{\sigma}_x^m(E_{n+1}^*)}{\bar{\sigma}_x^m(E_n^*)}\right)}{\ell n\left(\frac{E_{n+1}^*}{E_n^*}\right)} \qquad \text{(IV.69)}$$

The averaging of Eq.IV.68 using the ℓn - ℓn interpolation of Eq.IV.69 is performed analytically in the same manner as used in the MC^2 code.[10]

V. RABANL, HYPER-FINE GROUP INTEGRAL TRANSPORT THEORY NEUTRON SLOWING DOWN

A. Introduction

The RABANL algorithms provide rigorous resolved resonance cross sections and are intended for use in the lower energy ranges for which the narrow resonance approximation of the MC^2-2 module CSC006 is not valid. The methods used in RABANL are based on the earlier work of Kier and Robba in the RABBLE code[5] and the improvements afforded for slab geometry by Olson in the RABID code[6]. The present coding represents an improvement over these earlier codes with regard to accuracy and numerical stability, and also provides a fully variably dimensioned and CCCC compatible package which can be used in a standalone mode, (as with RABBLE or RABID), or in conjunction with a full MC^2-2 execution. In the latter case, elastic scattering sources as well as inelastic, (n,2n), and fission sources are supplied by the ultra-fine-group MC^2-2 calculation. In either mode of operation, RABANL uses the standard MC^2-2 library as derived from ENDF/B data. Thus, e.g., resonance parameters are library supplied as opposed to being provided by the code user as is the case for the earlier codes. The user may also optionally include unresolved resonance cross sections derived from the MC^2-2 module CSC005 in the RABANL calculation as described below.

RABANL may be used for homogeneous one region calculations or for multi-region cylindrical or slab heterogeneous geometries. In the latter cases, the spatial flux distribution is obtained using integral transport theory methods involving calculation of cylindrical or slab collision probabilities.

Section B discusses the algorithms used in computing the elastic slowing down sources. Section C discusses the calculation of the collision rates and fluxes for both homogeneous one region and for multi-region problems. The algorithms used for the calculation of the cross sections are presented in Section D. Finally, in Section E, the calculation of the edited broad group fluxes and cross sections is described.

B. Calculation of Elastic Slowing-Down Sources

In order to accurately calculate the neutron slowing down in the presence of rapidly varying resonance cross sections, the hyper-fine-group (hfg) width used in the calculation must be extremely narrow. By the same token the hfg width should be small compared with the maximum lethargy gained per collision with the heaviest of the nuclides in the mixture so that the assumption of only one collision per group is valid.

The code determines the hfg width relative to the resolved resonance Doppler width Δ

where

$$\Delta = \left[\frac{4kTE}{A}\right]^{\frac{1}{2}} \qquad (V.1)$$

for temperature T, energy E, mass A, and with the Boltzmann constant k equal to 8.61708×10^{-5} eV/degree Kelvin. In particular

$$\Delta u_J^{hfg} = \frac{\Delta}{NE_J} \tag{V.2}$$

for the hfg width appropriate to broad group J where E_J is the upper energy of broad group J, N is specified by the user on card type 14 of data set A.MCC2 with a default value of 4, and Δ is obtained from Eq.V.1 using T = 293 degrees Kelvin, E = E_J, and A = 250. The hfg width is generally broad group dependent. The user may however specify that a fixed hfg width be used for the entire problem. In that case, E_J corresponds to the upper energy of the highest broad group in the problem.

In any case, the code requires that Eq.V.2 yield a width not greater than 0.001. Δu^{hfg} is then finally adjusted to correspond to an integral sub-multiple of the ultra-fine group (ufg) width. This adjustment may result in a lethargy width somewhat larger than 0.001. Thus, for example, for the current Δu^{ufg} of 1/120, the largest possible Δu^{hfg} is 0.00141667. For a broad group with upper energy of 275.36 eV, for example, Δu^{hfg} is 0.00030864. A nucleus of mass 250 could elastically scatter neutrons a maximum lethargy width of 0.016 which corresponds to about 11.3 times the largest hyper-fine group width. Lighter nuclei of course can scatter down a greater lethargy span and hence would contain more hyper-fine groups in their scattering band. For example, a nucleus of mass 23 contains about 62.8 of the maximum width hyper-fine groups within its scattering lethargy band.

The probability per unit lethargy that a neutron is scattered from lethargy u' to lethargy u by a nucleus of mass ratio A is given by

$$P(u' \to u) = \begin{cases} \frac{1}{1-\alpha} e^{-(u-u')}, & u \geq u' \geq u - \varepsilon \\ 0 & u' < u - \varepsilon \end{cases} \tag{V.3}$$

where

$$\alpha = \left[\frac{A-1}{A+1}\right]^2 \tag{V.4}$$

$$\varepsilon = \ln(1/\alpha) \tag{V.5}$$

and A is the ratio of target nuclide mass to the mass of the neutron. Note that for hydrogen, the code uses the actual A ($\sim$ 0.99917) rather than the approximation A = 1.0.

In particular, the probability of scattering down ℓ hfg each of width Δu into the group having lower lethargy u_o is given by

$$P_\ell \Delta u = \frac{1}{1-\alpha} \int_{u_o}^{u_o+\Delta u} du \int_{u_o-\ell\Delta u}^{u_o-(\ell-1)\Delta u} du'\, e^{-(u-u')}$$

$$= \frac{(1 - e^{-\Delta u})^2}{1 - \alpha} e^{-(\ell-1)\Delta u}$$

$$= P_1 \Delta u\, e^{-(\ell-1)\Delta u} \qquad (V.6)$$

Equation V.6 must be corrected for scattering into the lowest energetically possible hfg as indicated below.

The scattering band ε is adjusted by making small changes to the mass A so that

$$L = \varepsilon/\Delta u \qquad (V.7)$$

is an integer. Thus a given hfg may scatter down into the next L hfg. The probability of scattering down into the lowest hfg is given by

$$P_{lowest} \Delta u = \frac{1}{1-\alpha} \int_{u_o}^{u_o+\Delta u} du \int_{u-\varepsilon}^{u_o-\varepsilon+\Delta u} du'\, e^{-(u - u')}$$

$$= \frac{\alpha}{1-\alpha} \left\{ - \Delta u + 1 + e^{\Delta u} \right\} \qquad (V.8)$$

where the limits on the second integral account for the fact that not all parts of the source hfg may energetically be able to scatter into the lowest hfg.

The ingroup scattering is given by

$$P_s \Delta u = \frac{1}{1-\alpha} \int_{u_o}^{u_o+\Delta u} du \int_{u_o}^{u} du'\, e^{-(u - u')}$$

$$= \frac{1}{1-\alpha} (\Delta u - 1 + e^{-\Delta u}) \ . \qquad (V.9)$$

Now if ℓ is set equal to L in Eq.V.6, we obtain

$$P_L \Delta u = \frac{\alpha}{1-\alpha} (e^{\Delta u} - 2 + e^{-\Delta u}) \qquad (V.10)$$

where we make use of the fact that

$$\alpha = e^{-L\Delta u} \ . \qquad (V.11)$$

By comparing Eqs.V.8, V.9, and V.10, we see that

$$P_{lowest}\Delta u = P_L\Delta u - \alpha P_s\Delta u \tag{V.12}$$

If we denote the hfg flux per unit lethargy in hfg k by ϕ_k and the macroscopic scattering cross section for that group by Σ_{s_k}, the source of neutrons per unit lethargy into group k due to elastic scattering-in from all energetically possible lower lethargy hfg is given by

$$S_{o_k} = \sum_{\ell=1}^{L} \Sigma_{s_{k-\ell}} \phi_{k-\ell} P_1 e^{\Delta u} e^{\ell\Delta u} - \alpha\Sigma_{s_{k-L}} \phi_{k-L} P_s \tag{V.13}$$

where P_ℓ and P_s are obtained from Eqs.V.6 and V.9, respectively. Similarly, the ingroup or self-scattering source of neutrons per unit lethargy is given by

$$S_{s_k} = \Sigma_{s_k} \phi_k P_s \ . \tag{V.14}$$

In the case of a mixture of various mass nuclides, the previous equations will have a contribution from each of the constituents of the composition in question. In particular, for a heterogeneous problem these equations will have contributions from the constituents appropriate to the particular spatial mesh involved.

Note that in the previous equations, Δu, P_ℓ, and P_s have not contained a subscript relating to hfg number. This is appropriate so long as the hfg width is a constant. Since in the normal problem Δu changes from broad group to broad group, P_ℓ and P_s become broad group dependent quantities.

The direct evaluation of S_{o_k} for each hfg using the summation in Eq.V.13 would be too time consuming since hundreds, and for light nuclides thousands, of lower lethargy hfg contribute to the scattering-in source for each hfg. By noting from Eq.V.6 that

$$P_\ell = e^{-\Delta u} P_{\ell-1} \tag{V.15}$$

and making use of Eq.V.11, one can show that Eq.V.13 may be rewritten in the form

$$S_{o_k} = e^{-\Delta u} S_{o_{k-1}} - (P_1 - e^{-\Delta u} P_s)\alpha(\Sigma_s\phi)_{k-1-L} + P_1(\Sigma_s\phi)_{k-1} \tag{V.16}$$

$$- \alpha P_s(\Sigma_s\phi)_{k-L} \ .$$

Thus, the scattering source into hfg k requires only the source into the previous hfg $S_{o_{k-1}}$, and the scattering rates $\Sigma_s\phi$ for hyper-fine groups k-1, k-L, and k-L-1.

When a variable hfg lethargy width is used, the lower lethargy scattering rates required in Eq.V.16 may occur in a broad group having a different hfg width from that of the receptor group k. In that case, the required $\Sigma_s\phi$ is in general obtained by a three point interpolation formula, namely

$$f(x_o+ph) = \frac{p(p-1)}{2} f_{-1} + (1-p^2) f_o + \frac{p(p+1)}{2} f_1 \qquad (V.17)$$

where the scattering rates f_{-1}, f_o, and f_1 are assigned to a lethargy at the center of the hfg involved. If the scattering source occurs within the first or last hfg of a broad group having a different hfg width from that of the receptor group, then the two point formula

$$f(x_o+ph) = (1-p)f_o+pf_1 \qquad (V.18)$$

is used for interpolation.

RABANL has provision for storing all energetically reachable lower lethargy scattering rates if the user specifies sufficient core storage. If this is not the case however, the code will store averages of the scattering rates over several hfg as necessary to accommodate the available storage. Results using averaged scattering rates will of course be less accurate than if all required hfg can be core contained. However, in practical problems, only slight changes have been observed in the resultant broad group cross sections if hfg averaging is used.

If scattering rates required in Eq.V.16 occur at energies above the top of the RABANL energy range, they are obtained in two ways depending upon whether RABANL is being run as a standalone or if the full MC^2-2 calculation is being made. In the former case, the code assumes $\phi = 1.0$ for all energies above the top of the RABANL energy range and takes Σ_s to be constant and equal to the homogenized hard sphere potential scattering cross sections for the materials in the composition involved. If the full MC^2-2 problem is run, the scattering rates $\Sigma_s\phi$ are provided to RABANL for all energetically reachable ultra-fine groups above the top of the RABANL energy range in a data set SRATES. RABANL assumes that $\Sigma_s\phi$ is constant within any ufg in obtaining the necessary $\Sigma_s\phi$ for use in Eq.V.16. If data set SRATES is saved from a previous MC^2-2 calculation, then a standalone RABANL calculation will similarly use these ufg $\Sigma_s\phi$ rather than the potential scattering cross sections and flat unit flux above the top of the RABANL calculation.

The source into the first, lowest lethargy hfg also depends upon whether RABANL is being run as a standalone code without access to a previously supplied data set SRATES, or rather if such data are available. If no SRATES data are available, from Eq.V.13 with ϕ=1.0 and Σ_s=Σ_p for all groups, one can show that

$$S_{o_1} = \Sigma_p \left\{ \frac{1 - e^{-\Delta u}}{\Delta u} - \alpha P_s \right\} \qquad (V.19)$$

where Δu is the hfg lethargy width of the first hfg in the RABANL energy range. As before, for a mixture of materials, Eq.V.19 receives a contribution from each of the constituents with appropriate Σ_p, α, and P_s for each.

When data set SRATES is available, the source into hfg number 1 is derived by directly performing the sum in Eq.V.13 and assuming that $\Sigma_s\phi$ is constant within each of the ufg above the top of the RABANL energy range.

In order to minimize numerical roundoff problems, Eq.V.13 is used to obtain S_o for the first hfg of each broad group rather than using the Eq.V.16 recursion relationship throughout all hfg in the problem. This has been found to be essential for heavily absorbing compositions for which exclusive use of Eq.V.16 for all hfg has led to the generation of negative sources.

If ingroup scattering is omitted, on user option, then P_s=0 and Eq.V.16 becomes

$$S_{o_k} = e^{-\Delta u} S_{o_{k-1}} - \alpha P_1 (\Sigma_s\phi)_{k-1-L} + P_1 (\Sigma_s\phi)_{k-1} \quad . \qquad (V.20)$$

In this case, the P_1 as defined in Eq.V.16 must be altered in order to conserve neutrons. In particular, one can show that

$$\sum_{\ell=1}^{L} P_\ell - \alpha P_s + P_s = 1.0 \qquad (V.21)$$

using Eqs.V.6, V.9, and V.11. That is the sum of the scattering-in source (corrected for scattering from the highest hfg) plus the ingroup self-scattering is normalized to unity. On the other hand if P_s=0, then one finds using Eq.V.6 that

$$\sum_{\ell=1}^{L} P_\ell \Delta u = 1 - e^{-\Delta u} \quad . \qquad (V.22)$$

Hence if ingroup scattering is deleted so that Eq.V.20 is pertinent, then to force normalization of all scattering to unity, P_1 as defined in Eq.V.6 must be divided by $1 - e^{-\Delta u}$ so that

$$P_\ell = \frac{P_1 \, e^{-(\ell-1)\Delta u}}{1 - e^{-\Delta u}} \text{ , if } P_s = 0. \tag{V.23}$$

The reason why the user might choose to accept this more approximate treatment is to reduce running time in the case of heterogeneous problems as discussed later. For homogeneous problems, there is no running time advantage in deleting the self-scattering.

C. Calculation of Collision Rates

1. One Region (Homogeneous) Problems

From neutron balance, the collision rate in a particular hfg k, CR_k is given by

$$CR_k = P_{n\ell_k} \left\{ S_{o_k} + S_{s_k} \right\} \tag{V.24}$$

where $P_{n\ell_k}$ is the non-leakage probability, and S_{o_k} and S_{s_k} are respectively the scattering-in and self-scattering sources. Using Eq.V.14, Eq.V.24 can be rewritten as

$$CR_k = P_{n\ell_k} \left\{ S_o + (\Sigma_s \phi)_k \, P_s \right\}$$

$$= P_{n\ell_k} \left\{ S_{o_k} + \frac{\Sigma_{s_k} P_s}{\Sigma_{t_k}} (\Sigma_t \phi)_k \right\}$$

$$= P_{n\ell_k} \left\{ S_{o_k} + R_k \cdot CR_k \right\}$$

where Σ_{t_k} is the macroscopic total cross section for hfg k,

$$R_k = \frac{\Sigma_{s_k} P_s}{\Sigma_{t_k}} \text{ ,} \tag{V.25}$$

and from neutron balance, $CR_k = \Sigma_{t_k} \phi_k$.

Solving then for CR_k, we have

$$CR_k = \frac{P_{n\ell_k} \, S_{o_k}}{1 - P_{n\ell_k} \, R_k} \tag{V.26}$$

For the special case of an infinite medium, $P_{n\ell_k}=1.0$. As discussed earlier, P_s will depend upon hfg for the case in which the hfg widths are variable. The hfg index has been omitted here for simplicity.

The non-leakage probability $P_{n\ell_k}$ is taken to be

$$P_{n\ell_k} = \frac{\Sigma_{t_k}}{\Sigma_{t_k}+D_k B^2} \tag{V.27}$$

where again Σ_{t_k} is the hfg k total macroscopic cross section for the mixture,

$$D_k = \frac{1}{3\Sigma_{tr_k}} \tag{V.28}$$

and Σ_{tr_k} is the macroscopic transport cross section for the mixture where we assume

$$\Sigma_{tr_k} = \sum_{i=1}^{M} n_i \frac{\sigma^i_{t_k}}{\upsilon^i_{s_k}} (\sigma^i_{t_k} - \bar{\mu}^i \sigma^i_{s_k}). \tag{V.29}$$

In Eq.V.29 the sum extends over all isotopes in the mixture, each with atom density N_i and microscopic total and scattering cross sections given by $\sigma^i_{t_k}$ and $\sigma^i_{s_k}$ respectively. $\bar{\mu}^i$ is $2/3A^i$ where A^i is the ratio of nuclide i mass to neutron mass. The buckling, B^2, is user specified on the A.MCC2 type 09 card.

The calculation of the S_{o_k} has been discussed earlier for the case of elastic slowing down. In addition to the elastic scattering sources, neutrons can also appear in a hfg due to inelastic and (n,2n) scattering or to fissions at energies above the top of the RABANL energy range, or due to external sources specified by the user on the A.MCC2 type 08 cards. The former are referred to as fixed source neutrons in that they do not depend upon the RABANL fluxes, while the latter are referred to as external sources. The fixed sources are supplied on data set SRATES which is generated by an MC^2-2 ufg calculation. These sources, as in the case of the external sources are specified at an ufg level. RABANL creates equivalent hfg values for these ufg data by a linearization algorithm as specified below.

Suppose ufg data are available for ufg numbers 1 to NG where Y_I is the ufg datum for ufg I. Defining

$$\Delta_1 = Y_2 - Y_1$$

$$\Delta_I = \frac{Y_{I+1} - Y_I}{2}, \quad I = 2, \text{ NG-1} \tag{V.30}$$

$$\Delta_{NG} = Y_{NG} - Y_{NG-1},$$

then the value assigned to a hfg j lying within ufg I, assuming there are exactly N hfg per ufg, is given by

$$y_j = (Y_I - \Delta_I/2) + f_j \Delta_I$$

where

$$f_j = \frac{2j - 1}{2N}, \quad j = 1,2, \ldots, N \tag{V.31}$$

An example is shown in Fig. 6 for the case of N = 5 and NG = 4. The dashed line represents the linearized hfg histogram equivalent to the solid line ufg histogram.

The fixed sources as supplied on data set SRATES are given for each isotope in the mixture. RABANL homogenizes these sources according to the atom densities of the materials contained in the mixture. If we denote the homogenized hfg fixed sources as S_{fix_k} and the external hfg sources as S_{ext_k}, Eq. V.26 is modified to

$$CR_k = \frac{P_{n\ell_k} S_{t_k}}{1 - P_{n\ell_k} R_k} \tag{V.32}$$

where

$$S_{t_k} = S_{o_k} + S_{fix_k} + S_{ext_k}. \tag{V.33}$$

From Eq. V.32 and the macroscopic total cross section in hfg k, we have then the hfg k flux per unit lethargy

$$\phi_k = \frac{CR_k}{\Sigma_{t_k}}. \tag{V.34}$$

The calculation of the ϕ_k thus proceeds hfg by hfg: the elastic slowing down source is calculated for the hfg in question using the methods in Section B; this source is augmented by S_{fix} and S_{ext} and the collision rate is calculated as shown above; the hfg flux is then obtained from Eq. V.34 and the scattering rate $(\Sigma_s \phi)_k$ is stored for use in later slowing down source calculations as required in Eq. V.16.

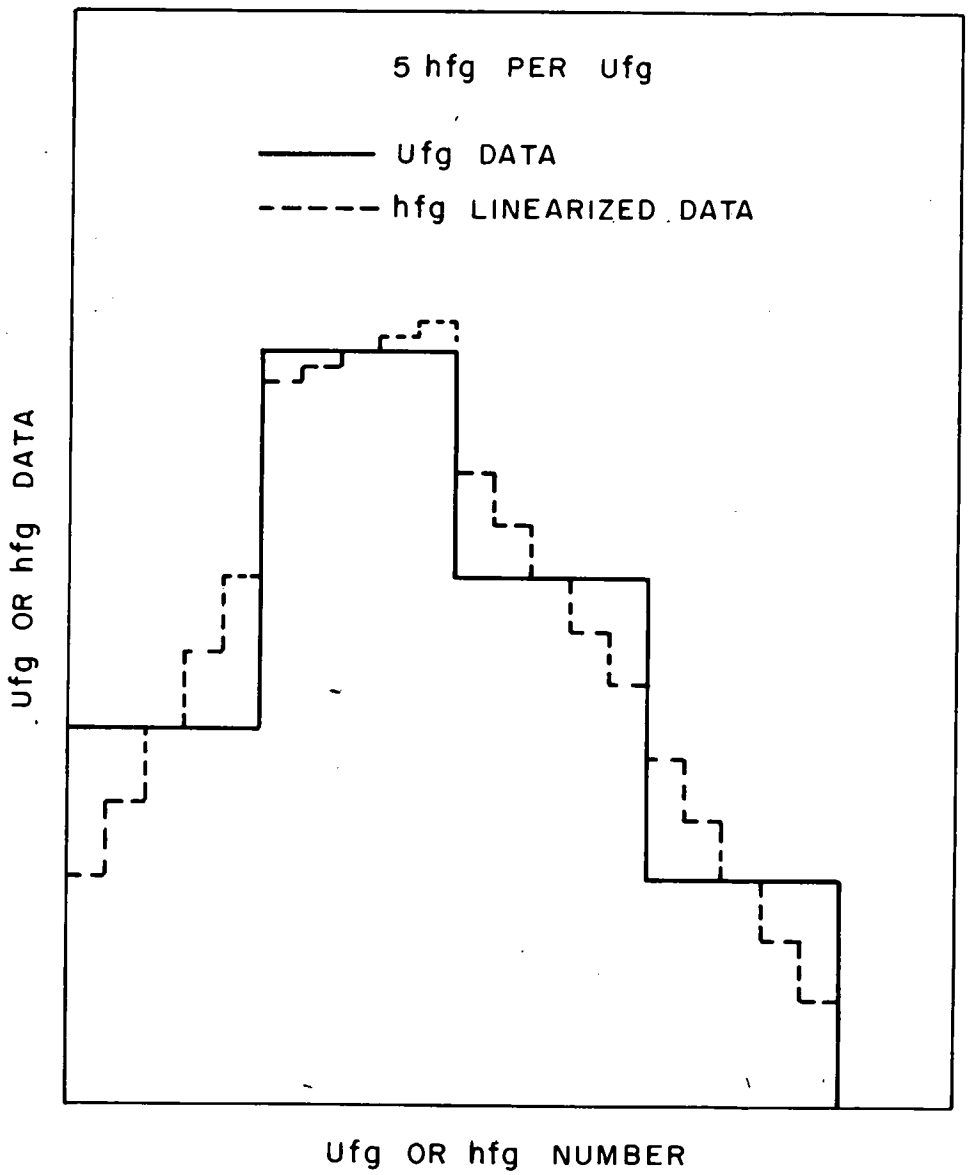

Fig. 6. Linearization of Ultra-Fine-Group Data.

RABANL also provides for calculation of cross sections of foils immersed in the flux of the homogeneous composition. The foil material is assumed to have a negligible influence on the spectrum. The expressions for the collision rate in the foil and hence the flux in the foil are presented at the end of Section C.2.a.

2. Multi-region (Heterogeneous) Problems

The integral transport form of the Boltzmann equation can be written in general terms as

$$\phi(\bar{r},u) = \iiint d\bar{r}' \int_0^u du' \, \Sigma_s(u')\phi(\bar{r}',u') \, P(u'\to u) \, T(u,\bar{r}'\to\bar{r})$$

$$= \iiint d\bar{r}' \, S(u,\bar{r}') \, T(u,\bar{r}'\to\bar{r}) \qquad (V.35)$$

where $\phi(\bar{r},u)$ is the flux per unit lethargy at space point $\bar{r}$, $\Sigma_s(u')$ is the scattering cross section at lethargy u', $P(u'\to u)$ is the probability of a lethargy change of u' to u due to the scattering event at $\bar{r}'$, $S(u,\bar{r}')$ is the source of neutrons of lethargy u at space point $\bar{r}'$, and $T(u,\bar{r}'\to\bar{r})$ is the transport kernel giving the probability that neutrons of lethargy u at space point $\bar{r}'$ will reach space point $\bar{r}$ without suffering a collision. $P(u'\to u)$ is defined in Eq.V.3. The transport kernel depends upon the geometry of the problem since it involves the geometric distance $|\bar{r}-\bar{r}'|$, namely

$$T(u,\bar{r}'\to\bar{r}) = \frac{\exp -\left[\Sigma_t(u,\bar{r}')|\bar{r}-\bar{r}'|\right]}{4\pi|\bar{r}-\bar{r}'|^2}. \qquad (V.36)$$

RABANL provides solutions for multi-region slab or cylindrical geometries as described below.

a. Slab Geometry

In the case of infinite slab geometry, with reference to Fig. 7 , the spatial integral in Eq.V.35 can be expressed as

$$\iiint d\bar{r}' \, \Sigma_s(u')\phi(\bar{r}',u') \, \frac{\exp\left[-\Sigma_t(u,\bar{r}')|\bar{r}-\bar{r}'|\right]}{4\pi|\bar{r}-\bar{r}'|^2}$$

$$= \int dx' \, \Sigma_s(u')\phi(x',u') \int_0^\infty \frac{2\pi\rho d\rho \, \exp\left[-\Sigma_t(u,x')\left\{\rho^2+|x-x'|^2\right\}^{\frac{1}{2}}\right]}{4\pi\left\{\rho^2+|x-x'|^2\right\}}$$

$$= \tfrac{1}{2}\int dx' \, \Sigma_s(u')\phi(x',u') \int_1^\infty dt \, \frac{\exp\left[-\Sigma_t(u,x')|x-x'|t\right]}{t}$$

$$= \tfrac{1}{2}\int dx' \, \Sigma_s(u')\phi(x',u') \, E_1\left\{\Sigma_t(u,x')|x-x'|\right\} \qquad (V.37)$$

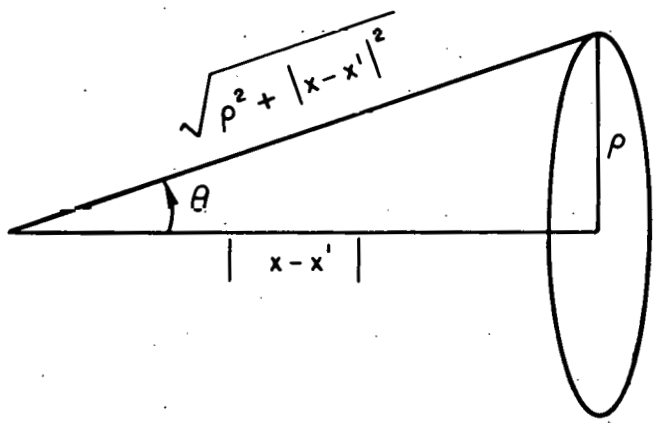

Fig. 7. Slab Geometry Coordinates.

where E_1 is the exponential integral defined in Eq.A.37 of Appendix A. The t used in transforming the variable of integration in Eq.V.37 is $1/\cos\theta$ where θ is shown in Fig. 7 .

The flux is therefore given by

$$\phi(x,u) = \tfrac{1}{2} \int dx' \int_0^u du' \; \Sigma_s(u')\phi(x',u')P(u'\to u)E_1 \left\{\Sigma_t(u,x')\left|x-x'\right|\right\} \tag{V.38}$$

Now since the current is $\phi \cos\theta$, from the definition of the exponential integrals, the current is given by

$$\vec{J}(x,u) = \tfrac{1}{2} \int dx' \int_0^u du' \; \Sigma_s(u')\phi(x',u')P(u'\to u)E_2 \left\{\Sigma_t(u,x')\left|x-x'\right|\right\} . \tag{V.39}$$

If now the continuous-lethargy expressions in Eqs.V.38 and V.39 are transformed into the equivalent hyper-fine multigroup form, Eq.V.39 can be written as

$$\bar{J}_k(x) = \tfrac{1}{2} \int dx' \; S_k(x') \; E_2 \left\{\Sigma_{t_k}(x')\left|x-x'\right|\right\} \tag{V.40}$$

where $\bar{J}_k(x)$ is the hfg k current at x, $S_k(x')$ is the hfg k source at x', and $\Sigma_{t_k}(x')$ is the total macroscopic cross section for hfg k and spatial point x'. The calculation of the S_k has been described earlier in Section B, and S_k contains the source into hfg k due to slowing down from all other hfg plus the ingroup or self-scatter source for hfg k

$$S_k(x') = S_{o_k}(x') + S_{s_k}(x') \tag{V.41}$$

Noting that the optical thickness τ_k is given by $\Sigma_{t_k} x$, the current at τ_k mean free paths beyond a slab of optical thickness τ_{k_1} is given by

$$\vec{J}_k(\tau_k,\tau_{k_1}) = \tfrac{1}{2} \int_0^{t_o} dx' \left[S_{o_k}(x') + S_{s_k}(x')\right] E_2(\tau_k + \Sigma_{t_k} x') \tag{V.42}$$

where Σ_{t_k} is the total macroscopic cross section in the slab for hfg k. Assuming that the self-scatter source and the in-scattered source have the same dependence on x' and assuming that the spatial source per unit length in the slab is given by a flat component plus a linearly varying component

$$S_k(x') = \frac{1}{t_1}\left[\bar{S}_k + \frac{\Delta S_k}{t_1}(t_1/2 - x')\right] \tag{V.43}$$

as shown in Fig. 8, Eq.V.42 may be rewritten as

$$\vec{J}_k(\tau_k,\tau_{k_1}) = \frac{\bar{S}_k}{2t_1}\int_0^{t_1} dx'\, E_2(\tau_k + \Sigma_{t_k} x')$$

$$- \frac{\Delta S}{2t_1^2}\int_0^{t_1} dx' x' E_2(\tau_k + \Sigma_{t_k} x')$$

$$+ \frac{\Delta S}{4t_1}\int_0^{t_1} dx' E_2(\tau_k + \Sigma_{t_k} x') \quad . \tag{V.44}$$

The first and last integrals of Eq.V.44 are easily evaluated using Eq.A.60 of Appendix A. The second integral may be evaluated by noting that[29]

$$\int x^m E_n(ax + b)\, dx = - \sum_{i=0}^{m} \frac{m!}{(m-i)!} \frac{x^{m-i}}{a^{i+1}} E_{n+i+1}(ax + b). \tag{V.45}$$

Finally, one may show that the current

$$\vec{J}_k(\tau_k,\tau_{k_1}) = \frac{\bar{S}}{2\tau_1}\left[E_3(\tau_k) - E_3(\tau_k+\tau_{k_1})\right]$$

$$+ \frac{\Delta S}{2\tau_1}\left\{\left[E_3(\tau_k) + E_3(\tau_k+\tau_{k_1})\right] \Big/ 2 - \frac{1}{\tau_1}\left[E_4(\tau_k) - E_4(\tau_k+\tau_{k_1})\right]\right\} \quad . \tag{V.46}$$

Now the collision rate in a slab is the difference between the uncollided current into the slab and the uncollided current out of the slab. Thus the collision rate in a slab of optical thickness τ_{k_2} due to the source in a slab of opical thickness τ_{k_1}, when slabs 1 and 2 are separated by τ_k mean free paths is, using the notation of Eq.V.46

$$\vec{CR}_k(1\to2) = \vec{J}_k(\tau_k,\tau_{k_1}) - \vec{J}_k(\tau_k+\tau_{k_2},\tau_{k_1}). \tag{V.47}$$

The arrow above CR in Eq.V.47 implies that slab 2 lies to the right of slab 1.

Now if there exists an infinite array of unit cells each made up of a number of slab mesh intervals, then the collision rate in all type 2 slabs which lie to the right of the type 1 slabs is given by the infinite sum

$$\vec{CR}_{\infty_k}(1\to2) = \sum_{m=0}^{\infty}\left[\vec{J}_k(\tau_k+mh,\tau_{k_1}) - \vec{J}(\tau_k+\tau_{k_2}+mh,\tau_{k_1})\right] \tag{V.48}$$

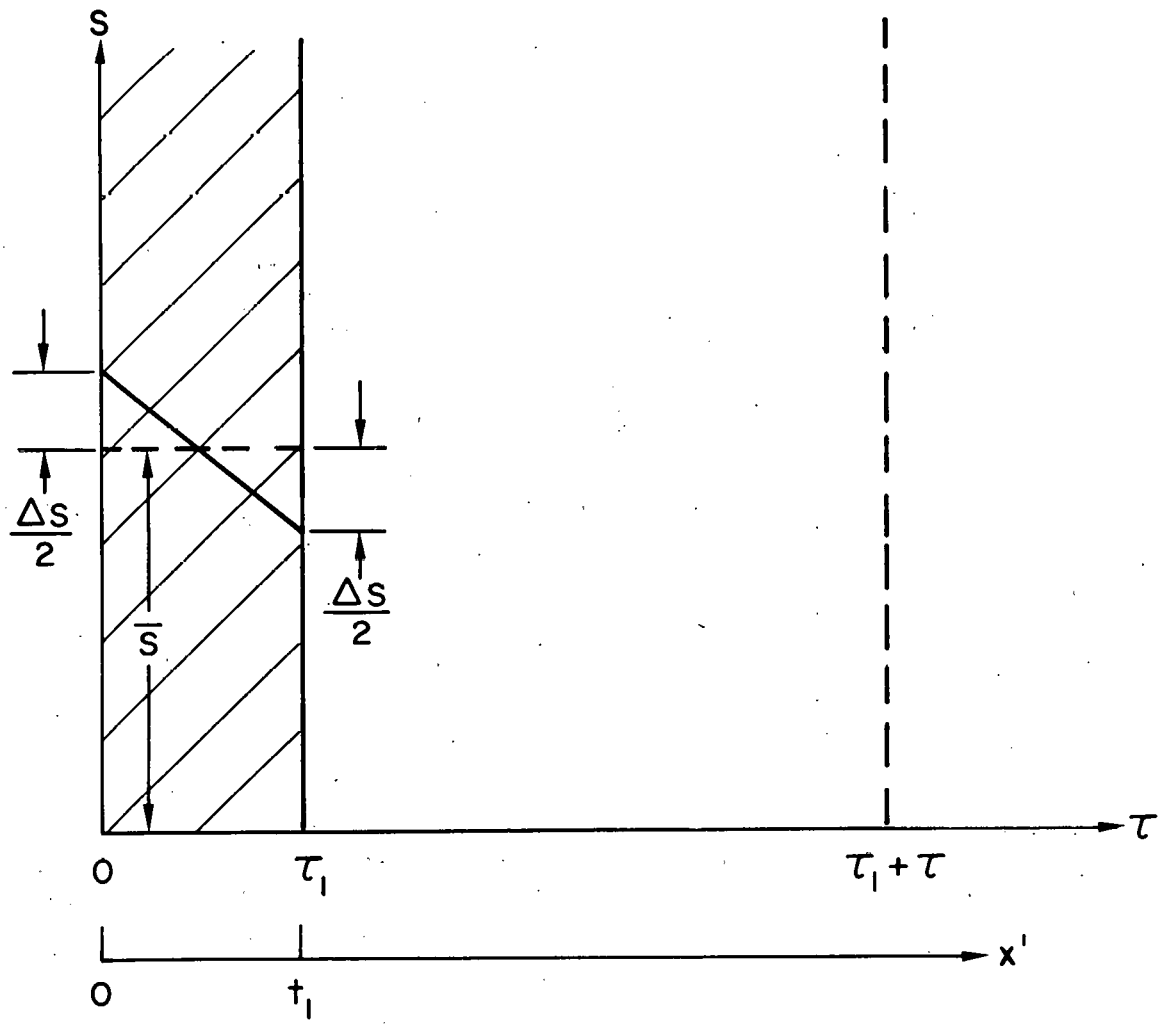

Fig. 8. Slab Geometry Optical Distance

where h is the optical thickness of the unit cell.

Since neutrons proceed both to the right and to the left, the total collision rate in slab j due to sources in slab i is given by

$$CR_{\infty_k}(i\to j) = \vec{CR}_{\infty_k}(i\to j) + \overleftarrow{CR}_{\infty_k}(j\leftarrow i) \tag{V.49}$$

where the arrows above the CR denote the direction of neutron motion. Appendix A describes the numerical methods used in evaluating the infinite sums of E_n functions involved in obtaining Eq.V.49.

Thus, for the neutron source S_{i_k} in mesh interval i, the collision probability from region i to k and hfg k is given by

$$C_{k_{ij}} = CR_{\infty_k}(i\to j)/S_{i_k} \tag{V.50}$$

The unit cell may have either periodic or reflective boundary conditions as specified by the user. Thus if a four mesh interval cell having compositions ordered as ABCD is specified to have periodic boundary conditions, the infinite lattice will have the compositions ... ABCDABCDABCD... If instead reflective boundary conditions are specified, the infinite lattice will correspond to ... DCBAABCDDCBAABCD...

We will now drop the hfg index to simplify the notation. If the unit cell consists of N slab mesh intervals, then the collision probability can be represented by an NxN square matrix $\underline{C}$. Similarly, the collision rate, the scattering-in sources, and the self-scattering sources are all N dimensional vectors, and are represented by $\underline{CR}$, $\underline{S_o}$, and $\underline{S_s}$ respectively.

Using matrix arithmetic then one has from neutron balance

$$\underline{CR} = \underline{C}\left[\underline{S_o} + \underline{S_s}\right] \tag{V.51}$$

Again, as for the case of the homogeneous one region calculation, the $\underline{S_o}$ are augmented by the fixed and external sources as in Eq.V.33 so that we rewrite Eq.V.51 as

$$\underline{CR} = \underline{C}\left[\underline{S_t} + \underline{S_s}\right] \tag{V.52}$$

where $\underline{S_t}$ is the N dimensional vector representation of Eq.V.30. Now from Eqs.V.25 and V.34, we can replace the self-scattering source $\underline{S_s}$ by

$$\underline{S_s} = \underline{R}\cdot\underline{CR}\ . \tag{V.53}$$

In matrix notation, $\underline{R}$ will be a square, NxN diagonal matrix with elements given by Eq.V.25 for each slab mesh interval. Thus we have

$$\underline{CR} = \underline{C}\left[\underline{S_t} + \underline{R}\ \underline{CR}\right] \tag{V.54}$$

Solving Eq.V.54 for CR we have

$$[\underline{I} - \underline{C}\ \underline{R}]\underline{CR} = \underline{C}\ \underline{S_t}$$

and hence

$$\underline{CR} = [I - \underline{C}\ \underline{R}]^{-1}\ \underline{C}\ \underline{S_t} \tag{V.55}$$

where $\underline{I}$ is the unit matrix.

Note that the solution of Eq.V.55 requires the inversion of an NxN matrix. Also, if self-scattering is ignored so that $\underline{R}$ is the null matrix, then Eq.V.54 reduces to

$$\underline{CR} = \underline{C}\ \underline{S_t} \quad , \text{ if } P_s = 0. \tag{V.56}$$

Now to this point, the algorithms for the slab geometry problem have referred to infinite geometry. If however the user choose to specify a buckling and permit leakage from each mesh interval, the code calculates the non-leakage probabilities as in Eq.V.27. Expressing these in the form of a square NxN diagonal matrix $\underline{PNL}$ where each diagonal element is the non-leakage probability for the particular mesh interval, we may rewrite Eq.V.54 as

$$\underline{CR} = \underline{C}\ \underline{PNL}\left[\underline{S_t} + \underline{R}\ \underline{CR}\right]. \tag{V.57}$$

Again, solving for $\underline{CR}$, we have in place of Eq.V.55

$$\underline{CR} = [\underline{I} - \underline{C}\ \underline{PNL}\ \underline{R}]^{-1}\ \underline{C}\ \underline{PNL}\ \underline{S_t} \tag{V.58}$$

and if self-scattering is omitted,

$$\underline{CR} = \underline{C}\ \underline{PNL}\ \underline{S_t} \quad , P_s = 0. \tag{V.59}$$

Thus, as noted earlier, the execution time is reduced if the user chooses to omit the self-scattering contribution because the matrix inversion is eliminated.

The calculation of the spatially integrated hfg flux per unit lethargy $\phi(i)$ where i denotes spatial mesh interval proceeds as for the homogeneous case, hfg by hfg: the elastic slowing down sources are calculated for each spatial mesh interval; these sources are augmented by the linearized fixed and external sources; the collision probability is calculated as in Eq.V.50 where however the self-scatter source is not included in S_{i_k}; the collision

rate is computed using Eq. V.55 or V.56 as appropriate; the hfg spatially integrated flux for each mesh interval is calculated using Eq.V.34; the scattering rates $\Sigma_s\phi$ are computed and stored for use in calculating lower energy slowing sources.

As mentioned above, in computing the collision probability as in Eq.V.50, the self-scattering source is not included since the hfg k flux is not yet available. Since the self-scattering contribution is always a very small part of the total source in a hfg, the alternative procedure requiring an iteration procedure to compute the true collision probability is not justified.

As in the case of the homogeneous calculation, the slab geometry problem provides for the calculation of foil cross sections. The code calculates the cross section for each foil specified at the interface between each spatial mesh interval and that immediately to its right. A foil is also place at the rightmost boundary of the unit cell.

The same procedure is used for the foil calculations as indicated above for the calculation of the collision rates in the slab mesh intervals. Thus, for example, by analogy with Eq.V.48, the collision rate in a foil f due to the sources in all intervals i in the infinite lattice lying to the left of the foil is given by

$$\vec{CR}_\infty(i\rightarrow foil) = \sum_{m=0}^{\infty}\left[\vec{J}(\tau+mh,\tau_i) - \vec{J}(\tau+\tau_f+mh,\tau_i)\right] \qquad (V.60)$$

where the arrows indicate that the current is right directed. The foil with optical thickness τ_f is separated from the interval of optical thickness τ_i by the distance $\tau+mh$ where again h is the unit cell optical thickness. Similar contributions to the collision rate are provided by the left directed currents which when add to Eq.V.60 yield the total collision rate $CR_\infty(foil)$.

Since the collision rate in the foil is given by

$$CR_\infty(foil) = \int_{foil}\phi(x)\,\Sigma_{t_f}\,dx = \bar{\phi}_{foil}\,\tau_f \qquad (V.61)$$

where Σ_{t_f} is the total foil macroscopic cross section, the average flux in the foil can be written as

$$\bar{\phi}_{foil} = \frac{CR_\infty(foil)}{\tau_f}\,. \qquad (V.62)$$

Now for a homogeneous one region problem, the current into the left surface of a foil due to all sources to the left is given by Eq.V.40 as

$$\vec{J}_L = \tfrac{1}{2}\int_0^\infty dx'\; S\; E_2(\Sigma_t x')$$

$$= \frac{S}{4\Sigma_t} \qquad (V.63)$$

where S is the space independent source of neutrons in the homogenous mixture and Σ_t is the macroscopic total cross section. Similarly, the current at the right surface of the foil due to the region to the left of the foil is given by

$$\vec{J}_R = \tfrac{1}{2} \int_0^\infty dx' \; S \; E_2(\Sigma_t x' + \tau_f)$$

$$= \frac{S}{2\Sigma_t} E_3(\tau_f) \qquad \text{(V.64)}$$

Hence the collision rate in the foil due to the incident flux from the left half space is

$$CR_\infty(\text{foil}) = \vec{J}_L - \vec{J}_R = \frac{S}{2\Sigma_t} \left[0.5 - E_3(\tau_f) \right] \; . \qquad \text{(V.65)}$$

Since the same contribution is provided by the incident flux from the right half space, the total collision rate then is given by

$$CR_\infty(\text{foil}) = \frac{S}{\Sigma_t} \left[0.5 - E_3 \; (\tau_f) \right] \; . \qquad \text{(V.66)}$$

Finally, Eq.V.66 in Eq.V.62 yields the average flux in the foil.

b. Cylindrical Geometry

RABANL makes the same approximation as does the RABBLE[5] code in the case of cylindrical geometry. Namely, the flux at the surface of any cylindrical mesh interval is assumed to be isotropic so that neutron currents at an interface vary as the cosine of the incident angle (the so called cosine current approximation). In this case, the collision rate in an interval need be related only to the neutron currents impinging on its inner and outer surfaces so that, the collision rate is dependent only upon the adjacent mesh intervals.

Following the notation of Ref. 5, let

J_i^+ = the current impinging on the inner surface of the (i + 1)th cylindrical interval (in the increasing radial direction)

J_i^- = the current impinging on the outer surface of the ith interval (in the decreasing radial direction)

P_i^+ = the probability of escape through the outer surface of interval i due to a flat volume source

P_i^- = the probability of escape through the inner surface of interval i due to a flat volume source

T_i^{OI} = the transmission probability from the inner to the outer surface of interval i

T_i^{IO} = the transmission probability from the outer to the inner surface of interval i

T_i^{OO} = the transmission probability from the outer to the outer surface of interval i.

If mesh interval 1 is the center interval and if isotropic return is assumed as the outer boundary condition for the cylindrical unit cell (the so called white boundary condition), then by neutron balance we have for an N cylindrical mesh interval unit cell

$$J_i^+ = \begin{cases} T_i^{OO} J_i^- + P_i^+ S_i & i = 1 \\ T_i^{OI} J_{i-1}^+ + T_i^{OO} J_i^- + P_i^+ S_i & i = 2, N \end{cases} \tag{V.67}$$

$$J_i^- = \begin{cases} T_i^{OI} J_{i+1}^- + P_{i+1}^- S_{i+1} & i = 1, N-1 \\ J_i^+ & i = N \end{cases} \tag{V.68}$$

If we define the column vector $\underline{J}$ having 2N elements J_1^+, J_1^-, J_2^+, J_2^-, J_3^+, ..., J_N^- and the column vector $\underline{PS}$ having 2N elements $P_1^+S_1$, $P_2^-S_2$, $P_2^+S_2$, $P_3^-S_3$, $P_3^+S_3$, ..., $P_N^-S_N$, $P_N^+S_N$, 0, then the 2N Eqs. V.67 plus V.68 may be represented in matrix notation as

$$\underline{T}\,\underline{J} = \underline{PS} \tag{V.69}$$

where $\underline{T}$ is a 2N+2N square matrix whose elements involve the T_i^{OO}, T_i^{OI}, and T_i^{IO}.

The set of Eqs. V.69 may be solved for the J_i^+ and J_i^- either by inverting the T matrix, or equivalently by the method of forward elimination, backward substitution. RABANL uses the latter procedure.

Having solved for the J_i^+ and J_i^-, the collision rates for each interval i can be obtained from neutron balance as

$$CR_i = \begin{cases} S_1 + J_1^- - J_1^+ & i = 1 \\ S_i + J_i^- - J_i^+ + J_{i-1}^+ - J_{i-1}^- & i = z, N \end{cases} \tag{V.70}$$

The above procedure is used if self-scattering is ignored. If this approximation is not made, the code first must compute the collision probabilities. In order to compute the collision probabilities C_{ij}, RABANL proceeds as indicated above by setting $S_i = 1$, setting all other $S_j = 0$, and solving for

$$C_{ij} = CR_j \qquad S_{i=1},\ S_{j=0},\ j \neq i. \tag{V.71}$$

This procedure is repeated for each interval i to complete the evaluation of the C_{ij}.

Having obtained the C_{ij}, the collision rates are calculated as indicated above for slab geometries using Eq. V.55 which requires a matrix inversion. Note that infinite geometry is assumed for the cylindrical geometry option so that the non-leakage probability is always 1.0.

The T^{OI} and T^{OO} are obtained as described in Section VII of Appendix A. The other quantities needed in the evaluation of the CR can be expressed in terms of these transmission probabilities as shown in Ref.5. In particular, define

$$x_i = \frac{r_{i-1}}{r_i} \tag{V.72}$$

where $r_o = 0$ and

$$z_i = \Sigma_{t_i}(r_i - r_{i-1}) \tag{V.73}$$

where r_i is the outer radius of mesh interval i and Σ_{t_i} is the total macroscopic cross section in interval i. Then

$$T_i^{IO} = x_i T_i^{OI} \tag{V.74}$$

$$P_i^- = \frac{x_i(1 - T_i^{OI})}{2z_i(1 + x_i)} \tag{V.75}$$

$$P_i^+ = \frac{1 - T_i^{OO} - T_i^{IO}}{2z_i\ (1 + x_i)}\ . \tag{V.76}$$

The foil capability described earlier for homogeneous or slab geometry problems is not provided in the case of cylindrical cells.

D. Calculation of Hyper-fine Group Cross Sections

The cross sections for a particular material in a given hfg are made up of both smooth and resonance contributions. The smooth data are available at an ufg detail from the library as provided by ETOE-2. At user option, as specified on card type 02 of data set A.STP015, the contribution from ufg unresolved resonance cross sections as prepared by the modules CSC004 and CSC008 will be added to the other library provided smooth data. These ufg smooth data are linearized as in the case of the fixed and external sources using the algorithms given in Eqs.V.30 and V.31 to generate the hfg cross sections to be added to the resolved resonance cross sections.

The contributions due to the resolved resonances are computed in RABANL during the sweep down through the hfg. The code will accept Breit-Wigner single level resonance parameters, or multilevel parameters in either the Adler-Adler or Breit-Wigner representations. The resolved resonance cross sections for a given hfg are evaluated at the energy corresponding to the average lethargy of the hfg.

1. Resonance Selection

Due to the large number of hfg, the calculation of the resonance cross sections in each due to all resolved resonance in the problem mixture may be rather time consuming. The user has the option of specifying a resolved resonance selection criterion using the type 14 card of data set A.MCC2. An intermediate group is specified corresponding to an integral number of ufg, with the default number being two. The contribution of any resonance falling within the intermediate group is automatically included in each hfg contained in the intermediate group in question. Those resonances lying outside the intermediate group, whose resonant total cross sections at the intermediate group boundary equal or exceed the criterion specified on the type 14 card, are also included for all hfg contained in the intermediate group. The default for this criterion is 0.05. All other resonances are ignored for that intermediate group. In calculating the total resonant cross sections during the selection process, the resonances are Doppler broadened using the temperature of the hottest composition in the problem.

By specifying a criterion of 0.0 on the type 14 card, the user may include the contributions of all resonances in each of the hfg in the calculation. This option, which is the most rigorous is also the most time consuming.

2. Resolved Resonance Algorithms

a. Single Level Breit-Wigner

Single level Breit-Wigner s-wave resonance scattering, capture, and fission cross sections are respectively evaluated using the expressions

$$\sigma_s^s(E) = \sigma_o^s \left\{ \frac{\Gamma_n^s}{\Gamma_t^s} \psi(\xi,x) + \left[\frac{\sigma_p g_J^s \Gamma_n^s}{\sigma_o^s \Gamma_t^s} \right]^{\frac{1}{2}} \chi(\xi,x) \right\}$$

$$= \sigma_o^s \left\{ \frac{\Gamma_n^s}{\Gamma_t^s} \psi(\xi,x) + a^s \chi(\xi,x) \right\} \qquad (V.77)$$

$$\sigma_c^s(E) = \sigma_o^s \left[\frac{|E_o|}{E}\right]^{\frac{1}{2}} \frac{\Gamma_\gamma^s}{\Gamma_t^s} \psi(\xi,x) \qquad (V.78)$$

$$\sigma_f^s(E) = \sigma_o^s \left[\frac{|E_o|}{E}\right]^{\frac{1}{2}} \frac{\Gamma_f^s}{\Gamma_t^s} \psi(\xi,x) \ . \qquad (V.79)$$

In the above,

σ_o^s = the peak cross section of the s-wave resonance

$= \dfrac{2.6039953 \times 10^6}{|E_o|} \left(\dfrac{A+1}{A}\right)^2 g_J^s \dfrac{\Gamma_n^s}{\Gamma_t^s}$

E_o = the resonance energy in eV

A = the mass number of the target nucleus

$g_J^s = \dfrac{2J+1}{2(2I+1)}$ where J is the total spin of the compound nucleus and I is the spin of the target nucleus

Γ_t^s = the s-wave total line width

Γ_γ^s = the s-wave radiation line width

Γ_f^s = the s-wave fission line width

$\Gamma_n^s = \Gamma_t^s - \Gamma_\gamma^s - \Gamma_f^s$

E = the laboratory neutron energy in eV corresponding to the average lethargy for the hfg in question

σ_p = the target nucleus potential scattering cross section

$\psi(\xi,x)$ = the Doppler-broadened symmetric line shape function

$= \dfrac{\xi\sqrt{\pi}}{2} \mathrm{ReW}\left(\dfrac{\xi x}{2}, \dfrac{\xi}{2}\right)$

$\chi(\xi,x)$ = the Doppler-broadened anti-symmetric line shape function

$= \xi\sqrt{\pi}\ \mathrm{ImW}\left(\dfrac{\xi x}{2}, \dfrac{\xi}{2}\right)$

$W(z)$ = the error function for complex arguments

$= \exp(-z^2)\ \mathrm{erfc}(-iz)$ where $z = x + iy$

$\xi = \Gamma_t^s/\Delta$ and Δ is defined in Eq. V.1 with E defined above and with the Boltzmann constant equal to 8.6168×10^{-5} eV/degree Kelvin

$x = 2(E - E_o)/\Gamma_t^s$.

The ψ and χ functions are obtained from bivariate interpolation in prestored tables as described in Section III of Appendix A.

Single level Breit-Wigner p-wave resonance scattering, capture, and fission cross sections are, respectively evaluated using the expressions

$$\sigma_s^p(E) = \sigma_o^p \frac{\Gamma_n^p}{\Gamma_t^p}\left\{\psi(\xi,x) + \frac{\Gamma_t^p}{2E_o}\chi(\xi,x) + \left[\frac{\Gamma_t^p}{2E_o}\right]^2 \left[1 - \psi(\xi,x)\right]\right\} \quad (V.80)$$

$$\sigma_c^p(E) = \sigma_o^p \left[\frac{|E_o|}{E}\right]^{\frac{1}{2}} \frac{\Gamma_\gamma^p}{\Gamma_t^p}\left[\psi(\xi,x) + \frac{\Gamma_t^p}{4E_o}\chi(\xi,x)\right] \quad (V.81)$$

$$\sigma_f^p(E) = \sigma_o^p \left[\frac{|E_o|}{E}\right]^{\frac{1}{2}} \frac{\Gamma_f^p}{\Gamma_t^p}\left[\psi(\xi,x) + \frac{\Gamma_t^p}{4E_o}\chi(\xi,x)\right] . \quad (V.82)$$

In the above,

σ_o^p = the peak cross section of the p-wave resonance evaluated as before but using the parameters for the p-wave resonance

Γ_t^p = the p-wave total line width

$\Gamma_n^p = \Gamma_t^p - \Gamma_\gamma^p - \Gamma_f^p$

Γ_γ^p = the p-wave radiation line width

Γ_f^p = the p-wave fission line width

$\xi = \Gamma_t^p/\Delta$

$x = 2(E - E_o)/\Gamma_t^p$.

b. Multilevel Breit-Wigner

Multilevel Breit-Wigner s-wave resonance scattering, capture, and fission cross sections are, respectively evaluated using the expressions

$$\sigma_s^{s,bw}(E) = \frac{\sigma_o^{bw}}{|G_t^{bw}|}\left\{G_t^{bw}\,\psi(\xi,x) + |G_t^{bw}|\,a^{bw}\,\chi(\xi,x) - G_\gamma^{bw}\,\psi(\xi,x) - G_f^{bw}\,\psi(\xi\right. \tag{V.83}$$

$$\sigma_c^{s,bw}(E) = \sigma_o^{bw}\,\frac{G_\gamma^{bw}}{|G_t^{bw}|}\left[\frac{|E_o|}{E}\right]^{\frac{1}{2}}\psi(\xi,x) \tag{V.84}$$

$$\sigma_f^{s,bw}(E) = \sigma_o^{bw}\,\frac{G_f^{bw}}{|G_t^{bw}|}\left[\frac{|E_o|}{E}\right]^{\frac{1}{2}}\psi(\xi,x)\ . \tag{V.85}$$

In the above

σ_o^{bw} = $\sigma_o^s G_t$ where σ_o^s is defined below Eq.V.79

G_t^{bw} = Breit-Wigner multilevel symmetric parameter for the total reaction which is 1 plus the symmetric level-level interference contribution

a^{bw} = a^s as defined in Eq.V.77 plus the asymmetric level-level interference contribution, all divided by G_t

G_γ^{bw} = Breit-Wigner multilevel symmetric parameter for the radiative capture reaction

= $\Gamma_\gamma^s/\Gamma_t^{bw}$

Γ_t^{bw} = the Breit-Wigner multilevel total line width

G_f^{bw} = Breit-Wigner multilevel symmetric parameter for the fission reaction

= Γ_f^s/Γ_t^{bw}

x = $2(E - E_o)/\Gamma_t^{bw}$

ξ = Γ_t^{bw}/Δ.

Multilevel Breit-Wigner p-wave resonance scattering, capture, and fission cross sections are, respectively evaluated using the single level expressions given by Eqs. V.80, V.81 and V.82 where σ_o^p is replaced by σ_o^{bw}, Γ_t^p is replaced by Γ_t^{bw}, Γ_γ^p is replaced by $G_\gamma^{bw}\,\Gamma_t^{bw}$, Γ_f^p is replaced by $G_f^{bw}\,\Gamma_t^{bw}$, and Γ_n^p is replaced by $\Gamma_t^{bw}(1 - G_\gamma^{bw} - G_f^{bw})$.

c. Multilevel Adler-Adler

Multilevel Adler-Adler resonance scattering, capture, and fission cross sections are, respectively evaluated using the expressions

$$\sigma_s^{aa} = \left[\frac{|E_o|}{E}\right]^{\frac{1}{2}} \frac{\sigma_o^{aa}}{|G_t^{aa}|} \left\{ G_t^{aa}\, \psi(\xi,x) + |G_t^{aa}|\, a^{aa}\, \chi(\xi,x) \right.$$

$$\left. - G_\gamma^{aa} \left[\psi(\xi,x) + b_\gamma\, \chi(\xi,x)\right] - \left[G_f^{aa}\ \psi(\xi,x) + b_f\, \chi(\xi,x)\right] \right\} \qquad \text{(V.86)}$$

$$\sigma_c^{aa}(E) = \sigma_o^{aa} \frac{G_\gamma^{aa}}{|G_t^{aa}|} \left[\frac{|E_o|}{E}\right]^{\frac{1}{2}} \left\{\psi(\xi,x) + b_\gamma\, \chi(\xi,x)\right\} \qquad \text{(V.87)}$$

$$\sigma_f^{aa}(E) = \sigma_o^{aa} \frac{G_f^{aa}}{|G_t^{aa}|} \left[\frac{|E_o|}{E}\right]^{\frac{1}{2}} \left\{\psi(\xi,x) + b_f\, \chi(\xi,x)\right\} \ . \qquad \text{(V.88)}$$

In the above

$$\sigma_o^{aa} = \frac{2.6039953 \times 10^6}{|E_o|} \left(\frac{A+1}{A}\right)^2 \frac{|G_t^{aa}|}{2\Gamma_t^{aa}}$$

$$G_t^{aa} = \sqrt{|E_o|}\left[G^T \cos 2\phi_\ell + H^T \sin 2\phi_\ell\right]$$

G^T = Adler-Adler symmetric total cross section parameter from ENDF/B

H^T = Adler-Adler antisymmetric total cross section parameter from ENDF/B

ϕ_ℓ = phase shift

Γ_t^{aa} = S- matrix total line width for the Adler-Adler formulation

$$a^{aa} = -0.5 \left\{\frac{H^T \cos 2\phi_\ell - G^T \sin 2\phi_\ell}{|G_t^{aa}|}\right\} \sqrt{|E_o|}$$

$$G_\gamma^{aa} = \sqrt{|E_o|}\left[G^c \cos 2\phi_\ell + H^c \sin 2\phi_\ell\right]$$

G^c = Adler-Adler symmetric capture cross section parameter from ENDF/B

H^c = Adler-Adler antisymmetric capture cross section parameter from ENDF/B

$$b_\gamma = -0.5 \left\{ \frac{H^c \cos 2\phi_\ell - G^c \sin 2\phi_\ell}{G_\gamma^{aa}} \right\} \sqrt{|E_o|}$$

$$G_f^{aa} = \sqrt{|E_o|} \left[G^F \cos 2\phi_\ell + H^F \sin 2\phi_\ell \right]$$

G^F = Adler-Adler symmetric fission cross section parameter from ENDF/B

H^F = Adler-Adler antisymmetric fission cross section parameter from ENDF/B

$$b_f = -0.5 \left\{ \frac{H^F \cos 2\phi_\ell - G^F \sin 2\phi_\ell}{G_f^{aa}} \right\} \sqrt{|E_o|}$$

$$x = 2(E - E_o)/\Gamma_t^{aa}$$

$$\xi = \Gamma_t^{aa}/\Delta$$

The various G and H parameters as obtained from ENDF/B are assumed to include the factor $2g_J/\sqrt{|E_o|}$. Thus the factor g_J does not appear explicitly in the expression for σ_o^{aa}.

E. Broad Group Edits

The hfg spatially integrated fluxes per unit lethargy as calculated from Eq. V.34 are summed over the corresponding ufg to obtain the ufg fluxes and these in turn are summed over the broad group involved to obtain the broad group fluxes. Thus the broad group J flux in mesh interval i is given by

$$\phi_J^{bg}(i) = \sum_j \phi_j(i)\, \Delta u. \qquad \text{(V.89)}$$

where the sum over hfg j extends over all hfg contained in bg J. The code edits the broad group fluxes per unit volume by dividing each of the $\phi_J^{bg}(i)$ by the corresponding mesh interval volume.

Each spatial region is made up of one or more spatial mesh intervals each of which contains the same mixture of isotopes. The region R integrated bg fluxes are obtained by summing Eq. V.89 to yield

$$\Phi_J^{bg}(R) = \sum_i \phi_J^{bg}(i) \qquad \text{(V.90)}$$

where the sum over i extends over all mesh intervals contained in region R.

The broad group, region dependent microscopic capture, fission, and scattering cross sections for each material m are obtained by dividing the reaction rate by the integrated flux. Therefore

$$\sigma^m_{x_J}(R) = \frac{\sum_i \sum_j \sigma^m_{x_j}(i)\ \phi_j(i)\ \Delta u}{\Phi^{bg}_J(R)} \qquad (V.91)$$

where x corresponds to capture, fission, or scattering. $\sigma^m_{x_j}(i)$ is the microscopic cross section for material m in mesh interval i and hfg j evaluated as described in Section D above. The sums over j and i as above extend over all hfg contained in bg J and all mesh intervals contained in region R.

Now in order to calculate the scattering cross section from broad group J to braod group K, we require the probability of scattering from each hfg j in bg J to bg K.

If we let u_j be the lower lethargy of hfg j in bg J, Δu_j be the lethargy width of hfg j, U_K be the lower lethargy of bg K, and ΔU_K be the lethargy width of bg K, then the probability of scattering by material m from hfg j into bg K, if all parts of bg K can be reached by scattering from hfg j, is given by

$$P^m(j \to K)\ \Delta u_j = \frac{1}{1-\alpha^m} \int_{U_K}^{U_K+\Delta U_K} du \int_{u_j}^{u_j+\Delta u_j} du'\ e^{-(u-u')}$$

$$= \frac{e^{\Delta u_j}-1}{1-\alpha^m} \left\{ e^{u_j} e^{-U_K} (1 - e^{-\Delta U_K}) \right\} . \qquad (V.92)$$

In the case of the lowest broad group, say bg L which can be reached by scattering from hfg J, since not all parts of bg L may be energetically reachable by scattering from hfg j,

$$P^m(j \to L) = \frac{1}{1-\alpha^m} \int_{u_j}^{u_j+\Delta u_j} du' \int_{U_L}^{u'+\varepsilon} du\ e^{-(u-u')}$$

$$= \frac{e^{\Delta u_j}-1}{1-\alpha^m} e^{u_j} e^{-U_L} - \frac{\alpha^m \Delta u_j}{1-\alpha^m} . \qquad (V.93)$$

In Eqs. V.92 and V.93, contributions are made from each of the materials in the mixture.

Using Eqs. V.92 or V.93 as appropriate, the scattering from broad group J to broad group K for material m in region R is given by

$$\sigma^m_{J\to K}(R) = \frac{\sum_i \sum_j \sigma^m_{s_j}(i)\ \phi_j(i)\ P^m(j\to K)}{\Phi^{bg}_J(R)} \qquad (V.94)$$

where the sums over i and j are as above.

For foil materilas, the capture, fission, and scattering cross sections are obtained as in Eq. V.91 where now the fluxes used are the averaged fluxes in each foil as given by Eq. V.62.

In addition to the region dependent cross sections, the code also edits quantities needed to calculate cell averaged macroscopic cross sections.

The all volume-averaged atom densities for each material m are computed as

$$N^m(C) = \frac{\sum_R n^m(R)\ V(R)}{\sum_R V(R)} \qquad (V.95)$$

where $n^m(R)$ is the atom density of material m in the composition contained in region R and V(R) is the volume of region R. The sums extend over all regions in the cell.

Spatial self-shielding factors are computed for each broad group J and material m as

$$F_J^m = \frac{\sum_R n^m(R)\ \Phi_J^{bg}(R)\ V(R)}{N^m(C) \sum_R \Phi_J^{bg}(R)\ V(R)} \quad . \qquad (V.96)$$

The product of $N^m(C)$ and F_J^m represents the effective cell averaged atom density for use in creating effective cell averaged macroscopic cross sections. The consistent cell averaged microscopic cross sections for use with the effective atom densities $N^m(C)F_J^m$ are given by

$$\bar{\sigma}_{x_J}^m(C) = \frac{\sum_R \Phi_J^{bg}(R)\ \sigma_{x_J}^m(R)\ n^m(R)\ V(R)}{\sum_R \Phi_J^{bg}(R)\ n^m(R)\ V(R)} \quad . \qquad (V.97)$$

Thus the effective cell averaged macroscopic cross sections can be obtained from the product $N^m(C)\ F_J^m\ \bar{\sigma}_{x_J}^m(C)$. Equation V.97 is used for capture, fission, scattering, and for transfer between broad groups.

VI. A GUIDE TO USER APPLICATION

A. Standard Path STP015

STP015 is a path driver of the ARC System which invokes the following modules to provide the MC^2-2 capability.

CSI010 (Area 4)	Processes BCD input from files A.MCC2 and A.NIP
CSC004 (Area 5)	Performs the unresolved resonance calculation
CSC005 (Area 6)	Performs the resolved resonance calculation
CSC006 (Area 65)	Calculates Σ_p and performs resolved-unresolved resonance overlap calculations
CSC008 (Area 7)	Calculates homogenized ultra-fine-group (ufg) cross sections, elastic scattering matrices, and moderating parameters
CSC009 (Area 8)	Calculates the ufg real spectrum using multigroup and continuous slowing down (CSD) algorithms, obtains a critical buckling, and prepares broad group (bg) cross sections
CSC010 (Area 9)	Calculates the bg fundamental mode real and adjoint spectra and obtains a critical buckling.
CSC011 (RABANL)	Performs a hyper-fine-group (hfg) integral transport calculation and prepares rigorous resolved resonance cross sections
CSE009	Edits broad group cross sections from data set ISOTXS
CSE007	Prepares a single or double precision ARC System XS.ISO data set from the CCCC data set ISOTXS
CSE012	Edits data set XS.ISO

The flow through the code as shown in the flow diagram, Fig. 9 is controlled by standard path STP015 in conjunction with the user supplied data in the A.STP015 BCD data set (Appendix B). As can be seen, the various code areas may be selectively included or excluded on user option. As a specific example, the user may select only CSI010 and RABANL, thereby effecting the equivalent of a RABBLE[5] or RABID[6] standalone calculation. Similarly if only module CSE012 is selected, a standalone XS.ISO editor capability is effected. Also e.g., if data sets related to the unresolved resonance calculation CSC004 are saved, a subsequent related execution of STP015 could reduce execution time by eliminating execution of this module.

A listing of the path STP015 is provided in Fig. 10.

B. Job Control Language Procedure ARCSP015

The Job Control Language procedure ARCSP015 is listed in Fig. 11. The procedure is consistent with IBM JCL conventions and with release 3.1 of the Attached Support Processor (ASP). The data set blocking is oriented toward use with 3330 magnetic disks.

The symbolic parameters used for the various datasets, their default values, usage, and corresponding DDNAME are given within the listing of the procedure. In addition, the contents of each of the datasets is given on comment cards in the procedure.

The parameters FULLBLK, HALFBLK, and UNITS which are used in many of the datasets are defined with the other symbolic parameters. The block size defaults of 12280 and 6136 for FULLBLK and HALFBLK are consistent with use of 3330 disks, and with the fact that IBM allocates space for buffers in blocks of 2K contiguous bytes (256 real*8 words). In the case of unformatted Fortran data sets (double buffered by default), the number of bytes of core required for buffers is given by 2*BLKSIZE+8 where BLKSIZE is given on the DD card and is rounded up to the nearest double word boundary. Thus, for example in the case of FULLBLK, 24576 bytes would be allocated for buffer space which corresponds to exactly 12, 2K blocks. This is only 8 bytes more than is required for the two buffers. The use of very closely an integral number of 2K byte blocks avoids the problem of possible core fragmentation when data sets are written, closed (rewound) and then read again several times during a run.

The use of SASCR and BATCHDSK for the UNIT parameter throughout the procedure correspond to ANL conventions for generic names corresponding to the class of units involved. SASCR is used to designate permanently resident disk packs for scratch data. BATCHDSK corresponds to both permanently resident and setup disk packs and is used for those files which may be saved on user option for later use. The default names for parameters MCC2F1, MCC2F2, ..., MCC2F8 correspond to the eight MC^2-2 library files currently in use. The PRELIB and POSTLIB parameters used in the STEPLIB DD statement are provided to simplify concatenation of program library data sets. They default to empty partitioned data sets.

Through use of the catalogued procedure, the amount of JCL which must be provided by the user is vastly decreased. In particular, Fig. 12 lists the minimal JCL required to execute a problem using the catalogued procedure ARCSP015. Further illustrations of the use of this procedure and of the symbolic parameters are given in Section D, Sample Problem Input.

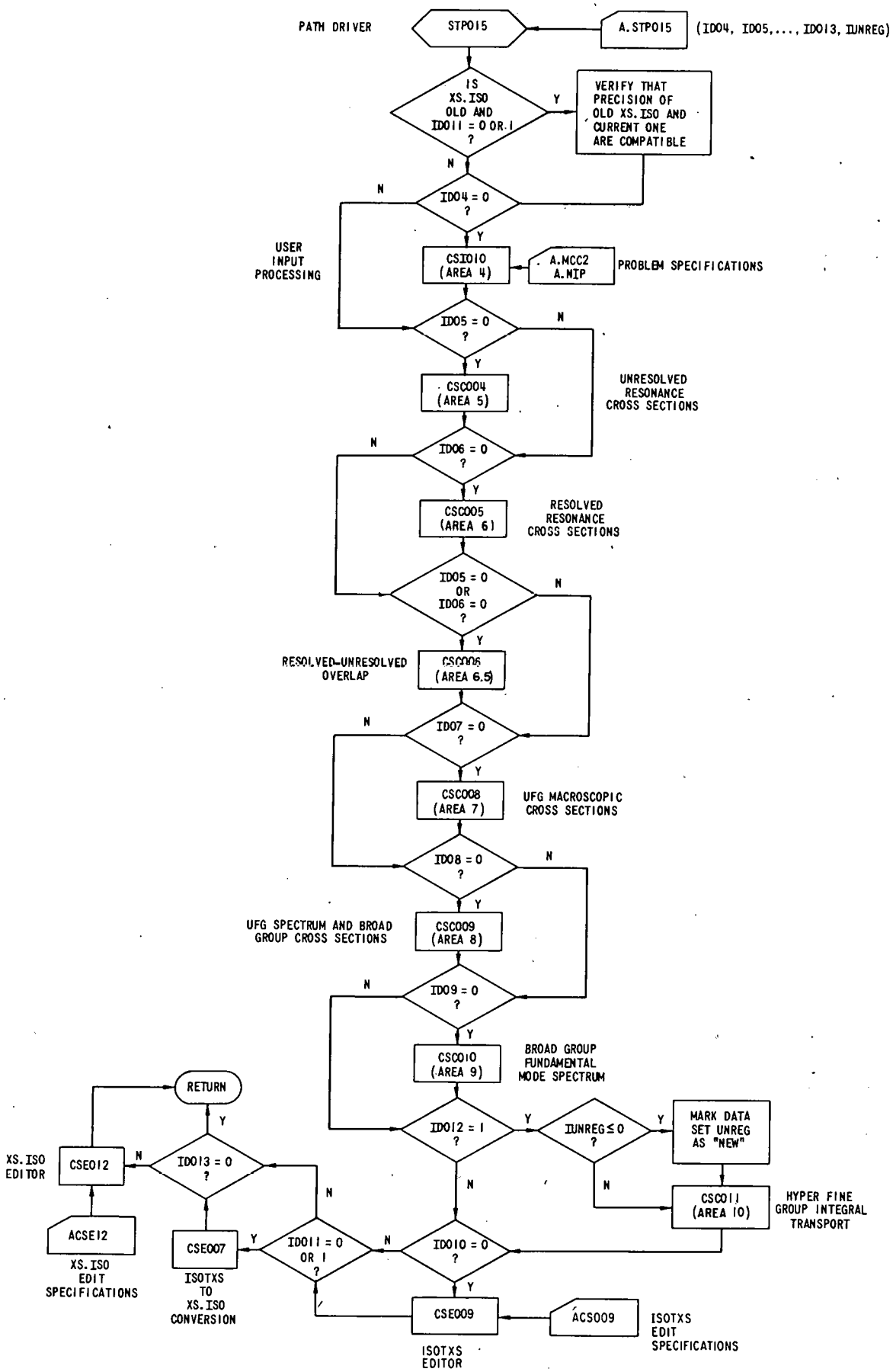

Fig. 9. MC^2-2 Module Flow Diagram

```
C
C     STP015 IS A STANDARD PATH DRIVER OF THE ARC SYSTEM WHICH
C     CONTROLS THE MCC-2 CROSS SECTION PREPARATION CAPABILITY.
C
C     MODULES INVOKED BY STP015
C
C     CSI010            MCC-2 INPUT PROCESSOR
C     CSC004            MCC-2/SDX UNRESOLVED RESONANCE CALCULATION
C     CSC005            MCC-2/SDX RESOLVED RESONANCE CALCULATION
C     CSC006            RESOLVED-UNRESOLVED RESONANCE OVERLAP
C     CSC008            MCC-2 ULTRA-FINE-GROUP MACROSCOPIC DATA
C                       PROCESSOR
C     CSC009            MCC-2 ULTRA-FINE-GROUP SPECTRUM CALCULATION
C                       AND BROAD GROUP COLLAPSE
C     CSC010            BROAD-GROUP PL SPECTRUM CALCULATION
C     CSC011            HYPER-FINE-GROUP INTEGRAL TRANSPORT SPECTRUM
C                       CALCULATION
C     CSE009            EDITOR OF FILE ISOTXS
C     CSE007            ISOTXS TO XS.ISO FORMAT CONVERSION
C     CSE012            EDITOR OF FILE XS.ISO
C     NUE003            SIMPLOTTER LINE PRINTER GRAPHICS
C
C
C     DECLARE ALL LITERAL VARIABLES TO BE DOUBLE PRECISION
C
CIBM
      DOUBLE PRECISION DSNAME,CSI010,CSC004,CSC005,CSC006,NUE003,
     1                 CSC008,CSC009,CSC010,CSE009,STP015,APATH,CSE007,
     2                 XSISO,CSC011,UNREG,PREC,CSE012
CIBM
      DIMENSION NSTAND(6),PREC(2),DSNAME(89)
      COMMON /OUTPUT/NOUT
C
C     SET LITERAL VARIABLES IN DATA STATEMENTS
C
      DATA CSI010/6HCSI010/,CSC004/6HCSC004/,CSC005/6HCSC005/,
     1     CSC006/6HCSC006/,CSC008/6HCSC008/,CSC009/6HCSC009/,
     2     CSC010/6HCSC010/,CSE009/6HCSE009/,STP015/6HSTP015/,
     3     NUE003/6HNUE003/,CSE007/6HCSE007/,APATH/8HA.STP015/,
     4     XSISO/6HXS.ISO/,CSC011/6HCSC011/,UNREG/6HUNREG /,
     5     CSE012/6HCSE012/
      DATA PREC/6HDOUBLE,6HSINGLE/
      DATA DSNAME/
     16HA.MCC2,6HA.NIP ,8HA.STP015,6HATNUAT,6HBC    ,6HBGRES ,
     26HGEOM1 ,6HGRPORD,6HISOTXS,6HLORENZ,6HMACTOT,6HMCC2F1,
     36HMCC2F2,6HMCC2F3,6HMCC2F4,6HMCC2F5,6HMCC2F6,6HMCC2F7,
     46HMCC2F8,6HMICTOT,6HOLDSGS,6HOPTICL,6HPLOTIT,6HPRBCHI,
     56HPRBSPC,6HRESINT,6HSCR001,6HSCR002,6HSCR003,6HSCR004,
     66HSCR005,6HSIGMAP,6HSMSIGS,6HSPECTR,6HSPECXS,6HSRATES,
     76HUNREG ,6HUNRES ,6HXS.ISO,6HXSISO2,6HIRESCS,
```

Fig. 10. MC^2-2 Path Driver Listing

```
     86HBIGXS1,6HBIGXS2,6HBIGXS3,6HBIGXS4,6HBIGXS5,6HBIGXS6,
     96HBIGXS7,6HBIGXS8,6HBIGXS9,6HBIGXSA,6HBIGXSB,6HBIGXSC,
     A6HBIGXSD,6HBIGXSE,6HBIGXSF,6HBIGXSG,6HBIGXSH,6HBIGXSI,
     B6HBIGXSJ,6HBIGXSK,6HBIGXSL,6HBIGXSM,6HBIGXSN,6HBIGXSO,
     C6HBIGXSP,6HRANDOM,6HRESDAT,6HACS009,6HACSE12,6H$     /
      DATA I0/0/,IDO4/0/,IDO5/0/,IDO6/0/,IDO7/0/,IDO8/0/,IDO9/0/,
     1     IDO10/0/,IDO11/0/,I1/1/,I2/2/,IDO12/0/,NSTAND/2*0/,IDO13/0/,
     2     IUNREG/0/
      NOUT=6
      CALL SYSTEM(DSNAME)
      CALL BCDDS(STP015,N1)
      IF (N1.LE.-2) GO TO 500
C
C     ESTABLISH LOGICAL UNIT NUMBERS FOR FILES MCC2F1-MCC2F8
C     IN ORDER TO AVOID THE NEED FOR THEIR SPECIFICATION IN BLOCK=OLD
C
      DO 10 I=12,19
      CALL SNIFF(DSNAME(I),IDUM,I1)
   10 CONTINUE
      CALL SNIFF(XSISO,IXSISO,I0)
      CALL SNIFF(APATH,IAPATH,I0)
      IF (IAPATH.LE.0) GO TO 110
C
C     READ DATA SET A.STP015
C
      READ (IAPATH,1000) APATH,JJ,KK,(NSTAND(I),I=1,JJ)
      IF (NSTAND(1).LE.0) GO TO 100
      READ (IAPATH,1100) IDO4,IDO5,IDO6,IDO7,IDO8,IDO9,IDO10,IDO11,
     1                   IDO12,IDO13
  100 CONTINUE
      IF (NSTAND(2).GT.0) READ (IAPATH,1100) IUNREG
C*********************************************************************
      REWIND IAPATH
C*********************************************************************
  110 CONTINUE
C
C     CHECK ON PRECISION OF EXISTING XS.ISO FILE
C
      IF (IXSISO.LE.0.OR.(IDO11.NE.0.AND.IDO11.NE.1)) GO TO 130
      NWDS=6
      NSTAND(6)=0
C
C     READ RECORD 1 OF DATA SET XS.ISO
C
      CALL REED(IXSISO,I1,NSTAND,NWDS,I0)
C
C     REWIND DATA SET XS.ISO
C
      CALL REED(IXSISO,I0,DUM,I0,I0)
      IF (NSTAND(6).EQ.IDO11) GO TO 130
```

Fig. 10. MC^2-2 Path Driver Listing (Contd.)

```
      WRITE (NOUT,1200) PREC(IDO11+1),PREC(2-IDO11),PREC(2-IDO11)
      IDO11=NSTAND(6)
  130 CONTINUE
C
C     INVOKE AREA 4
C
      IF (IDO4.EQ.0) CALL LINK(CSI010)
C
C     INVOKE AREA 5
C
      IF (IDO5.EQ.0) CALL LINK(CSC004)
C
C     INVOKE AREA 6
C
      IF (IDO6.EQ.0) CALL LINK(CSC005)
C
C     INVOKE AREA 6.5
C
      IF (IDO5.EQ.0.OR.IDO6.EQ.0) CALL LINK(CSC006)
C
C     INVOKE AREA 7
C
      IF (IDO7.EQ.0) CALL LINK(CSC008)
C
C     INVOKE AREA 8
C
      IF (IDO8.EQ.0) CALL LINK(CSC009)
C
C     INVOKE AREA 9
C
      IF (IDO9.EQ.0) CALL LINK(CSC010)
      IF (IDO12.NE.1) GO TO 120
      IF (IUNREG.LE.0) CALL SNIFF(UNREG,IUNREG,I2)
C
C     INVOKE AREA 10
C
      CALL LINK(CSC011)
  120 CONTINUE
C
C     EDIT BROAD GROUP CROSS SECTIONS
C
      IF (IDO10.EQ.0) CALL LINK(CSE009)
C
C     PREPARE A DOUBLE PRECISION OR SINGLE PRECISION VERSION OF
C     DATA SET XS.ISO ACCORDING TO WHETHER IDO11 IS 0 OR 1, RESPECTIVELY
C
      IF (IDO11.EQ.0.OR.IDO11.EQ.1) CALL LINK(CSE007,IDO11)
C
C     EDIT DATA SET XS.ISO
C
```

Fig. 10. MC^2-2 Path Driver Listing (Contd.)

```
      IF(IDO13.NE.0) CALL LINK(CSE012)
C
C     INVOKE THE SIMPLOTTER PRINTER GRAPHICS PACKAGE
C
      CALL LINK(NUE003,I0)
  500 CONTINUE
 1000 FORMAT(A8,2I5/(16I5))
 1100 FORMAT(6X,11I6)
 1200 FORMAT(1H0,129(1H*)/1H ,1H*,3X,A6,46H PRECISION CROSS SECTIONS MAY
     1 NOT BE ADDED TO ,A6,45H PRECISION XS.ISO. NEW DATA ARE PROCESSED
     2IN ,A6,11H PRECISION.,4X,1H*/1H ,129(1H*))
      RETURN
      END
```

Fig. 10. MC^2-2 Path Driver Listing (Contd.)

```
//ARCSP015 PROC ATNUAT='&ATNUAT',DEST=A,                                X
//              DMPDEST=F,                                              X
//              FULLBLK=12280,GRPDSP='(NEW,DELETE)',                    X
//              GRPJCL=',UNIT=(SASCR,SEP=(DUMMY1,DUMMY2))',             X
//              GRPORD='&GRPORD',HALFBLK=6136,                          X
//              ISOCYL=1,ISODSP='(NEW,DELETE)',                         X
//              ISOJCL=',UNIT=SASCR',ISOTXS='&ISOTXS',                  X
//              MCC2F1='C116.MCC2F1.MEV14.V4',                          X
//              MCC2F2='C116.MCC2F2',                                   X
//              MCC2F3='C116.MCC2F3.MEV14.V4',                          X
//              MCC2F4='C116.MCC2F4.MEV14.V4',                          X
//              MCC2F5='C116.MCC2F5.MEV14.V4',                          X
//              MCC2F6='C116.MCC2F6.MEV14.V4',                          X
//              MCC2F7='C116.MCC2F7.MEV14.V4',                          X
//              MCC2F8='C116.MCC2F8.MEV14.V4',                          X
//              MCC2VOL=,MICRDSP='(NEW,DELETE)',MICRVOL=,               X
//              MICRXS1='&MICRXS1',MICRXS2='&MICRXS2',                  X
//              MODLIB1='C116.B09202.MODLIB',                           X
//              MODLIB2='C116.ARC.MODLIB',                              X
//              OLDSGS=NULLFILE,OLDSVOL=,PATH=STP015,                   X
//              POSTLIB='SYS1.DUMMYLIB',PRELIB='SYS1.DUMMYLIB',         X
//              REGN=700K,RESBLK=12280,RESDSP='(NEW,DELETE)',           X
//              RESINT='&RESINT',RESJCL=',UNIT=SASCR',                  X
//              SCATBLK=12280,SCATDSP='(NEW,DELETE)',                   X
//              SCATJCL=',SUBALLOC=(CYL,(20,3),DUMMY2)',                X
//              SMSIGS='&SMSIGS',SPECDSP='(NEW,DELETE)',                X
//              SPECTR='&SPECTR',SPECJCL=',UNIT=SASCR',                 X
//              TIMLIM='(600,0)',UNITS=BATCHDSK,UNITSCR=SASCR,          X
//              UNRES='&UNRES',XSBLK1=3156,XSBLK2=6447
//*
//*     ****************************************************************
//*     *                                                              *
//*     *          CATALOGED PROCEDURE FOR MC**2-2 PROBLEMS            *
//*     *                                                              *
//*     ****************************************************************
//*
//*  ********************************************************************************
//*
//*  PARAMETER        DEFAULT VALUE                  USAGE                FTNNF001
//*  =========        =============                  =====                ========
//*
//*   PATH          STP015                      PROGRAM NAME              EXEC
//*   TIMLIM        (600,0)                     STEP TIME LIMIT           EXEC
//*   REGN          700K                        STEP REGION SIZE          EXEC
//*   MODLIB1       C116.B09202.MODLIB          FIRST REAL LIBRARY      STEPLIB
//*   MODLIB2       C116.ARC.MODLIB             ARC SYSTEM LIBRARY      STEPLIB
//*   PRELIB        SYS1.DUMMYLIB               FIRST STEP LIBRARY      STEPLIB
//*   POSTLIB       SYS1.DUMMYLIB               LAST STEP LIBRARY       STEPLIB
//*   DEST          A                           OUTPUT DEST. (PRINTER)    06
//*   DMPDEST       F                           ROUTE DUMP TO FICHE     SYSUDUMP
```

Fig. 11. MC^2-2 JCL Procedure

```
//*   GRPORD      &GRPORD                          DSN FOR FILE GRPORD      18
//*   GRPDSP      (NEW,DELETE)                     DISPOSITION OF GRPORD    18
//*   GRPJCL      ,UNIT=(SASCR,SEP=(DUMMY1,DUMMY2))  GRPORD UNIT & VOL     18
//*   ISOTXS      &ISOTXS                          DSN FOR FILE ISOTXS      19
//*   ISODSP      (NEW,DELETE)                     DISPOSITION OF ISOTXS    19
//*   ISOJCL      ,UNIT=SASCR                      ISOTXS UNIT AND VOLUME   19
//*   ISOCYL      1                                NO. CYL FOR X SECTIONS   19,50
//*   XSBLK2      6447                             X SECTION BLOCKING       19,50
//*   MCC2F1      C116.MCC2F1.MEV14.V4             LIBRARY FILE 1 DSN       22
//*   MCC2F2      C116.MCC2F2                      LIBRARY FILE 2 DSN       23
//*   MCC2F3      C116.MCC2F3.MEV14.V4             LIBRARY FILE 3 DSN       24
//*   MCC2F4      C116.MCC2F4.MEV14.V4             LIBRARY FILE 4 DSN       25
//*   MCC2F5      C116.MCC2F5.MEV14.V4             LIBRARY FILE 5 DSN       26
//*   MCC2F6      C116.MCC2F6.MEV14.V4             LIBRARY FILE 6 DSN       27
//*   MCC2F7      C116.MCC2F7.MEV14.V4             LIBRARY FILE 7 DSN       28
//*   MCC2F8      C116.MCC2F8.MEV14.V4             LIBRARY FILE 8 DSN       29
//*   MCC2VOL     ------                           LIBRARY VOLUME         22-29
//*   OLDSGS      NULLFILE                         RESTART ELASTIC MATRICES 31
//*   OLDSVOL     ------                           VOLUME FOR OLDSGS        31
//*   SMSIGS      &SMSIGS                          PROBLEM ELASTIC MATRICES 43
//*   SCATBLK     12280                            BLKSIZE FOR SMSIGS       43
//*   SCATDSP     (NEW,DELETE)                     DISPOSITION OF SMSIGS    43
//*   SCATJCL     ,SUBALLOC=(CYL,(20,3),DUMMY2)    SMSIGS UNIT,SPACE & VOL  43
//*   SPECTR      &SPECTR                          DSN FOR SPECTRUM FILE    44
//*   SPECDSP     (NEW,DELETE)                     DISPOSITION OF SPECTRUM  44
//*   SPECJCL     ,UNIT=SASCR                      SPECTRUM UNIT AND VOLUME 44
//*   MICRXS1     &MICRXS1                         XS.ISO FILE 1 DSN        49
//*   XSBLK1      3156                             BLOCKING FOR &MICRXS1    49
//*   MICRXS2     &MICRXS2                         XS.ISO FILE 2 DSN        50
//*   MICRDSP     (NEW,DELETE)                     DISPOSITION OF XS.ISO  49-50
//*   MICRVOL     ------                           VOLUME OF FILE XS.ISO  49-50
//*   ATNUAT      &ATNUAT                          DSN FOR FILE ATNUAT      14
//*   RESINT      &RESINT                          DSN FOR FILE RESINT      36
//*   UNRES       &UNRES                           DSN FOR FILE UNRES       48
//*
//*   THE FOLLOWING THREE PARAMETERS ARE APPLICABLE TO THE THREE
//*   RESONANCE FILES ATNUAT, RESINT AND UNRES
//*
//*   RESBLK      12280                            FILE BLKSIZE          14,36,48
//*   RESDSP      (NEW,DELETE)                     FILE DISPOSITION      14,36,48
//*   RESJCL      ,UNIT=SASCR                      FILE UNIT AND VOLUME  14,36,48
//*
//*   THE FOLLOWING THREE PARAMETERS DEFINE UNIT AND BLKSIZE FOR A
//*   VARIETY OF FILES
//*
//*   FULLBLK     12280                            FULL TRACK BLOCKING
//*   HALFBLK     6136                             HALF TRACK BLOCKING
//*   UNITS       BATCHDSK                         GENERIC UNIT NAME
//*   UNITSCR     SASCR                            GENERIC SCRATCH UNIT
//*
```

Fig. 11. MC^2-2 JCL Procedure (Contd.)

```
//*  ************************************************************************
//*
//STP015 EXEC PGM=&PATH,TIME=&TIMLIM,REGION=&REGN
//STEPLIB DD DSN=&PRELIB,DISP=SHR
//         DD DSN=&MODLIB1,DISP=SHR
//         DD DSN=&MODLIB2,DISP=SHR
//         DD DSN=&POSTLIB,DISP=SHR
//DUMMY1 DD DSN=&DUM1,UNIT=&UNITSCR,SPACE=(CYL,27,,CONTIG)
//DUMMY2 DD DSN=&DUM2,UNIT=&UNITSCR,SPACE=(CYL,55,,CONTIG)
//FT05F001 DD DDNAME=SYSIN
//*            BCD INPUT
//FT06F001 DD SYSOUT=&DEST,
//            DCB=(RECFM=FBA,LRECL=133,BLKSIZE=1596)
//*            PRINTED OUTPUT
//FT07F001 DD SYSOUT=B
//*            PUNCHED OUTPUT
//FT09F001 DD UNIT=&UNITSCR,SPACE=(CYL,(1,1)),
//            DCB=(RECFM=FBS,LRECL=80,BLKSIZE=3040)
//*            ARC SYSTEM SPOOLED INPUT FILE
//FT11F001 DD DSN=&AMCC2,UNIT=&UNITSCR,SPACE=(TRK,(1,1)),
//            DCB=(RECFM=FBS,LRECL=80,BLKSIZE=3040)
//*            MCC-2 ALPHANUMERIC INPUT
//FT12F001 DD DSN=&ANIP,UNIT=&UNITSCR,SPACE=(TRK,(1,1)),
//            DCB=(RECFM=FBS,LRECL=80,BLKSIZE=3040)
//*            GENERAL NEUTRONICS ALPHANUMERIC INPUT
//FT13F001 DD DSN=&APATH,UNIT=&UNITSCR,SPACE=(TRK,(1,1)),
//            DCB=(RECFM=FBS,LRECL=80,BLKSIZE=320)
//*            MCC-2 PATH ALPHANUMERIC INPUT
//FT14F001 DD DSN=&ATNUAT,
//            DISP=&RESDSP&RESJCL,
//            DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&RESBLK),
//            SPACE=(CYL,(1,1))
//*            UNRESOLVED RESONANCE ATTENUATION FACTORS
//FT15F001 DD DSN=&BC,UNIT=&UNITSCR,SPACE=(TRK,(1,1)),
//            DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*            BOUNDARY CONDITIONS
//FT16F001 DD DSN=&BGRES,UNIT=&UNITSCR,SPACE=(CYL,(1,1)),
//            DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*            BROAD GROUP RESONANCE CROSS SECTIONS
//FT17F001 DD DSN=&GEOM1,UNIT=&UNITSCR,SPACE=(TRK,(3,1),RLSE),
//            DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*            GEOMETRY DATA WRITTEN BY MCC-2 INPUT PROCESSOR
//FT18F001 DD DSN=&GRPORD,
//            DISP=&GRPDSP&GRPJCL,
//            SPACE=(CYL,(50,5),RLSE),
//            DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK,DEN=3)
//*            GROUP ORDERED INELASTIC AND (N,2N) DATA
//FT19F001 DD DSN=&ISOTXS,
//            DISP=&ISODSP&ISOJCL,
//            SPACE=(CYL,(&ISOCYL,1)),
```

Fig. 11. MC^2-2 JCL Procedure (Contd.)

```
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&XSBLK2)
//*            BROAD GROUP CROSS SECTION FILE IN CCCC FORMAT ISOTXS
//FT20F001 DD DSN=&LORENZ,UNIT=&UNITSCR,SPACE=(CYL,(1,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*            LORENTZIAN J-INTEGRALS FOR WIDE RESONANCES
//FT21F001 DD DSN=&MACTOT,UNIT=&UNITSCR,SPACE=(CYL,(1,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*            MACROSCOPIC TOTAL CROSS SECTION
//FT22F001 DD DSN=&MCC2F1,
//             UNIT=&UNITS,DISP=SHR,
//             VOL=(,RETAIN,SER=&MCC2VOL)
//*            FILE 1 OF MCC-2 LIBRARY
//FT23F001 DD DSN=&MCC2F2,
//             UNIT=&UNITS,DISP=SHR,
//             VOL=(,RETAIN,SER=&MCC2VOL)
//*            FILE 2 OF MCC-2 LIBRARY
//FT24F001 DD DSN=&MCC2F3,
//             UNIT=&UNITS,DISP=SHR,
//             VOL=(,RETAIN,SER=&MCC2VOL)
//*            FILE 3 OF MCC-2 LIBRARY
//FT25F001 DD DSN=&MCC2F4,
//             UNIT=&UNITS,DISP=SHR,
//             VOL=(,RETAIN,SER=&MCC2VOL)
//*            FILE 4 OF MCC-2 LIBRARY
//FT26F001 DD DSN=&MCC2F5,
//             UNIT=&UNITS,DISP=SHR,
//             VOL=(,RETAIN,SER=&MCC2VOL)
//*            FILE 5 OF MCC-2 LIBRARY
//FT27F001 DD DSN=&MCC2F6,
//             UNIT=&UNITS,DISP=SHR,
//             VOL=(,RETAIN,SER=&MCC2VOL)
//*            FILE 6 OF MCC-2 LIBRARY
//FT28F001 DD DSN=&MCC2F7,
//             UNIT=&UNITS,DISP=SHR,
//             VOL=(,RETAIN,SER=&MCC2VOL)
//*            FILE 7 OF MCC-2 LIBRARY
//FT29F001 DD DSN=&MCC2F8,
//             UNIT=&UNITS,DISP=SHR,
//             VOL=(,RETAIN,SER=&MCC2VOL)
//*            FILE 8 OF MCC-2 LIBRARY
//FT30F001 DD DSN=&MICTOT,UNIT=&UNITSCR,SPACE=(CYL,(1,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*            MICROSCOPIC TOTAL CROSS SECTIONS
//FT31F001 DD DSN=&OLDSGS,
//             UNIT=&UNITS,DISP=(OLD,KEEP),
//             VOL=(,RETAIN,SER=&OLDSVOL)
//*            MICROSCOPIC SCATTERING MATRICES SAVED FROM PREVIOUS
//*            EXECUTION FOR RESTART PURPOSES
//FT32F001 DD DSN=&OPTICL,UNIT=&UNITSCR,SPACE=(CYL,(1,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
```

Fig. 11. MC^2-2 JCL Procedure (Contd.)

```
//*              OPTICAL THICKNESS DATA
//FT33F001 DD DSN=&PLOTIT,UNIT=&UNITSCR,SPACE=(TRK,(1,1)),
//              DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*              SIMPLOTTER DATA FILE
//FT34F001 DD DSN=&PRBCHI,UNIT=&UNITSCR,SPACE=(CYL,(1,1)),
//              DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*              FISSION SPECTRUM DATA
//FT35F001 DD DSN=&PRBSPC,UNIT=&UNITSCR,SPACE=(TRK,(1,1)),
//              DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*              MCC-2 GENERAL PROBLEM SPECIFICATIONS
//FT36F001 DD DSN=&RESINT,
//              DISP=&RESDSP&RESJCL,
//              DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&RESBLK),
//              SPACE=(CYL,(1,1))
//*              RESOLVED RESONANCE J-INTEGRALS
//FT37F001 DD DSN=&SCR001,SUBALLOC=(CYL,(1,1),DUMMY1),
//              DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*              SCRATCH DATA
//FT38F001 DD DSN=&SCR002,SUBALLOC=(CYL,(1,1),DUMMY1),
//              DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*              SCRATCH DATA
//FT39F001 DD DSN=&SCR003,SUBALLOC=(CYL,(23,1),DUMMY1),
//              DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*              SCRATCH DATA
//FT40F001 DD DSN=&SCR004,SUBALLOC=(CYL,(1,1),DUMMY1),
//              DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*              SCRATCH DATA
//FT41F001 DD DSN=&SCR005,SUBALLOC=(CYL,(1,1),DUMMY1),
//              DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*              SCRATCH DATA
//FT42F001 DD DSN=&SIGMAP,UNIT=&UNITSCR,SPACE=(CYL,(1,1)),
//              DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*              POTENTIAL SCATTERING CROSS SECTIONS
//FT43F001 DD DSN=&SMSIGS,
//              DISP=&SCATDSP&SCATJCL,
//              DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&SCATBLK)
//*              MICROSCOPIC ELASTIC SCATTERING MATRICES
//FT44F001 DD DSN=&SPECTR,
//              DISP=&SPECDSP&SPECJCL,SPACE=(TRK,(1,1)),
//              DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//*              ULTRA-FINE-GROUP FLUX AND CURRENT SPECTRA
//FT45F001 DD DSN=&SPECXS,UNIT=&UNITSCR,SPACE=(CYL,(1,1)),
//              DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*              ULTRA-FINE-GROUP MACROSCOPIC CROSS SECTIONS AND
//*              MODERATING PARAMETERS
//FT46F001 DD DSN=&SRATES,UNIT=&UNITSCR,SPACE=(TRK,(1,1)),
//              DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*              SCATTERING COLLISION DENSITY AND EXTERNAL SOURCE
//*              FOR INTEGRAL TRANSPORT CALCULATION
//FT47F001 DD DSN=&UNREG,UNIT=&UNITSCR,SPACE=(CYL,(1,1)),
```

Fig. 11. MC^2-2 JCL Procedure (Contd.)

```
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*            UNRESOLVED MICROSCOPIC ULTRA-FINE-GROUP CROSS SECTIONS
//FT48F001 DD DSN=&UNRES,
//             DISP=&RESDSP&RESJCL,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&RESBLK),
//             SPACE=(CYL,(1,1))
//*            UNRESOLVED RESONANCE CROSS SECTION-ESTAR PAIRS
//FT49F001 DD DSN=&MICRXS1,
//             UNIT=&UNITS,VOL=(,RETAIN,SER=&MICRVOL),
//             DISP=&MICRDSP,SPACE=(TRK,(1,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&XSBLK1)
//*            FILE 1 OF BROAD GROUP XS.ISO CROSS SECTION FILE
//FT50F001 DD DSN=&MICRXS2,
//             UNIT=&UNITS,VOL=(,RETAIN,SER=&MICRVOL),
//             DISP=&MICRDSP,SPACE=(CYL,(&ISOCYL,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&XSBLK2)
//*            FILE 2 OF BROAD GROUP XS.ISO CROSS SECTION FILE
//FT51F001 DD DSN=&IRESCS,UNIT=&UNITSCR,SPACE=(TRK,(1,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)
//*            BROAD GROUP INTEGRAL TRANSPORT RESONANCE CROSS SECTIONS
//*   ************************************************************
//*   THE FOLLOWING 25 FILES (BIGXS1-BIGXSP) ARE SCRATCH FILES TO
//*   CONTAIN THE MACROSCOPIC ELASTIC SCATTERING MATRICES
//*   ************************************************************
//FT52F001 DD DSN=&BIGXS1,SUBALLOC=(CYL,(2,1),DUMMY2),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT53F001 DD DSN=&BIGXS2,SUBALLOC=(CYL,(2,1),DUMMY2),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT54F001 DD DSN=&BIGXS3,SUBALLOC=(CYL,(2,1),DUMMY2),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT55F001 DD DSN=&BIGXS4,SUBALLOC=(CYL,(2,1),DUMMY2),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT56F001 DD DSN=&BIGXS5,SUBALLOC=(CYL,(2,1),DUMMY2),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT57F001 DD DSN=&BIGXS6,SUBALLOC=(CYL,(2,1),DUMMY2),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT58F001 DD DSN=&BIGXS7,SUBALLOC=(CYL,(2,1),DUMMY2),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT59F001 DD DSN=&BIGXS8,SUBALLOC=(CYL,(2,1),DUMMY2),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT60F001 DD DSN=&BIGXS9,SUBALLOC=(CYL,(2,1),DUMMY2),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT61F001 DD DSN=&BIGXSA,SUBALLOC=(CYL,(2,1),DUMMY2),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT62F001 DD DSN=&BIGXSB,SPACE=(CYL,(0,1)),UNIT=&UNITSCR,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT63F001 DD DSN=&BIGXSC,SPACE=(CYL,(0,1)),UNIT=&UNITSCR,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT64F001 DD DSN=&BIGXSD,SPACE=(CYL,(0,1)),UNIT=&UNITSCR,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
```

Fig. 11. MC^2-2 JCL Procedure (Contd.)

```
//FT65F001 DD DSN=&BIGXSE,SPACE=(CYL,(0,1)),UNIT=&UNITSCR,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT66F001 DD DSN=&BIGXSF,SPACE=(CYL,(0,1)),UNIT=&UNITSCR,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT67F001 DD DSN=&BIGXSG,SPACE=(CYL,(0,1)),UNIT=&UNITSCR,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT68F001 DD DSN=&BIGXSH,SPACE=(CYL,(0,1)),UNIT=&UNITSCR,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT69F001 DD DSN=&BIGXSI,SPACE=(CYL,(0,1)),UNIT=&UNITSCR,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT70F001 DD DSN=&BIGXSJ,SPACE=(CYL,(0,1)),UNIT=&UNITSCR,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT71F001 DD DSN=&BIGXSK,SPACE=(CYL,(0,1)),UNIT=&UNITSCR,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT72F001 DD DSN=&BIGXSL,SPACE=(CYL,(0,1)),UNIT=&UNITSCR,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT73F001 DD DSN=&BIGXSM,SPACE=(CYL,(0,1)),UNIT=&UNITSCR,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT74F001 DD DSN=&BIGXSN,SPACE=(CYL,(0,1)),UNIT=&UNITSCR,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT75F001 DD DSN=&BIGXSO,SPACE=(CYL,(0,1)),UNIT=&UNITSCR,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT76F001 DD DSN=&BIGXSP,SPACE=(CYL,(0,1)),UNIT=&UNITSCR,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//FT77F001 DD DSN=&RANDOM,SUBALLOC=(CYL,(15,1),DUMMY2),DCB=RECFM=U
//FT78F001 DD DSN=&RESDAT,UNIT=&UNITSCR,SPACE=(TRK,(1,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)
//*            RESOLVED RESONANCE PARAMETERS
//FT79F001 DD DSN=&ACS009,UNIT=&UNITSCR,SPACE=(TRK,(1,1)),
//             DCB=(RECFM=FBS,LRECL=80,BLKSIZE=3040)
//*            ALPHANUMERIC INPUT FOR ISOTXS EDITOR MODULE CSE009
//FT80F001 DD DSN=&ACSE12,UNIT=&UNITSCR,SPACE=(TRK,(1,1)),
//             DCB=(RECFM=FBS,LRECL=80,BLKSIZE=3040)
//*            ALPHANUMERIC INPUT FOR XS.ISO EDITOR MODULE CSE012
//SYSUDUMP DD SYSOUT=&DMPDEST
//*            CORE DUMP FROM ABNORMAL TERMINATION
//*
//*      ****************************************************************
//*
//*
//*      ****************************************************************
//*
// PEND
```

Fig. 11. MC^2-2 JCL Procedure (Contd.)

C. Problem Specification

The user input to the MC^2-2 code is supplied on various card types from the BCD data sets A.STP015, A.MCC2, A.NIP, ACS009, and ACSE12. These data sets are described in the listings given in Appendix B. Table III summarizes the use of the various BCD data sets. This first release of MC^2-2 lacks a full heterogeneous treatment in that heterogeneous broad group cross sections are not yet generated by CSC009.

The input data deck for the execution of MC^2-2 follows the general ARC System format as described on pages 42-45 of Reference 1. A data set initialization block (DSIB) given the block name "OLD" is used if any data sets are to be used which were generated in previous jobs. In the case of the eight MC^2-2 library files (MCC2F1-MCC2F8), the path driver STP015 has been written so that these files need not be named in a DSIB. The format of these library files which are normally written by the ETOE-2 code are given in Appendix C. One common use of the DSIB with MC^2-2 is the addition of material cross sections to an existing XS.ISO file by the module CSE007. In this case the card DATASET=XS.ISO appears in the dataset initialization block.

The DSIB, if any, is followed in the input deck by a data block given the name STP015. This block may include the path dependent data set A.STP015 and the data sets A.MCC2, A.NIP, ACS009, and ACSE12. These data sets are discussed below in greater detail and examples of BCD input data are given in Section D, Sample Problems.

The BCD input processor has been written with particular attention to easing the burden on the user when preparing problem input. By using defaults, many of the card types may be omitted for a given problem. Thus for example, as a minimum for homogeneous problems, only type 06 cards of data set A.MCC2 need be supplied if the defaults supplied are acceptable to the user. Similarly, for heterogeneous problems, as a minimum one type 03 card of data set A.MCC2 and the type 06, 14, and 15 cards of data set A.NIP need be supplied.

In order to ease user specification work load, eleven prestored broad group structures are available on option in MC^2-2. These structures are selected as indicated on card type 03, cols. 31-36. If any type 05 or type 07 cards are supplied, the card type 03 selection, if any, is ignored. Similarly, if an old XS.ISO data set is included in the DSIB as discussed above, the card type 03 selection is ignored. If card type 03 is not supplied or if cols. 31-36 are blank and no type 05 or 07 cards are supplied, a built in default structure will be used.

The group structures for each of the eleven sets are given in Table IV which lists the broad group lethargy widths and upper energy boundaries. The upper energy of all of the sets is 10 MeV except for set USS226 which has an upper energy of 14.190675 MeV. Note that the last group for the BOND26 and the last two groups for the HANS16 sets have been changed relative to the original structures. This was required due to the fact that the current MC^2-2 library has a lower energy of 0.41399 eV. Also, the third from the last group in the sets USS212 and USS226 was altered slightly in order to fall on an integral multiple of an MC^2-2 ultra fine group.

TABLE III. BCD Input Data Sets

Data Set Name	Condition
A.STP015	Needed only if various of the code Areas 4 - 9 are to be omitted, if RABANL is to be executed, if broad group cross sections are not to be edited, if data set XS.ISO is not to be written, or if XS.ISO is to be edited.
A.MCC2	Always present unless only data set XS.ISO and/or ISOTXS is to be edited.
A.NIP	Needed only if a heterogeneous problem is involved.
ACSE12	Needed only if data set XS.ISO is to be edited, and then only if a non-standard edit is desired.
ACS009	Needed only if data set ISOTXS is to be edited, and then only if a non-standard edit is desired.

TABLE IV. Prestored Broad Group Structures

ANL9		ANL11		ANL27		ANL28		BOND26	
Group	Lethargy Width	Group	Lethargy Width	Group	Lethargy Width	Group	Lethargy Width	Group	Lethargy Width
1	1.5	1	1.0	1	0.5	1	0.5	1	0.425
2	1.0	2	1.0	2	0.5	2	0.5	2	0.483333
3	1.5	3	1.0	3	0.5	3	0.5	3	0.475
4	1.5	4	1.0	4	0.5	4	0.5	4	0.575
5	1.5	5	1.0	5	0.5	5	0.5	5	0.56666
6	1.5	6	1.0	6	0.5	6	0.5	6	0.6916666
7	1.5	7	1.0	7	0.5	7	0.5	7	0.6916666
8	4.5	8	1.0	8	0.5	8	0.5	8	0.6916666
9	∞	9	2.0	9	0.5	9	0.5	9	0.76666
		10	7.0	10	0.5	10	0.5	10	0.775
		11	∞	11	0.5	11	0.5	11	0.758333
				12	0.5	12	0.5	12	0.76666
				13	0.5	13	0.5	13	0.775
				14	0.5	14	0.5	14	0.76666
				15	0.5	15	0.5	15	0.76666
				16	0.5	16	0.5	16	0.76666
				17	0.5	17	0.5	17	0.76666
				18	0.5	18	0.5	18	0.76666
				19	0.5	19	0.5	19	0.775
				20	0.5	20	0.5	20	0.758333
				21	0.5	21	0.5	21	0.76666
				22	1.0	22	0.5	22	0.775
				23	1.0	23	0.5	23	0.766666
				24	1.0	24	0.5	24	0.766666
				25	1.0	25	0.5	25	0.116666
				26	1.0	26	0.5	26	∞
				27	∞	27	1.5		
						28	∞		

TABLE IV . Contd.

FFTF30		HANS16		USS212*					
Group	Lethargy Width	Group	Lethargy Width	Group	Lethargy Width	Group	Lethargy Width	Group	Lethargy Width
1	0.5	1	1.2	1	0.025	34	0.05	67	0.05
2	0.5	2	0.758333	2	0.025	35	0.05	68	0.05
3	0.5	3	0.441666	3	0.025	36	0.05	69	0.025
4	0.5	4	0.81666	4	0.025	37	0.05	70	0.025
5	0.5	5	1.38333	5	0.025	38	0.025	71	0.05
6	0.5	6	1.775	6	0.025	39	0.025	72	0.05
7	0.5	7	1.73333	7	0.025	40	0.025	73	0.05
8	0.5	8	1.691666	8	0.025	41	0.025	74	0.025
9	0.5	9	1.708333	9	0.025	42	0.05	75	0.016667
10	0.5	10	1.208333	10	0.025	43	0.05	76	0.008333
11	0.5	11	1.091666	11	0.025	44	0.05	77	0.05
12	0.5	12	1.208333	12	0.025	45	0.05	78	0.05
13	0.5	13	1.1	13	0.025	46	0.016667	79	0.05
14	0.5	14	0.766666	14	0.025	47	0.016667	80	0.05
15	0.5	15	0.116666	15	0.025	48	0.008333	81	0.05
16	0.5	16	∞	16	0.025	49	0.008333	82	0.05
17	0.5			17	0.008333	50	0.016667	83	0.05
18	0.5			18	0.008333	51	0.016667	84	0.05
19	0.5			19	0.008333	52	0.016667	85	0.05
20	0.5			20	0.025	53	0.05	86	0.05
21	0.5			21	0.025	54	0.05	87	0.05
22	0.5			22	0.025	55	0.025	88	0.025
23	0.5			23	0.025	56	0.025	89	0.025
24	0.5			24	0.025	57	0.025	90	0.025
25	0.5			25	0.05	58	0.025	91	0.025
26	1.0			26	0.05	59	0.05	92	0.05
27	1.0			27	0.05	60	0.05	93	0.05
28	1.0			28	0.025	61	0.025	94	0.05
29	1.0			29	0.025	62	0.025	95	0.05
30	∞			30	0.025	63	0.025	96	0.05
				31	0.025	64	0.025	97	0.05
				32	0.05	65	0.05	98	0.05
				33	0.05	66	0.05	99	0.05

TABLE IV. Contd.

USS212*

Group	Lethargy Width	Group	Lethargy Width	Group	Lethargy Width	Group	Lethargy Width
100	0.05	133	0.05	166	0.058333	199	0.25
101	0.025	134	0.075	167	0.041667	200	0.25
102	0.025	135	0.125	168	0.05	201	0.25
103	0.025	136	0.125	169	0.05	202	0.25
104	0.025	137	0.125	170	0.1	203	0.25
105	0.025	138	0.025	171	0.1	204	0.25
106	0.025	139	0.025	172	0.1	205	0.25
107	0.05	140	0.075	173	0.1	206	0.25
108	0.05	141	0.125	174	0.05	207	0.05
109	0.05	142	0.075	175	0.05	208	0.2
110	0.05	143	0.05	176	0.1	209	0.08333
111	0.05	144	0.025	177	0.1	210	0.16667
112	0.05	145	0.025	178	0.25	211	0.25
113	0.05	146	0.025	179	0.25	212	∞
114	0.05	147	0.025	180	0.25		
115	0.05	148	0.1	181	0.25		
116	0.025	149	0.125	182	0.25		
117	0.025	150	0.125	183	0.25		
118	0.025	151	0.125	184	0.25		
119	0.025	152	0.125	185	0.25		
120	0.05	153	0.125	186	0.25		
121	0.05	154	0.125	187	0.25		
122	0.05	155	0.125	188	0.25		
123	0.05	156	0.125	189	0.25		
124	0.05	157	0.125	190	0.25		
125	0.05	158	0.125	191	0.25		
126	0.05	159	0.1	192	0.25		
127	0.125	160	0.1	193	0.25		
128	0.125	161	0.05	194	0.25		
129	0.125	162	0.05	195	0.25		
130	0.125	163	0.1	196	0.25		
131	0.075	164	0.1	197	0.25		
132	0.05	165	0.1	198	0.25		

*USS226 is the same as USS212 except that an additional 14 groups with $\Delta u = 0.025$ are added above group 1 up to an upper energy of 14.190675 MeV.

TABLE IV. Contd.

SDX156		WARD9	
Group	Lethargy Width	Group	Lethargy Width
1	0.1	1	1.5
2	0.1	2	1.0
3	0.1	3	1.5
.	.	4	1.5
.	.	5	1.5
.	.	6	1.5
155	0.1	7	1.5
156	∞	8	6.5
		9	∞

D. Sample Problems

A number of examples of typical MC^2-2 problems will be given in this section along with a listing of the user supplied BCD data.

1. Homogeneous Reference Problem

The user input deck is shown in Fig. 13 .

This problem creates the XS.ISO data set having the data set names C116.BXXXXX.XSISOF1 and C116.BXXXXX.XSISOF2 for files 1 and 2 respectively as specified in the symbolic parameters MICRXS1 and MICRXS2. The data set will be catalogued as specified in the symbolic parameter MICRDSP. No data set initialization block is specified.

The type 01 card of data set A.STP015 is set to execute Areas 4, 5, 6, 6.5, 7, 8, and 9, to edit the broad group cross sections, and to create a double precision XS.ISO data set. This could also have been accomplished by supplying a card with only 01 in columns 1 and 2. Also, these same choices could have been selected by omitting the DATASET=A.STP015 card and the type 01 card which follows it since the standard defaults are used.

The data set A.MCC2 type 01 cards provide title information desired by the user.

The type 02 card specifies a BPOINTER main core container of 25000 real*8 words.

The type 03 card uses defaults for all fields except for columns 7-12 and 31-36 in which a consistent P1 fundamental mode calculation and the standard ANL27 broad group structure are specified.

The type 06 cards specify the five isotopes in the problem along with their atom densities. The problem material names were omitted from columns 19-24 and will default to the names given in columns 13-18. Also, the temperatures all default to 300 degrees K and all cross sections will be added to the output cross section data set.

The type 16 card specifies that the fission spectrum of PU2394 be used for all fissionable nuclides.

The type 22 cards classify the problem isotopes and assign values for MeV/fission for U-2384 and PU2394.

2. Hyper-fine Group Homogeneous Integral Transport Problem

The user input deck is shown in Fig. 14.

This problem corresponds to a standalone RABID[6] calculation for the homogeneous composition given in the previous example.

The type 01 card of data set A.STP015 is set to execute only the input processor Area 4 and the RABANL module.

As in example 1, a container of 25000 real*8 words is specified on card type 02 of data set A.MCC2.

The same type 06 cards are used as in example 1.

A fixed buckling of 0.0011466 is specified on the type 09 card.

The type 14 card specifies 3354.4 eV as the upper energy for the calculation with all other fields on that card using the default values specified.

The mixture temperature is specified as 300 degress K on the type 21 card.

3. Hyper-fine Group Heterogeneous Integral Transport Problem

The user input deck is shown in Fig. 15.

This problem corresponds to a standalone RABID[6] calculation for a six slab region heterogeneous problem.

As in example 2, the data set A.STP015 type 01 card is set to execute only Area 4 and RABANL.

A larger container of 30000 real*8 words is specified on the data set A.MCC2 type 02 card. Since this is the default, the type 02 card could have been omitted.

The type 03 card again specifies the ANL27 broad group structure and 1 in column 42 indicates slab geometry.

No data set A.MCC2 type 06 cards are supplied so that the mixture composition will be derived from the data set A.NIP input.

The upper energy of the problem is specified to be 275.36425 electron volts on the type 14 card.

The type 15 cards define two foils.

The type 21 card assigns a temperature of 293 degrees K to each of the compositions defined in the data set A.NIP type 14 cards.

The data set A.NIP type 04 card indicates that the left and right cell boundaries have reflective boundary conditions.

The A.NIP type 06 cards define the dimensions of the three regions in the problem. Because of the reflective boundary conditions, both regions MATX and CLAD 1 will have double the thicknesses as given on the type 06 cards.

The three compositions MATX, U308, and CLADA are defined on the type 14 cards.

The composition - region assignments are made on the type 15 cards.

E. Error Messages

Error messages issued by various subroutines of the modules of MC^2-2 are listed in Table V. The subroutines are presented alphabetically within each module, and the error messages for each subroutine are listed in numerical order.

The convention used is that fatal errors are negative, while non-fatal errors are positive.

As a general rule, fatal errors will not halt execution until the particular module involved has been completed. This will not be true in those cases in which the error results in some subsequent computer system error such as a divide check, core region violation, etc.

Also included are the error messages issued by the ANL version of the CCCC compatible I/O routine REED/RITE.[2]

Figure 12

Minimum JCL Execution Deck

```
//MINJCL JOB (FXXXXX,20,,MM),'YOUR CHOICE',MSGLEVEL=1,CLASS=A,
//             REGION=600K
 ACCOUNTING INFORMATION
// EXEC ARCSP015
//SYSIN DD *
 PROBLEM INPUT DATA
/*
```

Figure 13

Input for Sample Problem 1

```
//SAMPLE1 JOB (FXXXXX,20,,05),'YOUR CHOICE',MSGLEVEL=1,CLASS=A,
//             REGION=550K
 ACCOUNTING INFORMATION
// EXEC ARCSP015,
//             MICRXS1='C116.BXXXXX.XSISOF1',
//             MICRXS2='C116.BXXXXX.XSISOF2',
//             MICRDSP='(NEW,CATLG)'
//SYSIN DD *
BLOCK=STP015
DATASET=A.STP015
01         0     0     0     0     0     0     0     0     0     0
DATASET=A.MCC2
01    ************************************************************************
01    *     ENDF/B-IV DATA                                                   *
01    *     FIVE ISOTOPE HOMOGENEOUS REFERENCE PROBLEM                       *
01    *     BPOINTER CONTAINER IS SET TO 25000 WORDS                         *
01    *     CONSISTENT P1 FUNDAMENTAL MODE CALCULATION                       *
01    *     STANDARD ANL27 BROAD GROUP STRUCTURE                             *
01    *     DEFAULT TEMPERATURES OF 300 DEGREES K                            *
01    *     ALL FISSIONABLE ISOTOPES USE PU239 FISSION SPECTRUM              *
01    *     MEV/FISSION SET TO 201.8150613 FOR U238                          *
01    *     MEV/FISSION SET TO 215.7333414 FOR PU239                         *
01    ************************************************************************
02     25000
03         3                  ANL27
06          U-2384      .006383
06          PU2394      .001086
06          NA23 4      .01041
06          O-16 4      .01419
06          FE   4      .01814
16    PU2394
22          U-2384      2 201.8150613
22          PU2394      1 215.7333414
22          NA23 4      6
22          O-16 4      0
22          FE   4      5
/*
```

Figure 14

Input for Sample Problem 2

```
//SAMPLE2 JOB (FXXXXX,20,,05),'YOUR CHOICE',MSGLEVEL=1,CLASS=C,
//             REGION=550K
 ACCOUNTING INFORMATION
// EXEC ARCSP015
//SYSIN DD *
BLOCK=STP015
DATASET=A.STP015
01         0     1     1     1     1     1     1    -1     1
DATASET=A.MCC2
01    ************************************************************************
01    *     ENDF/B-IV DATA                                                   *
01    *     FIVE ISOTOPE HOMOGENEOUS REFERENCE PROBLEM                       *
01    *     STANDALONE HYPER-FINE-GROUP INTEGRAL TRANSPORT (RABANL)          *
01    *     CALCULATION                                                      *
01    *     BPOINTER CONTAINER IS SET TO 25000 WORDS                         *
01    *     STANDARD ANL27 BROAD GROUP STRUCTURE                             *
01    *     FIXED BUCKLING IS SET TO .0011466                                *
01    *     TOP ENERGY OF PROBLEM IS SET TO 3354.4 ELECTRON VOLTS            *
01    *     MIXTURE TEMPERATURE IS SET TO 300 DEGREES KELVIN                 *
01    ************************************************************************
02     25000
03                              ANL27
06          U-2384       .006383
06          PU2394       .001086
06          NA23 4       .01041
06          O-16 4       .01419
06          FE   4       .01814
09          .0011466
14          3354.4
21                 300.0
/*
```

Figure 15

Input for Sample Problem 3

```
//SAMPLE3 JOB (FXXXXX,20,,08),'YOUR CHOICE',MSGLEVEL=1,CLASS=C,
//             REGION=650K
 ACCOUNTING INFORMATION
// EXEC ARCSP015
//SYSIN DD *
BLOCK=STP015
DATASET=A.STP015
01         0     1     1     1     1     1     1    -1     1
DATASET=A.MCC2
01     ************************************************************************
01     *      ENDF/B-IV DATA                                                  *
01     *      SIX REGION HETEROGENEOUS PROBLEM                                *
01     *      STANDALONE HYPER-FINE-GROUP INTEGRAL TRANSPORT (RABANL)         *
01     *      CALCULATION                                                     *
01     *      BPOINTER CONTAINER IS SET TO 30000 WORDS                        *
01     *      STANDARD ANL27 BROAD GROUP STRUCTURE                            *
01     *      TOP ENERGY OF PROBLEM IS SET TO 275.36426 EV                    *
01     *      ALL COMPOSITION TEMPERATURES SET TO 293 DEGREES K               *
01     ************************************************************************
02      30000
03                              ANL27     1
14           275.36425
15     FOILA U-2354  .00003                          .00036
15     FOILB PU2394  .00015    PU2414 .000025        .00044
21           MATX   293.          U308  293.       CLADA   293.
DATASET=A.NIP
04                10    10
06       MATX     0.0        0.286          1
06       U308     0.286      0.921          1
06     CLAD 1     0.921      0.959          1
14           MATX  MO    4 0.00005    O-16 4 0.00025    FE    4 0.04474
14           MATX  NI    4 0.005479   CR   4 0.01257    MN55 4 0.00101
14           U308  U-2354 0.0000336  U-2384 0.01572    O-16 4 0.04201
14           CLADA NI    4  0.009832  CR   4  0.01939   MN55 4  0.00147
14           CLADA MO    4  0.000075  O-16 4  0.00038   FE   4  0.06811
15     MATX     MATX
15     U308   U308
15     CLADA CLAD 1
/*
```

TABLE V. MC^2-2 Error Messages

CSI010 (AREA 4)

Subroutine CARD05

Fatal Error -10100.	CARD PRESUMED TO BE TYPE 05 NOT FOUND
Fatal Error -10200.	THE FIRST GROUP NUMBER AND UPPER ENERGY OF THAT GROUP MUST BE GIVEN ON THE FIRST TYPE 05 CARD
Fatal Error -10300.	BROAD GROUP ENERGIES MUST ALL BE SPECIFIED
Fatal Error -10400.	THE HIGHEST ENERGY BROAD GROUP IN THE PROBLEM MAY NOT LIE ABOVE THE HIGHEST ENERGY IN THE LIBRARY
Fatal Error -10500.	ALL GROUPS MUST BE SPECIFIED
Fatal Error -10600.	BROAD GROUP ENERGIES MUST ALL BE UNIQUE
Fatal Error -10700.	THE SPECIFIED BROAD GROUP STRUCTURE EXTENDS BELOW THE BOTTOM OF THE LIBRARY GROUP STRUCTURE
Fatal Error -10800.	IF ONLY ONE UPPER ENERGY IS GIVEN, IT MUST CORRESPOND TO GROUP 1
Fatal Error -10900.	THE HIGHEST BORAD GROUP SPECIFIED LIES BELOW THE LOWEST ENERGY IN THE LIBRARY
Fatal Error -11000.	THE ADJUSTED BROAD GROUP ENERGY BOUNDARIES MUST ALL BE UNIQUE.

Subroutine CARD06

Fatal Error -10100.	CARD PRESUMED TO BE TYPE 06 NOT FOUND
Fatal Error -10200.	EACH MATERIAL MUST CORRESPOND TO SOME LIBRARY MATERIAL
Fatal Error -10400.	MATERIAL NAMES MUST BE NON-BLANK

Subroutine CARD07

Fatal Error -10100.	CARD PRESUMED TO BE TYPE 07 NOT FOUND
Fatal Error -10200.	LETHARGY WIDTHS SPECIFIED ON TYPE 07 CARDS MUST BE GREATER THAN ZERO
Fatal Error -10300.	FINAL BROAD GROUP NUMBERS IN COLS. 31-36 ON TYPE 07 CARDS MUST BE .GE. INITIAL BROAD GROUP NUMBERS GIVEN IN COLS. 25-30

TABLE V. Contd.

CSI010 (AREA 4) (Contd.)

Subroutine CARD07 (contd.)

Fatal Error -10400.	FINAL BROAD GROUP NUMBERS IN COLS. 55-60 ON TYPE 07 CARDS MUST BE .GE. INITIAL BROAD GROUP NUMBERS GIVEN IN COLS. 49-54
Fatal Error -10500.	THE FIRST BROAD GROUP NUMBER MUST BE 1
Fatal Error -10600.	THE BROAD GROUP NUMBERS MUST ALL BE SPECIFIED
Fatal Error -10700.	THERE MAY BE NO MORE BROAD GROUPS THAN THERE ARE ULTRA FINE GROUPS IN THE LIBRARY
Fatal Error -10800.	THE PRESTORED BROAD GROUP STRUCTURE SELECTED IS NOT CONSISTENT WITH THE LIBRARY ENERGY STRUCTURE
Fatal Error -10900.	THE PRESTORED BROAD GROUP STRUCTURE SELECTED IS NOT CONSISTENT WITH THE LIBRARY ENERGY STRUCTURE

Subroutine CARD08

Fatal Error -10100.	CARD PRESUMED TO BE TYPE 08 NOT FOUND
Fatal Error -10200.	LOWER ENERGY BROAD GROUP NUMBER IN COLS. 31-36 ON TYPE 08 CARDS MUST BE .GE. HIGHER ENERGY BROAD GROUP NUMBER IN COLS. 25-30
Fatal Error -10300.	LOWER ENERGY BROAD GROUP NUMBERS IN COLS. 55-60 ON TYPE 08 CARDS MUST BE .GE. HIGHER ENERGY BROAD GROUP NUMBERS IN COLS. 49-54
Fatal Error -10400.	MATERIAL SPECIFIED IN COLS. 25-30 ON TYPE 08 CARD DOES NOT CORRESPOND TO ANY FISSION SPECTRUM MATERIAL NAME ON DATA SET MCC2F7
Fatal Error -10500.	ONLY INITIAL ENERGY INDEPENDENT FISSION SPECTRA MAY BE SPECIFIED ON TYPE 08 CARDS
Fatal Error -10600.	MATERIAL SPECIFIED IN COLS. 25-30 ON TYPE 08 CARD DOES NOT CORRESPOND TO ANY PROBLEM MATERIAL

Subroutine CARD09

Fatal Error -10100.	CARD PRESUMED TO BE TYPE 09 NOT FOUND
Fatal Error -10200.	THE ULTRA FINE GROUP NUMBER IN COLS. 55-60 ON TYPE 09 CARDS MUST BE GREATER THAN OR EQUAL TO THE ULTRA FINE GROUP NUMBER IN COLS. 49-54
Fatal Error -10300.	CARD PRESUMED TO BE TYPE 09 NOT FOUND

TABLE V. Contd.

CSI010 (AREA 4) Contd.

Subroutine CARD09 (contd.)

Fatal Error -10400.	THE ULTRA FINE GROUP NUMBERS IN COLS. 49-54 ON TYPE 09 CARDS MUST BE .GT.0
Fatal Error - 10500.	THE ULTRA FINE GROUP NUMBER IN COLS. 55-60 ON TYPE 09 CARDS MUST BE GREATER THAN OR EQUAL TO THE ULTRA FINE GROUP NUMBER IN COLS. 49-54
Error 10600.	THE CONVERGENCE CRITERION ON THE TYPE 09 CARD MUST BE .GE. 0.
Fatal Error -10700.	BUCKLING ITERATION IS NOT POSSIBLE FOR AN INHOMOGENEOUS SOURCE PROBLEM
Fatal Error -10800.	BUCKLING ITERATION IS NOT ALLOWED FOR GROUP DEPENDENT BUCKLINGS
Fatal Error -10900.	BUCKLING ITERATION IS NOT ALLOWED FOR INHOMOGENEOUS SOURCE PROBLEMS

Subroutine CARD10

Fatal Error -10100.	CARD PRESUMED TO BE TYPE 10 NOT FOUND
Fatal Error -10200.	NUCLIDE IDENTIFICATION LABELS ON TYPE 10 CARDS MUST CORRESPOND TO SOME PROBLEM MATERIAL

Subroutine CARD11

Fatal Error -10100.	CARD PRESUMED TO BE TYPE 11 NOT FOUND
Fatal Error -10200.	NUCLIDE IDENTIFICATION LABELS ON TYPE 11 CARDS MUST CORRESPOND TO SOME PROBLEM MATERIAL

Subroutine CARD12

Fatal Error -10100.	CARD PRESUMED TO BE TYPE 12 NOT FOUND
Fatal Error -10200.	MATERIAL NAMES MUST BE NON-BLANK
Error 10300.	MATERIALS SPECIFIED ON TYPE 12 CARDS MUST BE PRESENT IN THE PIN REGION
Error 10400.	MATERIALS SPECIFIED ON TYPE 12 CARDS MUST BE RESONANCE MATERIALS
Fatal Error -10500.	ALL MATERIALS SPECIFIED ON TYPE 12 CARDS MUST CORRESPOND TO SOME PROBLEM MATERIAL
Fatal Error -10600.	CARD PRESUMED TO BE TYPE 12 NOT FOUND

TABLE V. Contd.

CSI010 (AREA 4) Contd.

Subroutine CARD12 (contd.)

Fatal Error -10700.	MATERIAL NAMES MUST BE NON-BLANK
Fatal Error -10800.	CARD PRESUMED TO BE TYPE 12 NOT FOUND
Fatal Error -10900.	MATERIAL NAMES MUST BE NON-BLANK
Error 11000.	ONLY ONE TYPE 12 CARD MAY BE SUPPLIED FOR A GIVEN MATERIAL WITH COLS. 13-18 BLANK
Fatal Error -11100.	ALL REGIONS REFERRED TO IN COLS. 19-24, 31-36, 43-48, 55-60, AND 67-72 ON TYPE 12 CARDS MUST CORRESPOND TO SOME REGION ON THE DATA SET A.NIP TYPE 06 CARDS
Fatal Error -11200.	ALL MATERIALS REFERRED TO ON TYPE 12 CARDS MUST CORRESPOND TO SOME PROBLEM MATERIAL
Fatal Error -11300.	ALL REGIONS REFERRED TO IN COLS. 13-18, 25-30, 37-42, 49-54, AND 61-66 ON TYPE 12 CARDS MUST CORRESPOND TO SOME REGION DEFINED ON THE DATA SET A.NIP TYPE 06 CARDS
Fatal Error -11400.	NO REGION REFERRED TO IN COLS. 19-24, 31-36, 43-48, 55-60, OR 67-72 ON TYPE 12 CARDS MAY ALSO BE REFERRED TO IN COLS. 13-18, 25-30, 37-42, 49-57, OR 61-66

Subroutine CARD14

Fatal Error -10100.	CARD PRESUMED TO BE TYPE 14 NOT FOUND
Fatal Error -10300.	THE ENERGY SPECIFIED IN COLS. 13-25 OF CARD TYPE 14 OR THE DEFAULT VALUE OF 300.0 VOLTS FALLS INTO THE THERMAL GROUP
Fatal Error -10400.	THE ENERGY SPECIFIED IN COLS. 13-25 OF CARD TYPE 14 OR THE DEFAULT VALUE OF 300.0 VOLTS FALLS ABOVE THE HIGHEST ENERGY IN THE PROBLEM

Subroutine CARD15

Fatal Error -10100.	CARD PRESUMED TO BE TYPE 15 NOT FOUND
Fatal Error -10200.	FOIL LABELS MUST BE NON-BLANK
Fatal Error -10300.	THE FIRST MATERIAL LABEL ON A TYPE 15 CARD WAS BLANK
Fatal Error -10400.	MATERIALS IN FOILS MUST CORRESPOND TO LIBRARY MATERIAL
Fatal Error -10500.	MATERIALS MAKING UP A GIVEN FOIL MUST BE DISTINCT
Fatal Error -10600.	CARD PRESUMED TO BE TYPE 15 NOT FOUND

TABLE V. Contd.

CSI010 (AREA 4) Contd.

Subroutine CARD15 (contd.)

Fatal Error -10700.	FOIL LABELS MUST BE NON-BLANK
Fatal Error -10800.	THE FIRST MATERIAL LABEL ON A TYPE 15 CARD WAS BLANK
Fatal Error -10900.	POSITIVE FOIL THICKNESSES MUST BE SPECIFIED
Fatal Error -11000.	POSITIVE FOIL THICKNESSES MUST BE SPECIFIED

Subroutine CARD16

Fatal Error -10100.	CARD PRESUMED TO BE TYPE 16 NOT FOUND
Fatal Error -10200.	FISSION SPECTRUM NUCLIDE IDENTIFICATION LABELS ON TYPE 16 CARDS MUST CORRESPOND TO LIBRARY FISSION SPECTRA LABELS
Fatal Error -10300.	ONLY ONE TYPE 16 CARD MAY BE SPECIFIED WITH COLS. 13-18 BLANK
Fatal Error -10400.	FISSIONABLE NUCLIDE IDENTIFICATION LABELS ON TYPE 16 CARDS MUST CORRESPOND TO PROBLEM NUCLIDE IDENTIFICATION LABELS

Subroutine CARD17

Fatal Error -10100.	CARD PRESUMED TO BE TYPE 17 NOT FOUND
Fatal Error -10200.	LETHARGY WIDTHS SPECIFIED ON TYPE 17 CARDS MUST BE GREATER THAN ZERO
Fatal Error -10300.	FINAL FIXED MESH POINT NUMBERS IN COLS. 31-36 ON TYPE 17 CARDS MUST BE .GE. INITIAL FIXED MESH POINT NUMBERS GIVEN IN COLS. 25-30
Fatal Error -10400.	FIXED MESH POINT NUMBERS IN COLS. 55-60 ON TYPE 17 CARDS MUST BE .GE. INITIAL MESH POINT NUMBERS GIVEN IN COLS. 49-54
Fatal Error -10500.	THE FIRST FIXED MESH POINT NUMBER MUST BE 1
Fatal Error -10600.	THE FIXED MESH POINT NUMBERS MUST ALL BE SPECIFIED
Fatal Error -10700.	A MAXIMUM OF 500 FIXED ENERGY MESH POINTS ARE PERMITTED
Fatal Error -10800.	THE UNRESOLVED ENERGY REGION FALLS BELOW THE FIXED ENERGY GRID

TABLE V. Contd.

CSI010 (AREA 4) Contd.

Subroutine CARD18

Fatal Error -10100.	CARD PRESUMED TO BE TYPE 18 NOT FOUND
Error 10200.	ALL MATERIALS NAMED ON TYPE 18 CARDS MUST CORRESPOND TO SOME PROBLEM MATERIAL

Subroutine CARD21

Fatal Error -10100.	CARD PRESUMED TO BE TYPE 21 NOT FOUND
Fatal Error -10200.	CARD PRESUMED TO BE TYPE 21 NOT FOUND
Fatal Error -10300.	EACH COMPOSITION LABEL ON TYPE 21 CARDS MUST CORRESPOND TO SOME COMPOSITION LABEL ON DATA SET A.NIP TYPE 14 CARDS
Fatal Error -10400.	THE FIRST COMPOSITION LABEL ON THE TYPE 21 CARDS MUST BE NON-BLANK

Subroutine CARD22

Fatal Error -10100.	CARD PRESUMED TO BE TYPE 22 NOT FOUND
Fatal Error -10200.	MATERIAL LABELS ON TYPE 22 CARDS MUST CORRESPOND TO LIBRARY MATERIALS

Subroutine CARD23

Fatal Error -10100.	CARD PRESUMED TO BE TYPE 23 NOT FOUND
Fatal Error -10200.	MORE THAN NPRMAT+MSORS FISSION SPECTRA TEMPERATURES WERE SPECIFIED ON THE TYPE 23 CARDS
Fatal Error -10300.	THE MATERIALS NAMED ON THE TYPE 23 CARDS MUST CORRESPOND TO MATERIALS SPECIFIED ON THE TYPE 06 CARDS AND/OR THE MATERIALS SPECIFIED ON THE DATA SET A.NIP TYPE 14 CARDS, OR THE LABELS FOR THE LIBRARY FISSION SPECTRA DATA

Subroutine CSI010 (MAIN)

Fatal Error -10100.	INPUT DATA SET A.MCC2 NOT FOUND
Fatal Error -10200.	CARD PRESUMED TO BE TYPE 02 NOT FOUND
Fatal Error -10300.	CARD PRESUMED TO BE TYPE 04 NOT FOUND
Fatal Error -10400.	CARD PRESUMED TO BE TYPE 03 NOT FOUND
Fatal Error -10500.	INPUT DATA SET A.NIP NOT FOUND

TABLE V. Contd.

CSI010 (AREA 4) Contd.

CSI010 (MAIN) (contd.)

Fatal Error -10600.	CARD PRESUMED TO BE TYPE 01 NOT FOUND
Fatal Error -10700.	TYPE 06 CARDS MUST BE SUPPLIED FOR HOMOGENEOUS PROBLEMS
Fatal Error -10800.	CARD PRESUMED TO BE TYPE 19 NOT FOUND
Fatal Error -10900.	EXTENDED TRANSPORT APPROXIMATION ORDER MUST BE 1 FOR INCONSISTENT FUNDAMENTAL MODE OPTION
Fatal Error -11000.	LEGENDRE ELASTIC SCATTERING TRANSPORT APPROXIMATION PERMITTED ONLY FOR NON-CONSISTENT FUNDAMENTAL MODE OPTIONS
Fatal Error -11100.	CARD PRESUMED TO BE TYPE 20 NOT FOUND
Fatal Error -11200.	THE BROAD GROUP STRUCTURE SPECIFIED ON THE TYPE 03 CARD DOES NOT CORRESPOND TO ONE OF THE PRESTORED GROUP STRUCTURES

Subroutine RDANIP

Fatal Error -10100.	CARD PRESUMED TO BE TYPE 04 OF DATA SET A.NIP NOT FOUND
Error 10200.	ONLY REFLECTIVE OR PERIODIC BOUNDARY CONDITIONS ARE ALLOWED AND THE SAME CONDITION APPLIES TO BOTH SIDES OF THE CELL. THE PERIODIC CONDITION IS BEING USED
Fatal Error -10300.	DATA SET A.NIP TYPE 06 CARDS MUST BE SUPPLIED IF COLS. 37-42 ON CARD TYPE 03 OF DATA SET A.MCC2 ARE NON-ZERO
Fatal Error -10400.	DATA SET A.NIP TYPE 14 CARDS MUST BE SUPPLIED IF COLS. 37-42 ON CARD TYPE 03 OF DATA SET A.MCC2 ARE NON-ZERO
Fatal Error -10500.	DATA SET A.NIP TYPE 15 CARDS MUST BE SUPPLIED IF COLS. 37-42 ON TYPE 03 CARD OF DATA SET A.MCC2 ARE NON-ZERO
Error 10600.	ONLY THE REFLECTIVE BOUNDARY CONDITION IS ALLOWED AT THE LEFT BOUNDARY OF A CYLINDRICAL CELL
Error 10700.	ONLY WHITE BOUNDARY CONDITIONS ARE ALLOWED FOR THE RIGHT BOUNDARY OF A CYLINDRICAL CELL.

TABLE V. Contd.

CSI010 (AREA 4) Contd.

Subroutine STRTCH	
Fatal Error -10100.	IF THE ATOMIC DENSITY OF SOME MATERIAL IS NOT SUPPLIED ON THE TYPE 06 CARDS, THE MATERIAL MUST APPEAR IN SOME HETEROGENEOUS REGION
Fatal Error -10200.	EACH MATERIAL MUST CORRESPOND TO SOME LIBRARY MATERIAL
Subroutine TESTBG	
Fatal Error -10100.	THE HIGHEST BROAD GROUP AS READ FROM DATA SET XS.ISO MAY NOT LIE ABOVE THE HIGHEST ENERGY IN THE LIBRARY
Fatal Error -10300.	THE HIGHEST BROAD GROUP ENERGY AS READ FROM DATASET XS.ISO DOES NOT FALL ON AN ULTRA-FINE-GROUP BOUNDARY
Fatal Error -10500.	THE SPECIFIED BROAD GROUP STRUCTURE AS READ FROM DATASET XS.ISO DOES NOT FALL ON ULTRA-FINE-GROUP BOUNDARIES
Subroutine TYPE06	
Fatal Error -10100.	CARD PRESUMED TO BE TYPE 06 OF DATA SET A.NIP NOT FOUND
Fatal Error -10200.	REGION LABELS MUST BE NON-BLANK
Fatal Error -10300.	INVALID REGION BOUNDARY COORDINATES GIVEN ON DATA SET A.NIP TYPE 06 CARDS. EACH REGION LOWER BOUNDARY COORDINATE MUST BE .GE.0. AND .LT. THE CORRESPONDING UPPER BOUNDARY COORDINATE FOR THAT REGION
Fatal Error -10400.	THE LOWEST MESH POINT FOR CYLINDERS MUST FALL AT 0.
Fatal Error -10500.	REGION BOUNDARIES FOR SEQUENTIAL REGIONS MUST AGREE TO AT LEAST 1.E-4
Subroutine TYPE14	
Fatal Error -10100.	CARD PRESUMED TO BE TYPE 14 OF DATA SET A.NIP NOT FOUND
Fatal Error -10200.	COMPOSITION LABELS MUST BE NON-BLANK
Fatal Error -10300.	THE FIRST MATERIAL LABEL ON A TYPE 14 CARD OF DATA SET A.NIP WAS BLANK
Fatal Error -10400.	MATERIALS IN HETEROGENEOUS REGIONS MUST CORRESPOND TO LIBRARY MATERIALS

TABLE V. Contd.

CSI010 (AREA 4) Contd.

Subroutine TYPE14 (contd.)

Fatal Error -10500.	MATERIALS MAKING UP A GIVEN COMPOSITION MUST BE DISTINCT
Fatal Error -10600.	CARD PRESUMED TO BE TYPE 14 OF DATA SET A.NIP NOT FOUND
Fatal Error -10700.	COMPOSITION LABELS MUST BE NON-BLANK
Fatal Error -10800.	THE FIRST MATERIAL LABEL ON A TYPE 14 CARD OF DATA SET A.NIP WAS BLANK

Subroutine TYPE15

Fatal Error -10100.	CARD PRESUMED TO BE TYPE 15 OF DATA SET A.NIP NOT FOUND
Fatal Error -10200.	COMPOSITION LABELS MUST BE NON-BLANK
Fatal Error -10300.	THE FIRST REGION LABEL ON A TYPE 15 CARD OF DATA SET A.NIP MUST BE NON-BLANK
Fatal Error -10400.	A COMPOSITION REFERRED TO ON A DATA SET A.NIP TYPE 15 CARD MUST CORRESPOND TO SOME COMPOSITION DEFINED ON A TYPE 14 CARD
Fatal Error -10500.	A REGION REFERRED TO ON A DATA SET A.NIP TYPE 15 CARD MUST CORRESPOND TO SOME REGION DEFINED ON THE TYPE 06 CARDS
Fatal Error -10600.	ONLY ONE COMPOSITION MAY BE ASSIGNED TO A GIVEN REGION
Fatal Error -10700.	CARD PRESUMED TO BE TYPE 15 OF DATA SET A.NIP NOT FOUND
Fatal Error -10800.	COMPOSITION LABELS MUST BE NON-BLANK
Fatal Error -10900.	A COMPOSITION REFERRED TO ON A DATA SET A.NIP TYPE 15 CARD MUST CORRESPOND TO SOME COMPOSITION DEFINED ON A TYPE 14 CARD
Fatal Error -11000.	THE FIRST REGION LABEL ON A TYPE 15 CARD OF DATA SET A.NIP MUST BE NON-BLANK
Fatal Error -11100.	A REGION REFERRED TO ON A DATA SET A.NIP TYPE 15 CARD MUST CORRESPOND TO SOME REGION DEFINED ON THE TYPE 06 CARDS
Fatal Error -11200.	EVERY REGION ON AN A.NIP TYPE 06 CARD MUST ALSO BE PRESENT ON A TYPE 15 CARD

TABLE V. Contd.

CSC004 (AREA 5)

Subroutine CSC004 (MAIN)

Fatal Error -10100.	PROBLEM MATERIAL NOT IN THE LIBRARY
Fatal Error -10200.	PROBLEM MATERIAL IS NOT IN THE LIBRARY

Subroutine MATRIX

Fatal Error -10100.	DETERMINANT IS SINGULAR

CSC005 (AREA 6)

Subroutine ADMSTR

Fatal Error -10100.	PROBLEM MATERIAL IS NOT IN THE LIBRARY

Subroutine CSC005 (MAIN)

Fatal Error -10100.	PROBLEM MATERIAL NOT IN THE LIBRARY

CSC006 (AREA 6.5)

Subroutine CSC006 (MAIN)

Fatal Error -10100.	PROBLEM MATERIAL IS NOT IN THE LIBRARY

CSC008 (AREA 7)

Subroutine CSC008 (MAIN)

Fatal Error -999	ERROR IN BPOINTER ALLOCATION

Subroutine SETCHI

Fatal Error -1	THE FISSION DISTRIBUTION SPECIFIED FOR THE PROBLEM IS NOT ON THE LIBRARY
Fatal Error -2	ALL FISSION DISTRIBUTIONS WERE NOT FOUND
Fatal Error -3	ALL FISSION DISTRIBUTIONS WERE NOT FOUND

Subroutine SETSCT

Fatal Error -1	ALL PROBLEM MATERIALS COULD NOT BE FOUND

TABLE V. Contd.

CSC008 (AREA 7) Contd.

Subroutine SETSCT (contd.)	
Error 2	NONE OF THE MATERIALS ON THE OLD DATASET OLDSGS ARE USED IN THIS PROBLEM. ALL MICROSCOPIC CROSS SECTIONS MUST BE CALCULATED
Error 3	THE OLD DATASET OLDSGS HAS A DIFFERENT ENERGY STRUCTURE THAN THE PRESENT PROBLEM (DIFFERENT NUMBER OF GROUPS OR DIFFERENT STARTING ENERGY). MICROSCOPIC CROSS SECTIONS WILL BE RECALCULATED
Error 4	FIRST ORDER SCATTERING MATRICES ARE REQUIRED BY PROBLEM BUT ARE NOT AVAILABLE ON OLD DATASET OLDSGS. ALL MICROSCOPIC CROSS SECTIONS MUST BE RECALCULATED
Fatal Error -999	ERROR IN BPOINTER ALLOCATION
Subroutine SIGMAC	
Fatal Error -1	ALL PROBLEM MATERIALS COULD NOT BE FOUND ON LIBRARY FILE

CSC009 (AREA 8)

Subroutine BGFLE1	
Fatal Error -170	ALL PROBLEM MATERIALS COULD NOT BE FOUND
Subroutine BGFLE2	
Fatal Error -200	ALL PROBLEM MATERIALS COULD NOT BE FOUND ON FILE MCC2F5
Fatal Error -320	NO CORRESPONDENCE CAN BE FOUND BETWEEN PROBLEM MATERIAL AND INELASTIC MATERIAL
Fatal Error -500	ALL PROBLEM MATERIALS TO BE EDITED COULD NOT BE FOUND
Subroutine BSQITR	
Error 1001	BUCKLING ITERATION NOT FEASIBLE-ZERO BUCKLING IS ASSUMED
Subroutine DRIVER	
Error 515	INHOMOGENEOUS SOURCE CALCULATION IS MEANINGFUL ONLY FOR SUBCRITICAL CONFIGURATION

TABLE V. Contd.

CSC009 (AREA 8) Contd.

Subroutine FILE1	
Fatal Error -1000	ALL PROBLEM MATERIALS COULD NOT BE FOUND
Subroutine FILE6	
Fatal Error -9000	ALL PROBLEM MATERIALS COULD NOT BE FOUND
Fatal Error -9010	ALL PROBLEM MATERIALS WITH INELASTIC AND/OR (N,2N) DATA COULD NOT BE FOUND
Fatal Error -9020	ALL PROBLEM MATERIALS WITH INELASTIC AND/OR (N,2N) DATA COULD NOT BE FOUND
Subroutine INIT	
Fatal Error -1000	ALL FISSION SPECTRA MUST BE VECTORS
Error 1001	PROBLEM CHI VECTORS ARE NOT PROPERLY NORMALIZED
Subroutine ISOCHI	
Fatal Error -500	FISSION SPECTRUM FOR PROBLEM MATERIAL M COULD NOT BE FOUND
Subroutine CSC009 (MAIN)	
Fatal Error -999	AN ERROR HAS OCCURRED IN ALLOCATING VARIABLY DIMENSIONED ARRAYS
Subroutine REORDR	
Fatal Error -1000.	ALL UNRESOLVED RESONANCES WERE NOT PROCESSED
Subroutine RESCAT	
Fatal Error -300	ALL RESOLVED RESONANCE MATERIALS COULD NOT BE FOUND
Subroutine RESCS	
Error 1001	THERE ARE UNRESOLVED MATERIALS IN PROBLEM BUT UNRESOLVED ULTRA-FINE-GROUP CROSS SECTIONS ARE NOT AVAILABLE FROM FILE UNREG
Subroutine SETBG	
Error 200	FIXED SOURCE CANNOT BE WRITTEN TO FILE SRATES
Fatal Error -999	ERROR IN BPOINTER ALLOCATIONS

TABLE V. Contd.

CSC010 (AREA 9)

Subroutine SETIN

Fatal Error -999	AN ERROR HAS OCCURRED IN ALLOCATING VARIABLY DIMENSIONED ARRAYS

Subroutine BGPN

Error 280	INHOMOGENEOUS PROBLEM IS POSSIBLE ONLY IF EIGENVALUE IS LESS THAN UNITY

Subroutine BSQTR

Error 1001	BUCKLING ITERATION NOT FEASIBLE-ZERO BUCKLING IS ASSUMED

Subroutine HOMOG

Error 1	AT LEAST TWO ISOTOPES ON FILE ISOTXS HAVE THE SAME NAME. ONLY THE CROSS SECTIONS OF THE FIRST ARE PROCESSED
Fatal Error -2	SCATTERING TYPE IS NOT DEFINED
Error 3	NO UPSCATTER IS PERMITTED. UPSCATTER MATRIX ELEMENTS WILL NOT BE PROCESSED
Fatal Error -4	ALL PROBLEM ISOTOPES COULD NOT BE FOUND ON FILE ISOTXS

Subroutine CSC010 (MAIN)

Fatal Error -1	SET FISSION VECTOR MUST BE PRESENT ON FILE ISOTXS IF NO EXTERNAL SOURCE IS PROVIDED
Fatal Error -999	ERROR IN BPOINTER ALLOCATION

CSC011 (RABANL)

Subroutine CSC011 (MAIN)

Fatal Error -10100.	PROBLEM MATERIAL NOT IN THE LIBRARY
Fatal Error -10200.	FOIL MATERIAL NOT IN THE LIBRARY

Subroutine MANAGR

Fatal Error -10100.	INSUFFICIENT STORAGE PROVIDED FOR AREA 10 EXECUTION

Subroutine MATRIX

Fatal Error -10100.	DETERMINANT IS SINGULAR

TABLE V. Contd.

CSC011 (RABANL) Contd.

Subroutine MERGER

Fatal Error -10100.	THE PROBLEM CONTAINS NO RESOLVED RESONANCES
Fatal Error -10200.	THE DATA SET SRATES IS NOT CONSISTENT WITH THE AREA 10 UPPER ENERGY OF THE CURRENT PROBLEM
Fatal Error -10300.	THE DATA SET SRATES IS NOT CONSISTENT WITH THE NUMBER OF ULTRA FINE GROUPS IN THE CURRENT PROBLEM

Subroutine RATES

Fatal Error -10100.	A NEGATIVE COLLISION RATE HAS BEEN ENCOUNTERED

Subroutine SOARCE

Fatal Error -10100.	A NEGATIVE SOURCE HAS BEEN COMPUTED

CSE009 (ISOTXS Editor)

Subroutine CSE009 (MAIN)

Error 10000	CARD IS OF WRONG TYPE. SHOULD BE CARD OF TYPE 01

Subroutine XSEDIT

Fatal Error -10000	CARD IS OF WRONG TYPE. SHOULD BE CARD OF TYPE 02
Fatal Error -20000	REQUESTED ISOTOPE NOT FOUND IN LIBRARY

CSE007 (Generate XS.ISO from ISOTXS)

Subroutine CTD

Fatal Error -998	SET YOU HAVE ASKED TO ADD TO IS INCOMPATIBLE IN ENERGY STRUCTURE OR GROUPS
Fatal Error -999	ERROR IN BPOINTER ALLOCATION

Subroutine CTS

Fatal Error -998	SET YOU HAVE ASKED TO ADD TO IS INCOMPATIBLE IN ENERGY STRUCTURE OR GROUPS
Fatal Error -999	ERROR IN BPOINTER ALLOCATION

Subroutine PRINXD

Error 500	FILE ISOTXS CONTAINS UNDEFINED SCATTERING TYPE

TABLE V. Contd.

CSE007 (Generate XS.ISO from ISOTXS) Contd.

Subroutine PRINXS

Error 500	FILE ISOTXS CONTAINS UNDEFINED SCATTERING TYPE

CSE012 (XS.ISO Editor)

Subroutine CSE012

Fatal Error -10000.	DATA SET XS.ISO NOT PROVIDED
Fatal Error -10100.	TYPE 01 CARD NOT FOUND
Fatal Error -10200.	TYPE 02 CARD NOT FOUND

Subroutine SORTNM

Fatal Error -10000.	CARD TYPE 01 NOT FOUND
Fatal Error -10100.	CARD TYPE 01 NOT FOUND
Fatal Error -10200.	ISOTOPE LABELS MUST BE NON-BLANK
Fatal Error -10300.	EACH ISOTOPE SPECIFIED ON AN ACSE12 CARD MUST CORRESPOND TO SOME ISOTOPE IN THE XS.ISO DATA SET

REED/RITE

Fatal Error -900	LOGICAL UNIT NUMBER IS OUT OF RANGE
Fatal Error -910	MODE INDEX OUT OF RANGE
Fatal Error -920	RECORD NUMBER OUT OF RANGE
Fatal Error -930	NUMBER OF WORDS IS NEGATIVE
Fatal Error -940	MISSING DD CARD FOR FILE LUN
Fatal Error -950	SIO ACCESS ERROR
Error 960	WRITING A RECORD WITH NWDS=0
Fatal Error -999	ATTEMPTING TO READ PAST END OF FILE

VII. PROGRAMMING INFORMATION

The MC^2-2 code system was developed within the ARC System modular environment[1] on IBM hardware with an OS operating system. Great care was taken in the programming to limit the degree of system dependence. A number of local conventions were adopted to permit ease of code conversion. These local conventions supplemented the procedures adopted by the CCCC[2]. Two standalone versions of MC^2-2 were created based on the ARC System modular program; (i) an IBM version for use on any IBM 360 or 370 operating system with at least 600K bytes of storage and (ii) a CDC version for use on CDC 7600 hardware with 50K words of SCM, 60K words of directly addressable LCM, and SECMENTATION LOADER capability as offered with SCOPE 3.4. In this chapter some of the details of the MC^2-2 code are given along with a description of the differences between the IBM and CDC versions of the code. A guide for the implementation of both standalone versions of the code is provided.

A. Program Structure

The standalone versions of the MC^2-2 code were adapted from the ARC System modular programs by creating a primary overlay for each of the MC^2-2 modules (c.f. Chapter VI). Figure 16 shows the overlay control cards for the IBM version and Figure 17 shows the directives required for a segmented load of the CDC version of the code. The segmentation loader available with the SCOPE 3.4 operating system was used by MC^2-2 to avoid the need to insert special OVERLAY and PROGRAM statements and to permit the passing of arguments across overlays.

The programming language used in MC^2-2 is almost entirely FORTRAN. The few machine language subprograms used are discussed in Section D below. There is a one-to-one correspondence between the FORTRAN source code of the IBM and CDC versions. Changes required to account for word length differences, large core memory use, or ENTRY point differences, for example, are flagged by CDC* and/or CIBM comment cards. Testing of the FORTRAN code was performed using the IBM FORTRAN H, OPT=2, compiler whereas the CDC code was compiled using the FTN 4.5, OPT=1 compiler. Extensive use is made of comment cards throughout the FORTRAN source code in an attempt to make the code as self-documenting as possible.

B. ARC System Routines

The user specified BCD (card) input to MC^2-2 follows the ARC System conventions[1] as discussed in Chapter VI. The FORTRAN routines SCAN and STUFF read and process the input as discussed in Reference 1.

```
ENTRY MAIN
INSERT MAIN
INSERT SNIFF,SEEK,REED,TIMER,ERROR
INSERT POINTR,PUTPNT,BULK,FREE,WIPOUT,GETPNT,IGET,IPT2,PUTM
INSERT IPTERR,ILAST,REDEF,REDEFM,PURGE,STATUS,PRTI1,PRTI1E
INSERT PRTI2,PRTI2E,PRTR1,PRTR1E,PRTR2,PRTR2E
INSERT ALLOC$,LOCF,TIME,CLOCK#,DATE,ABEND,TRACER,SECOND,JOBID
INSERT PRNT1E,PRNT1A,PRNT1I
INSERT MIXER,SIGMAX,QUICK1,CSLAB1,SIGESC
INSERT QL,FXP1,GRAPH
INSERT MATRIX
INSERT LENGTH,OUTPUT,NUMBER,ARRAY,SPECS,EDITS,REAIMW,INTEGL
INSERT TIMING,OPTUNR,IOPUT,STFARC,LOCATE,TABLES,PTERR,LCMSIZ,BFLAGS
OVERLAY ALPHA
INSERT CODE
INSERT SCAN
INSERT STUFF,STUFF1
OVERLAY ALPHA
INSERT CSI010,SPACER,PRNT1D,PRNTAE,DISPOS,GOWEST
INSERT UNITS,CRDCNT,LBSPEC
OVERLAY BETA
INSERT TESTBG,CARD05,CARD06,CARD07,CARD09
OVERLAY BETA
INSERT RDANIP,TYPE06,TYPE14,TYPE15,EDGEOM,GEOM
OVERLAY BETA
INSERT STRTCH,HETERO,CARD10,CARD11,CARD12,SXLSXR,CSDMGI,CARD14
INSERT CARD15,CARD16,CARD17,CARD18,FOILS,CARD21,CARD22,CARD08,CARD23
OVERLAY BETA
INSERT WRITER,EDTPRB
INSERT REC1
OVERLAY ALPHA
INSERT CSC004,SETUPU,UNRINT,DRCTOR,EDITUN
INSERT ESMESH,PACKER
INSERT WZERO,QUICKJ,INTERP
INSERT RATION,MULTIP,FILE3,BOUNDY,DRCUNR
OVERLAY ALPHA
INSERT CSC005,ADMSTR,SETUPR,SIFTER,RATNL
INSERT REORDR,STUFIT,NSIG0
INSERT JINT,OVRLAP,WINNER,JINTGL,TRIPLE,LORENT,EDITLZ
INSERT BOUNDE,PHILE1,FILE4
INSERT TRIPIN
OVERLAY ALPHA
INSERT CSC006,EDITSP,EDITAT,EDITRS,POTNTL,WRISIT,INTRAC
INSERT MAININ
OVERLAY ALPHA
INSERT CSC008
INSERT NSCR7
OVERLAY BETA
INSERT SIGAVG,SIGMAC,SETCHI
```

Fig. 16. IBM Overlay Control

```
OVERLAY BETA
INSERT SETSCT,SETCSD,CALCFN,FNAVG,ELSCAT,XTRN,MODPAR
OVERLAY BETA
INSERT EDIT1,EDIT2
OVERLAY ALPHA
INSERT CSC009,DRIVER,SETBG,TABINT,PROBIN
INSERT NSCR8,RESINF,LUN8,INDATA,THDATA,ARGUE
OVERLAY BETA
INSERT ATNSRC,REORDR,EGRID
OVERLAY BETA
INSERT SETIN,FILE1,FILE6,MATCH,INIT
OVERLAY BETA
INSERT INSCAT,MGSPEC,CSDSPC,FISSOR,BSQITR,PARAB
OVERLAY BETA
INSERT EDTUFG,ORIGIN
OVERLAY BETA
INSERT BGSPEC,INSBG,DOIO
OVERLAY BETA
INSERT BGFLE1,FILEID,RESCS,RESCAT
OVERLAY BETA
INSERT BGFLE2,PRINXS,CVD,BGSCAT,ISOCHI
OVERLAY BETA
INSERT SRATE
OVERLAY ALPHA
INSERT CSC010,HOMOG,BGPN,BSQTR,CRAMER,BGSORS
INSERT NSCR9,LUN9
OVERLAY ALPHA
INSERT CSE009,XSEDIT
INSERT CONT,INPUT,NUMBRE,ISOCNT
OVERLAY ALPHA
INSERT CSC011,E2E3E4,FREEUP
OVERLAY BETA
INSERT MERGER,SPOOL,FLIPIT,SYM
OVERLAY BETA
INSERT SIFTIT
OVERLAY GAMMA
INSERT STUFER,REARNG
OVERLAY GAMMA
INSERT RESXSC,RATES,SOARCE,MANAGR,EZ3,YZ3,YZ4,XTRAP,PFUNC
INSERT GAUSS,EXTRNL,RTS3S4
OVERLAY GAMMA
INSERT PREEDT,EDTICS,PREFOL,EDTFOL,DRIVED
INSERT BIGLUN
OVERLAY GAMMA
INSERT PREEDI,EDTICI,PREFOI,EDTFOI,DRIVEI
```

Fig. 16. IBM Overlay Control (Contd.)

```
 ROOT       TREE     ALLOC1-(CODE,M4,INTERP,EDITLZ,PRTECS,M7,M8,BGPN,XSEDT
,T,M10)
 M4         TREE     GOWEST-(CA-D09,EDGEOM,CARD23,EDTPRB)
 M7         TREE     CSC008-(SETCHI,MODPAR,EDIT2)
 M8         TREE     PROBIN-(EGRID,INIT,PARAB,EDTUFG,DOIO,RESCAT,ISOCHI,SR
,ATE)
 M10        TREE     FREEUP-(SYM,M10A21)
 M10A21     TREE     SIFTIT-(REARNG,PFUNC,DRIVED,DRIVEI)
 ALLOC1     INCLUDE MCC2,PRNT1E,PRNT1A,ERF,CVD,SNIFF,SEEK,REED,DRED,TIMER
,,WIPOUT,GETPNT,IGET,IPT2,PUTM,IPTERR,ILAST,REDEFM,PURGE,PRTI1,PRTI1E,PR
,TI2,PRTI2E,PRTR1,PRTR1E,PRTR2,PRTR2E,PRNT1I,ERROR,ABEND,POINTR,PUTPNT,B
,ULK,FREE,FREE1,MEMGET,BUOPEN,ZEROIO,MATRIX,STATUS,QUICK1,FXP1,QL,MIXER,
,GRAPH,SIGMAX,CSLAB1,SIGESC
 CODE       INCLUDE SCAN,STUFF,STUFF1
 GOWEST     INCLUDE CSI010,SPACER,PRNT1D,PRNTAE,DISPOS
 CARD09     INCLUDE TESTBG,CARD05,CARD06,CARD07
 EDGEOM     INCLUDE RDANIP,TYPE06,TYPE14,TYPE15
 CARD23     INCLUDE STRTCH,HETERO,CARD10,CARD11,CARD12,SXLSXR,CSDMGI,CARD
,14,CARD15,CARD16,CARD17,CARD18,FOILS,CARD21,CARD22,CARD08
 EDTPRB     INCLUDE WPITER
 INTERP     INCLUDE CSC004,SETUPU,DRCTOR,EDITUN,UNRINT,ESMESH,PACKER,WZER
,O,QUICKJ
 EDITLZ     INCLUDE CSC005,ADMSTR,SETUPR,SIFTER,RATNL,REORDR,STUFIT,NSIG0
,,SIGMAX,JINT,OVRLAP,WINNER,JINTGL,TRIPLE,LORENT
 PRTECS     INCLUDE CSC006,EDITSP,EDITAT,EDITRS,POTNTL,WRISIT,INTRAC
 SETCHI     INCLUDE SIGMAC,SIGAVG
 MODPAR     INCLUDE SETSCT,SETCSD,CALCFN,FNAVG,ELSCAT,XTRN
 EDIT2      INCLUDE EDIT1
 PROBIN     INCLUDE CSC009,DRIVER,SETBG,TABINT
 EGRID      INCLUDE ATNSRC,REORDR
 INIT       INCLUDE SETIN,FILE1,FILE6,MATCH
 PARAB      INCLUDE INSCAT,MGSPEC,CSDSPC,FISSOR,BSQITR
 DOIO       INCLUDE BGSPEC,INSBG
 RESCAT     INCLUDE BGFLE1,FILEID,RESCS
 ISOCHI     INCLUDE PRINXS,BGFLE2,BGSCAT
 BGPN       INCLUDE CSC010,HOMOG,BSQTR,CRAMER,BGSOPS
 XSEDIT     INCLUDE CSE009
 FREEUP     INCLUDE CSC011,E2E3E4
 SYM        INCLUDE MERGER,SPOOL,FLIPIT
 REARNG     INCLUDE STUFER
 PFUNC      INCLUDE RESXSC,RATES,SOARCE,MANAGR,EZ3,YZ3,YZ4,XTRAP
 DRIVED     INCLUDE PREEDT,EDTICS,PREFOL,EDTFOL
 DRIVEI     INCLUDE PREEDI,EDTICI,PREFOI,EDTFOI
            GLOBAL  LENGTH,OUTPUT,NUMBER,ARRAY,SPECS,EDITS,INTEGL,TIMING,
,OPTUNR,UNITS,LBSPEC,CRDCNT,ARRAY2,CRALOC,STFARC,BFLAGS,LCMSIZ,PTERR,TAB
,LES,LOCATE,INITIO,NSCR7,ARGUE,THDATA,INDATA,LUN8,RESINF,NSCR9,IOPUT,REA
,IMW,NSCR10,SAVER,FINDER,LGUNIT,WPNTRS,GEOMBC
            END      MCC2
```

Fig. 17. CDS Segmentation Loader Directives

The code MC^2-2 uses the dynamic storage capability, BPOINTER, described in Reference 1, to manage all variable dimension array allocations. A one-to-one correspondence between the IBM and CDC versions of this subprogram package has been retained except for the machine dependent routines ALLOC and LOCF which are discussed in Section D below. The bulk storage capability of the IBM version of BPOINTER has been modified to manage arrays in large core memory of the CDC 7600. Appendix E describes some of the characteristics of the BPOINTER subprogram package.

The ARC System routine SNIFF is used throughout the code to assign logical unit numbers to named data files. Both the IBM and CDC standalone versions of the code use a modification of the routine SNIFF which calls the CCCC subroutine SEEK described in Section C below.

C. CCCC Standard Subroutines

The Committee on Computer Code Coordination has specified a number of standard routines[2] to be used in RRD funded code development. In principle the routines may be installation dependent. The MC^2-2 code uses the standard routines REED, RITE, TIMER and SEEK as specified in Reference 2. While it is possible to substitute installation dependent code, simple versions of these routines are provided with both the IBM and CDC standalone versions of MC^2-2.

1. SEEK

The subroutine SEEK is used by MC^2-2 to return the logical unit number associated with a named data file. With only two exceptions, all files referenced by MC^2-2 are assigned unit numbers through calls to subroutine SEEK. The two exceptions are the BCD files input (5) and printed output (6). While it should be possible to use installation dependent versions of SEEK, it is obvious that any changes in unit allocation must also be reflected in the Job Control Language required for the IBM version of MC^2-2 (Fig. 11) or the program card of the CDC version. A single initialization call to SEEK is made from the main program driver of MC^2-2. In Table VI information is provided about the various files referenced by MC^2-2. Detailed formats for the interface files MCC2F1 - MCC2F8, ISOTXS and XSISO, card input files A.MCC2, A.NIP, A.STP015, ACS009 and ACSE12, and some of the other important files are given in the Appendices B, C and D. It should be noted from Table VI that each named file in the IBM version of the program is assigned a unique logical unit number. Restrictions on the number of unit definitions permitted by CDC 7600 software made it necessary to use the same unit number for more than one file. This equivalencing of files was specified to retain full program generality. The file assignment is specified in the initialization call to SEEK from the main program driver. In spite of the large number of files required, even the largest problem requires that a maximum of seven files be open at any particular time in the calculation.

In Table VI there is a column indicating the modules (overlays) which reference a particular file for reading and/or writing. Many of these references are conditional and depend upon the particular problem specifications. Extensive use is made of the various SEEK options to determine whether a particular file is available for reading and/or writing.

TABLE VI. MC^2-2 File Information

Name	Logical Unit Number IBM (CDC)	Contents	Modules Referencing File*
Input	5 (5)	BCD Input-Not Referenced by SEEK	CSI010 (R)
Output	6 (6)	Printed Output-Not Referenced by SEEK	All Modules (W)
ARC	9 (56)	Processed BCD Input-Not Referenced by SEEK	SCAN (W) STUFF (R)
A.MCC2	11 (11)	MC^2-2 General BCD Input	STUFF (W) CSI010 (R)
A.NIP	12 (12)	Geometry and composition BCD Input	STUFF (W) CSI010 (R)
A.STP015	13 (13)	Path BCD Input	STUFF (W) DRIVER (R) CSI010 (R)
ATNUAT	14 (14)	Unresolved Attenuation Factors	CSC004 (W) CSC006 (R,W) CSC009 (R)
BC	15 (15)	Boundary Conditions	CSI010 (R,W) CSC004 (R) CSC005 (R) CSC006 (R) CSC011 (R)
BGRES	16 (16)	Broad Group Resonance Cross Sections	CSC009 (R,W)

TABLE VI. MC^2-2 File Information (Contd.)

Name	Logical Unit Number IBM (CDC)	Contents	Modules Referencing File*
GEOM1	17 (17)	Geometry Data	CSI010 (R,W) CSC004 (R) CSC005 (R) CSC006 (R) CSC011 (R)
GRPORD	18 (18)	Group Ordered Inelastic Data	CSC009 (R,W)
ISOTXS	19 (19)	Interface Broad Group Cross Sections	CSC009 (W) CSC010 (R) CSE009 (R) CSE007 (R)
LORENZ	20 (20)	Lorenzian Distribution	CSC005 (R,W)
MACTOT	21 (21)	Ultra-Fine-Group Macroscopic Total Cross Section	CSC004 (R,W) CSC005 (R,W) CSC006 (R,W) CSC011 (R,W)
MCC2F1	22 (22)	Administrative Data	CSI010 (R) CSC004 (R) CSC005 (R) CSC006 (R) CSC008 (R) CSC009 (R) CSC011 (R)
MCC2F2	23 (23)	Tabulated Data	CSC004 (R) CSC005 (R) CSC006 (R) CSC009 (R) CSC011 (R)
MCC2F3	24 (24)	Unresolved Resonance Data	CSI010 (R) CSC004 (R) CSC006 (R)

TABLE VI. MC^2-2 File Information (Contd.)

Name	Logical Unit Number IBM (CDC)	Contents	Modules Referencing File*
MCC2F4	25 (25)	Resolved Resonance Data	CSI010 (R) CSC005 (R) CSC006 (R) CSC011 (R)
MCC2F5	26 (26)	Ultra-Fine-Group Non-Resonance Cross Sections	CSC004 (R) CSC005 (R) CSC006 (R) CSC008 (R) CSC009 (R) CSC011 (R)
MCC2F6	27 (27)	Inelastic and (n,2n) Data	CSC009 (R)
MCC2F7	28 (28)	Fission Spectrum Data	CSI010 (R) CSC008 (R)
MCC2F8	29 (29)	Elastic Scattering Distribution Data	CSC008 (R)
MICTOT	30 (30)	Ultra-Fine-Group Microscopic Total Cross Section	CSC004 (R,W) CSC005 (R,W) CSC006 (R,W)
OLDSGS	31 (31)	Ultra-Fine-Group Elastic Matrices for Restart	CSC008 (R)
OPTICL	32 (32)	Optical Distance Data	CSC004 (R,W) CSC005 (R,W) CSC006 (R)
PLOTIT**	33 (33)	Dummy File for Plotting Output	CSC008 (W) CSC009 (W)

TABLE VI. MC^2-2 File Information (Contd.)

Name	Logical Unit Number IBM (CDC)	Contents	Modules Referencing File*
PRBCHI	34 (34)	Problem Dependent Fission Spectrum Data	CSC008 (W) CSC009 (R,W)
PRBSPC	35 (35)	Problem Specifications	CSI010 (R,W) CSC004 (R) CSC005 (R) CSC006 (R) CSC008 (R) CSC009 (R) CSC010 (R) CSC011 (R) CSE009 (R) CSE007 (R)
RESINT	36 (38)	Resolved Resonance Integrals	CSC005 (W) CSC006 (R,W) CSC009 (R)
SCR001	37 (39)	Scratch	CSC005 (R,W) CSC008 (R,W) CSC009 (R,W) CSC011 (R,W)
SCR002	38 (40)	Scratch	CSC005 (R,W) CSC008 (R,W) CSC009 (R,W) CSC011 (R,W)
SCR003	39 (41)	Scratch	CSC004 (R,W) CSC005 (R,W) CSC006 (R,W) CSC009 (R,W) CSC011 (R,W)
SCR004	40 (42)	Scratch	CSC009 (R,W) CSC011 (R,W)

TABLE VI. MC^2-2 File Information (Contd.)

Name	Logical Unit Number IBM (CDC)	Contents	Modules Referencing File*
SCR005	41 (43)	Scratch	CSC009 (R,W) CSC011 (R,W)
SIGMAP	42 (44)	Ultra-Fine-Group Background Cross Section	CSC006 (R,W)
SMSIGS	43 (45)	Ultra-Fine-Group Elastic Transfer Matrices	CSC008 (R,W) CSC009 (R)
SPECTR	44 (46)	Ultra-Fine-Group Spectrum	CSC009 (W) CSC010 (R)
SPECXS	45 (47)	Ultra-Fine-Group Cross Sections and Moderating Parameters	CSC008 (R,W) CSC009 (R)
SRATES	46 (48)	Ultra-Fine-Group Microscopic Scattering Collision Density and Sources	CSC009 (W) CSC011 (R)
UNREG	47 (49)	Unresolved Resonance Ultra-Fine-Group Cross Sections	CSC008 (W) CSC009 (R) CSC011 (R)
UNRES	48 (50)	Unresolved Cross Sections at E* Points	CSC004 (R,W) CSC008 (R)
XSISO	49 (51)	File 1 of ARC System Broad Group File	CSI010 (R) CSE007 (R,W) CSE012 (R)
XSISO5	50 (52)	File 2 of ARC System Broad Group File	CSE007 (R,W) CSE012 (R)
IRESCS	51 (53)	Integral Transport Derived Broad Group Cross Sections	CSC011 (R,W)

TABLE VI. MC^2-2 File Information (Contd.)

Name	Logical Unit Number IBM (CDC)	Contents	Modules Referencing File*
BIGXS1	52 (54)	Ultra-Fine-Group Macroscopic Scattering Data, Foil Data in Integral Transport Module For IBM 25 Files are defined BIGXS1 - BIGXSP with unit Numbers 52-76 For CDC 14 Files are defined BIGXS1 - BIGXSE with unit Numbers 54, 55, 11, 12, 13, 20, 21, 30, 32, 33, 44, 51, 52, 53	CSC008 (R,W) CSC009 (R) CSC011 (R,W)
RANDOM**	77 (-)	Random Access Data File Not Used In Standalone Code Releases	CSC009 (R,W)
RESDAT	78 (37)	Selected Resonance Parameters	CSC005 (W) CSC009 (R)
ACS009	79 (36)	BCD Input for ISOTXS Editor	STUFF (W) CSE009 (R)
ACSE12**	80 (-)	BCD Input for XS.ISO Editor	STUFF (W) CSE012 (R)

*R Read
W Write

** Not Referenced in Standalone Version of MC^2-2

2. REED/RITE

The standard routines REED and RITE are used to perform the non-formatted (binary) I/O operations for MC^2-2. The ARC System modular version of REED/RITE makes use of three access methods, standard FORTRAN, asynchronous FORTRAN and a special random access I/O package SIO[40]. The IBM and CDC standalone versions of MC^2-2 contain a far simpler version of REED/RITE which uses standard FORTRAN I/O. The CCCC specifications of REED and RITE did not account for the possibility of multilevel data transfers as required by the CDC version of MC^2-2 to permit the transfer of data between large core memory and disk files without use of a buffer array in small core memory. In order to permit such transfers the routines DRED and DRIT were used in the CDC version of the code. The argument lists to DRED/DRIT are precisely the same as the calls to REED/RITE but the array address into (from) which data are transferred is assumed to be in large core memory. This convention differs from a recent proposal to the CCCC where a pointer rather than an address was recommended. Changes to conform with the recommended versions of DRED/DRIT would be quite simple because of the limited number of calls to these routines.

3. TIMER

The standard subroutine TIMER is used by MC^2-2 to provide timing and problem identification information. These data are not essential to the execution of the MC^2-2 program. As a consequence, the CDC version of TIMER is in large part a dummy program. It calls only the standard CDC system code SECOND to provide CPU timing data. The IBM version of TIMER makes use of a number of assembler language routines to provide time and edit information. These assembler routines are described in Section D below.

D. Machine Language Routines

Machine language routines are used in MC^2-2 to provide capability which does not exist in the FORTRAN language. A brief description of these subprograms is provided in this section.

1. ALLOC

The subroutine POINTR of the dynamic allocation subprogram package BPOINTER assigns storage dynamically at run time based on user input specifications. The routine ALLOC is called to assign and free this storage. The IBM version of the code ALLOC makes use of the OS macros GETMAIN and FREEMAIN to perform this function. The CDC version of ALLOC is a FORTRAN function which calls the COMPASS routine MEMGET to perform the allocation.

2. LOCF

The function subprogram LOCF is used by subroutine POINTR to obtain the address of the dynamic storage container and the common block /ARRAY/. This function is a standard routine of CDC FORTRAN. The IBM version of the function is coded in assembler language. Since the CDC version of LOCF does not obtain the address of LCM variables, the CDC version of POINTR assumes that the LCM common block /ARRAY2/ is located at the start of LCM (address 1).

3. GOWEST

The subroutine GOWEST is used to left-justify Hollerith variables. The IBM version of the routine is written in assembler language. The CDC version of the routine is written in FORTRAN and uses the standard CDC FORTRAN version of the function SHIFT.

4. FILEID

The subroutine FILEID is used in subroutine BGFLE1 of module CSC009 to obtain the dataset name associated with the file ISOTXS. It is an assembler language routine in the IBM version of the code and a dummy FORTRAN routine in the CDC code.

5. CVD

The subroutine CVD is used in subroutine BGFLE2 of module CSC009 to convert a variable from integer to Hollerith format. The IBM version of CVD is written in assembler language and the CDC version of the routine uses the FORTRAN ENCODE capability.

6. TIME

TIME is used by the IBM version of subroutine TIMER to return the wall clock time in the form HH.MM.SS. TIME is not referenced in the CDC version of the code.

7. CLOCK

CLOCK is used by the IBM version of subroutine TIMER to return the wall clock time in units of .01 seconds. CLOCK is not referenced in the CDC version of the code.

8. DATE

The function subprogram DATE is called by the IBM version of subroutine TIMER to return the current date in the form MM/DD/YY. DATE is not referenced by the CDC version of the code.

9. SECOND

The subroutine SECOND is called by TIMER to return the elapsed CPU time in seconds. An IBM assembler language version of SECOND which uses the STIMER and TTIMER macro-instructions is provided. The CDC version of the code requires the standard system version of the subroutine SECOND.

10. ABEND

The subroutine ABEND is called by subroutine ERROR to force an abnormal termination of the job with a DUMP. The IBM version of ABEND is an assembler language routine which invokes the macro-instruction ABEND. An abnormal termination code USER 16 is given and a dump is written to the file SYSUDUMP or SYSABEND. The CDC version of ABEND is a FORTRAN routine which calls the FORTRAN routine EXIT.

11. JOBID

JOBID is used by the IBM version of subroutine TIMER to return the job name supplied on the user's job card. JOBID is not referenced by the CDC version of the code.

12. FXP

FXP is a fast exponential function. The algorithm is described in Appendix A. The IBM version of FXP is programmed in assembler language. An equivalent FORTRAN routine is provided with the CDC version of the code.

13. DISPOS

The subroutine DISPOS is used by the module CSI010 to determine whether the file SRATES is given a permanent or temporary disposition. The IBM version of DISPOS is programmed in assembler language. The CDC version of DISPOS is a dummy FORTRAN routine which returns a flag to the calling routine indicating a temporary disposition for the file.

14. TRACER

TRACER is used by the IBM version of REED/RITE to provide trace-back information in case of an error in REED/RITE. The IBM version of TRACER is programmed in assembler language. TRACER is not referenced in the CDC version of the code.

E. Program Implementation

Both the IBM and CDC versions of the program MC^2-2 are available from the Argonne Code Center. Each version of the code requires a program tape and a library tape. A description of the tapes along with a step-by-step implementation strategy for each version of the program is described below.

1. IBM Code Implementation

The IBM program tape is written as described in Table VII. The source code for MC^2-2 is contained on Files 1 and 2 of the program tape. A brief description of each of the subprograms of File 1 is given in Table VIII. The assembler language subprograms on File 2 of the tape were discussed in Section D above. Creation of object code for input to the linkage editor is the first step required for implementation of the MC^2-2 program. It is recommended that this step be performed in the following manner: (i) preallocate an object module dataset; (ii) compile File 1 Fortran code; (iii) assemble File 2 assembler code. The preallocation may be performed by submitting the job shown in Fig. 18. The user may clearly specify any DSN, VOL or UNIT information consistent with local naming conventions. In all of the examples which follow, ANL conventions will be used but the essential nature of each step is intended to be system independent. The compilation of the File 1 subprograms should be performed using the highest level of optimization available. Routinely this means use of the FORTRAN H compiler with OPT=2 specified. It should be noted that FORTRAN compilers are often system dependent in the sense of release identification and system generation (SYSGEN) options. The Level 21.7

compiler is currently in use at ANL but other releases of IBM compilers have been used without problem. The SIZE parameter on the standard ANL Fortran H compiler was set at 215K at SYSGEN time. Several of the MC^2-2 subroutines are too large to compile with this specification. A second Fortran H compiler is available at ANL which was specified with SIZE=450K at SYSGEN time. This compiler is used at ANL to compile the subroutines CSI010, DRCTOR, ELSCAT, CSC009, SETBG, CSC011, RATES and SIFTIT since these routines will not compile (ADCON TABLE EXCEEDED) with the smaller compiler. The compilation of File 1 code may be performed in one job step as shown in Fig. 19 or by breaking up the code into a number of smaller blocks. The latter procedure is recommended as it permits one to work with smaller blocks of source code. In order to break up the file into such manageable blocks, one can use the IBM utility IEBGENER to create a partitioned data set (PDS) and then compile each member of the PDS separately into the PDS created by the preallocation step of Fig. 18. If this mode of operation is used, a recommended breakup of the source language is by module as indicated in Table VIII. Whether one uses a PDS or the tape as input, it is recommended that the code be compiled and link edited (with NCAL specified) as shown in Fig. 19. The final step in the processing of the source language tape is the assembly of the assembler language routines on File 2 of the tape. This is done in a straightforward manner as illustrated in Fig. 20. The File 2 routines should not be broken into blocks although all of File 2 (944 source cards) may be copied as a single member of the source language PDS if desired.

If the user does not wish to work directly with source code as recommended above, an object library PDS is available on File 3 of the program tape. One may bypass the steps above and use the IBM utility IEHMOVE to load the object library to a disk pack as shown in Fig. 21. The blocksize of the object module was set to 6K so that it may be moved to either a 2314 or 3330 disk pack. This is not the recommended procedure unless there are particular problems involved in operating with the two files of source code.

A sample problem input deck is provided on File 4 of the program tape. Prior to executing this sample problem three further steps are required: (i) preparation of MC^2-2 binary libraries; (ii) modification of sample problem linkage editor instructions to conform with the object library preparation completed above; (iii) modification of the JCL procedure provided with sample problem.

A library tape is provided along with the MC^2-2 program tape. This second tape contains eight binary sequential files in the format of files MCC2F1 - MCC2F8 described in Appendix C. These files must be copied to a direct access device (e.g. disk pack) as the next step in program implementation. A sample of the job control required to copy these files is given in Fig. 22. The space requirements for these files (on a 3330 disk pack) are given in Table VII. The data available on these library files were processed from the ENDF/B-IV data files by the code ETOE-II. A summary of the library specifications is given in Table IX. The Argonne Code Center also has available four BCD tapes which contain this same eight file library in BCD format along with a Fortran program, MC^2-2 LIBGEN, which reads the BCD files and writes the eight binary files. This library generation program is described in Appendix F.

Having copied the eight library files to a direct access device, the only remaining steps in implementation involve modification of the sample problem linkage edit and JCL procedure to conform with local conventions. The linkage edit step of the sample problem deck builds an executable load module from the object library segments created by compilation and assembly of Files 1 and 2 of the library tape respectively (or alternatively copy of File 3). The user must modify the sample problem deck to reference this object library on the JCL card with the DDNAME MYLIB. Following the linkage edit SYSIN card the user must INCLUDE all members of the object library. The INCLUDE cards provided with the sample problem deck reference the members available on the PDS of File 3 of the library tape. It is obvious that the user must also modify the procedure name FTHEP and step names to conform with local conventions. If desired the load module created in this step may be given a permanent disposition so that the edit step may be bypassed on future problem executions thus saving a considerable amount ($\sim$ 2 minutes) of I/O time.

The JCL procedure (c.f. Fig. 11) ARCSP015, which follows the linkage edit step of the sample problem input must be modified to conform with local conventions. Symbolic parameters have been provided to ease the burden of this modification. For example the parameter UNITSCR should be changed in the PROC statement to reference the standard system direct access scratch unit, FULLBLK should be set to 6136 if 3330 disk packs are not available, etc. In addition the parameters MCC2F1 through MCC2F8 should be modified to conform with the data set names assigned to the eight MC^2-2 library files copied from the library tape. The parameter PRELIB should be set to the data set name (permanent or temporary) assigned to the MC^2-2 load module.

Table VII

IBM Code Center Tape Description

1) Program Tape (Non-Labelled, 9 trk, 800 bpi)

File	Description	RFCFM	LRECL	BLKSIZE
1	Fortran Source (EBCDIC)	FB	80	3200
2	Assembler Source(EBCDIC)	FB	80	3200
3	Load Module (Binary)	FB	80	800
4	Sample Problem (EBCDIC) Input	FB	80	3200

2) Library Tape (Non-Labelled, 9 trk, 1600 bpi)

File	Space (units of 3330 Tracks)	RECFM	LRECL	BLKSIZE
1	1	VBS	X	6447
2	9	VBS	X	6447
3	6	VBS	X	6447
4	11	VBS	X	6447
5	223	VBS	X	6447
6	289	VBS	X	6447
7	1	VBS	X	6447
8	334	VBS	X	6447

Figure 18

Preallocation of Object Library

```
// EXEC PGM=IEFBR14
//OBJECT DD DSN=MCC2.OBJLIB,DISP=(NEW,CATLG),UNIT=SHRT3330,
//   SPACE=(CYL,(5,3,1)),VOL=SER=,DCB=BLKSIZE=6144
/*
```

Figure 19

Compilation of Fortran Subprograms

```
// EXEC FTHCEP,OPTIONS='OPT=2',COMPILE=FORTH450,
//     EDTOPTS='LET,LIST,MAP,DCBS,NCAL'
//FTH.SYSIN DD UNIT=TAPE9TRK,DISP=OLD,LABEL=(1,NL),
//     VOL=(,RETAIN,SER=nnnnnn),
//     DCB=(RECFM=FB,LRECL=80,BLKSIZE=3200,DEN=2)
//EDT.SYSLMOD DD DISP=OLD,DCB=BLKSIZE=6144,
//     DSN=MCC2.OBJLIB(anyname1)
/*
```

Figure 20

Assembly of File 2 CSECTS

```
// EXEC ASMCEP,EDTOPTS='LIST,MAP,DCBS'
//ASM.SYSIN DD UNIT=TAPE9TRK,DISP=OLD,LABEL=(2,NL),
//     VOL=(,RETAIN,SER=nnnnnn),
//     DCB=(RECFM=FB,LRECL=80,BLKSIZE=3200,DEN=2)
//EDT.SYSLMOD DD DISP=OLD,DCB=BLKSIZE=6144,
//     DSN=MCC2.OBJLIB(anyname2)
/*
```

Figure 21

Copy Object Module from File 3 of Program Tape to Disk

```
// EXEC PGM=IEHMOVE
//SYSPRINT DD SYSOUT=A
//SYSUT1 DD DISP=SHR,UNIT=3330,VOL=SER=SCR001
//OBJECT DD DISP=OLD,UNIT=3330,VOL=SER=PACKxx
//TAPE DD DISP=(OLD,PASS),UNIT=TAPE9TRK,VOL=(,RETAIN,SER=nnnnnn),
//             DCB=(RECFM=FB,LRECL=80,BLKSIZE=800,DEN=2),
//             LABEL=(3,NL),DSN=FILE3
//SYSIN DD *
 COPY FROM=2400=(nnnnnn,3),TO=3330=PACKxx,FROMDD=TAPE,                *
             DSNAME=MCC2.OBJLIB
/*
```

```
//LIBCOPY PROC TAPE=119361,TUNIT=TAPE1600,FILE=1,NAME=,
//            PRIMARY=1,SPCE=TRK,UN=3330,DSP=KEEP
// EXEC PGM=IEBGENER
//SYSPRINT DD SYSOUT=A
//SYSUT1 DD DISP=OLD,DCB=(RECFM=VBS,LRECL=X,BLKSIZE=6447),
//            UNIT=&TUNIT,LABEL=(&FILE,NL),VOL=(,RETAIN,SER=&TAPE)
//SYSUT2 DD DSN=&NAME,UNIT=&UN,DISP=(NEW,&DSP),DCB=*.SYSUT1,
//            SPACE=(&SPCE,(&PRIMARY,1))
//SYSIN DD DUMMY
// PEND
// EXEC LIBCOPY,NAME=MCC2F1
// EXEC LIBCOPY,NAME=MCC2F2,FILE=2,PRIMARY=9
// EXEC LIBCOPY,NAME=MCC2F3,FILE=3,PRIMARY=6
// EXEC LIBCOPY,NAME=MCC2F4,FILE=4,PRIMARY=11
// EXEC LIBCOPY,NAME=MCC2F5,FILE=5,PRIMARY=12,SPCE=CYL
// EXEC LIBCOPY,NAME=MCC2F6,FILE=6,PRIMARY=16,SPCE=CYL
// EXEC LIBCOPY,NAME=MCC2F7,FILE=7
// EXEC LIBCOPY,NAME=MCC2F8,FILE=8,PRIMARY=18,SPCE=CYL
```

Fig. 22. Copy of MC^2-2 IBM Binary Library Files

TABLE VIII. Function of MC^2-2 Subprograms

Driver and System Subprograms

MAIN (000010 - 002110)*

Main program driver for MC^2-2. Initializes SEEK, calls system routines to read and spool BCD input and calls all modules.

SEEK (002120 - 004290)

CCCC routine returns logical unit numbers associated with named data file.

REED/RITE (004300 - 006500)

CCCC routine performs all binary I/O data transfer operations.

TIMER (006510 - 007830)

CCCC routine performs all timing and system dependent editing (date, ID, etc.) operations.

ERROR (007840 - 008450)

Prints error numbers and calls ABEND for job termination in case of FATAL error.

SNIFF (008460 - 008700)

Dummy ARC System interface routine calls SEEK to obtain unit information.

BPOINTER (008710 - 021230)

Dynamic allocation subprogram package - c.f. Appendix .

CODE (021240 - 022650)

Reads a BCD card image and inspects it; called by SCAN and STUFF modules.

SCAN (022660 - 024880)

Reads entire BCD input stream from logical unit number 5 and spools the data to file ARC. Calls SEEK to initialize files in BLOCK=OLD.

*Numbers in brackets are sequence numbers of routine on MC^2-2 program tape.

TABLE VIII. Function of MC^2-2 Subprograms (Contd.)

STUFF (024890 - 026270)

Locates next block of data from file ARC for processing.

STUFF1 (026280 - 029800)

Reads and process next block of BCD data from file ARC.

PRNT1A (029810 - 031020)

Edits one-dimensional Hollerith arrays.

PRNT1E (031030 - 032250)

Edits one-dimensional floating point single precision arrays.

PRNT1I (032260 - 033470)

Edits one-dimensional integer arrays.

MIXER (033480 - 034950)

Homogenizes smooth u.f.g. total cross sections for homogeneous mixture and each heterogeneous region.

SIGMAX (034960 - 036560)

Calculates optical thickness to left and right of each slab region.

QUICK1/QUICKW (036570 - 038070)

Calculates the real and imaginary parts of the complex W function.

MATRIX (038080 - 039830)

Matrix inversion routine.

CSLAB1/CSLAB (039840 - 040460)

Calculates Dancoff factor for slab region.

SIGESC (040470 - 040800)

Calculates escape cross section for cylindrical two-region pin cells.

TABLE VIII. Function of MC^2-2 Subprograms (Contd.)

QL (040810 - 043580)

Calculates ratio of Legendre functions of the second kind, Q_{N+1}/Q_N - c.f. Appendix A.

GRAPH (043590 - 043650)

Dummy routine to substitute for Simplotter driver.

****

CSI010 (043660 - 060380)

Main program driver for MC^2-2 input processor.

CARD06 (060390 - 062630)

Reads type 06 cards of file A.MCC2 and orders materials consistent with library.

CARD15 (062640 - 066460)

Reads and processes type 15 cards of file A.MCC2.

CARD22 (066470 - 068170)

Reads type 22 cards of file A.MCC2 and loads arrays.

CARD09 (068180 - 071100)

Reads and processes type 09 cards of file A.MCC2.

CARD14 (071110 - 072970)

Reads and processes type 14 cards of file A.MCC2.

CARD18 (072980 - 074070)

Reads and processes type 18 cards of file A.MCC2.

CARD10 (074080 - 075330)

Reads and processes type 10 cards of file A.MCC2.

TYPE06 (075340 - 078580)

Reads and processes type 06 cards of file A.NIP.

TYPE14 (078590 - 081610)

Reads and processes type 14 cards of file A.NIP.

TABLE VIII. Function of MC^2-2 Subprograms (Contd.)

TYPE15 (081620 - 086030)

Reads and processes type 15 cards of file A.NIP.

CARD16 (086040 - 087860)

Reads and processes type 16 cards of file A.MCC2.

CARD21 (087870 - 089690)

Reads and processes type 21 cards of file A.MCC2.

SPACER (089700 - 090260)

Reads past cards in a BCD file.

CARD23 (090270 - 091960)

Reads and processes type 23 cards of file A.MCC2.

CARD11 (091970 - 093130)

Reads and processes type 11 cards of file A.MCC2.

CARD08 (093140 - 097070)

Reads and processes type 08 cards of file A.MCC2.

HETERO (097080 - 098250)

Generates homogeneous atom densities from A.NIP data.

CARD17 (098260 - 102370)

Reads and processes type 17 cards of file A.MCC2.

CSDMGI (102380 - 103130)

Determines interface energy between multigroup and continuous slowing down solution algorithms.

PRNTAE (103140 - 103860)

Edits Hollerith and single precision floating point arrays.

TESTBG (103870 - 105610)

Tests broad group energy structure for compatibility with ultra-fine-group energies.

TABLE VIII. Function of MC^2-2 Subprograms (Contd.)

CARD12 (105620 - 112160)

Reads and processes type 12 cards of file A.MCC2.

CARD07/SETGRP (112170 - 117750)

Reads and processes type 07 cards of file A.MCC2; processes prestored broad-group structures.

CARD05 (117760 - 122280)

Reads and processes type 05 cards of file A.MCC2.

RDANIP (122290 - 127690)

Controls the reading of type 06, 14, 15 cards of file A.NIP.

EDGEOM (127700 - 129190)

Edits binary file GEOM1

FOILS (129200-129640)

Loads foil atom density array FOILDN

STRTCH (129650 - 131600)

Assures that all materials in heterogeneous problem appear in homogeneous mixture.

PRNT1D (131610 - 132830)

Edits one-dimensional double precision floating point array.

WRITER (132840 - 135310)

Writes the binary file PRBSPC.

SXLSXR (135320 - 137340)

Calculates arrays SXL, SXR used to obtain slab optical thickness.

EDTPRB (137350 - 145270)

Edits file PRBSPC.

****

CSC004 (145280 - 152910)

Main driver for MC^2-2 unresolved resonance calculation.

TABLE VIII. Function of MC^2-2 Subprograms (Contd.)

UNRINT/UNRUNT (152920 - 165770)

Calculates the single level unresolved resonance integral including interference scattering and self overlap.

PACKER (165780 - 167120)

Reads unresolved resonance data from library file MCC2F3 and processes data.

INTERP (167130 - 168290)

Linearly interpolates input array onto a second array on a different energy grid.

SETUPU (168300 - 168760)

Identifies mixture materials with unresolved data.

QUICKJ (168770 - 171960)

Calculates the isolated J integral with or without interference scattering using a single level representation.

DRCTOR (171970 - 180300)

Allocates, loads arrays and directs calculation of unresolved resonance cross sections.

EDITUN (180310 - 182320)

Edits file UNRES.

ESMESH (182330 - 183710)

Sets up correspondence between input and collapsed energy mesh.

WZERO (183720 - 184170)

Calculates real part of the function W(o,x) using a rational approximation.

****

CSC005 (184180 - 187700)

Main driver for MC^2-2 resolved resonance calculation.

TABLE VIII. Function of MC^2-2 Subprograms (Contd.)

ADMSTR (187710 - 191750)

Reads MC^2-2 library data and controls calculation of resolved resonance integrals.

STUFIT (191760 - 193860)

Reads resolved data from file MCC2F4 and loads arrays in compressed form.

JINT (193870 - 204290)

Calculates isolated resonance integrals including interference scattering using either single level or multi-level formalisms.

EDITLZ (204300 - 205880)

Edits file LORENZ.

NSIGO (205890 - 206950)

Calculates $N\sigma_o$ for homogeneous and heterogeneous mixtures.

LORENT/LORANT (206960 - 209070)

Calculates ultra-fine-group integrals of Lorentzian shape resonance integrals.

WINNER (209080 - 210390)

Determines which neighboring resolved resonances contribute to overlap integral.

OVRLAP/OVRLOP (210400 - 216960)

Calculates overlap integrals for each resolved resonance.

RATNL (216970 - 217510)

Calculates real part of W(o,x) using a rational approximation.

SETUPR (217520 - 217990)

Identifies mixures with resolved resonance data.

TRIPLE (218000 - 219450)

Calculates infinite integrals of products of ψ and χ.

TABLE VIII. Function of MC^2-2 Subprograms (Contd.)

JINTGL (219460 - 222330)

Calculates isolated J integral including interference scattering for the single level representation.

SIFTER (222340 - 228020)

Selects materials from resolved data file MCC2F4, controls reordering of resonances and selects overlap candidates.

REORDR (228030 - 231250)

Arranges resolved resonances in order of decreasing energy and deletes those that fall outside range of problem.

****

CSC006 (231260 - 239090)

Main driver for resolved-unresolved resonance interaction module.

INTRAC (239100 - 242260)

Reads files ATNUAT and RESINT and calculates interaction factors.

POTNTL (242270 - 245890)

Calculates resonance background cross sections and writes file SIGMAP.

EDITAT (245900 - 248660)

Edits file ATNUAT.

EDITRS (248670 - 250540)

Edits file RESINT.

WRISIT (250550 - 251560)

Calculates resolved overlap factors to be associated with each grid point.

EDITSP (251570 - 252880)

Edits file SIGMAP.

****

CSC008 (252890 - 259500)

Main driver for macroscopic data calculations.

TABLE VIII. Function of MC^2-2 Subprograms (Contd.)

SIGMAC (259510 - 265370)

Calculates macroscopic total, elastic and $\nu\Sigma_f$ ultra-fine-group cross sections.

SETCHI (265380 - 269330)

Calculates fission spectra distributions and writes file PRBCHI.

SETSCT (269340 - 278160)

Controls calculation of elastic matrices, transport cross sections and moderating parameters.

ELSCAT/ELSCT1 (278170 - 290780)

Calculates P_o and P_1 ultra-fine-group elastic transfer matrices.

CALCFN (290790 - 292630)

Calculates $(2n+1)f_n(u)$ at all hyper-fine-group boundaries.

FNAVG (292640 - 294260)

Calculates group averaged values of elastic expansion coefficients.

SIGAVG (294270 - 296400)

Calculates group averaged cross sections from data pairs using interpolation laws.

SETCSD (296410 - 298790)

Prepares coefficients for calculation of moderating parameters.

MODPAR (298800 - 305270)

Calculates continuous slowing down moderating parameters.

XTRN (305280 - 308120)

Calculates ultra-fine-group extended transport cross sections.

EDIT1 (308130 - 309270)

Edits elastic transfer matrices.

EDIT2 (309280 - 311930)

Edits macroscopic ultra-fine-group vectors.

****

TABLE VIII. Function of MC^2-2 Subprograms (Contd.)

CSC009 (311940 - 322980)

Main program driver for ultra-fine-group spectrum and broad-group cross section calculation.

FILE1 (322990 - 324560)

Loads data from record 5 of file MCC2F1 to determine storage requirements for inelastic data.

FILE6 (324570 - 331140)

Reads the file MCC2F6 inelastic and (n,2n) data and writes the file GRPORD.

ATNSRC (331150 - 332070)

Reads file ATNUAT to determine number of spin states and resonances.

EGRID (332080 - 333080)

Sets up energies at which unresolved attenuation factors act.

REORDR (333090 - 336350)

Reads unresolved resonance integrals from file ATNUAT and orders them by energy.

MATCH (336360 - 339070)

Reads resolved resonance integrals from file RESINT and sets up problem material - resonance material correspondence.

INIT (339080 - 340870)

Sets initial fission source distribution.

SETIN (340880 - 347570)

Sets up storage for inelastic and (n,2n) data.

DRIVER (347580 - 354540)

Controls ultra-fine-group spectrum calculation.

MGSPEC/MGSPC1 (354550 - 358240)

Solves multigroup spectrum equations.

CSDSPC/CSDSP1 (358250 - 363430)

Solves continuous slowing down spectrum equations.

TABLE VIII. Function of MC^2-2 Subprograms (Contd.)

FISSOR/FISOR1 (363440 - 366990)

Calculates ultra-fine-group fission source and eigenvalue.

BSQITR (367000 - 368940)

Tests on convergence of buckling search and sets next buckling guess.

PARAB (368950 - 369350)

Computes coefficients for parabolic fit to three points.

INSCAT/INSCT1 (369360 - 376090)

Calculates inelastic and (n,2n) ultra-fine-group scattering source.

PROBIN (376100 - 378370)

Calculates discrete inelastic scattering source taking account of energy-angle correlation.

TABINT (378380 - 381170)

Calculates inelastic (n,2n) scattering probability from tabulated function.

EDTUFG (381180 - 381600)

Edits ultra-fine values of array input.

SETBG (381610 - 391130)

Controls calculation of broad-group cross sections.

BGSPEC (391140 - 394860)

Calculates broad-group fluxes and currents; sets correspondence between broad- and ultra-fine-groups.

INSBG (394870 - 402660)

Calculates inelastic and (n,2n) broad group scattering source.

RESCS (402670 - 408030)

Calculates homogeneous broad group resonance capture, fission and total cross sections.

TABLE VIII. Function of MC^2-2 Subprograms (Contd.)

RESCAT (408040 - 412060)

Calculates resolved resonance broad group elastic transfer matrices.

BGFLE1 (412070 - 415090)

Sets data and writes first three records of file ISOTXS.

BGFLE2 (415100 - 421560)

Writes isotope dependent data to file ISOTXS.

ISOCHI (421570 - 422650)

Calculates broad-group chi vectors by isotope.

PRINXS/PRNXS1 (422660 - 429660)

Calculates broad-group non-resonance cross section vectors.

BGSCAT (429670 - 434230)

Calculates non-resolved resonance broad-group elastic scattering transfer matrices.

SRATE (434240 - 435890)

Writes the file SRATES for use by RABANL.

DOIO/DOIO1/DOIO2/DOIO3 (435900 - 438780)

Prepares data for file SRATES.

ORIGIN (438790 - 438840)

Dummy routine to replace SIMPLOTTER subroutine.

****

CSCO10 (438850 - 444400)

Main driver for broad-group fundamental mode spectrum calculation.

HOMOG (444410 - 448100)

Prepares macroscopic broad group data.

TABLE VIII. Function of MC^2-2 Subprograms (Contd.)

BGPN (448110 - 451640)

Solves broad-group P_N equations.

BSQTR (451650 - 453570)

Controls buckling search calculation.

CRAMER (453580 - 453980)

Calculates coefficients for parabolic fit to three sets data points.

BGSORS (453990 - 454540)

Calculates inhomogeneous broad-group source by summing ultra-fine-group sources.

****

CSE009 (454550 - 458210)

Main driver for editor of broad-group cross section file ISOTXS.

XSEDIT (458220 - 463840)

Edits isotope cross section data from file ISOTXS.

****

CSC011 (463850 - 481310)

Main driver for integral transport theory resolved resonance calculation.

E2E3E4/E2/E3/E4 (481320 - 483230)

This function obtains the exponential integrals E2(X), E3(X), and E4(X) by interpolation on tabular values or asymptotic expansions as appropriate.

FREEUP (483240 - 483760)

Closes data sets MCC2F1, MCC2F4, and SRATES.

MERGER (483770 - 489790)

Forms the union of all unique problem and foil materials and computes arrays.

TABLE VIII. Function of MC^2-2 Subprograms (Contd.)

SPOOL (489800 - 495000)

Reads in the elastic, fission, capture, and total ultra fine group cross sections from scratch data sets.

FLIPIT (495010 - 495630)

Converts a slab cell with reflective boundary conditions to the equivalent cell with periodic boundaries.

SYM (495040 496320)

Determines symmetrical mesh interval pairs for slab geometry.

SIFTIT (496330 - 507750)

Selects materials from data set MCC2F4, calls STUFER to load arrays, and calls MANAGR to proceed with the integral theory resolved resonance calculation.

STUFER (507760 - 510000)

Reads data set MCC2F4, loads arrays, multiplies SIGO by the isotope abundances, and obtains the square roots of the resolved resonance energies.

REARNG (510010 - 511040)

Arranges resonances in order of decreasing energy.

EZ3/EZ4 (511050 - 511840)

This function obtains S3(Z,H) defined as the sum of E3(Z+KH) for K between zero and infinity. EZ3 is used for optically thin unit cells.

YZ3 (511850 - 512940)

Obtains the difference in the sums of E3(Y+KH) and E3(Y+DEL+KH) for K equal zero to infinity, S3(Y,H) - S3(Y+DEL,H).

YZ4 (512950 - 513790)

Obtains the difference in the sums of E4(Y+KH) and E4(Y+DEL+KH) for K equal zero to infinity, S4(Y,H) - S4(Y+DEL,H).

XTRAP/XTRAP4 (513800 - 514510)

Obtains S3(Z3,H) defined as the sum of E3(Z3+KH) for K between zero and infinity using gaussian quadrature.

TABLE VIII. Function of MC^2-2 Subprograms (Contd.)

PFUNC (514520 - 515070)

Obtains the slab collision escape probability.

SOARCE/SORCE1/SORCEF (515080 - 523730)

Computes the scattering source into the current hyper-fine-group.

MANAGR (523740 - 539000)

Acts as the driver to complete the integral transport theory calculation.

RESXSC/RESTES/XSECT (539010 - 544420)

Determines the resolved resonances to be included for the calculation of the hyper-fine-groups within each intermediate group, and computes the resolved resonance related cross sections for each hyper-fine-group.

RATES/RATESF (544430 - 559260)

Obtains the collision rates for the current hyper-fine-group and for each mesh interval of each region in the cell.

PREEDT (559270 - 561730)

Reads the data set IRESCS and writes out the rearranged data onto scratch data sets, one for each region, in preparation for editing the integral transport resonance cross sections.

EDTICS (561740 - 567650)

Reads scratch data sets, loads arrays, and edits the resolved resonance cross sections.

PREFOL (567660 - 569850)

Reads data set SCR005 and writes out the rearranged data onto scratch data sets, one for each foil, in preparation for editing the resonance foil cross section.

EDTFOL (569860 - 572050)

Reads scratch data sets, load arrays, and edits the resolved resonance cross sections for foil materials.

TABLE VIII. Function of MC^2-2 Subprograms (Contd.)

DRIVED (572060 - 576610)

Acts as the driver for the editing functions of the integral transport theory calculation.

PREEDI (576620 - 577880)

Reads the data set IRESCS and loads arrays for the case when arrays can be core contained in preparation for editing the integral transport theory resonance cross sections.

EDTICI (577890 - 583220)

Edits the resolved resonance transport theory resonance cross sections when arrays can be core contained.

PREFOI (583230 - 584500)

Reads scratch data set and loads arrays for the case when arrays can be core contained in preparation for editing foil cross sections.

EDTFOI (584510 - 585960)

Edits resolved resonance cross sections for foil material when arrays can be core contained.

DRIVEI (585970 - 589070)

Acts as the driver for the editing functions of the integral transport theory calculation when arrays can be core contained.

TABLE IX. MC^2-2 ENDF/B-IV Library Files

Maximum Energy - 1.419×10^7 eV
Lethargy Width - 1/120
Number of groups - 2082
Number of Materials - 104

MC^2-2 ID	ENDF/B Mat Number	Comments
TA1824	1127	U, R
W-1824	1128	U, R
W-1834	1129	U, R
W-1844	1130	U, R
W-1864	1131	U, R
U-238B	1262	U, R, F, ENDF/B-IV Mat 1262 plus background corrections
U-238M	1262	U, R, F, ENDF/B-IV Mat 1262 with MLBW resolved resonance flag
PU2404	1265	U, R, F
TA1814	1285	U, R
H-3 4	1169	
CA 4	1195	
HE 4	1270	
DY1644	1031	U, R
LU1754	1032	U, R
LU1764	1033	U, R
H-2 4	1120	
HE3 4	1146	
XE1244	1170	R
XE1264	1171	R
XE1284	1172	R
XE1294	1173	R
XE1304	1174	R
XE1314	1175	R
XE1324	1176	R
XE1344	1177	R

TABLE IX. MC^2-2 ENDF/B-IV Library Files (Cont'd.)

MC^2-2 ID	ENDF/B Mat Number	Comments
XE1364	1178	
KR78 4	1181	
KR80 4	1182	
KR82 4	1183	
KR83 4	1184	
KR84 4	1185	
KR86 4	1186	
V 4	1196	
AL27 4	1193	
SI 4	1194	
MG 4	1280	
NI 4	1190	
CR 4	1191	
FE 4	1192	
SM1494	1027	U, R
GD 4	1030	R
RE1854	1083	U, R
RE1874	1084	U, R
RH1034	1125	U, R
TC99 4	1137	
AG1074	1138	R
AG1094	1139	R
CS1334	1141	R
CL 4	1149	
K 4	1150	
NA23 4	1156	
B-11 4	1160	
MN55 4	1197	
U-2384	1262	U, R, F
NP2374	1263	U, R, F
TI 4	1286	
MO 4	1287	
CO59 4	1199	
EU1514	1290	U, R

TABLE IX. MC^2-2 ENDF/B-IV Library Files (Cont'd.)

MC^2-2 ID	ENDF/B Mat Number	Comments
EU1534	1291	U, R
EU1524	1292	U, R
EU1544	1293	U, R
CU 4	1295	
NB93 4	1189	
F 4	1277	
CD 4	1281	
CD1134	1282	
AU1974	1283	U, R
ZIRC 4	1284	
U-2354	1261	U, R, F
PU2394	1264	U, R, F
PU2414	1266	U, R, F
PA2334	1297	U, R, F
C-12 4	1274	
N-14 4	1275	
O-16 4	1276	
PB 4	1288	
U-2344	1043	U, R, F
PU2384	1050	U, R, F
AM2414	1056	U, R, F
AM2434	1057	U, R, F
PU2424	1161	U, R, F
CM2444	1162	U, R, F
U-2464	1163	U, R, F
LI-6 4	1271	
LI-7 4	1272	
B-10 4	1273	
XE1354	1294	
TH2324	1296	U, R, F
U3FP13	1042	
U5FP13	1045	

TABLE IX. MC^2-2 ENDF/B-IV Library Files (Cont'd.)

MC^2-2 ID	ENDF/B Mat Number	Comments
P9FP13	1052	
U3FP23	1066	
U3FP33	1067	
U5FP23	1068	
U5FP33	1069	
P9FP23	1070	
P9FP33	1071	
BE-9 3	1154	
CS1353	1229	
SM1503	1244	
PM148M	1254	
U-2334	1260	R, F, ENDF/B-III Fission Spectrum
HYDRGN	1269	

U This material has unresolved resonance data

R This material has resolved resonance data

F This material has fission spectrum data

2. CDC Code Implementation

The implementation of the MC^2-2 code has been performed at two CDC computer laboratories - Lawrence Berkeley Laboratory and Brookhaven National Laboratory. Each laboratory has one CDC 7600 computer with 65,536 (60-bit) words of small core memory and 512,000 (60-bit) words of large core memory. Also each laboratory has two CDC 6600 computers with 65,536 (60-bit) words of central memory. MC^2-2 was implemented only on the CDC 7600 computers. The examples in this section display the control cards suitable for each installation. The essential nature of each step is intended to be system independent. Each CDC installation has local conventions but Brookhaven National Laboratory adheres almost entirely to standard CDC conventions. The user will find all the necessary CDC control card information and FORTRAN usage in the following four manuals.

1. FORTRAN Extended 4 Reference Manual (Publication No. 60305600, Rev. G)

2. SCOPE 2.1 Reference Manual (Publication No. 60342600, Rev. H)

3. Loader Reference Manual (Publication No. 60344200, Rev. G)

4. Update Reference Manual (Publication No. 60342500, Rev. E)

The CDC program tape is written as described in Table X. The source code for MC^2-2 is contained on Files 1 and 2 of the program tape. A brief description of each of the FORTRAN subprograms of File 1 is given in Table VIII, and the subprograms and sequence numbers in this table are the same for both IBM and CDC codes. The source code differs in that all cards between two cards with CDC* in columns 1-4 have a C in column 1 on the IBM tape and a blank in column 1 on the CDC tape. The opposite change is true of cards between two cards with CIBM in columns 1-4. The 14 subprograms on File 2 of the tape are discussed in Table XI. The first 13 subprograms are written in FORTRAN, and the last subprogram, MEMGET, is a COMPASS routine. Creation of object code for input to the segmentation loader is the first step required for implementation of the MC^2-2 program. The compilation of File 1 subprograms and the first 13 subprograms of File 2 should be performed using the highest level of optimization available that will give the correct object code. Currently, this means use of the FORTRAN extended compiler with OPT=1 specified. The FORTRAN extended compiler is necessary because of the presence of LEVEL 2 statements. At the present time there are errors in code generated with the OPT=2 FORTRAN extended compiler. Also the CDC FORTRAN compiler release of 4.4 or later was used. Earlier releases generated incorrect object code for all available optimizations. Figure 23 displays the control cards necessary for reading the two files of the source program tape, compilation of the FORTRAN code, assembly of the one COMPASS routine and writing of the object code onto a magnetic tape. Depending on the installation, it may be necessary to isolate the one COMPASS routine in File 2 before assembly.

This is currently a requirement at the Berkeley site because of interface problems with their FORTRAN extended compiler. Therefore the CDC UPDATE routine was used to separate the FORTRAN and COMPASS source code. Generally for CDC computers, source code can be mixed FORTRAN and COMPASS subprograms. The FORTRAN compiler will recognize COMPASS routines and invoke the COMPASS assembler and then control will be returned to the FORTRAN compiler.

Figure 24 displays the control cards which read the generated object code from the magnetic tape. The segmented loader is then invoked and it builds the segments from the object code in accordance with the directives issued to the segmented loader. These directives are provided on File 3 of the program tape. The INCLUDE directives must be specified in a manner which is dependent on the CDC 7600 computer operating system. For an operating system less (greater) than SCOPE 2.0, a subroutine specified in the verb field must (must not) be specified in the specification field. For example, if subroutines A, B, and C are to appear in the same segment, then the directive statement under a SCOPE operating system equal or greater than 2.0 will be expressed as

```
A  INCLUDE  B,C
```

For a 7600 computer operating system less than 2.0 or the Berkeley 'BKY' operating system, the equivalent directive statement must be stated as

```
A  INCLUDE  B,C,A
```

The segmented loader resolves I/O routines and mathematical subroutines with the system library called FTN4LIB (Berkeley) or FORTRAN (Brookhaven). The executable code now resides on the file designated as MCCA. This file is written onto a magnetic tape.

Two library tapes are provided along with the MC^2-2 program tape. These library tapes contain eight binary sequential files with a total of 4559 records and 2,767,155 words in the format of the files MCC2F1-MCC2F8 described in Appendix C . These library tapes were written at the Berkeley Laboratory on 7 track unlabeled tapes at a density of 800 BPI and x-mode binary. Appendix F describes the process used for generating the MC^2-2 library files on a single 1600 BPI tape from these two 7 track tapes. These files must be copied to a direct access device (e.g. disk pack) as the next step in program implementation. Since no private disk space was available, the library was copied from tape to disk for each problem execution as illustrated in Fig. 25. The data set names assigned to the eight binary MC^2-2 library files are TAPE22-TAPE29 as displayed in Fig. 25. The data available on these library files were processed from the ENDF/B-IV data files by the code ETOE-2. A summary of the library specifications is given in Table IX. The Argonne Code Center also has available four BCD tapes which contain this same eight file library in BCD format along with a FORTRAN program, MC^2-2 LIBGEN, which reads the BCD files and writes the eight binary files. Appendix F illustrates this process. The binary library tapes generated at Berkeley Laboratory were made from the FORTRAN program MC^2-2 LIBGEN.

The control cards used to execute an MC^2-2 problem are given in Fig. 25. The executable code generated by the segmented loader and the eight binary library files are copied from tape to a disk pack. Note that the eight

binary library files are copied from tape to disk for every problem execution. For the Berkeley example the TAPE control card and its appropriate directives require 34 charge units (one charge unit costs the user about 7 cents) to transfer the binary library files from tape to disk pack and assign a data set name to each file. Brookhaven does not have a comparable control card. The control cards used to transfer the library files from tape to disk pack in the Brookhaven example are very inefficient. Staging the data and using the COPYBF control cards to assign a data set name to each of the eight files requires twice the disk space since two copies of the library exist on disk packs. When this method was used at Berkeley for comparison purposes the STAGE command required 8 charge units to transfer all the binary data from tape to disk and the COPYBF control cards which assign data set names to each file require an additional 267 charge units. The user should be aware of the BPOINTER container array size allocated in SCM and LCM and the appropriate field length specified on the CDC control card preceding MC^2-2 problem execution. The size of the dynamic storage capability, BPOINTER, described in Reference 1 and briefly in Appendix E, used to manage all variable dimension array allocations, is provided for on card type 02 of data set A.MCC2. For the CDC version of the code, a container array is allocated in SCM (up to 22,000 decimal words available in small core plus another 10,000 decimal words if no small core buffers exist) as well as a container array in LCM (up to 131,072 decimal words in directly addressable large core memory). Almost all of the large BPOINTER arrays in the CDC version of the MC^2-2 code are placed in the container array in LCM. At this time, no known limitations due to core size are placed upon executions of the CDC version of this code.

Two BCD sample problem input decks are provided on File 4 of the program tape. The first problem displays the execution of a homogeneous consistent P_1 problem. The type 01 card of data set A.STP015 is set to execute Areas 4, 5, 6, 6.5, 7, 8, and 9 and to edit the broad group cross sections. The second sample problem shows the execution of a homogeneous resolved resonance integral transport calculation. The type 01 card of data set A.STP015 is set to execute Areas 4 and 10. Data set UNREG, the unresolved resonance ultra-fine-group cross sections, (called TAPE 49) was saved from the first problem. This data set is input to the second problem by specifying DATASET=UNREG under the data set initialization BLOCK=OLD.

TABLE X. CDC Code Center Tape Description

File Number	Contents	Number of Card Images
1	MC^2-2 Subprograms See Table VIII	58907
2	MC^2-2 Subprograms for CDC Code See Table XI	654
3	Directives Required for Segmented Loader See Fig. 17	48
4	Two Sample MC^2-2 Problem Input Decks	150

TABLE XI. Function of MC^2-2 Subprograms for CDC Code

ALLOC1/ALLOC2† (000010 - 000760)*

Assign storage for the dynamic allocation subprogram package BPOINTER.

FREE1/FREE2 (000770 - 001010)

Dummy FORTRAN routine that releases the storage of the dynamic storage container array that was allocated by the subroutine ALLOC1/ALLOC2.

ABEND/ABSTOP† (001020 - 001080)

Called by subroutine ERROR to force an abnormal termination of the job with a DUMP.

FXP1/FXP† (001090 - 001580)

Fast exponential function.

GOWEST† (001590 - 001840)

Left-justify Hollerith variables.

DISPOS† (001850 - 001950)

Used by module CSI010 to determine whether the file SRATES is given a permanent or temporary disposition. CDC code always sets a temporary disposition to the file.

FILEID† (001960 - 002110)

A dummy routine that is used in subroutine BGFLE1 of module CSC009 to obtain the dataset name associated with the file ISOTXS.

CVD† (002120 - 002240)

Used in subroutine BGFLE2 of module CSC009 to convert a variable from integer to Hollerith format.

DRED/DRIT (002250 - 004040)

FORTRAN routine that performs the non-formatted (binary) I/O operations between LCM and disk files without use of a buffer array in small core memory.

ZEROIO (004050 - 004150)

FORTRAN routine that initializes the common block /INITIO/ which is common to subroutines REED and DRED.

TABLE XI. Function of MC^2-2 Subprograms for CDC Code (Contd.)

BUOPEN/BUCLOSE (004160 - 004200)

A dummy FORTRAN routine that is intended to open/close dataset buffers.

ERF (004210 - 005130)

A FORTRAN written function that evaluates the error function.

PRTECS (005140 - 006320)

A FORTRAN subroutine that edits a one-dimensional floating point single precision array located in LCM.

MEMGET/MEMGET1 (006330 - 006540)

A COMPASS routine that performs the allocation for ALLOC1/ALLOC2.

*Numbers in brackets are sequence numbers of routine on File 2 of CDC program tape.

†This is a FORTRAN routine for the CDC code. See Section D above for a further description of this routine.

BERKELEY

```
(JOBCARD)
SCF(R=BCDIN,RL=80,BF=40,D8,nnnnn)
COPYBF(BCDIN,TAPE1,1)
COPYBF(BCDIN,TAPE2,1)
REWIND(BCDIN,TAPE1,TAPE2)
RFL,100000,100000.
FTN4,I=TAPE1,OPT=1,L=0,B=FILE1.
REWIND(TAPE1,FILE1)
UPDATE(N)
UPDATE(F,P=NEWPL)
REWIND(COMP)
FTN4,I=COMP,OPT=1,B=FILE2A.
REWIND(COMP,NEWPL,FILE2A)
UPDATE(F,P=NEWPL)
REWIND(COMP)
COMPASS,I=COMP,B=FILE2B.
REWIND(COMP,FILE2B)
COPY(FILE1,1FXF,FILE2A,1FXF,FILE2B,1F,PG)
REWIND(PG)
STAGE(PG,D9,NT,P3,W,nnnnn,1F)
7/8/9
*DECK MC
*READ TAPE2
7/8/9
*COPY MC,MC.2,MC.633,COMP
7/8/9
*COPY MC,MC.634,MC.655,COMP
7/8/9
6/7/8/9
```

BROOKHAVEN

```
(JOBCARD)
ACCOUNT(Name,NNNN)
STAGE(BCDIN,HY,VSN=Nnnnnn)
STAGE(PG,POST,PE,E,VSN=Knnn)
FILE(BCDIN,RT=F,FL=80,RB=40,BT=K,CM=YES)
COPYBF(BCDIN,TAPE1,1)
COPYBF(BCDIN,TAPE2,1)
REWIND(TAPE1,TAPE2)
RETURN(BCDIN)
FTN(I=TAPE1,OPT=1,L=0,B=FILE1,SYSEDIT,PL=70000)
REWIND(TAPE1,FILE1)
FTN(I=TAPE2,OPT=1,B=FILE2,SYSEDIT,PL=70000)
REWIND(TAPE2,FILE2)
COPYBF(FILE1,PG,1)
COPYBF(FILE2,PG,1)
REWIND(FILE1,FILE2,PG)
6/7/8/9
```

Fig. 23. Compilation and Assembly of CDC Source Code to Generate Object Code

BERKELEY

```
(JOBCARD)
STAGE,PG,D9,NTP3,R,nnnnn.
RFL,100000,1000.
SEGLINK(F=PG,P=FTN4LIB,B=MCCA,LO=BEX)
REWIND(MCCA)
STAGE,MCCA,D9,NT,P3,W,nnnnn.
7/8/9
   (Insert directives required for
    the segmented loader.  See Fig. 17)
7/8/9
6/7/8/9
```

BROOKHAVEN

```
(JOBCARD)
ACCOUNT (Name,NNNN)
STAGE(FLE1,PE,E,VSN=Knnn)
STAGE(MCCB,POST,PE,E,VSN=Knnn)
COPYBF(FLE1,PG1,1)
COPYBF(FLE1,PG2,1)
REWIND(PG1,PG2)
RETURN(FLE1)
RFL(140000,L=1)
SEGLOAD(B=MCCA)
LOAD(PG1)
LOAD(PG2)
NOGO.
REWIND(MCCA)
COPY(MCCA,MCCB)
REWIND(MCCB)
7/8/9
   (Insert directives required for the
    segmented loader.  See Fig. 17)
7/8/9
6/7/8/9
```

Fig. 24. Build the Segments from Object Code Using the Segmentation Loader

BERKELEY

```
(JOBCARD)
DISKHOG,12000.
TAPE,TAPE22,D9,X,NT,R,nnnnn.
STAGE,MCCB,D9,NT,P3,R,nnnnn.
RFL,170000,400000.
MCCB(PL=70000)
7/8/9
*READ
*FILE,TAPE23
*READ
*FILE,TAPE24
*READ
*FILE,TAPE25
*READ
*FILE,TAPE26
*READ
*FILE,TAPE27
*READ
*FILE,TAPE28
*READ
*FILE,TAPE29
*READ
7/8/9
   (BCD MC²-2 problem input deck)
7/8/9
6/7/8/9
```

BROOKHAVEN

```
(JOBCARD)
ACCOUNT(Name,NNNN)
STAGE(LIB,PE,E,VSN=Knnn)
STAGE(MCCA,PE,E,VSN=Knnn)
COPYBF(LIB,TAPE22,1)
COPYBF(LIB,TAPE23,1)
COPYBF(LIB,TAPE24,1)
COPYBF(LIB,TAPE25,1)
COPYBF(LIB,TAPE26,1)
COPYBF(LIB,TAPE27,1)
COPYBF(LIB,TAPE28,1)
COPYBF(LIB,TAPE29,1)
REWIND(TAPE22,TAPE23,TAPE24,TAPE25,TAPE26,TAPE27)
REWIND(TAPE28,TAPE29)
RETURN(LIB)
COPY(MCCA,MCCB)
REWIND(MCCB)
RETURN(MCCA)
RFL(160000,L=400)
MCCB.
7/8/9
   (BCD MC²-2 problem input deck)
7/8/9
6/7/8/9
```

Fig. 25. Execution of MC²-2 Problem

APPENDIX A

SPECIAL FUNCTION EVALUATIONS

I. Legendre Functions of the Second Kind

In the B_N approximation the extended transport cross section depends on a ratio of Legendre functions of the second kind,

$$R \equiv \frac{Q_{N+1}(z)}{Q_N(z)}$$

where

$$1 \leq N \leq 9$$

$$z \equiv \frac{i\Sigma_t}{B}$$

and the buckling B can be either real or imaginary. The calculation of the ratio R depends upon both N and z. In Table XII the computational option is identified with the values of N and z. In the expressions below defining the options B is used to represent the real or imaginary part of $\sqrt{B^2}$.

1) Option 1 (Analytic)

$$R_1 = \frac{i}{2} \frac{\left[\left(1 + \frac{3\Sigma_t^2}{B^2}\right) \tan^{-1} \frac{B}{\Sigma_t} - \frac{3\Sigma_t}{B} \right]}{\frac{\Sigma_t}{B} \tan^{-1} \frac{B}{\Sigma_t} - 1}$$

2) Option 2 (Analytic)

$$R_2 = \frac{\left[\frac{3\Sigma_t^2}{B^2} - 1 \right] \ell n \left| \frac{1 + B/\Sigma_t}{1 - B/\Sigma_t} \right| - \frac{3\Sigma_t}{B}}{\frac{\Sigma_t}{2B} \ell n \left| \frac{1 + B/\Sigma_t}{1 - B/\Sigma_t} \right| - 1}$$

3) Option 3 (Hypergeometric Series)

Q_N and Q_{N+1} are calculated using an eleven term hypergeometric series expansion,[30]

$$Q_N(x) = B(N, 0, x)\ F\left(\frac{1}{2}, \frac{1}{2}; N + \frac{3}{2}; -t\right)$$

$$x = \frac{\Sigma_t}{B}, \quad t = \frac{x - (x^2 - 1)^{\frac{1}{2}}}{2(x^2 - 1)^{\frac{1}{2}}}$$

$$B(N, 0, x) = \frac{\Gamma(\frac{1}{2})\ \Gamma(N+1)}{\Gamma(N+\frac{3}{2})\ \sqrt{2}\ (x^2-1)^{\frac{1}{4}}\ (x+(x^2-1)^{\frac{1}{2}})^{N+\frac{1}{2}}}$$

$$F(\tfrac{1}{2}, \tfrac{1}{2}; N+\tfrac{3}{2}; -t) = \sum_{k=0}^{\infty} \frac{\Gamma(\frac{1}{2}+k)\ \Gamma(\frac{1}{2}+k)\ \Gamma(N+\frac{3}{2})}{k!\ \Gamma(\frac{1}{2})\ \Gamma(\frac{1}{2})\ \Gamma(N+\frac{3}{2}+k)}\ (-t)^k$$

with the coefficients of the eleven term summation precalculated. The ratio, R_3, is then calculated from $Q_{N+1}(x)/Q_N(x)$.

4) Option 4 (Backward Recursion)

The ratio R_4 is calculated using Gautschi's backward recursion relation[31]. Setting

$$\nu = N + 9$$

$$S = -\frac{B^2}{|B^2|}$$

$$r_o = 0$$

the recursive relationship

$$r_n = \frac{\frac{(\nu - n + 1)}{(\nu - n + 2)}}{\frac{\Sigma_t}{B}\left[1 + \frac{\nu - n + 1}{\nu - n + 2}\right] + S\ r_{n-1}} \qquad n = 1, 2, \ldots, 9$$

is used to define r_9. The ratio R is then given by

$$R_4 = \begin{cases} -ir_9 & B^2 > 0 \\ r_9 & B^2 < 0 \end{cases}$$

5) Option 5 (Forward Recursion)

The ratio R_5 is calculated using the standard forward recursion relation. Setting

$$r_o = \begin{cases} -\tan^{-1}\frac{B}{\Sigma_t} & B^2 > 0 \\ \frac{1}{2}\,\ell n\left|\frac{1+\Sigma_t/B}{1-\Sigma_t/B}\right| & B^2 < 0 \end{cases}$$

$$r_1 = \frac{\Sigma_t}{B}\, S\, r_o - 1$$

$$S = -\frac{B^2}{|B^2|}$$

the recursive relationship

$$r_{n+1} = \frac{\Sigma_t}{B} S^{n+1} r_n - r_{n-1} + \frac{\Sigma_t}{B} S^{n+1} r_n$$

$$- \left(\frac{\Sigma_t}{B} S^{n+1} r_n - r_{n-1} \right) / (n + 1) \qquad n = 1, 2, \ldots, N$$

is used and R is defined

$$R_5 = \begin{cases} \dfrac{r_{N+1}}{r_N} & B^2 < 0 \\ i \dfrac{r_{N+1}}{r_N} & B^2 < 0 \end{cases}$$

6) Option 6 (Relationship with P_N)

Use is made of the relationship between Legendre functions of the first kind $P_n(z)$ and the second kind $Q_N(z)$ to calculate the ratio R_6. Since the forward recursion relation is stable for all P_n, the Legendre functions of the first kind are calculated directly from it,

$$P_0(z) = 1$$

$$|P_1(z)| = \frac{\Sigma_t}{B}$$

$$|P_n(z)| = (-)^{n+1} \frac{\Sigma_t}{B} |P_{n-1}(z)| - |P_{n-2}(z)| + (-)^{n+1} \frac{\Sigma_t}{B} |P_{n-1}(z)|$$

$$- \left[(-)^{n+1} \frac{\Sigma_t}{B} |P_{n-1}(z)| - |P_{n-2}(z)| \right] / (n - 1)$$

$$n = 2, 3, \ldots, N + 1$$

From the $P_n(z)$, the non-singular part of $Q_N(z)$ and $Q_{N+1}(z)$ is calculated,

$$(-)^{\left[\frac{N}{2} + 1\right]} W_N = \frac{2N + 1}{N + 1} P_N - \frac{2N - 3}{3N} P_{N-2} + \frac{2N - 7}{5(N - 1)} P_{N-4} + \ldots$$

$$(-)^{\left[\frac{N+1}{2} + 2\right]} W_{N-1} = \frac{2N - 1}{N} P_{N-1} + \frac{2N - 5}{3(N - 1)} P_{N-3} + \ldots$$

The functions Q_N and Q_{N+1} are then calculated as,

$$Q_{N+1} = (-)^{\left[\frac{N+1}{2} + 2\right]} \left(\frac{\pi}{2} - \tan^{-1}\frac{\Sigma_t}{B}\right) \left| P_{N+1}\left(\frac{i\Sigma_t}{B}\right)\right| + W_N$$

$$Q_N = (-)^{\left[\frac{N}{2} + 2\right]} \left(\frac{\pi}{2} - \tan^{-1}\frac{\Sigma_t}{B}\right) \left| P_N\left(\frac{i\Sigma_t}{B}\right)\right| + W_{N-1}$$

and

$$R_6 = \frac{Q_{N+1}}{Q_N}$$

TABLE XII Legendre Function Evaluation

N	B^2	$\lvert\Sigma_t/B\rvert$	Option	
1	> 0	all	1	Analytic
1	< 0	all	2	Analytic
> 1	< 0	(1.0, 1.15]	3	Hypergeometric series
> 1	< 0	1.15	4	Backward recursion
> 1	> 0	> 1.0	4	Backward recursion
> 1	< 0	$\leq$ 1.0	5	Forward recursion
< 4	> 0	$\leq$ 1.0	5	Forward recursion
> 1	> 0	(0.0, 0.45]	5	Forward recursion
$\geq$ 4	> 0	(0.45, 1.0]	6	Relationship with P_N

II. A Fast Exponential Subroutine - FXP

Approximately half of the central processor time in a heterogeneous slab calculation in the RABANL module of MC^2-2 is devoted to the calculation of exponentials, $e^{-|x|}$. In the ultra-fine-group calculation, about 25% of the CPU time for a problem with many isotopes is spent in the calculation of exponentials to treat the inelastic and (n,2n) evaporation laws. The standard IBM Fortran exponential function is quite general with regard to permissable arguments and quite accurate. On the other hand it is relatively slow ($\sim 9 \times 10^{-6}$ sec. on a 360/195). Large gains in speed at the expense of accuracy and core storage are obtained by use of an assembler language routine FXP. For arguments in the range $0 \leq x \leq 18$, the program FXP uses a linear interpolation scheme

$$e^{-x} \approx y_i - m_i x \qquad 0 \leq i < 1022$$

where

$$y_i = y_i^* + i\Delta m_i \qquad 0 \leq i \leq 1022$$

$$m_i = \frac{y_i^* - y_{i+1}^*}{\Delta} \qquad 0 \leq i \leq 1022$$

$$y_i^* = e^{-\Delta}\, y_{i-1}^* \qquad 0 < i \leq 1022$$

$$y_o^* = \frac{2}{\Delta}\frac{(1 - e^{-\Delta})}{(1 + e^{-\Delta})}$$

$$\Delta = 18.0/1022$$

This approximation was shown by Olson[22] to be sufficiently accurate for calculations of collision probabilities in the RABID code[6]. The programming of the assembler language routine FXP was optimized to a 195 by A. Hinds of ANL. Computation times less than half that of the Fortran exponential functions are typical of FXP on an IBM 370/195. A Fortran equivalent of FXP is available with the CDC code. The Fortran routine is approximately 20% faster than the CDC library exponential routine.

III. Calculation of Doppler-Broadened Line Shape Functions

In the computation of Doppler-broadened resonance cross sections, use is made of the symmetric and anti-symmetric line shape functions. These functions, usually denoted as ψ and χ, are defined in terms of the real and imaginary parts of the error function for complex arguments as

$$\psi(a,b) = \frac{a\sqrt{\pi}}{2} \text{ Re } W(\frac{ab}{2}, \frac{a}{2}) \tag{A.1}$$

$$\chi(a,b) = a\sqrt{\pi} \text{ Im } W(\frac{ab}{2}, \frac{a}{2}) \tag{A.2}$$

where

$$W(z) = W(x,y) = \exp(-z^2) \text{ erfc}(-iz) \tag{A.3}$$

and $z = x + iy$.

ReW(x,y) and ImW(x,y) were precalculated using the methods described in Ref. 32 and stored in coarse and fine mesh tables as indicated below. In the fine mesh tables, y ranges between -0.02 and 0.5 with the mesh -0.02(0.02)0.5 while in the coarse mesh tables y ranges between 0.4 and 3.0 with the mesh 0.4(0.1)3.0. In both tables, x ranges between -0.1 and 3.9 with the mesh -0.1(0.1)3.9.

If $|x| \leq 3.9$ and $y \leq 3.0$, the ReW and ImW are obtained using the six-point bivariate interpolation formula (25.2.67) of Ref. 33 in either the fine or coarse mesh tables as appropriate to the value of y.

If $|x| > 3.9$ or $y > 3.0$ but $|x| \leq 6.0$ and $y \leq 6.0$, W(z) is approximated by[34]

$$W(z) = iz \sum_{i=1}^{3} \frac{a_i}{z^2 - b_i} \tag{A.4}$$

where

$a_1 = 0.4613135$
$b_1 = 0.1901635$
$a_2 = 0.09999216$
$b_2 = 1.7844927$
$a_3 = 0.002883894$
$b_3 = 5.5253437$

Setting $z = x + iy$, Eq. A.4 yields

$$\mathrm{ReW} = \sum_{i=1}^{3} \frac{a_i \left[-y\,(x^2 - y^2 - b_i) + 2\,x^2\,y\right]}{(x^2 - y^2 - b_i)^2 + 4\,x^2\,y^2} \tag{A.5}$$

$$\mathrm{ImW} = \sum_{i=1}^{3} \frac{a_i \left[x\,(x^2 - y^2 - b_i) + 2\,xy^2\right]}{(x^2 - y^2 - b_i)^2 + 4\,x^2\,y^2} \,. \tag{A.6}$$

If $|x| > 6.0$ or $y > 6.0$ but $|x| \leq 100.0$ and $y \leq 100.0$, W(z) is approximated by[34]

$$W(z) = iz \sum_{i=1}^{2} \frac{c_i}{z^2 - d_i} \tag{A.7}$$

where

$$c_1 = 0.5124242$$
$$d_1 = 0.2752551$$
$$c_2 = 0.05176536$$
$$d_2 = 2.724745 \,.$$

Thus

$$\mathrm{ReW} = \sum_{i=1}^{2} \frac{c_i \left[-y\,(x^2 - y^2 - d_i) + 2\,x^2\,y\right]}{(x^2 - y^2 - d_i)^2 + 4\,x^2\,y^2} \tag{A.8}$$

$$\mathrm{ImW} = \sum_{i=1}^{2} \frac{c_i \left[x\,(x^2 - y^2 - d_i) + 2\,x\,y^2\right]}{(x^2 - y^2 - d_i)^2 + 4\,x^2\,y^2} \,. \tag{A.9}$$

If $|x| > 100.0$ or $y > 100.0$, the code uses an asymptotic approximation. The integral representation of W(z) is given by formula 7.1.4 of Ref. 33 as

$$W(z) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}\,dt}{z - t} \tag{A.10}$$

$$\approx \frac{i}{\pi} \sum_{j=1}^{N} \frac{w_j}{z - t_j} \tag{A.11}$$

where the w_j and t_j are the weights and abscissae for the Hermite quadrature. In particular, for very large x or y, we set N = 2 and ignore t_i relative to z so that

$$W(z) \approx \frac{2i}{\pi} \frac{w}{z} \tag{A.12}$$

where $w = \sqrt{\pi}/2$. Setting $z = x + iy$, we have finally

$$\mathrm{ReW} = \frac{y}{\sqrt{\pi}\ (x^2 + y^2)} \tag{A.13}$$

$$\mathrm{ImW} = \frac{x}{\sqrt{\pi}\,(x^2 + y^2)} \quad . \tag{A.14}$$

For the special case of $x = 0$, Eq. A.3 becomes

$$W(o,y) = e^{y^2}\ \mathrm{erfc}(y). \tag{A.15}$$

If $y < 2.0$, Eq.A.15 is evaluated using the rational approximation (7.1.26) of Ref. 33. If $2.0 \leq y \leq 6.0$, Eq.A.15 is evaluated using Eq.A.5 with x set equal to zero. If $6.0 < y \leq 100.0$, Eq.A.15 is evaluated using Eq.A.8 with x set equal to zero. Finally, for $y > 100.0$, Eq.A.15 is evaluated using Eq.A.13 with x set equal to zero.

IV. Numerical Methods Used in Calculating the Isolated Resonance Integral

The three terms of the factored isolated resonance integral $J(\beta,\theta, 0, 0)$, $I(\beta,\theta, a)$, and $M(\beta,\theta, a)$ given respectively in Eqs. III.46-III.48 are evaluated using fixed point Gauss-Jacobi quadrature or asymptotic algorithms depending upon the value of β. The code calculates the quantity

$$T1 = \frac{\beta + \psi(\theta, 0)}{\psi(\theta, 0)} . \tag{A.16}$$

If $T1 > 4.5$, asymptotic expressions are evaluated as described later. Otherwise, the code evaluates the integrals as follows.[25]

The variable of integration is changed from x to u using the transformation

$$x = K \frac{u}{\sqrt{1 - u^2}} \tag{A.17}$$

so that in general

$$\int_0^\infty f(x)dx = \frac{1}{K}\int_0^1 \frac{du}{\sqrt{1 - u^2}} \cdot \frac{f(x(u))}{1 - u^2}$$

$$= \frac{\pi/N}{K}\left\{\frac{1}{2} f(0) + \sum_{i=2}^{(N-1)/2} \frac{f(x(u_i))}{1 - u_i^2}\right\} + R_N . \tag{A.18}$$

The Gauss-Jacobi quadrature points u_i are given by

$$u_i = \cos \frac{(2i - 1)\,\pi}{2N} \tag{A.19}$$

the quadrature weights are constant and equal to π/N, and the remainder is given

$$R_N = \frac{\pi}{(2N)!\; 2^{2N-1}} f^{(2N)}(\xi), \quad 0 < \xi < 1 . \tag{A.20}$$

The value selected for N (either 9 or 13) and the value for K is determined[25] as shown in Fig. 26 based upon the values of θ and β.

Now when $T1 \geq 4.5$, Hwang has shown[25] that one may write

$$J(\beta,\theta, 0, 0) = T \int_0^\infty dx \frac{\psi(\theta,x)}{\beta + S\,\psi(\theta,x)}$$

$$\approx T \left\{\frac{\frac{\pi}{2}}{\beta + \rho} + S^2 \frac{\int_0^\infty \psi^3(\theta,x)\, dx}{(\beta + \rho)^3} - \frac{\frac{\pi}{2}\rho^2}{(\beta + \rho)^3}\right\} \tag{A.21}$$

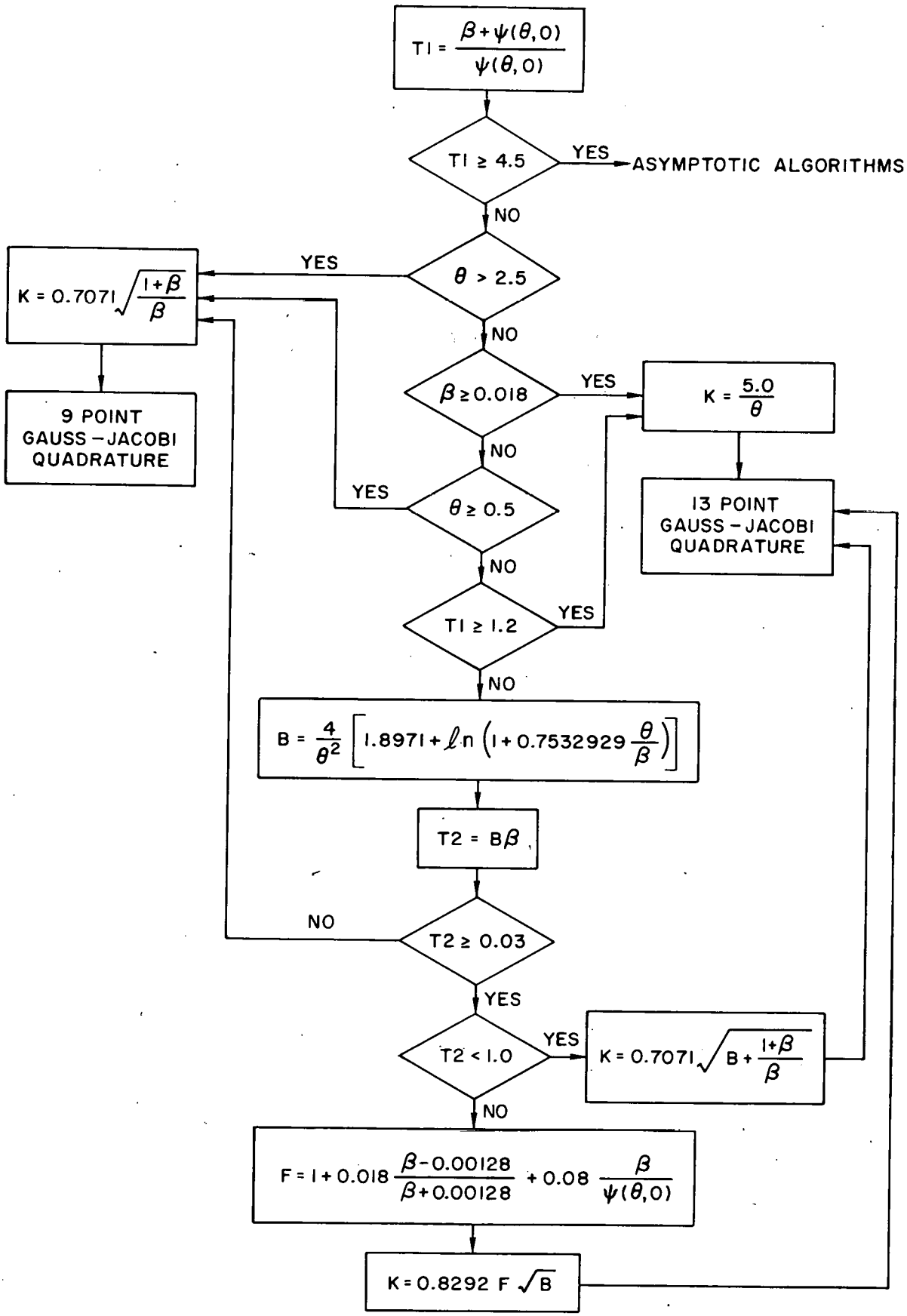

Fig. 26. Gauss-Jacobi Quadrature Selection

$$I(\beta,\theta,\ a) = Ta^2 \int_0^\infty dx\ \frac{\psi}{\beta + S\psi} \cdot \frac{\chi^2}{(\beta + S\psi)^2 - a^2\chi^2}$$

$$\approx \frac{4a^2}{3}\ T\ \frac{\int_0^\infty \psi^3\ dx}{(\beta + \rho)^3} \qquad (A.22)$$

$$M(\beta,\theta,\ a) = a \int_0^\infty dx\ \frac{\chi^2}{(\beta + S\psi)^2 - a^2\chi^2}$$

$$\approx \frac{2\pi a(\beta + 3\rho)\rho}{S(\beta + \rho)^3} - \frac{8aS}{3(\beta + \rho)^3} \int_0^\infty \psi^3\ dx\ . \qquad (A.23)$$

In Eqs.A.21-A.23,

$$\rho = \frac{S}{2}\ \psi(\sqrt{2}\ \theta,\ 0) \qquad (A.24)$$

and $\psi(\sqrt{2}\ \theta,\ 0)$ is evaluated using Eq.A.15.

The third order integral which appears in Eqs. A.21-A-23 is evaluated using a power series expansion, or if $\theta > 2.5$, an asymptotic expansion.

For $\theta \leq 2.5$

$$\int_0^\infty \psi^3(\theta,x)\ dx \approx \frac{\pi}{2} \left\{ \frac{\rho}{S} \left[3\ \psi(\sqrt{2/3}\ \theta,\ 0) - \sqrt{3\pi/2}\ \theta\ e^{\frac{\theta^2}{6}} \right] + \frac{3}{2}\ \theta^2\ S_1 \right\} \qquad (A.25)$$

where

$$S_1 = \frac{1}{4} + \sum_{n=1}^{6} A_n \left[\frac{1}{4} + \sum_{m=1}^{n} B_m\ \theta^{2m} \right] \qquad (A.26)$$

and

$$A_n = \frac{n!}{1 \cdot 3 \cdot 5 \cdots (2n + 1)}\ \frac{1}{2^n}$$

$$B_m = \frac{1}{(\frac{3}{2})^m \cdot 4 \cdot m!}\ . \qquad (A.27)$$

For $\theta > 2.5$

$$\int_0^\infty \psi^3(\theta,x)\ dx \approx \frac{\pi}{8} \left\{ \frac{3}{2} \left[\frac{2}{3}\ \theta^2\ e^{\frac{2}{3}\theta^2}\ E_1(\tfrac{2}{3}\ \theta^2) - h_1 + h_2 - h_3 + h_4 \right] \right\} \qquad (A.28)$$

where

E_1 is the exponential integral defined in Eq. A.37 and

$$h_1 = 1 - \frac{2}{3}\theta^2 e^{\frac{2}{3}\theta^2} E_1(\tfrac{2}{3}\theta^2)$$

$$h_2 = \frac{1}{\frac{2}{3}\theta^2} - h_1 \qquad (A.29)$$

$$h_3 = \frac{5}{\theta^4} - \frac{10}{9} h_2$$

$$h_4 = \frac{105}{4\theta^6} - \frac{7}{6} h_3 \quad .$$

For $x < 10$, $E_1(x)$ is evaluated using the rational expression 5.1.54 of Ref. 33 and for $x \geq 10$, the rational expression 5.1.55 of Ref. 33.

For the case of $\beta \geq 10^{10}$, the code uses the first term in Eq. A.21 for J and sets I and M equal to 0.

V. Quadratures for Statistical Integration

In the calculation of unresolved resonance cross sections, integrals of the form

$$\langle f(x,y)\rangle = \int_0^\infty P_\mu(x)\,dx \int_0^\infty P_\nu(y) f(x,y)\,dy \tag{A.30}$$

are required where P_μ is the Chi-squared distribution of order μ given by

$$P_\mu(x)\,dx = \frac{\mu}{2} \frac{1}{\Gamma\left(\frac{\mu}{2}\right)} \left(\frac{\mu x}{2}\right)^{\frac{\mu}{2}-1} \exp\left(-\frac{\mu x}{2}\right). \tag{A.31}$$

Eq.A.30 is evaluated using the method described by Hwang[35] as

$$\langle f(x,y)\rangle = \sum_{j=1}^{10}\sum_{k=1}^{10} A_j A_k f(X_j, Y_k) \tag{A.32}$$

where the A_j and X_j have been calculated for $\mu = 1,2,3$, and 4. The ten point quadrature is used for both neutron and fission width distributions.

For odd μ

$$X_j = 2Z_j^{\,2}/\mu \tag{A.33}$$

$$A_j = 2W_j^{\,S} Z_j^{\,\mu-1}/\Gamma(\mu/2) \tag{A.34}$$

while for even μ

$$X_j = (1-S_j)/(1+S_j) \tag{A.35}$$

$$A_j = \mu W_j^{\,L} \left(\frac{\mu}{2} X_j\right)^{\mu/2-1} \exp\left(-\frac{\mu}{2}X_j\right) / [\Gamma(\mu/2)(1+S_j)^2]. \tag{A.36}$$

In Eqs.A.33 and A.34, Z_j and W_j^S are respectively the ordinates and weights of the half-range Gauss-Hermite quadrature derived by Steen, et al.[36] while in Eqs.A.35 and A.36, S_j and W_j^L are respectively the usual Gauss-Legendre ordinates and weights.

Table XIII lists A_j and X_j for $\nu = 1,2,3$, and 4 and $j = 1,2,\ldots,10$.

Table XIII. Ten Point Quadrature Weights and Abscissae for Statistical Integration

	One Degree of Freedom		Two Degrees of Freedom	
	Weight	Abscissa	Weight	Abscissa
1	1.1120413E-01	3.0013465E-03	3.3773418E-02	1.3219203E-02
2	2.3546798E-01	7.8592886E-02	7.9932171E-02	7.2349624E-02
3	2.8440987E-01	4.3282415E-01	1.2835937E-01	1.9089473E-01
4	2.2419127E-01	1.3345267E+00	1.7652616E-01	3.9528842E-01
5	1.0967668E-01	3.0481846E+00	2.1347043E-01	7.4083443E-01
6	3.0493789E-02	5.8263198E+00	2.1154965E-01	1.3498293E+00
7	4.2930874E-03	9.9452656E+00	1.3365186E-01	2.5297983E+00
8	2.5827047E-04	1.5782128E+01	2.2630659E-02	5.2384894E+00
9	4.9031965E-06	2.3996824E+01	1.6313638E-05	1.3821772E+01
10	1.4079206E-08	3.6216208E+01	0.0	7.5647525E+01

	Three Degrees of Freedom		Four Degrees of Freedom	
	Weight	Abscissa	Weight	Abscissa
1	3.3376214E-04	1.0004488E-03	1.7623788E-03	1.3219203E-02
2	1.8506108E-02	2.6197629E-02	2.1517749E-02	7.2349624E-02
3	1.2309946E-01	1.4427472E-01	8.0979849E-02	1.9089473E-01
4	2.9918923E-01	4.4484223E-01	1.8797998E-01	3.9528842E-01
5	3.3431475E-01	1.0160615E+00	3.0156335E-01	7.4083443E-01
6	1.7766657E-01	1.9421066E+00	2.9616091E-01	1.3498293E+00
7	4.2695894E-02	3.3150885E+00	1.0775649E-01	2.5297983E+00
8	4.0760575E-03	5.2607092E+00	2.5171914E-03	5.2384894E+00
9	1.1766115E-04	7.9989414E+00	8.9630388E-10	1.3821772E+01
10	5.0989546E-07	1.2072069E+01	0.0	7.5647525E+01

VI. Numerical Methods Used in Calculating Slab Collision Rates

a. Exponential Integrals

The exponential integral $E_n(x)$ is defined as

$$E_n(x) = \int_1^\infty \frac{e^{-xt}}{t^n}\, dt \tag{A.37}$$

The integrals $E_2(x)$, $E_3(x)$, and $E_4(x)$ are obtained using the following algorithms.

$E_2(x)$ is evaluated using the series expansion (5.1.11) of the Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables[33] for $E_1(s)$ along with the recursion relationship

$$E_{n+1}(x) = \frac{1}{n}\left[e^{-x} - x\, E_n(x)\right] \tag{A.38}$$

to yield

$$E_2(x) \approx 1 - x\,(1 - \gamma - \ln x) - \frac{x^2}{1\cdot 2!} + \frac{x^3}{2\cdot 3!} - \frac{x^4}{3\cdot 4!} \tag{A.39}$$

where Euler's constant γ has the value $\gamma = 0.5772156649\ldots$

For $x < 0.6$, $E_3(x)$ as in the case of $E_2(x)$ uses (5.1.11) of Ref.33 with successive application of Eq.A.38 to yield

$$E_3(x) \approx 0.5 - x + \frac{x^2}{2}\,(1.5 - \gamma - \ln x) + \frac{x^3}{3!} - \frac{x^4}{2\cdot 4!} + \frac{x^5}{3\cdot 5!} - \frac{x^6}{4\cdot 6!}\,. \tag{A.40}$$

For $0.6 \le x \le 6.4$, $E_3(x)$ is obtained by linear interpolation in a table of E_3 with tabular entries 0(0.01)2(0.02)4(0.08)6.4. The table values are calculated using the polynomial approximation (5.1.53) of Ref. 33 if $0 \le x \le 1$ and the rational approximation (5.1.56) of Ref. 33 if $x > 1$ to obtain $E_1(x)$, and successive application of Eq.A.38.

For $6.4 < x \le 80$, $E_3(x)$ is evaluated using the first three terms of the series representation of $E_n(x)$ for large n (5.1.52) of Ref. 33 so that

$$E_3(x) \approx \frac{e^{-x}}{x+3}\left[1 + \frac{3}{(x+3)^2} + \frac{3(3-2x)}{(x+3)^4}\right] \tag{A.41}$$

Beyond $x = 80$, E_3 is assumed to be zero.

For $0 \leq x \leq 6.4$, $E_4(x)$ is obtained by linear interpolation in a Table of E_4 with table entries the same as for the E_3 table mentioned above. The table values were obtained as in the case of E_3 with one more application of the recursion relation Eq.A.38.

For $6.4 < x \leq 80$, E_4 is evaluated as in the case of E_3 using (5.1.52) of Ref. 33 so that

$$E_4(x) \approx \frac{e^{-x}}{x+4}\left[1 + \frac{4}{(x+4)^2} + \frac{4(4-2x)}{(x+4)^4}\right] \tag{A.42}$$

Beyond $x = 80$, E_4 is assumed to be zero.

b. Slab Collision Escape Probability

The probability of escape without a collision from a slab with optical thickness x is given by

$$P = \frac{0.5 - E_3(x)}{x} \quad . \tag{A.43}$$

If $x \geq 0.6$, P is evaluated with $E_3(x)$ being obtained as described earlier using table interpolation or using Eq.A.41 as appropriate to the range of x.

For $x < 0.6$, use of Eq.A.40 in Eq.A.43 yields

$$P \approx 1 - \frac{x}{2}(1.5 - \gamma - \ln x) - \frac{x^2}{3!} + \frac{x^3}{2\cdot 4!} - \frac{x^4}{3\cdot 5!} + \frac{x^5}{4\cdot 6!} - \frac{x^6}{5\cdot 7!} \tag{A.44}$$

c. Infinite Sums of Exponential Integrals

In the case of a unit cell of optical thickness h, the collision rate calculation involves evaluation of infinite sums of exponential integrals. Numerical procedures have been developed[6] for evaluating the functions

$$S_n(z,h) = \sum_{k=0}^{\infty} E_n(z + kh) = \int_1^{\infty} \frac{e^{-zt}}{(1 - e^{-ht})t^n}\, dt \tag{A.45}$$

which make use of fast and accurate Gaussian quadrature formulas.

The code evaluates $S_3(z,h)$ using

$$S_3(z,h) \approx \sum_{i=1}^{M}\left[\frac{w_{i,3}\exp(t_{i,3})}{1 - \exp(-ht_{i,3})}\right]\exp(-zt_{i,3}) + C(z,h) \tag{A.46}$$

where

$$C(z,h) = \left\{0.004126 + 0.00628\exp(-19.8h)\right\}\exp(-18.2z), \quad z < 0.3$$
$$= 0, \quad z \geq 0.3 \tag{A.47}$$

and the abscissae $t_{i,3}$ and weights $w_{i,3}$ are precalculated as described in Ref. 37 data and stored as data in the code.

The number of terms M used in the sum in Eq.A.46 lay between 1 and 4 depending upon the value of z. If

$z \leq 3.16$, M is determined by truncating to an integer

$$M = 0.633\ (7.89 - z). \tag{A.48}$$

For $3.16 < z \leq 13.7$, M is determined from

$$M = 1.0 + 6.2/z. \tag{A.49}$$

For $z > 13.7$, $S_3(z,H)$ is assumed to be zero.

$S_4(z,h)$ is evaluated as

$$S_4(z,h) \approx \sum_{i=1}^{N} \left[\frac{w_{i,4}\ \exp(t_{i,4})}{1 - \exp(-\ ht_{i,4})}\right] \exp(-\ zt_{i,4}) \tag{A.50}$$

with the abscissae and weights again precalculated and stored.

N lay between 1 and 4 depending upon z. If $z \leq 3.64$, M is determined by truncating to an integer

$$N = 0.549\ (9.10 - z)\ . \tag{A.51}$$

For $3.64 < N \leq 15.6$, M is determined from

$$N = 1.0 + 6.81/z. \tag{A.52}$$

For $z > 15.6$, $S_4(z,H)$ is assumed to be zero.

In addition to the infinite sums $S_n(z,h)$, the code requires differences of these sums

$$D_n(y,\Delta,h) = S_n(y,\ h) - S_n(y + \Delta,\ h)\ . \tag{A.53}$$

The $D_n(y,\Delta,h)$ are evaluated using various algorithms depending upon the cell optical thickness and the incremental length Δ. In particular, the method of Gaussian quadrature for the evaluation of the S_n described above is least accurate for either z or h small.

For $\Delta > 0.02$ and $h \leq 0.2$, if $z > 1.147h^{1.4}$, the $S_3(z,h)$ of Eq.A.53 are evaluated using the Euler-Maclaurin series

$$S_3(z,h) \approx \frac{1}{12}\left\{e^{-z}\left[\frac{4 - 2z}{h} + 3 - \frac{h^3}{60z}\left\langle 1 - \frac{h^2}{21z2}\ (1 + z + \frac{z^2}{2})\right\rangle\right]\right.$$

$$\left. + E_2(z)\left[h - 3z + \frac{2z^2}{h}\right]\right\}. \tag{A.54}$$

If $z \leq 1.147h^{1.4}$ but $z + h > 1.147h^{1.4}$,

$$S_3(z,h) = E_3(z) + S_3(z + h, h) \tag{A.55}$$

where $S_3(z + h, h)$ is evaluated using Eq.A.54.

If $z + h \leq 1.147h^{1.4}$ but $z + 2h > 1.147h^{1.4}$,

$$S_3(z,h) = E_3(z) + E_3(z + h) + S_3(z + 2h, h) \tag{A.56}$$

where again $S_3(z + 2h, h)$ uses Eq.A.54. In Eqs.A.54-A.56, the $E_2(z)$ and $E_3(z)$ are obtained using the methods described above for obtaining the exponential integrals.

If $\Delta > 0.02$ and $h > 0.2$, the $S_3(z, h)$ of Eqs.A.53 are evaluated using Gaussian quadrature as described earlier in the discussion relating to Eq.A.46 with the number of terms used in the quadrature determined using Eqs.A.48 and A.49.

If Δ is ≤ 0.02, a Taylor series expansion is used to obtain

$$D_3(y,\Delta,h) = S_3(y, h) - S_3(y + \Delta, h) = S_3(z - \tfrac{\Delta}{2}, h) - S_3(z + \tfrac{\Delta}{2}, h)$$

$$\approx \Delta \cdot \left[S_2(y + \Delta/2,h) + \frac{\Delta^2}{24} S_o(y + \Delta/2,h) + \frac{\Delta^4}{1920} S_{-2}(y + \Delta/2,h) \right]. \tag{A.57}$$

For $y + \Delta/2 < 0.6$, only the S_2 and the S_o are retained and the first few terms of the series in Eq.A.57 are evaluated by directly summing the E_2 and E_o functions as

$$S_1 = \Delta \cdot \left\{ E_2(y + \Delta/2) + E_2(y + \Delta/2 + h) + E_2(y + \Delta/2 + 2h) + \ldots \right.$$
$$\left. + \frac{\Delta^2}{24} \left[E_o(y + \Delta/2) + E_o(y + \Delta/2 + h) + E_2(y + \Delta/2 + 2h) + \ldots \right] \right\} \tag{A.58}$$

where the direct summation in Eq.A.58 is continued as long as $y + \Delta/2 + kh < 0.6$, and $E_o(z) = \exp(-z)/z$.

When $y + \Delta/2 + kh \geq 0.6$, the remainder of the series of Eq.A.57 is obtained as follows. S_2 is obtained using the Gaussian quadrature algorithm

$$S_2(y + \Delta/2 + kh, h) = \sum_{i=1}^{4} \left[\frac{w_{i,2} \exp(t_{i,2})}{1 - \exp(-ht_{i,2})} \right] \exp\left\{ -(y + \Delta/2 + kh)t_{i,2} \right\} \tag{A.59}$$

using precalculated and stored weights and abscissae. Then, using the fact that

$$\frac{\partial E_n(z)}{\partial z} = - E_{n-1}(z) \tag{A.60}$$

we may rewrite Eq. A.57 as

$$S_2 = \Delta \cdot S_2(y + \Delta/2 + kh,\ h) \left\{1 + \frac{\Delta^2}{24} t_{i,2}^2 + \frac{\Delta^4}{1920} t_{i,2}^4\right\} \tag{A.61}$$

with Eq. 23 used to obtain S_2. Thus finally

$$D_3(y,\Delta,h) = S_1 + S_2 \ . \tag{A.62}$$

The $D_4(y,\Delta,h)$ are similarly evaluated using various algorithms depending upon the cell optical thickness h and the incremental length Δ.

For $\Delta > 0.02$ and $h \leq 0.2$, if $z > 1.818h^{2.5}$, the $S_4(z,h)$ of Eq.A.53 are evaluated using the Euler-Maclaurin series

$$S_4(z,h) \approx \frac{1}{12} \left\{ e^{-z} \left[\frac{3 - z}{h} + 2 + \frac{h^3}{60z^2} (1 - z)\right] + E_3(z) \left[\frac{z^2}{h} - h - 2z - \frac{h^3}{30z^2}\right]\right\} \ . \tag{A.63}$$

If $z \leq 1.818h^{2.5}$ but $z + h > 1.818h^{2.5}$,

$$S_4(z,h) = E_4(z) + S_4(z + h,\ h) \tag{A.64}$$

where $S_4(z + h,\ h)$ is evaluated using Eq.A.63. In Eqs.A.63 and A.64, the $E_3(z)$ and $E_4(z)$ are obtained using the methods described earlier for obtaining the exponential integrals.

If $\Delta > 0.02$ and $h > 0.2$, the $S_4(z,h)$ of Eq.A.53 are evaluated using Gaussian quadrature as described earlier in the discussion relating to Eq.A.50 with the number of terms used in the quadrature determined using Eqs.A.51 and A.52.

If Δ is ≤ 0.02, a Taylor series expansion is used as in the case of $D_3(y,\Delta,h)$ to obtain

$$D_4(y,\Delta,h) = S_4(y,\ h) - S_4(y + \Delta,\ h) \approx \Delta \cdot S_3(y + \Delta/2,\ h) \left\{1 + \frac{\Delta^2}{24} t_{i,3}^2\right\} \tag{A.65}$$

with S_3 being obtained using the Gaussian quadrature of Eq.A.46.

VII. Cylindrical Transmission Probabilities

As given in Ref. 5, for a cylindrical region i having outer radius r_i, inner radius r_{i-1}, and macroscopic cross section Σ_i, the transmission probabilities from inner surface to outer surface T_i^{OI} and from outer surface to outer surface T_i^{OO} are given by

$$T_i^{OI} = \frac{4}{\pi} \int_0^{\pi/2} d\phi \cos \phi \, K_{i_3}\left\{\Sigma_i f_i(\phi)\right\} \tag{A.66}$$

$$T_i^{OO} = \frac{4}{\pi} \int_0^{\pi/2} d\phi \cos \phi \left[K_{i_3}\left\{\Sigma_i g_i(\phi)\right\} - \frac{r_{i-1}}{r_i} K_{i_3}\left\{\Sigma_i h_i(\phi)\right\}\right] \tag{A.67}$$

where

$$K_{i_3}(\xi) = \int_0^{\pi/2} e^{-\xi \csc\theta} \sin^2 \theta \, d\theta \tag{A.68}$$

$$f_i(\phi) = - r_{i-1} \cos \phi + \left\{r_i^2 - r_{i-1}^2 \sin^2 \phi\right\}^{\frac{1}{2}} \tag{A.69}$$

$$g_i(\phi) = 2r_i \cos \phi \tag{A.70}$$

$$h_i(\phi) = 2\left\{r_i^2 - r_{i-1}^2 \sin^2 \phi\right\}^{\frac{1}{2}} \tag{A.71}$$

The T^{OI} and T^{OO} are tabulated as a function of x and z where

$$x_i = \frac{r_{i-1}}{r_i} \tag{A.72}$$

$$z_i = \Sigma_i (r_i - r_{i-1}) \tag{A.73}$$

with x ranging between 0.0 and 1.0 and z between 0.0 and 8.0. For both T^{OI} and T^{OO}, the mesh for z is 0(0.01)0.4(0.02)1.0(0.04)2.6(0.06)5.0(0.10)8.0. For T^{OI}, the x mesh increment is 0.04, and for T^{OO}, the x mesh increment is 0.02.

The K_{i_3} used in Eqs. A.66 and A.67 were obtained from an extended precision (real*16) function KIN which computes $K_{i_N}(x)$ for $1 \leq N \leq 10$ and $x \geq 0$ using the following algorithms.

For $x > 39.0$, KIN returns the value 0.0 for all N. For $0.0 < x \leq 39.0$, K_{i_2} and K_{i_3} are evaluated using the rational expressions given by I. Gargantine and T. Pomentale[38].

For $0.0 < x \leq 2.0$, $K_{i_o}(x) = K_o(x)$ is obtained from the polynomial approximations (9.8.5) and (9.8.1) of the Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables[33] and for $x > 2.0$, K_{i_o} is obtained from the polynomial approximation (9.8.6) of Ref.33.

K_{i_1} is obtained for $0.0 < x \leq 7.0$ in terms of $K_{i_{-1}}$ and K_{i_2} as

$$K_{i_1}(x) = K_{i_{-1}}(x) - \frac{1}{x} K_{i_2}(x) \tag{A.74}$$

where K_{i_2} is obtained as indicated above and $K_{i_{-1}}(x) = K_1(x)$ is obtained using the polynomial approximations (9.8.7) and (9.8.3) of Ref.33 when $0.0 < x \leq 2.0$, and using the polynomial approximation (9.8.8) of Ref.33 when $x > 2.0$. For $x > 7.0$, K_{i_1} is obtained from the polynomial approximation (11.1.18) of Ref.33.

For $n > 3$, the recursion relationship

$$n\, K_{i_{n+1}}(x) = (n-1)\, K_{i_{n-1}}(x) + x\left[K_{i_{n-2}}(x) - K_{i_n}(x)\right] \tag{A.75}$$

is used.

For $x = 0.0$, KIN uses stored precalculated data to return

$$K_{i_n}(0) = \frac{(\pi)^{\frac{1}{2}}}{2} \frac{\Gamma\left[\frac{n}{2}\right]}{\Gamma\left[\frac{n}{2} + \frac{1}{2}\right]} \tag{A.76}$$

where

$$\Gamma(\tfrac{1}{2}) = (\pi)^{\frac{1}{2}}$$

$$\Gamma(\tfrac{3}{2}) = \tfrac{1}{2}\,(\pi)^{\frac{1}{2}}$$

$$\Gamma(n + \tfrac{1}{2}) = \frac{1 \cdot 3 \cdot 5 \cdot 7 \cdots (2n-1)}{2^n}\,(\pi)^{\frac{1}{2}}$$

$$\Gamma(n+1) = n!$$

$$(-\tfrac{1}{2})! = (\pi)^{\frac{1}{2}}$$

$$(\tfrac{1}{2})! = \tfrac{1}{2}\,(\pi)^{\frac{1}{2}}$$

The extended precision (real*16) numerical integration of Eqs.A.66 and A.67 was accomplished using an adaptive Simpson's rule quadrature with convergence criteria adjusted for different ranges of x and z to achieve at least six significant figure agreement with very small convergence criterion results.

For a given x and z, T^{0I} and T^{00} are obtained using the six point bivariate interpolation formula (25.2.67) of Ref.33 within the body of the table and the four point formula (25.2.66) of Ref.33 in the first x or z intervals.

Outside the range of the table T^{0I} is set to zero and an approximate polynomial fit similar to that used in the RABBLE code[5] is used for T^{00}.

APPENDIX B

MC^2-2 BCD INPUT FILES

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2

```
C*****************************************************************
C                                                                -
C                        PREPARED 3/8/76 AT ANL                  -
C                                                                -
CF          A.MCC2                                               -
CE          GENERAL BCD INPUT FOR MC**2-II AND SDX CALCULATIONS  -
C                                                                -
CN                      THIS IS A USER SUPPLIED BCD DATA SET.    -
CN                      THE LIST FOR EACH RECORD IS GIVEN IN TERMS -
CN                      OF THE BCD FORMAT OF THAT DATA CARD.     -
CN                      COLUMNS 1-2 CONTAIN THE CARD TYPE NUMBER. -
CN                      BLANK FIELDS PRODUCE THE DEFAULT OPTIONS.
C                                                                -
C*****************************************************************


C----------------------------------------------------------------
CR          PROBLEM TITLE (TYPE 01)                              -
C                                                                -
CL    FORMAT-----(I2,4X,11A6)                                    -
C                                                                -
CD    COLUMNS           CONTENTS...IMPLICATIONS, IF ANY          -
CD    =======   ==================================================-
CD    1-2       01                                               -
CD                                                               -
CD    7-72      ANY ALPHANUMERIC CHARACTERS.                     -
C                                                                -
CN              ANY NUMBER OF TYPE 01 CARDS MAY BE USED.         -
C                                                                -
C----------------------------------------------------------------


C----------------------------------------------------------------
CR          CONTAINER ARRAY SPECIFICATIONS (TYPE 02)             -
C                                                                -
CL    FORMAT-----(I2,4X,3I6)                                     -
C                                                                -
CD    COLUMNS           CONTENTS...IMPLICATIONS, IF ANY          -
CD    =======   ==================================================-
CD    1-2       02                                               -
CD                                                               -
CD    7-12      SIZE OF MAIN CORE CONTAINER ARRAY IN 8 BYTE WORDS, -
CD              TYPICALLY 30000 (DEFAULT=30000).                 -
CD              FOR CDC USERS TYPICALLY 20000 (DEFAULT=20000).   -
CD                                                               -
CD    13-18     SIZE OF BULK CORE CONTAINER ARRAY IN 8 BYTE WORDS, -
CD              TYPICALLY 0, (DEFAULT=0).                        -
CD              FOR CDC USERS TYPICALLY 100000 (DEFAULT=100000). -
CD              MAXIMUM ALLOWABLE=131072.                        -
CD
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
CD     19-24      POINTR DEBUGGING EDIT, TYPICALLY 0.                    -
CD                0...NO DEBUGGING PRINTOUT (DEFAULT).                   -
CD                1...DEBUGGING DUMP PRINTOUT.                           -
CD                2...DEBUGGING TRACE PRINTOUT.                          -
CD                3...FULL DEBUGGING PRINTOUT.                           -
C                                                                        -
CN                NO TYPE 02 CARD WILL GIVE THE FOLLOWING DEFAULT        -
CN                VALUES FOR IBM USERS.                                  -
CN                MAIN CORE CONTAINER=30000                              -
CN                BULK CORE CONTAINER=0                                  -
CN                PRINT OPTION FLAG=0                                    -
CN                FOR THE DEFAULT VALUES ON THE TYPE 02 CARD, THE        -
CN                REGION PARAMETER OF THE JOB CARD SHOULD BE             -
CN                REGION=700K                                            -
CN                                                                       -
CN                NO TYPE 02 CARD WILL GIVE THE FOLLOWING DEFAULT        -
CN                VALUES FOR CDC USERS.                                  -
CN                MAIN CORE CONTAINER=20000                              -
CN                BULK CORE CONTAINER=100000                             -
CN                PRINT OPTION FLAG=0                                    -
CN                FOR THE DEFAULT VALUES ON THE TYPE 02 CARD, THE        -
CN                REDEFINE FIELD LENGTH CONTROL CARD SHOULD SPECIFY      -
CN                RFL(160000,L=400)                                      -
C                                                                        -
C------------------------------------------------------------------------

C------------------------------------------------------------------------
CR           GENERAL PROBLEM SPECIFICATIONS (TYPE 03)                    -
C                                                                        -
CL     FORMAT-----(I2,4X,4I6,A6,6I6)                                     -
C                                                                        -
CD     COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                 -
CD     =======    ========================================================-
CD     1-2        03                                                     -
CD                                                                       -
CD     7-12       FUNDAMENTAL MODE TYPE.                                 -
CD                1...P1 (DEFAULT).                                      -
CD                2...B1.                                                -
CD                3...CONSISTENT P1.                                     -
CD                4...CONSISTENT B1.                                     -
CD                                                                       -
CD     13-18      ORDER OF EXTENDED TRANSPORT APPROXIMATION (DEFAULT=1). -
CD                                                                       -
CD     19-24      CONTINUOUS SLOWING DOWN MODERATING PARAMETER OPTION.   -
CD                0...IMPROVED GREULING GOERTZEL (DEFAULT).              -
CD                1...GREULING GOERTZEL.                                 -
CD                                                                       -
CD     25-30      MAXIMUM NUMBER OF HYPERFINE GROUPS PER ULTRAFINE GROUP -
CD                USED IN EVALUATION OF ELASTIC SCATTERING MATRICES      -
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
CD              (DEFAULT=1).                                            -
CD                                                                      -
CD    31-36     BROAD GROUP STRUCTURE TYPE.                             -
CD              ANL9...ANL 9 GROUP STRUCTURE.                           -
CD              ANL11...ANL 11 GROUP STRUCTURE.                         -
CD              ANL27...ANL 27 GROUP STRUCTURE.                         -
CD              ANL28...ANL 28 GROUP STRUCTURE.                         -
CD              BOND26...BONDARENKO 26 GROUP STRUCTURE.                 -
CD              FFTF30...FFTF 30 GROUP STRUCTURE.                       -
CD              HANS16...HANSEN-ROACH 16 GROUP STRUCTURE.               -
CD              SDX156...SDX 156 GROUP STRUCTURE.                       -
CD              USS212...UNIVERSAL SUPERGROUP 212 GROUP STRUCTURE.      -
CD              USS226...UNIVERSAL SUPERGROUP 226 GROUP STRUCTURE.      -
CD              WARD9...WARD 9 GROUP STRUCTURE.                         -
CD                                                                      -
CD    37-42     FUEL GEOMETRY.                                          -
CD              0...HOMOGENEOUS.                                        -
CD              1...SLAB.                                               -
CD              2...CYLINDER.                                           -
CD                                                                      -
CD    43-48     RESOLVED RESONANCE OVERLAP OPTION.                      -
CD              0...INCLUDE OVERLAP CALCULATION FOR THE NUMBER OF       -
CD                  NEIGHBORING RESONANCES DESIGNATED IN COLS. 55-60    -
CD                  (DEFAULT).                                          -
CD              1...OMIT OVERLAP CALCULATION.                           -
CD                                                                      -
CD    49-54     UNRESOLVED RESONANCE SELF-OVERLAP OPTION.               -
CD              0...INCLUDE SELF-OVERLAP CALCULATION (DEFAULT).         -
CD              1...OMIT SELF-OVERLAP CALCULATION.                      -
CD                                                                      -
CD    55-60     NUMBER OF RESOLVED RESONANCES TO BE TESTED FOR OVERLAP  -
CD              ON EACH SIDE OF EACH RESOLVED RESONANCE (DEFAULT=4).    -
CD              THIS FIELD IS IGNORED IF COLS. 43-48 ARE 1.             -
CD                                                                      -
CD    61-66     RESERVED FOR FUTURE USE                                 -
CD                                                                      -
CD    67-72     INELASTIC AND (N,2N) ULTRA-FINE-GROUP TREATMENT.        -
CD              0...APPROXIMATE TREATMENT (DEFAULT).                    -
CD              1...RIGOROUS ENERGY-ANGLE CORRELATION ACCOUNTED FOR.    -
C                                                                       -
CN              IF CARD TYPE 03 IS NOT SUPPLIED, ALL DEFAULT OPTIONS    -
CN              WILL BE UTILIZED.                                       -
CN              IF COLS. 37-42 ARE NON-ZERO, CARD TYPES 04, 06, 14, AND-
CN              15 OF DATA SET A.NIP MUST BE SUPPLIED TO SPECIFY THE    -
CN              HETEROGENEOUS PROBLEM GEOMETRY AND COMPOSITIONS.        -
CN              IF COLS. 7-12 ARE 1 OR 2, COLS. 13-18 MUST BE 1.        -
CN              COLS. 31-36 ARE IGNORED IF ANY TYPE 05 OR 07 CARDS      -
CN              ARE SUPPLIED OR IF THE DATA SET XS.ISO IS DECLARED TO   -
CN              BE OLD IN THE EXECUTION DECK.
C
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
C-----------------------------------------------------------------

C-----------------------------------------------------------------
CR          GENERAL PROBLEM CONSTANTS (TYPE 04)                  -
C                                                                -
CL    FORMAT-----(I2,10X,5E12.5)                                 -
C                                                                -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY           -
CD    =======    ========================================================-
CD    1-2        04                                             -
CD                                                              -
CD    13-24      CONTINUOUS SLOWING DOWN INTEGRATION FACTOR THETA -
CD               (DEFAULT=0.5).                                 -
CD                                                              -
CD    25-36      MASS OF MATERIAL USED IN DETERMINATION OF THE DATA -
CD               MANAGEMENT STRATEGY FOR THE SPECTRUM CALCULATION. -
CD               COLS 25-36 SHOULD BE LESS THAN OR EQUAL TO THE MASS OF -
CD               THE LIGHTEST MATERIAL IN THE PROBLEM (EXCLUDING H). -
CD               IF COLS. 25-36 ARE BLANK, THE MANAGEMENT STRATEGY IS -
CD               SELECTED BY THE BUILT IN ALGORITHM.  IF COLS. 25-36 -
CD               CONTAIN A VALUE LARGER THAN THE LIGHTEST MASS MATERIAL -
CD               IN THE PROBLEM, THE LATTER WILL BE USED INSTEAD. -
CD                                                              -
CD    37-48      BOUNDARY ENERGY IN EV. BETWEEN THE MULTIGROUP FLUX -
CD               SOLUTION AND THE CONTINUOUS SLOWING DOWN FLUX  -
CD               SOLUTION. THE BOUNDARY ENERGY MUST BE GREATER THAN -
CD               THE ENERGY OF THE HIGHEST RESOLVED RESONANCE IN THE -
CD               PROBLEM.  THE DEFAULT VALUES WILL SATISFY THIS -
CD               REQUIREMENT.                                   -
CD                                                              -
CD    49-60      CONSTANT A1 USED IN THE EQUIVALENCE PRINCIPLE. -
CD                                                              -
CD    61-72      CONSTANT A2 USED IN THE EQUIVALENCE PRINCIPLE. -
C                                                               -
CN               IF COLS. 49-60 ARE BLANK, COLS. 49-60 AND      -
CN               COLS. 61-72 ARE SET EQUAL TO 1.35 IF COLS 37-42 ON -
CN               CARD TYPE 03 CONTAIN A 2 AND THEY ARE SET EQUAL TO -
CN               1.09 IF COLS. 37-42 ON CARD TYPE 03 CONTAIN A 1. -
CN               IF COLS. 49-60 ARE NON-BLANK AND COLS. 61-72 ARE -
CN               BLANK, COLS. 61-72 ARE SET EQUAL TO COLS. 49-60. -
CN               IF NO CARD TYPE 04 IS SUPPLIED, ALL DEFAULT OPTIONS -
CN               WILL BE UTILIZED.                              -
C                                                               -
C-----------------------------------------------------------------

C-----------------------------------------------------------------
 R           BROAD GROUP ENERGIES (TYPE 05)                     -
                                                                -
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
CL     FORMAT-----(I2,10X,3(I6,E12.5))                                  -
C                                                                       -
CD     COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                 -
CD     =======  ==================================================     -
CD     1-2      05                                                      -
CD                                                                      -
CD     13-18    BROAD GROUP NUMBER.                                     -
CD                                                                      -
CD     19-30    UPPER ENERGY OF GROUP (EV).                             -
CD                                                                      -
CD     31-36    BROAD GROUP NUMBER.                                     -
CD                                                                      -
CD     37-48    UPPER ENERGY OF GROUP (EV).                             -
CD                                                                      -
CD     49-54    BROAD GROUP NUMBER.                                     -
CD                                                                      -
CD     55-66    UPPER ENERGY OF GROUP (EV).                             -
C                                                                       -
CN              THE BROAD GROUP STRUCTURE MAY BE SPECIFIED USING TYPE   -
CN              05 CARDS OR TYPE 07 CARDS OR A COMBINATION OF EACH.     -
CN              ALTERNATIVELY, ONE OF THE PRESTORED GROUP STRUCTURES    -
CN              SPECIFIED IN COLS. 31-36 ON THE TYPE 03 CARD OR THE     -
CN              BUILT IN DEFAULT DESCRIBED BELOW MAY BE USED.           -
CN              GROUP 1 IS THE GROUP OF HIGHEST ENERGY. THE THERMAL     -
CN              GROUP HAVING THE LARGEST GROUP NUMBER HAS AS UPPER      -
CN              ENERGY THE INTERFACE BETWEEN THE THERMAL GROUP AND      -
CN              EPI-THERMAL GROUPS. AS MANY TYPE 05 CARDS ARE USED AS   -
CN              ARE NECESSARY TO SPECIFY THE ENERGIES. IF COLS. 31-36   -
CN              OR 49-54 ARE BLANK, THE REST OF THE DATA ON THE TYPE 05-
CN              CARDS ARE IGNORED.                                      -
CN              IF ONLY THE BROAD GROUP NUMBER ONE UPPER ENERGY IS       -
CN              SPECIFIED AND IF NO TYPE 07 CARDS ARE SUPPLIED, A FIXED-
CN              0.5 LETHARGY WIDTH BROAD GROUP STRUCTURE IS CONSTRUCTED-
CN              EXTENDING DOWN FROM THE SPECIFIED ENERGY TO THE LOWEST  -
CN              ENERGY IN THE LIBRARY. IF TYPE 07 CARDS ARE SUPPLIED,   -
CN              THE TYPE 07 DATA ARE USED WITH THE SPECIFIED UPPER      -
CN              ENERGY TO CONSTRUCT THE BROAD GROUP STRUCTURE.          -
CN              IF MORE THAN ONE BROAD GROUP ENERGY BOUNDARY IS          -
CN              SPECIFIED ON THE TYPE 05 CARDS, ANY TYPE 07 CARDS       -
CN              SUPPLIED WILL BE IGNORED.                               -
CN              IF COLS. 31-36 ON CARD TYPE 03 ARE BLANK AND            -
CN              IF NO TYPE 05 CARDS ARE SUPPLIED AND NO TYPE 07 CARDS   -
CN              ARE SUPPLIED, A FIXED 0.5 LETHARGY WIDTH BROAD GROUP    -
CN              STRUCTURE IS CONSTRUCTED COVERING THE ENERGY RANGE      -
CN              OF THE LIBRARY.                                         -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
CR          HOMOGENEOUS COMPOSITION SPECIFICATIONS (TYPE 06)                -
C                                                                           -
CL    FORMAT-----(I2,10X,2A6,3E12.5,I6)                                     -
C                                                                           -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                      -
CD    =======  ========================================================     -
CD    1-2      06                                                           -
CD                                                                          -
CD    13-18    NUCLIDE IDENTIFICATION LABEL ON LIBRARY.                     -
CD                                                                          -
CD    19-24    PROBLEM MATERIAL LABEL. THIS LABEL CAN BE ANY ALIAS          -
CD             NAME. IF COLS. 19-24 ARE BLANK, THE MATERIAL NAMED           -
CD             IN COLS. 13-18 WILL BE USED.                                 -
CD                                                                          -
CD    25-36    MATERIAL ATOMIC CONCENTRATION USED TO COMPUTE                -
CD             HOMOGENEOUS CROSS SECTIONS FOR USE IN THE                    -
CD             SPECTRUM CALCULATION (ATOMS/CC*1.E-24).                      -
CD                                                                          -
CD    37-48    MATERIAL TEMPERATURE IN DEGREES K (DEFAULT=300.).            -
CD                                                                          -
CD    49-60    EPSHET, USED TO DETERMINE NEAREST NEIGHBORING PLATE          -
CD             CONTAINING MATERIAL NAMED IN COLUMNS 13-18.IF A PLATE K-     -
CD             CONTAINS MATERIAL I, THEN NEIGHBORING PLATES ARE             -
CD             SEARCHED TO FIND THE NEAREST PLATE M WHICH SATISFIES         -
CD             THE CONDITION N(I,M)*DX(M).GE.EPSHET*N(I,K)*DX(K),           -
CD             WHERE N(I,M) IS THE ATOM DENSITY OF MATERIAL I IN            -
CD             PLATE M AND DX(M) IS THE THICKNESS OF PLATE M.               -
CD             (DEFAULT VALUE=0.1).                                         -
CD                                                                          -
CD    61-66    OUTPUT CROSS SECTION DATA SET FLAG. IF COLS. 61-66 ARE       -
CD             BLANK, THE MATERIAL NAMED IN COLS. 13-18 WILL BE ADDED       -
CD             TO THE OUTPUT CROSS SECTION DATA SET. IF COLS. 61-66         -
CD             ARE NON-BLANK, THE BROAD GROUP CROSS SECTIONS FOR THE        -
CD             MATERIAL NAMED WILL NOT BE CALCULTED AND HENCE NOT BE        -
CD             ADDED TO THE OUTPUT DATA SET.                                -
C                                                                           -
CN             ONE TYPE 06 CARD MUST BE GIVEN FOR EACH MATERIAL             -
CN             PRESENT IN THE MACROSCOPIC MIXTURE OF THE SPECTRUM           -
CN             COMPOSITION IF COLS. 37-42 ON CARD TYPE 03 ARE ZERO          -
CN             OR IF CARD TYPE 03 IS NOT SUPPLIED. IF NO TYPE 06 CARD       -
CN             IS GIVEN, THE MACROSCOPIC MIXTURE IS DERIVED FROM            -
CN             THE DATA ON THE A.NIP CARD TYPES 06, 14, AND 15. IN          -
CN             THIS CASE, ALL MATERIALS WILL BE ASSUMED TO HAVE A           -
CN             TEMPERATURE OF 300 DEGREES K AND LIBRARY NUCLIDE             -
CN             IDENTIFICATION LABELS WILL BE USED FOR THE PROBLEM           -
CN             MATERIAL LABELS. IF COLS. 25-36 ARE BLANK OR ZERO FOR        -
CN             ANY MATERIAL THE ATOMIC DENSITY FOR THAT MATERIAL            -
CN             IS DERIVED FROM THE A.NIP DATA FOR THE REGIONS               -
CN             ALTHOUGH MATERIAL LABELS AND TEMPERATURES WILL BE            -
 N             SET BY THE TYPE 06 DATA. ANY ATOMIC DENSITY WHICH IS         -
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
CN              GIVEN AS LESS THAN 1. E-20 WILL BE SET TO 1. E-20.      -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          EPI-THERMAL BROAD GROUP LETHARGY WIDTHS (TYPE 07)           -
C                                                                       -
CL    FORMAT-----(I2,10X,2(E12.5,I6,I6))                                -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    =======  ========================================================-
CD    1-2      07                                                       -
CD                                                                      -
CD    13-24    LETHARGY WIDTH.                                          -
CD                                                                      -
CD    25-30    INITIAL BROAD GROUP NUMBER.                              -
CD                                                                      -
CD    31-36    FINAL BROAD GROUP NUMBER.                                -
CD                                                                      -
CD    37-48    LETHARGY WIDTH.                                          -
CD                                                                      -
CD    49-54    INITIAL BROAD GROUP NUMBER.                              -
CD                                                                      -
CD    55-60    FINAL BROAD GROUP NUMBER.                                -
C                                                                       -
CN             SEE NOTES FOR THE TYPE 05 CARDS.                         -
CN             DATA SHOULD BE SUPPLIED FOR ONLY THE EPI-THERMAL         -
CN             GROUPS.  THUS, NO LETHARGY WIDTH SHOULD BE GIVEN         -
CN             FOR THE THERMAL GROUP.                                   -
CN             AS MANY TYPE 07 CARDS AS NECESSARY MAY BE USED.          -
CN             AS A MAXIMUM, THERE MAY BE AS MANY BROAD EPI-THERMAL     -
CN             GROUPS AS THERE ARE ULTRA FINE GROUPS IN THE LIBRARY.    -
CN             THE LETHARGY WIDTH SPECIFIED IN COLS. 13-24 IS USED      -
CN             FOR BROAD GROUPS SPECIFIED IN COLS. 25-30 THROUGH        -
CN             31-36. THE LETHARGY WIDTH SPECIFIED IN COLS. 37-48 IS    -
CN             USED FOR BROAD GROUPS SPECIFIED IN COLS. 49-54 THROUGH   -
CN             55-60. IF COLS. 25-30 OR 49-54 ARE BLANK, THE LETHARGY   -
CN             WIDTH SPECIFIED IN COLS. 13-24 OR 37-48 IS USED FOR ALL  -
CN             REMAINING BROAD GROUPS DOWN TO THE THE BOTTOM OF THE     -
CN             LIBRARY ENERGY STRUCTURE AND THE REST OF THE DATA ON     -
CN             THE TYPE 07 CARDS ARE IGNORED. IF NO TYPE 05 CARDS ARE   -
CN             SUPPLIED, THE BROAD GROUPS BEGIN AT THE TOP OF THE       -
CN             LIBRARY. IF AN UPPER ENERGY IS SPECIFIED ON A            -
CN             TYPE 05 CARD, THE BROAD GROUPS WILL EXTEND DOWN FROM     -
CN             THAT ENERGY. IF COLS. 31-36 AND/OR COLS. 55-60 ARE       -
CN             BLANK, THE VALUE SPECIFIED IN COLS. 13-24 AND/OR 37-48   -
CN             IS USED FOR THE BROAD GROUPS SPECIFIED IN COLS. 25-30     -
CN             AND/OR COLS. 49-54. LETHARGY WIDTHS SPECIFIED IN COLS.
CN             13-24 AND 37-48 ARE ADJUSTED TO CORRESPOND TO A
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
CN              MULTIPLE OF THE LIBRARY GROUP LETHARGY WIDTH.
C
C-----------------------------------------------------------------


C-----------------------------------------------------------------
CR          EXTERNAL SOURCE SPECIFICATIONS (TYPE 08)
C
CL    FORMAT-----(I2,10X,2(E12.5,2I6)) OR (I2,10X,E12.5,A6)
C
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY
CD    =======    ==================================================
CD    1-2        08
CD
CD    13-24      MAGNITUDE OF EXTERNAL SOURCE.
CD
CD    25-30      HIGHER ENERGY ULTRAFINE GROUP NUMBER TO WHICH SOURCE
CD               IN COLS. 13-24 APPLIES.
CD
CD    31-36      LOWER ENERGY ULTRAFINE GROUP NUMBER TO WHICH SOURCE
CD               IN COLS. 13-24 APPLIES.
CD
CD    37-48      MAGNITUDE OF EXTERNAL SOURCE.
CD
CD    49-54      HIGHER ENERGY ULTRAFINE GROUP NUMBER TO WHICH SOURCE
CD               IN COLS. 37-48 APPLIES.
CD
CD    55-60      LOWER ENERGY ULTRAFINE GROUP NUMBER TO WHICH SOURCE
CD               IN COLS. 37-48 APPLIES.
C
CN               IF COLS. 13-24 OF THE FIRST TYPE 08 CARD ARE BLANK OR
CN               ZERO THEN COLS. 25-30 OF THIS CARD MUST CONTAIN THE
CN               FISSION SPECTRUM NUCLIDE IDENTIFICATION LABEL ON THE
CN               LIBRARY (A6 FORMAT) SPECIFYING THE EXTERNAL SOURCE.
CN               THIS OPTION SHOULD BE USED WHEN A FISSION SPECTRUM
CN               SOURCE IS DESIRED FOR A PROBLEM WHICH CONTAINS NO
CN               FISSIONABLE NUCLIDES.  ALL OTHER TYPE 08 CARDS ARE
CN               NEGLECTED IF COLS. 13-24 OF THE FIRST TYPE 08 CARD
CN               ARE BLANK OR ZERO.
CN               IF COLS. 37-48 OR 49-54 ON ANY TYPE 08 CARD ARE BLANK
CN               OR ZERO, OR IF COLS. 13-24 OR 25-30 ON ANY TYPE 08 CARD
CN               AFTER THE FIRST ARE BLANK OR ZERO, THE REST OF THE
CN               TYPE 08 DATA ARE IGNORED.
CN               IF COLS. 25-30 ARE BLANK ON THE FIRST TYPE 08 CARD
CN               ENCOUNTERED, THE SOURCE SPECIFIED IN COLS.
CN               13-24 IS ASSIGNED TO ALL ULTRAFINE GROUPS AND THE REST
CN               OF THE CARD TYPE 08 DATA IS IGNORED. IF COLS. 31-36
CN               AND/OR 55-60 ARE BLANK, THE SOURCE VALUE GIVEN IN
 N               COLS. 13-24 AND/OR 37-48 APPLIES TO THE GROUP
 N               GIVEN IN COLS. 25-30 AND/OR 49-54. ANY GROUP NOT
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
CN              COVERED BY THIS DATA WILL BE ASSIGNED THE EXTERNAL      -
CN              SOURCE VALUE 0. AS MANY TYPE 08 CARDS AS NECESSARY MAY  -
CN              USED SPECIFY THE EXTERNAL SOUPCE DATA.                  -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          BUCKLING SPECIFICATIONS (TYPE 09)                           -
C                                                                       -
CL    FORMAT-----(I2,10X,3E12.5,2I6,E12.5)                              -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    =======    ========================================================-
CD    1-2        09                                                     -
CD                                                                      -
CD    13-24      INITIAL BUCKLING GUESS.                                -
CD                                                                      -
CD    25-36      SECOND BUCKLING GUESS.                                 -
CD                                                                      -
CD    37-48      CONVERGENCE CRITERION, EPS, FOR BUCKLING ITERATION     -
CD               TO KEFF=1. ABSOLUTE VALUE OF (KEFF-1.).LE.EPS.         -
CD                                                                      -
CD    49-54      HIGHER ENERGY ULTRAFINE GROUP NUMBER TO WHICH          -
CD               VALUES OF BUCKLING APPLY.                              -
CD                                                                      -
CD    55-60      LOWER ENERGY ULTRAFINE GROUP NUMBER TO WHICH           -
CD               VALUES OF BUCKLING APPLY.                              -
CD                                                                      -
CD    61-72      EXTENDED TRANSPORT APPROXIMATION BUCKLING, KAPPA       -
CD               SQUARED.                                               -
C                                                                       -
CN               AS MANY TYPE 09 CARDS MAY BE USED AS NECESSARY TO      -
CN               SPECIFY THE BUCKLING DATA. IF COLS. 49-54 ARE BLANK,   -
CN               THE BUCKLING DATA WILL BE ASSUMED TO BE GROUP          -
CN               INDEPENDENT. IF COLS. 55-60 ARE BLANK, THE             -
CN               DATA IN COLS. 13-24 WILL APPLY TO                      -
CN               THE ULTRAFINE GROUP GIVEN IN COLS. 49-54. IF COLS.     -
CN               61-72 ARE BLANK, THE BUCKLING GIVEN IN COLS. 13-24     -
CN               ON THE FIRST TYPE 09 CARD ENCOUNTERED WILL             -
CN               BE USED FOR KAPPA SQUARED. NOTE THAT THE SECOND        -
CN               BUCKLING GUESS IN COLS. 25-36 AND THE CONVERGENCE      -
CN               CRITERION IN COLS. 37-48 ARE PERTINENT ONLY FOR        -
CN               ENERGY INDEPENDENT BUCKLING PROBLEMS WHICH WILL        -
CN               ITERATE ON BUCKLING TO KEFF=1. IF COLS. 37-48 ARE BLANK-
CN               OR ZERO, THE SECOND BUCKLING GUESS IS IGNORED AND NO   -
CN               BUCKLING ITERATION IS PERFORMED. COLS. 25-48 WILL      -
CN               BE IGNORED IF COLS. 49-54 ARE NON-BLANK.               -
CN               ANY GROUP NOT COVERED BY THIS DATA WILL BE ASSIGNED    -
CN               THE BUCKLING VALUE 0.
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
CN              COLS. 61-72 ARE IGNORED AFTER READING THE FIRST
CN              TYPE 09 CARD.
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          THERMAL GROUP CROSS SECTION DATA (TYPE 10)
C
CL    FORMAT-----(I2,4X,A6,5E12.5)
C
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY
CD    =======   ==================================================
CD    1-2       10
CD
CD    7-12      NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY
CD              (COLS. 13-18 ON TYPE 06 CARDS).
CD
CD    13-24     MICROSCOPIC THERMAL GROUP CAPTURE CROSS SECTION (BARNS)
CD
CD    25-36     MICROSCOPIC THERMAL GROUP FISSION CROSS SECTION (BARNS)
CD
CD    37-48     NUMBER OF NEUTRONS EMITTED PER FISSION IN THE
CD              THERMAL GROUP.
CD
CD    49-60     MICROSCOPIC THERMAL GROUP TOTAL CROSS SECTION (BARNS).
CD
CD    61-72     THERMAL GROUP AVERAGE RECIPROCAL VELOCITY (SEC/CM)
CD              (DEFAULT=1./2.2E+5).
C
CN              AS MANY TYPE 10 CARDS ARE USED AS NECESSARY TO
CN              SPECIFY THE THERMAL GROUP VALUES. ANY MATERIAL NOT
CN              SPECIFIED ON A TYPE 10 CARD WILL BE ASSIGNED THERMAL
CN              GROUP CROSS SECTIONS EQUAL TO THE LAST EPI-THERMAL
CN              GROUP VALUES.
CN              THE FIRST POSITIVE VALUE ENCOUNTERED IN COLS. 61-72
CN              OF ANY TYPE 10 CARD WILL BE USED FOR THE AVERAGE
CN              THERMAL GROUP RECIPROCAL VELOCITY. THE THERMAL GROUP
CN              VELOCITY IS NOT MATERIAL DEPENDENT.
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          AUXILIARY THERMAL GROUP CROSS SECTION DATA (TYPE 11)
C
CL    FORMAT-----(I2,4X,A6,5E12.5)
C
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY
CD    =======   ==================================================
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
CD     1-2         11                                                    -
CD                                                                       -
CD     7-12        NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY           -
CD                 (COLS. 13-18 ON TYPE 06 CARDS).                       -
CD                                                                       -
CD     13-24       MICROSCOPIC THERMAL GROUP N-ALPHA CROSS SECTION (BARNS)-
CD                                                                       -
CD     25-36       MICROSCOPIC THERMAL GROUP N-P CROSS SECTION (BARNS).  -
CD                                                                       -
CD     37-48       MICROSCOPIC THERMAL GROUP N-D CROSS SECTION (BARNS).  -
CD                                                                       -
CD     49-60       MICROSCOPIC THERMAL GROUP N-H3 CROSS SECTION (BARNS). -
CD                                                                       -
CD     61-72       MICROSCOPIC THERMAL GROUP N-HE3 CROSS SECTION (BARNS). -
C                                                                        -
CN                 AS MANY TYPE 11 CARDS ARE USED AS NECESSARY TO        -
CN                 SPECIFY THE AUXILIARY THERMAL GROUP DATA. ANY MATERIAL -
CN                 NOT SPECIFIED ON A TYPE 11 CARD WILL BE ASSIGNED      -
CN                 THERMAL GROUP CROSS SECTIONS EQUAL TO THE LAST        -
CN                 EPI-THERMAL GROUP VALUES.                             -
C                                                                        -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR           RESONANCE HETEROGENEITY SPECIFICATIONS (TYPE 12)            -
C                                                                        -
CL     FORMAT-----(I2,4X,A6,5(2A6))                                      -
C                                                                        -
CD     COLUMNS              CONTENTS...IMPLICATIONS, IF ANY              -
CD     =======    ==========================================================-
CD     1-2         12                                                    -
CD                                                                       -
CD     7-12        NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY           -
CD                 (COLS. 13-18 ON TYPE 06 CARDS OR IF NO TYPE 06 CARDS  -
CD                 ARE SUPPLIED, COLS. 19-24, 37-42, AND 55-60 ON DATA   -
CD                 SET A.NIP TYPE 14 CARDS).                             -
CD                                                                       -
CD     13-18       REGION LABEL.                                         -
CD                                                                       -
CD     19-24       REGION LABEL.                                         -
CD                                                                       -
CD     25-30       REGION LABEL.                                         -
CD                                                                       -
CD     31-36       REGION LABEL.                                         -
CD                                                                       -
CD     37-42       REGION LABEL.                                         -
CD                                                                       -
CD     43-48       REGION LABEL.
CD
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
CD     49-54      REGION LABEL.                                          -
CD                                                                       -
CD     55-60      REGION LABEL.                                          -
CD                                                                       -
CD     61-66      REGION LABEL.                                          -
CD                                                                       -
CD     67-72      REGION LABEL.                                          -
C                                                                        -
CN                MATERIALS NOT SPECIFIED ON THE TYPE 12 CARDS WILL      -
CN                RECEIVE A HOMOGENEOUS RESONANCE TREATMENT.             -
CN                FOR CYLINDRICAL GEOMETRY (NGEOM=2) ONLY COLS. 1-2      -
CN                AND 7-12 ARE PERTINENT. MATERIALS NAMED                -
CN                IN COLS. 7-12 WILL RECEIVE A RESONANCE HETEROGENEITY   -
CN                TREATMENT IN THE CENTRAL PIN REGION OF THE CYLINDRICAL -
CN                CELL IF THEY ARE PRESENT IN THE PIN REGION AND IF      -
CN                THEY ARE RESONANCE MATERIALS.                          -
CN                FOR SLAB GEOMETRY (NGEOM=1) ONE OR MORE                -
CN                TYPE 12 CARDS ARE SUPPLIED FOR EACH MATERIAL           -
CN                NAMED IN COLS. 7-12 WHICH IS TO RECEIVE                -
CN                A RESONANCE HETEROGENEITY TREATMENT. IF MORE THAN      -
CN                ONE CARD IS NEEDED FOR A GIVEN MATERIAL, THE MATERIAL  -
CN                LABEL IS REPEATED ON EACH CARD. THE REGION LABELS      -
CN                APPEAR IN PAIRS STARTING WITH THE PAIR IN COLS. 13-18  -
CN                AND 19-24. IF COLS. 13-18 ARE BLANK, THE REST OF THE   -
CN                DATA ON THE CARD IS IGNORED AND THE MATERIAL NAMED     -
CN                IN COLS. 7-12 WILL BE TREATED HETEROGENEOUSLY          -
CN                IN ALL REGIONS IN WHICH IT APPEARS. REGIONS NAMED IN   -
CN                COLS. 13-18, 25-30, 37-42, 49-54, AND 61-66 INDICATE  -
CN                REGIONS IN WHICH THE MATERIAL IS NOT TO BE TREATED     -
CN                HETEROGENEOUSLY. IF ANY OF THESE COLUMNS ARE BLANK,    -
CN                THE REST OF THE DATA ON THE CARD IS IGNORED.           -
CN                IF COLUMNS 19-24, 31-36, 43-48, 55-60,                 -
CN                OR 67-72 ARE NON-BLANK, THEN THE MATERIAL WILL         -
CN                RECEIVE THE SAME TREATMENT IN THE REGION NAMED IN      -
CN                COLS. 13-18 AS IN THE REGION NAMED IN COLS. 19-24, THE -
CN                SAME IN REGION 25-30 AS IN THE REGION 31-36, ETC.      -
CN                NO REGION NAMED IN COLS. 19-24, 31-36, 43-48, 55-60,   -
CN                OR 67-72 MAY BE NAMED IN COLS. 13-18, 25-30, 36-42     -
CN                46-54, OR 61-66.                                       -
CN                AS AN EXAMPLE, LET MATERIAL M1 APPEAR IN REGIONS       -
CN                R1, R2, R3, R4, AND R5. IF M1 IS TO BE TREATED         -
CN                HOMOGENEOUSLY IN REGIONS R2 AND R5 AND IF IT IS        -
CN                TO RECEIVE THE SAME HETEROGENEITY TREATMENT IN REGION  -
CN                R1 AS IN R3, THEN CARD TYPE 12 WOULD CONTAIN THE       -
CN                FOLLOWING:                                             -
CN                COLUMNS       CONTENTS                                 -
CN                -------       --------                                 -
CN                  1-2           12                                   -
CN                  7-12          M1                                   -
CN                  13-18         R2                                   -
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
CN              19-24                          (BLANK)                  -
CN              25-30          R5                                       -
CN              31-36                          (BLANK)                  -
CN              37-42          R1                                       -
CN              43-48          R3                                       -
CN              49-54                          (BLANK)                  -
CN            SINCE REGION R4 IS NOT MENTIONED, MATERIAL M1 WILL         -
CN            BE TREATED HETEROGENEOUSLY IN REGION R4. SINCE COLS.       -
CN            49-54 ARE BLANK, THE REST OF THE DATA, IF ANY, ON THE      -
CN            CARD ARE IGNORED.                                          -
CN            THE RESONANCE REGION MODULES WILL NOT GENERATE             -
CN            RESONANCE CROSS SECTIONS FOR MATERIAL M1 IN REGION R1      -
CN            BUT WILL GENERATE RESONANCE CROSS SECTIONS FOR             -
CN            MATERIAL M1 IN REGION R3.                                  -
CN            NOTE THAT ANY MATERIAL IN A GIVEN REGION WHICH IS          -
CN            EITHER TO RECEIVE A HOMOGENEOUS TREATMENT OR IS TO         -
CN            RECEIVE THE SAME HETEROGENEOUS TREATMENT AS IN SOME        -
CN            OTHER REGION WILL NOT HAVE ANY RESONANCE OVERLAP           -
CN            INFLUENCE ON ANY OTHER RESONANCE MATERIALS IN THE          -
CN            REGION IN QUESTION.                                        -
C                                                                        -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR          INTEGRAL TRANSPORT SPECIFICATIONS (TYPE 14)                  -
C                                                                        -
CL    FORMAT-----(I2,10X,2E12.5,4I6)                                     -
C                                                                        -
CD    COLUMNS            CONTENTS...IMPLICATIONS, IF ANY                 -
CD    =======    ========================================================-
CD    1-2        14                                                      -
CD                                                                       -
CD    13-24      ENERGY AT WHICH INTEGRAL TRANSPORT THEORY TREATMENT     -
CD               BEGINS. (DEFAULT=300.0 EV).                             -
CD                                                                       -
CD    25-36      CRITERION USED FOR TESTING FOR INCLUSION OF RESONANCES  -
CD               FOR HYPER FINE GROUPS WITHIN AN INTERMEDIATE GROUP      -
CD               (DEFAULT=0.05). A 0.0 MUST BE SPECIFIED IN COLS.        -
CD               25-36 IF ALL RESONANCES ARE TO BE INCLUDED.             -
CD                                                                       -
CD    37-42      NUMBER OF ULTRA FINE GROUPS PER INTERMEDIATE GROUP      -
CD               (DEFAULT=2).                                            -
CD                                                                       -
CD    43-48      NUMBER OF HYPER FINE GROUPS PER DOPPLER WIDTH           -
CD               (DEFAULT=4).                                            -
CD                                                                       -
CD    49-54      TRANSVERSE LEAKAGE OPTION.                              -
CD               0...OMIT TRANSVERSE LEAKAGE CORRECTION (DEFAULT).       -
CD               1...INCLUDE TRANSVERSE LEAKAGE CORRECTION USING THE
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
CD                BUCKLING SPECIFIED IN COLS. 61-72 ON THE TYPE 09   -
CD                CARD.                                              -
CD                                                                   -
CD    55-60       INGROUP SCATTERING OPTION.                         -
CD                0...INCLUDE INGROUP SCATTERING (DEFAULT).          -
CD                1...OMIT INGROUP SCATTERING.                       -
C                                                                    -
CN                IF INVOKED BY THE PATH DRIVER, RESOLVED RESONANCE BROAD-
CN                GROUP CROSS SECTIONS WILL BE RECOMPUTED USING      -
CN                INTEGRAL TRANSPORT THEORY ALGORITHMS FOR ALL BROAD -
CN                GROUPS WHOSE LOWER ENERGIES ARE .LT. THE VALUE     -
CN                SPECIFIED.  THE INTERMEDIATE GROUPS ARE USED TO    -
CN                DETERMINE WHICH RESONANCES ARE TO BE INCLUDED FOR THE -
CN                HYPER FINE GROUPS CONTAINED IN THAT INTERMEDIATE GROUP -
CN                USING THE CRITERION SPECIFIED IN COLS. 25-36.       -
CN                THE CODE WILL ADJUST THE HYPER FINE GROUP WIDTH TO BE -
CN                AN INTEGRAL SUB-MULTIPLE OF THE ULTRA FINE GROUP WIDTH -
CN                WITH A MAXIMUM HYPER FINE GROUP WIDTH OF 0.001.    -
CN                IF COLS. 43-48 ARE NEGATIVE, A CONSTANT HYPER FINE -
CN                GROUP WIDTH IS USED FOR ALL BROAD GROUPS BASED ON THE -
CN                ABSOLUTE VALUE OF THE QUANTITY GIVEN IN COLS. 43-48. -
CN                IF THE PATH INVOKES AREA 10, THE PROBLEM MIXTURE MUST -
CN                CONTAIN MATERIALS HAVING RESOLVED RESONANCES.       -
C                                                                    -
C--------------------------------------------------------------------

C--------------------------------------------------------------------
CR          FOIL SPECIFICATIONS (TYPE 15)                            -
C                                                                    -
CL    FORMAT-----(I2,4X,A6,2(A6,E12.5),2E12.5)                       -
C                                                                    -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY               -
CD    =======    ==================================================-
CD    1-2        15                                                 -
CD                                                                   -
CD    7-12       FOIL IDENTIFICATION LABEL.                         -
CD                                                                   -
CD    13-18      NUCLIDE IDENTIFICATION IN THE LIBRARY.             -
CD                                                                   -
CD    19-30      NUCLIDE ATOMIC DENSITY (ATOMS/CC*1.E-24).          -
CD                                                                   -
CD    31-36      NUCLIDE IDENTIFICATION IN THE LIBRARY.             -
CD                                                                   -
CD    37-48      NUCLIDE ATOMIC DENSITY (ATOMS/CC*1.E-24).          -
CD                                                                   -
CD    49-60      FOIL THICKNESS IN CM.                              -
CD                                                                   -
CD    61-72      FOIL TEMPERATURE IN DEGREES K. (DEFAULT=300.0).    -
 D                                                                   -
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
C                                                                       -
CN              AS MANY TYPE 15 CARDS MAY BE USED AS NECESSARY TO       -
CN              SPECIFY THE FOILS.  IF MORE THAN ONE TYPE 15 CARD IS    -
CN              NEEDED TO SPECIFY A PARTICULAR FOIL, THE FOIL LABEL     -
CN              MUST BE REPEATED IN COLS. 7-12 ON SUBSEQUENT CARDS.     -
CN              COLS. 49-72 ARE PERTINENT ONLY FOR THE FIRST TYPE 15    -
CN              CARD FOR A GIVEN FOIL.  ALL FOILS SPECIFIED ON TYPE 15  -
CN              CARDS WILL BE EDITED AT EACH MESH INTERVAL BOUNDARY AS  -
CN              SPECIFIED ON THE DATA SET A.NIP TYPE 06 CARDS FOR       -
CN              HETEROGENEOUS PROBLEMS, OR FOR THE HOMOGENEOUS SPECTRUM-
CN              FOR HOMOGENEOUS PROBLEMS WHEN RESOLVED RESONANCE CROSS -
CN              SECTIONS ARE RECOMPUTED USING INTEGRAL TRANSPORT        -
CN              THEORY.                                                 -
CN              IF THE PATH INVOKES AREA 10, THE PROBLEM MIXTURE MUST   -
CN              CONTAIN MATERIALS HAVING RESOLVED RESONANCES.           -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          FISSION SPECTRUM SPECIFICATIONS (TYPE 16)                   -
C                                                                       -
CL    FORMAT-----(I2,4X,11A6)                                           -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    =======   ========================================================-
CD    1-2       16                                                      -
CD                                                                      -
CD    7-12      FISSION SPECTRUM NUCLIDE IDENTIFICATION LABEL ON        -
CD              THE LIBRARY.                                            -
CD                                                                      -
CD    13-18     FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY-
CD                                                                      -
CD    19-24     FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY-
CD                                                                      -
CD    25-30     FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY-
CD                                                                      -
CD    31-36     FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY-
CD                                                                      -
CD    37-42     FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY-
CD                                                                      -
CD    43-48     FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY-
CD                                                                      -
CD    49-54     FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY-
CD                                                                      -
CD    55-60     FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY-
CD                                                                      -
CD    61-66     FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY-
CD
CD    67-72     FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
C                                                                       -
CN              IF NO TYPE 16 CARDS ARE GIVEN, THE FISSION SPECTRUM     -
CN              WILL BE OBTAINED FROM A MIXTURE OF ALL SPECTRA          -
CN              REPRESENTED BY THE MATERIALS PRESENT IN THE SPECTRUM    -
CN              COMPOSITION. THE FISSION SPECTRUM SPECIFIED IN          -
CN              COLS. 7-12 WILL BE USED FOR THE FISSIONABLE NUCLIDES    -
CN              SPECIFIED IN COLS. 13-18,19-24,ETC. IF COLS. 13-18 OF   -
CN              ANY TYPE 16 CARD ARE BLANK, THE REST OF THAT TYPE 16    -
CN              CARD IS IGNORED AND THE FISSION SPECTRUM SPECIFIED IN    -
CN              COLS. 7-12 WILL BE USED FOR ANY FISSIONABLE NUCLIDES    -
CN              NOT SPECIFIED ON OTHER TYPE 16 CARDS. ONLY ONE TYPE 16  -
CN              CARD WITH A BLANK FIELD IN COLS. 13-18 IS PERMITTED.    -
CN              IF NO SUCH CARD IS GIVEN ANY FISSIONABLE                -
CN              NUCLIDE NOT SPECIFIED ON A TYPE 16 CARD WILL BE         -
CN              ASSIGNED ITS OWN FISSION SPECTRUM. AS MANY TYPE 16      -
CN              CARDS AS NECESSARY MAY BE USED. THE FISSION SPECTRUM    -
CN              IDENTIFICATION LABEL SHOULD BE REPEATED ON              -
CN              ADDITIONAL CARDS. COLS. 13-18, 19-24, ETC. SHOULD       -
CN              CONTAIN LABELS CORRESPONDING TO LABELS IN COLS. 13-18   -
CN              OF THE TYPE 06 CARDS.                                   -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          UNRESOLVED RESONANCE FIXED ENERGY MESH (TYPE 17)            -
C                                                                       -
CL    FORMAT-----(I2,10X,2(E12.5,I6,I6))                                -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    =======    ========================================================-
CD    1-2        17                                                     -
CD                                                                      -
CD    12-24      LETHARGY WIDTH.                                        -
CD                                                                      -
CD    25-30      INITIAL FIXED MESH POINT NUMBER.                       -
CD                                                                      -
CD    31-36      FINAL FIXED MESH POINT NUMBER.                         -
CD                                                                      -
CD    37-48      LETHARGY WIDTH.                                        -
CD                                                                      -
CD    49-54      INITIAL FIXED MESH POINT NUMBER.                       -
CD                                                                      -
CD    55-60      FINAL FIXED MESH POINT NUMBER.                         -
C                                                                       -
CN              A MAXIMUM OF 500 FIXED ENERGY MESH POINTS MAY BE USED.  -
CN              AS MANY TYPE 17 CARDS AS NECESSARY MAY BE USED. IF NO   -
CN              TYPE 17 CARD IS SUPPLIED, THE BUILT IN FIXED ENERGY     -
 I              MESH STRUCTURE IS USED. THE LETHARGY WIDTH SPECIFIED    -
 I              IN COLS. 12-24 IS USED FOR POINTS SPECIFIED IN COLS.    -
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
CN              25-30 THROUGH 31-36. THE LETHARGY WIDTH SPECIFIED       -
CN              IN COLS. 37-48 IS USED FOR POINTS SPECIFIED IN COLS.    -
CN              49-54 THROUGH 55-60. IF COLS. 25-30 OR 49-54 ARE BLANK,-
CN              THE LETHARGY WIDTH SPECIFIED IN COLS. 12-24 OR 37-48 IS-
CN              USED FOR ALL REMAINING POINTS                           -
CN              AND THE REST OF THE DATA ON THE TYPE 17                 -
CN              CARDS ARE IGNORED. THE FIXED ENERGY MESH COVERS THE     -
CN              ENTIRE ENERGY RANGE AS SPECIFIED ON THE TYPE 05 CARDS. -
CN              IF COLS. 31-36 AND/OR COLS. 55-60 ARE BLANK, THE        -
CN              VALUE SPECIFIED IN COLS. 12-24 AND/OR COLS. 37-48 IS    -
CN              USED FOR THE MESH POINT SPECIFIED IN COLS. 25-30 AND/OR-
CN              COLS. 49-54.                                            -
C                                                                       -
C---------------------------------------------------------------------

C---------------------------------------------------------------------
CR          HOMOGENEOUS INFINITELY DILUTE SPECIFICATIONS (TYPE 18)      -
C                                                                       -
CL    FORMAT-----(I2,4X,11A6)                                           -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    =======  ========================================================-
CD    1-2      18                                                       -
CD                                                                      -
CD    7-12     NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY              -
CD             (COLS. 13-18 ON TYPE 06 CARDS).                          -
CD                                                                      -
CD    13-18    NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY              -
CD             (COLS. 13-18 ON TYPE 06 CARDS).                          -
CD                                                                      -
CD    19-24    NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY              -
CD             (COLS. 13-18 ON TYPE 06 CARDS).                          -
CD                                                                      -
CD    25-30    NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY              -
CD             (COLS. 13-18 ON TYPE 06 CARDS).                          -
CD                                                                      -
CD    31-36    NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY              -
CD             (COLS. 13-18 ON TYPE 06 CARDS).                          -
CD                                                                      -
CD    37-42    NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY              -
CD             (COLS. 13-18 ON TYPE 06 CARDS).                          -
CD                                                                      -
CD    43-48    NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY              -
CD             (COLS. 13-18 ON TYPE 06 CARDS).                          -
CD                                                                      -
CD    49-54    NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY              -
CD             (COLS. 13-18 ON TYPE 06 CARDS).                          -
CD
CD    55-60    NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
CD              (COLS. 13-18 ON TYPE 06 CARDS).                          -
CD                                                                       -
CD     61-66    NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY              -
CD              (COLS. 13-18 ON TYPE 06 CARDS).                          -
CD                                                                       -
CD     67-72    NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY              -
CD              (COLS. 13-18 ON TYPE 06 CARDS).                          -
C                                                                        -
CN              MATERIALS NAMED ON THE TYPE 18 CARDS WILL BE ASSUMED     -
CN              TO BE INFINITELY DILUTE FOR THE HOMOGENEOUS RESOLVED     -
CN              RESONANCE CALCULATION.  MATERIALS WHICH ARE ASSUMED TO   -
CN              BE INFINITELY DILUTE WILL NOT BE INVOLVED IN THE         -
CN              OVERLAP CALCULATION FOR ANY OTHER MATERIAL.              -
CN              THEIR RESONANCE INTEGRALS WILL BE SET TO THE             -
CN              INFINITELY DILUTE LIMIT OF PI/(2.*BETA).                 -
CN              SEE CARD TYPE 12 FOR THE HETEROGENEOUS SPECIFICATIONS.   -
C                                                                        -
C--------------------------------------------------------------------------

C--------------------------------------------------------------------------
CR          RESONANCE EDIT OPTIONS (TYPE 19)                             -
C                                                                        -
CL    FORMAT-----(I2,4X,6I6)                                             -
C                                                                        -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                   -
CD    =======    ==================================================      -
CD    1-2        19                                                      -
CD                                                                       -
CD    7-12       DATA SET UNRES EDIT FLAG.                               -
CD                                                                       -
CD    13-18      DATA SET ATNUAT EDIT FLAG.                              -
CD                                                                       -
CD    19-24      DATA SET RESINT EDIT FLAG.                              -
CD                                                                       -
CD    25-30      DATA SET SIGMAP EDIT FLAG.                              -
CD                                                                       -
CD    31-36      DATA SET LORENZ EDIT FLAG.                              -
CD                                                                       -
CD    37-42      BROAD GROUP RESONANCE CROSS SECTION FLAG.               -
CD               0...INCLUDE RESONANCE CROSS SECTIONS IN THE BROAD GROUP  -
CD                   CROSS SECTIONS (DEFAULT).                           -
CD               1...OMIT ALL RESONANCE CROSS SECTIONS FROM THE BROAD     -
CD                   GROUP CROSS SECTIONS.                               -
CD               2...OMIT RESONANCE CAPTURE AND FISSION CROSS SECTIONS    -
CD                   FROM THE BROAD GROUP CROSS SECTIONS.                -
C                                                                        -
CN               EACH DATA SET WHOSE EDIT FLAG IS NON-ZERO WILL BE       -
 N               EDITED. OTHERWISE IT WILL NOT BE EDITED.                -
                                                                         -
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          GENERAL PROBLEM EDIT OPTIONS (TYPE 20)                 -
C                                                                  -
CL    FORMAT-----(I2,4X,6I6)                                       -
C                                                                  -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY             -
CD    =======   ========================================================-
CD    1-2       20                                                 -
CD                                                                 -
CD    7-12      ULTRA-FINE-GROUP MACROSCOPIC FISSION, TOTAL, TRANSPORT -
CD              AND SCATTERING CROSS SECTIONS.                     -
CD              0...DO NOT EDIT DATA (DEFAULT).                    -
CD              1...EDIT DATA.                                     -
CD                                                                 -
CD    13-18     ULTRA-FINE-GROUP MACROSCOPIC MODERATING PARAMETERS. -
CD              0...DO NOT EDIT DATA (DEFAULT).                    -
CD              1...EDIT DATA.                                     -
CD                                                                 -
CD    19-24     ULTRA-FINE-GROUP MICROSCOPIC PL SCATTERING CROSS   -
CD              SECTIONS, P0 AND P1 ELASTIC TRANSFER MATRICES.     -
CD              0...DO NOT EDIT DATA (DEFAULT).                    -
CD              N...EDIT DATA AT ULTRA-FINE-GROUPS 1,N+1,2*N+1,... -
CD                                                                 -
CD    25-30     ULTRA-FINE-GROUP SPECTRUM.                         -
CD              0...EDIT DATA (DEFAULT).                           -
CD              1...DO NOT EDIT DATA.                              -
CD                                                                 -
CD    31-36     BROAD GROUP RESONANCE CROSS SECTION EDIT FLAG.     -
CD              0...DO NOT EDIT DATA (DEFAULT).                    -
CD              1...EDIT DATA.                                     -
CD                                                                 -
CD    37-42     BROAD GROUP REACTION RATE EDIT FLAG.               -
CD              0...EDIT DATA.                                     -
CD              1...DO NOT EDIT DATA.                              -
C                                                                  -
CN              COLS. 19-24 SHOULD ROUTINELY BE SET AT ZERO (DEFAULT) -
CN              AS THE EDIT OF TRANSFER MATRICES PRODUCES A GREAT  -
CN              DEAL OF PAPER OUTPUT.                              -
C                                                                  -
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          COMPOSITION TEMPERATURES (TYPE 21)                     -
C                                                                  -
CL    FORMAT-----(I2,10X,3(A6,E12.5))                              -
C
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
CD     COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                -
CD     =======   ========================================================-
CD     1-2       21                                                     -
CD                                                                      -
CD     13-18     COMPOSITION LABEL.                                     -
CD                                                                      -
CD     19-30     TEMPERATURE IN DEGREES K (DEFAULT=300.0).              -
CD                                                                      -
CD     31-36     COMPOSITION LABEL.                                     -
CD                                                                      -
CD     37-48     TEMPERATURE IN DEGREES K (DEFAULT=300.0).              -
CD                                                                      -
CD     49-54     COMPOSITION LABEL.                                     -
CD                                                                      -
CD     55-66     TEMPERATURE IN DEGREES K (DEFAULT=300.0).              -
C                                                                       -
CN               AS MANY TYPE 21 CARDS AS NECESSARY MAY BE USED TO      -
CN               SPECIFY THE COMPOSITION TEMPERATURES.                  -
CN               COMPOSITION LABELS IN COLS. 13-18, 31-36, AND 49-54    -
CN               MUST CORRESPOND TO LABELS GIVEN IN COLS. 13-18 ON DATA -
CN               SET A.NIP TYPE 14 CARDS.  THE COMPOSITION TEMPERATURES -
CN               ARE USED ONLY FOR THE INTEGRAL TRANSPORT THEORY        -
CN               CALCULATIONS.                                          -
CN               IN THE CASE OF HOMOGENEOUS PROBLEMS FOR WHICH COLS.    -
CN               37-42 ON THE TYPE 03 CARD ARE ZERO, THE TEMPERATURE    -
CN               USED FOR AN INTEGRAL TRANSPORT THEORY CALCULATION WILL -
CN               BE THE VALUE SPECIFIED IN COLS 19-30 ON THE FIRST      -
CN               TYPE 21 CARD PROVIDED.  IF NO TYPE 21 CARDS ARE GIVEN, -
CN               THE TEMPERATURE FOR A HOMOGENEOUS PROBLEM WILL BE THAT -
CN               SPECIFIED ON THE TYPE 06 CARD FOR THE FIRST MATERIAL   -
CN               AFTER THE INPUT IS REORDERED TO CORRESPOND TO THE      -
CN               ORDER OF MATERIALS IN THE LIBRARY.                     -
CN               IF THE PATH INVOKES AREA 10, THE PROBLEM MIXTURE MUST  -
CN               CONTAIN MATERIALS HAVING RESOLVED RESONANCES.          -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          ISOTOPE IDENTIFICATION (TYPE 22)                           -
C                                                                       -
CL     FORMAT-----(I2,10X,A6,I6,2E12.5)                                -
C                                                                       -
CD     COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                -
CD     =======   ========================================================-
CD     1-2       22                                                     -
CD                                                                      -
CD     13-18     NUCLIDE IDENTIFICATION LABEL ON LIBRARY.               -
CD                                                                      -
       19-24     ISOTOPE CLASSIFICATION.                                -
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
CD              0...UNDEFINED (DEFAULT).
CD              1...FISSILE.
CD              2...FERTILE.
CD              3...OTHER ACTINIDE.
CD              4...FISSION PRODUCT.
CD              5...STRUCTURAL.
CD              6...COOLANT.
CD              7...CONTROL.
CD
CD    25-36     TOTAL THERMAL ENERGY YIELD/FISSION (MEV/FISSION).
CD
CD    37-48     TOTAL THERMAL ENERGY YIELD/CAPTURE (MEV/CAPTURE).
C
CN              IF COLS. 25-36 OR 37-48 ARE BLANK, THE CORRESPONDING
CN              DATA IS OBTAINED FROM DATA SET MCC2F1.
C
C---------------------------------------------------------------------

C---------------------------------------------------------------------
CR          FISSION SPECTRA TEMPERATURES (TYPE 23)
C
CL    FORMAT-----(I2,4X,3(A6,E12.5))
C
CD    COLUMNS           CONTENTS...IMPLICATIONS, IF ANY
CD    =======   ==========================================================
CD    1-2       23
CD
CD    7-12      NUCLIDE IDENTIFICATION LABEL ON LIBRARY.
CD
CD    13-24     FISSION SPECTRUM TEMPERATURE, E.V.
CD
CD    25-30     NUCLIDE IDENTIFICATION LABEL ON LIBRARY.
CD
CD    31-42     FISSION SPECTRUM TEMPERATURE, E.V.
CD
CD    43-48     NUCLIDE IDENTIFICATION LABEL ON LIBRARY.
CD
CD    49-60     FISSION SPECTRUM TEMPERATURE, E.V.
C
CN              NOTE THAT THE TYPE 23 DATA ARE PERTINENT ONLY FOR
CN              FISSIONABLE ISOTOPES.
CN              THE TEMPERATURES ON THE TYPE 23 CARDS ARE USED TO
CN              OVERRIDE THE CORRESPONDING TEMPERATURES OF PROBLEM
CN              MATERIALS ON THE LIBRARY FOR USE IN GENERATING
CN              FISSION SPECTRA.  IF AN EXTERNAL SOURCE IS SPECIFIED
CN              SUCH THAT ON THE TYPE 08 CARD COLS. 13-24 ARE BLANK
CN              AND COLS. 25-30 CONTAIN THE FISSION SPECTRUM NUCLIDE
CN              IDENTIFICATION LABEL ON THE LIBRARY, THEN THAT LABEL
CN              AND THE CORRESPONDING LABEL IN COLS. 7-12 ON THE TYPE
```

APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

```
CN              23 CARD NEED NOT CORRESPOND TO ONE OF THE PROBLEM       -
CN              MATERIALS.  ANY LIBRARY MATERIAL NOT REFERENCED         -
CN              ON THE TYPE 23 CARDS WILL USE THE LIBRARY SPECIFIED     -
CN              FISSION SPECTRUM TEMPERATURE.                           -
CN              IF COLS. 7-12, 25-30, OR 43-48 ARE BLANK ON ANY TYPE    -
CN              23 CARD, THE REST OF ANY SUPPLIED TYPE 23 DATA WILL BE  -
CN              IGNORED.                                                -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX B. MC^2-2 BCD Input Files. A.NIP

```
C*****************************************************************
C                                                                -
C                        PREPARED 6/13/75 AT ANL                 -
C                                                                -
CF          A.NIP                                                -
CE          BCD INPUT FOR HETEROGENEOUS MC**2-II AND SDX CALCULATIONS -
C                                                                -
CN                       THIS IS A USER-SUPPLIED BCD DATA SET. IT IS -
CN                       AN ABBREVIATED VERSION OF THE DATA SET  -
CN                       A.NIP.                                  -
CN                       THE LIST FOR EACH RECORD IS GIVEN IN TERMS OF -
CN                       THE BCD FORMAT OF THE DATA CARD.        -
CN                       COLUMNS 1 2 CONTAIN THE CARD TYPE NUMBER. -
C                                                                -
C*****************************************************************


C----------------------------------------------------------------
CR          EXTERNAL BOUNDARY CONDITIONS (TYPE 04)               -
C                                                                -
CL    FORMAT-----(I2,10X,216)                                    -
C                                                                -
CD    COLUMNS            CONTENTS...IMPLICATIONS, IF ANY         -
CD    =======    ========================================================-
CD    1-2        04                                             -
CD                                                               -
CD    13-18      BOUNDARY CONDITION AT LOWER "X" BOUNDARY OF CELL. -
CD                                                               -
CD    19-24      BOUNDARY CONDITION AT UPPER "X" BOUNDARY OF CELL. -
CD                                                               -
CD               10...REFLECTIVE.                                -
CD               11...PERIODIC.                                  -
CD               12...WHITE.                                     -
CD                                                               -
CN               THE LEFT BOUNDARY CONDITION MUST BE REFLECTIVE AND -
CN               THE RIGHT BOUNDARY CONDITION MUST BE WHITE FOR  -
CN               CYLINDRICAL GEOMETRY.  THE LEFT AND RIGHT BOUNDARY -
CN               CONDITIONS MUST BE THE SAME AND MAY BE ONLY REFLECTIVE -
CN               OR PERIODIC FOR SLAB GEOMETRIES.                -
C                                                                -
C----------------------------------------------------------------


C----------------------------------------------------------------
CR          REGION BOUNDARY COORDINATES AND MESH STRUCTURE       -
CR          (TYPE 06)                                            -
C                                                                -
CL    FORMAT-----(I2,4X,A6,2E12.5,I6)                            -
C                                                                -
CD    COLUMNS            CONTENTS...IMPLICATIONS, IF ANY         -
```

APPENDIX B. MC^2-2 BCD Input Files. A.NIP (Contd.)

```
CD     =======   ==================================================-
CD     1-2       06                                                -
CD                                                                 -
CD     7-12      REGION LABEL (REPEATED ON ADDITIONAL TYPE 06 CARDS).-
CD                                                                 -
CD     13-24     "X"-DIRECTION LOWER-BOUNDARY COORDINATE.          -
CD                                                                 -
CD     25-36     "X"-DIRECTION UPPER-BOUNDARY COORDINATE.          -
CD                                                                 -
CD     37-42     NUMBER OF INTERVALS IN "X" DIRECTION.             -
CD                                                                 -
CN               "X" REPRESENTS X OR R.                            -
CN                                                                 -
CN               REGIONS MAY BE DEFINED USING THE OVERLAY PROCEDURE,-
CN               WITH THE LATEST REGION ASSIGNMENT OVERLAYING THE   -
CN               PREVIOUS CONFIGURATION, OR USING THE USUSAL PRECEDURE,-
CN               WITH EACH REGION'S BOUNDARIES GIVEN EXPLICITLY.    -
CN               REGION LABELS MUST BE NON-BLANK.                  -
CN               ONLY THE "X"-DIRECTION UPPER BOUNDARIES NEED      -
CN               BE GIVEN FOR REGIONS AFTER THE FIRST.             -
C                                                                  -
C------------------------------------------------------------------

C------------------------------------------------------------------
CR          COMPOSITION SPECIFICATIONS (TYPE 14)                   -
C                                                                  -
CL     FORMAT-----(I2,10X,A6,3(A6,E12.5))                         -
C                                                                  -
CD     COLUMNS          CONTENTS...IMPLICATIONS, IF ANY           -
CD     =======   ==================================================-
CD     1-2       14                                                -
CD                                                                 -
CD     13-18     COMPOSITION LABEL (REPEATED ON ADDITIONAL TYPE 14 -
CD               CARDS).                                           -
CD                                                                 -
CD     19-24     ISOTOPE LABEL.                                    -
CD                                                                 -
CD     25-36     ISOTOPE ATOM DENSITY.                             -
CD                                                                 -
CD     37-42     ISOTOPE LABEL.                                    -
CD                                                                 -
CD     43-54     ISOTOPE ATOM DENSITY.                             -
CD                                                                 -
CD     55-60     ISOTOPE LABEL.                                    -
CD                                                                 -
CD     61-72     ISOTOPE ATOM DENSITY.                             -
CD                                                                 -
CN               COMPOSITION LABELS MUST BE NON-BLANK.             -
 N               ISOTOPE LABELS IN COLS. 19-24, 37-42, AND 55-60 MUST -
```

APPENDIX B. MC^2-2 BCD Input Files. A.NIP (Contd.)

```
CN              CORRESPOND TO NUCLIDE IDENTIFICATION LABELS ON THE      -
CN              LIBRARY IF THEY DO NOT CORRESPOND TO ANY OF THE         -
CN              MATERIALS NAMED ON THE DATA SET A.MCC2 TYPE 06 CARDS.   -
CN              IN OTHER CASES, THEY MUST CORRESPOND TO SOME PROBLEM    -
CN              MATERIAL LABEL IN COLS. 19-24 ON THE DATA SET A.MCC2    -
CN              TYPE 06 CARDS.                                          -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          COMPOSITION AND REGION ASSIGNMENTS (TYPE 15)                -
C                                                                       -
CL    FORMAT-----(I2,4X,11A6)                                           -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    =======    ========================================================-
CD    1-2        15                                                     -
CD                                                                      -
CD    7-12       COMPOSITION LABEL (REPEATED ON ADDITIONAL TYPE 15       -
CD               CARDS).                                                -
CD                                                                      -
CD    13-18      REGION LABEL OF REGION CONTAINING SPECIFIED             -
CD               COMPOSITION.                                           -
CD                                                                      -
CD    19-24      REGION LABEL OF REGION CONTAINING SPECIFIED             -
CD               COMPOSITION.                                           -
CD                                                                      -
CD    25-30      REGION LABEL OF REGION CONTAINING SPECIFIED             -
CD               COMPOSITION.                                           -
CD                                                                      -
CD    31-36      REGION LABEL OF REGION CONTAINING SPECIFIED             -
CD               COMPOSITION.                                           -
CD                                                                      -
CD    37-42      REGION LABEL OF REGION CONTAINING SPECIFIED             -
CD               COMPOSITION.                                           -
CD                                                                      -
CD    43-48      REGION LABEL OF REGION CONTAINING SPECIFIED             -
CD               COMPOSITION.                                           -
CD                                                                      -
CD    49-54      REGION LABEL OF REGION CONTAINING SPECIFIED             -
CD               COMPOSITION.                                           -
CD                                                                      -
CD    55-60      REGION LABEL OF REGION CONTAINING SPECIFIED             -
CD               COMPOSITION.                                           -
CD                                                                      -
CD    61-66      REGION LABEL OF REGION CONTAINING SPECIFIED             -
CD               COMPOSITION.                                           -
CD                                                                      -
CD    67-72      REGION LABEL OF REGION CONTAINING SPECIFIED
```

APPENDIX B. MC^2-2 BCD Input Files. A.NIP (Contd.)

```
CD                COMPOSITION.                                          -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX B. MC^2-2 BCD Input Files. A.STP015

```
C*****************************************************************
C                                                                -
C                        PREPARED 2/25/76 AT ANL                 -
C                                                                -
CF          A.STP015                                             -
CE          GENERAL BCD INPUT FOR MC**2-II PATH DRIVER           -
C                                                                -
CN                      THIS IS A USER SUPPLIED BCD DATA SET.    -
CN                      THE LIST FOR EACH RECORD IS GIVEN IN TERMS -
CN                      OF THE BCD FORMAT OF THAT DATA CARD.     -
CN                      COLUMNS 1-2 CONTAIN THE CARD TYPE NUMBER. -
CN                      BLANK FIELDS PRODUCE THE DEFAULT OPTIONS. -
C                                                                -
C*****************************************************************


C----------------------------------------------------------------
CR          PATH OPTIONS (TYPE 01)                               -
C                                                                -
CL    FORMAT-----(I2,4X,9I6)                                     -
C                                                                -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY           -
CD    =======   ========================================================-
CD    1-2       01                                               -
CD                                                               -
CD    7-12      MC**2-II INPUT PROCESSOR CALCULATION             -
CD              AREA 4 (CSI010).                                 -
CD              0... INVOKE INPUT PROCESSOR (DEFAULT).           -
CD              1...DO NOT INVOKE INPUT PROCESSOR.               -
CD                                                               -
CD    13-18     UNRESOLVED RESONANCE CALCULATION                 -
CD              AREA 5 (CSC004).                                 -
CD              0...DO UNRESOLVED RESONANCE CALCULATION (DEFAULT). -
CD              1...DO NOT DO UNRESOLVED RESONANCE CALCULATION.  -
CD                                                               -
CD    19-24     RESOLVED RESONANCE CALCULATION                   -
CD              AREA 6 (CSC005).                                 -
CD              0...DO RESOLVED RESONANCE CALCULATION (DEFAULT). -
CD              1...DO NOT DO RESOLVED RESONANCE CALCULATION.    -
CD                                                               -
CD    25-30     MACROSCOPIC CROSS SECTION AND MODERATING PARAMETER -
CD              CALCULATION                                      -
CD              AREA 7 (CSC008).                                 -
CD              0...DO CALCULATION OF MACROSCOPIC CROSS SECTIONS -
CD                  AND CONTINUOUS SLOWING DOWN MODERATING PARAMETERS -
CD                  (DEFAULT).                                   -
CD              1...DO NOT CALCULATE MODERATING PARAMETERS AND   -
CD                  MACROSCOPIC CROSS SECTIONS.                  -
CD                                                               -
CD    31-36     UFG SPECTRUM AND BROAD GROUP CROSS SECTIONS      -
```

APPENDIX B. MC^2-2 BCD Input Files. A.STP015 (Contd.)

```
CD              AREA 8 (CSC009).                                        -
CD              0...DO ULTRA-FINE-GROUP CALCULATION AND BROAD GROUP     -
CD                  CROSS SECTIONS (DEFAULT).                           -
CD              1...DO NOT DO ULTRA-FINE-GROUP CALCULATION AND BROAD    -
CD                  GROUP CROSS SECTIONS.                               -
CD                                                                      -
CD    37-42     BROAD GROUP SPECTRUM CALCULATION                        -
CD              AREA 9 (CSC010).                                        -
CD              0...DO BROAD GROUP SPECTRUM CALCULATION (DEFAULT).      -
CD              1...DO NOT DO BROAD GROUP SPECTRUM CALCULATION.         -
CD                                                                      -
CD    43-48     BROAD GROUP CROSS SECTION EDITS (CSE009).               -
CD              0...EDIT BROAD GROUP CROSS SECTION FILE ISOTXS          -
CD                  (DEFAULT).                                          -
CD              1...DO NOT EDIT BROAD GROUP CROSS SECTION FILE ISOTXS.  -
CD                                                                      -
CD    49-54     ISOTXS TO XS.ISO CONVERSION (CSE007).                   -
CD              0...CREATE EQUIVALENT OF DATA SET ISOTXS IN THE DOUBLE  -
CD                  PRECISION DATA SET XS.ISO (DEFAULT).                -
CD              1...CREATE EQUIVALENT OF DATA SET ISOTXS IN A SINGLE    -
CD                  PRECISION VERSION OF DATA SET XS.ISO.               -
CD              -1...DO NOT CREATE DATA SET XS.ISO.                     -
CD              (OPTION NOT AVAILABLE IN ARGONNE CODE CENTER VERSION    -
CD               OF MC**2-II.)                                          -
CD                                                                      -
CD    55-60     HYPER FINE GROUP INTEGRAL TRANSPORT CALCULATION         -
CD              AREA 10 (CSC011).                                       -
CD              0...DO NOT DO HYPER FINE GROUP INTEGRAL TRANSPORT       -
CD                  CALCULATION (DEFAULT).                              -
CD              1...DO HYPER FINE GROUP INTEGRAL TRANSPORT CALCULATION. -
CD                                                                      -
CD    61-66     DATA SET XS.ISO EDIT (CSE012).                          -
CD              0...DO NOT EXECUTE CSE012 (XS.ISO EDITOR).              -
CD              1...EXECUTE CSE012.                                     -
CD              (OPTION NOT AVAILABLE IN ARGONNE CODE CENTER VERSION    -
CD               OF MC**2-II.)                                          -
C                                                                       -
CN              IF COLS. 13-18 OR COLS. 19-24 ARE 1, AREA 6.5 WILL BE   -
CN              EXECUTED TO OBTAIN THE RESOLVED-UNRESOLVED OVERLAP      -
CN              CALCULATION.                                            -
C                                                                       -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          UNRESOLVED RESONANCE OPTION (TYPE 02)                       -
C                                                                       -
CL    FORMAT-----(I2,4X,I6)                                             -
                                                                        -
 D    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
```

APPENDIX B. MC^2-2 BCD Input Files. A.STP015 (Contd.)

```
CD     =======   ==================================================-
CD     1-2       02                                                -
CD                                                                 -
CD     7-12      AREA 10 UNRESOLVED RESONANCE OPTION (CSC011).     -
CD               0...EXCLUDE UNRESOLVED RESONANCE CROSS SECTIONS FROM -
CD                   THE HYPER FINE GROUP INTEGRAL TRANSPORT       -
CD                   CALCULATION (DEFAULT).                        -
CD               1...INCLUDE UNRESOLVED RESONANCE CROSS SECTIONS IN THE -
CD                   HYPER FINE GROUP INTEGRAL TRANSPORT CALCULATION. -
C                                                                  -
C------------------------------------------------------------------

CEOF
```

APPENDIX B. MC^2-2 BCD Input Files. ACSE12

```
C*****************************************************************
C                                                                -
C                        PREPARED 12/09/74 AT ANL                -
C                                                                -
CF          ACSE12                                               -
CE          BCD INPUT FOR XS.ISO EDITOR CSE012                   -
C                                                                -
CN                       THIS IS A USER-SUPPLIED BCD DATA SET.   -
CN                       THE LIST FOR EACH RECORD IS GIVEN IN TERMS OF -
CN                       THE BCD FORMAT OF THE DATA CARD.        -
CN                       COLUMNS 1-2 CONTAIN THE CARD TYPE NUMBER. -
C                                                                -
C*****************************************************************


C----------------------------------------------------------------
CR          EDIT SPECIFICATIONS (TYPE 01)                        -
C                                                                -
CL    FORMAT-----(I2,4X,A6,I6)                                   -
C                                                                -
CD    COLUMNS            CONTENTS...IMPLICATIONS, IF ANY         -
CD    =======    ========================================================-
CD    1-2        01                                              -
CD                                                               -
CD    7-12       ISOTOPE LABEL.                                  -
CD                                                               -
CD    13-18      EDIT FLAG.                                      -
CD                                                               -
CN               IF COLS. 7-12 ON THE FIRST TYPE 01 CARD ARE BLANK, THE -
CN               ENTIRE XS.ISO DATA SET WILL BE EDITED.  IF COLS. 13-18 -
CN               ARE 0, ALL CROSS SECTION TYPES WILL BE EDITED.  IF -
CN               COLS. 13-18 ARE 1, ONLY THE PRINCIPAL CROSS SECTIONS -
CN               WILL BE EDITED.  IF COLS. 13-18 ARE 2, ONLY THE -
CN               SCATTERING ARRAYS WILL BE EDITED.  IF COLS. 13-18 ARE -
CN               3, ONLY FILE 1 OF DATA SET XS.ISO WILL BE EDITED. -
CN               IF COLS. 7-12 ARE BLANK ON THE FIRST TYPE 01 CARD BUT -
CN               ADDITIONAL TYPE 01 CARDS ARE SUPPLIED, THE ISOTOPE -
CN               NAMED IN COLS. 7-12 OF EACH ADDITIONAL CARD WILL BE -
CN               EDITED ACCORDING TO THE FLAG SET IN COLS. 13-18 OF THAT-
CN               SAME CARD. ANY ISOTOPE NOT SPECIFICALLY REFERENCED WILL-
CN               BE EDITED ACCORDING TO THE VALUE IN COLS. 13-18 ON THE -
CN               FIRST TYPE 01 CARD (WHICH HAS COLS. 7-12 BLANK).  IF -
CN               COLS. 13-18 ON AN ADDITIONAL TYPE 01 CARD ARE -1, THE -
CN               ISOTOPE NAMED IN COLS. 7-12 OF THAT CARD WILL NOT BE -
CN               EDITED.  IF THE FIRST TYPE 01 CARD IS NON-BLANK IN -
CN               COLS. 7-12, ONLY THE ISOTOPES NAMED ON THE TYPE 01 -
CN               CARDS WILL BE EDITED, EACH ACCORDING TO THE FLAG IN -
CN               COLS. 13-18 ON THE SAME CARD.  IF DATA SET ACSE12 IS -
CN               NOT SUPPLIED, THE ENTIRE SET IS EDITED AND ALL CROSS -
CN               SECTION TYPES ARE EDITED FOR EACH ISOTOPE.      -
```

APPENDIX B. MC^2-2 BCD Input Files. ACSE12 (Contd.)

```
CN              IF NO TYPE 01 CARDS ARE SUPPLIED, THE EDIT WILL        -
CN              CORRESPOND TO HAVING PUT IN A SINGLE BLANK TYPE 01     -
CN              CARD.                                                  -
C                                                                      -
C---------------------------------------------------------------------

C---------------------------------------------------------------------
CR          BPOINTER EDIT OPTION (TYPE 02)                             -
C                                                                      -
CL    FORMAT-----(I2,4X,I6)                                            -
C                                                                      -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                 -
CD    =======   ==================================================-
CD    1-2       02                                                     -
CD                                                                     -
CD    7-12      BPOINTER EDIT FLAG.                                    -
CD              0...NO BPOINTER DEBUGGING PRINTS.                      -
CD              1...DEBUGGING DUMP PRINTOUT.                           -
CD              2...DEBUGGING TRACE PRINTOUT.                          -
CD              3...FULL DEBUGGING PRINTOUT.                           -
C                                                                      -
C---------------------------------------------------------------------

CEOF
```

APPENDIX B. MC^2-2 BCD Input Files. ACS009

```
C*****************************************************************
C                                                                -
C                        PREPARED 2/27/75 AT ANL                 -
C                                                                -
CF          ACS009                                               -
CF          BCD INPUT FOR EDITING ISOTXS DATA SET (CSF009)       -
C                                                                -
CN                       THIS IS A USER SUPPLIED BCD DATA SET.   -
CN                       THE LIST FOR EACH RECORD IS GIVEN IN TERMS -
CN                       OF THE BCD FORMAT OF THAT DATA CARD.    -
CN                       COLUMNS 1-2 CONTAIN THE CARD TYPE NUMBER. -
CN                       BLANK FIELDS PRODUCE THE DEFAULT OPTIONS. -
C                                                                -
C*****************************************************************


C----------------------------------------------------------------
CR          COMPUTER CONTAINER ARRAY (TYPE 01)                   -
C                                                                -
CC          OPTIONAL CARD TYPE                                   -
C                                                                -
CL     FORMAT-----(I2,4X,3I6)                                    -
C                                                                -
CD     COLUMNS          CONTENTS...IMPLICATIONS, IF ANY          -
CD     =======    ========================================================-
CD     1-2        01                                             -
CD                                                               -
CD     7-12       SIZE OF MAIN STORAGE ARRAY IN REAL*8 WORDS     -
CD                (DEFAULT=30000).                               -
CD                                                               -
CD     13-18      SIZE OF BULK CORE STORAGE ON REAL*8 WORDS (DEFAULT=0). -
CD                                                               -
CD     19-24      POINTR DEBUGGING EDIT.                         -
CD                0...NO DEBUGGING PRINTOUT (DEFAULT).           -
CD                1...DEBUGGING DUMP PRINTOUT.                   -
CD                2...DEBUGGING TRACE PRINTOUT.                  -
CD                3...FULL DEBUGGING PRINTOUT.                   -
C                                                                -
CN                THIS CARD TYPE IS USED ONLY AFTER THE BPOINTER -
CN                CONTAINER ARRAY CAN NOT BE ALLOCATED BY:       -
CN                (1) ATTEMPTING TO CALCULATE THE SIZE OF THE CONTAINER -
CN                    ARRAY FROM THE FILE CONTROL RECORD OF THE ISOTXS -
CN                    DATA SET, OR                               -
CN                (2) OBTAINING THE SIZE OF THE CONTAINER ARRAY SPECIFIED-
CN                    IN DATA SET PRBSPC (IF IT EXISTS) WHICH CONTAINS -
CN                    THE SIZE OF THE CONTAINER ARRAY SPECIFIED BY THE -
CN                    DATA SET A.MCC2.                           -
C                                                                -
C----------------------------------------------------------------
```

APPENDIX B. MC^2-2 BCD Input Files. ACS009 (Contd.)

```
C-----------------------------------------------------------------------
CR          ISOTOPES TO BE EDITED (TYPE 02)                            -
C                                                                      -
CC          OPTIONAL CARD TYPE                                         -
C                                                                      -
CL    FORMAT------(I2,4X,12A6)                                         -
C                                                                      -
CD    COLUMNS            CONTENTS...IMPLICATIONS, IF ANY               -
CD    =======   ========================================================-
CD    1-2       02                                                     -
CD                                                                     -
CD    7-12      ISOTOPE TO BE EDITED.                                  -
CD                                                                     -
CD    13-18     ISOTOPE TO BE EDITED.                                  -
CD                                                                     -
CD    19-24     ISOTOPE TO BE EDITED.                                  -
CD                                                                     -
CD    25-30     ISOTOPE TO BE EDITED.                                  -
CD                                                                     -
CD    31-36     ISOTOPE TO BE EDITED.                                  -
CD                                                                     -
CD    37-42     ISOTOPE TO BE EDITED.                                  -
CD                                                                     -
CD    43-48     ISOTOPE TO BE EDITED.                                  -
CD                                                                     -
CD    49-54     ISOTOPE TO BE EDITED.                                  -
CD                                                                     -
CD    55-60     ISOTOPE TO BE EDITED.                                  -
CD                                                                     -
CD    61-66     ISOTOPE TO BE EDITED.                                  -
CD                                                                     -
CD    67-72     ISOTOPE TO BE EDITED.                                  -
CD                                                                     -
CD    73-80     ISOTOPE TO BE EDITED.                                  -
C                                                                      -
CN              ISOTOPE NAME MUST BE LEFT-JUSTIFIED IN FORMAT FIELD    -
CN              WITH IMBEDDED BLANKS PRESERVED.                        -
CN              AS MANY TYPE 02 CARDS AS NECESSARY MAY BE USED.        -
CN              NO TYPE 02 CARD WILL RESULT IN ALL THE ISOTOPES IN     -
CN              THE ISOTXS DATA SET TO BE EDITED.                      -
CN              A TYPE 02 CARD WITH NO ISOTOPE NAMES WILL RESULT IN    -
CN              ONLY ISOTOPE INDEPENDENT DATA TO BE EDITED E.G., AN    -
CN              EDIT OF THE FIRST THREE OR FOUR RECORDS OF DATA SET    -
CN              ISOTXS.                                                -
C                                                                      -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX C

MC^2-2 BINARY INTERFACE FILES

APPENDIX C. MC^2-2 Binary Interface Files. ISOTXS

```
C*****************************************************************
C                                                                 -
C                        PREPARED 03/03/75                        -
C                                                                 -
CF          ISOTXS                                                -
CE          MICROSCOPIC GROUP NEUTRON CROSS SECTIONS              -
C                                                                 -
CN                      THIS FILE PROVIDES A BASIC BROAD GROUP    -
CN                      LIBRARY, ORDERED BY ISOTOPE               -
C                                                                 -
C*****************************************************************


CD    MULT              2 FOR IBM MACHINES, 1 OTHERWISE


C-----------------------------------------------------------------
CS          FILE STRUCTURE                                        -
CS                                                                -
CS             RECORD TYPE                          PRESENT IF    -
CS             ================================     ==========    -
CS             FILE IDENTIFICATION                  ALWAYS        -
CS             FILE CONTROL                         ALWAYS        -
CS             FILE DATA                            ALWAYS        -
CS             SET CHI DATA                         ICHIST.GT.1   -
CS    *********** (REPEAT FOR ALL ISOTOPES)                       -
CS    *        ISOTOPE CONTROL AND GROUP            ALWAYS        -
CS    *        INDEPENDENT DATA                                   -
CS    *        PRINCIPAL CROSS SECTIONS             ALWAYS        -
CS    *        ISOTOPE CHI DATA                     ICHI.GT.1     -
CS    *  ******** (REPEAT TO NSCMAX SCATTERING BLOCKS)            -
CS    *  *  ***** (REPEAT FROM 1 TO NSBLOK)                       -
CS    *  *  *  SCATTERING SUB-BLOCK                LORD(N).GT.0  -
CS    ***********                                                 -
C                                                                 -
C-----------------------------------------------------------------


C-----------------------------------------------------------------
CR          FILE IDENTIFICATION (TYPE 1)                          -
C                                                                 -
CL    HNAME,(HUSE(I),I=1,2),IVERS                                 -
C                                                                 -
CW    1+3*MULT                                                    -
C                                                                 -
CD    HNAME             HOLLERITH FILE NAME - ISOTXS - (A6)       -
CD    HUSE              HOLLERITH USER IDENTIFICATION (A6)        -
CD    IVERS             FILE VERSION NUMBER                       -
C                                                                 -
C-----------------------------------------------------------------
```

APPENDIX C. MC^2-2 Binary Interface Files. ISOTXS (Contd.)

```
C-----------------------------------------------------------------------
CR          FILE CONTROL (TYPE 2)                                      -
C                                                                      -
CL    NGROUP,NISO,MAXUP,MAXDN,MAXORD,ICHIST,NSCMAX,NSBLOK              -
C                                                                      -
CW    8                                                                -
C                                                                      -
CD    NGROUP            NUMBER OF ENERGY GROUPS IN SET                 -
CD    NISO              NUMBER OF ISOTOPES IN SET                      -
CD    MAXUP             MAXIMUM NUMBER OF UPSCATTER GROUPS             -
CD    MAXDN             MAXIMUM NUMBER OF DOWNSCATTER GROUPS           -
CD    MAXORD            MAXIMUM NUMBER OF SCATTERING ORDERS            -
CD    ICHIST            SET FISSION SPECTRUM FLAG                      -
CD                      ICHIST.EQ.0, NO SET FISSION SPECTRUM           -
CD                      ICHIST.EQ.1, SET VECTOR                        -
CD                      ICHIST.GT.1, SET MATRIX                        -
CD    NSCMAX            MAXIMUM NUMBER OF BLOCKS OF SCATTERING DATA    -
CD    NSBLOK            BLOCKING CONTROL FOR SCATTER MATRICES. THE     -
CD                      SCATTERING DATA ARE BLOCKED INTO NSBLOK        -
CD                      RECORDS PER SCATTERING BLOCK                   -
C                                                                      -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          FILE DATA (TYPE 3)                                         -
C                                                                      -
CL    (HSETID(I),I=1,12),(HISONM(I),I=1,NISO),                         -
CL   1(CHI(J),J=1,NGROUP),(VEL(J),J=1,NGROUP),                         -
CL   2(EMAX(J),J=1,NGROUP),EMIN,(LOCA(I),I=1,NISO)                     -
C                                                                      -
CW    (12+NISO)*MULT+1+NISO+(2+ICHIST*(2/(ICHIST+1)))*NGROUP           -
C                                                                      -
CD    HSETID            HOLLERITH IDENTIFICATION OF SET (A6)           -
CD    HISONM(I)         HOLLERITH ISOTOPE LABEL FOR ISOTOPE I (A6)     -
CD    CHI(J)            SET FISSION SPECTRUM (PRESENT IF ICHIST.EQ.1)  -
CD    VEL(J)            MEAN NEUTRON VELOCITY IN GROUP J (CM/SEC)      -
CD    EMAX(J)           MAXIMUM ENERGY BOUND OF GROUP J (EV)           -
CD    EMIN              MINIMUM ENERGY BOUND OF SET (EV)               -
CD    LOCA(I)           NUMBER OF RECORDS TO BE SKIPPED TO READ DATA   -
CD                      FOR ISOTOPE I. LOCA(1)=0                       -
C                                                                      -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          SET CHI DATA (TYPE 4)                                      -
C                                                                      -
```

APPENDIX C. MC^2-2 Binary Interface Files. ISOTXS (Contd.)

```
CC          PRESENT IF ICHIST.GT.1                                          -
C                                                                           -
CL    ((CHI(K,J),K=1,ICHIST),J=1,NGROUP),(ISSPEC(I),I=1,NGROUP)             -
C                                                                           -
CW    NGROUP*(ICHIST+1)                                                     -
C                                                                           -
CD    CHI(K,J)          FRACTION OF NEUTRONS EMITTED IN GROUP J AS A        -
CD                      RESULT OF FISSION IN ANY GROUP USING SPECTRUM K     -
CD    ISSPEC            ISSPEC(I)=K IMPLIES THAT SPECTRUM K IS USED         -
CD                      TO CALCULATE EMISSION SPECTRUM FROM FISSION         -
CD                      IN GROUP I                                          -
C                                                                           -
C---------------------------------------------------------------------------

C---------------------------------------------------------------------------
CR          ISOTOPE CONTROL AND GROUP INDEPENDENT DATA (TYPE 5)             -
C                                                                           -
CL    HABSID,IDENT,MAT,AMASS,EFISS,ECAPT,TEMP,SIGPOT,ADENS,KBR,ICHI,        -
CL   1IFIS,IALF,INP,IN2N,IND,INT,LTOT,LTRN,ISTRPD,                          -
CL   2(IDSCT(N),N=1,NSCMAX),(LORD(N),N=1,NSCMAX),                           -
CL   3((JBAND(J,N),J=1,NGROUP),N=1,NSCMAX),                                 -
CL   4((IJJ(J,N),J=1,NGROUP),N=1,NSCMAX)                                    -
C                                                                           -
CW    (2*NGROUP+2)*NSCMAX+17+MULT*3                                         -
C                                                                           -
CD    HABSID            HOLLERITH ABSOLUTE ISOTOPE LABEL - SAME FOR         -
CD                      ALL VERSIONS OF THE SAME ISOTOPE IN SET (A6)        -
CD    IDENT             IDENTIFIER OF LIBRARY FROM WHICH BASIC DATA         -
CD                      CAME (E.G. ENDF/B) (A6)                             -
CD    MAT               ISOTOPE IDENTIFICATION (E.G. ENDF/B MAT NO.)        -
CD                      (A6)                                                -
CD    AMASS             GRAM ATOMIC WEIGHT                                  -
CD    EFISS             TOTAL THERMAL ENERGY YIELD/FISSION (W.SEC/FISS)     -
CD    ECAPT             TOTAL THERMAL ENERGY YIELD/CAPTURE (W.SEC/CAPT)     -
CD    TEMP              ISOTOPE TEMPERATURE (DEGREES KELVIN)                -
CD    SIGPOT            AVERAGE EFFECTIVE POTENTIAL SCATTERING IN           -
CD                      RESONANCE RANGE (BARNS/ATOM)                        -
CD    ADENS             DENSITY OF ISOTOPE IN MIXTURE IN WHICH ISOTOPE      -
CD                      CROSS SECTIONS WERE GENERATED (A/BARN.CM)           -
CD    KBR               ISOTOPE CLASSIFICATION                              -
CD                      KBR=0, UNDEFINED                                    -
CD                         =1, FISSILE                                      -
CD                         =2, FERTILE                                      -
CD                         =3, OTHER ACTINIDE                               -
CD                         =4, FISSION PRODUCT                              -
CD                         =5, STRUCTURE                                    -
CD                         =6, COOLANT                                      -
CD                         =7, CONTROL
CD    ICHI              ISOTOPE FISSION SPECTRUM FLAG
```

APPENDIX C. MC^2-2 Binary Interface Files. ISOTXS (Contd.)

```
CD                      ICHI.EQ.0, USE SET CHI                                -
CD                      ICHI.EQ.1, ISOTOPE CHI VECTOR                         -
CD                      ICHI.GT.1, ISOTOPE CHI MATRIX                         -
CD    IFIS              (N,F) CROSS SECTION FLAG                              -
CD                      IFIS=0, NO FISSION DATA IN PRINCIPAL CROSS            -
CD                           SECTION RECORD                                   -
CD                         =1, FISSION DATA PRESENT IN PRINCIPAL              -
CD                           CROSS SECTION RECORD                             -
CD    IALF              (N,ALPHA) CROSS SECTION FLAG                          -
CD                        SAME OPTIONS AS IFIS                                -
CD    INP               (N,P) CROSS SECTION FLAG                              -
CD                        SAME OPTIONS AS IFIS                                -
CD    IN2N              (N,2N) CROSS SECTION FLAG                             -
CD                        SAME OPTIONS AS IFIS                                -
CD    IND               (N,D) CROSS SECTION FLAG                              -
CD                        SAME OPTIONS AS IFIS                                -
CD    INT               (N,T) CROSS SECTION FLAG                              -
CD                        SAME OPTIONS AS IFIS                                -
CD    LTOT              NUMBER OF MOMENTS OF TOTAL CROSS SECTION              -
CD                      PROVIDED IN PRINCIPAL CROSS SECTIONS RECORD           -
CD    LTRN              NUMBER OF MOMENTS OF TRANSPORT CROSS SECTION          -
CD                      PROVIDED IN PRINCIPAL CROSS SECTIONS RECORD           -
CD    ISTRPD            NUMBER OF COORDINATE DIRECTIONS FOR WHICH             -
CD                      COORDINATE DEPENDENT TRANSPORT CROSS SECTIONS         -
CD                      ARE GIVEN. IF ISTRPD=0, NO COORDINATE DEPENDENT       -
CD                      TRANSPORT CROSS SECTIONS ARE GIVEN                    -
CD    IDSCT(N)          SCATTERING MATRIX TYPE IDENTIFICATION FOR             -
CD                      SCATTERING BLOCK N. SIGNIFICANT ONLY IF               -
CD                      LORD(N).GT.0                                          -
CD                      IDSCT(N)=000 + NN, TOTAL SCATTERING                   -
CD                              =100 + NN, ELASTIC SCATTERING                 -
CD                              =200 + NN, INELASTIC SCATTERING               -
CD                              =300 + NN, (N,2N) SCATTERING PER              -
CD                                         EMITTED NEUTRON,                   -
CD                      WHERE NN IS THE LEGENDRE EXPANSION INDEX OF           -
CD                      THE FIRST MATRIX IN BLOCK N                           -
CD    LORD(N)           NUMBER OF SCATTERING ORDERS IN BLOCK N. IF            -
CD                      LORD(N)=0, THIS BLOCK IS NOT PRESENT FOR THIS         -
CD                      ISOTOPE. IF NN IS THE VALUE TAKEN FROM                -
CD                      IDSCT(N), THEN THE MATRICES IN THIS BLOCK             -
CD                      HAVE LEGENDRE EXPANSION INDICES OF NN, NN+1,          -
CD                      NN+2,...,NN+LORD(N)-1                                 -
CD    JBAND(J,N)        SCATTERING BANDWIDTH FOR GROUP J, SCATTERING          -
CD                      BLOCK N                                               -
CD    IJJ(J,N)          POSITION OF IN-GROUP SCATTERING CROSS SECTION         -
CD                      IN SCATTERING DATA FOR GROUP J, SCATTERING            -
CD                      BLOCK N, COUNTED FROM THE FIRST WORD OF               -
CD                      GROUP J DATA                                          -
C                                                                             -
C-------------------------------------------------------------------------------
```

APPENDIX C. MC^2-2 Binary Interface Files. ISOTXS (Contd.)

```
C-------------------------------------------------------------------
CR          PRINCIPAL CROSS SECTIONS (TYPE 6)                      -
C                                                                  -
CL    ((STRPL(J,L),J=1,NGROUP),L=1,LTRN),                          -
CL   1((STOTPL(J,L),J=1,NGROUP),L=1,LTOT),(SNGAM(J),J=1,NGROUP),   -
CL   2(SFIS(J),J=1,NGROUP),(SNUTOT(J),J=1,NGROUP),                 -
CL   3(CHIISO(J),J=1,NGROUP),(SNALF(J),J=1,NGROUP),                -
CL   4(SNP(J),J=1,NGROUP),(SN2N(J),J=1,NGROUP),                    -
CL   5(SND(J),J=1,NGROUP),(SNT(J),J=1,NGROUP),                     -
CL   6((STRPD(J,I),J=1,NGROUP),I=1,ISTRPD)                         -
C                                                                  -
CW    (1+LTRN+LTOT+IALF+INP+IN2N+IND+INT+ISTRPD+2*IFIS+            -
CW    ICHI*(2/(ICHI+1)))*NGROUP                                    -
C                                                                  -
CD    STRPL             PL WEIGHTED TRANSPORT CROSS SECTION        -
CD                      THE FIRST ELEMENT OF ARRAY STRPL IS THE    -
CD                      CURRENT (P1) WEIGHTED TRANSPORT CROSS SECTION -
CD    STOTPL            PL WEIGHTED TOTAL CROSS SECTION            -
CD                      THE FIRST ELEMENT OF ARRAY STOTPL IS THE   -
CD                      FLUX (P0) WEIGHTED TOTAL CROSS SECTION     -
CD    SNGAM             (N,GAMMA)                                  -
CD    SFIS              (N,F)                (PRESENT IF IFIS.GT.0) -
CD    SNUTOT            TOTAL NEUTRON YIELD/ (PRESENT IF IFIS.GT.0) -
CD                      FISSION                                    -
CD    CHISO             ISOTOPE CHI          (PRESENT IF ICHI.EQ.1) -
CD    SNALF             (N,ALPHA)            (PRESENT IF IALF.GT.0) -
CD    SNP               (N,P)                (PRESENT IF INP.GT.0)  -
CD    SN2N              (N,2N)               (PRESENT IF IN2N.GT.0) -
CD    SND               (N,D)                (PRESENT IF IND.GT.0)  -
CD    SNT               (N,T)                (PRESENT IF INT.GT.0)  -
CD    STRPD             COORDINATE DIRECTION (PRESENT IF ISTRPD.GT.0) -
CD                      I TRANSPORT CROSS                          -
CD                      SECTION                                    -
C                                                                  -
C-------------------------------------------------------------------


C-------------------------------------------------------------------
CR          ISOTOPE CHI DATA (TYPE 7)                              -
C                                                                  -
CC          PRESENT IF ICHI.GT.1                                   -
C                                                                  -
CL    ((CHIISO(K,J),K=1,ICHI),J=1,NGROUP),(ISOPEC(I),I=1,NGROUP)   -
C                                                                  -
CW    NGROUP*(ICHI+1)                                              -
C                                                                  -
CD    CHIISO            ISOTOPE FISSION SPECTRUM
CD    ISOPEC            FISSION SPECTRUM USED FOR A GIVEN SOURCE GROUP
```

APPENDIX C. MC^2-2 Binary Interface Files. ISOTXS (Contd.)

```
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          SCATTERING SUB-BLOCK (TYPE 8)                               -
C                                                                       -
CC          PRESENT IF LORD(N).GT.0                                     -
C                                                                       -
CL    ((SCAT(K,L),K=1,KMAX),L=1,LORDN)                                  -
C                                                                       -
CC    KMAX=SUM OVER J OF JBAND(J) WITHIN THE J-GROUP RANGE OF THIS      -
CC    SUB-BLOCK. IF M IS THE INDEX OF THE SUB-BLOCK, THE J-GROUP        -
CC    RANGE CONTAINED WITHIN THIS SUB-BLOCK IS                          -
CC    JL=(M-1)*((NGROUP-1)/NSBLOK+1)+1 TO JU=M*((NGROUP-1)/NSBLOK+1)    -
CC    LORDN=LORD(N)                                                     -
C                                                                       -
CW    KMAX*LORDN                                                        -
C                                                                       -
CD    SCAT(K,L)          SCATTERING MATRIX OF SCATTERING ORDER L, FOR   -
CD                       REACTION TYPE IDENTIFIED BY IDSCT(N) FOR THIS  -
CD                       BLOCK. JBAND(J) VALUES FOR SCATTERING INTO     -
CD                       GROUP J ARE STORED AT LOCATIONS K=SUM FROM 1   -
CD                       TO (J-1) OF JBAND(I) PLUS 1 TO K+JBAND(J)-1.   -
CD                       THE SUM IS ZERO WHEN J=1. J-TO-J SCATTER IS    -
CD                       THE IJJ(J)-TH ENTRY IN THE RANGE JBAND(J).     -
CD                       VALUES ARE STORED IN THE ORDER (J+MAXUP),      -
CD                       (J+MAXUP-1),...,(J+1),J,(J-1),...,(J-MAXDN),   -
CD                       WHERE MAXUP=IJJ(J)-1 AND MAXDN=JBAND(J)-IJJ(J) -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F1

```
C*****************************************************************************
C                                                                              -
C                        PREPARED 2/11/75 AT ANL                               -
C                                                                              -
CF          MCC2F1                                                             -
CE          ADMINISTRATIVE                                                     -
C                                                                              -
C*****************************************************************************


CD    MMAT              NUMBER OF MATERIALS IN THE LIBRARY WITH
CD                      INELASTIC AND/OR (N,2N) DATA (C.F. DATA SET
CD                      MCC2F6)
CD    MULT              2 FOR IBM MACHINES, 1 OTHERWISE
CD    NMAT              NUMBER OF MATERIALS IN LIBRARY
CD    NMAX              MAXIMUM NUMBER OF GROUPS OF INELASTIC OR
CD                      (N,2N) DATA FOR ANY MATERIAL IN THE LIBRARY
CD                      (.EQ.MAX (NINEL,N2NTH) WHERE NINEL AND
CD                      N2NTH ARE THE THRESHHOLD GROUP NUMBERS FOR
CD                      INELASTIC AND (N,2N) SCATTERING RESPECTIVELY)
CD    NRESMT            NUMBER OF MATERIALS IN LIBRARY WITH RESOLVED
CD                      RESONANCE PARAMETERS (C.F. DATA SET MCC2F4)
CD    NUNRMT            NUMBER OF MATERIALS IN LIBRARY WITH
CD                      UNRESOLVED RESONANCE PARAMETERS
CD                      (C.F. DATA SET MCC2F3)


C-----------------------------------------------------------------------------
CR          SPECIFICATIONS (TYPE 1)                                            -
C                                                                              -
CC          ALWAYS PRESENT                                                     -
C                                                                              -
CL    NMAT,NGROUP,NRESMT,NUNRMT,MSORS,NPASS,NPL,IPTMAX,ETOP,DELTAU,            -
CL   1MANY1,MMAT,NMAX                                                          -
C                                                                              -
CW    13                                                                       -
C                                                                              -
CD    NGROUP            NUMBER OF ENERGY GROUPS IN LIBRARY                     -
CD    MSORS             NUMBER OF FISSION SPECTRA SPECIFIED IN LIBRARY         -
CD                      (C.F. DATA SET MCC2F7)                                 -
CD    NPASS             NUMBER OF 'BLOCKS' OF LEGENDRE DATA IN LIBRARY         -
CD                      (C.F. DATA SET MCC2F8)                                 -
CD    NPL               HIGHEST ORDER PERMITTED FOR EXTENDED                   -
CD                      TRANSPORT APPROXIMATION                                -
CD                      (C.F. DATA SET MCC2F8)                                 -
CD    IPTMAX            MAXIMUM NUMBER OF LEGENDRE COMPONENTS                  -
CD                      PROVIDED IN THE LIBRARY                                -
CD                      (C.F. DATASET MCC2F8)                                  -
CD    ETOP              HIGHEST ENERGY POINT IN LIBRARY, I.E. ENERGY           -
CD                      AT TOP OF FIRST ENERGY GROUP
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F1 (Contd.)

```
CD    DELTAU              GROUP LETHARGY WIDTH FOR ALL ENERGY GROUPS      -
CD                        IN LIBRARY                                      -
CD    MANY1               NUMBER OF ENERGY LEVELS FOR EACH 'BLOCK'        -
CD                        OF DATA                                         -
C                                                                         -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR          MATERIAL NAMES (TYPE 2)                                       -
C                                                                         -
CC          ALWAYS PRESENT                                                -
C                                                                         -
CL    (NAME(I),I=1,NMAT)                                                  -
C                                                                         -
CW    MULT*NMAT                                                           -
C                                                                         -
CD    NAME                DOUBLE PRECISION (R*8) MATERIAL IDENTIFICATION -
C                                                                         -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR          MATERIAL IDENTIFICATION (TYPE 3)                              -
C                                                                         -
CC          ALWAYS PRESENT                                                -
C                                                                         -
CL    (A(I),I=1,NMAT),(IZ(I),I=1,NMAT),(MAT(I),I=1,NMAT),                 -
CL   1(EFISS(I),I=1,NMAT),(ECAPT(I),I=1,NMAT)                             -
C                                                                         -
CW    5*NMAT                                                              -
C                                                                         -
CD    A                   MATERIAL MASS/NEUTRON MASS                      -
CD    IZ                  ATOMIC NUMBER OF MATERIAL                       -
CD    MAT                 ENDF/B MATERIAL IDENTIFICATION NUMBER           -
CD    EFISS               MEV/FISSION FOR EACH MATERIAL                   -
CD    ECAPT               MEV/CAPTURE FOR EACH MATERIAL WHERE CAPTURE      -
CD                        REFERS TO NON-FISSION ABSORPTION                -
C                                                                         -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR          RESONANCE CONTROL INFORMATION (TYPE 4)                        -
C                                                                         -
CC          PRESENT IF NRESMT.GT.0 OR IF NUNRMT.GT.0                      -
C                                                                         -
CL    (NRES(I),I=1,NRESMT),(NREC(I),I=1,NRESMT),                          -
CL   1(EMAXR(I),I=1,NRESMT),(EMAXU(I),I=1,NUNRMT),                        -
CL   2(EMINU(I),I=1,NUNRMT)                                               -
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F1 (Contd.)

```
C                                                                       -
CW     3*NRESMT+2*NUNRMT                                                -
C                                                                       -
CD     NRES              NUMBER OF RESOLVED RESONANCES FOR EACH         -
CD                       RESOLVED RESONANCE MATERIAL. NRES INCLUDES ALL -
CD                       RESONANCES FOR ALL ISOTOPES OF A MULTI-ISOTOPE -
CD                       MATERIAL                                       -
CD     NREC              NUMBER OF RECORDS FOR EACH RESOLVED RESONANCE  -
CD                       MATERIAL                                       -
CD     EMAXR             ENERGY OF THE HIGHEST RESOLVED RESONANCE       -
CD                       FOR EACH MATERIAL                              -
CD     EMAXU             ENERGY OF THE HIGHEST POINT AT WHICH           -
CD                       UNRESOLVED RESONANCE CALCULATIONS ARE          -
CD                       PERFORMED, FOR EACH MATERIAL                   -
CD     EMINU             ENERGY OF THE LOWEST POINT AT WHICH UNRESOLVED -
CD                       RESONANCE CALCULATIONS ARE PERFORMED,          -
CD                       FOR EACH MATERIAL                              -
C                                                                       -
CN                       THE INFORMATION IN THIS RECORD REFERS TO THE   -
CN                       STRUCTURE OF DATA SETS MCC2F3 AND MCC2F4       -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR           INELASTIC AND N2N DISTRIBUTIONS CONTROL INFORMATION        -
CR           (TYPE 5)                                                   -
C                                                                       -
CC           PRESENT IF MMAT.GT.0                                       -
C                                                                       -
CL     (ANAME(I),I=1,MMAT),(NINEL(I),I=1,MMAT),(N2NTH(I),I=1,MMAT),     -
CL    1(NLEVLS(I),I=1,MMAT),(N2NLEV(I),I=1,MMAT),(MAX1(I),I=1,MMAT),    -
CL    2(MAX2(I),I=1,MMAT),(MAX3(I),I=1,MMAT),(MAX4(I),I=1,MMAT),        -
CL    3(NSINK1(I),I=1,MMAT),(NSINK2(I),I=1,MMAT),                       -
CL    4(NUMREC(I),I=1,NMAX),MAXREC                                      -
C                                                                       -
CW     10*MMAT+MUIT*MMAT+1+NMAX                                         -
C                                                                       -
CD     ANAME             DOUBLE PRECISION (R*8) MATERIAL IDENTIFICATION -
CD     NINEL             THRESHOLD GROUP NUMBER FOR INELASTIC           -
CD                       SCATTERING (=0 IF NO INELASTIC SCATTERING)     -
CD     N2NTH             THRESHOLD GROUP NUMBER FOR (N,2N)              -
CD                       SCATTERING (=0 IF NO (N,2N) SCATTERING)        -
CD     NLEVLS            NUMBER OF DISCRETE INELASTIC SCATTERING        -
CD                       LEVELS FOR EACH MATERIAL                       -
CD     N2NLEV            NUMBER OF DISCRETE (N,2N) SCATTERING           -
CD                       LEVELS FOR EACH MATERIAL                       -
CD     MAX1              MAXIMUM NUMBER OF INELASTIC EVAPORATION        -
CD                       SPECTRA FOR EACH MATERIAL
CD     MAX2              MAXIMUM NUMBER OF TABULATED INELASTIC
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F1 (Contd.)

```
CD                      DISTRIBUTIONS FOR EACH MATERIAL                 -
CD                      MAX2.EQ. ZERO OR ONE                            -
CD     MAX3             MAXIMUM NUMBER OF (N,2N) EVAPORATION            -
CD                      SPECTRA FOR EACH MATERIAL                       -
CD     MAX4             MAXIMUM NUMBER OF TABULATED (N,2N)              -
CD                      DISTRIBUTIONS FOR EACH MATERIAL                 -
CD                      MAX4.EQ. ZERO OR ONE                            -
CD     NSINK1           NUMBER OF ENERGIES PROVIDED IN TABULATED        -
CD                      INELASTIC DISTRIBUTIONS FOR EACH MATERIAL       -
CD                      IF MAX2.EQ.0 THEN NSINK1.EQ.0                   -
CD     NSINK2           NUMBER OF ENERGIES PROVIDED IN TABULATED        -
CD                      (N,2N) DISTRIBUTIONS FOR EACH MATERIAL          -
CD                      IF MAX4.EQ.0 THEN NSINK2.EQ.0                   -
CD     MAXREC           MAXIMUM RECORD LENGTH (WORDS) IN FILE MCC2F6    -
CD                      FOR ANY RECORD TYPE                             -
CD     NUMREC           NUMBER OF RECORDS OF INELASTIC AND (N,2N)       -
CD                      DATA FOR EACH GROUP. EQUAL TO 2 OR 3            -
CD                      FOR EACH GROUP                                  -
C                                                                       -
CN                      THE INFORMATION IN THIS RECORD REFERS TO        -
CN                      THE STRUCTURE OF DATA SET MCC2F6                -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CF          HARD SPHERE POTENTIAL SCATTERING CROSS SECTIONS (TYPE 6)    -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL     (SIGP(I),I=1,NMAT)                                               -
C                                                                       -
CW     NMAT                                                             -
C                                                                       -
CD     SIGP             HARD SPHERE POTENTIAL SCATTERING CROSS SECTIONS-
C                                                                       -
CN                      THE SIGP ARE THE ENERGY INDEPENDNT VALUES       -
CN                      OBTAINED FROM THE NUCLEAR RADIUS USING          -
CN                      4*PI*(RADIUS)**2                                -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F2

```
C*****************************************************************
C                                                                -
C                        PREPARED 12/15/73 AT ANL                -
C                                                                -
CF          MCC2F2                                               -
CE          FUNCTION TABLE                                       -
C                                                                -
C*****************************************************************


C----------------------------------------------------------------
CR          REAL W COARSE (TYPE 1)                               -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL    ((WRC(I,J),I=1,41),J=1,27)                                 -
C                                                                -
CW    1107                                                       -
C                                                                -
CD    WRC               REAL PART OF W(X,Y) TABULATED AT INCREMENTS OF -
CD                      0.1 FOR -0.1.LE.X.LE.3.9 AND 0.4.LE.Y.LE.3.0   -
C                                                                -
C----------------------------------------------------------------


C----------------------------------------------------------------
CR          IMAGINARY W COARSE (TYPE 2)                          -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL    ((WIC(I,J),I=1,41),J=1,27)                                 -
C                                                                -
CW    1107                                                       -
C                                                                -
CD    WIC               IMAGINARY PART OF W(X,Y) TABULATED AT    -
CD                      INCREMENTS OF 0.1 FOR -0.1.LE.X.LE.3.9 AND -
CD                      0.4.LE.Y.LE.3.0                          -
C                                                                -
C----------------------------------------------------------------


C----------------------------------------------------------------
CR          REAL W FINE (TYPE 3)                                 -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL    ((WRF(I,J),I=1,41),J=1,27)                                 -
C                                                                -
CW    1107                                                       -
C
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F2 (Contd.)

```
CD     WRF                  REAL PART OF W(X,Y) TABULATED AT INCREMENTS     -
CD                          OF 0.1 FOR -0.1.LE.X.LE.3.9 AND AT INCREMENTS   -
CD                          OF 0.02 FOR -0.02.LE.Y.LE.0.5                   -
C                                                                           -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR           IMAGINARY W FINE (TYPE 4)                                      -
C                                                                           -
CC           ALWAYS PRESENT                                                 -
C                                                                           -
CL     ((WIF(I,J),I=1,41),J=1,27)                                           -
C                                                                           -
CW     1107                                                                 -
C                                                                           -
CD     WIF                  IMAGINARY PART OF W(X,Y) TABULATED AT          -
CD                          INCREMENTS OF 0.1 FOR -0.1.LE.X.LE.3.9 AND     -
CD                          AT INCREMENTS OF 0.02 FOR -0.02.LE.Y.LE.0.5    -
C                                                                           -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR           EXPONENTIAL INTEGRAL E3 (TYPE 5)                               -
C                                                                           -
CC           ALWAYS PRESENT                                                 -
C                                                                           -
CL     (E3(I),I=1,1001)                                                     -
C                                                                           -
CW     1001                                                                 -
C                                                                           -
CD     E3                   EXPONENTIAL INTEGRAL, E3(X), TABULATED AT      -
CD                          INCREMENTS OF 0.01 FOR 0.0.LE.X.LE.10.0        -
C                                                                           -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR           EXPONENTIAL FUNCTION (TYPE 6)                                  -
C                                                                           -
CC           ALWAYS PRESENT                                                 -
C                                                                           -
CL     (EXPON(I),I=1,K1)                                                    -
C                                                                           -
CW     2*NGROUP-1                                                           -
C                                                                           -
CC           K1=2*NGROUP-1 WHERE NGROUP IS THE NUMBER OF LIBRARY            -
 C           ENERGY GROUPS AS SPECIFIED IN THE ADMINISTRATIVE FILE          -
 C           MCC2F1                                                         -
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F2 (Contd.)

```
C                                                                       -
CD     EXPON              EXPON(I)=(1.+(1./C)**(NGROUP-I))*             -
CD                        EXP(-(1./C)**(NGROUP-I)) WHERE                -
CD                        C=EXP(-DELTAU) AND DELTAU IS THE LIBRARY      -
CD                        GROUP LETHARGY WIDTH AS SPECIFIED IN THE      -
CD                        ADMINISTRATIVE FILE MCC2F1                    -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR            FIRST FLIGHT TRANSMISSION PROBABILITIES                   -
CR            (TYPE 7)                                                  -
C                                                                       -
CC            ALWAYS PRESENT                                            -
C                                                                       -
CL     ((T1(I,J),I=1,181),J=1,26),((T2(I,J),I=1,181),J=1,51)            -
C                                                                       -
CW     13937                                                            -
C                                                                       -
CD     T1(I,J)            TRANSMISSION PROBABILITY, INNER TO OUTER      -
CD                        SURFACE FOR ANNULAR REGION, FOR I-TH VALUE OF -
CD                        Z AND J-TH VALUE OF X, WHERE THE X INCREMENT  -
CD                        IS 0.04                                       -
CD     T2(I,J)            TRANSMISSION PROBABILITY, OUTER TO OUTER      -
CD                        SURFACE FOR ANNULAR REGION, FOR I-TH VALUE OF -
CD                        Z AND J-TH VALUE OF X, WHERE THE X INCREMENT  -
CD                        IS 0.02                                       -
C                                                                       -
CN                        Z=TOTAL CROSS SECTION * (OUTER RADIUS-INNER   -
CN                        RADIUS), AND                                  -
CN                        X=(INNER RADIUS)/(OUTER RADIUS).              -
CN                        X TAKES ON VALUES BETWEEN 0.0 AND 1.0         -
CN                                                                      -
CN                        RANGE OF Z          Z INCREMENT               -
CN                        ----------          -----------               -
CN                        0.0 TO 0.4             0.01                   -
CN                        0.4 TO 1.0             0.02                   -
CN                        1.0 TO 2.6             0.04                   -
CN                        2.6 TO 5.0             0.06                   -
CN                        5.0 TO 8.0             0.10                   -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR            EXPONENTIAL INTEGRALS AND FUNCTIONS (TYPE 8)              -
C                                                                       -
CC            ALWAYS PRESENT
C
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F2 (Contd.)

```
CL     (EXPY(I),I=1,1023),(EXPM(I),I=1,1022),(E3(I),I=1,331),          -
CL    1(E4(I),I=1,331)                                                 -
C                                                                      -
CW     2707                                                            -
C                                                                      -
CD     E3                  EXPONENTIAL INTEGRAL, E3(X), TABULATED AT   -
CD                         0(0.01)2(0.02)4(0.08)6.4.                   -
CD     E4                  EXPONENTIAL INTEGRAL, E4(X), TABULATED AT   -
CD                         0(0.01)2(0.02)4(0.08)6.4.                   -
CD     EXPY                ORDINATES Y(I) FOR EXP(-X)=Y(I)-M(I)*X      -
CD                         TABULATED FOR 0.0.LE.X.LE.18.0 WITH TABULAR -
CD                         INTERVAL 18.0/1022.                         -
CD     EXPM                SLOPES M(I) FOR EXP(-X)=Y(I)-M(I)*X         -
CD                         TABULATED FOR 0.0.LE.X.LE.18.0 WITH TABULAR -
CD                         INTERVAL 18.0/1022.                         -
C                                                                      -
C----------------------------------------------------------------------

CEOF
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F3

```
C*****************************************************************
C                                                                 -
C                      PREPARED 2/11/75 AT ANL                    -
C                                                                 -
CF          MCC2F3                                                -
CE          UNRESOLVED RESONANCE DATA                             -
C                                                                 -
C*****************************************************************


CD     JST                  NUMBER OF CHANNEL SPIN STATES ASSOCIATED WITH
CD                          A PARTICULAR ANGULAR MOMENTUM STATE IN
CD                          UNRESOLVED RESONANCE CALCULATION
CD     LST                  NUMBER OF ANGULAR MOMENTUM STATES CONSIDERED
CD                          FOR A GIVEN ISOTOPE IN UNRESOLVED CALCULATION
CD     MULT                 2 FOR IBM MACHINES, 1 OTHERWISE
CD     NISO                 NUMBER OF ISOTOPES IN MATERIAL
CD     NPT                  NUMBER OF ENERGIES AT WHICH UNRESOLVED
CD                          CALCULATION IS DONE
CD     NUNRMT               NUMBER OF MATERIALS WITH UNRESOLVED RESONANCE
CD                          PARAMETERS AS SPECIFIED IN THE ADMINISTRATIVE
CD                          FILE MCC2F1


C-----------------------------------------------------------------
CS          FILE STRUCTURE                                        -
CS                                                                -
CS          RECORD TYPE                          PRESENT IF       -
CS          ===================================  ================-
CS          UNRESOLVED RESONANCE MATERIAL NAMES  ALWAYS           -
CS          MATERIAL SPECIFICATIONS              ALWAYS           -
CS     ******** (REPEAT FOR ALL MATERIALS WITH                    -
CS     *          UNRESOLVED RESONANCE PARAMETERS)                -
CS     *     ISOTOPE CONTROL                     ALWAYS           -
CS     *  ***** (REPEAT FOR ALL ISOTOPES)                         -
CS     *  *  UNRESOLVED SPIN STATE AND          ALWAYS           -
CS     *  *  ENERGY DATA                                          -
CS     *  *  STATISTICAL UNRESOLVED RESONANCE    ALWAYS           -
CS     *  *  INFORMATION                                          -
CS     ********                                                  -
C                                                                 -
C-----------------------------------------------------------------


C-----------------------------------------------------------------
CR          UNRESOLVED RESONANCE MATERIAL NAMES (TYPE 1)          -
C                                                                 -
CC          ALWAYS PRESENT                                        -
C                                                                 -
CL     (NAME(I),I=1,NUNRMT)                                       -
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F3 (Contd.)

```
C                                                                       -
CW     MULT*NUNRMT                                                      -
C                                                                       -
CD     NAME              DOUBLE PRECISION (R*8) MATERIAL IDENTIFICATION -
C                                                                       -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR           MATERIAL SPECIFICATIONS (TYPE 2)                           -
C                                                                       -
CC           ALWAYS PRESENT                                             -
C                                                                       -
CL     (NISO(I),I=1,NUNRMT),(IFI(I),I=1,NUNRMT),                       -
CI    1(ISK(I),I=1,NUNRMT),LSTMAX,JSTMAX,NPTMAX                         -
C                                                                       -
CW     3*NUNRMT+3                                                       -
C                                                                       -
CD     IFI               FISSILE ISOTOPE INDEX                        -
CD                       IFI=0 FOR NON-FISSILE MATERIAL               -
CD                       IFI=1 FOR FISSILE MATERIAL                   -
CD     ISK               NUMBER OF LOGICAL RECORDS OF UNRESOLVED      -
CD                       RESONANCE DATA FOR EACH MATERIAL             -
CD     LSTMAX            MAXIMUM VALUE OF LST OVER ALL MATERIALS IN FILE-
CD     JSTMAX            MAXIMUM VALUE OF JST OVER ALL MATERIALS IN FILE-
CD     NPTMAX            MAXIMUM VALUE OF NPT OVER ALL MATERIALS IN FILE-
C                                                                       -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR           ISOTOPE CONTROL DATA (TYPE 3)                              -
C                                                                       -
CC           ALWAYS PRESENT                                             -
C                                                                       -
CL     (ABUN(I),I=1,NISO),(A(I),I=1,NISO),(RPF(I),I=1,NISO),            -
CL    1(LST(I),I=1,NISO),(NPT(I),I=1,NISO),(RPS(I),I=1,NISO)            -
C                                                                       -
CW     6*NISO                                                           -
C                                                                       -
CD     ABUN              ABUNDANCE OF EACH ISOTOPE                    -
CD     A                 ISOTOPIC MASS/NEUTRON MASS                   -
CD     RPF               RPF=K*R/SQRT(E), K= WAVE NUMBER,             -
CD                       R=CHANNEL RADIUS,E=ENERGY. FOR USE IN        -
CD                       OBTAINING P AND D WAVE PENETRATION FACTOR    -
CD     RPS               RPS=K*R/SQRT(E), K= WAVE NUMBER,             -
CD                       R=EFFECTIVE SCATTERING RADIUS,E=ENERGY. FOR USE-
CD                       IN OBTAINING THE S,P, AND D WAVE PHASE SHIFTS -
C                                                                       -
C-----------------------------------------------------------------------
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F3 (Contd.)

```
C-----------------------------------------------------------------------
CR          UNRESOLVED SPIN STATE AND ENERGY DATA (TYPE 4)             -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL    (ES(I),I=1,NPT),(DEL(I),I=1,NPT),(JST(I),I=1,LST)                -
C                                                                      -
CW    2*NPT+LST                                                        -
C                                                                      -
CD    ES                ENERGIES AT WHICH UNRESOLVED CALCULATION     -
CD                      IS TO BE DONE, IN EV. AND ORDER OF DECREASING -
CD                      ENERGY, ES(I).GT.ES(I+1)                     -
CD    DEL               DOPPLER WIDTH/(SQUARE ROOT OF THE TEMPERATURE) -
C                                                                      -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          STATISTICAL UNRESOLVED RESONANCE INFORMATION (TYPE 5)      -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL     (((GA(I,J,L),I=1,NPT),J=1,JST),L=1,LST),                        -
CL    1(((D(I,J,L),I=1,NPT),J=1,JST),L=1,LST),                         -
CL    2(((GF(I,J,L),I=1,NPT),J=1,JST),L=1,LST),                        -
CL    3(((GNO(I,J,L),I=1,NPT),J=1,JST),L=1,LST),                       -
CL    4((G(J,L),J=1,JST),L=1,LST),((NDFF(J,L),J=1,JST),L=1,LST),       -
CL    5((NDFN(J,L),J=1,JST),L=1,LST)                                   -
C                                                                      -
CW     (4*NPT+3)*(JST(1)+JST(2)+...+JST(LST))                          -
C                                                                      -
CD    GA                AVERAGE RADIATION WIDTH, EV.,                -
CD                      FOR EACH ENERGY ES                           -
CD    D                 AVERAGE SPACING, EV., FOR EACH ENERGY ES     -
CD    GF                AVERAGE FISSION WIDTH, EV., FOR EACH ENERGY ES -
CD    GNO               AVERAGE REDUCED NEUTRON WIDTH, EV.,          -
CD                      FOR EACH ENERGY ES                           -
CD    NDFF              NUMBER OF DEGREES OF FREEDOM IN FISSION WIDTH -
CD                      DISTRIBUTION (1,2,3 OR 4)                    -
CD    G                 STATISTICAL FACTOR                           -
CD    NDFN              NUMBER OF DEGREES OF FREEDOM IN NEUTRON WIDTH -
CD                      DISTRIBUTION (1 OR 2). NUMBER OF ENTRANCE    -
CD                      CHANNELS FOR NEUTRONS IN AN L,J SEQUENCE     -
C                                                                      -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F4

```
C*****************************************************************-
C                                                                 -
C                      PREPARED 1/13/76 AT ANL                    -
C                                                                 -
CF          MCC2F4                                                -
CE          RESOLVED RESONANCE DATA                               -
C                                                                 -
C*****************************************************************

CD     GIT,GIF,GIC          RESPECTIVELY, THE ASYMMETRICAL ADLER-ADLER
CD                          TOTAL, FISSION, AND CAPTURE CROSS SECTION
CD                          PARAMETERS SUPPLIED BY ENDF/B
CD     GRT,GRF,GRC          RESPECTIVELY, THE SYMMETRICAL ADLER-ADLER
CD                          TOTAL, FISSION, AND CAPTURE CROSS SECTION
CD                          PARAMETERS SUPPLIED BY ENDF/B
CD     IWR                  RESOLVED RESONANCE PARAMETER INDEX
CD                          IWR=1  MATERIAL HAS RESOLVED RESONANCE
CD                                 SINGLE-LEVEL BREIT-WIGNER PARAMETERS
CD                          IWR=2  MATERIAL HAS MULTI-LEVEL ADLER-ADLER
CD                                 RESOLVED RESONANCE PARAMETERS
CD                          IWR=3  MATERIAL HAS MULTI-LEVEL BREIT-WIGNER
CD                                 RESOLVED RESONANCE PARAMETERS
CD     MULT                 2 FOR IBM MACHINES, 1 OTHERWISE
CD     NISO                 NUMBER OF ISOTOPES IN MATERIAL
CD     NRESMT               NUMBER OF MATERIALS WITH RESOLVED RESONANCE
CD                          PARAMETERS AS SPECIFIED IN THE ADMINISTRATIVE
CD                          FILE MCC2F1
CD     NRGYS                NUMBER OF RESOLVED RESONANCES FOR AN ISOTOPE
CD     PHI                  S WAVE PHASE SHIFT EQUAL TO K*R. THE NEUTRON
CD                          WAVE NUMBER K=2.196771E-3*(A/(A+1))*SQUARE
CD                          ROOT OF RESONANCE ENERGY, A IS THE RATIO OF
CD                          THE MASS OF THE PARTICULAR ISOTOPE TO THAT OF
CD                          THE NEUTRON, AND R IS THE EFFECTIVE SCATTERING
CD                          RADIUS. A AND R ARE SUPPLIED BY ENDF/B

C-----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                          PRESENT IF      -
CS          ===================================  ================-
CS          RESOLVED RESONANCE MATERIAL NAMES    ALWAYS          -
CS          MATERIAL SPECIFICATIONS              ALWAYS          -
CS     ******** (REPEAT FOR ALL MATERIALS WITH                    -
CS     *          RESOLVED RESONANCE PARAMETERS)                 -
CS     *    ISOTOPE CONTROL                      ALWAYS          -
CS     *  ***** (REPEAT FOR ALL ISOTOPES)                        -
CS     *  *  RESOLVED RESONANCE ENERGY DATA      IWR.GE.1        -
CS     *  *  RESOLVED RESONANCE PEAK CROSS       IWR.GE.1        -
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F4 (Contd.)

```
CS     *   *  SECTION                                                  -
CS     *   *  MODIFIED RESONANCE NATURAL TO          IWR.GE.1          -
CS     *   *  DOPPLER WIDTH                                            -
CS     *   *  INTERFERENCE SCATTERING FACTOR         IWR.GE.1          -
CS     *   *  RESOLVED RESONANCE TOTAL AND           IWR.EQ.1          -
CS     *   *  NEUTRON LINE WIDTHS                                      -
CS     *   *  RESONANCE RADIATION LINE WIDTH         IWR.EQ.1          -
CS     *   *  RESONANCE FISSION LINE WIDTH           IWR.EQ.1          -
CS     *   *  S-MATRIX TOTAL LINE WIDTH              IWR.EQ.2          -
CS     *   *  SYMMETRIC PARAMETER FOR CAPTURE        IWR.EQ.2          -
CS     *   *  REACTION                                                 -
CS     *   *  SYMMETRIC PARAMETER FOR FISSION        IWR.EQ.2          -
CS     *   *  REACTION                                                 -
CS     *   *  SYMMETRIC PARAMETER FOR TOTAL          IWR.EQ.2          -
CS     *   *  REACTION                                                 -
CS     *   *  ADLER-ADLER FACTOR FOR J CAPTURE       IWR.EQ.2          -
CS     *   *  INTEGRAL                                                 -
CS     *   *  ADLER-ADLER FACTOR FOR J FISSION       IWR.EQ.2          -
CS     *   *  INTEGRAL                                                 -
CS     *   *  BREIT-WIGNER MULTI-LEVEL TOTAL LINE    IWR.EQ.3          -
CS     *   *  WIDTH                                                    -
CS     *   *  BREIT-WIGNER MULTI-LEVEL SYMMETRIC     IWR.EQ.3          -
CS     *   *  PARAMETER FOR CAPTURE REACTION                           -
CS     *   *  BREIT-WIGNER MULTI-LEVEL SYMMETRIC     IWR.EQ.3          -
CS     *   *  PARAMETER FOR FISSION REACTION                           -
CS     *   *  BREIT-WIGNER MULTI-LEVEL SYMMETRIC     IWR.EQ.3          -
CS     *   *  PARAMETER FOR TOTAL REACTION                             -
CS     *   *  BREIT-WIGNER MULTI-LEVEL RELATIVE      IWR.EQ.3          -
CS     *   *  ASYMMETRIC CONTRIBUTION TO CAPTURE                       -
CS     *   *  REACTION                                                 -
CS     *   *  BREIT-WIGNER MULTI-LEVEL RELATIVE      IWR.EQ.3          -
CS     *   *  ASYMMETRIC CONTRIBUTION TO FISSION                       -
CS     *   *  REACTION                                                 -
CS     *******                                                         -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR           RESOLVED RESONANCE MATERIAL NAMES (TYPE 1)                -
C                                                                      -
CC           ALWAYS PRESENT                                            -
C                                                                      -
CI     (NAME(I),I=1,NRESMT)                                            -
C                                                                      -
CW     MULT*NRESMT                                                     -
C                                                                      -
CD     NAME              DOUBLE PRECISION (R*8) MATERIAL IDENTIFICATION -
C                                                                      -
C-----------------------------------------------------------------------
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F4 (Contd.)

```
C-----------------------------------------------------------------------
CR          MATERIAL SPECIFICATIONS (TYPE 2)                           -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL    (NISO(I),I=1,NRESMT),(IWR(I),I=1,NRESMT),(EL(I),I=1,NRESMT),     -
CL   1(EU(I),I=1,NRESMT)                                               -
C                                                                      -
CW    4*NRESMT                                                         -
C                                                                      -
CD    EL                LOWEST ENERGY FOR WHICH RESONANCE PARAMETERS   -
CD                      APPLY FOR ANY ISOTOPE OF EACH MATERIAL         -
CD    EU                HIGHEST ENERGY FOR WHICH RESONANCE PARAMETERS  -
CD                      APPLY FOR ANY ISOTOPE OF EACH MATERIAL         -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          ISOTOPE CONTROL DATA (TYPE 3)                              -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL    (ABUN(I),I=1,NISO),(NRGYS(I),I=1,NISO)                           -
C                                                                      -
CW    2*NISO                                                           -
C                                                                      -
CD    ABUN              ABUNDANCE OF EACH ISOTOPE                      -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          RESOLVED RESONANCE ENERGY DATA (TYPE 4)                    -
C                                                                      -
CC          PRESENT IF IWR.GE.1                                        -
C                                                                      -
CL    (EN(J),J=1,NRGYS)                                                -
C                                                                      -
CW    NRGYS                                                            -
C                                                                      -
CD    EN                RESONANCE ENERGY EN(J).GT.EN(J+1)              -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
 R          RESOLVED RESONANCE PEAK CROSS SECTION (TYPE 5)             -
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F4 (Contd.)

```
C                                                                       -
CC          PRESENT IF IWR.GE.1                                         -
C                                                                       -
CL    (SIG0(J),J=1,NRGYS)                                               -
C                                                                       -
CW    NRGYS                                                             -
C                                                                       -
CD    SIG0              CROSS SECTION AT RESONANCE                      -
C                                                                       -
CN                      FOR IWR.EQ.1, SIG0 IS 4*PI*G*LAMBDA-BAR SQUARED-
CN                      *((GAMT-GAMGAM-GAF)/GAMT)*((A+1)/A) SQUARED.    -
CN                      (SEE RECORD TYPES 8,9, AND 10)                  -
CN                                                                      -
CN                      FOR IWR.EQ.2, SIG0 IS 4*PI*LAMBDA-BAR SQUARED*  -
CN                      ((A+1)/A) SQUARED*ABS(GT)/(2*GAMS). (SEE        -
CN                      RECORD TYPES 11 AND 14)                         -
CN                                                                      -
CN                      FOR IWR.EQ.3, SIG0 IS THE VALUE COMPUTED FOR    -
CN                      IWR.EQ.1 MULTIPLIED BY GT. (SEE RECORD          -
CN                      TYPE 20)                                        -
C                                                                       -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          RATIO OF RESONANCE NATURAL TO DOPPLER WIDTH (TYPE 6)        -
C                                                                       -
CC          PRESENT IF IWR.GE.1                                         -
C                                                                       -
CL    (THETAP(J),J=1,NRGYS)                                             -
C                                                                       -
CW    NRGYS                                                             -
C                                                                       -
CD    THETAP            RATIO OF NATURAL WIDTH TO DOPPLER WIDTH *     -
CD                      SQRT(TEMPERATURE) IF IWR.EQ.1 OR IWR.EQ.3.    -
CD                      RATIO OF S-MATRIX TOTAL LINE WIDTH TO DOPPLER -
CD                      WIDTH*SQRT(TEMPERATURE) IF IWR.EQ.2           -
C                                                                       -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          INTERFERENCE SCATTERING FACTOR (TYPE 7)                     -
C                                                                       -
CC          PRESENT IF IWR.GE.1                                         -
C                                                                       -
CL    (AFAC(J),J=1,NRGYS)                                               -
C                                                                       -
CW    NRGYS                                                             -
C
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F4 (Contd.)

```
CD    AFAC                FACTOR TO MULTIPLY CHI TO OBTAIN INTERFERENCE  -
CD                        SCATTERING                                     -
C                                                                        -
CN                        FOR IWR.EQ.1, AFAC IS THE SQUARE ROOT OF       -
CN                        (G*((GAMT-GAMGAM-GAF)/GAMT)* ATOM POTENTIAL    -
CN                        SCATTERING CROSS SECTION /SIG0). G, THE        -
CN                        STATISTICAL FACTOR, IS (2J+1)/(4I+2) WHERE J   -
CN                        IS THE SPIN OF THE COMPOUND NUCLEUS RESONANCE  -
CN                        AND I IS THE TARGET NUCLEUS SPIN.              -
CN                        (SEE RECORD TYPES 5,8,9,AND 10)                -
CN                        AFAC IS SET TO 0 FOR P AND D WAVE RESONANCES    -
CN                                                                       -
CN                        FOR IWR.EQ.2, AFAC IS -0.5*(GIT*COS(2*PHI)-    -
CN                        GRT*SIN(2*PHI))/(GRT*COS(2*PHI)+GIT*SIN(2*PHI))-
CN                                                                       -
CN                        FOR IWR.EQ.3, AFAC IS THE VALUE COMPUTED FOR   -
CN                        IWR.EQ.1 PLUS THE ASYMMETRIC LEVEL-LEVEL       -
CN                        INTERFERENCE CONTRIBUTION, ALL DIVIDED BY      -
CN                        GT. (SEE RECORD TYPE 20)                       -
CN                        AFAC IS SET TO 0 FOR P AND D WAVE RESONANCES    -
C                                                                        -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR          RESOLVED RESONANCE TOTAL AND NEUTRON LINE WIDTHS (TYPE 8)    -
C                                                                        -
CC          PRESENT IF IWR.EQ.1                                          -
C                                                                        -
CL    (GAMT(J),J=1,NRGYS),(GAMN(J),J=1,NRGYS)                            -
C                                                                        -
CW    2*NRGYS                                                            -
C                                                                        -
CD    GAMT                RESOLVED RESONANCE TOTAL LINE WIDTH            -
CD    GAMN                RESOLVED RESONANCE NEUTRON LINE WIDTH          -
C                                                                        -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR          RESONANCE RADIATION LINE WIDTH (TYPE 9)                      -
C                                                                        -
CC          PRESENT IF IWR.EQ.1                                          -
C                                                                        -
CL    (GAMGAM(J),J=1,NRGYS)                                              -
C                                                                        -
CW    NRGYS                                                              -
C                                                                        -
CD    GAMGAM              RESOLVED RESONANCE RADIATION LINE WIDTH        -
                                                                         -
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F4 (Contd.)

```
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          RESONANCE FISSION LINE WIDTH (TYPE 10)                     -
C                                                                      -
CC          PRESENT IF IWR.EQ.1                                        -
C                                                                      -
CL    (GAF(J),J=1,NRGYS)                                               -
C                                                                      -
CW    NRGYS                                                            -
C                                                                      -
CD    GAF               RESOLVED RESONANCE FISSION LINE WIDTH        -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          S-MATRIX TOTAL LINE WIDTH (TYPE 11)                        -
C                                                                      -
CC          PRESENT IF IWR.EQ.2                                        -
C                                                                      -
CL    (GAMS(J),J=1,NRGYS)                                              -
C                                                                      -
CW    NRGYS                                                            -
C                                                                      -
CD    GAMS              S-MATRIX TOTAL LINE WIDTH FOR ADLER-ADLER    -
CD                      FORMULATION (.EQ.2.0*NU)                     -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          SYMMETRIC PARAMETER FOR CAPTURE RFACTION (TYPE 12)         -
C                                                                      -
CC          PRESENT IF IWR.EQ.2                                        -
C                                                                      -
CL    (GC(J),J=1,NRGYS)                                                -
C                                                                      -
CW    NRGYS                                                            -
C                                                                      -
CD    GC                SYMMETRIC PARAMETER FOR CAPTURE REACTION     -
C                                                                      -
CN                      GC = (GRC*COS(2*PHI)+GIC*SIN(2*PHI)) * SQUARE -
CN                           ROOT OF THE RESONANCE ENERGY              -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F4 (Contd.)

```
CR          SYMMETRIC PARAMETER FOR FISSION REACTION (TYPE 13)
C
CC          PRESENT IF IWR.EQ.2
C
CL    (GF(J),J=1,NRGYS)
C
CW    NRGYS
C
CD    GF                SYMMETRIC PARAMETER FOR FISSION REACTION
C
CN                      GF = (GRF*COS(2*PHI)+GIF*SIN(2*PHI)) * SQUARE
CN                           ROOT OF THE RESONANCE ENERGY
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          SYMMETRIC PARAMETER FOR TOTAL REACTION (TYPE 14)
C
CC          PRESENT IF IWR.EQ.2
C
CL    (GT(J),J=1,NRGYS)
C
CW    NRGYS
C
CD    GT                SYMMETRIC PARAMETER FOR TOTAL REACTION
C
CN                      GT = (GRT*COS(2*PHI)+GIT*SIN(2*PHI)) * SQUARE
CN                           ROOT OF THE RESONANCE ENERGY
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          ADLER-ADLER FACTOR FOR J CAPTURE INTEGRAL (TYPE 15)
C
CC          PRESENT IF IWR.EQ.2
C
CL    (BC(J),J=1,NRGYS)
C
CW    NRGYS
C
CD    BC                -0.5*(GIC*COS(2*PHI)-GRC*SIN(2*PHI)) * SQUARE
CD                      ROOT OF THE RESONANCE ENERGY/GC, WHERE GC IS
CD                      DEFINED IN RECORD TYPE 12
C
C-------------------------------------------------------------------
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F4 (Contd.)

```
CR          ADLER-ADLER FACTOR FOR J FISSION INTEGRAL (TYPE 16)
C
CC          PRESENT IF IWR.EQ.2
C
CL    (BF(J),J=1,NRGYS)
C
CW    NRGYS
C
CD    BF                -0.5*(GIF*COS(2*PHI)-GRF*SIN(2*PHI)) * SQUARE
CD                      ROOT OF THE RESONANCE ENERGY/GF, WHERE GF IS
CD                      DEFINED IN RECORD TYPE 13
C
CN                      BF IS SET TO ZERO FOR UNFISSIONABLE
CN                      MULTI-LEVEL MATERIALS
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          BREIT-WIGNER MULTI-LEVEL TOTAL LINE WIDTH (TYPE 17)
C
CC          PRESENT IF IWR.EQ.3
C
CL    (GAMS(J),J=1,NRGYS)
C
CW    NRGYS
C
CD    GAMS              BREIT-WIGNER MULTI-LEVEL TOTAL LINE WIDTH
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          BREIT-WIGNER MULTI-LEVEL SYMMETRIC PARAMETER FOR
CR          CAPTURE REACTION (TYPE 18)
C
CC          PRESENT IF IWR.EQ.3
C
CL    (GC(J),J=1,NRGYS)
C
CW    NRGYS
C
CD    GC                BREIT-WIGNER MULTI-LEVEL SYMMETRIC PARAMETER
CD                      FOR CAPTURE REACTION, THE RATIO OF GAMGAM TO
CD                      GAMS. (SEE RECORD TYPE 9 AND 17)
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F4 (Contd.)

```
CR          BREIT-WIGNER MULTI-LEVEL SYMMETRIC PARAMETER FOR          -
CR          FISSION REACTION (TYPE 19)                                -
C                                                                     -
CC          PRESENT IF IWR.EQ.3                                       -
C                                                                     -
CL    (GF(J),J=1,NRGYS)                                               -
C                                                                     -
CW    NRGYS                                                           -
C                                                                     -
CD    GF              BREIT-WIGNER MULTI-LEVEL SYMMETRIC PARAMETER    -
CD                    FOR FISSION REACTION, THE RATIO OF GAF TO GAMS. -
CD                    (SEE RECORD TYPE 10 AND 17)                     -
C                                                                     -
C---------------------------------------------------------------------


C---------------------------------------------------------------------
CR          BREIT-WIGNER MULTI-LEVEL SYMMETRIC PARAMETER FOR          -
CR          TOTAL REACTION (TYPE 20)                                  -
C                                                                     -
CC          PRESENT IF IWR.EQ.3                                       -
C                                                                     -
CL    (GT(J),J=1,NRGYS)                                               -
C                                                                     -
CW    NRGYS                                                           -
C                                                                     -
CD    GT              BREIT-WIGNER MULTI-LEVEL SYMMETRIC PARAMETER    -
CD                    FOR TOTAL REACTION, 1 PLUS THE SYMMETRIC        -
CD                    LEVEL-LEVEL INTERFERENCE CONTRIBUTION           -
C                                                                     -
C---------------------------------------------------------------------


C---------------------------------------------------------------------
CR          BREIT-WIGNER MULTI-LEVEL RELATIVE ASYMMETRIC CONTRIBUTION -
CR          TO CAPTURE REACTION (TYPE 21)                             -
C                                                                     -
CC          PRESENT IF IWR.EQ.3                                       -
C                                                                     -
CL    (BC(J),J=1,NRGYS)                                               -
C                                                                     -
CW    NRGYS                                                           -
C                                                                     -
CD    BC              BREIT-WIGNER MULTI-LEVEL RELATIVE ASYMMETRIC    -
CD                    CONTRIBUTION TO CAPTURE REACTION                -
C                                                                     -
CN                    NOTE THAT BC IS IDENTICALLY 0.0 FOR BREIT-      -
CN                    WIGNER MULTI-LEVEL FORMALISM                    -
C                                                                     -
C---------------------------------------------------------------------
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F4 (Contd.)

```
C-----------------------------------------------------------------------
CR          BREIT-WIGNER MULTI-LEVEL RELATIVE ASYMMETRIC CONTRIBUTION -
CR          TO FISSION REACTION (TYPE 22)                             -
C                                                                     -
CC          PRESENT IF IWR.EQ.3                                       -
C                                                                     -
CL    (BF(J),J=1,NRGYS)                                               -
C                                                                     -
CW    NRGYS                                                           -
C                                                                     -
CD    BF                BREIT-WIGNER MULTI-LEVEL RELATIVE ASYMMETRIC -
CD                      CONTRIBUTION TO FISSION REACTION              -
C                                                                     -
CN                      NOTE THAT BF IS IDENTICALLY 0.0 FOR BREIT-    -
CN                      WIGNER MULTI-LEVEL FORMALISM                  -
C                                                                     -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F5

```
C*****************************************************************
C                                                                -
C                        PREPARED 2/11/75 AT ANL                 -
C                                                                -
CF          MCC2F5                                               -
CF          SMOOTH (TABULATED) NON-RESONANT DATA                 -
C                                                                -
C*****************************************************************

CD    MULT              2 FOR IBM MACHINES, 1 OTHERWISE
CD    NREAC             NREAC=NUMBER OF REACTION TYPES FOR A
CD                      GIVEN MATERIAL

C----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                          PRESENT IF      -
CS          ===================================  ==============-
CS    ******** (REPEAT FOR ALL MATERIALS)                        -
CS    *     MATERIAL NAME                        ALWAYS          -
CS    *     SPECIFICATIONS                       ALWAYS          -
CS    *  ***** (REPEAT FOR NREAC REACTION TYPES)                 -
CS    *  *  CROSS SECTIONS                       NREAC.GT.0      -
CS    ********                                                   -
C                                                                -
C----------------------------------------------------------------

C----------------------------------------------------------------
CR          MATERIAL NAME (TYPE 1)                               -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL    NAME                                                       -
C                                                                -
CW    MULT*1                                                     -
C                                                                -
CD    NAME              DOUBLE PRECISION (R*8) MATERIAL IDENTIFICATION -
C                                                                -
C----------------------------------------------------------------

C----------------------------------------------------------------
CR          SPECIFICATIONS (TYPE 2)                              -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL    NREAC,NEL,NF,NGAM,NP,ND,NH3,NHE3,NALPHA,NTOT,A0,A1,A2,A3   -
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F5 (Contd.)

```
C                                                                       -
CW     14                                                               -
C                                                                       -
CD     NEL                 FLAG FOR ELASTIC CROSS SECTIONS              -
CD     NF                  FLAG FOR FISSION CROSS SECTIONS              -
CD     NGAM                FLAG FOR (N,GAMMA) CROSS SECTIONS            -
CD     NP                  FLAG FOR (N,P) CROSS SECTIONS                -
CD     ND                  FLAG FOR (N,D) CROSS SECTIONS                -
CD     NH3                 FLAG FOR (N,H3) CROSS SECTIONS               -
CD     NHE3                FLAG FOR (N,HE3) CROSS SECTIONS              -
CD     NALPHA              FLAG FOR (N,ALPHA) CROSS SECTIONS            -
CD     NTOT                FLAG FOR TOTAL CROSS SECTIONS                -
CD                                                                      -
CD                         FOR EACH OF THE ABOVE REACTION TYPES THE     -
CD                         FLAGS ARE ZERO IF NO CROSS SECTION DATA ARE  -
CD                         GIVEN AND EQUAL TO THE HIGHEST ENERGY GROUP  -
CD                         NUMBER (LOWEST ENERGY) FOR WHICH CROSS SECTION -
CD                         DATA ARE GIVEN                               -
CD                                                                      -
CD     A0,A1,A2,A3         COEFFICIENTS FOR CALCULATION OF NU(E), THE    -
CD                         NUMBER OF NEUTRONS PER FISSION. IF THE       -
CD                         ISOTOPE IS NOT FISSIONABLE, THEN THE         -
CD                         COEFFICIENTS WILL BE SET TO ZERO             -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR           CROSS SECTIONS (TYPE 3)                                    -
C                                                                       -
CC           PRESENT IF NREAC.GT.0                                      -
C                                                                       -
CL     (XSIG(J),J=1,NLAST)                                              -
C                                                                       -
CW     NGROUP                                                           -
C                                                                       -
CD     XSIG                CROSS SECTION ASSOCIATED WITH ULTRAFINE      -
CD                         GROUP J FOR A GIVEN REACTION TYPE            -
CD     NLAST               FLAG FOR REACTION TYPE IN QUESTION. (THAT    -
CD                         IS, NEL,NF,ETC.)                             -
CD     NGROUP              NUMBER OF ENERGY GROUPS IN LIBRARY           -
C                                                                       -
CN                         THE CROSS SECTION RECORDS FOR THE DIFFERENT  -
CN                         REACTION TYPES WHICH ARE PRESENT WILL BE IN THE-
CN                         FOLLOWING ORDER: ELASTIC,FISSION,(N,GAMMA),  -
CN                         (N,P),(N,D),(N,H3),(N,HE3),(N,ALPHA),        -
CN                         AND TOTAL.                                   -
CN                         THE TOTAL CROSS SECTION FOR ULTRA-           -
CN                         FINE GROUP J =ELASTIC SCATTERING+INELASTIC
CN                         SCATTERING+(N,2N)SCATTERING+FISSION+(N,GAMMA)+
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F5 (Contd.)

```
CN                    (N,P)+(N,D)+(N,H3)+(N,HE3)+(N,ALPHA).  THE      -
CN                    ELASTIC SCATTERING=SMOOTH(TABULATED) ELASTIC    -
CN                    SCATTERING+UNRESOLVED RESONANCE SCATTERING+     -
CN                    RESOLVED RESONANCE SCATTERING. THE ELASTIC      -
CN                    SCATTERING DOES NOT INCLUDE THE UNRESOLVED      -
CN                    RESONANCE SCATTERING AND RESOLVED RESONANCE     -
CN                    SCATTERING CONTRIBUTIONS FOR MATERIALS WITH     -
CN                    'HEAVY' MASSES. A 'HEAVY' MASS MATERIAL IS      -
CN                    DESIGNATED BY THE USER. ELASTIC SCATTERING      -
CN                    EXPLICITLY INCLUDES THE POTENTIAL SCATTERING    -
CN                    CROSS SECTION                                   -
CN                                                                    -
CN                    ONE CROSS SECTION RECORD IS PRESENT FOR EACH    -
CN                    NON-ZERO FLAG                                   -
C                                                                     -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F6

```
C*****************************************************************
C                                                                 -
C                      PREPARED 10/27/75 AT ANL                   -
C                                                                 -
CF          MCC2F6                                                -
CE          INELASTIC AND N2N DISTRIBUTIONS                       -
C                                                                 -
C*****************************************************************


CD    MMAT          NUMBER OF MATERIALS IN THE LIBRARY WITH
CD                  INELASTIC AND/OR (N,2N) DATA AS SPECIFIED IN
CD                  THE ADMINISTRATIVE FILE MCC2F1
CD    MMAT1         NUMBER OF MATERIALS THAT HAVE INELASTIC AND/OR
CD                  (N,2N) DATA FOR THE ENERGY GROUP BEING
CD                  PROCESSED. IF THE VALUE OF NINEL OR N2NTH
CD                  FOR A MATERIAL IS LESS THAN THE ENERGY GROUP
CD                  NUMBER BEING PROCESSED, THEN NO DATA ARE
CD                  PRESENT FOR THIS MATERIAL. THE CONTROL
CD                  INFORMATION NINEL AND N2NTH ARE SPECIFIED IN
CD                  RECORD TYPE 5 OF MCC2F1
CD    NEND1         NUMBER OF LAST SINK ENERGY POINT (EIN) FOR
CD                  WHICH THE TABULATED INELASTIC PROBABILITY
CD                  IS NON-ZERO FOR THE SOURCE GROUP IN QUESTION
CD    NEND2         NUMBER OF LAST SINK ENERGY POINT (EN2N) FOR
CD                  WHICH THE TABULATED (N,2N) PROBABILITY
CD                  IS NON-ZERO FOR THE SOURCE GROUP IN QUESTION
CD    NINEVP        NUMBER OF INELASTIC EVAPORATION SPECTRA
CD                  FOR ENERGY GROUP IN QUESTION
CD    NINTAB        NUMBER OF TABULATED INELASTIC DISTRIBUTIONS
CD                  FOR ENERGY GROUP IN QUESTION
CD                  NINTAB.EQ.ZERO OR ONE
CD    NLVS          NUMBER OF DISCRETE INELASTIC SCATTERING LEVELS
CD                  FOR EACH MATERIAL FOR THE ENERGY GROUP IN
CD                  QUESTION
CD    NMAX          MAXIMUM NUMBER OF GROUPS OF INELASTIC OR
CD                  (N,2N) DATA FOR ANY MATERIAL IN THE LIBRARY
CD                  (.EQ.MAX(NINEL,N2NTH) AS SPECIFIED IN THE
CD                  ADMINISTRATIVE FILE MCC2F1)
CD    NSINK1        NUMBER OF ENERGIES PROVIDED IN TABULATED
CD                  INELASTIC DISTRIBUTIONS FOR EACH MATERIAL
CD                  AS SPECIFIED IN THE ADMINISTRATIVE FILE MCC2F1
CD    NSINK2        NUMBER OF ENERGIES PROVIDED IN TABULATED
CD                  (N,2N) DISTRIBUTIONS FOR EACH MATERIAL
CD                  AS SPECIFIED IN THE ADMINISTRATIVE FILE MCC2F1
CD    NSTRT1        NUMBER OF FIRST SINK ENERGY POINT (EIN) FOR
CD                  WHICH THE TABULATED INELASTIC PROBABILITY
CD                  IS NON-ZERO FOR THE SOURCE GROUP IN QUESTION
CD    NSTRT2        NUMBER OF FIRST SINK ENERGY POINT (EN2N) FOR
CD                  WHICH THE TABULATED (N,2N) PROBABILITY
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F6 (Contd.)

```
CD                      IS NON-ZERO FOR THE SOURCE GROUP IN QUESTION
CD     N2NEVP           NUMBER OF (N,2N) EVAPORATION SPECTRA
CD                      FOR ENERGY GROUP IN QUESTION
CD     N2NLV            NUMBER OF DISCRETE (N,2N) SCATTERING LEVELS
CD                      FOR EACH MATERIAL FOR THE ENERGY GROUP IN
CD                      QUESTION
CD     N2NTAB           NUMBER OF TABULATED (N,2N) DISTRIBUTIONS
CD                      FOR ENERGY GROUP IN QUESTION
CD                      N2NTAB.EQ.ZERO OR ONE


C-----------------------------------------------------------------------
CS           FILE STRUCTURE                                            -
CS                                                                     -
CS           RECORD TYPE                              PRESENT IF       -
CS           ================================         ================-
CS           GROUP INDEPENDENT INELASTIC              MMAT.GT.0        -
CS           AND (N,2N) DATA                                           -
CS     ******** (REPEAT FOR NMAX GROUPS)                               -
CS     *     CONTROL INFORMATION AND CROSS            NMAX.GT.0        -
CS     *     SECTION DATA                                              -
CS     *     SECONDARY DISTRIBUTION DATA              (NLVS.GT.0) OR   -
CS     *                                              (N2NLV.GT.0) OR  -
CS     *                                              (NINEVP.GT.0) OR -
CS     *                                              (N2NEVP.GT.0)    -
CS     *                                              FOR ANY MATERIAL -
CS     *     TABULATED INELASTIC AND (N,2N)           (NINTAB.GT.0) OR -
CS     *     PROBABILITIES                            (N2NTAB.GT.0)    -
CS     *                                              FOR ANY MATERIAL -
CS     ********                                                        -
C                                                                      -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR           GROUP INDEPENDENT INELASTIC AND (N,2N) DATA (TYPE 1)      -
C                                                                      -
CC           PRESENT IF MMAT.GT.0                                      -
C                                                                      -
CL     ((EGAM(I,J),I=1,NLSJ),(U(I,J),I=1,MAX1J),                       -
CL    1(GAMN2N(I,J),I=1,N2NLJ),(EIN(I,J),I=1,NSNK1J),                  -
CL    2(EN2N(I,J),I=1,NSNK2J),J=1,MMAT)                                -
C                                                                      -
CW     SUMJ                                                            -
C                                                                      -
CD     EGAM             GAMMA RAY ENERGY ASSOCIATED WITH THE L'TH     -
CD                      RESOLVED SCATTERING LEVEL.  IF Q IS THE       -
CD                      ASSOCIATED Q-VALUE OF THE REACTION, THEN      -
CD                      EGAM=-Q (EGAM.GT.0)                           -
CD                      EGAM IS ORDERED SUCH THAT EGAM(1).LE.EGAM(2)...-
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F6 (Contd.)

```
CD     U                  DEFINES INELASTIC UPPER ENERGY LIMIT FOR THE   -
CD                        SECONDARY NEUTRON ENERGY E' SUCH THAT          -
CD                        0.LE.E'.LE.E-U (GIVEN IN THE LABORATORY) WHERE -
CD                        E IS THE INCOMING NEUTRON ENERGY               -
CD     GAMN2N             GAMMA RAY ENERGY ASSOCIATED WITH THE L'TH      -
CD                        (N,2N) RESOLVED SCATTERING LEVEL. IF Q IS THE  -
CD                        ASSOCIATED Q-VALUE OF THE REACTION, THEN       -
CD                        GAMN2N=-Q (GAMN2N.GT.0)                        -
CD                        GAMN2N IS ORDERED SUCH THAT                    -
CD                        GAMN2N(1).LE.GAMN2N(2).LE.GAMN2N(3).....       -
CD     EIN                SINK ENERGIES FOR WHICH TABULATED INELASTIC    -
CD                        SCATTERING PROBABILITIES ARE GIVEN             -
CD     EN2N               SINK ENERGIES FOR WHICH TABULATED (N,2N)       -
CD                        SCATTERING PROBABILITIES ARE GIVEN             -
CD     SUMJ               SUM OF (NLSJ+MAX1J+N2NLJ+NSNK1J+NSNK2J) OVER   -
CD                        ALL MMAT MATERIALS                             -
CD     NLSJ               = NLEVLS(J) FOR CURRENT MATERIAL J             -
CD     MAX1J              = MAX1(J) FOR CURRENT MATERIAL J               -
CD     N2NLJ              = N2NLEV(J) FOR CURRENT MATERIAL J             -
CD     NSNK1J             = NSINK1(J) FOR CURRENT MATERIAL J             -
CD     NSNK2J             = NSINK2(J) FOR CURRENT MATERIAL J             -
C                                                                        -
CN                        THE INELASTIC AND (N,2N) CONTROL INFORMATION   -
CN                        NLEVLS, MAX1, N2NLEV, NSINK1, AND NSINK2 ARE   -
CN                        SPECIFIED IN RECORD TYPE 5 OF MCC2F1            -
CN                                                                       -
CN                        DATA ARE PRESENT ONLY FOR MATERIALS THAT HAVE  -
CN                        EITHER INELASTIC OR (N,2N) DATA                -
C                                                                        -
C-------------------------------------------------------------------------


C-------------------------------------------------------------------------
CR           CONTROL INFORMATION AND CROSS SECTION DATA (TYPE 2)         -
C                                                                        -
CC           PRESENT IF NMAX.GT.0                                        -
C                                                                        -
CL     (SIGIN(I),SIGN2N(I),NINEVP(I),NINTAB(I),N2NEVP(I),N2NTAB(I),      -
CL    1NSTRT1(I),NEND1(I),NSTRT2(I),NEND2(I),KT1(I),KT2(I),              -
CL    2NLVS(J),N2NLV(I),I=1,MMAT1)                                       -
C                                                                        -
CW     SUMJ                                                            -
C                                                                        -
CD     SIGIN              GROUP TOTAL INELASTIC SCATTERING CROSS SECTION -
CD     SIGN2N             GROUP (N,2N) SCATTERING CROSS SECTION          -
CD     KT1                INTERPOLATION LAW FOR CALCULATING GROUP TO     -
CD                        GROUP TABULATED INELASTIC SCATTERING           -
CD                        PROBABILITIES FROM THE GROUP TO ENERGY (PINTAB)-
CD                        PROBABILITIES GIVEN IN RECORD TYPE 4
CD                        KT=0  CONSTANT PROBABILITY
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F6 (Contd.)

```
CD                    KT=1  LN(ENERGY) VS. LN(PROBABILITY)                -
CD                    KT=2  LN(ENERGY) VS. PROBABILITY                    -
CD                    KT=3  ENERGY VS. PROBABILITY                        -
CD                    KT=4  ENERGY VS. LN(PROBABILITY)                    -
CD    KT2             INTERPOLATION LAW FOR CALCULATING GROUP TO          -
CD                    GROUP TABULATED (N,2N) SCATTERING                   -
CD                    PROBABILITIES FROM THE GROUP TO ENERGY (PNNTAB)     -
CD                    PROBABILITIES GIVEN IN RECORD TYPE 4                -
CD                    KT=0  CONSTANT PROBABILITY                          -
CD                    KT=1  LN(ENERGY) VS. LN(PROBABILITY)                -
CD                    KT=2  LN(ENERGY) VS. PROBABILITY                    -
CD                    KT=3  ENERGY VS. PROBABILITY                        -
CD                    KT=4  ENERGY VS. LN(PROBABILITY)                    -
CD    SUMI            SUM OVER I FOR ALL 14 ARRAYS FOR ALL                -
CD                    MMAT1 MATERIALS                                     -
C                                                                         -
CN                    CROSS SECTION DATA AND CONTROL INFORMATION          -
CN                    DATA ARE PRESENT FOR A MATERIAL ONLY IF THE         -
CN                    MATERIAL HAS THESE DATA PRESENT AS SPECIFIED        -
CN                    IN RECORD TYPE 5 OF MCC2F1. ALSO THESE DATA         -
CN                    ARE PRESENT ONLY IF THE GROUP BEING PROCESSED       -
CN                    IS ABOVE THE THRESHOLD ENERGY OF THE REACTION       -
CN                    BEING CONSIDERED                                    -
CN                                                                        -
CN                    SIGIN IS PRESENT FOR MATERIALS THAT HAVE            -
CN                    INELASTIC DATA FOR THE ENERGY GROUP BEING           -
CN                    PROCESSED. NINEVP IS PRESENT FOR ALL MATERIALS      -
CN                    THAT HAVE MAX1.GT.0. NLVS IS PRESENT FOR ALL        -
CN                    MATERIALS THAT HAVE NLEVLS.GT.0. IN ADDITION        -
CN                    SIGIN, NINEVP, AND NLVS ARE PRESENT ONLY FOR        -
CN                    GROUPS.LE.NINEL                                     -
CN                                                                        -
CN                    SIGN2N IS PRESENT FOR MATERIALS THAT HAVE           -
CN                    (N,2N) DATA FOR THE ENERGY GROUP BEING              -
CN                    PROCESSED. N2NEVP IS PRESENT FOR ALL MATERIALS      -
CN                    THAT HAVE MAX3.GT.0. N2NLV IS PRESENT FOR ALL       -
CN                    MATERIALS THAT HAVE N2NLEV.GT.0. IN ADDITION        -
CN                    SIGN2N, N2NEVP, AND N2NLV ARE PRESENT ONLY          -
CN                    FOR GROUPS.LE.N2NTH                                 -
CN                                                                        -
CN                    NINTAB, NSTRT1, NEND1, AND KT1 ARE PRESENT FOR      -
CN                    ALL MATERIALS THAT HAVE MAX2.GT.0. DATA             -
CN                    PRESENT FOR ALL GROUPS.LE.NINEL                     -
CN                                                                        -
CN                    N2NTAB, NSTRT2, NEND2, AND KT2 ARE PRESENT          -
CN                    FOR ALL MATERIALS THAT HAVE MAX4.GT.0. DATA         -
CN                    PRESENT FOR ALL GROUPS.LE.N2NTH                     -
CN                                                                        -
CN                    NINEL, N2NTH, NLEVLS, N2NLEV, MAX1, MAX2,           -
CN                    MAX3, AND MAX4 ARE PRESENT IN RECORD 5              -
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F6 (Contd.)

```
CN                        OF MCC2F1                                      -
C                                                                        -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR          SECONDARY DISTRIBUTION DATA (TYPE 3)                         -
C                                                                        -
CC          PRESENT IF (NLVS.GT.0) OR (N2NLV.GT.0) OR                    -
CC                     (NINEVP.GT.0) OR (N2NEVP.GT.0)                    -
CC                     FOR ANY MATERIAL                                  -
C                                                                        -
CL    ((SIGLEV(I,J),I=1,NLVSJ),(AVGMU(I,J),I=1,NLVSJ),                   -
CL   1(SIGN(I,J),I=1,N2NLVJ),(TSTAT(I,J),I=1,NINVPJ),                    -
CL   2(PIN(I,J),I=1,NINVPJ),(TN2N(I,J),I=1,N2NVPJ),                      -
CL   3(PN2N(I,J),I=1,N2NVPJ),J=1,MMAT1)                                  -
C                                                                        -
CW    SUMJ                                                               -
C                                                                        -
CD    SIGLEV            GROUP CROSS SECTION ASSOCIATED WITH THE          -
CD                      L'TH RESOLVED INELASTIC SCATTERING LEVEL         -
CD    SIGN              GROUP CROSS SECTION ASSOCIATED WITH THE          -
CD                      L'TH RESOLVED (N,2N) SCATTERING LEVEL            -
CD    AVGMU             AVERAGE COSINE OF THE SCATTERING ANGLE IN        -
CD                      THE CENTER OF MASS SYSTEM FOR THE GROUP IN       -
CD                      QUESTION FOR DISCRETE INELASTIC SCATTERING       -
CD    TSTAT             GROUP AVERAGED "STATISTICAL" INELASTIC           -
CD                      TEMPERATURE                                      -
CD    PIN               FRACTIONAL PROBABILITY THAT THE I'TH INELASTIC   -
CD                      EVAPORATION LAW CAN BE USED FOR THE GROUP IN     -
CD                      QUESTION                                         -
CD    TN2N              AVERAGE GROUP TEMPERATURE ASSOCIATED WITH A      -
CD                      STATISTICAL CALCULATION OF (N,2N) SCATTERING     -
CD                      FOR THE I'TH DISTRIBUTION                        -
CD    PN2N              FRACTIONAL PROBABILITY THAT THE I'TH (N,2N)      -
CD                      EVAPORATION LAW CAN BE USED FOR THE GROUP IN     -
CD                      QUESTION                                         -
CD    SUMJ              SUM OF (2*(NLVSJ+NINVPJ+N2NVPJ)+N2NLVJ) OVER     -
CD                      ALL MMAT MATERIALS                               -
CD    NLVSJ             = NLVS(J) FOR CURRENT MATERIAL J                 -
CD    N2NLVJ            = N2NLV(J) FOR CURRENT MATERIAL J                -
CD    NINVPJ            = NINEVP(J) FOR CURRENT MATERIAL J               -
CD    N2NVPJ            = N2NEVP(J) FOR CURRENT MATERIAL J               -
C                                                                        -
CN                      THE INELASTIC AND (N,2N) CONTROL INFORMATION     -
CN                      NLVS, N2NLV, NINEVP, AND N2NEVP ARE SPECIFIED    -
CN                      IN RECORD TYPE 2 OF MCC2F6                       -
CN                                                                       -
CN                      IF FOR A GIVEN MATERIAL J, THE VALUE OF NLVSJ,   -
CN                      N2NLVJ, NINVPJ, OR N2NVPJ ARE ZERO, THEN THE
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F6 (Contd.)

```
CN                      DATA IN THE ARRAY IN QUESTION ARE NOT PRESENT  -
C                                                                      -
C----------------------------------------------------------------------

C----------------------------------------------------------------------
CR          TABULATED INELASTIC AND (N,2N) PROBABILITIES (TYPE 4)      -
C                                                                      -
CC           PRESENT IF (NINTAB.GT.0) OR (N2NTAB.GT.0)                 -
CC                      FOR ANY MATERIAL                               -
C                                                                      -
CL     ((PINTAB(I,J),I=1,K1),(PNNTAB(I,J),I=1,K2),J=1,MMAT1)           -
C                                                                      -
CW     (K1+K2)*MMAT1                                                   -
C                                                                      -
CD     PINTAB              TABULATED PROBABILITY OF A NEUTRON BEING    -
CD                         INELASTICALLY SCATTERED FROM THE GROUP IN   -
CD                         QUESTION TO ALL POSSIBLE SINK ENERGIES (EIN).-
CD                         PINTAB(1)=PROBABILITY OF SCATTERING FROM    -
CD                         GROUP IN QUESTION TO ENERGY EIN(NSTRT1)     -
CD                         PINTAB(K1)=PROBABILITY OF SCATTERING FROM GROUP-
CD                         IN QUESTION INTO ENERGY EIN(NEND1)          -
CD                         PINTAB IS CALCULATED AS THE SUM OVER ALL    -
CD                         (ENDF/B) GIVEN TABULATED INELASTIC          -
CD                         DISTRIBUTIONS OF THE PARTIAL ENERGY         -
CD                         DISTRIBUTION*FRACTIONAL PROBABILITY         -
CD     K1                  NEND1(J)-NSTRT1(J)+1                        -
CD     PNNTAB              TABULATED PROBABILITY OF A NEUTRON BEING    -
CD                         (N,2N) SCATTERED FROM THE GROUP IN          -
CD                         QUESTION INTO ALL POSSIBLE SINK ENERGIES (EN2N)-
CD                         PNNTAB(1)=PROBABILITY OF SCATTERING FROM    -
CD                         GROUP IN QUESTION TO ENERGY EN2N(NSTRT2)    -
CD                         PNNTAB(K2)=PROBABILITY OF SCATTERING FROM GROUP-
CD                         IN QUESTION INTO ENERGY EN2N(NEND2)         -
CD                         PNNTAB IS CALCULATED AS THE SUM OVER ALL    -
CD                         (ENDF/B) GIVEN TABULATED (N,2N)             -
CD                         DISTRIBUTIONS OF THE PARTIAL ENERGY         -
CD                         DISTRIBUTION*FRACTIONAL PROBABILITY         -
CD     K2                  NEND2(J)-NSTRT2(J)+1                        -
C                                                                      -
CN                         PINTAB IS PRESENT ONLY IF NINTAB.GT.0       -
CN                         PNNTAB IS PRESENT ONLY IF N2NTAB.GT.0       -
CN                                                                     -
CN                         NEND1, NSTRT1, NEND2, NSTRT2, NINTAB, AND   -
CN                         N2NTAB ARE SPECIFIED IN RECORD TYPE 2       -
CN                         OF MCC2F6                                   -
C                                                                      -
C----------------------------------------------------------------------

:EOF
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F7

```
C*****************************************************************
C                                                                -
C                       PREPARED 2/11/75 AT ANL                  -
C                                                                -
CF          MCC2F7                                               -
CE          FISSION SPECTRA DATA                                 -
C                                                                -
C*****************************************************************


CD    ICHI              FLAG INDICATING WHETHER PARAMETERS IN
CD                      GENERALIZED FISSION SPECTRUM ARE ENERGY
CD                      (GROUP) DEPENDENT OR NOT
CD                      ICHI=1  PARAMETERS NOT ENERGY DEPENDENT
CD                      ICHI=NGROUP  PARAMETERS ARE ENERGY DEPENDENT
CD                                   AND NGROUP, THE NUMBER OF GROUPS
CD                                   IN THE LIBRARY IS SPECIFIED IN THE
CD                                   ADMINISTRATIVE FILE MCC2F1
CD    MSORS             NUMBER OF FISSION SPECTRA IN LIBRARY
CD                      AS SPECIFIED IN THE ADMINISTRATIVE
CD                      FILE MCC2F1
CD    MULT              2 FOR IBM MACHINES, 1 OTHERWISE


C-----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                          PRESENT IF      -
CS          ===================================  ================-
CS          MATERIAL NAMES                       ALWAYS          -
CS          SPECIFICATIONS                       ALWAYS          -
CS    ******** (REPEAT MSORS TIMES)                             -
CS    *     FISSION SPECTRA                      ALWAYS          -
CS    ********                                                  -
C                                                                -
C-----------------------------------------------------------------


C-----------------------------------------------------------------
CR          MATERIAL NAMES (TYPE 1)                              -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL    (NAME(I),I=1,MSORS)                                        -
C                                                                -
CW    MULT*MSORS                                                 -
C                                                                -
CD    NAME              DOUBLE PRECISION (R*8) MATERIAL IDENTIFICATION -
CD                      ASSOCIATED WITH THE GIVEN FISSION SPECTRUM      -
CD                      PARAMETERS
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F7 (Contd.)

```
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          SPECIFICATIONS (TYPE 2)                                     -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    (ICHI(I),I=1,MSORS)                                               -
C                                                                       -
CW    MSORS                                                             -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          FISSION SPECTRA (TYPE 3)                                    -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    (BETA(I),I=1,ICHI),(ALPHA(I),I=1,ICHI),(TAU(I),I=1,ICHI)          -
C                                                                       -
CW    3*ICHI                                                            -
C                                                                       -
CD    BETA,ALPHA,TAU    PARAMETERS IN GENERALIZED FISSION SPECTRUM       -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F8

```
C*****************************************************************
C                                                                 -
C                        PREPARED 2/11/75 AT ANL                  -
C                                                                 -
CF          MCC2F8                                                -
CE          LEGENDRE DATA                                         -
C                                                                 -
C*****************************************************************


CD    IL                NUMBER OF BLOCKS OF DATA FOR A GIVEN MATERIAL
CD                      NO DATA ARE PROVIDED FOR ENERGIES BELOW
CD                      WHICH SCATTERING IS ISOTROPIC
CD    IPT               NUMBER OF LEGENDRE COEFFICIENTS PROVIDED FOR
CD                      EACH BLOCK OF DATA BY MATERIAL
CD    IR                NUMBER OF INTERPOLATION REGIONS FOR LEGENDRE
CD                      DATA RECORD
CD    MULT              2 FOR IBM MACHINES, 1 OTHERWISE
CD    NPL               HIGHEST ORDER PERMITTED FOR EXTENDED TRANSPORT
CD                      APPROXIMATION AS SPECIFIED IN THE
CD                      ADMINISTRATIVE FILE MCC2F1


C-----------------------------------------------------------------
CS          FILE STRUCTURE                                        -
CS                                                                -
CS          RECORD TYPE                          PRESENT IF       -
CS          ===================================  ================-
CS          SPECIFICATIONS                       ALWAYS           -
CS    ******** (REPEAT FOR ALL MATERIALS)                         -
CS    *     MATERIAL IDENTIFICATION              ALWAYS           -
CS    *     T MATRIX AND INTERPOLATION DATA      ALWAYS           -
CS    *  ***** (REPEAT IL TIMES)                                  -
CS    *  *  LEGENDRE COEFFICIENTS                IL.GT.0          -
CS    ********                                                    -
C                                                                 -
C-----------------------------------------------------------------


C-----------------------------------------------------------------
CR          SPECIFICATIONS (TYPE 1)                               -
C                                                                 -
CC          ALWAYS PRESENT                                        -
C                                                                 -
CL    (LGTH(I),I=1,NMAT),(IR(I),I=1,NMAT),(IL(I),I=1,NMAT),       -
CL   1((IPT(I,J),I=1,NPASS),J=1,NMAT)                             -
C                                                                 -
CW    NMAT*(3+NPASS)                                              -
C                                                                 -
CD    LGTH              LENGTH (IN WORDS) OF
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F8 (Contd.)

```
CD                      T MATRIX AND INTERPOLATION DATA RECORD          -
CD    NMAT              NUMBER OF MATERIALS IN LIBRARY AS SPECIFIED     -
CD                      IN THE ADMINISTRATIVE FILE MCC2F1               -
CD    NPASS             NUMBER OF 'BLOCKS' OF LEGENDRE DATA             -
CD                      AS SPECIFIED IN THE ADMINISTRATIVE FILE         -
CD                      MCC2F1                                          -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          MATERIAL IDENTIFICATION (TYPE 2)                            -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    NAME                                                            -
C                                                                       -
CW    MULT*1                                                          -
C                                                                       -
CD    NAME              DOUBLE PRECISION (R*8) MATERIAL IDENTIFICATION -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          T MATRIX AND INTERPOLATION DATA (TYPE 3)                    -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    (KT(I),I=1,IR),(NG(I),I=1,IR),                                    -
CL   1((TLJ(L,J),L=1,NPL),J=1,MAX(IPT)+1),                              -
CL   2((TLJ1(L,J),L=1,2),J=1,MAX(IPT)+1),                               -
CL   3((TLJ2(L,J),L=1,2),J=1,6),((FACK(I,J),I=1,6),J=1,6),              -
CL   4((FAC(I,J),I=1,4),J=1,MAX(IPT)+1)                                 -
C                                                                       -
CW    2*IR+MULT*(54+MAX(IPT)*(NPL+6)+NPL)   FOR DELTAU.GE.Q (SEE BELOW) -
CW    2*IR+MULT*(50+MAX(IPT)*(NPL+2)+NPL)   FOR DELTAU.LT.Q (SEE BELOW) -
C                                                                       -
CD    KT                INTERPOLATION LAW USED TO OBTAIN HYPERFINE     -
CD                      GROUP VALUES OF THE LEGENDRE COEFFICIENTS,     -
CD                      F1,F2,...,FN, IN THE INTERPOLATION REGION I    -
CD                      KT=0  CONSTANT                                 -
CD                      KT=1  LN E VS. LN FN                           -
CD                      KT=2  LN E VS. FN                              -
CD                      KT=3  E VS. FN                                 -
CD                      KT=4  E VS. LN FN                              -
CD    NG                LOWEST ENERGY GROUP NUMBER (HIGHEST ENERGY)    -
CD                      FOR WHICH INTERPOLATION LAW APPLIES            -
CD    TLJ               STANDARD ZERO ORDER T MATRIX ELEMENTS          -
CD    TLJ1              STANDARD FIRST ORDER T MATRIX ELEMENTS         -
```

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F8 (Contd.)

```
CD     TLJ2                STANDARD SECOND ORDER T MATRIX ELEMENTS          -
CD     FACK                MASS DEPENDENT CONSTANTS USED IN CALCULATION     -
CD                         OF CONTINUOUS SLOWING DOWN MODERATING            -
CD                         PARAMETERS                                       -
CD     FAC                 'INCOMPLETE' T MATRIX ELEMENTS                   -
CD                         THE ARRAY FAC IS PRESENT ONLY FOR THOSE          -
CD                         ELEMENTS THAT HAVE                               -
CD                         DELTAU.GE.Q                                      -
CD                         WHERE Q=LOG(((A+1)/(A-1))**2)/3.                 -
CD                         DELTAU AND A ARE THE GROUP LETHARGY              -
CD                         WIDTH AND MATERIAL MASS/NEUTRON MASS             -
CD                         RESPECTIVELY. BOTH ARE SPECIFIED IN THE          -
CD                         ADMINISTRATIVE FILE MCC2F1                       -
C                                                                           -
CN                         ALL REAL ARRAYS, TLJ,TLJ1,TLJ2,FACK, AND FAC     -
CN                         ARE WRITTEN IN DOUBLE PRECISION (REAL*8)         -
C                                                                           -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR           LEGENDRE COEFFICIENTS (TYPE 4)                                 -
C                                                                           -
CC           PRESENT IF IL.GT.0                                             -
C                                                                           -
CL     (F1(J),F2(J),...,FN(J),J=1,MANY1)                                    -
C                                                                           -
CW     MANY1*IPT                                                            -
C                                                                           -
CD     F1,F2,...,FN        FIRST,SECOND,...,N'TH ORDER EXPANSION            -
CD                         COEFFICIENT AT THE ENERGY LEVEL SPECIFIED        -
CD                         BY THE INDEX J.  FOR EXAMPLE, ON THE THIRD       -
CD                         PASS, THE THIRD BLOCK OF DATA, F1(1) WOULD       -
CD                         BE THE FIRST ORDER COEFFICIENT FOR ENERGY        -
CD                         LEVEL 2*MANY1-1                                  -
CD                         THE NUMBER OF COEFFICIENTS (N) FOR A GIVEN       -
CD                         'BLOCK' OF DATA IS GIVEN BY THE ARRAY IPT        -
CD                         IN THE TABLE OF CONTENTS. NOTE THAT              -
CD                         F0(J)=1.0 AND IS THEREFORE NOT TABULATED. THIS   -
CD                         RECORD IS NOT PROVIDED FOR THOSE ENERGY BLOCKS   -
CD                         CORRESPONDING TO ENERGIES BELOW WHICH            -
CD                         SCATTERING IS ISOTROPIC IN THE CENTER OF         -
CD                         MASS SYSTEM.                                     -
CD     MANY1               NUMBER OF ENERGY LEVELS FOR EACH 'BLOCK' OF      -
CD                         DATA (EXCEPT THE LAST) AS SPECIFIED IN THE       -
CD                         ADMINISTRATIVE FILE MCC2F1                       -
CD                         RECOMMENDED MAXIMUM VALUE FOR MANY1 WOULD BE     -
CD                         MANY1=126                                        -
C
C-------------------------------------------------------------------------

CEOF
```

APPENDIX C. MC^2-2 Binary Interface Files. XS.ISO

```
C*****************************************************************
C                                                                -
C                        PREPARED 3/11/76 AT ANL                 -
C                                                                -
CF          XS.ISO                                               -
CE          MICROSCOPIC GROUP CROSS SECTIONS, FILE 1             -
C                                                                -
CN                      THIS IS FILE 1 OF A TWO-FILE DATA SET    -
CN                      CONTAINING MICROSCOPIC GROUP CROSS SECTIONS. -
C                                                                -
C*****************************************************************


CD    NGROUP            NUMBER OF BROAD ENERGY GROUPS IN SET.
CD    NISO              NUMBER OF ISOTOPES IN SET.
CD    MULT              2 FOR IBM MACHINES, 1 OTHERWISE.


C-----------------------------------------------------------------
CR          FILE SIZE (TYPE 1)                                   -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL    NGROUP,NISO,MAXUP,MAXDN,MAXORD,IPREC                       -
C                                                                -
CW    6                                                          -
C                                                                -
CD    MAXUP             MAXIMUM NUMBER OF GROUPS OF UPSCATTER IN THE -
CD                      SET.                                     -
CD    MAXDN             MAXIMUM NUMBER OF GROUPS OF DOWNSCATTER IN THE -
CD                      SET.                                     -
CD    MAXORD            (MAXIMUM OF LEL, LIN, OR LN2N FOR THE SET)-1 -
CD                      (SEE ISOTOPE HEADING RECORD OF DATA SET XS.ISO, -
CD                      FILE 2).                                 -
CD    IPREC             0 FOR DOUBLE PRECISION VERSION OF DATA SET -
CD                      XS.ISO, 1 FOR SINGLE PRECISION VERSION OF THE -
CD                      DATA SET.                                -
C                                                                -
C-----------------------------------------------------------------


C-----------------------------------------------------------------
CR          ISOTOPE NAMES (TYPE 2)                               -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL    (ISONAM(I),I=1,NISO),(LOCA(I),I=1,NISO1),(TEMP(I),I=1,NISO), -
CL   1(TNAME(I),I=1,NISO),(AMASS(I),I=1,NISO)                    -
C                                                                -
CC    NISO1=NISO+1                                               -
```

APPENDIX C. MC^2-2 Binary Interface Files. XS.ISO (Contd.)

```
C                                                                       -
CW     NTSO+1+2*MULT*NISO+2*NISO*(2-IPREC)                              -
C                                                                       -
CD     ISONAM(I)          LOCAL NAME OF I-TH ISOTOPE (REAL*8).          -
CD     LOCA(I)            NUMBER OF RECORDS IN FILE 2 OF XS.ISO TO BE   -
CD                        SKIPPED TO READ DATA FOR ISOTOPE I. LOCA(1)=0. -
CD     TEMP(I)            TEMPERATURE OF I-TH ISOTOPE.                  -
CD     TNAME              I-TH ISOTOPE NAME AS GIVEN IN ENDF/B FILES.   -
CD     AMASS              GRAM ATOMIC WEIGHTS OF THE ISOTOPES.          -
C                                                                       -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR           GROUP STRUCTURE (TYPE 3)                                   -
C                                                                       -
CC           ALWAYS PRESENT                                             -
C                                                                       -
CL     ICHI,(E(I),I=1,NGP1),(U(I),I=1,NGP1),(VEL(I),I=1,NGROUP)         -
C                                                                       -
CC     NGP1=NGROUP+1                                                    -
C                                                                       -
CW     1+(3*NGROUP+2)*(2-IPREC)                                         -
C                                                                       -
CD     ICHI               FISSION SPECTRUM FLAG FOR SET.                -
CD                        ICHI=0, NO SET CHI.                           -
CD                            =1, SET CHI VECTOR.                       -
CD                            =NGROUP, SET CHI MATRIX.                  -
CD     E(I)               ENERGY BOUNDARIES OF GROUPS. E(1) IS          -
CD                        THE MAXIMUM ENERGY.                           -
CD     U(I)               LETHARGY BOUNDARIES OF GROUPS. U(1)=0.        -
CD     VEL(I)             NEUTRON SPEED FOR GROUP I,                    -
CD                        SPEED   1./(1./V).                            -
C                                                                       -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR           SET FISSION SPECTRUM (TYPE 4)                              -
C                                                                       -
CC           PRESENT IF ICHI.NE.0                                       -
C                                                                       -
CL     ((CHI(I,J),I=1,ICHI),J=1,NGROUP)                                 -
C                                                                       -
CW     ICHI*NGROUP*(2-IPREC)                                            -
C                                                                       -
CD     CHI(I,J)           PROMPT FISSION FRACTION INTO GROUP J          -
CD                        FROM GROUP I.                                 -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX C. MC^2-2 Binary Interface Files. XS.ISO (Contd.)

```
C*****************************************************************
C                                                                -
C                        PREPARED 3/11/76 AT ANL                 -
C                                                                -
CF          XSISO2                                               -
CE          MICROSCOPIC GROUP CROSS SECTIONS, FILE 2             -
C                                                                -
CN                      THIS IS FILE 2 OF A TWO-FILE DATA SET    -
CN                      CONTAINING MICROSCOPIC GROUP CROSS SECTIONS. -
C                                                                -
C*****************************************************************


C----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS             RECORD TYPE                          PRESENT IF   -
CS             ================================     ============-
CS     ************(REPEAT FOR ALL ISOTOPES)                     -
CS     *       ISOTOPE NAME                         ALWAYS       -
CS     *       ISOTOPE HEADING                      ALWAYS       -
CS     *       ISOTOPE FISSION SPECTRUM             ICHI.GT.0    -
CS     *  *********(REPEAT FOR ALL GROUPS)                       -
CS     *  *    PRINCIPAL CROSS SECTIONS             ALWAYS       -
CS     *  *********                                             -
CS     *                                                        -
CS     *  *********(REPEAT FOR EACH SCATTERING ORDER             -
CS     *  *          L=1,LMAX, WHERE LMAX IS THE                -
CS     *  *          LARGEST OF LIN, LEL, AND LN2N.             -
CS     *  *          SEE ISOTOPE HEADING RECORD.)               -
CS     *  *  ******(REPEAT FOR ALL GROUPS)                      -
CS     *  *  *  INDEX FOR SCATTERING GROUP        ALWAYS       -
CS     *  *  *  INELASTIC SCATTERING              LIN.GE.L     -
CS     *  *  *  ELASTIC SCATTERING                LEL.GE.L     -
CS     *  *  *  (N,2N) SCATTERING                 LN2N.GE.L    -
CS     ************                                             -
C                                                                -
C----------------------------------------------------------------


CD     LELDN            NUMBER OF ELASTIC DOWNSCATTER GROUPS.
CD     LELUP            NUMBER OF ELASTIC UPSCATTER GROUPS.
CD     LINDN            NUMBER OF INELASTIC DOWNSCATTER GROUPS.
CD     LINUP            NUMBER OF INELASTIC UPSCATTER GROUPS.
CD     LN2NDN           NUMBER OF (N,2N) DOWNSCATTER GROUPS.
CD     LN2NUP           NUMBER OF (N,2N) UPSCATTER GROUPS.
CD     NGROUP           NUMBER OF ENERGY GROUPS IN THE SET.
CD     MULT             2 FOR IBM MACHINES, 1 OTHERWISE.
CD     IPREC            0 FOR DOUBLE PRECISION VERSION OF DATA SET
CD                      XS.ISO, 1 FOR SINGLE PRECISION VERSION OF THE
```

APPENDIX C. MC^2-2 Binary Interface Files. XS.ISO (Contd.)

```
CD                          DATA SET.

C-------------------------------------------------------------------
CR          ISOTOPE NAME (TYPE 1)                                  -
C                                                                  -
CC          ALWAYS PRESENT                                         -
C                                                                  -
CL    ISONAM                                                       -
C                                                                  -
CW    MULT                                                         -
C                                                                  -
CD    ISONAM              ISOTOPE NAME (REAL*8).                 -
C                                                                  -
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          ISOTOPE HEADING RECORD (TYPE 2)                        -
C                                                                  -
CC          ALWAYS PRESENT                                         -
C                                                                  -
CL    ICHI,LIN,LEL,LN2N,EFISS,ECAPT                                -
C                                                                  -
CW    4+2*(2-IPREC)                                                -
C                                                                  -
CD    ICHI                ISOTOPE FISSION SPECTRUM FLAG.         -
CD                        ICHI=-1, ISOTOPE USES PROMPT FISSION SPECTRUM -
CD                                 FOR SET.                        -
CD                            =0, ISOTOPE IS NOT FISSIONABLE.     -
CD                            =1, ISOTOPE USES OWN PROMPT FISSION -
CD                                 SPECTRUM WHICH IS NOT INCIDENT-ENERGY- -
CD                                 DEPENDENT (VECTOR).             -
CD                           =NGROUP, ISOTOPE USES OWN PROMPT FISSION -
CD                                 SPECTRUM WHICH IS INCIDENT-ENERGY- -
CD                                 DEPENDENT (MATRIX).             -
CD    LIN                 MAXIMUM ORDER OF INELASTIC SCATTERING. -
CD                        LIN=0, NO SCATTERING.                   -
CD                           =1, ISOTROPIC SCATTERING.            -
CD                           =2, LINEAR ANISOTROPIC SCATTERING.   -
CD                           =N, ORDER N-1 ANISOTROPIC SCATTERING. -
CD    LEL                 MAXIMUM ORDER OF ELASTIC SCATTERING.   -
CD                        LEL=0, NO SCATTERING.                   -
CD                           =1, ISOTROPIC SCATTERING.            -
CD                           =2, LINEAR ANISOTROPIC SCATTERING.   -
CD                           =N, ORDER N-1 ANISOTROPIC SCATTERING. -
CD    LN2N                MAXIMUM ORDER OF (N,2N) SCATTERING.    -
CD                        LN2N=0, NO SCATTERING.                  -
CD                            =1, ISOTROPIC SCATTERING.           -
CD                            =2, LINEAR ANISOTROPIC SCATTERING.
```

APPENDIX C. MC^2-2 Binary Interface Files. XS.ISO (Contd.)

```
CD                          =N, ORDER N-1 ANISOTROPIC SCATTERING.
CD     EFISS                WATT-SECONDS/FISSION.
CD     ECAPT                WATT-SECONDS/CAPTURE WHERE CAPTURE REFERS TO
CD                          NON-FISSION ABSORPTION.
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR           ISOTOPE FISSION SPECTRUM (TYPE 3)
C
CC           PRESENT IF ICHI.GT.0 (SEE ISOTOPE HEADING RECORD)
C
CL     ((CHI(I,J),I=1,ICHI),J=1,NGROUP) ,
C
CW     ICHI*NGROUP*(2-IPREC)
C
CD     CHI(I,J)             FISSION SPECTRUM INCIDENT IN GROUP J, BORN
CD                          IN GROUP I.
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR           PRINCIPAL CROSS SECTIONS (TYPE 4)
C
CC           ALWAYS PRESENT
C
CL     J,STR,SCAP,SNALF,SNP,ANISO,SFIS,FISNU
C
CW     1+7*(2-IPREC)   IF ICHI.NE.0
CW     1+5*(2-IPREC)   IF ICHI.EQ.0
C
CD     J                    GROUP INDEX.
CD     STR                  TRANSPORT CROSS SECTION.
CD     SCAP                 RADIATIVE CAPTURE (N,GAMMA) CROSS SECTION.
CD     SNALF                (N,ALPHA) CROSS SECTION.
CD     SNP                  (N,P) CROSS SECTION.
CD     ANISO                ISOTROPIC ELASTIC SELF-SCATTERING CONSISTENT
CD                          WITH ANISOTROPIC TOTAL CROSS SECTION.
CD                          ANISO, WHEN ADDED TO THE SUM OF ALL EVENTS
CD                          WHICH REMOVE A NEUTRON FROM THE GROUP,
CD                          YIELDS THE TOTAL GROUP CROSS SECTION.
CD     SFIS                 FISSION CROSS SECTION, PRESENT IF ICHI.NE.0.
CD     FISNU                NUMBER OF FISSION NEUTRONS PER FISSION TIMES
CD                          FISSION CROSS SECTION, PRESENT IF ICHI.NE.0.
C
C-------------------------------------------------------------------
```

APPENDIX C. MC^2-2 Binary Interface Files. XS.ISO (Contd.)

```
C-----------------------------------------------------------------------
CR          INDEX FOR SCATTERING GROUP (TYPE 5)                        -
C                                                                      -
CC          PRESENT IF LIN+LEL+LN2N.NE.0                               -
CC          (SEE ISOTOPE HEADING RECORD)                               -
C                                                                      -
CL    LINUP,LINDN,LELUP,LELDN,LN2NUP,LN2NDN                            -
C                                                                      -
CW    6                                                                -
C                                                                      -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          INELASTIC SCATTERING (TYPE 6)                              -
C                                                                      -
CC          PRESENT IF LIN.GE.CURRENT SCATTERING ORDER                 -
CC          (SEE ISOTOPE HEADING RECORD)                               -
C                                                                      -
CL    SINL(J+LINUP),SINL(J+LINUP-1),...,SINL(J),...,SINL(J-LINDN)      -
C                                                                      -
CW    (LINUP+LINDN+1)*(2-IPREC)                                        -
C                                                                      -
CD    SINL(K)           INELASTIC SCATTERING, GROUP K TO GROUP J.      -
C                                                                      -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          ELASTIC SCATTERING (TYPE 7)                                -
C                                                                      -
CC          PRESENT IF LEL.GE.CURRENT SCATTERING ORDER                 -
CC          (SEE ISOTOPE HEADING RECORD)                               -
C                                                                      -
CL    SELT(J+LELUP),SELT(J+LELUP-1),...,SELT(J),...,SELT(J-LELDN)      -
C                                                                      -
CW    (LELUP+LELDN+1)*(2-IPREC)                                        -
C                                                                      -
CD    SELT(K)           ELASTIC SCATTERING, GROUP K TO GROUP J.        -
C                                                                      -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          (N,2N) SCATTERING (TYPE 8)                                 -
C                                                                      -
CC          PRESENT IF LN2N.GE.CURRENT SCATTERING ORDER                -
CC          (SEE ISOTOPE HEADING RECORD)                               -
C                                                                      -
CL    SN2N(J+LN2NUP),SN2N(J+LN2NUP-1),...,SN2N(J),...,SN2N(J-LN2NDN)
```

APPENDIX C. MC^2-2 Binary Interface Files. XS.ISO (Contd.)

```
C                                                                       -
CW     (LN2NUP+LN2NDN+1)*(2-IPREC)                                      -
C                                                                       -
CD     SN2N(K)              (N,2N) SCATTERING, GROUP K TO GROUP J.      -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX D

MC^2-2 BINARY FILES

APPENDIX D. MC^2-2 Binary Files. ATNUAT

```
C*****************************************************************
C                                                                -
C                        PREPARED 3/05/75 AT ANL                 -
C                                                                -
CF          ATNUAT                                               -
CE          UNRESOLVED RESONANCE INTEGRALS                       -
C                                                                -
CN                       THIS DATA SET IS WRITTEN BY MC**2-II AREA 5    -
CN                       (CSC004) IF UNRESOLVED MATERIALS ARE PRESENT   -
C                                                                -
C*****************************************************************


CD     IFI               FISSILE MATERIAL INDEX
CD                       IFI=0 FOR NON-FISSILE MATERIAL
CD                       IFI=1 FOR FISSILE MATERIAL
CD     JL                NUMBER OF SPIN STATES FOR CURRENT ISOTOPE
CD     MULT              2 FOR IBM MACHINES, 1 OTHERWISE
CD     NESF              NUMBER OF FIXED ENERGY MESH POINTS
CD     NREG              NUMBER OF REGIONS
CD                       NREG=1 FOR HOMOGENEOUS PREOBLEMS (NGEOM=0)
CD                       NREG=2 FOR PIN CELLS (NGEOM=2) AND IF
CD                              MAXHTM.GT.0
CD                       NREG=1 + NUMBER OF SLAB REGIONS FOR SLAB
CD                              PROBLEMS (NGEOM=1) AND IF MAXHTM.GT.0
CD                       (MAXHTM IS THE MAXIMUM NUMBER OF MATERIALS IN
CD                        ANY HETEROGENEOUS REGION)
CD     NUMRES            NUMBER OF UNRESOLVED RESONANCE MATERIALS
CD     NUNRES            NUNRES=0 IF UNRESOLVED RESONANCE CROSS SECTIONS
CD                       ARE GENERATED. NUNRES=1 IF UNRESOLVED RESONANCE
CD                       INTEGRALS ARE GENERATED


C----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS             RECORD TYPE                          PRESENT IF   -
CS             ================================     ============-
CS             SPECIFICATIONS                       ALWAYS       -
CS             MATERIAL NAMES                       ALWAYS       -
CS             FIXED UNRESOLVED RESONANCE           ALWAYS       -
CS             ENERGY MESH                                       -
CS    ********** (REPEAT FOR NUMRES MATERIALS)                   -
CS    *        MATERIAL SPECIFICATIONS              ALWAYS       -
CS    *  ******** (REPEAT FOR NISO ISOTOPES)                     -
CS    *  *     SPIN STATE DATA                      ALWAYS       -
CS    *  *     LEVEL SPACING                        ALWAYS       -
CS    *  *  ***** (REPEAT FOR 1+NO. OF REGIONS                   -
CS    *  *  *       IN WHICH MATERIAL IS TREATED                -
CS    *  *  *       HETEROGENEOUSLY)                            -
```

APPENDIX D. MC^2-2 Binary Files. ATNUAT (Contd.)

```
CS     *  *  *  CAPTURE J INTEGRAL                    ALWAYS
CS     *  *  *  TOTAL J INTEGRAL                      ALWAYS
CS     *  *  *  FISSION J INTEGRAL                    IFI.EQ.1
CS     **********
CS              TOTAL FLUX CORRECTION FACTOR          ALWAYS
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          SPECIFICATIONS (TYPE 1)
C
CC          ALWAYS PRESENT
C
CL     NUMRES,NESF,NREG,JLMAX,MAXISO
C
CW     5
C
CD     JLMAX              LSTMAX*JSTMAX WHERE LSTMAX IS THE MAXIMUM
CD                        VALUE OF THE NUMBER OF ANGULAR MOMENTUM
CD                        STATES OVER ALL MATERIALS IN THE FILE AND
CD                        JSTMAX IS THE MAXIMUM VALUE OF THE NUMBER OF
CD                        CHANNEL SPIN STATES ASSOCIATED WITH A
CD                        PARTICULAR ANGULAR MOMENTUM STATE OVER ALL
CD                        MATERIALS IN THE FILE
CD     MAXISO             MAXIMUM NUMBER OF ISOTOPES IN THE MIXTURE
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          MATERIAL NAMES (TYPE 2)
C
CC          ALWAYS PRESENT
C
CL     (UNRMAT(I),I=1,NUMRES)
C
CW     MULT*NUMRES
C
CD     UNRMAT             DOUBLE PRECISION (R*8) UNRESOLVED RESONANCE
CD                        MATERIAL NAMES
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          FIXED UNRESOLVED RESONANCE ENERGY MESH (TYPE 3)
C
CC          ALWAYS PRESENT
C
```

APPENDIX D. MC^2-2 Binary Files. ATNUAT (Contd.)

```
CL     (ESF(I),I=1,NESF)                                                -
C                                                                       -
CW     NESF                                                             -
C                                                                       -
CD     ESF                 FIXED ENERGY MESH POINTS GIVEN IN ORDER OF   -
CD                         DECREASING ENERGY                            -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR           MATERIAL SPECIFICATIONS (TYPE 4)                           -
C                                                                       -
CC           ALWAYS PRESENT                                             -
C                                                                       -
CL     NISO,IFI                                                         -
C                                                                       -
CW     2                                                                -
C                                                                       -
CD     NISO                NUMBER OF ISOTOPES                           -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR           SPIN STATE DATA (TYPE 5)                                   -
C                                                                       -
CC           ALWAYS PRESENT                                             -
C                                                                       -
CL     JL                                                               -
C                                                                       -
CW     1                                                                -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR           LEVEL SPACING (TYPE 6)                                     -
C                                                                       -
CC           ALWAYS PRESENT                                             -
C                                                                       -
CL     ((D(I,J),I=1,NESF),J=1,JL)                                       -
C                                                                       -
CW     NESF*JL                                                          -
C                                                                       -
CD     D                   AVERAGE LEVEL SPACING                        -
C                                                                       -
C-----------------------------------------------------------------------
```

APPENDIX D. MC^2-2 Binary Files. ATNUAT (Contd.)

```
C-----------------------------------------------------------------------
CR          CAPTURE J INTEGRAL (TYPE 7)                                -
C                                                                      -
CC          ALWAYS PRESENT FOR THE HOMOGENEOUS MIXTURE.                -
CC          ALSO PRESENT FOR EACH HETEROGENEOUS REGION IN WHICH        -
CC          CURRENT MATERIAL IS TREATED HETEROGENEOUSLY                -
C                                                                      -
CL    ((UCJ(I,J),I=1,NESF),J=1,JL)                                     -
C                                                                      -
CW    NESF*JL                                                          -
C                                                                      -
CD    UCJ               UNRESOLVED RESONANCE CAPTURE INTEGRAL          -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          TOTAL J INTEGRAL (TYPE 8)                                  -
C                                                                      -
CC          ALWAYS PRESENT FOR THE HOMOGENEOUS MIXTURE.                -
CC          ALSO PRESENT FOR EACH HETEROGENEOUS REGION IN WHICH        -
CC          CURRENT MATERIAL IS TREATED HETEROGENEOUSLY                -
C                                                                      -
CL    ((UTJ(I,J),I=1,NESF),J=1,JL)                                     -
C                                                                      -
CW    NESF*JL                                                          -
C                                                                      -
CD    UTJ               UNRESOLVED RESONANCE TOTAL INTEGRAL            -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          FISSION J INTEGRAL (TYPE 9)                                -
C                                                                      -
CC          IF IFI.EQ.1, ALWAYS PRESENT FOR THE HOMOGENEOUS MIXTURE.   -
CC          ALSO PRESENT FOR EACH HETEROGENEOUS REGION IN WHICH        -
CC          CURRENT MATERIAL IS TREATED HETEROGENEOUSLY                -
C                                                                      -
CL    ((UFJ(I,J),I=1,NESF),J=1,JL)                                     -
C                                                                      -
CW    NESF*JL                                                          -
C                                                                      -
CD    UFJ               UNRESOLVED RESONANCE FISSION INTEGRAL          -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          TOTAL FLUX CORRECTION FACTOR (TYPE 10)
```

APPENDIX D. MC^2-2 Binary Files. ATNUAT (Contd.)

```
C
CC          ALWAYS PRESENT
C
CL     (TOTFCF(I,J),I=1,NESF),J=1,NREG)
C
CW     NESF*NREG
C
CD     TOTFCF              TOTAL FLUX CORRECTION FACTOR
C
C-------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. BC

```
C*****************************************************************
C                                                                 -
C                        PREPARED 6/13/75 AT ANL                  -
C                                                                 -
CF          BC                                                    -
CE          BOUNDARY CONDITION SPECIFICATIONS                     -
C                                                                 -
CN                       THIS IS AN ABBREVIATED VERSION OF THE    -
CN                       DATA SET BC. IT IS USED FOR MC**2-II     -
CN                       CALCULATIONS.                            -
C                                                                 -
C*****************************************************************

C-----------------------------------------------------------------
CR          SPECIFICATIONS (TYPE 1)                               -
C                                                                 -
CL     NBCL,NBCR                                                  -
C                                                                 -
CW     2                                                          -
C                                                                 -
CD     NBCL              BOUNDARY CONDITION TYPE NUMBER FOR LEFT  -
CD                       BOUNDARY OF THE CELL (SEE BELOW).        -
CD     NBCR              BOUNDARY CONDITION TYPE NUMBER FOR RIGHT -
CD                       BOUNDARY OF THE CELL (SEE BELOW).        -
CD                                                                -
CD                       TYPE            DESCRIPTION              -
CD                       ----   ------------------------------    -
CD                         8    REFLECTIVE                        -
CD                         9    PERIODIC                          -
CD                        10    WHITE                             -
C                                                                 -
C-----------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. BIGXS(I)

```
C*****************************************************************
C                                                                 -
C                       PREPARED 3/10/75 AT ANL                   -
C                                                                 -
CF          BIGXS1 THROUGH BIGXSP                                 -
CE          MACROSCOPIC ELASTIC SCATTERING                        -
C                                                                 -
CN                      THESE FILES ARE WRITTEN BY MC**2-II AREA 7 -
CN                      (CSC008)                                  -
C                                                                 -
C*****************************************************************


CD    NDOWN             NUMBER OF SOURCE GROUPS OF DATA
CD                      REPRESENTED IN EACH CROSS SECTION RECORD
CD    NDOWN1            NUMBER OF GROUPS OF DOWNSCATTER CHARACTERISTIC
CD                      OF THE PROBLEM ISOTOPE OF LIGHTEST MASS


C-----------------------------------------------------------------
CR          SPECIFICATIONS (TYPE 1)                               -
C                                                                 -
CC          ALWAYS PRESENT FOR FILE BIGXS1                        -
CC          NEVER PRESENT FOR FILES BIGXS2 THROUGH BIGCSP         -
C                                                                 -
CL    NDOWN,NDOWN1,NUMSPC                                       -
C                                                                 -
CW    3                                                         -
C                                                                 -
CD    NUMSPC            NUMBER OF BIGXS (I.E. BIGXS1 THROUGH BIGXSP)  -
CD                      FILES REQUIRED FOR PROBLEM. THE MAX. NUMBER OF -
CD                      FILES ALLOWED IS 25. THE VALUE OF NUMSPC      -
CD                      DEPENDS UPON THE NUMBER OF ULTRA-FINE-GROUPS  -
CD                      IN THE MULTIGROUP PORTION OF THE SPECTRUM      -
CD                      CALCULATION AND THE MASS OF THE MATERIAL      -
CD                      USED TO DETERMINE THE DATA MANAGEMENT STRATEGY.-
CD                      THE VALUE OF NUMSPC IS SET BY THE CODE AT RUN -
CD                      TIME                                          -
C                                                                 -
C-----------------------------------------------------------------


C-----------------------------------------------------------------
CR          CROSS SECTION (TYPE 2)                                -
C                                                                 -
CC          ALWAYS PRESENT                                        -
C                                                                 -
CL     ((SIGS(I),I=1,NORD1),(SIG0(I),I=1,NDN1),(SIG1(I),I=1,NDN1),   -
CL    1J=1,NDOWN)                                                -
C                                                                 -
```

APPENDIX D. MC^2-2 Binary Files. BIGXS(I) (Contd.)

```
CW     NDOWN*(NORD1+ISP*NDN1)                                          -
C                                                                      -
CD     ISP=1 FOR INCONSISTENT SPECTRUM OPTIONS (ISPOPT.LE.2)           -
CD     ISP=2 FOR CONSISTENT SPECTRUM OPTIONS (ISPOPT.GE.3)             -
CD     NORD1              ORDER OF EXTENDED TRANSPORT APPROXIMATION+1  -
CD     NDN1=NDOWN1+1                                                   -
CD                                                                     -
CD     SIGS               LEGENDRE MOMENTS OF MACROSCOPIC SCATTERING   -
CD                        CROSS SECTION THE THE J'TH GROUP.            -
CD                        I=1 CORRESPONDS TO THE NORDER COMPONENT      -
CD                        I=NORDER CORRESPONDS TO THE P1 COMPONENT     -
CD                        I=NORD1 CORRESPONDS TO THE P0 COMPONENT      -
CD     SIG0               MACROSCOPIC P0 SCATTERING MATRIX ORDERED AS  -
CD                        J TO J+I-1 SO THAT I=1 IS THE IN-GROUP TERM  -
CD     SIG1               MACROSCOPIC P1 SCATTERING MATRIX ORDERED AS  -
CD                        J TO J+I-1 SO THAT I=1 IS THE IN-GROUP TERM  -
C                                                                      -
CN                        THE J'TH GROUP IN THE ABOVE LISTS CORRESPONDS -
CN                        TO A PARTICULAR ULTRA-FINE-GROUP IN THE      -
CN                        PROBLEM. THAT IS, FOR BIGXS1 THE J'TH        -
CN                        GROUP CORRESPONDS TO THE J'TH ULTRA-FINE GROUP.-
CN                        FOR BIGXS2 THE J'TH GROUP CORRESPONDS TO THE -
CN                        ULTRA-FINE-GROUP IN THE PROBLEM OF J+NDOWN,   -
CN                        AND SO ON THROUGH BIGXSP.                    -
CN                        THE ARRAY SIG1 IS PRESENT ONLY FOR ISP=2     -
C                                                                      -
C----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. GEOM1

```
C*****************************************************************
C                                                                 -
C                        PREPARED 6/13/75 AT ANL                  -
C                                                                 -
CF          GEOM1                                                 -
CE          GEOMETRY DATA                                         -
C                                                                 -
CN                       THIS IS AN ABBREVIATED VERSION OF THE    -
CN                       DATA SET GEOM. IT IS USED FOR MC**2-II   -
CN                       CALCULATIONS.                            -
CN                       ALL NON-INTEGER QUANTITIES IN THIS FILE ARE -
CN                       REAL*8.                                  -
C                                                                 -
C*****************************************************************


CD     MULT              2 FOR IBM MACHINES, 1 OTHERWISE.
CD     NCMP              NUMBER OF COMPOSITIONS.
CD     NINTI             NUMBER OF MESH INTERVALS.
CD     NPTI              NUMBER OF MESH INTERVAL LINES.
CD     NREG              NUMBER OF REGIONS.


C-----------------------------------------------------------------
CR          SPECIFICATIONS (TYPE 1)                               -
C                                                                 -
CL     NDIM,NGEOM,NPTI,NDUM,NINTI,NDUM,NREG,NCMP,NDUM,NDUM,NDUM,  -
CL    1NDUM,NDUM,NDUM                                            -
C                                                                 -
CW     14                                                         -
C                                                                 -
CD     NDIM              NUMBER OF DIMENSIONS=1.                 -
CD     NGEOM             GEOMETRY.                               -
CD                       NGEOM=1, ONE-DIMENSIONAL SLAB.          -
CD                            =2, ONE-DIMENSIONAL CYLINDER.      -
CD     NDUM              DUMMY VARIABLE SET TO 0.                -
C                                                                 -
C-----------------------------------------------------------------


C-----------------------------------------------------------------
CR          MESH INTERVAL BOUNDARIES (TYPE 2)                     -
C                                                                 -
CL     (XMESH(I),I=1,NPTI)                                        -
C                                                                 -
CW     MULT*NPTI                                                  -
C                                                                 -
CD     XMESH             MESH BOUNDARIES (REAL*8).               -
C                                                                 -
C-----------------------------------------------------------------
```

APPENDIX D. MC^2-2 Binary Files. GEOM1 (Contd.)

```
C-----------------------------------------------------------------------
CR          REGION-INTERVAL CORRESPONDENCE (TYPE 3)                    -
C                                                                      -
CL    (MR(I),I=1,NINTI)                                                -
C                                                                      -
CW    NINTI                                                            -
C                                                                      -
CD    MR                REGION INDEX. IF MR(I)=N, THEN REG(N) IS       -
CD                      THE REGION LABEL IN INTERVAL I                 -
CD                      (SEE LABELS RECORD BELOW).                     -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          COMPOSITION-INTERVAL CORRESPONDENCE (TYPE 4)                -
C                                                                      -
CL    (MC(I),I=1,NINTI)                                                -
C                                                                      -
CW    NINTI                                                            -
C                                                                      -
CD    MC                COMPOSITION INDEX. IF MC(I)=N, THEN CNAME(N)   -
CD                      IS THE COMPOSITION LABEL IN INTERVAL I         -
CD                      (SEE LABELS RECORD BELOW).                     -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          COMPOSITION-REGION CORRESPONDENCE (TYPE 5)                  -
C                                                                      -
CL    (NC(I),I=1,NREG)                                                 -
C                                                                      -
CW    NREG                                                             -
C                                                                      -
CD    NC                COMPOSITION INDEX. IF NC(I)=N, THEN CNAME(N)   -
CD                      IS THE COMPOSITION LABEL IN REGION I           -
CD                      (SEE LABELS RECORD BELOW).                     -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          LABELS (TYPE 6)                                            -
C                                                                      -
CL    (REG(I),I=1,NREG),(CNAME(I),I=1,NCMP)                            -
C                                                                      -
CW    MULT*(NREG+NCMP)
```

APPENDIX D. MC^2-2 Binary Files. GEOM1 (Contd.)

```
C                                                                       -
CD     REG                 REGION LABELS (REAL*8).                      -
CD     CNAME               COMPOSITION LABELS (REAL*8).                 -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR           REGION VOLUMES (TYPE 7)                                    -
C                                                                       -
CL     (VOL(I),I=1,NREG)                                                -
C                                                                       -
CW     MULT*NREG                                                        -
C                                                                       -
CD     VOL                 VOLUME OF REGION REG(I) (REAL*8) (SEE LABELS -
CD                         RECORD ABOVE). VOL EQUALS THE VOLUME PER     -
CD                         UNIT HEIGHT IN THE TRANSVERSE DIRECTION.     -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. IRESCS

```
C*****************************************************************
C                                                                 -
C                        PREPARED 4/26/76 AT ANL                  -
C                                                                 -
CF          IRESCS                                                -
CE          INTEGRAL TRANSPORT RESONANCE CROSS SECTIONS           -
C                                                                 -
CN                       BROAD GROUP RESONANCE CAPTURE, FISSION,  -
CN                       SCATTERING AND TRANSFER CROSS SECTIONS AS -
CN                       CALCULATED IN MC**2-II AREA 10 (CSC011)  -
CN                       INTEGRAL TRANSPORT THEORY                -
C                                                                 -
C*****************************************************************


CD     MULT              2 FOR IBM MACHINES, 1 OTHERWISE
CD     NBROAD            NUMBER OF BROAD GROUPS IN THE RABANL (CSC011)
CD                       ENERGY RANGE
CD     NCNTM             NUMBER OF RESOLVED RESONANCE MATERIALS IN THE
CD                       PROBLEM MIXTURE EXCLUDING ANY UNIQUE FOIL
CD                       MATERIALS
CD     NGEOM             GEOMETRY TYPE
CD                       NGEOM=0 FOR HOMOGENEOUS PROBLEM
CD                       NGEOM=1 FOR SLAB GEOMETRY
CD                       NGEOM=2 FOR CYLINDRICAL GEOMETRY
CD     NREG              NUMBER OF REGIONS IN THE CELL.  NREG=1 FOR
CD                       HOMOGENEOUS PROBLEMS


C-----------------------------------------------------------------
CS          FILE STRUCTURE                                        -
CS                                                                -
CS          RECORD TYPE                          PRESENT IF       -
CS          ===================================  ================-
CS          SPECIFICATIONS                       ALWAYS PRESENT   -
CS          MATERIAL NAMES                       ALWAYS PRESENT   -
CS          REGION NAMES                         NGEOM.GT.0       -
CS     ******** (REPEAT NBROAD TIMES)                             -
CS     *    DOWNSCATTERS                         ALWAYS PRESENT   -
CS     *    RESONANCE CROSS SECTIONS             ALWAYS PRESENT   -
CS     *    TRANSFER CROSS SECTIONS              ALWAYS PRESENT   -
CS     ********                                                   -
CS          CELL CROSS SECTIONS                  NGEOM.GT.0       -
CS          GROUPS SCATTERED                     NGEOM.GT.0       -
CS          CELL TRANSFER CROSS SECTIONS         NGEOM.GT.0       -
C                                                                 -
C-----------------------------------------------------------------


C-----------------------------------------------------------------
```

APPENDIX D. MC^2-2 Binary Files. IRESCS (Contd.)

```
CR          SPECIFICATIONS (TYPE 1)                                    -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL     NCNTM,NREG,NBROAD,NGEOM                                         -
C                                                                      -
CW     4                                                               -
C                                                                      -
C----------------------------------------------------------------------

C----------------------------------------------------------------------
CR          MATERIAL NAMES (TYPE 2)                                    -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL     RESNAM(M),M=1,NCNTM                                             -
C                                                                      -
CW     MULT*NCNTM                                                      -
C                                                                      -
CD     RESNAM            REAL*8 NAMES OF RESONANCE MATERIALS HAVING    -
CD                       AN INTEGRAL TRANSPORT TREATMENT BY AREA 10    -
CD                       (CSC011)                                      -
C                                                                      -
C----------------------------------------------------------------------

C----------------------------------------------------------------------
CR          REGION NAMES (TYPE 3)                                      -
C                                                                      -
CC          PRESENT IF NGEOM.GT.0                                      -
C                                                                      -
CL     RLABEL(N),N=1,NREG                                              -
C                                                                      -
CW     MULT*NREG                                                       -
C                                                                      -
CD     RLABEL            REAL*8 NAMES OF REGIONS                       -
C                                                                      -
C----------------------------------------------------------------------

C----------------------------------------------------------------------
CR          DOWNSCATTERS (TYPE 4)                                      -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL     NBGMAX(M),M=1,NCNTM                                             -
C                                                                      -
CW     NCNTM                                                           -
C                                                                      -
```

APPENDIX D. MC^2-2 Binary Files. IRESCS (Contd.)

```
CD    NBGMAX            MAXIMUM NUMBER OF BROAD GROUPS DOWN-SCATTERED -
CD                      FOR EACH MATERIAL AND CURRENT BROAD GROUP      -
C                                                                     -
C---------------------------------------------------------------------


C---------------------------------------------------------------------
CR          RESONANCE CROSS SECTIONS (TYPE 5)                         -
C                                                                     -
CC          ALWAYS PRESENT                                            -
C                                                                     -
CL    ((RESCAP(M,K),M=1,NCNTM),K=1,NREG),((RESFIS(M,K),M=1,NCNTM),    -
CL   1  J=1,NREG),((RESSCT(M,K),M=1,NCNTM),K=1,NREG)                  -
C                                                                     -
CW    3*NCNTM*NREG                                                    -
C                                                                     -
CD    RESCAP(M,K)       RESONANCE CAPTURE CROSS SECTION FOR MATERIAL M -
CD                      AND REGION K FOR THE CURRENT BROAD GROUP      -
CD    RESFIS(M,K)       RESONANCE FISSION CROSS SECTION FOR MATERIAL M -
CD                      AND REGION K FOR THE CURRENT BROAD GROUP      -
CD    RESSCT(M,K)       RESONANCE SCATTERING CROSS SECTIONS FOR       -
CD                      MATERIAL M AND REGION K FOR THE CURRENT BROAD -
CD                      GROUP                                         -
C                                                                     -
C---------------------------------------------------------------------


C---------------------------------------------------------------------
CR          TRANSFER CROSS SECTIONS (TYPE 6)                          -
C                                                                     -
CC          ALWAYS PRESENT                                            -
C                                                                     -
CL    (((TRNSFR(M,K,J),M=1,NCNTM),K=1,NREG),J=1,NMAX)                 -
C                                                                     -
CW    NCNTM*NREG*NMAX                                                 -
C                                                                     -
CD    TRNSFR(M,K,J)     RESONANCE MATERIAL M TRANSFER CROSS SECTION   -
CD                      FOR REGION K FROM THE CURRENT BROAD GROUP, SAY -
CD                      I, TO BROAD GROUP I+J                         -
CD    NMAX              LARGEST OF THE NBGMAX FOR THE CURRENT BROAD   -
CD                      GROUP  FOR ANY OF THE NCNTM MATERIALS         -
C                                                                     -
C---------------------------------------------------------------------


C---------------------------------------------------------------------
CR          CELL CROSS SECTIONS (TYPE 7)                              -
C                                                                     -
CC          PRESENT IF NGEOM.GT.0                                     -
C
```

APPENDIX D. MC^2-2 Binary Files. IRESCS (Contd.)

```
CL    ((CELCAP(M,K),M=1,NCNTM),K=1,NBROAD),((CELFIS(M,K),M=1,NCNTM),    -
CL   1K=1,NBROAD),((CELSCT(M,K),M=1,NCNTM),K=1,NBROAD)                  -
C                                                                       -
CW    3*NCNTM*NBROAD                                                    -
C                                                                       -
CD    CELCAP(M,K)       CELL AVERAGED RESOLVED RESONANCE CAPTURE        -
CD                      CROSS SECTION FOR MATERIAL M AND BROAD GROUP K -
CD    CELFIS(M,K)       CELL AVERAGED RESOLVED RESONANCE FISSION        -
CD                      CROSS SECTION FOR MATERIAL M AND BROAD GROUP K -
CD    CELSCT(M,K)       CELL AVERAGED RESOLVED RESONANCE SCATTERING     -
CD                      CROSS SECTION FOR MATERIAL M AND BROAD GROUP K -
C                                                                       -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          GROUPS SCATTERED (TYPE 8)                                   -
C                                                                       -
CC          PRESENT IF NGEOM.GT.0                                       -
C                                                                       -
CL    ((NGRPDN(M,K),M=1,NCNTM),K=1,NBROAD)                              -
C                                                                       -
CW    NCNTM*NBROAD                                                      -
C                                                                       -
CD    NGRPDN(M,K)       NUMBER OF BROAD GROUPS DOWNSCATTERED BY         -
CD                      MATERIAL M IN BROAD GROUP K                     -
C                                                                       -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          CELL TRANSFER CROSS SECTIONS (TYPE 9)                       -
C                                                                       -
CC          PRESENT IF NGEOM.GT.0                                       -
C                                                                       -
CL    (((CELTFR(M,K,J),M=1,NCNTM),K=1,NBROAD),J=1,MOST)                 -
C                                                                       -
CW    NCNTM*NBROAD*MOST                                                 -
C                                                                       -
CD    CELTFR(M,K,J)     CELL AVERAGED TRANSFER CROSS SECTION FOR        -
CD                      MATERIAL M FROM BROAD GROUP K TO BROAD GROUP    -
CD                      K+J                                             -
CD    MOST              LARGEST OF THE NBGMAX FOR ANY BROAD GROUP       -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. LORENZ

```
C*****************************************************************
C                                                                -
C                        PREPARED 3/05/75 AT ANL                 -
C                                                                -
CF          LORENZ                                               -
CE          LORENTZIAN SHAPE RESONANCE INTEGRALS                 -
C                                                                -
CN                      THIS INTERFACE DATA SET IS WRITTEN       -
CN                      BY MC**2-II AREA 6 (CSC005)              -
CN                      THIS DATA SET IS PRESENT ONLY IF MAXNOL.GT.0  -
C                                                                -
C*****************************************************************


CD    NOLINT            NUMBER OF ULTRA FINE GROUPS HAVING
CD                      LORENTZIAN SHAPE RESONANCE INTEGRALS FOR
CD                      EACH RESONACE SO TREATED
CD    NOLRES            NUMBER OF RESONANCES GIVEN A LORENTZIAN SHAPE
CD                      TREATMENT FOR EACH REGION
CD    NREG1             1 FOR HOMOGENEOUS PROBLEMS, 2 FOR CYLINDRICAL
CD                      PROBLEMS, 1+THE NUMBER OF SLAB REGIONS FOR
CD                      SLAB GEOMETRY PROBLEMS


C---------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                          PRESENT IF      -
CS          ===================================  ==============-
CS          SPECIFICATIONS                       ALWAYS          -
CS    ******** (REPEAT NREG1 TIMES)                              -
CS    *     RESONANCE SPECIFICATIONS             ALWAYS          -
CS    *     RESONANCE NUMBERS                    NOLRES.GT.0     -
CS    *  ***** (REPEAT NOLRES TIMES)                            -
CS    *  *  ULTRA FINE GROUP NUMBERS             NOLRES.GT.0     -
CS    *  *  LORENTZIAN RESONANCE INTEGRALS        NOLRES.GT.0     -
CS    ********                                                   -
C                                                                -
C---------------------------------------------------------------


C---------------------------------------------------------------
CR          SPECIFICATIONS (TYPE 1)                              -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL    MAXNOL,MAXGRP,MAXGPH                                       -
C                                                                -
CW    3                                                          -
C                                                                -
```

APPENDIX D. MC^2-2 Binary Files. LORENZ (Contd.)

```
CD     MAXNOL              MAXIMUM VALUE OF NOLRES OVER ALL REGIONS       -
CD     MAXGRP              MAXIMUM VALUE OF NOLINT OVER ALL REGIONS       -
CD     MAXGPH              MAXIMUM VALUE OF NOLINT OVER THE HOMOGENEOUS   -
CD                         MIXTURE (REGION 1)                             -
C                                                                         -
C-------------------------------------------------------------------------


C-------------------------------------------------------------------------
CR           RESONANCE SPECIFICATIONS (TYPE 2)                            -
C                                                                         -
CC           ALWAYS PRESENT                                               -
C                                                                         -
CL     NOLRES,N1MIN,N2MAX                                                 -
C                                                                         -
CW     3                                                                  -
C                                                                         -
CD     N1MIN               HIGHEST ENERGY ULTRA FINE GROUP HAVING         -
CD                         LORENTZIAN SHAPE RESONANCE INTEGRALS           -
CD     N2MAX               LOWEST ENERGY ULTRA FINE GROUP HAVING          -
CD                         LORENTZIAN SHAPE RESONANCE INTEGRALS           -
C                                                                         -
C-------------------------------------------------------------------------


C-------------------------------------------------------------------------
CR           RESONANCE NUMBERS (TYPE 3)                                   -
C                                                                         -
CC           PRESENT ONLY IF NOLRES.GT.0                                  -
C                                                                         -
CL     LRESNO(I),I=1,NOLRES                                               -
C                                                                         -
CW     NOLRES                                                             -
C                                                                         -
CD     LRESNO              RESOLVED RESONANCE NUMBERS FOR RESONANCES      -
CD                         HAVING A LORENTZIAN SHAPE TREATMENT            -
C                                                                         -
C-------------------------------------------------------------------------


C-------------------------------------------------------------------------
CR           ULTRA FINE GROUP NUMBERS (TYPE 4)                            -
C                                                                         -
CC           PRESENT ONLY IF NOLRES.GT.0                                  -
C                                                                         -
CL     NOLINT,N1,N2                                                       -
C                                                                         -
CW     3                                                                  -
C                                                                         -
CD     N1                  HIGHEST ENERGY ULTRA FINE GROUP HAVING         -
```

APPENDIX D. MC^2-2 Binary Files. LORENZ (Contd.)

```
CD                      LORENTZIAN SHAPE RESONANCE INTEGRALS            -
CD     N2               LOWEST ENERGY ULTRA FINE GROUP HAVING           -
CD                      LORENTZIAN SHAPE RESONANCE INTEGRALS            -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          LORENTZIAN RESONANCE INTEGRALS (TYPE 5)                     -
C                                                                       -
CC          PRESENT ONLY IF NOLRES.GT.0                                 -
C                                                                       -
CL     CJINTL(I),I=1,NOLINT                                             -
C                                                                       -
CW     NOLINT                                                           -
C                                                                       -
CD     CJINTL           LORENTZIAN SHAPE RESONANCE INTEGRALS            -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. MACTOT

```
C*****************************************************************
C                                                                -
C                       PREPARED 3/06/75 AT ANL                  -
C                                                                -
CF          MACTOT                                               -
CE          MACROSCOPIC TOTAL CROSS SECTIONS                     -
C                                                                -
CN                      THIS DATA SET IS WRITTEN BY MC**2-II AREA 5
CN                      (CSC004), AREA 6 (CSC005) AND/OR AREA 6.5
CN                      (CSC006)                                 -
C                                                                -
C*****************************************************************


CD    NREC              NUMBER OF RECORDS IN THE DATA SET
CD                      NREC=1 FOR HOMOGENEOUS PROBLEMS
CD                      NREC=3 FOR CYLINDRICAL GEOMETRY
CD                      NREC=1 + THE NUMBER OF SLAB REGIONS FOR
CD                             SLAB GEOMETRY


C----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                          PRESENT IF      -
CS          ===================================  ==============-
CS    ******** (REPEAT NREC TIMES)                               -
CS    *     MACROSCOPIC TOTAL CROSS SECTION      ALWAYS          -
CS    ********                                                   -
C                                                                -
C----------------------------------------------------------------


C----------------------------------------------------------------
CR          MACROSCOPIC TOTAL CROSS SECTION (TYPE 1)             -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL    (SIGMAT(I),I=1,NGROUP)                                     -
C                                                                -
CW    NGROUP                                                     -
C                                                                -
CD    SIGMAT            MACROSCOPIC TOTAL CROSS SECTION (1/CM)   -
CD    NGROUP            NUMBER OF ENERGY GROUPS                  -
C                                                                -
C----------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. MACTOT (Contd.)

```
C*****************************************************************
C                                                                -
C                     PREPARED 3/10/75 AT ANL                    -
C                                                                -
CF          MACTOT                                               -
CE          ULTRA FINE GROUP TOTAL CROSS SECTIONS                -
C                                                                -
CN                      BOTH CONFIGURATIONS OF THIS SCRATCH DATA SET -
CN                      MACTOT ARE WRITTEN BY MC**2-II AREA 10   -
CN                      (CSC011). THE FIRST CONFIGURATION CONTAINS -
CN                      ULTRA FINE GROUP MICROSCOPIC TOTAL CROSS -
CN                      SECTIONS. THE SECOND CONFIGURATION CONTAINS -
CN                      ULTRA FINE GROUP MACROSCOPIC TOTAL CROSS -
CN                      SECTIONS                                 -
C                                                                -
C*****************************************************************

CD     I1               FIRST ULTRA FINE GROUP READ FOR CURRENT PASS
CD     I2               LAST ULTRA FINE GROUP READ FOR CURRENT PASS
CD     NPASS            NUMBER OF TYPE 1 RECORDS PRESENT IN THE FILE.
CD                      IF NULTRA.GT.NUFGRD*NPASS, THERE WILL BE ONE
CD                      ADDITIONAL RECORD READ FOR THE REMAINING
CD                      NULTRA-NPASS*NUFGRD ULTRA FINE GROUPS
CD     NPRMTO           NUMBER OF MATERIALS IN THE PROBLEM MIXTURE
CD                      WHICH HAVE TABULATED TOTAL CROSS SECTIONS
CD                      IN THE AREA 10 (CSC011) ENERGY RANGE
CD     NUFGRD           NUMBER OF ULTRA FINE GROUPS READ PER PASS.
CD                      NUFGRD=I2-I1+1

C         ********************************
C         *                              *
C=========*    FIRST CONFIGURATION       *================================
C         *                              *
C         ********************************

C----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                          PRESENT IF      -
CS          ==================================   ================-
CS     ******** (REPEAT NPRMTO TIMES)                            -
CS     *                                         THE CURRENT MATERIAL -
CS     *      ULTRA FINE GROUP TOTAL             HAS TOTAL CROSS -
CS     *      CROSS SECTIONS                     SECTIONS IN THE AREA -
CS     *                                         10 (CSC011) ENERGY -
CS     *                                         RANGE           -
CS     ********
```

APPENDIX D. MC^2-2 Binary Files. MACTOT (Contd.)

```
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          ULTRA FINE GROUP TOTAL CROSS SECTIONS (TYPE 1)              -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    (SIGTOT(I),I=NITUFG,NGROUP)                                       -
C                                                                       -
CW    NGROUP-NITUFG+1                                                   -
C                                                                       -
CD    SIGTOT(I)          ULTRA FINE GROUP MICROSCOPIC TOTAL CROSS       -
CD                       SECTION FOR ULTRA FINE GROUP I                 -
CD    NITUFG             HIGHEST ENERGY ULTRA FINE GROUP ON THE AREA 10 -
CD                       (CSC011) ENERGY RANGE                          -
CD    NGROUP             LOWEST ENERGY ULTRA FINE GROUP IN THE PROBLEM  -
C                                                                       -
C-----------------------------------------------------------------------

CEOF

C       *********************************
C       *                               *
C=======*    SECOND CONFIGURATION       *================================
C       *                               *
C       *********************************


C-----------------------------------------------------------------------
CS          FILE STRUCTURE                                              -
CS                                                                      -
CS          RECORD TYPE                          PRESENT IF             -
CS          ===================================  =======================-
CS    ******** (REPEAT NPASS TIMES)                                     -
CS    *     ULTRA FINE GROUP MACROSCOPIC TOTAL    ALWAYS PRESENT       -
CS    *     CROSS SECTIONS                                             -
CS    ********                                                         -
CS          ULTRA FINE GROUP MACROSCOPIC TOTAI    NULTRA.GT.           -
CS          CROSS SECTIONS                        NUFGRD*NPASS         -
C                                                                       -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          ULTRA FINE GROUP MACROSCOPIC TOTAL CROSS SECTIONS (TYPE 1)  -
C                                                                       -
CC          ALWAYS PRESENT                                              -
```

APPENDIX D. MC^2-2 Binary Files. MACTOT (Contd.)

```
C                                                                       -
CL     ((SIGTOT(M,I),M=1,NCMPFL),I=I1,I2)                               -
C                                                                       -
CW     NCMPFL*NUFGRD                                                    -
C                                                                       -
CD     SIGTOT(M,I)          ULTRA FINE GROUP MACROSCOPIC TOTAL CROSS    -
CD                          SECTION FOR COMPOSITION M AND ULTRA FINE    -
CD                          GROUP I                                     -
CD     NCMPFL               NUMBER OF COMPOSITIONS PLUS NUMBER OF FOILS -
CD                          IN THE PROBLEM                              -
C                                                                       -
CN                          NUFGRD ULTRA FINE GROUPS ARE READ FOR EACH PASS-
CN                          WHERE NUFGRD=I2-I1+1.  THERE WILL BE        -
CN                          ONE ADDITIONAL RECORD AFTER THE NPASS RECORDS -
CN                          WHICH CONTAINS NULTRA-NPASS*NUFGRD ULTRA FINE -
CN                          GROUPS IF NULTRA IS NOT AN INTEGRAL MULTIPLE OF-
CN                          NUFGRD.  NULTRA IS THE NUMBER OF ULTRA FINE -
CN                          GROUPS IN THE AREA 10 (CSC011) ENERGY RANGE -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. MICTOT

```
C*****************************************************************
C                                                                -
C                        PREPARED 3/06/75 AT ANL                 -
C                                                                -
CF          MICTOT                                               -
CE          MICROSCOPIC TOTAL CROSS SECTIONS                     -
C                                                                -
CN                       THIS DATA SET IS WRITTEN BY MC**2-II AREA 5  -
CN                       (CSC004), AREA 6 (CSC005) AND/OR AREA 6.5   -
CN                       (CSC006)                                -
C                                                                -
C*****************************************************************

CD    NPRMAT             NUMBER OF PROBLEM MATERIALS

C-----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                          PRESENT IF      -
CS          ===================================  ================-
CS    ******** (REPEAT FOR NPRMAT MATERIALS)                     -
CS    *     MICROSCOPIC TOTAL CROSS SECTION      ALWAYS          -
CS    ********                                                   -
C                                                                -
C-----------------------------------------------------------------

C-----------------------------------------------------------------
CR          MICROSCOPIC TOTAL CROSS SECTION (TYPE 1)             -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL    (SIGMAT(I),I=1,NGROUP)                                     -
C                                                                -
CW    NGROUP                                                     -
C                                                                -
CD    SIGMAT             MICROSCOPIC TOTAL CROSS SECTION (BARNS) -
CD    NGROUP             NUMBER OF ENERGY GROUPS                 -
C                                                                -
C-----------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. OLDSGS

```
C*************************************************************************
C                                                                        -
C                        PREPARED 3/19/75 AT ANL                         -
C                                                                        -
CF          OLDSGS                                                       -
CE          MICROSCOPIC ELASTIC SCATTERING                               -
C                                                                        -
CN                      THIS FILE IS READ BY MC**2-II AREA 7 (CSC008).   -
CN                      THE FORMAT OF THIS DATA SET IS IDENTICAL         -
CN                      TO THAT OF DATA SET SMSIGS                       -
C                                                                        -
C*************************************************************************

CEOF
```

APPENDIX D. MC^2-2 Binary Files. OPTICL

```
C*****************************************************************
C                                                                -
C                        PREPARED 3/06/75 AT ANL                 -
C                                                                -
CF          OPTICL                                               -
CE          SLAB GEOMETRY OPTICAL THICKNESSES                    -
C                                                                -
CN                      THIS DATA SET IS WRITTEN BY MC**2-II AREA 5  -
CN                      (CSC004), AREA 6 (CSC005) AND/OR AREA 6.5   -
CN                      (CSC006) AND IS PRESENT IF NGEOM.EQ.1       -
CN                      (SLAB GEOMETRY)                          -
C                                                                -
C*****************************************************************


CD    NREG              NUMBER OF SLAB REGIONS


C-----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                          PRESENT IF      -
CS          ===================================  ================-
CS    ******** (REPEAT FOR NREG SLAB REGIONS)                    -
CS    *     SIGLXL SIGRXR                        ALWAYS          -
CS    ********                                                   -
C                                                                -
C-----------------------------------------------------------------


C-----------------------------------------------------------------
CR          SIGLXL SIGRXR (TYPE 1)                               -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL     ((SIGLXL(I,K),I=1,MAXHTM),K=1,NGROUP),                    -
CL    1((SIGRXR(I,K),I=1,MAXHTM),K=1,NGROUP)                     -
C                                                                -
CW     MAXHTM*NGROUP*2                                           -
C                                                                -
CD     SIGLXL            OPTICAL THICKNESS TO THE LEFT OF THE CURRENT  -
CD                       SLAB REGION FOR MATERIAL I AND GROUP K. THE   -
CD                       CONNECTION BETWEEN I AND PROBLEM MATERIAL     -
CD                       IS DETERMINED BY THE ARRAY MATHET (SEE        -
CD                       DATA SET PRBSPC)                              -
CD     SIGRXR            OPTICAL THICKNESS TO THE RIGHT OF THE CURRENT -
CD                       SLAB REGION FOR MATERIAL I AND GROUP K. THE   -
CD                       CONNECTION BETWEEN I AND PROBLEM MATERIAL IS  -
CD                       DETERMINED BY THE ARRAY MATHET (SEE           -
CD                       DATA SET PRBSPC)                              -
```

APPENDIX D. MC^2-2 Binary Files. OPTICL (Contd.)

```
CD     MAXHTM              MAXIMUM NUMBER OF MATERIALS IN ANY              -
CD                         HETEROGENEOUS REGION                            -
CD     NGROUP              NUMBER OF ENERGY GROUPS                         -
C                                                                          -
CN                         SOME REGIONS WILL HAVE SIGLXL AND SIGRXR        -
CN                         FILLED OUT WITH ZEROS IF THERE ARE FEWER        -
CN                         MATERIALS THAN MAXHTM TREATED HETEROGENEOUSLY   -
CN                         IN THAT REGION                                  -
C                                                                          -
C--------------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. PRBCHI

```
C*****************************************************************
C                                                                -
C                       PREPARED 3/12/75 AT ANL                  -
C                                                                -
CF          PRBCHI                                               -
CE          FISSION SPECTRUM DATA                                -
C                                                                -
CN                      THIS FILE IS WRITTEN BY MC**2-II AREA 7  -
CN                      (CSC008)                                 -
C                                                                -
C*****************************************************************


CD     NCHI             FISSION SPECTRUM VECTOR OR MATRIX FLAG
CD                      NCHI=1 FOR VECTOR CHI
CD                      NCHI.GT.1 FOR MATRIX CHI
CD     NGROUP           NUMBER OF UFG IN MC**2 LIBRARY
CD     NGRP             NUMBER OF UFG IN PROBLEM
CD     NUMCHI           NUMBER OF FISSION SPECTRA IN PROBLEM


C----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                          PRESENT IF      -
CS          ===================================  ================-
CS          SPECIFICATIONS                       ALWAYS          -
CS          PROBLEM MATERIAL CORRESPONDENCE      ALWAYS          -
CS          FISSION SPECTRUM FLAG                ALWAYS          -
CS          FISSION SPECTRUM USE COUNT           ALWAYS          -
CS     ******** (REPEAT FOR NUMCHI SPECTRA)                      -
CS     *    FISSION SPECTRUM VALUES              NCHI.EQ.1       -
CS     *    FISSION SPECTRUM PARAMETERS          NCHI.GT.1       -
CS     *  ***** (REPEAT FOR ALL ISOTOPES USING                   -
CS     *  *       SPECTRUM)                                      -
CS     *  *  FISSION CROSS SECTIONS             NUMCHI.GT.1     -
CS     ********                                                  -
C                                                                -
C----------------------------------------------------------------


C----------------------------------------------------------------
CR          SPECIFICATIONS (TYPE 1)                              -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL     NUMCHI                                                    -
C                                                                -
CW     1                                                         -
C                                                                -
```

APPENDIX D. MC^2-2 Binary Files. PRBCHI (Contd.)

```
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          PROBLEM MATERIAL CORRESPONDENCE (TYPE 2)                    -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    (IFIS(I),I=1,NPRMAT)                                              -
C                                                                       -
CW    NPRMAT                                                            -
C                                                                       -
CD    IFIS              FISSION SPECTRUM IDENTIFICATION                 -
CD                      IFIS=0 PROBLEM MATERIAL IS NOT FISSIONABLE      -
CD                      IFIS=N PROBLEM MATERIAL USES THE N'TH FISSION   -
CD                             SPECTRUM                                 -
C                                                                       -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          FISSION SPECTRUM FLAG (TYPE 3)                              -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    (NCHI(I),I=1,NUMCHI)                                              -
C                                                                       -
CW    NUMCHI                                                            -
C                                                                       -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          FISSION SPECTRUM USE COUNT (TYPE 4)                         -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    (LCHI(I),I=1,NUMCHI)                                              -
C                                                                       -
CW    NUMCHI                                                            -
C                                                                       -
CD    LCHI              NUMBER OF PROBLEM MATERIALS USING A GIVEN     -
CD                      FISSION SPECTRUM DISTRIBUTION                   -
C                                                                       -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          FISSION SPECTRUM VALUES (TYPE 5)                            -
C
```

APPENDIX D. MC^2-2 Binary Files. PRBCHI (Contd.)

```
CC          PRESENT IF NCHI.EQ.1                                          -
C                                                                         -
CL     (CHI(I),I=1,NGRP)                                                  -
C                                                                         -
CW     NGRP                                                               -
C                                                                         -
CD     CHI                 FRACTION OF FISSION NEUTRONS BORN IN GROUP     -
C                                                                         -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR          FISSION SPECTRUM PARAMETERS (TYPE 6)                          -
C                                                                         -
CC          PRESENT IF NCHI.GT.1                                          -
C                                                                         -
CL     (BETA(I),I=1,NGROUP),(ALPHA(I),I=1,NGROUP),                        -
CL    1(TAU(I),I=1,NGROUP),(ANORM(I),I=1,NGRP)                            -
C                                                                         -
CW     3*NGROUP+NGRP                                                      -
C                                                                         -
CD     ALPHA               FRACTIONAL PROBABILITY OF USING EVAPORATION    -
CD                         SPECTRUM LAW. 1-ALPHA IS FRACTIONAL            -
CD                         PROBABILITY OF USING FISSION DISTRIBUTION LAW. -
CD     BETA                NUCLEAR TEMPERATURE (EV.) FOR EVAPORATION      -
CD                         SPECTRUM LAW                                   -
CD     TAU                 NUCLEAR TEMPERATURE (EV.) FOR FISSION          -
CD                         DISTRUBUTION LAW                               -
CD     ANORM               FISSION SPECTRUM NORMALIZAYION FACTOR          -
C                                                                         -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR          FISSION CROSS SECTIONS (TYPE 7)                               -
C                                                                         -
CC          PRESENT IF NUMCHI.GT.1                                        -
C                                                                         -
CL     (BSIGF(I),I=1,NGRP)                                                -
C                                                                         -
CW     NGRP                                                               -
C                                                                         -
CD     BSIGF               ISOTOPIC ATOM DENSITY*NUMBER OF NEUTRONS       -
CD                         PER FISSION*MICROSCOPIC FISSION CROSS SECTION  -
C                                                                         -
C-------------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. PRBSPC

```
C*****************************************************************************
C                                                                              -
C                          PREPARED 10/29/75 AT ANL                            -
C                                                                              -
CF          PRBSPC                                                             -
CE          BINARY VERSION OF MC**2-II BCD INPUT DATA                          -
C                                                                              -
C                                                                              -
C*****************************************************************************


CD    BSQ1              FIXED OR FIRST GUESS FOR BUCKLING
CD    ICHI              ICHI=0, USE LIBRARY FISSION SPECTRA FOR ALL
CD                              MATERIALS IN THE PROBLEM
CD                          =1, USE FISSION SPECTRUM OF MATERIAL
CD                              IDENTIFIED IN FISSION SPECTRUM RECORD
CD                              FOR ALL MATERIALS IN THE PROBLEM
CD                         =NPRMAT, USE FISSION SPECTRUM OF MATERIAL
CD                                  GIVEN IN FISSION SPECTRUM RECORD
CD                                  FOR THE PROBLEM MATERIAL I
CD    MAXHTM            MAXIMUM NUMBER OF MATERIALS TREATED
CD                      HETEROGENEOUSLY IN ANY REGION. FOR
CD                      CYLINDRICAL PROBLEMS, ONLY REGION 1 IS
CD                      CONSIDERED
CD    MULT              2 FOR IBM MACHINES, 1 OTHERWISE
CD    NBG1              1+THE NUMBER OF EPI-THERMAL BROAD GROUPS
CD    NCMP              NUMBER OF COMPOSITIONS FOR USE IN HETEROGENOUS
CD                      REGIONS AS DEFINED ON DATA SET A.NIP TYPE 14
CD                      CARDS
CD    NESF              NUMBER OF POINTS IN THE FIXED UNRESOLVED
CD                      RESONANCE ENERGY MESH
CD    NFLMAT            NUMBER OF MATERIALS USED IN FOILS IN THE
CD                      INTEGRAL TRANSPORT THEORY CALCULATION
CD    NFOILS            NUMBER OF FOILS TO BE EDITED IN THE INTEGRAL
CD                      TRANSPORT THEORY CALCULATION
CD    NGROUP            NUMBER OF UFG IN THE PROBLEM
CD    NPRMAT            NUMBER OF MATERIALS IN THE HOMOGENEOUS
CD                      MIXTURE OF THE PROBLEM
CD    NREG              NUMBER OF HETEROGENEOUS REGIONS. NREG=1 FOR
CD                      A HOMOGENEOUS PROBLEM (NGEOM=0), NREG=2 FOR
CD                      CYLINDRICAL GEOMETRY (NGEOM=2), AND NREG EQUALS
CD                      THE NUMBER OF PLATES FOR SLAB GEOMETRY (NGEOM=1)


C-----------------------------------------------------------------------------
CD          SPECIFICATIONS (TYPE 1)                                            -
C                                                                              -
CC          ALWAYS PRESENT                                                     -
C                                                                              -
CL    NPRMAT,NGROUP,MGCSD,NGROP,NORDER,ISPOPT,ICSOPT,ITRANS,NGEOM,
```

APPENDIX D. MC^2-2 Binary Files. PRBSPC (Contd.)

```
CL    1NREG,NHFG,ICHI,IBSQ,MAXSIZ,MAXBLK,THETA,CAPSQR,AMIN,MAXHTM,      -
CL    2MATSLB,NOHET,NESF,NUNRES,NBG1,NOVRLP,NCAND,IPRINT,NCSD,NCMP,     -
CL    3A1,A2,ISORS,NITBG,NUFGIG,NHFGDW,NFOILS,NINGRP,NLEAK,NFLMAT,      -
CL    4RESTST,HOMTEM,INELAS,NHYDRO                                      -
C                                                                       -
CW    43                                                                -
C                                                                       -
CD    MGCSD             UFG NUMBER AT WHICH THE CONTINUOUS SLOWING     -
CD                      CALCULATION BEGINS                            -
CD    NGROP             LIBRARY UFG NUMBER CORRESPONDING TO THE        -
CD                      HIGHEST UFG OF THE PROBLEM                    -
CD    NORDER            ORDER OF THE EXTENDED TRANSPORT APPROXIMATION  -
CD    ISPOPT            SPECTRUM OPTION                               -
CD                      ISPOPT=1, P1                                  -
CD                            =2, B1                                  -
CD                            =3, CONSISTENT P1                       -
CD                            =4, CONSISTENT B1                       -
CD    ICSOPT            CONTINUOUS SLOWING DOWN PARAMETER OPTION      -
CD                      ICSOPT=0, IMPROVED GOERTZEL-GREULING          -
CD                            =1, ORDINARY GOERTZEL-GREULING          -
CD    ITRANS            TRANSPORT APPROXIMATION                       -
CD                      ITRANS=0, USE ALL LEGENDRE COMPONENTS         -
CD                            =1, USE STANDARD TRANSPORT APPROXIMATION -
CD                            =2, USE IMPROVED TRANSPORT APPROXIMATION -
CD    NGEOM             GEOMETRY OPTION                               -
CD                      NGEOM=0, HOMOGENEOUS                          -
CD                           =1, SLAB GEOMETRY                        -
CD                           =2, CYLINDRICAL GEOMETRY                 -
CD    NHFG              MAXIMUM NUMBER OF HYPER FINE GROUPS PER       -
CD                      ULTRA FINE GROUP TO BE USED IN CALCULATING    -
CD                      ELASTIC SCATTERING MATRICES                   -
CD    IBSQ              BUCKLING OPTION                               -
CD                      IBSQ=-1, DO NOT ITERATE ON BUCKLING AND       -
CD                               BUCKLING IS NOT ENERGY DEPENDENT     -
CD                          =0, ITERATE ON BUCKLING AND BUCKLING IS   -
CD                              NOT ENERGY DEPENDENT                  -
CD                          =1, DO NOT ITERATE ON BUCKLING AND        -
CD                              BUCKLING IS GROUP DEPENDENT           -
CD    MAXSIZ            NUMBER OF REAL*8 WORDS ASSIGNED TO THE MAIN    -
CD                      CORE CONTAINER ARRAY                          -
CD    MAXBLK            NUMBER OF REAL*8 WORDS ASSIGNED TO THE BULK    -
CD                      CORE CONTAINER ARRAY                          -
CD    THETA             CONTINUOUS SLOWING DOWN INTEGRATING FACTOR    -
CD    CAPSQR            KAPPA SQUARED, THE BUCKLING USED IN           -
CD                      CALCULATING THE EXTENDED TRANSPORT CROSS      -
CD                      SECTION AND THE LEAKAGE TERM FOR THE          -
CD                      RESONANCE INTEGRAL CALCULATIONS               -
CD    AMIN              MASS OF MATERIAL USED IN DETERMINATION OF THE -
CD                      DATA MANAGEMENT STRATEGY FOR THE SPECTRUM      -
CD                      CALCULATION. AMIN.LE. THE MASS OF THE         -
```

APPENDIX D. MC^2-2 Binary Files. PRBSPC (Contd.)

```
CD                    LIGHTEST MATERIAL IN THE PROBLEM (EXCLUDING H) -
CD     MATSLB         MATSLB=NPRMAT IF NGEOM.EQ.1. OTHERWISE MATSLB=1-
CD     NOHET          NOHET=NPRMAT IF NGEOM.GT.0. OTHERWISE NOHET=1  -
CD     NUNRES         RESOLVED RESONANCE OVERLAP OPTION              -
CD                    NUNRES=0, INCLUDE OVERLAP CALCULATION FOR UP   -
CD                              TO NCAND NEIGHBORING RESONANCES      -
CD                          =1, OMIT OVERLAP CALCULATION             -
CD     NOVRLP         UNRESOLVED RESONANCE SELF-OVERLAP OPTION       -
CD                    NOVRLP=0, INCLUDE SELF-OVERLAP CALCULATION     -
CD                          =1, OMIT SELF-OVERLAP CALCULATION        -
CD     NCAND          NUMBER OF RESOLVED RESONANCES TO BE TESTED     -
CD                    FOR OVERLAP ON EACH SIDE OF EACH RESOLVED      -
CD                    RESONANCE. NCAND WILL BE 1 IF NUNRES=1         -
CD     IPRINT         BPOINTER DEBUGGING PRINT FLAG                  -
CD                    IPRINT=0, NO DEBUGGING PRINTOUT                -
CD                          =1, DEBUGGING DUMP PRINTOUT              -
CD                          =2, DEBUGGING TRACE PRINTOUT             -
CD                          =3, FULL DEBUGGING PRINTOUT              -
CD     NCSD           NUMBER OF ULTRA FINE GROUPS PER CONTINUOUS     -
CD                    SLOWING DOWN GROUP                             -
CD     A1             CONSTANT USED IN THE EQUIVALENCE PRINCIPLE     -
CD     A2             CONSTANT USED IN THE EQUIVALENCE PRINCIPLE     -
CD     ISORS          IF 0, NO EXTERNAL SOURCES ARE USED. IF 1,      -
CD                    EXTERNAL SOURCES ARE USED                      -
CD     NITBG          HIGHEST ENERGY BROAD GROUP NUMBER FOR WHICH    -
CD                    INTEGRAL TRANSPORT THEORY RESOLVED RESONANCE   -
CD                    CROSS SECTIONS MAY BE CALCULATED.  IF NITBG=0, -
CD                    THE INTEGRAL TRANSPORT THEORY CALCULATION WILL -
CD                    NOT BE INVOKED.                                -
CD     NUFGIG         NUMBER OF ULTRA FINE GROUPS PER INTERMEDIATE   -
CD                    GROUP FOR THE INTEGRAL TRANSPORT CALCULATION   -
CD     NHFGDW         NUMBER OF HYPER FINE GROUPS PER DOPPLER WIDTH  -
CD                    USED FOR THE INTEGRAL TRANSPORT CALCULATION    -
CD     NINGRP         INGROUP SCATTERING OPTION                      -
CD                    NINGRP=0, INCLUDE INGROUP SCATTERING IN THE    -
CD                              INTEGRAL TRANSPORT CALCULATION       -
CD                          =1, OMIT THE INGROUP SCATTERING          -
CD     NLEAK          TRANSVERSE LEAKAGE OPTION                      -
CD                    NLEAK=0, OMIT THE TRANSVERSE LEAKAGE CORRECTION-
CD                             IN THE INTEGRAL TRANSPORT CALCULATION -
CD                          =1, INCLUDE TRANSVERSE LEAKAGE CORRECTION -
CD                             USING CAPSOR FOR THE BUCKLING         -
CD     RESTST         CRITERION USED FOR SELECTION OF RESONANCES TO  -
CD                    BE INCLUDED IN THE INTEGRAL TRANSPORT          -
CD                    CALCULATION                                    -
CD     HOMTEM         TEMPERATURE OF HOMOGENEOUS MIXTURE FOR INTEGRAL-
CD                    TRANSPORT CALCULATIONS                         -
CD     INELAS         INELASTIC AND (N,2N) ULTRA-FINE-GROUP TREATMENT-
CD                    INELAS=0, RIGOROUS TREATMENT
CD                          =1, APPROXIMATE TREATMENT
```

APPENDIX D. MC^2-2 Binary Files. PRBSPC (Contd.)

```
CD     NHYDRO              HYDROGEN TREATMENT                                -
CD                         NHYDRO=0, HYDROGEN IS NOT IN THE PROBLEM          -
CD                                   MIXTURE                                 -
CD                               =1, HYDROGEN IS PRESENT IN THE PROBLEM      -
CD                                   MIXTURE                                 -
C                                                                            -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR           PROBLEM NAMES (TYPE 2)                                          -
C                                                                            -
CC           ALWAYS PRESENT                                                  -
C                                                                            -
CL     (PRBNAM(I),I=1,NPRMAT),(ALIAS(I),I=1,NPRMAT),                         -
CL    1(IEDIT(I),I=1,NPRMAT),(ISTYPE(I),I=1,NPRMAT),                         -
CL    2(EFISS(I),I=1,NPRMAT),(ECAP(I),I=1,NPRMAT)                            -
C                                                                            -
CW     2*MULT*NPRMAT+4*NPRMAT                                                -
C                                                                            -
CD     PRBNAM              REAL*8 NAMES OF LIBRARY NUCLIDES CORRESPONDING    -
CD                         TO PROBLEM MATERIALS                              -
CD     ALIAS               REAL*8 ALIAS NAMES OF PROBLEM MATERIALS           -
CD     IEDIT(I)            0 IF MATERIAL I IS TO BE ADDED TO THE OUTPUT      -
CD                         CROSS SECTION DATA SET, 1 IF MATERIAL I IS NOT    -
CD                         TO BE ADDED TO THE OUTPUT DATA SET                -
CD     ISTYPE              MATERIAL TYPES                                    -
CD                         ISTYPE=1, FISSILE                                 -
CD                               =2, FERTILE                                 -
CD                               =3, OTHER ACTINIDE                          -
CD                               =4, FISSION PRODUCT                         -
CD                               =5, STRUCTURAL                              -
CD                               =6, COOLANT                                 -
CD                               =7, CONTROL                                 -
CD     EFISS               ENERGY RELEASE FOR FISSION (MEV/FISSION)          -
CD     ECAP                ENERGY RELEASE FOR CAPTURE (MEV/CAPTURE)          -
C                                                                            -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR           HOMOGENEOUS ATOM DENSITIES (TYPE 3)                             -
C                                                                            -
CC           ALWAYS PRESENT                                                  -
C                                                                            -
CL     (ATMDEN(I),I=1,NPRMAT)                                                -
C                                                                            -
CW     NPRMAT                                                                -
C                                                                            -
CD     ATMDEN              ATOMIC DENSITIES OF PROBLEM MATERIALS IN THE      -
```

APPENDIX D. MC^2-2 Binary Files. PRBSPC (Contd.)

```
CD                        HOMOGENOUS MIXTURE                                -
C                                                                           -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR          TEMPERATURES (TYPE 4)                                           -
C                                                                           -
CC          ALWAYS PRESENT                                                  -
C                                                                           -
CL    (TEMP(I),I=1,NPRMAT),(CHITEM(I),I=1,NPRMAT)                           -
C                                                                           -
CW    2*NPRMAT                                                              -
C                                                                           -
CD    TEMP              TEMPERATURES OF PROBLEM MATERIALS, DEGREES K
CD    CHITEM            FISSION SPECTRUM TEMPERATURES IN E.V. FOR THE      -
CD                      PROBLEM MATERIALS.  CHITEM(I)=0.0 IF MATERIAL      -
CD                      I WAS NOT SPECIFIED ON THE DATA SET A.MCC2          -
CD                      TYPE 23 CARDS                                      -
C                                                                           -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR          HETEROGENOUS ATOM DENSITIES (TYPE 5)                            -
C                                                                           -
CC          PRESENT ONLY IF MAXHTM.GT.0                                     -
C                                                                           -
CL    ((HETDEN(I,K),I=1,NPRMAT),K=1,NREG)                                   -
C                                                                           -
CW    NPRMAT*NREG                                                           -
C                                                                           -
CD    HETDEN            ATOMIC DENSITIES OF MATERIALS IN HETEROGENOUS      -
CD                      REGIONS                                            -
C                                                                           -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR          HETEROGENOUS MATERIAL DESIGNATIONS (TYPE 6)                     -
C                                                                           -
CC          PRESENT ONLY IF NGEOM.GT.0                                      -
C                                                                           -
CL    ((MATHET(I,K),I=1,NPRMAT),K=1,NREG1)                                  -
C                                                                           -
CW    NPRMAT*NREG1                                                          -
C                                                                           -
CD    MATHET            MATHET(I,K) IS .GT.0 IF MATERIAL I IS              -
CD                      A RESONANCE MATERIAL AND IS TREATED                -
CD                      HETEROGENOUSLY IN REGION K. OTHERWISE MATHET=(
```

APPENDIX D. MC^2-2 Binary Files. PRBSPC (Contd.)

```
CD                      MATHET(I,K) IS INDEXED BY 1 FOR EACH MATERIAL  -
CD                      I TO BE TREATED HETEROGENOUSLY IN EACH REGION  -
CD                      K. ANY MATERIAL HAVING MATHET=0 WILL NOT       -
CD                      BE INVOLVED IN THE CALCUALTION OF RESONANCE    -
CD                      OVERLAP FOR ANY OTHER MATERIAL IN THAT REGION  -
CD    NREG1             1 IF NGEOM=2, NREG IF NGEOM=1                  -
C                                                                      -
C---------------------------------------------------------------------

C---------------------------------------------------------------------
CR          ATOM DENSITIES TIMES LEFT SLAB THICKNESSES (TYPE 7)        -
C                                                                      -
CC          PRESENT ONLY IF NGEOM.EQ.1 AND MAXHTM.GT.0                 -
C                                                                      -
CL    (((SXL(I,J,K),I=1,MAXHTM),J=1,NPRMAT),K=1,NREG)                  -
C                                                                      -
CW    MAXHTM*NPRMAT*NREG                                               -
C                                                                      -
CD    SXL               SUM OF ATOM DENSITY*THICKNESS OF SLAB REGIONS  -
CD                      FOR ALL MATERIALS AND REGIONS TO THE LEFT      -
CD                      OF EACH SLAB REGION. SXL(I,J,K) IS THE VALUE   -
CD                      FOR MATERIAL I IN SLAB REGION K, FOR ALL       -
CD                      MATERIALS J IN ALL SLAB REGIONS TO THE LEFT    -
CD                      OF REGION K. SXL IS FILLED WITH ZEROS IN       -
CD                      REGIONS K IN WHICH THERE ARE FEWER THAN MAXHTM -
CD                      MATERIALS TREATED HETEROGENEOULSY              -
C                                                                      -
C---------------------------------------------------------------------

C---------------------------------------------------------------------
CR          ATOM DENSITIES TIMES RIGHT SLAB THICKNESSES (TYPE 8)       -
C                                                                      -
CC          PRESENT ONLY IF NGEOM.EQ.1 AND MAXHTM.GT.0                 -
C                                                                      -
CL    (((SXR(I,J,K),I=1,MAXHTM),J=1,NPRMAT),K=1,NREG)                  -
C                                                                      -
CW    MAXHTM*NPRMAT*NREG                                               -
C                                                                      -
CD    SXR               SUM OF ATOM DENSITY*THICKNESS OF SLAB REGIONS  -
CD                      FOR ALL MATERIALS AND REGIONS TO THE RIGHT     -
CD                      OF EACH SLAB REGION. SXR(I,J,K) IS THE VALUE   -
CD                      FOR MATERIAL I IN SLAB REGION K, FOR ALL       -
CD                      MATERIALS J IN ALL SLAB REGIONS TO THE RIGHT   -
CD                      OF REGION K. SXR IS FILLED WITH ZEROS IN       -
CD                      REGIONS K IN WHICH THERE ARE FEWER THAN MAXHTM -
CD                      MATERIALS TREATED HETEROGENEOULSY              -
C                                                                      -
C---------------------------------------------------------------------
```

APPENDIX D. MC^2-2 Binary Files. PRBSPC (Contd.)

```
C-----------------------------------------------------------------------
CR          REGION OUTER BOUNDARIES (TYPE 9)                           -
C                                                                      -
CC          PRESENT ONLY IF MAXHTM.GT.0                                -
C                                                                      -
CL    (R(I),I=1,NREG)                                                  -
C                                                                      -
CW    NREG                                                             -
C                                                                      -
CD    R                 R(I) IS THE OUTER DIMENSION OF REGION I. THE   -
CD                      OUTER DIMENSIONS ARE MEASURED RELATIVE TO THE  -
CD                      CENTER OF REGION 1 FOR CYLINDERS, AND          -
CD                      RELATIVE TO THE LEFT BOUNDARY OF REGION 1 FOR  -
CD                      SLABS                                          -
C                                                                      -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          FISSION SPECTRUM (TYPE 10)                                 -
C                                                                      -
CC          PRESENT IF ICHI.GE.1                                       -
C                                                                      -
CL    (CHINAM(I),I=1,ICHI)                                             -
C                                                                      -
CW    MULT*ICHI                                                        -
C                                                                      -
CD    CHINAM(I)         REAL*8 LIBRARY NUCLIDE IDENTIFICATION LABEL    -
CD                      WHOSE FISSION SPECTRUM WILL BE USED FOR        -
CD                      PROBLEM MATERIAL I. IF ONLY ONE VALUE IS GIVEN,-
CD                      THE FISSION SPECTRUM OF THE GIVEN NUCLIDE      -
CD                      WILL BE USED FOR ALL FISSIONABLE MATERIALS IN  -
CD                      THE PROBLEM                                    -
C                                                                      -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          FIXED UNRESOLVED RESONANCE ENERGY MESH (TYPE 11)           -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL    (ESF(I),I=1,NESF)                                                -
C                                                                      -
CW    NESF                                                             -
C                                                                      -
CD    ESF               FIXED ENERGY MESH FOR UNRESOLVED RESONANCE     -
CD                      CALCULATIONS. (ES(I).GT.ES(I+1))
```

APPENDIX D. MC^2-2 Binary Files. PRBSPC (Contd.)

```
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          HETEROGENOUS MATERIAL EDITS (TYPE 12)                       -
C                                                                       -
CC          PRESENT ONLY IF MAXHTM.GT.0                                 -
C                                                                       -
CL    ((LOCHET(I,K),I=1,NPRMAT),K=1,NREG)                               -
C                                                                       -
CW    NPRMAT*NREG                                                       -
C                                                                       -
CD    LOCHET(I,K)       LOCHET(I,K)=0, IF MATERIAL I IS NOT A RESONANCE-
CD                                     MATERIAL OR IS NOT PRESENT IN    -
CD                                     REGION K                         -
CD                                =-1, IF MATERIAL I IN REGION K USES   -
CD                                     THE HOMOGENEOUS CROSS SECTIONS   -
CD                                     FOR MATERIAL I                   -
CD                                =L,  IF MATERIAL I IN REGION K USES   -
CD                                     THE HETEROGENOUS CROSS SECTIONS  -
CD                                     FOR MATERIAL I IN REGION L       -
C                                                                       -
CN                      IF LOCHET(I,K).NE.K THEN MATHET(I,K).EQ.0       -
CN                      NOTE ALSO THAT FOR NGEOM=2, LOCHET(I,2) IS      -
CN                      EQUAL TO 0 OR -1. MATHET IS NOT DEFINED FOR     -
CN                      K=2 IN THIS CASE                                -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          FIXED BUCKLING GUESS (TYPE 13)                              -
C                                                                       -
CC          PRESENT ONLY IF IBSQ=-1                                     -
C                                                                       -
CL    BSQ1                                                              -
C                                                                       -
CW    1                                                                 -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          VARIABLE BUCKLING GUESSES (TYPE 14)                         -
C                                                                       -
CC          PRESENT ONLY IF IBSQ=0                                      -
C                                                                       -
CL    BSQ1,BSQ2,EPS                                                     -
C                                                                       -
```

APPENDIX D. MC^2-2 Binary Files. PRBSPC (Contd.)

```
CW    3
C
CD    BSQ2              SECOND GUESS FOR BUCKLING
CD    EPS               CONVERGENCE CRITERION FOR BUCKLING ITERATION
C
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          GROUP DEPENDENT BUCKLINGS (TYPE 15)
C
CC          PRESENT ONLY IF IBSQ=1
C
CL    (BSQ(I),I=1,NGROUP)
C
CW    NGROUP
C
CD    BSQ               BUCKLINGS FOR ULTRA FINE GROUPS
C
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          COMPOSITION DENSITIES (TYPE 16)
C
CC          PRESENT ONLY IF NCMP.GT.0
C
CL    ((COMDEN(I,K),I=1,NPRMAT),K=1,NCMP),(COMTEM(K),K=1,NCMP)
C
CW    (NPRMAT+1)*NCMP
C
CD    COMDEN(I,K)       ATOM DENSITY OF MATERIAL I IN COMPOSITION K
CD    COMTEM(K)         COMPOSITION TEMPERATURES IN DEGREES K
C
CN                      COMTEM IS USED ONLY BY THE INTEGRAL TRANSPORT
CN                      THEORY CALCULATION.  ALL MATERIALS IN A REGION
CN                      CONTAINING A PARTICULAR COMPOSITION ARE
CN                      ASSIGNED THE TEMPERATURE OF THAT COMPOSITION.
CN                      NOTE THAT NOT ALL DEFINED COMPOSITIONS NEED
CN                      BE ASSIGNED TO REGIONS IN A GIVEN PROBLEM.
CN                      THE COMPOSITION-REGION ASSIGNMENTS ARE GIVEN
CN                      IN DATA SET GEOM
C
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          EXTERNAL SOURCES (TYPE 17)
C
CC          PRESENT ONLY IF ISORS.GT.0
```

APPENDIX D. MC^2-2 Binary Files. PRBSPC (Contd.)

```
C                                                                       -
CL     (SOURCE(I),I=1,NGROUP)                                           -
C                                                                       -
CW     NGROUP                                                           -
C                                                                       -
CD     SOURCE              EXTERNAL SOURCES FOR EACH ULTRA FINE GROUP   -
C                                                                       -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR           BROAD GROUP ENERGIES (TYPE 18)                             -
C                                                                       -
CC           ALWAYS PRESENT                                             -
C                                                                       -
CL     (EBG(I),I=1,NBG1)                                                -
C                                                                       -
CW     NBG1                                                             -
C                                                                       -
CD     EBG(I)              UPPER ENERGY OF BROAD GROUP I. EBG(NBG1) IS THE-
CD                         ENERGY AT THE INTERFACE BETWEEN THE THERMAL   -
CD                         GROUP AND LOWEST EPI-THERMAL BROAD GROUP      -
C                                                                       -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR           THERMAL GROUP CROSS SECTIONS (TYPE 19)                     -
C                                                                       -
CC           ALWAYS PRESENT                                             -
C                                                                       -
CL     (SIGCAP(I),I=1,NPRMAT),(SIGFIS(I),I=1,NPRMAT),                   -
CL    1(GNU(I),I=1,NPRMAT),(SIGTOT(I),I=1,NPRMAT),                      -
CL    2(SIGNA(I),I=1,NPRMAT),(SIGNP(I),I=1,NPRMAT),                     -
CL    3(SIGND(I),I=1,NPRMAT),(SIGNH3(I),I=1,NPRMAT),                    -
CL    4(SIGHE3(I),I=1,NPRMAT),RECVEL)                                   -
C                                                                       -
CW     9*NPRMAT+1                                                       -
C                                                                       -
CD     SIGCAP              THERMAL GROUP CAPTURE CROSS SECTIONS         -
CD     SIGFIS              THERMAL GROUP FISSION CROSS SECTIONS         -
CD     GNU                 THERMAL GROUP NUMBER OF NEUTRONS PER FISSION -
CD     SIGTOT              THERMAL GROUP TOTAL CROSS SECTIONS           -
CD     SIGNA               THERMAL GROUP N-ALPHA CROSS SECTIONS         -
CD     SIGNP               THERMAL GROUP N-P CROSS SECTIONS             -
CD     SIGND               THERMAL GROUP N-D CROSS SECTIONS             -
CD     SIGNH3              THERMAL GROUP N-H3 CROSS SECTIONS            -
CD     SIGHE3              THERMAL GROUP N-HE3 CROSS SECTIONS           -
CD     RECVEL              THERMAL GROUP RECIPROCAL VELOCITY            -
                                                                        -
```

APPENDIX D. MC^2-2 Binary Files. PRBSPC (Contd.)

```
CN                      ANY QUANTITY HAVING THE VALUE -1.0E-20 WILL BE -
CN                      ASSIGNED THE CORRESPONDING LAST EPI-THERMAL    -
CN                      GROUP VALUE FOR THE THERMAL GROUP              -
C                                                                      -
C----------------------------------------------------------------------

C----------------------------------------------------------------------
CR          HOMOGENEOUS INFITITELY DILUTE SPECIFICATIONS (TYPE 20)     -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL    (INFINT(I),I=1,NPRMAT)                                           -
C                                                                      -
CW    NPRMAT                                                           -
C                                                                      -
CD    INFINT            IF 0, MATERIAL I IS NOT INFITELY DILUTE.       -
CD                      IF 1, MATERIAL I IS ASSUMED TO BE INFINITELY   -
CD                      DILUTE FOR THE HOMOGENEOUS RESOLVED RESONANCE  -
CD                      CALCULATION. MATERIALS HAVING INFINT=1 ARE     -
CD                      NOT INVOLVED IN THE OVERLAP CALCULATION OF ANY -
CD                      OTHER RESONANCES. THEIR RESONANCE INTEGRALS    -
CD                      WILL BE SET TO THE INFINITELY DILUTE LIMIT     -
CD                      OF PI/(2.*BETA)                                -
C                                                                      -
C----------------------------------------------------------------------

C----------------------------------------------------------------------
CR          EDIT OPTIONS (TYPE 21)                                     -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL    KUNRES,KATNUA,KRESIN,KSIGMA,KLORNZ,KUFGCS,KUFGMP,KUFGPL,KRESED,  -
CL   1KSPEC,KBGRES,KBGRR                                               -
C                                                                      -
CW    12                                                               -
C                                                                      -
CD    KUNRES            IF 0, DO NOT EDIT DATA SET UNRES. OTHERWISE    -
CD                      EDIT THE DATA SET                              -
CD    KATNUA            IF 0, DO NOT EDIT DATA SET ATNUAT. OTHERWISE   -
CD                      EDIT THE DATA SET                              -
CD    KRESIN            IF 0, DO NOT EDIT DATA SET RESINT. OTHERWISE   -
CD                      EDIT THE DATA SET                              -
CD    KSIGMA            IF 0, DO NOT EDIT DATA SET SIGMAP. OTHERWISE   -
CD                      EDIT THE DATA SET                              -
CD    KLORNZ            IF 0, DO NOT EDIT DATA SET LORENZ. OTHERWISE   -
CD                      EDIT THE DATA SET                              -
CD    KUFGCS            IF 0 EDIT ULTRA FINE GROUP MACROSCOPIC         -
CD                      FISSION, TOTAL, TRANSPORT, AND SCATTERING CRO--
```

APPENDIX D. MC^2-2 Binary Files. PRBSPC (Contd.)

```
CD                      SECTIONS. OTHERWISE DO NOT EDIT THESE DATA      -
CD     KUFGMP           IF 0 EDIT ULTRA FINE GROUP MACROSCOPIC          -
CD                      MODERATING PARAMETERS. OTHERWISE DO NOT         -
CD                      EDIT THESE DATA                                 -
CD     KUFGPL           IF 0, DO NOT EDIT ULTRA FINE GROUP MICROSCOPIC -
CD                      PL SCATTERING CROSS SECTIONS, P0 AND P1         -
CD                      ELASTIC TRANSFER MATRICES. OTHERWISE EDIT       -
CD                      THESE DATA                                      -
CD     KRESED           IF 0, RESONANCE CROSS SECTIONS ARE ADDED TO THE-
CD                      BROAD GROUP OUTPUT DATA SET.  IF 1, RESONANCE   -
CD                      CROSS SECTIONS ARE OMITTED FROM THE BROAD GROUP-
CD                      CROSS SECTIONS. IF 2, RESONANCE CAPTURE AND     -
CD                      FISSION CROSS SECTIONS ARE OMITTED FROM THE     -
CD                      BROAD GROUP CROSS SECTIONS                      -
CD     KSPEC            IF 0, EDIT ULTRA-FINE-GROUP FLUX, CURRENT AND   -
CD                      SLOWING DOWN DENSITIES. OTHERWISE DO NOT EDIT   -
CD                      THESE DATA                                      -
CD     KBGRES           IF 0, DO NOT EDIT BROAD GROUP RESONANCE CROSS   -
CD                      SECTIONS.  OTHERWISE EDIT THESE DATA            -
CD     KBGRR            IF 0, EDIT BROAD GROUP REACTION RATES.          -
CD                      OTHERWISE DO NOT EDIT THESE DATA                -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR           FOIL SPECIFICATIONS (TYPE 22)                              -
C                                                                       -
CC           PRESENT IF NFOILS.GT.0                                     -
C                                                                       -
CL     (FOILNM(K),K=1,NFOILS),(FOILMT(I),I=1,NFLMAT),                   -
CL    1(FOILDX(K),K=1,NFOILS),((FOILDN(I,K),I=1,NFLMAT),K=1,NFOILS),    -
CL    2(FOILTM(K),K=1,NFOILS)                                           -
C                                                                       -
CW     (NFLMAT+2)*NFOILS+MULT*(NFOILS+NFLMAT)                           -
C                                                                       -
CD     FOILNM           REAL*8 LABELS OF FOILS                         -
CD     FOILMT           REAL*8 LABELS OF LIBRARY NUCLIDES USED IN FOILS-
CD     FOILDX           FOIL THICKNESSES IN CM                         -
CD     FOILDN(I,K)      ATOMIC DENSITY OF MATERIAL I IN FOIL K         -
CD                      (ATOMS/CC*1.E-24)                              -
CD     FOILTM           FOIL TEMPERATURES IN DEGREES K                 -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR           NON-CELL AVERAGED CROSS SECTION SPECIFICATIONS (TYPE 23)   -
C                                                                       -
CC           PRESENT IF NGEOM .GT. 0                                    -
```

APPENDIX D. MC^2-2 Binary Files. PRBSPC (Contd.)

```
C                                                                       -
CL     ((ALEDIT(N,I),N=1,NREG2),I=1,NPRMAT)                             -
C                                                                       -
CW     NREG2*NPRMAT*MULT                                                -
C                                                                       -
CD     ALEDIT(N,I)          REAL*8 ALIAS NAME FOR PROBLEM MATERIAL I TO -
CD                          BE EDITED FOR REGION N                      -
CD     NREG2                NREG+1                                     -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. RESDAT

```
C*****************************************************************
C                                                                -
C                        PREPARED 3/07/75 AT ANL                 -
C                                                                -
CF          RESDAT                                               -
CE          RESOLVED RESONANCE DATA                              -
C                                                                -
CN                       THIS DATA SET IS WRITTEN BY MC**2-II AREA 6
CN                       (CSC005)                                -
C                                                                -
C*****************************************************************

CD    NRES               TOTAL NUMBER OF RESOLVED RESONANCES IN THE
CD                       PROBLEM. THE RESONANCES ARE ORDERED ACCORDING
CD                       TO DECREASING ENERGY

C----------------------------------------------------------------
CR          RESONANCE ENERGY - TOTAL WIDTH RATIOS (TYPE 1)       -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL    (X(I),I=1,NRES)                                            -
C                                                                -
CW    NRES                                                       -
C                                                                -
CD    X                  2.0*RESONANCE ENERGY/GAMMA, WHERE GAMMA IS THE -
CD                       TOTAL LINE WIDTH FOR SINGLE LEVEL RESONANCES -
CD                       OR THE S-MATRIX TOTAL LINE WIDTH FOR    -
CD                       ADLER-ADLER MULTILEVEL RESONANCES       -
C                                                                -
C----------------------------------------------------------------

C----------------------------------------------------------------
CR          TOTAL TO NEUTRON LINE WIDTH RATIOS (TYPE 2)          -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL    (GAMTN(I),I=1,NRES)                                        -
C                                                                -
CW    NRES                                                       -
C                                                                -
CD    GAMTN              IF A EQUALS ZERO, WHERE A IS THE FACTOR WHICH -
CD                       MULTIPLIES CHI TO OBTAIN THE INTERFERENCE -
CD                       SCATTERING (SEE RECORD TYPE 4), THEN GAMTN -
CD                       EQUALS ZERO                             -
CD                                                               -
CD                       FOR SINGLE LEVEL RESONANCES,            -
```

APPENDIX D. MC^2-2 Binary Files. RESDAT (Contd.)

```
CD                      GAMTN = GAMT/GAMN, WHERE GAMT AND GAMN ARE      -
CD                      RESPECTIVELY THE TOTAL AND NEUTRON LINE WIDTHS -
CD                                                                      -
CD                      FOR ADLER-ADLER MULTILEVEL RESONANCES,          -
CD                      GAMTN = -0.5*(HT-HC-HF)/(A*(GT-GC-GF)), WHERE   -
CD                      HT, HC, AND HF ARE ASYMMETRIC ADLER-ADLER       -
CD                      PARAMETERS FOR TOTAL, CAPTURE, AND FISSION,     -
CD                      AND GT, GC, AND GF ARE THE CORRESPONDING        -
CD                      SYMMETRIC PARAMETERS                            -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          RESOLVED RESONANCE PEAK CROSS SECTION (TYPE 3)              -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    (SIG0(I),I=1,NRES)                                                -
C                                                                       -
CW    NRES                                                              -
C                                                                       -
CD    SIG0              RESOLVED RESONANCE CROSS SECTION AT RESONANCE   -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          INTERFERENCE SCATTERING FACTOR (TYPE 4)                     -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    (A(I),I=1,NRES)                                                   -
C                                                                       -
CW    NRES                                                              -
C                                                                       -
CD    A                 FACTOR TO MUTLIPLY CHI TO OBTAIN INTERFERENCE   -
CD                      SCATTERING                                      -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. RESINT

```
C*****************************************************************
C                                                                -
C                       PREPARED 3/05/75 AT ANL                  -
C                                                                -
CF          RESINT                                               -
CE          RESONANCE INTERFACE DATA SET                         -
C                                                                -
CN                      THIS INTERFACE DATA SET IN WRITTEN       -
CN                      BY MC**2-II AREA 6 (CSC005)              -
C                                                                -
C*****************************************************************

CD    NREG              NUMBER OF REGIONS
CD                      NREG=1 FOR HOMOGENEOUS PROBLEMS
CD                      NREG=2 FOR CYLINDRICAL PIN PROBLEMS AND IF
CD                             MAXHTM.GT.0
CD                      NREG=1 + THE NUMBER OF SLAB REGIONS FOR
CD                             SLAB PROBLEMS AND IF MAXHTM.GT.0
CD    NRES              NUMBER OF RESOLVED RESONANCES

C----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                          PRESENT IF      -
CS          ===================================  ================-
CS          SPECIFICATIONS                       ALWAYS          -
CS          RESOLVED RESONANCE GROUPS            ALWAYS          -
CS          RESOLVED RESONANCE MATERIALS         ALWAYS          -
CS          RESOLVED RESONANCE ENERGIES          ALWAYS          -
CS    ******** (REPEAT NREG TIMES)                               -
CS    *     RESOLVED CAPTURE INTEGRALS           ALWAYS          -
CS    *     RESOLVED FISSION INTEGRALS           ALWAYS          -
CS    *     TOTAL RESONANCE INTEGRALS            ALWAYS          -
CS    ********                                                   -
CS    ******** (REPEAT NREG TIMES)                               -
CS    *     UNRESOLVED OVERLAP CORRECTED         UNRESOLVED DATA -
CS    *     CAPTURE INTEGRALS                    IS PRESENT      -
CS    *     UNRESOLVED OVERLAP CORRECTED         UNRESOLVED DATA -
CS    *     FISSION INTEGRALS                    IS PRESENT      -
CS    *     UNRESOLVED OVERLAP CORRECTED         UNRESOLVED DATA -
CS    *     TOTAL INTEGRALS                      IS PRESENT      -
CS    ********                                                   -
C                                                                -
C----------------------------------------------------------------

C----------------------------------------------------------------
CR          SPECIFICATIONS (TYPE 1)                              -
```

APPENDIX D. MC^2-2 Binary Files. RESINT (Contd.)

```
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    NRES,NREG,NRESMT                                                  -
C                                                                       -
CW    3                                                                 -
C                                                                       -
CD    NRESMT          NUMBER OF RESOLVED RESONANCE PROBLEM MATERIALS     -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          RESOLVED RESONANCE GROUPS (TYPE 2)                          -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    (NGPRES(I),I=1,NRES)                                              -
C                                                                       -
CW    NRES                                                              -
C                                                                       -
CD    NGPRES          NUMBER OF RESOLVED RESONANCE GROUPS               -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          RESOLVED RESONANCE MATERIALS (TYPE 3)                       -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    (MATRES(I),I=1,NRES)                                              -
C                                                                       -
CW    NRES                                                              -
C                                                                       -
CD    MATRES(I)       PROBLEM MATERIAL NUMBER CORRESPONDING TO          -
CD                    RESONANCE I                                       -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          RESOLVED RESONANCE ENERGIES (TYPE 4)                        -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    (EN(I),I=1,NRES)                                                  -
C                                                                       -
CW    NRES
C
```

APPENDIX D. MC^2-2 Binary Files. RESINT (Contd.)

```
CD    EN                RESOLVED RESONANCE ENERGIES                    -
C                                                                        -
C                                                                        -
C--------------------------------------------------------------------

C--------------------------------------------------------------------
CR          RESOLVED CAPTURE INTEGRALS (TYPE 5)                        -
C                                                                        -
CC          ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE. ALSO PRESENT       -
CC          FOR EACH HETEROGENEOUS REGION                              -
C                                                                        -
CL    (CJ(I),I=1,NRES)                                                 -
C                                                                        -
CW    NRES                                                             -
C                                                                        -
CD    CJ                RESOLVED CAPTURE INTEGRALS                     -
C                                                                        -
C--------------------------------------------------------------------

C--------------------------------------------------------------------
CR          RESOLVED FISSION INTEGRALS (TYPE 6)                        -
C                                                                        -
CC          ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE. ALSO PRESENT       -
CC          FOR EACH HETEROGENEOUS REGION                              -
C                                                                        -
CL    (FJ(I),I=1,NRES)                                                 -
C                                                                        -
CW    NRES                                                             -
C                                                                        -
CD    FJ                RESOLVED FISSION INTEGRALS                     -
C                                                                        -
C--------------------------------------------------------------------

C--------------------------------------------------------------------
CR          TOTAL RESONANCE INTEGRALS (TYPE 7)                         -
C                                                                        -
CC          ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE. ALSO PRESENT       -
CC          FOR EACH HETEROGENEOUS REGION                              -
C                                                                        -
CL    (TJ(I),I=1,NRES)                                                 -
C                                                                        -
CW    NRES                                                             -
C                                                                        -
CD    TJ                TOTAL RESONANCE INTEGRALS                      -
C                                                                        -
C--------------------------------------------------------------------
```

APPENDIX D. MC^2-2 Binary Files. RESINT (Contd.)

```
C-----------------------------------------------------------------------
CR          UNRESOLVED OVERLAP CORRECTED CAPTURE INTEGRALS (TYPE 8)    -
C                                                                      -
CC          PRESENT ONLY IF PROBLEM CONTAINS UNRESOLVED DATA           -
C                                                                      -
CL    (CJFL(I),I=1,NRES)                                               -
C                                                                      -
CW    NRES                                                             -
C                                                                      -
CD    CJFL              RESOLVED CAPTURE INTEGRALS MULTIPLIED BY       -
CD                      APPROPRIATE UNRESOLVED OVERLAP FACTORS         -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          UNRESOLVED OVERLAP CORRECTED FISSION INTEGRALS (TYPE 9)    -
C                                                                      -
CC          PRESENT ONLY IF PROBLEM CONTAINS UNRESOLVED DATA           -
C                                                                      -
CL    (FJFL(I),I=1,NRES)                                               -
C                                                                      -
CW    NRES                                                             -
C                                                                      -
CD    FJFL              RESOLVED FISSION INTEGRALS MULTIPLIED BY       -
CD                      APPROPRIATE UNRESOLVED OVERLAP FACTORS         -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          UNRESOLVED OVERLAP CORRECTED TOTAL INTEGRALS (TYPE 10)     -
C                                                                      -
CC          PRESENT ONLY IF PROBLEM CONTAINS UNRESOLVED DATA           -
C                                                                      -
CL    (TJFL(I),I=1,NRES)                                               -
C                                                                      -
CW    NRES                                                             -
C                                                                      -
CD    TJFL              TOTAL RESONANCE INTEGRALS MULTIPLIED BY        -
CD                      APPROPRIATE UNRESOLVED OVERLAP FACTORS         -
C                                                                      -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. SCR001

```
C*****************************************************************
C                                                                -
C                        PREPARED 3/05/75 AT ANL                 -
C                                                                -
CF          SCR001                                               -
CF          CSC005 SCRATCH DATA SET SCR001                       -
C                                                                -
CN                       THIS SCRATCH DATA SET IS WRITTEN BY     -
CN                       MC**2-II AREA 6 (CSC005)                -
C                                                                -
C*****************************************************************


CD     NOLINT            NUMBER OF ULTRA FINE GROUPS HAVING
CD                       LORENTZIAN SHAPE RESONANCE INTEGRALS FOR
CD                       EACH RESONACE SO TREATED
CD     NOLRES            NUMBER OF RESONANCES GIVEN A LORENTZIAN SHAPE
CD                       TREATMENT FOR EACH REGION. NOLRES IS WRITTEN
CD                       IN DATA SET SCR002


C-----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                          PRESENT IF      -
CS          ===================================  ================-
CS     ******** (REPEAT NOLRES TIMES)                            -
CS     *    ULTRA FINE GROUP NUMBERS             ALWAYS          -
CS     *    LORENTZIAN RESONANCE INTEGRALS       ALWAYS          -
CS     ********                                                  -
C                                                                -
C-----------------------------------------------------------------


C-----------------------------------------------------------------
CR          ULTRA FINE GROUP NUMBERS (TYPE 1)                    -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL     NOLINT,N1,N2                                              -
C                                                                -
CW     3                                                         -
C                                                                -
CD     N1                HIGHEST ENERGY ULTRA FINE GROUP HAVING -
CD                       LORENTZIAN SHAPE RESONANCE INTEGRALS   -
CD     N2                LOWEST ENERGY ULTRA FINE GROUP HAVING  -
CD                       LORENTZIAN SHAPE RESONANCE INTEGRALS   -
C                                                                -
C-----------------------------------------------------------------
```

APPENDIX D. MC^2-2 Binary Files. SCR001 (Contd.)

```
C-------------------------------------------------------------------------
CR            LORENTZIAN RESONANCE INTEGRALS (TYPE 2)                    -
C                                                                        -
CC            ALWAYS PRESENT                                             -
C                                                                        -
CL    CJINTL(I),I=1,NOLINT                                               -
C                                                                        -
CW    NOLINT                                                             -
C                                                                        -
CD    CJINTL              LORENTZIAN SHAPE RESONANCE INTEGRALS           -
C                                                                        -
C-------------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. SCR001 (Contd.)

```
C*****************************************************************
C                                                                -
C                        PREPARED 3/07/75 AT ANL                 -
C                                                                -
CF          SCR001                                               -
CE          ULTRA FINE GROUP SCATTERING CROSS SECTIONS           -
C                                                                -
CN                       BOTH CONFIGURATIONS OF THIS SCRATCH DATA SET -
CN                       SCR001 ARE WRITTEN BY MC**2-II AREA 10  -
CN                       (CSC011)                                -
C                                                                -
C*****************************************************************


CD     I1                FIRST ULTRA FINE GROUP READ FOR CURRENT PASS
CD     I2                LAST ULTRA FINE GROUP READ FOR CURRENT PASS
CD     NPASS             NUMBER OF TYPE 1 RECORDS PRESENT IN THE FILE.
CD                       IF NULTRA.GT.NUFGRD*NPASS, THERE WILL BE ONE
CD                       ADDITIONAL RECORD READ FOR THE REMAINING
CD                       NULTRA-NPASS*NUFGRD ULTRA FINE GROUPS
CD     NPRMSC            NUMBER OF MATERIALS IN THE PROBLEM MIXTURE
CD                       WHICH HAVE TABULATED SCATTERING CROSS SECTIONS
CD                       IN THE AREA 10 (CSC011) ENERGY RANGE
CD     NUFGRD            NUMBER OF ULTRA FINE GROUPS READ PER PASS.
CD                       NUFGRD=I2-I1+1


C          *********************************
C          *                               *
C=========*     FIRST CONFIGURATION       *================================
C          *                               *
C          *********************************


C----------------------------------------------------------------------
CS          FILE STRUCTURE                                           -
CS                                                                   -
CS          RECORD TYPE                          PRESENT IF          -
CS          ===================================  ====================-
CS     ******** (REPEAT NPRMSC TIMES)                                -
CS     *                                         THE CURRENT MATERIAL -
CS     *    ULTRA FINE GROUP SCATTERING          HAS SCATTERING CROSS -
CS     *    CROSS SECTIONS                       SECTIONS IN THE AREA -
CS     *                                         10 (CSC011) ENERGY   -
CS     *                                         RANGE                -
CS     ********                                                      -
C                                                                    -
C----------------------------------------------------------------------
```

APPENDIX D. MC^2-2 Binary Files. SCR001 (Contd.)

```
C-----------------------------------------------------------------------
CR          ULTRA FINE GROUP SCATTERING CROSS SECTIONS (TYPE 1)        -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL     (SIGSCT(I),I=NITUFG,NGROUP)                                     -
C                                                                      -
CW     NGROUP-NITUFG+1                                                 -
C                                                                      -
CD     SIGSCT(I)          ULTRA FINE GROUP MICROSCOPIC SCATTERING CROSS -
CD                        SECTION FOR ULTRA FINE GROUP I               -
CD     NITUFG             HIGHEST ENERGY ULTRA FINE GROUP ON THE AREA 10 -
CD                        (CSC011) ENERGY RANGE
CD     NGROUP             LOWEST ENERGY ULTRA FINE GROUP IN THE PROBLEM -
C                                                                      -
C-----------------------------------------------------------------------

CEOF


C         *********************************
C         *                               *
C========*    SECOND CONFIGURATION       *================================
C         *                               *
C         *********************************


C-----------------------------------------------------------------------
CS          FILE STRUCTURE                                             -
CS                                                                     -
CS          RECORD TYPE                              PRESENT IF        -
CS          =====================================    ================-
CS     ******** (REPEAT NPASS TIMES)                                   -
CS     *    ULTRA FINE GROUP SCATTERING CROSS       ALWAYS PRESENT    -
CS     *    SECTIONS                                                  -
CS     ********                                                       -
CS          ULTRA FINE GROUP SCATTERING CROSS       NULTRA.GT.        -
CS          SECTIONS                                NUFGRD*NPASS      -
C                                                                      -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          ULTRA FINE GROUP SCATTERING CROSS SECTIONS (TYPE 1)        -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL     ((SIGSCT(M,I),M=1,NPRMAT),I=I1,I2)                              -
C
CW     NPRMAT*NUFGRD
```

APPENDIX D. MC^2-2 Binary Files. SCR001 (Contd.)

```
C                                                                       -
CD     SIGSCT(M,I)          ULTRA FINE GROUP SCATTERING CROSS SECTION FOR  -
CD                          MATERIAL M AND ULTRA FINE GROUP I              -
CD     NPRMAT               NUMBER OF MATERIALS IN THE PROBLEM             -
C                                                                       -
CN                          NUFGRD ULTRA FINE GROUPS ARE READ FOR EACH     -
CN                          PASS WHERE NUFGRD=I2-I1+1.  THERE WILL BE      -
CN                          ONE ADDITIONAL RECORD AFTER THE NPASS RECORDS  -
CN                          WHICH CONTAINS NULTRA-NPASS*NUFGRD ULTRA FINE  -
CN                          GROUPS IF NULTRA IS NOT AN INTEGRAL MULTIPLE OF-
CN                          NUFGRD.  NULTRA IS THE NUMBER OF ULTRA FINE    -
CN                          GROUPS IN THE AREA 10 (CSC011) ENERGY RANGE    -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. SCR002

```
C*****************************************************************
C                                                                -
C                        PREPARED 3/05/75 AT ANL                 -
C                                                                -
CF          SCR002                                               -
CE          CSC005 SCRATCH DATA SET SCR002                       -
C                                                                -
CN                       THIS SCRATCH DATA SET IS WRITTEN BY     -
CN                       MC**2-II AREA 6 (CSC005)                -
C                                                                -
C*****************************************************************

CD     NOLRES            NUMBER OF RESONANCES GIVEN A LORENTZIAN SHAPE
CD     NREG1             1 FOR HOMOGENEOUS PROBLEMS, 2 FOR CYLINDRICAL
CD                       PROBLEMS, 1+THE NUMBER OF SLAB REGIONS FOR
CD                       SLAB GEOMETRY PROBLEMS

C----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                          PRESENT IF      -
CS          ===================================  ==============-
CS     ******** (REPEAT NREG1 TIMES)                            -
CS     *    RESONANCE SPECIFICATIONS             ALWAYS          -
CS     *    RESONANCE NUMBERS                    ALWAYS          -
CS     ********                                                 -
C                                                                -
C----------------------------------------------------------------

C----------------------------------------------------------------
CR          RESONANCE SPECIFICATIONS (TYPE 1)                    -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL     NOLRES,N1MIN,N2MAX                                        -
C                                                                -
CW     3                                                         -
C                                                                -
CD     N1MIN             HIGHEST ENERGY ULTRA FINE GROUP HAVING -
CD                       LORENTZIAN SHAPE RESONANCE INTEGRALS   -
CD     N2MAX             LOWEST ENERGY ULTRA FINE GROUP HAVING  -
CD                       LORENTZIAN SHAPE RESONANCE INTEGRALS   -
C                                                                -
C----------------------------------------------------------------

C----------------------------------------------------------------
```

APPENDIX D. MC^2-2 Binary Files. SCRQ02 (Contd.)

```
CR          RESONANCE NUMBERS (TYPE 2)                                  -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    LRESNO(I),I=1,NOLRES                                              -
C                                                                       -
CW    NOLRES                                                            -
C                                                                       -
CD    LRESNO            RESOLVED RESONANCE NUMBERS FOR RESONANCES       -
CD                      HAVING A LORENTZIAN SHAPE TREATMENT             -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. SCRQ02 (Contd.)

```
C*****************************************************************
C                                                                -
C                       PREPARED 3/10/75 AT ANL                  -
C                                                                -
CF          SCR002                                               -
CE          ULTRA FINE GROUP FISSION CROSS SECTIONS              -
C                                                                -
CN                      BOTH CONFIGURATIONS OF THIS SCRATCH DATA SET -
CN                      SCR002 ARE WRITTEN BY MC**2-II AREA 10   -
CN                      (CSC011)                                 -
C                                                                -
C*****************************************************************


CD     I1               FIRST ULTRA FINE GROUP READ FOR CURRENT PASS
CD     I2               LAST ULTRA FINE GROUP READ FOR CURRENT PASS
CD     NPASS            NUMBER OF TYPE 1 RECORDS PRESENT IN THE FILE.
CD                      IF NULTRA.GT.NUFGRD*NPASS, THERE WILL BE ONE
CD                      ADDITIONAL RECORD READ FOR THE REMAINING
CD                      NULTRA-NPASS*NUFGRD ULTRA FINE GROUPS
CD     NPRMFS           NUMBER OF MATERIALS IN THE PROBLEM MIXTURE
CD                      WHICH HAVE TABULATED FISSION CROSS SECTIONS
CD                      IN THE AREA 10 (CSC011) ENERGY RANGE
CD     NUFGRD           NUMBER OF ULTRA FINE GROUPS READ PER PASS.
CD                      NUFGRD=I2-I1+1


C         *********************************
C         *                               *
C=========*    FIRST CONFIGURATION        *================================
C         *                               *
C         *********************************


C---------------------------------------------------------------------
CS          FILE STRUCTURE                                           -
CS                                                                   -
CS          RECORD TYPE                              PRESENT IF      -
CS          =================================        ================-
CS     ******** (REPEAT NPRMFS TIMES)                                -
CS     *                                             THE CURRENT MATERIAL -
CS     *    ULTRA FINE GROUP FISSION                 HAS FISSION CROSS -
CS     *    CROSS SECTIONS                           SECTIONS IN THE AREA -
CS     *                                             10 (CSC011) ENERGY -
CS     *                                             RANGE           -
CS     ********                                                      -
C                                                                    -
C---------------------------------------------------------------------
```

APPENDIX D. MC^2-2 Binary Files. SCR002 (Contd.)

```
C-----------------------------------------------------------------------
CR          ULTRA FINE GROUP FISSION CROSS SECTIONS (TYPE 1)           -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL    (SIGFIS(I),I=NITUFG,NGROUP)                                      -
C                                                                      -
CW    NGROUP-NITUFG+1                                                  -
C                                                                      -
CD    SIGFIS(I)          ULTRA FINE GROUP MICROSCOPIC FISSION CROSS     -
CD                       SECTION FOR ULTRA FINE GROUP I                -
CD    NITUFG             HIGHEST ENERGY ULTRA FINE GROUP ON THE AREA 10 -
CD                       (CSC011) ENERGY RANGE                         -
CD    NGROUP             LOWEST ENERGY ULTRA FINE GROUP IN THE PROBLEM  -
C                                                                      -
C-----------------------------------------------------------------------

CEOF


C         *********************************
C         *                               *
C=========*    SECOND CONFIGURATION       *================================
C         *                               *
C         *********************************


C-----------------------------------------------------------------------
CS          FILE STRUCTURE                                             -
CS                                                                     -
CS          RECORD TYPE                              PRESENT IF        -
CS          =======================================  ================-
CS    ******** (REPEAT NPASS TIMES)                                    -
CS    *     ULTRA FINE GROUP FISSION CROSS         ALWAYS PRESENT     -
CS    *     SECTIONS                                                  -
CS    ********                                                        -
CS          ULTRA FINE GROUP FISSION CROSS         NULTRA.GT.         -
CS          SECTIONS                               NUFGRD*NPASS       -
C                                                                      -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          ULTRA FINE GROUP FISSION CROSS SECTIONS (TYPE 1)           -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL    ((SIGFIS(M,I),M=1,NPRMAT),I=I1,I2)                               -
C                                                                      -
CW    NPRMAT*NUFGRD                                                    -
```

APPENDIX D. MC^2-2 Binary Files. SCR002 (Contd.)

```
C                                                                      -
CD     SIGFIS(M,I)          ULTRA FINE GROUP FISSION CROSS SECTION FOR -
CD                          MATERIAL M AND ULTRA FINE GROUP I          -
CD     NPRMAT               NUMBER OF MATERIALS IN THE PROBLEM         -
C                                                                      -
CN                          NUFGRD ULTRA FINE GROUPS ARE READ FOR EACH PASS-
CN                          WHERE NUFGRD=I2-I1+1.  THERE WILL BE       -
CN                          ONE ADDITIONAL RECORD AFTER THE NPASS RECORDS -
CN                          WHICH CONTAINS NULTRA-NPASS*NUFGRD ULTRA FINE -
CN                          GROUPS IF NULTRA IS NOT AN INTEGRAL MULTIPLE OF-
CN                          NUFGRD.  NULTRA IS THE NUMBER OF ULTRA FINE -
CN                          GROUPS IN THE AREA TO (CSCUT1) ENERGY RANGE -
C                                                                      -
C----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. SCR003

```
C*****************************************************************************
C                                                                             -
C                        PREPARED 3/05/75 AT ANL                              -
C                                                                             -
CF          SCR003                                                            -
CE          CSC004 SCRATCH DATA SET SCR003                                    -
C                                                                             -
CN                       THIS SCRATCH DATA SET IS WRITTEN BY                  -
CN                       MC**2-II AREA 5 (CSC004) IF UNRESOLVED               -
CN                       MATERIALS ARE PRESENT                                -
C                                                                             -
C*****************************************************************************


CD     IFI               FISSILE MATERIAL INDEX
CD                       IFI=0 FOR NON-FISSILE MATERIAL
CD                       IFI=1 FOR FISSILE MATERIAL
CD     JL                NUMBER OF SPIN STATES FOR CURRENT ISOTOPE
CD     NESF              NUMBER OF FIXED ENERGY MESH POINTS
CD     NISO              NUMBER OF ISOTOPES
CD     NREG              NUMBER OF REGIONS
CD                       NREG=1 FOR HOMOGENEOUS PROBLEMS
CD                       NREG=2 FOR CYLINDRICAL GEOMETRY
CD                       NREG=1 + THE NUMBER OF SLAB REGIONS FOR
CD                              SLAB GEOMETRY


C-----------------------------------------------------------------------------
CS          FILE STRUCTURE                                                    -
CS                                                                            -
CS             RECORD TYPE                              PRESENT IF            -
CS             ================================         ======================-
CS     ********** (REPEAT FOR NPRMAT MATERIALS)                               -
CS     *       MATERIAL SPECIFICATIONS                  ALWAYS                -
CS     *  ******** (REPEAT FOR NISO ISOTOPES)                                 -
CS     *  *    SPIN STATE DATA                         ALWAYS                -
CS     *  *    LEVEL SPACING                           ALWAYS                -
CS     *  * ***** (REPEAT FOR 1+NO. OF REGIONS                               -
CS     *  *  *      IN WHICH MATERIAL IS TREATED                              -
CS     *  *  *      HETEROGENEOUSLY)                                          -
CS     *  *  *  CAPTURE J INTEGRAL                    ALWAYS                -
CS     *  *  *  TOTAL J INTEGRAL                      ALWAYS                -
CS     *  *  *  FISSION J INTEGRAL                    IFI.EQ.1              -
CS     **********                                                             -
C                                                                             -
C-----------------------------------------------------------------------------


C-----------------------------------------------------------------------------
CR          MATERIAL SPECIFICATIONS (TYPE 1)                                  -
```

APPENDIX D. MC^2-2 Binary Files. SCRQ03 (Contd.)

```
C                                                                       -
CC          PRESENT IF NUNRES.EQ.1                                      -
C                                                                       -
CL    NISO,IFI                                                          -
C                                                                       -
CW    2                                                                 -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          SPIN STATES (TYPE 2)                                        -
C                                                                       -
CC          PRESENT IF NUNRES.EQ.1                                      -
C                                                                       -
CL    JL                                                                -
C                                                                       -
CW    1                                                                 -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          LEVEL SPACING (TYPE 3)                                      -
C                                                                       -
CC          PRESENT IF NUNRES.EQ.1                                      -
C                                                                       -
CI    ((D(I,J),I=1,NESF),J=1,JL)                                        -
C                                                                       -
CW    NESF*JL                                                           -
C                                                                       -
CD    D                   AVERAGE LEVEL SPACING                       -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          CAPTURE J INTEGRAL (TYPE 4)                                 -
C                                                                       -
CC          ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE.                     -
CC          ALSO PRESENT FOR EACH HETEROGENEOUS REGION IN WHICH         -
CC          CURRENT MATERIAL IS TREATED HETEROGENEOUSLY                 -
C                                                                       -
CL    ((CJESF(I,J),I=1,NESF),J=1,JL)                                    -
C                                                                       -
CW    NESF*JL                                                           -
C                                                                       -
CD    CJESF               UNRESOLVED RESONANCE CAPTURE INTEGRAL         -
C
C-----------------------------------------------------------------------
```

APPENDIX D. MC^2-2 Binary Files. SCR003 (Contd.)

```
C-----------------------------------------------------------------------
CR          TOTAL J INTEGRAL (TYPE 5)                                  -
C                                                                      -
CC          ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE.                    -
CC          ALSO PRESENT FOR EACH HETEROGENEOUS REGION IN WHICH        -
CC          CURRENT MATERIAL IS TREATED HETEROGENEOUSLY                -
C                                                                      -
CL     ((TJESF(I,J),I=1,NESF),J=1,JL)                                  -
C                                                                      -
CW     NESF*JL                                                         -
C                                                                      -
CD     TJESF              UNRESOLVED RESONANCE TOTAL INTEGRAL          -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          FISSION J INTEGRAL (TYPE 6)                                -
C                                                                      -
CC          IF IFI.EQ.1, ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE.       -
CC          ALSO PRESENT FOR EACH HETEROGENEOUS REGION IN WHICH        -
CC          CURRENT MATERIAL IS TREATED HETEROGENEOUSLY                -
C                                                                      -
CL     ((FJESF(I,J),I=1,NESF),J=1,JL)                                  -
C                                                                      -
CW     NESF*JL                                                         -
C                                                                      -
CD     FJESF              UNRESOLVED RESONANCE FISSION INTEGRAL        -
C                                                                      -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. SCR003 (Contd.)

```
C*****************************************************************
C                                                                 -
C                        PREPARED 3/05/75 AT ANL                  -
C                                                                 -
CF          SCR003                                                -
CE          CSC005 SCRATCH DATA SET SCR003                        -
C                                                                 -
CN                     THIS SCRATCH DATA SET IS WRITTEN           -
CN                     BY MC**2-II AREA 6 (CSC005)                -
C                                                                 -
C*****************************************************************

CD    NREG             NUMBER OF REGIONS
CD                     NREG=1 FOR HOMOGENEOUS PROBLEMS
CD                     NREG=2 FOR CYLINDRICAL GEOMETRY
CD                     NREG=1 + THE NUMBER OF SLAB REGIONS
CD                            FOR SLAB GEOMETRY

C-----------------------------------------------------------------
CS          FILE STRUCTURE                                        -
CS                                                                -
CS          RECORD TYPE                          PRESENT IF       -
CS          ===================================  ================-
CS    ******** (REPEAT NREG TIMES)                                -
CS    *     PEAK CROSS SECTION                   ALWAYS PRESENT   -
CS    ********                                                    -
C                                                                 -
C-----------------------------------------------------------------

C-----------------------------------------------------------------
CR          PEAK CROSS SECTION (TYPE 1)                           -
C                                                                 -
CC          ALWAYS PRESENT                                        -
C                                                                 -
CL    (NSIG0(I),I=1,MAXRES)                                       -
C                                                                 -
CW    MAXRES                                                      -
C                                                                 -
CD    MAXRES           MAXIMUM NUMBER OF RESOLVED RESONANCES      -
CD    NSIG0            HOMOGENIZED MACROSCOPIC SIGMA ZERO,        -
CD                     PEAK RESONANCE CROSS SECTIONS              -
C                                                                 -
CN                     NSIG0 IS FILLED WITH ZEROS AS NECESSARY    -
C                                                                 -
C-----------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. SCR003 (Contd.)

```
C*****************************************************************
C                                                                -
C                        PREPARED 3/10/75 AT ANL                 -
C                                                                -
CF          SCR003                                               -
CE          ULTRA FINE GROUP CAPTURE CROSS SECTIONS              -
C                                                                -
CN                       BOTH CONFIGURATIONS OF THIS SCRATCH DATA SET  -
CN                       SCR003 ARE WRITTEN BY MC**2-II AREA 10  -
CN                       (CSC011)                                -
C                                                                -
C*****************************************************************


CD     I1                FIRST ULTRA FINE GROUP READ FOR CURRENT PASS
CD     I2                LAST ULTRA FINE GROUP READ FOR CURRENT PASS
CD     NPASS             NUMBER OF TYPE 1 RECORDS PRESENT IN THE FILE.
CD                       IF NULTRA.GT.NUFGRD*NPASS, THERE WILL BE ONE
CD                       ADDITIONAL RECORD READ FOR THE REMAINING
CD                       NULTRA-NPASS*NUFGRD ULTRA FINE GROUPS
CD     NPRMCP            NUMBER OF MATERIALS IN THE PROBLEM MIXTURE
CD                       WHICH HAVE TABULATED CAPTURE CROSS SECTIONS
CD                       IN THE AREA 10 (CSC011) ENERGY RANGE
CD     NUFGRD            NUMBER OF ULTRA FINE GROUPS READ PER PASS.
CD                       NUFGRD=I2-I1+1


C         *********************************
C         *                               *
C=========*    FIRST CONFIGURATION        *================================
C         *                               *
C         *********************************


C----------------------------------------------------------------------
CS          FILE STRUCTURE                                           -
CS                                                                   -
CS          RECORD TYPE                              PRESENT IF      -
CS          =======================================  ================-
CS     ******** (REPEAT NPRMCP TIMES)                                -
CS     *                                            THE CURRENT MATERIAL -
CS     *      ULTRA FINE GROUP CAPTURE              HAS CAPTURE CROSS    -
CS     *      CROSS SECTIONS                        SECTIONS IN THE AREA -
CS     *                                            10 (CSC011) ENERGY   -
CS     *                                            RANGE                -
CS     ********                                                      -
C                                                                    -
C---------------------------------------------------------------------
```

APPENDIX D. MC^2-2 Binary Files. SCR003 (Contd.)

```
C-----------------------------------------------------------------------
CR          ULTRA FINE GROUP CAPTURE CROSS SECTIONS (TYPE 1)           -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL     (SIGCAP(I),I=NITUFG,NGROUP)                                     -
C                                                                      -
CW     NGROUP-NITUFG+1                                                 -
C                                                                      -
CD     SIGCAP(I)          ULTRA FINE GROUP MICROSCOPIC CAPTURE CROSS   -
CD                        SECTION FOR ULTRA FINE GROUP I               -
CD     NITUFG             HIGHEST ENERGY ULTRA FINE GROUP ON THE AREA TO -
CD                        (CSC011) ENERGY RANGE                        -
CD     NGROUP             LOWEST ENERGY ULTRA FINE GROUP IN THE PROBLEM -
C                                                                      -
C-----------------------------------------------------------------------

CEOF


C         *********************************
C         *                               *
C=========*    SECOND CONFIGURATION       *================================
C         *                               *
C         *********************************


C-----------------------------------------------------------------------
CS          FILE STRUCTURE                                             -
CS                                                                     -
CS          RECORD TYPE                              PRESENT IF        -
CS          ===================================      ================-
CS     ******** (REPEAT NPASS TIMES)                                   -
CS     *    ULTRA FINE GROUP CAPTURE CROSS          ALWAYS PRESENT    -
CS     *    SECTIONS                                                  -
CS     ********                                                       -
CS          ULTRA FINE GROUP CAPTURE CROSS          NULTRA.GT.        -
CS          SECTIONS                                NUFGRD*NPASS      -
C                                                                      -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          ULTRA FINE GROUP CAPTURE CROSS SECTIONS (TYPE 1)           -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL     ((SIGCAP(M,I),M=1,NPRMAT),I=I1,I2)                              -
C
CW     NPRMAT*NUFGRD
```

APPENDIX D. MC^2-2 Binary Files. SCRQQ3 (Contd.)

```
C                                                                      -
CD     SIGCAP(M,I)          ULTRA FINE GROUP CAPTURE CROSS SECTION FOR -
CD                          MATERIAL M AND ULTRA FINE GROUP I          -
CD     NPRMAT               NUMBER OF MATERIALS IN THE PROBLEM         -
C                                                                      -
CN                          NUFGRD ULTRA FINE GROUPS ARE READ FOR EACH PASS-
CN                          WHERE NUFGRD=I2-I1+1.  THERE WILL BE       -
CN                          ONE ADDITIONAL RECORD AFTER THE NPASS RECORDS -
CN                          WHICH CONTAINS NULTRA-NPASS*NUFGRD ULTRA FINE -
CN                          GROUPS IF NULTRA IS NOT AN INTEGRAL MULTIPLE OF-
CN                          NUFGRD.  NULTRA IS THE NUMBER OF ULTRA FINE -
CN                          GROUPS IN THE AREA 10 (CSC011) ENERGY RANGE -
C                                                                      -
C----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. SCR003 (Contd.)

```
C*****************************************************************
C                                                                -
C                        PREPARED 10/29/75 AT ANL                -
C                                                                -
CF          SCR003                                               -
CE          CSC006   SCRATCH DATA SET                            -
C                                                                -
CN                   THIS SCRATCH DATA SET IS WRITTEN BY MC**2-II.  -
CN                   BOTH CONFIGURATIONS OF THIS SCRATCH DATA SET   -
CN                   SCR003 ARE WRITTEN BY MC**2-II AREA 6.5        -
CN                   (CSC006)                                    -
C                                                                -
C*****************************************************************


CD    IFI            FISSILE MATERIAL INDEX
CD                   IFI=0 FOR NON-FISSILE MATERIAL
CD                   IFI=1 FOR FISSILE MATERIAL
CD    JL             NUMBER OF SPIN STATES FOR CURRENT ISOTOPE
CD    NESF           NUMBER OF FIXED ENERGY MESH POINTS
CD    NREG           NUMBER OF REGIONS
CD                   NREG=1 FOR HOMOGENEOUS PROBLEMS
CD                   NREG=2 FOR CYLINDRICAL GEOMETRY
CD                   NREG=1 + THE NUMBER OF SLAB REGIONS FOR
CD                          SLAB GEOMETRY
CD    NRES           NUMBER OF RESOLVED RESONANCES
CD    NUMRES         NUMBER OF UNRESOLVED RESONANCE MATERIALS


C        ********************************
C        *                              *
C========*    FIRST CONFIGURATION       *================================
C        *                              *
C        ********************************

C----------------------------------------------------------------------
CS          FILE STRUCTURE                                           -
CS                                                                   -
CS          RECORD TYPE                              PRESENT IF      -
CS          ====================================     ================-
CS    ********** (REPEAT FOR NUMRES MATERIALS)                       -
CS    *        MATERIAL SPECIFICATIONS               ALWAYS          -
CS    *  ******** (REPEAT FOR NISO ISOTOPES)                        -
CS    *  *     SPIN STATE DATA                       ALWAYS          -
CS    *  *     LEVEL SPACING                         ALWAYS          -
CS    *  *  ***** (REPEAT FOR 1+NO. OF REGIONS                      -
CS    *  *  *       IN WHICH MATERIAL IS TREATED                    -
CS    *  *  *       HETEROGENEOUSLY)                                -
CS    *  *  *  CAPTURE J INTEGRAL                   ALWAYS          -
CS    *  *  *  TOTAL J INTEGRAL                     ALWAYS
```

APPENDIX D. MC^2-2 Binary Files. SCR003 (Contd.)

```
CS     *  *  *  FISSION J INTEGRAL                    IFI.EQ.1
CS     ***********
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR           MATERIAL SPECIFICATIONS (TYPE 1)
C
CC           ALWAYS PRESENT
C
CL     NISO,IFI
C
CW     2
C
CD     NISO                NUMBER OF ISOTOPES
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR           SPIN STATE DATA (TYPE 2)
C
CC           ALWAYS PRESENT
C
CL     JL
C
CW     1
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR           LEVEL SPACING (TYPE 3)
C
CC           ALWAYS PRESENT
C
CL     ((D(I,J),I=1,NESF),J=1,JL)
C
CW     NESF*JL
C
CD     D                   AVERAGE LEVEL SPACING
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR           CAPTURE J INTEGRAL (TYPE 4)
C
CC           ALWAYS PRESENT FOR THE HOMOGENEOUS MIXTURE.
```

APPENDIX D. MC^2-2 Binary Files. SCR003 (Contd.)

```
CC          ALSO PRESENT FOR EACH HETEROGENEOUS REGION IN WHICH          -
CC          CURRENT MATERIAL IS TREATED HETEROGENEOUSLY                  -
C                                                                        -
CL    ((UCJ(I,J),I=1,NESF),J=1,JL)                                       -
C                                                                        -
CW    NESF*JL                                                            -
C                                                                        -
CD    UCJ               UNRESOLVED RESONANCE CAPTURE INTEGRAL TIMES     -
CD                      THE TOTAL REOLVED OVERLAP FACTOR                -
C                                                                        -
C--------------------------------------------------------------------------

C--------------------------------------------------------------------------
CR          TOTAL J INTEGRAL (TYPE 5)                                    -
C                                                                        -
CC          ALWAYS PRESENT FOR THE HOMOGENEOUS MIXTURE.                  -
CC          ALSO PRESENT FOR EACH HETEROGENEOUS REGION IN WHICH          -
CC          CURRENT MATERIAL IS TREATED HETEROGENEOUSLY                  -
C                                                                        -
CL    ((UTJ(I,J),I=1,NESF),J=1,JL)                                       -
C                                                                        -
CW    NESF*JL                                                            -
C                                                                        -
CD    UTJ               UNRESOLVED RESONANCE TOTAL INTEGRAL TIMES       -
CD                      THE TOTAL RESOLVED OVERLAP FACTOR               -
C                                                                        -
C--------------------------------------------------------------------------

C--------------------------------------------------------------------------
CR          FISSION J INTEGRAL (TYPE 6)                                  -
C                                                                        -
CC          IF IFI.EQ.1, ALWAYS PRESENT FOR THE HOMOGENEOUS MIXTURE.     -
CC          ALSO PRESENT FOR EACH HETEROGENEOUS REGION IN WHICH          -
CC          CURRENT MATERIAL IS TREATED HETEROGENEOUSLY                  -
C                                                                        -
CL    ((UFJ(I,J),I=1,NESF),J=1,JL)                                       -
C                                                                        -
CW    NESF*JL                                                            -
C                                                                        -
CD    UFJ               UNRESOLVED RESONANCE FISSION INTEGRAL TIMES     -
CD                      THE TOTAL REOLVED OVERLAP FACTOR                -
C                                                                        -
C--------------------------------------------------------------------------

CEOF

C       ********************************
```

APPENDIX D. MC^2-2 Binary Files. SCR003 (Contd.)

```
C        *                                *
C========*    SECOND CONFIGURATION        *================================
C        *                                *
C        **********************************

C-------------------------------------------------------------------------
CS          FILE STRUCTURE                                               -
CS                                                                       -
CS          RECORD TYPE                                PRESENT IF        -
CS          ================================   ========================-
CS    ******** (REPEAT NREG TIMES)                                       -
CS    *     RESOLVED CAPTURE INTEGRALS           ALWAYS                -
CS    *     RESOLVED FISSION INTEGRALS           ALWAYS                -
CS    *     TOTAL RESONANCE INTEGRALS            ALWAYS                -
CS    ********                                                           -
C                                                                        -
C-------------------------------------------------------------------------


C-------------------------------------------------------------------------
CR          RESOLVED CAPTURE INTEGRAL (TYPE 1)                           -
C                                                                        -
CC          ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE. ALSO PRESENT         -
CC          FOR EACH HETEROGENEOUS REGION                                -
C                                                                        -
CL    (CJ(I),I=1,NRES)                                                   -
C                                                                        -
CW    NRES                                                               -
C                                                                        -
CD    CJ              RESOLVED CAPTURE INTEGRALS TIMES THE               -
CD                    APPROPRIATE UNRESOLVED OVERLAP FACTORS             -
C                                                                        -
C-------------------------------------------------------------------------


C-------------------------------------------------------------------------
CR          RESOLVED FISSION INTEGRAL (TYPE 2)                           -
C                                                                        -
CC          ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE. ALSO PRESENT         -
CC          FOR EACH HETEROGENEOUS REGION                                -
C                                                                        -
CL    (FJ(I),I=1,NRES)                                                   -
C                                                                        -
CW    NRES                                                               -
C                                                                        -
CD    FJ              RESOLVED FISSION INTEGRALS TIMES THE               -
CD                    APPROPRIATE UNRESOLVED OVERLAP FACTORS             -
C                                                                        -
C-------------------------------------------------------------------------
```

APPENDIX D. MC^2-2 Binary Files. SCR003 (Contd.)

```
C-----------------------------------------------------------------------
CR          TOTAL RESONANCE INTEGRAL (TYPE 3)                          -
C                                                                      -
CC          ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE. ALSO PRESENT       -
CC          FOR EACH HETEROGENEOUS REGION                              -
C                                                                      -
CL    (TJ(I),I=1,NRES)                                                 -
C                                                                      -
CW    NRES                                                             -
C                                                                      -
CD    TJ                  TOTAL RESONANCE INTEGRAL TIMES THE           -
CD                        APPROPRIATE OVERLAP FACTORS                  -
C                                                                      -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. SCR004

```
C*****************************************************************
C                                                                -
C                        PREPARED 3/10/75 AT ANL                 -
C                                                                -
CF          SCR004                                               -
CE          ULTRA FINE GROUP FIXED SOURCES                       -
C                                                                -
CN                       SCRATCH DATA SET WRITTEN BY MC**2-II AREA 10  -
CN                       (CSC011)                                -
C                                                                -
C*****************************************************************


CD     I1                FIRST ULTRA FINE GROUP READ FOR CURRENT PASS
CD     I2                LAST ULTRA FINE GROUP READ FOR CURRENT PASS
CD     NPASS             NUMBER OF TYPE 1 RECORDS PRESENT IN THE FILE.
CD                       IF NULTRA.GT.NUFGRD*NPASS, THERE WILL BE ONE
CD                       ADDITIONAL RECORD READ FOR THE REMAINING
CD                       NULTRA-NPASS*NUFGRD ULTRA FINE GROUPS
CD     NUFGRD            NUMBER OF ULTRA FINE GROUPS READ PER PASS.
CD                       NUFGRD=I2-I1+1


C----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                          PRESENT IF      -
CS          ===================================  ================-
CS     ******** (REPEAT NPASS TIMES)                             -
CS     *    ULTRA FINE GROUP FIXED SOURCES       ALWAYS PRESENT  -
CS     ********                                                  -
CS          ULTRA FINE GROUP FIXED SOURCES       NULTRA.GT.      -
CS                                                NUFGRD*NPASS    -
C                                                                -
C----------------------------------------------------------------


C----------------------------------------------------------------
CR          ULTRA FINE GROUP FIXED SOURCES (TYPE 1)              -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL     ((SFIX(M,I),M=1,NPRMAT),I=I1,I2)                          -
C                                                                -
CW     NPRMAT*NUFGRD                                             -
C                                                                -
CD     SFIX(M,I)         ULTRA FINE GROUP FIXED SOURCES FOR      -
CD                       MATERIAL M AND ULTRA FINE GROUP I       -
C                                                                -
CN                       NUFGRD ULTRA FINE GROUPS ARE READ FOR EACH PASS-
```

APPENDIX D. MC^2-2 Binary Files. SCR004 (Contd.)

```
CN                      WHERE NUFGRD=I2-I1+1.  THERE WILL BE            -
CN                      ONE ADDITIONAL RECORD AFTER THE NPASS RECORDS   -
CN                      WHICH CONTAINS NULTRA-NPASS*NUFGRD ULTRA FINE   -
CN                      GROUPS IF NULTRA IS NOT AN INTEGRAL MULTIPLE OF-
CN                      NUFGRD.  NULTRA IS THE NUMBER OF ULTRA FINE     -
CN                      GROUPS IN THE AREA 10 (CSC011) ENERGY RANGE     -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. SCR005

```
C*****************************************************************
C                                                                -
C                        PREPARED 3/10/75 AT ANL                 -
C                                                                -
CF          SCR005                                               -
CE          RESONANCE FOIL CROSS SECTIONS                        -
C                                                                -
C                                                                -
C*****************************************************************

CD    NBROAD              NUMBER OF BROAD GROUPS IN THE AREA 10 (CSC011)
CD                        ENERGY RANGE
CD    NCNTF               NUMBER OF RESONANCE FOIL MATERIALS
CD    NFOILS              NUMBER OF FOILS
CD    NINTI               NUMBER OF MESH INTERVALS IN THE CELL.  NINTI=1
CD                        FOR HOMOGENEOUS PROBLEMS

C----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                          PRESENT IF      -
CS          ===================================  ================-
CS    ******** (REPEAT NBROAD TIMES)                             -
CS    *     FOIL CAPTURE CROSS SECTIONS          ALWAYS          -
CS    *     FOIL FISSION CROSS SECTIONS          ALWAYS          -
CS    *     FOIL SCATTERING CROSS SECTIONS       ALWAYS          -
CS    ********                                                   -
C                                                                -
C----------------------------------------------------------------

C----------------------------------------------------------------
CR          FOIL CAPTURE CROSS SECTIONS (TYPE 1)                 -
C                                                                -
C                                                                -
CL    (((FOLCAP(M,K,L),M=1,NCNTF),K=1,NINTI),L=1,NFOILS)         -
C                                                                -
CW    NCNTF*NINTI*NFOILS                                         -
C                                                                -
CD    FOLCAP(M,K,L)       RESONANCE CAPTURE CROSS SECTION FOR MATERIAL -
CD                        M IN FOIL L AT THE RIGHT EDGE OF MESH  -
CD                        INTERVAL I                             -
C                                                                -
C----------------------------------------------------------------

C----------------------------------------------------------------
CR          FOIL FISSION CROSS SECTIONS (TYPE 2)                 -
```

APPENDIX D. MC^2-2 Binary Files. SCR005 (Contd.)

```
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    (((FOLFIS(M,K,L),M=1,NCNTF),K=1,NINTI),L=1,NFOILS)                -
C                                                                       -
CW    NCNTF*NINTI*NFOILS                                                -
C                                                                       -
CD    FOLFIS(M,K,L)     RESONANCE FISSION CROSS SECTION FOR MATERIAL    -
CD                      M IN FOIL L AT THE RIGHT EDGE OF MESH           -
CD                      INTERVAL I                                      -
C                                                                       -
C-------------------------------------------------------  ------------

C-------------------------------------------------------  ------------
CR          FOIL SCATTERING CROSS SECTIONS (TYPE 3)                     -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    (((FOLSCT(M,K,L),M=1,NCNTF),K=1,NINTI),L=1,NFOILS)                -
C                                                                       -
CW    NCNTF*NINTI*NFOILS                                                -
C                                                                       -
CD    FOLSCT(M,K,L)     RESONANCE SCATTERING CROSS SECTION FOR MATERIAL-
CD                      M IN FOIL L AT THE RIGHT EDGE OF MESH           -
CD                      INTERVAL I                                      -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. SIGMAP

```
C*****************************************************************
C                                                                -
C                        PREPARED 3/06/75 AT ANL                 -
C                                                                -
CF          SIGMAP                                               -
CE          BACKGROUND SMOOTH SCATTERING CROSS SECTIONS          -
C                                                                -
CN                      THIS DATA SET IS WRITTEN BY MC**2-II     -
CN                      AREA 6.5 (CSC006) AND PRESENT IF DATA SET -
CN                      RESINT HAS BEEN WRITTEN, OR IF DATA SET  -
CN                      ATNUAT HAS BEEN WRITTEN                  -
C                                                                -
C*****************************************************************


CD     MAXHTM           MAXIMUM NUMBER OF MATERIALS IN ANY
CD                      HETEROGENEOUS REGION
CD     MGCUT            UFG ABOVE THE HIGHEST RESONANCE ENERGY IN THE
CD                      PROBLEM (RESOLVED OR UNRESOLVED)
CD                      MULTIGROUP TO CONTINUOUS SLOWING DOWN
CD     NGROUP           NUMBER OF ENERGY GROUPS
CD     NPRMAT           NUMBER OF PROBLEM MATERIALS
CD     NREG1            REGION INDEX
CD                      NREG1=1 FOR CYLINDERS
CD                      NREG1=NUMBER OF SLAB REGIONS FOR SLABS


C-----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                          PRESENT IF      -
CS          ===================================  ================-
CS          SPECIFICATIONS                       ALWAYS          -
CS          HOMOGENEOUS SMOOTH SCATTERING        ALWAYS          -
CS          CROSS SECTIONS                                       -
CS     ******** (REPEAT FOR NREG1 HETEROGENEOUS                  -
CS     *         REGIONS)                                       -
CS     *  ***** (REPEAT FOR NPRMAT MATERIALS                    -
CS     *  *      OMITTING THOSE WHICH ARE NOT                   -
CS     *  *      TREATED HETEROGENEOUSLY IN THE                 -
CS     *  *      CURRENT REGION. FOR CYLINDERS,                 -
CS     *  *      ONLY 1 RECORD IS PRESENT SINCE                 -
CD     *  *      ALL MATERIALS HAVE THE SAME                    -
CD     *  *      ESCAPE CROSS SECTION)                          -
CS     *  *  HETEROGENEOUS SMOOTH SCATTERING      MAXHTM.GT.0     -
CS     *  *  CROSS SECTIONS                                      -
CS     ********                                                 -
C                                                                -
C-----------------------------------------------------------------
```

APPENDIX D. MC^2-2 Binary Files. SIGMAP

```
C-----------------------------------------------------------------------
CR          SPECIFICATIONS (TYPE 1)                                    -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL    NGROUP,MGCUT,NPRMAT,NGEOM,NREG1,MAXHTM                           -
C                                                                      -
CW    6                                                                -
C                                                                      -
CD    NGEOM             GEOMETRY TYPE                                  -
CD                      NGEOM=0 FOR HOMOGENEOUS PROBLEMS               -
CD                      NGEOM=1 FOR SLAB GEOMETRY                      -
CD                      NGEOM=2 FOR CYLINDRICAL GEOMETRY               -
C                                                                      -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          HOMOGENEOUS SMOOTH SCATTERING CROSS SECTIONS (TYPE 2)      -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL    (SIGMAP(I),I=MGCUT,NGROUP)                                       -
C                                                                      -
CW    NGROUP-MGCUT+1                                                   -
C                                                                      -
CD    SIGMAP            HOMOGENIZED SMOOTH UFG CROSS SECTIONS FOR      -
CD                      THE HOMOGENEOUS MIXTURE                        -
C                                                                      -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR          HETEROGENEOUS SMOOTH SCATTERING CROSS SECTIONS (TYPE 3)    -
C                                                                      -
CC          PRESENT IF MAXHTM.GT.0                                     -
C                                                                      -
CL    (SIGPP(I),I=MGCUT,NGROUP)                                        -
C                                                                      -
CW    NGROUP-MGCUT+1                                                   -
C                                                                      -
CD    SIGPP             HOMOGENIZED SMOOTH UFG CROSS SECTIONS PLUS     -
CD                      THE ESCAPE CROSS SECTION FOR THE REGION        -
CD                      IN QUESTION                                    -
C                                                                      -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. SMSIGS

```
C*****************************************************************
C                                                                -
C                       PREPARED 3/10/75 AT ANL                  -
C                                                                -
CF          SMSIGS                                               -
CE          MICROSCOPIC ELASTIC SCATTERING                       -
C                                                                -
CN                      THIS FILE IS WRITTEN BY MC**2-II AREA 7  -
CN                      (CSC008)                                 -
C                                                                -
C*****************************************************************

CD     ISPOPT           SPECTRUM OPTION
CD                      ISPOPT=1 FOR P1
CD                      ISPOPT=2 FOR B1
CD                      ISPOPT=3 FOR CONSISTENT P1
CD                      ISPOPT=4 FOR CONSISTENT B1
CD     MULT             2 FOR IBM MACHINES, 1 OTHERWISE
CD     NGRP             NUMBER OF GROUPS IN PROBLEM
CD     NORDER           ORDER OF EXTENDED TRANSPORT APPROXIMATION
CD     NPRMAT           NUMBER OF PROBLEM MATERIALS

C----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                          PRESENT IF      -
CS          ===================================  ==============-
CS          SPECIFICATIONS                       ALWAYS          -
CS          MATERIAL NAMES                       ALWAYS          -
CS     ******** (REPEAT FOR NPRMAT MATERIALS)                    -
CS     *  ***** (REPEAT FOR NGRP GROUPS)                        -
CS     *  *  ELASTIC SCATTERING DATA              ALWAYS        -
CS     ********                                                 -
C                                                                -
C----------------------------------------------------------------

C----------------------------------------------------------------
CR          SPECIFICATIONS (TYPE 1)                              -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL     NPRMAT,NGRP,ISPOPT,NORDER,NGROP,ITRANS                    -
C                                                                -
CW     6                                                         -
C                                                                -
CD     NGROP            LIBRARY UFG NUMBER CORRESPONDING TO THE -
CD                      HIGHEST UFG IN THE PROBLEM               -
```

APPENDIX D. MC^2-2 Binary Files. SMSIGS (Contd.)

```
CD     ITRANS              TRANSPORT APPROXIMATION                          -
CD                         ITRANS=0 USE ALL LEGENDRE COMPONENTS             -
CD                         ITRANS=1 USE STANDARD TRANSPORT APPROXIMATION    -
CD                         ITRANS=2 USE IMPROVED TRANSPORT APPROXIMATION    -
C                                                                           -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR           MATERIAL NAMES (TYPE 2)                                        -
C                                                                           -
CC           ALWAYS PRESENT                                                 -
C                                                                           -
CL     (PRBNAM(I),I=1,NPRMAT)                                               -
C                                                                           -
CW     MULT*NPRMAT                                                          -
C                                                                           -
CD     PRBNAM              PROBLEM MATERIAL NAMES                           -
C                                                                           -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR           ELASTIC SCATTERING DATA (TYPE 3)                               -
C                                                                           -
CC           ALWAYS PRESENT                                                 -
C                                                                           -
CL     (SIGS(I),I=1,NORD1),SIGUNR,BETA,(SIG0(I),I=1,NDN1),                  -
CL    1(SIG1(I),I=1,NDN1)                                                   -
C                                                                           -
CW     NORD1+ISP*NDN1+2                                                     -
C                                                                           -
CD     NORD1=NORDER+1                                                       -
CD     ISP=1 IF ISPOPT.LE.2                                                 -
CD     ISP=2 IF ISPOPT.GT.2                                                 -
CD     NDN1=NUMBER OF GROUPS OF DOWNSCATTER PLUS 1                          -
CD                                                                          -
CD     SIGS                LEGENDRE MOMENTS OF NONRESONANCE SCATTERING      -
CD                         CROSS SECTION                                    -
CD                         I=1 CORRESPONDS TO THE NORDER COMPONENT          -
CD                         I=NORDER CORRESPONDS TO THE P1 COMPONENT         -
CD                         I=NORD1 CORRESPONDS TO THE P0 COMPONENT          -
CD     SIGUNR              UNRESOLVED RESONANCE SCATTERING CROSS SECTION     -
CD     BETA                TRANSPORT CORRECTION FACTOR                      -
CD     SIG0                P0 SCATTERING MATRIX ORDERED AS                  -
CD                         J TO J+I-1 SO THAT I=1 IS THE IN-GROUP TERM      -
CD     SIG1                P1 SCATTERING MATRIX ORDERED AS                  -
CD                         J TO J+I-1 SO THAT I=1 IS THE IN-GROUP TERM      -
C
CN                         THE ARRAY SIG1 IS PRESENT ONLY FOR ISP=2
```

APPENDIX D. MC^2-2 Binary Files. SMSIGS (Contd.)

```
CN                    THE MATRIX ELEMENTS SIG0 AND SIG1 ARE          -
CN                    NORMALIZED TO THE TRANSPORT CORRECTED SMOOTH   -
CN                    PLUS UNRESOLVED SCATTERING CROSS SECTION,      -
CN                    THAT IS ((SIGS(NORD1)+SIGUNR)*(1.-BETA))       -
C                                                                    -
C--------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. SPECTR

```
C*****************************************************************
C                                                                -
C                        PREPARED 5/13/76 AT ANL                 -
C                                                                -
CF          SPECTR                                               -
CE          ULTRA FINE GROUP SPECTRUM                            -
C                                                                -
CN                       THIS FILE IS WRITTEN BY M**2-II AREA 8   -
CN                       (CSC009)                                -
C                                                                -
C*****************************************************************


CD     ISP               1 FOR INCONSISTENT SPECTRUM OPTIONS
CD                       2 FOR CONSISTENT SPECTRUM OPTIONS
CD     NGRP              NUMBER OF UFG IN PROBLEM


C----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                          PRESENT IF      -
CS          ===================================  ================-
CS          SPECIFICATIONS                       ALWAYS          -
CS          FLUX                                 ALWAYS          -
CS          CURRENT                              ISP.EQ.2        -
C                                                                -
C----------------------------------------------------------------


C----------------------------------------------------------------
CR          SPECIFICATIONS (TYPE 1)                              -
C                                                                -
CC          ALWAYS PRESENT                                       -
C                                                                -
CL     RHO,BSQ,EMQX,DELTAU,NGRP,MGCSD,NCSD                       -
C                                                                -
CW     7                                                         -
C                                                                -
CD     RHO               ULTRA FINE GROUP EIGENVALUE            -
CD     BSQ               B**2 FROM UFG CALCULATION              -
CD     EMAX              HIGHEST ENERGY IN PROBLEM              -
CD     DELTAU            UFG LETHARGY WIDTH                     -
CD     MGCSD             UFG NUMBER AT WHICH CONTINUOUS SLOWING DOWN -
CD                       CALCULATION BEGINS                     -
CD     NCSD              NUMBER OF UFG IN CONTINUOUS SLOWING DOWN -
CD                       CALCULATION                            -
C                                                                -
C----------------------------------------------------------------
```

APPENDIX D. MC^2-2 Binary Files. SPECTR (Contd.)

```
C-------------------------------------------------------------------
CR          FLUX (TYPE 2)                                          -
C                                                                  -
CC          ALWAYS PRESENT                                         -
C                                                                  -
CL    (PHI(I),I=1,NGRP)                                            -
C                                                                  -
CW    NGRP                                                         -
C                                                                  -
CD    PHI               ULTRA FINE GROUP FLUX                      -
C                                                                  -
C-------------------------------------------------------------------


C-------------------------------------------------------------------
CR          CURRENT (TYPE 3)                                       -
C                                                                  -
CC          PRESENT IF ISP.EQ.2                                    -
C                                                                  -
CL    (CURNT(I),I=1,NGRP)                                          -
C                                                                  -
CW    NGRP                                                         -
C                                                                  -
CD    CURNT             ULTRA FINE GROUP CURRENT                   -
C                                                                  -
C-------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. SPECXS

```
C*************************************************************************
C                                                                        -
C                        PREPARED 3/12/75 AT ANL                         -
C                                                                        -
CF          SPECXS                                                       -
CE          MACROSCOPIC CROSS SECTIONS AND MODERATING PARAMETERS         -
C                                                                        -
CN                       THIS FILE IS WRITTEN BY MC**2-II AREA 7         -
CN                       (CSC008)                                        -
C                                                                        -
C*************************************************************************


CD     ISP               SPECTRUM OPTION
CD                       ISP=1 FOR INCONSISTENT OPTION (ISPOPT.LE.2)
CD                       ISP=2 FOR CONSISTENT SPECTRUM OPTION
CD                             (ISPOPT.GE.3)
CD     NCSD              NUMBER OF ENERGY POINTS IN CONTINUOUS SLOWING
CD                       DOWN REGION (=NGRP-MGCSD+2)
CD     NGRP              NUMBER OF UFG IN PROBLEM


C------------------------------------------------------------------------
CR          NUSIGMA FISSION (TYPE 1)                                     -
C                                                                        -
CC          ALWAYS PRESENT                                               -
C                                                                        -
CL     (BNSIGF(I),I=1,NGRP)                                              -
C                                                                        -
CW     NGRP                                                              -
C                                                                        -
CD     BNSIGF            MACROSCOPIC UFG FISSION CROSS SECTION*         -
CD                       AVERAGE NUMBER OF NEUTRONS PER FISSION         -
C                                                                        -
C------------------------------------------------------------------------


C------------------------------------------------------------------------
CR          NU COEFFICIENTS (TYPE 2)                                     -
C                                                                        -
CC          ALWAYS PRESENT                                               -
C                                                                        -
CL     (A0(I),A1(I),A2(I),A3(I),I=1,NPRMAT)                              -
C                                                                        -
CW     4*NPRMAT                                                          -
C                                                                        -
CD     NPRMAT            NUMBER OF PROBLEM MATERIALS                    -
CD     A0,A1,A2,A3       MATERIAL DEPENDENT COEFFICIENTS USED IN        -
CD                       FIT OF AVERAGE NUMBER OF NEUTRONS PER FISSION  -
CD                       VERSUS ENERGY
```

APPENDIX D. MC^2-2 Binary Files. SPECXS (Contd.)

```
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          TOTAL CROSS SECTION (TYPE 3)                                -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    (BSIGT(I),I=1,NGRP)                                               -
C                                                                       -
CW    NGRP                                                              -
C                                                                       -
CD    BSIGT           MACROSCOPIC UFG TOTAL CROSS SECTION               -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          SCATTERING CROSS SECTION (TYPE 4)                           -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    (BSIGS(I),I=1,NGRP)                                               -
C                                                                       -
CW    NGRP                                                              -
C                                                                       -
CD    BSIGS           MACROSCOPIC UFG P0 SCATTERING CROSS SECTION        -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          EXTENDED TRANSPORT CROSS SECTION (TYPE 5)                   -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL    ((AL(I,K),I=1,NGRP),K=1,NORDER)                                   -
C                                                                       -
CW    NGRP*NORDER                                                       -
C                                                                       -
CD    NORDER          ORDER OF EXTENDED TRANSPORT APPROXIMATION         -
CD    AL              MACROSCOPIC UFG EXTENDED TRANSPORT CROSS          -
CD                    SECTION                                           -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          P1 SCATTERING (TYPE 6)                                      -
```

APPENDIX D. MC^2-2 Binary Files. SPECXS (Contd.)

```
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL     (SIGTRN(I),I=1,NGRP)                                             -
C                                                                       -
CW     NGRP                                                             -
C                                                                       -
CD     SIGTRN              MACROSCOPIC UFG P1 SCATTERING CROSS SECTION   -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          MODERATING PARAMETER ZETA (TYPE 7)                          -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL     ((ZETA(I,J),I=1,NCSD),J=1,ISP)                                   -
C                                                                       -
CW     ISP*NCSD                                                         -
C                                                                       -
CD     ZETA                CONTINUOUS SLOWING DOWN MODERATING PARAMETER -
CD                         ZETA AT EACH ENERGY POINT IN CSD REGION FOR  -
CD                         P0 AND P1 SCATTERING                         -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          MODERATING PARAMETER EPS (TYPE 8)                           -
C                                                                       -
CC          ALWAYS PRESENT                                              -
C                                                                       -
CL     ((EPS(I,J),I=1,NCSD),J=1,ISP)                                    -
C                                                                       -
CW     ISP*NCSD                                                         -
C                                                                       -
CD     EPS                 CONTINUOUS SLOWING DOWN MODERATING PARAMETER -
CD                         1./GAMMA AT EACH ENERGY POINT IN CSD REGION FOR-
CD                         P0 AND P1 SCATTERING                         -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. SRATES

```
C*****************************************************************
C                                                                -
C                       PREPARED 3/06/75 AT ANL                  -
C                                                                -
CF          SRATES                                               -
CE          SCATTERING RATES AND SOURCES                         -
C                                                                -
CN                      SCATTERING RATES AND SOURCES FOR USE IN  -
CN                      AREA 10 (CSC011) INTEGRAL TRANSPORT THEORY -
CN                      CALCULATIONS                             -
C                                                                -
C*****************************************************************


CD    MAXUFG            LOWEST ENERGY ULTRA FINE GROUP FOR WHICH
CD                      SCATTERING RATES ARE PROVIDED.  ULTRA FINE
CD                      GROUP MAXUFG IS THE ULTRA FINE GROUP
CD                      IMMEDIATELY ABOVE THE TOP OF THE HIGHEST
CD                      ENERGY BROAD GROUP IN THE AREA 10 (CSC011)
CD                      ENERGY RANGE
CD    MINUFG            HIGHEST ENERGY ULTRA FINE GROUP NUMBER FOR
CD                      WHICH SCATTERING RATES ARE PROVIDED
CD    NPASS             NUMBER OF TYPE 2 RECORDS PRESENT IN THE FILE
CD    NPRMAT            NUMBER OF MATERIALS IN THE PROBLEM
CD    NUFGRD            NUMBER OF ULTRA FINE GROUPS READ FOR EACH PASS
CD                      OF RECORD 2.  NUFGRD=I2-I1+1 (SEE RECORD 2)


C---------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                        PRESENT IF        -
CS          ================================   ================= -
CS          SPECIFICATIONS                     ALWAYS            -
CS    ******** (REPEAT NPASS TIMES)                             -
CS    *     SOURCES                            NPASS.GT.0        -
CS    ********                                                   -
CS          SCATTERING RATES                   ALWAYS PRESENT    -
CS          HYDROGEN SCATTERING RATES          PRESENT IF NHYDRO=1 -
CS                                             (SEE RECORD 1 OF DATA-
CS                                              SET PRBSPC)      -
C                                                                -
C---------------------------------------------------------------


C---------------------------------------------------------------
CR          SPECIFICATIONS (TYPE 1)                              -
C                                                                -
CL    MINUFG,MAXUFG,NUFGRD,NPASS                                 -
C                                                                -
```

APPENDIX D. MC^2-2 Binary Files. SRATES (Contd.)

```
CW     4
C
C-----------------------------------------------------------------

C-----------------------------------------------------------------
CR           SOURCES (TYPE 2)
C
CC           PRESENT IF NPASS.GT.0
C
CL     ((SFIX(M,I),M=1,NPRMAT),I=I1,I2)
C
CW     NUFGRD*NPRMAT
C
CD     SFIX(M,I)          MICROSCOPIC SOURCE INTO ULTRA FINE GROUP I
CD                        DUE TO FISSION, INELASTIC SCATTERING, AND
CD                        N,2N SCATTERING IN MATERIAL M.
CD                        I RANGES OVER THE ULTRA FINE GROUPS IN THE
CD                        AREA 10 (CSC011) ENERGY RANGE, MAXUFG+1
CD                        THROUGH NGROUP, WHERE NGROUP IS THE
CD                        LOWEST ENERGY ULTRA FINE GROUP IN THE PROBLEM.
CD                        NUFGRD ULTRA FINE GROUPS ARE INCLUDED FOR EACH
CD                        PASS.
CD     I1                 FIRST ULTRA FINE GROUP READ FOR CURRENT PASS
CD     I2                 LAST ULTRA FINE GROUP READ FOR CURRENT PASS
C
C-----------------------------------------------------------------

C-----------------------------------------------------------------
CR           SCATTERING RATES (TYPE 3)
C
CC           ALWAYS PRESENT
C
CL     ((SS(I,M),I=1,MINMAX),M=1,NPRO)
C
CW     NPRO*MINMAX
C
CD     SS                 PRODUCT OF MICROSCOPIC SCATTERING CROSS
CD                        SECTION TIMES ULTRA FINE GROUP FLUX DIVIDED BY
CD                        THE ULTRA FINE GROUP LETHARGY WIDTH FOR THE
CD                        FINE GROUPS MINUFG THROUGH MAXUFG FOR EACH
CD                        MATERIAL
CD     MINMAX             MAXUFG-MINUFG+1
CD     NPRO               NPRMAT IF HYDROGEN IS NOT PRESENT IN THE
CD                        PROBLEM MIXTURE.  NPRMAT-1 IF HYDROGEN IS IN
CD                        PROBLEM MIXTURE
C
C-----------------------------------------------------------------
```

APPENDIX D. MC^2-2 Binary Files. SRATES (Contd.)

```
C-----------------------------------------------------------------------
CR          HYDROGEN SCATTERING RATES (TYPE 4)                        -
C                                                                     -
CC          PRESENT IF NHYDRO=1 (SEE RECORD 1 OF DATA SET PRBSPC)     -
C                                                                     -
CL    (SHYDRO(I),I=1,MAXUFG)                                          -
C                                                                     -
CW    MAXUFG                                                          -
C                                                                     -
CD    SHYDRO            PRODUCT OF HYDROGEN MICROSCOPIC SCATTERING    -
CD                      CROSS SECTION TIMES ULTRA FINE GROUP FLUX     -
CD                      DIVIDED BY THE ULTRA FINE GROUP LETHARGY WIDTH -
CD                      FOR ALL ULTRA FINE GROUPS ABOVE THE AREA 10   -
CD                      (CSC011) ENERGY RANGE                         -
C                                                                     -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. UNREG

```
C*****************************************************************
C                                                                -
C                        PREPARED 3/10/75 AT ANL                 -
C                                                                -
CF          UNREG                                                -
CE          UNRESOLVED UFG CROSS SECTIONS                        -
C                                                                -
CN                       THIS FILE IS WRITTEN BY MC**2-II AREA 7 -
CN                       (CSC008)                                -
C                                                                -
C*****************************************************************

CD     IFI               FISSION FLAG
CD                       IFI=0 MATERIAL IS NOT FISSIONABLE
CD                       IFI=1 MATERIAL IS FISSIONABLE
CD     IMAX1             LOWEST ENERGY UFG FOR WHICH MATERIAL HAS
CD                       NON-ZERO UNRESOLVED CROSS SECTION
CD     IMIN1             HIGHEST ENERGY UFG FOR WHICH MATERIAL HAS
CD                       NON-ZERO UNRESOLVED CROSS SECTION
CD     MULT              2 FOR IBM MACHINES, 1 OTHERWISE
CD     NREG              NUMBER OF REGIONS
CD                       NREG=1 FOR HOMOGENEOUS PROBLEMS (NGEOM=0)
CD                       NREG=2 FOR PIN CELLS (NGEOM=2) AND IF
CD                              MAXHTM.GT.0
CD                       NREG=1 + NUMBER OF SLAB REGIONS FOR SLAB
CD                              PROBLEMS (NGEOM=1) AND IF MAXHTM.GT.0
CD                       (MAXHTM IS THE MAXIMUM NUMBER OF MATERIALS IN
CD                       ANY HETEROGENEOUS REGION)
CD     NUMRES            NUMBER OF UNRESOLVED RESONANCE MATERIALS

C-----------------------------------------------------------------
CS          FILE STRUCTURE                                       -
CS                                                               -
CS          RECORD TYPE                          PRESENT IF      -
CS          ===================================  ================-
CS          SPECIFICATIONS                       ALWAYS          -
CS          UNRESOLVED MATERIAL NAMES            ALWAYS          -
CS    ******** (REPEAT FOR NUMRES MATERIALS)                     -
CS    *     MATERIAL SPECIFICATIONS              ALWAYS          -
CS    *  ***** (REPEAT FOR 1+NO. OF REGIONS                      -
CS    *  *       IN WHICH MATERIAL IS TREATED                    -
CS    *  *       HETEROGENEOUSLY)                                -
CS    *  *  CAPTURE CROSS SECTION               IMIN1.GT.0      -
CS    *  *  FISSION CROSS SECTION               IMIN1.GT.0, IFI.GT.0
CS    *  *  TOTAL CROSS SECTION                 IMIN1.GT.0      -
CS    ********                                                   -
C                                                                -
C-----------------------------------------------------------------
```

APPENDIX D. MC^2-2 Binary Files. UNREG (Contd.)

```
C-------------------------------------------------------------------------
CR          SPECIFICATIONS (TYPE 1)                                      -
C                                                                        -
CC          ALWAYS PRESENT                                               -
C                                                                        -
CL    NUMRES,NREG                                                        -
C                                                                        -
CW    2                                                                  -
C                                                                        -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR          UNRESOLVED MATERIAL NAMES (TYPE 2)                           -
C                                                                        -
CC          ALWAYS PRESENT                                               -
C                                                                        -
CL    (UNRMAT(I),I=1,NUMRES)                                             -
C                                                                        -
CW    MULT*NUMRES                                                        -
C                                                                        -
CD    UNRMAT            NAME OF UNRESOLVED MATERIAL (DOUBLE PRECISION)   -
C                                                                        -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR          MATERIAL SPECIFICATIONS (TYPE 3)                             -
C                                                                        -
CC          ALWAYS PRESENT                                               -
C                                                                        -
CL    IFI,IMIN1,IMAX1                                                    -
C                                                                        -
CW    3                                                                  -
C                                                                        -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR          CAPTURE CROSS SECTION (TYPE 4)                               -
C                                                                        -
CC          PRESENT FOR HOMOGENEOUS MIXTURE IF IMIN1.GT.0.               -
CC          ALSO PRESENT FOR EACH HETEROGENEOUS REGION IN WHICH CURRENT- -
CC          MATERIAL IS TREATED HETEROGENEOUSLY                          -
C                                                                        -
CL    (SIGC(I),I=IMIN1,IMAX1)                                            -
C                                                                        -
CW    IMAX1-IMIN1+1                                                      -
```

APPENDIX D. MC^2-2 Binary Files. UNREG (Contd.)

```
C                                                                       -
CD    SIGC              UNRESOLVED RESONANCE CAPTURE CROSS SECTIONS      -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          FISSION CROSS SECTION (TYPE 5)                              -
C                                                                       -
CC          PRESENT FOR HOMOGENEOUS MIXTURE IF IMIN1.GT.0, IFI.GT.0.    -
CC          ALSO PRESENT FOR EACH HETEROGENEOUS REGION IN WHICH CURRENT-
CC          MATERIAL IS TREATED HETEROGENEOUSLY AND IFI.GT.0             -
C                                                                       -
CL    (SIGF(I),I=IMIN1,IMAX1)                                           -
C                                                                       -
CW    IMAX1-IMIN1+1                                                     -
C                                                                       -
CD    SIGF              UNRESOLVED RESONANCE FISSION CROSS SECTIONS      -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CP          TOTAL CROSS SECTION (TYPE 6)                                -
C                                                                       -
CC          PRESENT FOR HOMOGENEOUS MIXTURE IF IMIN1.GT.0.              -
CC          ALSO PRESENT FOR EACH HETEROGENEOUS REGION IN WHICH CURRENT-
CC          MATERIAL IS TREATED HETEROGENEOUSLY                         -
C                                                                       -
CL    (SIGT(I),I=IMIN1,IMAX1)                                           -
C                                                                       -
CW    IMAX1-IMIN1+1                                                     -
C                                                                       -
CD    SIGT              UNRESOLVED RESONANCE TOTAL CROSS SECTIONS       -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX D. MC^2-2 Binary Files. UNRES

```
C*****************************************************************************
C                                                                              -
C                        PREPARED 3/05/75 AT ANL                               -
C                                                                              -
CF          UNRES                                                              -
CE          UNRESOLVED RESONANCE CROSS SECTIONS                                -
C                                                                              -
CN                       THIS DATA SET IS WRITTEN BY MC**2-II AREA 5            -
CN                       (CSC004) IF UNRESOLVED MATERIALS ARE PRESENT          -
C                                                                              -
C*****************************************************************************


CD     MULT              2 FOR IBM MACHINES, 1 OTHERWISE
CD     NISO              NUMBER OF ISOTOPES FOR EACH MATERIAL
CD     NPTS              NUMBER OF ENERGY (ESTAR) POINTS FOR
CD                       EACH ISOTOPE
CD     NREG              NUMBER OF REGIONS
CD                       NREG=1 FOR HOMOGENEOUS PROBLEMS (NGEOM=0)
CD                       NREG=2 FOR PIN CELLS (NGEOM=2) AND IF
CD                              MAXHTM.GT.0
CD                      •NREG=1 + NUMBER OF SLAB REGIONS FOR SLAB
CD                              PROBLEMS (NGEOM=1) AND IF MAXHTM.GT.0
CD                       (MAXHTM IS THE MAXIMUM NUMBER OF MATERIALS IN
CD                       ANY HETEROGENEOUS REGION)
CD     NUMRES            NUMBER OF UNRESOLVED RESONANCE MATERIALS


C------------------------------------------------------------------------------
CS          FILE STRUCTURE                                                     -
CS                                                                             -
CS             RECORD TYPE                              PRESENT IF             -
CS             ================================         ======================-
CS             SPECIFICATIONS                           ALWAYS                 -
CS             MATERIAL NAMES                           ALWAYS                 -
CS     ********** (REPEAT FOR NUMRES                                           -
CS     *           MATERIALS)                                                  -
CS     *       MATERIAL SPECIFICATION                   ALWAYS                 -
CS     *       ENERGY POINT INDEX                       ALWAYS                 -
CS     *  ******** (REPEAT NISO TIMES)                                         -
CS     *  *     ENERGY SPECIFICATIONS                   ALWAYS                 -
CS     *  *  ***** (REPEAT FOR 1+NO. OF REGIONS                                -
CS     *  *  *       IN WHICH MATERIAL IS TREATED                              -
CS     *  *  *       HETEROGENEOUSLY)                                          -
CS     *  *  *  CAPTURE CROSS SECTIONS               ALWAYS                   -
CS     *  *  *  FISSION CROSS SECTIONS               IFI.EQ.1                 -
CS     *  *  *  TOTAL CROSS SECTIONS                 ALWAYS                   -
CS     **********                                                              -
C                                                                              -
C------------------------------------------------------------------------------
```

APPENDIX D. MC^2-2 Binary Files. UNRES (Contd.)

```
CR          ENERGY POINT INDEX (TYPE 4)                                  -
C                                                                        -
CC          ALWAYS PRESENT                                               -
C                                                                        -
CL    (NPTS(I),I=1,NISO)                                                 -
C                                                                        -
CW    NISO                                                               -
C                                                                        -
C-------------------------------------------------------------------------


C-------------------------------------------------------------------------
CR          ENERGY SPECIFICATIONS (TYPE 5)                               -
C                                                                        -
CC          ALWAYS PRESENT                                               -
C                                                                        -
CL    (ESTAR(I),I=1,NPTS)                                                -
C                                                                        -
CW    NPTS                                                               -
C                                                                        -
CD    ESTAR             ENERGY POINTS                                    -
C                                                                        -
C-------------------------------------------------------------------------


C-------------------------------------------------------------------------
CR          CAPTURE CROSS SECTIONS (TYPE 6)                              -
C                                                                        -
CC          ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE, ALSO PRESENT         -
CC          FOR EACH HETEROGENEOUS REGION IN WHICH CURRENT MATERIAL      -
CC          IS TREATED HETEROGENEOUSLY                                   -
C                                                                        -
CL    (SIGCAP(I),I=1,NPTS)                                               -
C                                                                        -
CW    NPTS                                                               -
C                                                                        -
CD    SIGCAP            UNRESOLVED RESONANCE CAPTURE CROSS SECTIONS     -
C                                                                        -
C-------------------------------------------------------------------------


C-------------------------------------------------------------------------
CR          FISSION CROSS SECTIONS (TYPE 7)                              -
C                                                                        -
CC          ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE IF IFI.EQ.1           -
CC          ALSO PRESENT FOR EACH HETEROGENEOUS REGIONS IF IFI.EQ.1       -
CC          AND CURRENT MATERIAL IS TREATED HETEROGENEOUSLY IN REGION    -
C                                                                        -
CL    (SIGFIS(I),I=1,NPTS)                                               -
C
```

APPENDIX D. MC^2-2 Binary Files. UNRES (Contd.)

```
C-----------------------------------------------------------------------
CR          SPECIFICATIONS (TYPE 1)                                    -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL    NUMRES,NREG,NPTMAX,MAXISO                                        -
C                                                                      -
CW    4                                                                -
C                                                                      -
CD    NPTMAX            MAXIMUM NUMBER OF POINTS FOR ANY MATERIAL      -
CD                      IN THE LIBRARY                                 -
CD    MAXISO            MAXIMUM NUMBER OF ISOTOPES IN THE MIXTURE      -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          MATERIAL NAMES (TYPE 2)                                    -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL    (UNRMAT(I),I=1,NUMRES)                                           -
C                                                                      -
CW    MULT*NUMRES                                                      -
C                                                                      -
CD    UNRMAT            DOUBLE PRECISION (R*8) UNRESOLVED RESONANCE    -
CD                      MATERIAL NAMES                                 -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          MATERIAL SPECIFICATION (TYPE 3)                            -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL    NISO,IFI                                                         -
C                                                                      -
CW    2                                                                -
C                                                                      -
CD    IFI               FISSILE MATERIAL INDEX                         -
CD                      IFI=0 FOR NON-FISSILE MATERIAL                 -
CD                      IFI=1 FOR FISSILE MATERIAL                     -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
```

APPENDIX D. MC^2-2 Binary Files. UNRES (Contd.)

```
CW    NPTS                                                              -
C                                                                       -
CD    SIGFIS            UNRESOLVED RESONANCE FISSION CROSS SECTIONS      -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          TOTAL CROSS SECTIONS (TYPE 8)                               -
C                                                                       -
CC          ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE, ALSO PRESENT        -
CC          FOR EACH HETEROGENEOUS REGION IN WHICH CURRENT MATERIAL     -
CC          IS TREATED HETEROGENEOUSLY                                  -
C                                                                       -
CL    (SIGTOT(I),I=1,NPTS)                                              -
C                                                                       -
CW    NPTS                                                              -
C                                                                       -
CD    SIGTOT            UNRESOLVED RESONANCE TOTAL CROSS SECTIONS      -
C                                                                       -
C-----------------------------------------------------------------------

CEOF
```

APPENDIX E

BPOINTER, A DYNAMIC STORAGE ALLOCATION PROGRAM

APPENDIX E

BPOINTER, A Dynamic Storage Allocation Program

1. Description of Subprogram Package

BPOINTER is a FORTRAN subprogram package which was developed to alleviate bookkeeping chores associated with the use of dynamic storage allocation techniques.[1]

Programs which use the BPOINTER capability tend to be structured in subroutine form. A control routine is used to define one or two large blocks of storage (called the container arrays), and make the appropriate calls to BPOINTER to control the allocation of storage within these block(s). Calls to calculational subroutines transmit pointers corresponding to appropriate array locations through the calling sequences. All BPOINTER capabilities are accessed through an appropriate call to an entry point, subroutine, or function subprogram. The following capabilities are available in the BPOINTER system:

(a) Storage of data in and retrieval of data from the container array, via user defined variable arrays.

(b) Purge of variable arrays stored in the container array.

(c) Automatic "cleanup" of the container array when more storage is required.

(d) Re-definition of array sizes without loss of data already stored in the array.

(e) Array dump of selected integer, floating point or BCD arrays in a prescribed format.

(f) Trace dumps of BPOINTER activities.

(g) Status reports of the BPOINTER tables.

Detailed program documentation including flow charts, common block information and subprogram descriptions is availabe in Reference 1. This Appendix is intended to provide a brief description of how the program package operates. The major differences between the IBM and CDC standalone versions of the program package are also noted.

The short example listed in Fig. 27 is intended to illustrate the structure of a program using the BPOINTER package. This example demonstrates the manner in which a container is allocated, pointers defined and used, and the container released.

Brief descriptions of all the BPOINTER entry points, subroutines and functions are given in Table XIV.

All dynamically allocated arrays are addressed relative to the common block /ARRAY/ which contains a single array element, BLK(1). In the IBM version of the code the element must be declared as DOUBLE PRECISION. A second common block /ARRAY2/ is used in the CDC version of BPOINTER to address arrays allocated to a large core memory container. This common block also contains a single array element BLKECS(1) which must be declared a LEVEL 2 variable. The equivalent of the large core memory container on IBM equipment is a second container which may be given a HIARCHY 1 location but is addressed in precisely the same manner as the first (SCM) container. The one word assigned to the container by the source language program provides a reference address. At execution time machine language routines (ALLOC1, ALLOC2 on IBM, MEMGET1, MEMGET2 on CDC) are used to obtain the addresses of core which are available to the program for the allocation of data arrays. These blocks of core are allocated in the following manner.

(a) IBM allocation

The standard IBM macro instructions GETMAIN and FREEMAIN are used to allocate and free consecutive words of core which are available to the program. The designations subpool 1 and 2 are assigned to the bulk (LCM) and fast (SCM) containers respectively. Since allocations are performed in units of 256 (eight byte) words, it is most efficient to request blocks of core in such multiplies;

(b) CDC allocation

The COMPASS routine MEMGET uses the standard CDC macro instruction MEMORY to determine the jobs SCM and LCM field length. The core available as a container for the BPOINTER SCM arrays is determined by subtracting the address of blank common from the SCM field length. Thus a program using the CDC version of BPOINTER should not use blank common. Blank common is used for this purpose because of the CDC loader convention which places blank common after all other program sections in core. Although blank common is used in this manner to determine the available core for a container, arrays in the container are addressed relative to the common block /ARRAY/ as noted above. The BPOINTER program package accounts for the offsets between the address of /ARRAY/ in core and the address of the container. It should also be noted that the conventions used by BPOINTER are such that the first word of the container is not in general set to the first word of blank common. This is important since the loader convention noted above is not adhered to by all CDC Systems. The user is therefore responsible for providing enough SCM memory to accommodate the program, any SCM buffers, and the BPOINTER container as there is currently no effective check to make sure that data stored in the BPOINTER container do not overlap code. It is assumed by the CDC version of BPOINTER that the LEVEL 2 common block /ARRAY2/ is addressed as the first word of LCM and the entire LCM field length is assumed to be available to BPOINTER for its LCM container.

The letters M and B are used as neumonics within BPOINTER to designate routines which operate on the SCM and LCM containers respectively. Thus PUTM allocates an array in the SCM container while PUTB allocates an array which must be referenced on CDC equipment as a LEVEL 2 array. On IBM equipment without HIARCHY support (e.g. 370/195) the two containers are equivalent. The distinctions noted above between the two dynamic containers are important on CDC equipment where the containers are addressed quite differently and on IBM equipment with HIARCHY support where access to the BULK core container (HIARCHY 1, subpool 1) is significantly slower than access to the MAIN core container (HIARCHY 0, subpool 2).

```
C  BPOINTER EXAMPLE
C  DEFINE CONTAINER COMMON BLOCK
C
      REAL*8 BLK, FLUX, POWER
      COMMON/ARRAY/BLK(1)
      DIMENSION BLK4(1)
      EQUIVALENCE (BLK(1),BLK4(1))
      DATA FLUX/6HFLUX  /, POWER/6HPOWER /, MAXSIZ/10000/
      DATA I4/4/, I8/8/, I0/0/, NG/27/
C
C  ALLOCATE CONTAINER WITH MAXSIZ WORDS OF SCM AND NO LCM
C
      CALL BULK(I0)
      CALL POINTR(BLK,MAXSIZ,I0)
C
C  ALLOCATE SPACE FOR ARRAYS POWER, FLUX AND CURRENT
C
      CALL PUTM(POWER,I8,NG,IPOWR)
      CALL PUTM(FLUX,I4,2*NG,IFLUX)
C
C  DETERMINE POINTER FOR SUB-ARRAY CURRENT WHICH FOLLOWS THE
C  NG SINGLE PRECISION WORDS FOR THE ARRAY FLUX
C
      ICURNT=IPT2(IFLUX,NG,I0)
C
C  CHECK ON BPOINTER ERROR
C
      IF( IPTERR(DUM).GT.0 ) PRINT 500
  500 FORMAT(1H0,14HBPOINTER ERROR)
C
C  CALL SUBROUTINE INIT TO USE THESE ARRAYS
C
      CALL INIT(BLK(IFLUX),BLK(IPOWR),BLK4(ICURNT),NG)
C
C  FREE CONTAINER AND RETURN
C
      CALL FREE
      RETURN
      END
      SUBROUTINE INIT(PHI,POWER,CURENT,NG)
C
C  USE BPOINTER ARRAYS JUST AS ANY OTHER VARIABLES
C
      REAL*8 POWER
      DIMENSION PHI(1),POWER(1),CURENT(1)
      DO 10 I=1,NG
      PHI(I)=1.0
      POWER(I)=3.1E+06
      CURENT(I)=.333
   10 CONTINUE
      RETURN
      END
```

Fig. 27. BPOINTER Example

TABLE XIV. BPOINTER Subprogram Descriptions

POINTR (008710 - 010270)*	Initializes tables of dynamic allocation program package and calls ALLOC1 and ALLOC2 to allocate container(s) for variably dimensioned arrays.
PUTPNT/PUTBLK (010280 - 010590)	Dummy routine calls PUTM to allocate array storage.
BULK (010600 - 010720)	Sets number of words of BULK(LCM) core to be allocated.
FREE (010730 - 011020)	Calls FREE1 and FREE2 to release containers allocated by calls from subroutine POINTR.
WIPOUT/CLEAR (011030 - 011780)	Deletes a named array from BPOINTER tables; zeroes all locations assigned to a named array.
GETPNT/GETN/DUMP (011790 - 013310)	Returns pointer for a named array; return index in BPOINTER tables of a named array; controls printing of a named array.
IGET (013320 - 013730)	Returns pointer for a named array.
IPT2 (013740 - 013870)	Returns pointer to a sub-array relative to a single precision word length container.
PUTM/PUTB (013880 - 015460)	Enters named arrays into fast and bulk(LCM) containers respectively.
IPTERR/NNAMSF (015470 - 015740)	Returns number of BPOINTER errors; returns number of named arrays in BPOINTER tables.
ILAST/ILASTB (015750 - 015940)	Returns word number of first available word in SCM/LCM container.
REDEF (015950 - 016130)	Dummy routine calls REDEFM to redefine size and/or location of named array.
REDEFM/REDEFB (016140 - 017990)	Redefine the size and/or location of named array within BPOINTER tables and containers.

*Numbers in brackets are card sequence numbers of routine on MC^2-2 program tape.

TABLE XIV. BPOINTER Subprogram Descriptions (Contd.)

PURGE/PURGEB	(018000 - 019270)	Sift storage in SCM/LCM containers to eliminate unused blocks created by WIPOUT calls.
STATUS	(019280 - 019660)	Edits status of BPOINTER tables.
PRTI1	(019670 - 019790)	Prints half word integer array from SCM container.
PRTI1E	(019800 - 020000)	Prints half word integer array from LCM container.
PRTI2	(020010 - 020090)	Prints full word integer array from SCM container.
PRTI2E	(020100 - 020270)	Prints full word integer array from LCM container.
PRTR1/PRTA1	(020280 - 020450)	Prints full word real array from SCM container.
PRTR1E/PRTA1E	(020460 - 020720)	Prints full word real array from LCM container.
PRTR2/PRTA2	(020730 - 020930)	Prints double word read array from SCM container.
PRTR2E/PRTA2E	(020940 - 021230)	Prints double word real array from LCM container.

APPENDIX F

MC^2-2 LIBRARY GENERATION

APPENDIX F

MC^2-2 Library Generation

The MC^2-2 library contains eight files, MCC2F1-MCC2F8, that were processed from the ENDF/B-IV data files by the code ETOE-II. Appendix C contains a description of these files. The user has the option of obtaining the binary MC^2-2 library or generating the MC^2-2 library from BCD card images on magnetic tapes. The library data are briefly summarized in Table IX.

The binary library for IBM users is contained on one 9 track, non-labeled, LRECL=X, RECFM=VBS, and BLKSIZE=6447 magnetic tape with a recording density of 1600 BPI. The eight files are written in sequential order MCC2F1-MCC2F8. A sample of the job control cards required to copy these files from tape to a direct access device (e.g. disk pack) is given in Fig. 22. The binary library for CDC users is contained on two 7 track, non-labeled, and x-mode binary tapes written with a recording density of 800 BPI. The first binary tape contains the files MCC2F1-MCC2F4, MCC2F7, and MCC2F8. The second tape contains the files MCC2F5 and MCC2F6. These two binary tapes were generated at BERKELEY. Figure 28 displays the control cards necessary to read the two 7 track x-mode binary tapes and write a 9 track 1600 BPI tape. The BERKELEY example displays the generation of a non-labeled, phase encoded, and x-mode binary-odd parity tape. The BROOKHAVEN example displays the generation of a labeled, SCOPE standard format tape. The 9 track tape which is generated in each case is used directly in the execution of the MC^2-2 problem as displayed in Fig. 25.

The user may generate the MC^2-2 library from three BCD data tapes which contain the same eight file library data in BCD format along with a BCD tape which contains a Fortran program, MC^2-2 LIBGEN, which reads the three BCD data tapes and writes the eight binary files. All four tapes are 7 track, unlabeled, 40 card images per physical block, and written at 800 BPI. Figure 29 displays the CDC control cards used to read the three BCD data tapes as well as the BCD program tape, MC^2-2 LIBGEN. The control cards also show the compilation and execution of this program which generates the eight binary MC^2-2 library files. The data tapes which are physically labeled MC2BCDLIB1, MC2BCDLIB2, and MC2BCDLIB3 are assigned the data set names TAPE11, TAPE12, and TAPE13 respectively in the program execution. The eight binary library files are written on one data set named TAPE21, and these data are written onto a 9 track 1600 BPI tape. This binary library tape is used directly in the execution of the MC^2-2 problem as shown in Fig. 25.

BERKELEY

```
(JOBCARD)
STAGE(IN1,D8,P3,MT,R,nnnnn,6F)
STAGE(IN2,D8,P3,MT,R,nnnnn,2F)
COPYBF(IN1,BINLIB,4)
COPYBF(IN2,BINLIB,2)
COPYBF(IN1,BINLIB,2)
REWIND(IN1,IN2,BINLIB)
STAGE(BINLIB,D9,P3,NT,W,nnnnn,8F)
6/7/8/9
```

BROOKHAVEN

```
(JOBCARD)
ACCOUNT(Name,NNNN)
STAGE(IN1,HY,VSN=Nnnnnn)
STAGE(IN2,HY,VSN=Nnnnnn)
STAGE(BINLIB,POST,E,PE,VSN=Knnn)
FILE(IN1,RT=X,BT=C,MBL=5120)
FILE(IN2,RT=X,BT=C,MBL=5120)
COPYBF(IN1,BINLIB,4)
COPYBF(IN2,BINLIB,2)
COPYFB(IN1,BINLIB,2)
REWIND(IN1,IN2,BINLIB)
6/7/8/9
```

Fig. 28. Generation of MC^2-2 Library from Two X-Mode Binary Library Tapes that were Generated at Berkeley

BERKELEY

```
(JOBCARD)
SCF(R=TAPE11,RL=80,BF=40,D8,nnnnn)
SCF(R=TAPE12,RL=80,BF=40,D8,nnnnn)
SCF(R=TAPE13,RL=80,BF=40,D8,nnnnn)
SCF(R=LIBGN,RL=80,BF=40,D8,nnnnn)
FTN(I=LIBGN,OPT=1)
LINK,X.
STAGE(TAPE21,D9,P3,NT,W,nnnnn,8F)
6/7/8/9
```

BROOKHAVEN

```
(JOBCARD)
ACCOUNT(Name,NNNN)
STAGE(TAPEA1,HY,VSN=Nnnnnn)
STAGE(TAPEA2,HY,VSN=Nnnnnn)
STAGE(TAPEA3,HY,VSN=Nnnnnn)
STAGE(LIBGN1,HY,VSN=Nnnnnn)
STAGE(TAPE21,POST,E,PE,VSN=Knnn)
FILE(TAPEA1,RT=F,FL=80,RB=40,BT=K,CM=YES)
FILE(TAPEA2,RT=F,FL=80,RB=40,BT=K,CM=YES)
FILE(TAPEA3,RT=F,FL=80,RB=40,BT=K,CM=YES)
FILE(LIBGN1,RT=F,FL=80,RB=40,BT=K,CM=YES)
COPYBF(TAPEA1,TAPE11,1)
COPYBF(TAPEA2,TAPE12,1)
COPYBF(TAPEA3,TAPE13,1)
COPYBF(LIBGN1,LIBGN,1)
REWIND(TAPE11,TAPE12,TAPE13,LIBGN)
RETURN(TAPEA1,TAPEA2,TAPEA3,LIBGN1)
FTN(I=LIBGN,OPT=1)
REWIND(LGO)
LOAD(LGO)
EXECUTE.
REWIND(TAPE21)
6/7/8/9
```

Fig. 29. Generation of MC^2-2 Library from Three BCD Data Tapes Using the Fortran Program MC^2-2 LIBGEN

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