Conf-780334--5

ETOE-2/MC^2-2/SDX MULTIGROUP CROSS-SECTION PROCESSING

By

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Prepared for

RSIC Seminar-Workshop on
Multigroup Cross Sections

Oak Ridge, TN

March 14, 1978

U of C-AUA-USDOE

ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

Operated under Contract W-31-109-Eng-38 for the
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ABSTRACT

The ETOE-2/MC^2-2/SDX multigroup cross-section processing codes have been designed to provide a comprehensive neutron cross-section processing capability for a wide range of applications including critical experiment analysis and core design calculations. Fundamental nuclear data from ENDF/B provide the primary input to the code system and the output consists of a user-specified CCCC ISOTXS multigroup cross-section data file. Great flexibility has been provided to the user in specifying the rigor of the calculation so that a unified cross-section processing system with a single data base is available which may be used for both preliminary survey scoping studies and rigorous design calculations.

The principal program blocks of the code system include: a library processor and format converter between ENDF/B data and the MC^2-2/SDX library; an ultra-fine-group fundamental mode calculation (MC^2-2) which provides a composition dependent spectrum calculation and broad-group collapsing capability; a rigorous hyper-fine-group spatially heterogeneous resolved resonance calculation (RABANL) to supplement the more approximate NR approximation used in the ultra-fine-group treatement; and an intermediate group space-dependent capability (SDX).

INTRODUCTION

The ETOE-2/MC^2-2/SDX multigroup cross-section processing codes have been designed to provide a comprehensive neutron cross-section generation capability for a wide range of applications including critical experiment analysis and core calculations. Fundamental nuclear data (ENDF/B) provide the primary input to the code system and the output consists of a user-specified multigroup cross-section data file (ISOTXS). Great flexibility is provided to the user in specifying the rigor of a calculation, thus providing a unified cross-section processing system with a single data base which may be used for both preliminary survey scoping and design calculations.

Work performed under the auspices of the U.S. Department of Energy.

The principal program blocks of the code system include a library processor (ETOE-2), an ultra-fine-group (ufg) fundamental mode calculation (MC^2-2), a rigorous hyper-fine-group (hfg) spatially heterogeneous resolved resonance capability (RABANL) and an intermediate-group space-dependent capability (SDX). A block diagram indicating the general program flow is given in Fig. 1. Brief descriptions of the physics methods and models incorporated in the ETOE-2/MC^2-2/SDX code system are presented below.

ETOE-2

The ETOE-2 program processes the fundamental nuclear data from an ENDF/B[1] data file and prepares eight binary library files for use by the computational modules of MC^2-2/SDX. Neither MC^2-2, RABANL, nor SDX reads the ENDF/B data directly. Thus, one could prepare MC^2-2/SDX library files from an alternative input data base (e.g., UKNDL, KEDAK) by either conversion of the basic data to the ENDF/B formats or by the replacement of the ETOE-2 code with a new processing code which generates the MC^2-2/SDX libraries.

The ETOE-2 program performs six basic functions: (1) reformat data; (2) preprocess "light" element ($A \approx 100$) resonance cross sections; (3) screen and preprocess "wide" and "weak" resolved resonances; (4) generate ultra-fine-group "floor" cross sections; (5) calculate function tables; and (6) convert all ENDF/B formats to laws which are allowed by MC^2-2/SDX.

The ENDF/B data files provide all data for a given material, whereas the MC^2-2/SDX computational modules require that the data be ordered by reaction type (e.g., resolved resonance parameters, scattering coefficients, etc.). The MC^2-2/SDX library structure has been designed to permit efficient access to data by the computational modules. The eight data files in the MC^2-2/SDX library include resolved resonance parameters, unresolved resonance parameters, ufg nonresonance cross sections, inelastic and (n,2n) scattering data, fission spectrum parameters, and elastic scattering distributions, as well as function tables and an administrative file.

At user option the ETOE-2 code calculates resonance cross sections from ENDF/B resonance parameters for all materials of mass less than an input value. Generally a mass of 100 is used. These "light" element resonance cross sections are then combined with the ENDF/B "floor" cross sections and integrated over ufg energy boundaries ($\Delta u \gtrsim 0.008$) to provide the ufg cross sections required by MC^2-2/SDX. It is assumed that "light" element resonance cross sections are composition-independent on the ultra-fine-group level.

With recent increasing emphasis on the use of the rigorous RABANL capability, much attention has been given to improving the computational efficiency of RABANL. One of the approaches taken has been to have

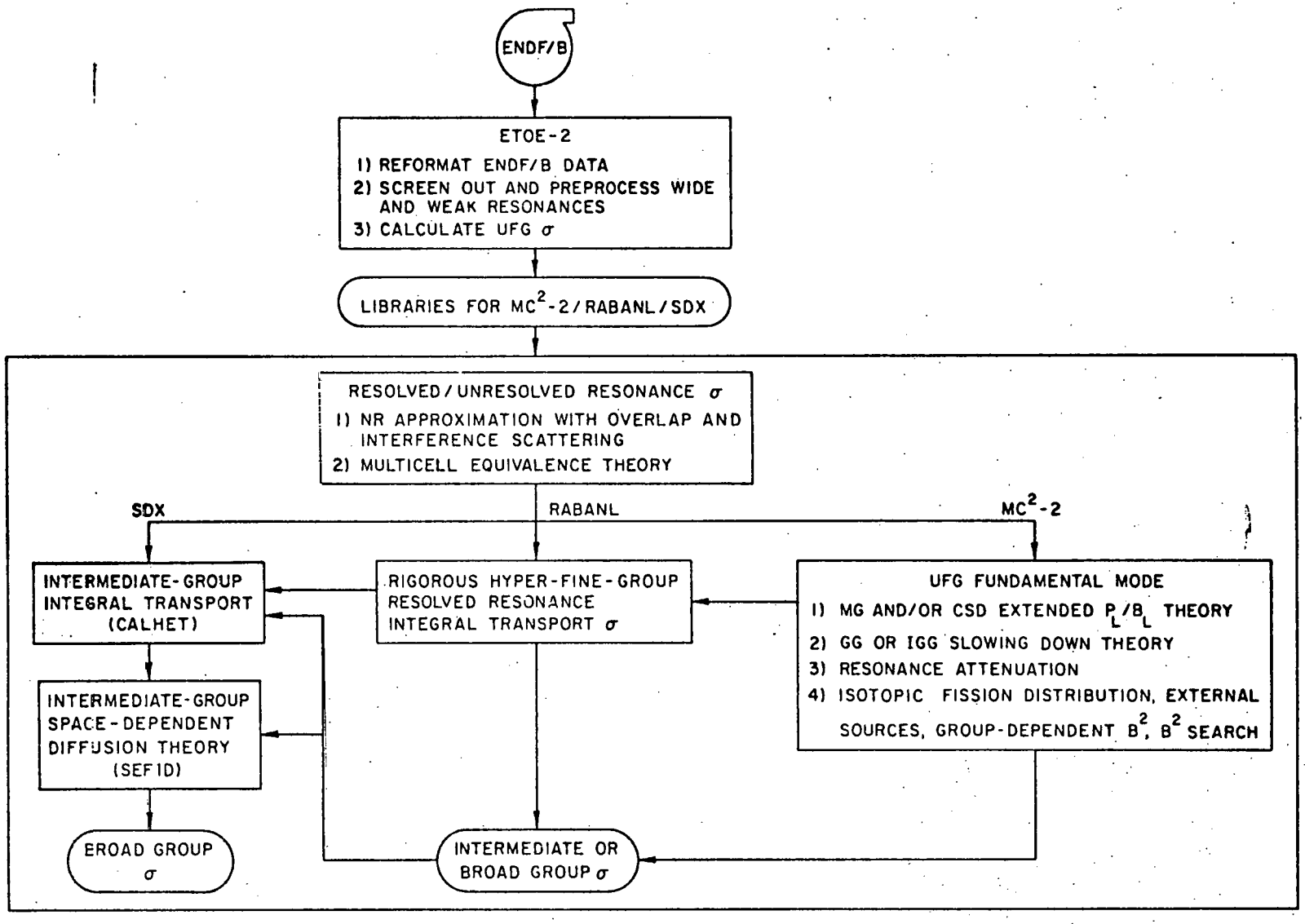

Fig. 1. ETOE-2/MC²-2/SDX

ETOE-2 screen out and preprocess a significant number of the resolved resonances into composition and temperature independent ufg "smooth" cross sections. Resolved resonances suitable for such screening can be characterized as belonging to one of two types. The first are the extremely wide resonances with natural widths much larger than both the corresponding Doppler width and the ufg width. The second type of resonance is typified by the extremely weak resonances belonging to the medium weight nuclei of low natural abundance, or the p-wave resonances of the heavy nuclei. This preprocessing by ETOE-2 has provided significant reductions in RABANL execution times, especially for problems involving structural material resonances.[2]

The ENDF/B formats permit a large number of options in describing the fundamental data. Many of these options have not been used in the four releases of ENDF/B to date and only a subset of the allowed ENDF/B laws are processed by MC^2-2/SDX. It is, therefore, necessary for the ETOE-2 code to process data given by any of the other laws and prepare these data in a format permitted by MC^2-2/SDX. The MC^2-2/SDX resolved resonance algorithms assume a single or multilevel Breit-Wigner or a multilevel Adler-Adler description whereas ENDF/B also permits R-Matrix (Reich-Moore) parameters. It is well known that equivalent multilevel Adler-Adler parameters may be derived from these models[3] and these equivalent parameters are calculated by ETOE-2. Similarly, ENDF/B permits six secondary energy distribution laws for inelastic and (n,2n) scattering, whereas MC^2-2 permits only three. The ETOE-2 code generates a tabulated function if data are provided for any of the three laws not processed by MC^2-2. Similar examples may be cited in the processing of elastic scattering distributions and fission spectrum data. In general, the format conversions performed by ETOE-2 do not alter the basic data input on the ENDF/B files. The unresolved parameters in ENDF/B may include data for the average competitive reaction width. These data have been ignored by ETOE-2 up to the present time. With the release of ENDF/B-V the ETOE-2 and MC^2-2/SDX codes will be modified to process the competitive width reaction data and the MC^2-2/SDX library files will be changed to include these data.

The ETOE-2 program thus provides an automated capability for the generation of MC^2-2/SDX library files from ENDF/B data. It performs the same functions for MC^2-2/SDX as the ETOE[4] and MERMC2[5] codes performed for the MC^2 cross-section preparation program.[6] Since the library files generated by ETOE-2 are not composition dependent, the program need be executed only when new fundamental data become available (e.g., each release of ENDF/B). A limited capability is also available to modify the data in the MC^2-2/SDX libraries, thus obviating the need to rerun ETOE-2 in order to study the sensitivity of multigroup cross sections to changes in fundamental data.

Since its introduction in 1967 and up to the present time, the MC² code has been used extensively for the preparation of multigroup cross sections. However, a number of recognized limitations and inconsistencies in the code pointed out the need for a new capability which could serve as a standard for fast reactor calculations. The MC²-2 code[7] has been developed to satisfy this need and represents a significant departure from the earlier MC² code. Recent advances in neutron slowing-down theory, resonance theory, and numerical methods have been incorporated into the ultra-fine-group fundamental mode MC²-2 calculation. The code algorithms and implementation strategy which are described in detail in Ref. 7 are briefly summarized below. A block diagram indicating the flow through the computational modules of MC²-2 is given in Fig. 2.

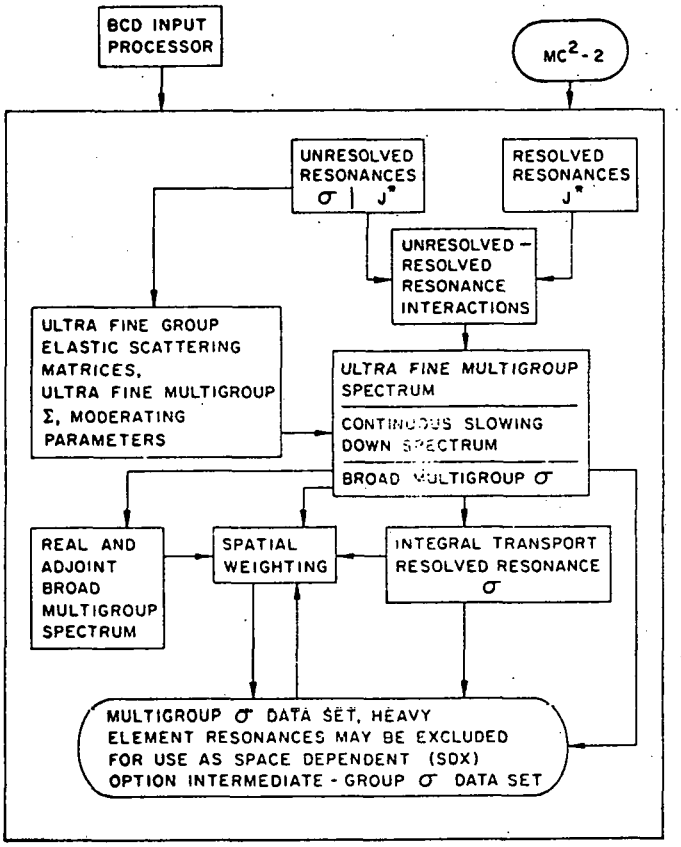

Fig. 2
MC²-2 Program Flow

The MC²-2 code solves the neutron slowing-down equations in the P_1, B_1, consistent P_1, and consistent B_1 approximations and makes use of the extended transport approximation to account for high-order transport and anisotropic scattering effects.[8,9] Both the continuous slowing down and multigroup forms of the slowing-down equations are solved using an ufg lethargy structure as depicted in Fig. 3.

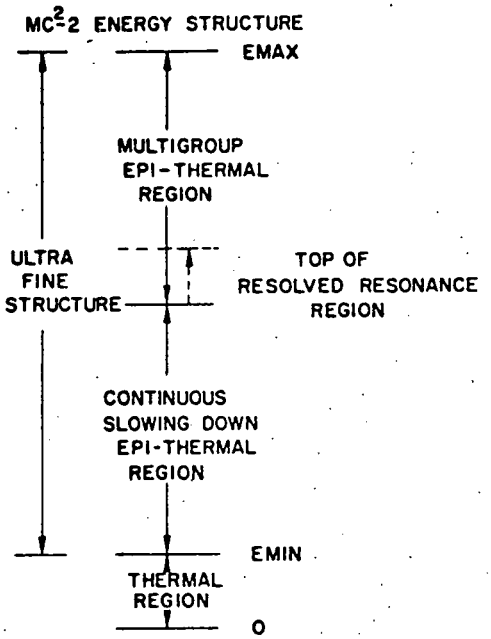

Fig. 3. MC^2-2 Energy Structure

The energy boundary between the multigroup and continuous slowing-down formulations is user-specified but must lie above the top of the resolved resonance energy region. This is a consequence of the resonance treatment discussed below. The moderating parameters, in the continuous slowing-down formulation may be calculated using either Greuling-Goertzel[10] or Improved Greuling-Goertzel[8] algorithms. Only elastic scattering is treated continuously in the continuous slowing-down formulation. Inhomogeneous sources along with fission, inelastic and (n,2n) sources are represented in the ufg multigroup form.

The resolved and unresolved resonance calculations of MC^2-2 are modeled after the work of Hwang[11] and represent a marked improvement in accuracy and a dramatic improvement in efficiency over the methods incorporated in the MC^2 code. The resonance algorithms make use of a generalized J*-integral formulation based on the narrow resonance approximation including overlap effects. The characteristics of these algorithms may be summarized briefly as follows:

(1) The integration procedure was optimized by utilizing the asymptotic properties of the integrands and the general characteristics of the Gauss-Jacobi quadrature. This was achieved by introducing a rational transformation of the variable of integration.

(2) For the relatively weak resonances which represent a significant portion in practical calculations, the J*-integral is evaluated analytically.

(3) For the resolved energy range, the new algorithms allow the use of the multilevel formalism in Adler-Adler form[12] and the multilevel and single level Breit-Wigner[13] forms.

(4) For the unresolved energy range, the algorithms provide an accurate estimate of the in-sequence overlap effect which accounts for the long-range correlation of levels described by Dyson[14] and include the influence of interference scattering.

As shown in Ref. 15, the J*-integral method provides an efficient means of accounting for resonance effects in the continuous slowing-down formulation. In particular, the continuous slowing-down equations are solved for the "asymptotic" neutron slowing-down density ignoring narrow resonances. Then the resonance reaction rates are computed using the flux resulting from the asymptotic slowing-down density

attentuated by absorption in higher energy resonances. The ultra-fine-group flux derived from the attentuated slowing-down is then used in the generation of broad-group cross sections by standard group-collapsing methods.

As noted above, the entire MC^2-2 calculation is performed on an ultra-fine-group mesh. Inelastic and (n,2n) secondary energy distributions may be described by discrete levels, evaporation spectra and/or tabulated functions according to the ENDF/B specifications. Detailed angular distributions are used in calculating ultra-fine-group P_0 and P_1 elastic transfer matrices for all materials. For light elements, an analytic integration over the sink group is combined with a detailed numerical integration over the source group.[16] Heavy element transfer matrices are calculated semi-analytically according to the methods described in Ref. 17.

Options available to the user of MC^2-2 include inhomogeneous group-dependent sources, group-dependent buckling, buckling search to critical, and isotope-dependent fission spectrum distributions. The user-specified cross-section file generated by MC^2-2 is appropriate for neutronics calculations ($\lesssim$50 groups) or for use in intermediate group ($\approx$50-300 groups) spectrum calculations. In particular, the intermediate group cross-section file may be used in the SDX capability described below.

A hyper-fine-group integral transport capability RABANL is also available at user option. The hfg width is defined to be small compared to the maximum lethargy gain on scattering by the heaviest isotope in the problem. RABANL was modeled after the RABID[18] and RABBLE[19] codes although significant modifications have been made to: (1) eliminate precision difficulties; (2) make use of the MC^2-2/SDX library data; (3) link the hyper-fine-group calculation to the ultra-fine-group calculations through the slowing-down souce; and (4) increase the overall efficiency of the codes.

Since hundreds of thousands of hfg may be involved, especially when including resonances of the structural materials which occur at tens or hundreds of keV, attention to algorithm efficiency was essential in order to permit RABANL to be used for routine calculations. The ETOE-2 screening mentioned above represents one such efficiency. Even more significant was recognizing and taking advantage of the asymptotic shape of the Doppler broadened resonance line shape functions to minimize calculations of these functions during the hfg sweep.[2]

An example of the improvement in accuracy of RABANL compared to the previous codes is the calculation of cylindrical transmission probabilities. By recognition of the asymptotic nature and analytic representation of the integrals involved, Hwang[20] has been able to eliminate the tabular interpolations required by earlier brute force methods with consequent improvements in storage requirements as well as accuracy.

Whereas initially RABANL was thought of as an option intended for use only in the low energy region ($\lesssim$300 eV) where the narrow resonance approximation assumed in the J*-integral formulation is known to be deficient, the algorithm improvements in RABANL have resulted in a code which is now used routinely for design and analysis activities with users frequently specifying a RABANL upper energy well above the heavy element resolved resonance range.

Figure 4 shows an example of the spectral detail provided by the MC^2-2 ufg capability for an inner core composition of ZPPR. The spectral detail below 4 keV is provided by the resolved resonance treatment described above, whereas the detail above 1 MeV is due primarily to the ufg treatment of the inelastic and (n,2n) scattering.

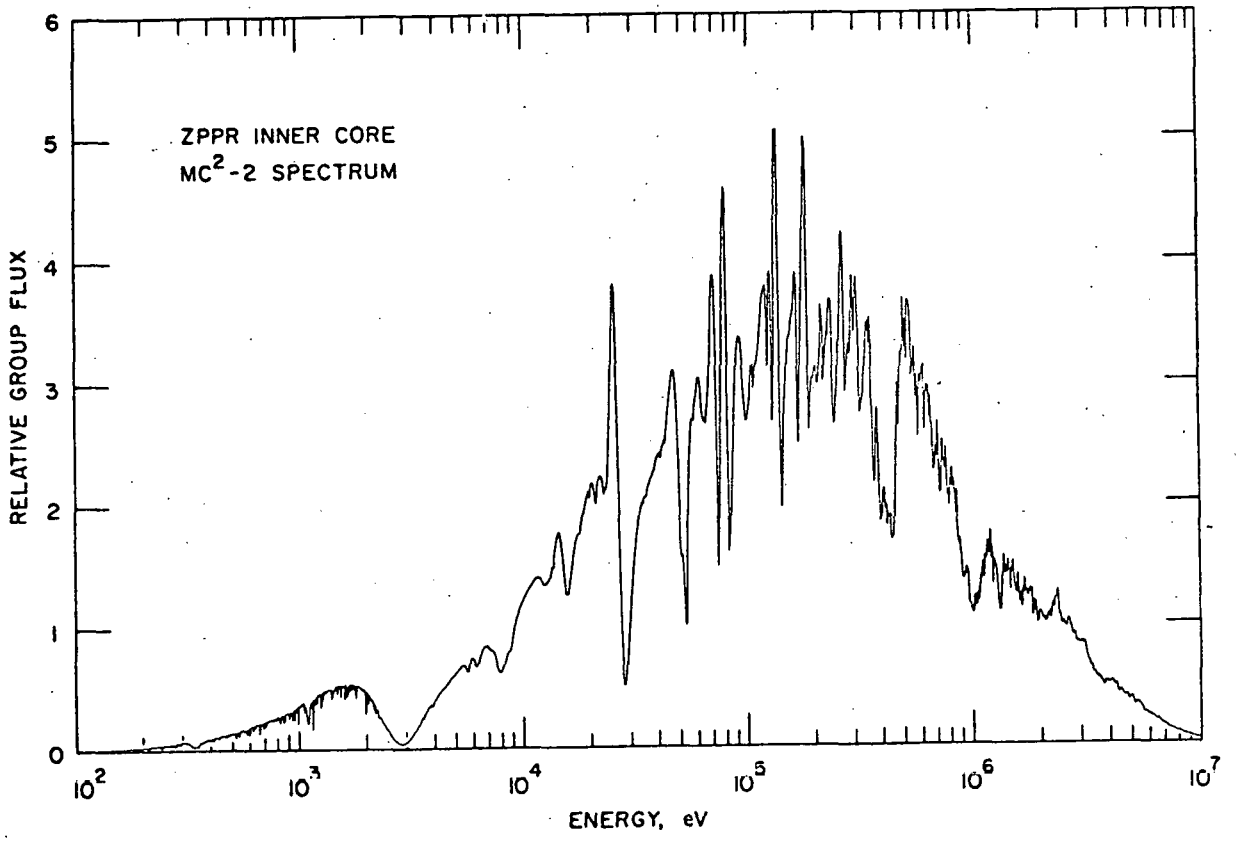

Fig. 4. MC^2-2 Spectrum, 0.0001-10 MeV

In order to illustrate the MC^2-2 execution times and compare IBM and CDC versions of the code, a sample problem as specified in Table 1 was run at ANL on the IBM/370-195 computer and at LRL Berkeley on the CDC 7600 computer. Table 2 compares the CPU execution times on the two machines for different areas of the code. The peripheral processor time is not available on the CDC 7600.

Table 1. MC^2-2 Sample Problem Specifications

Mixture: ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{235}U, ^{238}U, ^{12}C, ^{16}O, ^{23}Na, ^{27}Al, Fe, Cr, Ni, Mn, Cu, Mo, Si

Options: Δu^{ufg} = 1/120, 27 epi-thermal broad groups; inconsistent P_1 homogeneous spectrum; buckling iteration; 1740 ultra-fine groups; single fission spectrum; continuous slowing down below ~4 keV; improved Greuling-Goertzel moderating parameters; unresolved resonance self-overlap; four nearest resolved resonances; RABANL treatment below ~1.234 keV.

Table 2. MC^2-2 Sample Problem Timing

Code Area	IBM/370-195 CPU, sec	IBM/370-195 CPU + PP, sec	CDC-7600 CPU, sec
Input	0.5	4.1(0.5%)	0.1
NR Unresolved Resonance σ	42.7	66.8	24.3
NR Resolved Resonance σ	17.0	22.7	19.0
NR Interaction	0.3	2.8	0.1
NR Resonance Calculation	60.0	92.3(11.0%)	43.4
Tabulated σ	1.4	15.6	0.1
Elastic Matrices	36.0	136.6	19.4
Moderating Parameters	2.3	4.9	1.3
Macroscopic Data Processing	39.7	157.1(18.8%)	21.5
Ultra-fine Group Spectrum	143.8[a]	279.8[a]	106.7[a]
Broad Group σ Management	31.3	83.0	13.8
Inelastic σ Management	10.9	71.6	5.0
Ufg Spectrum and Broad Group σ	186.9[a]	448.8[a](53.6%)	148.2[a]
Broad Group Spectrum	0.6	1.5(0.2%)	0.2
RABANL Resolved Resonance σ	74.6	-	85.5
RABANL Slowing Down	15.1	-	11.6
RABANL Collision Rates	2.0	-	4.7
RABANL	111.3	130.4(15.6%)	113.0
TOTAL	401.4	836.7	327.6
Total CPU/Total		0.48	

[a]Three passes to obtain critical buckling.

A space-dependent cross-section generation capability is provided by the SDX option of the ETOE-2/MC^2-2/SDX code system. The SDX option may be characterized by three salient features:

(1) the use of an intermediate-group microscopic cross-section library for all cross sections except those represented by resonance formalisms;

(2) run time computation of intermediate-group resonance cross sections appropriate to the composition, cell structure, and temperature of the problem; and

(3) explicit treatment of all heterogeneity and multiregion spatial effects in one dimension.

The SDX option has been designed to provide the user great latitude in the rigor, complexity, and computational effort associated with a given problem. For example, it is possible, for each region in a multiregion problem, to obtain the intermediate-group cross sections, perform the resonance cross section and integral transport calculation for a heterogeneous cell model, and homogenize the intermediate-group cross sections. The homogenized cross sections for each region would then be used in a multiregion, intermediate-group diffusion theory calculation, and the resulting flux used to calculate broad-group spatially averaged cross sections on a cell-averaged and plate (pin)-wise basis. The rigor, and computational effort, of such a calculation could be relaxed by using a single set of intermediate-group cross sections for all regions, but still generating the resonance cross sections for each different region. The integral transport calculation could be omitted and volume-averaging used in the cell homogenization with or without the use of equivalence theory to account for heterogeneous effects in the calculation of resonance cross sections. A block diagram indicating the major program modules of SDX is given in Fig. 5.

At its most rigorous the SDX calculation is more rigorous, yet significantly more economical, than the most rigorous previously existing fast neutron multigroup cross-section preparation capability. On the other end of the spectrum, the simplest SDX calculation provides in less than 2 min a broad-group cross-section set which should be adequate for many analyses. In particular, the latter option is an improvement upon the self-shielding factor schemes because of the more accurate resonance cross-section and elastic removal treatments.

Broad-group microscopic cross sections are composition-dependent because of the composition-dependence of the neutron flux (and current) weighting spectrum. Elastic removal and heavy element resonance cross sections are generally the most sensitive to composition due to intermediate element scattering resonances and heavy element resonances. In the SDX option the resonance cross sections are calculated on an

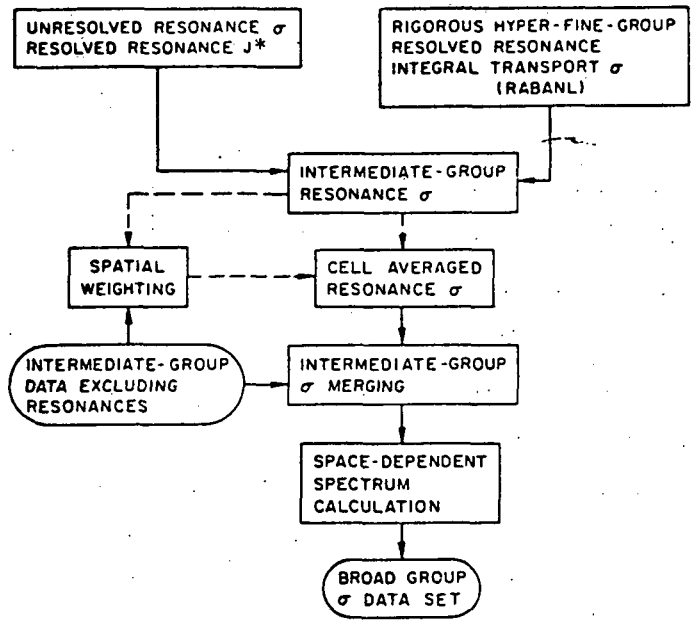

Fig. 5

SDX Program Flow

intermediate-group level for each plate or pin type (using equivalence theory) or homogeneous mixture in each region of a multiregion problem. As Fig. 1 indicates, the resonance calculation in SDX uses the same program modules as MC^2-2. In particular, either the narrow resonance J*-integral treatment or the rigorous RABANL treatment may be used to provide the composition and temperature dependent resonance cross sections. Intermediate-group resonance cross- sections are calculated assuming a constant collision density per unit lethargy in SDX rather than by use of the attenuation treatment described earlier in MC^2-2. Thus the resonance algorithms employed in the SDX calculation combine a high degree of accuracy with modest computational time. It is assumed in the SDX option that all the remaining cross sections are composition independent on the intermediate-group level and that the intermediate-group spectrum will adequately reflect the composition-dependence for the purpose of obtaining broad-group cross sections. For current applications, intermediate-group cross-section libraries on the order of 150 to 200 groups have been generated. These libraries adequately "trace out" the higher energy scattering resonances in intermediate mass nuclei. The intermediate-group cross-section libraries may be constructed from MC^2-2 ultra-fine group calculations as indicated in Fig. 1 or any other code which creates a cross-section file in the proper format.

Three options exist in SDX with respect to unit cell homogenization:

(1) A homogeneous mixture may be specified in which case resonance cross sections are computed for a homogeneous mixture and simply combined with the intermediate-group library data (i.e., no unit cell homogenization).

(2) If a heterogeneous unit cell is specified, heterogeneous resonance cross sections are computed for selected isotopes in the specified plate/pin types using equivalence theory or the rigorous RABANL heterogeneous treatment. These resonance cross sections are combined with the intermediate-group library data and an infinite slab or cylinder integral transport calculation is performed for the unit cell. Spatial self-shielding factors and cell-averaged intermediate-group cross sections are calculated. The integral transport calculation is based on a modified version of the code CALHET[21] which makes use of the collision probability methods developed for RABANL.

(3) The integral transport calculation described in item (2) may be omitted and volume averaging used to obtain all cross sections.

The intermediate-group library data and cell-averaged resonance cross sections are input to a one-dimensional diffusion theory calculation. The space-dependent calculation employs the space-energy factorization[22] approximation optionally as a final solution or as a means for accelerating the direct intermediate-group solution, and employs power iteration with Chebyshev acceleration. A fundamental mode option is available for space-independent solutions. A modified version of the SEF1D code[22] is used for the space-dependent calculation. Broad-group microscopic cross sections are averaged over the intermediate-group spectrum and over user-specified spatial regions with cross sections appropriate to individual plates/pins available on option.

SDX has also been extended to provide a γ-processing capability by interfacing AMPX[24] generated files with SDX and providing a γ-source module. Use of this capability permits a consistent calculation of γ-production data accounting for the resonance and spatial self-shielding of the capture and fission cross sections.

The computing time required for an SDX calculation is dependent upon the user options as discussed above. Three sample problems have been run on the IBM-370/195 at Argonne National Laboratory to provide an indication of time requirements. All problems were run with a single 156-group cross-section library. Both the unit cell calculation and the diffusion theory spectrum calculation depend upon the number of intermediate groups. In Table 3 timing results are presented for a single-region problem in both a homogeneous and heterogeneous (12-plate) representation. The computation times for the resolved and unresolved resonance calculations increase in the heterogeneous problem since the calculation must be performed for the homogeneous mixture as well as for each resonance material in each plate. In Table 4 timings are presented for a multiregion space-dependent calculation in which each region was treated homogeneously. The simplest SDX calculation is represented by the homogeneous problem of Table 3. The most detailed calculation would include multiregion effects as in Table 4 along with a heterogeneous cell model as in Table 3.

Table 3. Fundamental Mode SDX, 12 Isotopes (time in sec)

Code Area	Homogeneous		Heterogeneous[a]	
	CPU	PP	CPU	PP
Input processor	<1	2	<1	2
Unresolved resonances	18	14	28	32
Resolved resonances	13	4	22	6
Interaction and cross-section preparation	2	9	3	13
Unit cell	-	-	36	9
Spectrum	8	7	8	7
Total	43	50	98	81

[a]Twelve plates of which seven contained resonance isotopes.

Table 4. Homogeneous, Space-Dependent SDX - 16 Isotopes, 4 Regions (time in sec)

SEF1D		Remainder		Total	
CPU	PP	CPU	PP	CPU	PP
73	23	92	126	165	149

PROGRAMMING METHODS

The ETOE-2/MC^2-2/SDX code system was developed at Argonne National Laboratory on an IBM-370/195. All programming has been done in FORTRAN and has rigorously adhered to the standards established by the Committee on Computer Code Coordination (CCCC).[25] In addition, considerable effort was expended to produce a code which may be implemented as simply as possible on other computers.

The entire code is variably dimensioned through use of the subprogram package BPOINTER.[26] All binary I/O is performed by subroutine calls to the standard CCCC routines REED/RITE[25] so that great flexibility is provided in specifying installation-dependent data management strategies. The standard CCCC routine TIMER[25] has been used for installation-dependent timing function. Extensive use has been made of comment cards in order to make the codes as self-documenting as possible (approximately one-third of the more than 50,000 source cards of MC^2-2 are comments).

As ponted out above, the input to the code system is an ENDF/B data file. Broad-group cross-section files are output by the code system in either the ARC System XS.ISO format[25] or the ISOTXS format[24] specified by the CCCC. BCD input is prepared according to standard ARC System conventions.[26]

The code system is operational at ANL (IBM), SLAC (IBM), LRL Berkeley (CDC), BNL (CDC), and is available from the Argonne Code Center and the NEA ISPRA Code Center. The program package includes ETOE-2 processed data for the ENDF/B Version IV data. Modifications to ETOE-2 and MC^2-2 are underway to permit processing of ENDF/B Version V data which is scheduled for release during CY 1978. The modified code and data will be made available through the ANL and ISPRA Code Centers.

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