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AUS MODULE MIRANDA - A DATA PREPARATION CODE
BASED ON MULTIREGION RESONANCE THEORY

by

G.S. ROBINSON

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ABSTRACT

MIRANDA is a data preparation module of the AUS reactor neutronics scheme and is used to prepare multigroup cross-section data which are pertinent to a particular reactor system from a general purpose multigroup library of cross sections. The cross-section library has been prepared from ENDF/B and includes temperature dependent data and resonance cross sections represented by subgroup parameters. The MIRANDA module includes a multiregion resonance calculation in slab, cylinder or cluster geometry, a homogeneous B_L flux solution, and a group condensation facility. Interaction with other AUS modules, particularly for burnup calculations, is provided.

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GROUP CONSTANTS; RESONANCE; MATHEMATICAL MODELS: M CODES

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1. INTRODUCTION

The AUS scheme [Robinson 1975a] has been developed at the AAEC Research Establishment (AAECRE) for reactor neutronics computations of a wide range of thermal and fast reactor systems. The scheme consists of a number of large modules, each of which may be capable of performing several tasks, which communicate *via* standard data sets (data pools). MIRANDA has been developed as a cross-section preparation module which is suitable for both thermal and fast reactor computations. The term cross-section preparation is used in the restricted sense of preparing group cross-section data suitable for a particular subsystem of a reactor, from an input group cross-section library of wider application.

MIRANDA uses as input data, a multigroup cross-section library with group scattering matrices of any order P_n , resonance cross sections in the form of subgroup data, and scattering matrices dependent on potential scattering. All relevant quantities may be temperature dependent. The standard library for MIRANDA is the 128-group library AUS.ENDFB which contains data derived mainly from ENDF/B III and ENDF/B IV. The use of such a library with groups of 0.25 lethargy width above 10 eV for fast reactor calculations requires that structural and coolant materials as well as the fuel be represented as resonance materials.

The basic output of a MIRANDA calculation is a cross-section data pool containing cross sections for each region of a lattice for use in a transport theory calculation of the lattice. Thus MIRANDA is only the first phase of a normal lattice calculation. The major function of MIRANDA is the resonance theory calculation of nuclide cross sections, in the library group structure, appropriate to the system under study. The multiregion resonance calculation may be performed in slab, cylinder or cluster geometry using the method of subgroups. Preliminary group condensation may also be carried out following a homogeneous B_L flux solution.

As well as detailing the methods of calculation, including those used in preparing the library, and describing the input requirements of the module, this report gives the results of comparisons of the resonance theory with numerical solution of the neutron slowing down equation. Comparison of MIRANDA with integral experiments lies outside the scope of this report, but it will be given elsewhere.

2. HISTORICAL DEVELOPMENT

This section gives a brief history of the methods used for cross-section preparation at the AAECRE. It also reviews the manner in which the MIRANDA code depends on its predecessors, and the reasons for developing a new code.

The earliest methods at the AAECRE were incorporated in the MULGA code series [Clancy *et al.* 1963]. The MULGA codes were written to satisfy the requirements of the Australian High Temperature Gas Cooled Reactor (HTGCR) project which involved Pu-Th particles dispersed in BeO balls. The homogeneous nature of the concept has strongly influenced the development of methods. MULGA used continuous slowing down theory and the heavy gas equation to calculate a basic spectrum at 0.1 lethargy intervals for cross-section averaging. The resonance treatment was the intermediate resonance (IR) method of Goldstein & Cohen [1962] applied to resolved single-level resonance parameters. Output scatter matrices at thermal energies were evaluated using a gas scattering kernel. The cross-section data were obtained from the AAEC nuclear data card library [Doherty 1964] which was based mainly on the compilations of Buckingham *et al.* [1960], Hughes & Schwartz [1956] and Hughes *et al.* [1960]. The restrictions of MULGA can best be appreciated from the fact that it was written for an IBM1620 computer, which is of limited size and speed.

In the following years, the major theoretical effort was devoted to the calculation of resonance absorption in homogeneous systems and the subsequent derivation of cross sections. In addition, codes were obtained from the United States and Great Britain which were capable of generating many-group fast and thermal scattering matrices from more realistic models than those of MULGA. With the advent of a more powerful computer, the IBM7040, the GYMEA code [Pollard & Robinson 1966] was written to replace MULGA and a space-independent burnup code GIBBA [B.E. Clancy, A. Keane & J.P. Pollard (unpublished AAEC report)]. The requirements of the HTGCR project again dictated a homogeneous code.

GYMEA had a 120-group library of cross sections and P_0 scattering matrices, the group structure being basically 0.25 lethargy width groups above 10 eV and 0.1 lethargy width groups below 10 eV. Single-level resolved resonance parameters were also included. The resonance theory was an extension of the Hill & Schaefer method [McKay *et al.* 1965] and the derivation of multigroup cross sections followed Keane & Pollard [1966] and Pollard [1966]. The only allowance for heterogeneity was for particle shielding in the resonance treatment following Keane [1964]. An unusual feature of the code was the inclusion of a toy-FORTRAN capability which allowed the code to be extended by the user. Data sources and methods used in preparing the cross-section library are given by Cook [1966a] and further information is supplied by Gemmell *et al.* [1968]. It is merely noted here that the major codes used were GAM [Joanou & Dudek 1961], LEAP [McLatchie 1962], PIXSE [MacDougall 1963] and GUNYA [Cook 1966b], whereas the major additional data compilation used was that of Stehn *et al.* [1964, 1965].

GYMEA has remained in use until its recent replacement by MIRANDA. GYMEA evolved during this period from a code specific to the HTGCR project, to one that has been successfully applied to a wide selection of fast and thermal reactor systems. With the conversion to an IBM360 computer, the toy-FORTRAN approached the normal language by the use of the FORTRAN dialect, FOREX [Robinson 1968]. This FORTRAN capability was used to extend the code to a variety of situations with only minor modifications to the basic coding. It was also used to provide direct linkages to other codes, which enable simple lattice calculations (three-region fuel, clad and coolant) to be performed. In recent years, this ability to extend GYMEA was used to incorporate the code in the AUS scheme. The resonance equivalence relation finally adopted was that of Chiarella [1969]. Other improvements to GYMEA included an unresolved resonance treatment with suitably weighted average resonance parameters, and a more accurate J function for resonance integral evaluation. The data libraries have been updated many times and the number of groups extended to 127. Some of the major compilations that have been used are the UKAEA nuclear data file [Norton 1968], the AAEC fission product library [Bertram *et al.* 1971], and ENDF [Honeck 1964] for $S(\alpha, \beta)$ data.

Though the extensions to GYMEA made it applicable to a wide range of systems, it could not be used for the cluster geometry of pressure tube reactors. The British lattice codes WIMS [Askew *et al.* 1966] and METHUSELAH [Alpiar 1964] were obtained for assessment calculations of SGHW and CANDU reactors. In later years, the fast reactor code MURAL [MacDougall *et al.* 1968] was also obtained.

The development of approximate resonance treatments for lattice codes required 'exact' numerical methods against which the approximations could be tested. The codes which have been written for this purpose are PEAS [Pollard 1964] for homogeneous calculation of an isolated symmetric single-level resonance, and PEARLS [Chiarella 1971] for multiregion

calculations using a 124 000 point cross-section library below 20 keV. The initial PEARLS library was prepared for ^{238}U by Doherty [1968, AAEC unpublished report] with the codes RESP and GENEX [Brissenden & Durston 1968] and the resonance parameters of Schmidt [1966].

Summarising the position before the development of MIRANDA, a number of data preparation codes were available, each having its own data base. The British codes were not sufficiently documented for their libraries to be consistently updated, or for major code modifications to be applied in the light of local experience and requirements. On the other hand, GYMEA was basically a homogeneous code which had already been extended as far as possible. In addition, its use as an accurate general purpose data preparation code was prevented by the following deficiencies :

- (a) it was limited to P_0 scattering matrices;
- (b) the current library was prepared from a variety of sources (some very old) by a variety of methods, and methods to include ENDF/B data were not automated;
- (c) resonance contours were restricted to single-level Breit-Wigner without interference scattering;
- (d) the resonance integral was computed as the sum of J functions with no account taken of the overlap of resonances of a single nuclide;
- (e) there were difficulties arising from assigning a wide resonance entirely to one narrow group and this had never been overcome satisfactorily;
- (f) scatter matrices of resonance nuclides were not system dependent in any way;
- (g) no treatment was included for resonance scattering materials such as Na and Fe;
- (h) resonance treatment of heterogeneous systems was limited by the use of a two-region equivalence relation; and
- (i) resonance cross sections in a heterogeneous system were correctly prepared only in rather broad groups as the cross sections included the flux depression of the fuel.

Almost all the deficiencies related to the now inadequate resonance treatment which was the major task of the code.

Many of the deficiencies in the resonance treatment can be eliminated by tabulating group resonance integrals as a function of potential scattering and temperature; this is the approach adopted in the WIMS code. The group resonance integrals may be calculated by numerical solution of the slowing down equation in homogeneous mixtures of the resonance nuclide with hydrogen over a very fine energy grid, as in the PEARLS code, or they may be calculated by more approximate methods where appropriate. The dependence of the resonance integral on moderator nuclide can only be accounted for in an approximate manner. In MIRANDA, the method of McKay *et al.* [1965] used in GYMEA has been adapted to the tabulated integral approach by making use of 'group-averaged' resonance parameters.

The subgroup method [Nikolaev & Khokhlov 1967] has proved very useful in the treatment of resonance processes. A review of this method is given by Khairallah & Reclin [1972]. The subgroup method has been applied to fast reactor calculations in the MURAL code and, more recently, to thermal calculations by Roth [1974]. At the AAECRE, initial investigation of the method was carried out by Doherty [1972] who developed methods for fitting group

resonance integrals by subgroup parameters, and gave the general outline of a scheme of calculation. The subgroup method as applied in MIRANDA is a development of his work. The great advantage of the subgroup method is that the geometry of any complex system can be represented, as accurately as desired, by the provision of an appropriate collision probability routine.

Many of the features of the GYMEA code have been incorporated in MIRANDA in a modified form. The 127-group structure of the GYMEA library has been retained, but is supplemented by a group above 10 MeV. The initial MIRANDA library was prepared by reprocessing the GYMEA data, but this has been superseded by an ENDF/B-based library. The combination of a resonance treatment and a homogeneous flux calculation within the one code has been continued. The concept of calculating resonance group cross sections, which reproduce the reaction rates as calculated from the resonance theory, has also been adopted. Finally, the method of solution of the homogeneous group flux equations has been adapted to the B_L equations.

Another important consideration in the development of MIRANDA is the requirement for a data preparation module which could be fully integrated into the AUS scheme. A new code written as a module of the scheme is better suited to this purpose than one adapted to the requirements of the scheme. All data sets, which are used by MIRANDA, including the cross-section library, are in the form of AUS data pools.

3. OVERVIEW OF THE CODE

3.1 Introduction

MIRANDA is a module of the AUS system which has been written in the FORTRAN IV language for the IBM360 series of computers. The module is currently operational at the AAECRE on an IBM360/65 and has been tested for a running time of over 18 months on this machine and also on an IBM360/50. The code makes efficient use of core storage by program overlay and the dynamic allocation of data storage. The code employs a method of dynamic core procurement in order to make use of all available core storage. The 360 K bytes normally allocated to AUS runs are more than adequate, except in a few extreme situations. (The only such situation encountered to date is the generation of 128-group, P_3 cross sections as output from the code.) The execution time of the code is particularly dependent on the complexity of the geometry used in the resonance calculation and the number of resonance nuclides represented. A fairly standard 3-region calculation requires about half a minute CPU time on the model 65.

Input data takes the form of keyword-directed, free format data using the SCAN input routine [Bennett & Pollard 1967]. The burden of input data preparation is further eased by the use of default values for many code options. Complete input details are given in Section 9. The functions performed by MIRANDA may be conveniently divided into three sections. The first is the generation of group cross sections in the group structure of the library by the application of a multiregion resonance treatment. This is followed by the solution of the homogeneous B_L equations for a spatially smeared model of the lattice. The homogeneous group fluxes are used for a preliminary group condensation in the last section of the code, and this produces cross sections for each region of the cell. A general description of each of these functions is given in the following subsections. In addition, since a data preparation code is only as good as its cross-section library, a brief description of the current library is given.

3.2 Cross-section Library

The cross-section library is in the form of an AUS XSLIB data pool, the structure of which has been given by Robinson [1975a]. The current 128-group library AUS.ENDFB has been generated basically from ENDF/B, versions III and IV (version III data have been retained chiefly for moderators). The group structure of the library and the nuclides included are detailed in Appendix A. The library contains group scatter matrices, cross sections, subgroup parameters for resonance representation, fission spectra and other miscellaneous information including nuclide mass and burnup chains. All relevant data may be given as a function of temperature and, in general, have been prepared at two temperatures only.

As well as fuel nuclides, the resonance scatterers Na, Fe, Cr and Ni of fast reactor lattices have subgroup representation. The subgroup data have been obtained from group resonance integrals per unit lethargy l , tabulated as a function of effective potential scattering cross section $\hat{\sigma}_p$, by fits of the form

$$l(\hat{\sigma}_p) = \sum_i w_i \hat{\sigma}_p / (\sigma_i + \hat{\sigma}_p) \quad , \quad \dots(3.1)$$

where σ_i is a parameter representing the total cross section of the nuclide in the i th subgroup, and w_i is the subgroup weight. The resonance integrals have been obtained for the resolved resonance range by generating point cross sections on an extremely fine mesh and solving the slowing down equation numerically for mixtures of the resonance nuclide and hydrogen (with a constant hydrogen cross section). The calculation also provides the P_0 scattering matrix as a function of $\hat{\sigma}_p$. In the unresolved region, resonance integrals have generally been obtained from average parameters by an integration over the neutron and fission width distributions combined with J-function summation. For ^{238}U below 20 keV, an appropriate sequence of resonances has been generated in the unresolved region by sampling from the width and spacing distributions, in order to generate point cross sections for use as in the resolved region.

Non-resonance cross sections have been generated by the code SUPERTOG [Wright *et al.* 1969] except at thermal energies, where scattering data have been generated by PIXSE from ENDF $S(\alpha, \beta)$ data for moderators, or from a gas kernel for other nuclides. Scattering matrices have generally been generated up to P_3 order in SUPERTOG but, in the thermal and resonance region P_0 or P_1 data only have been generated.

Details of the methods used to generate the library, particularly in the resonance region, are given in Appendix B.

3.3 Resonance Treatment

The resonance treatment of MIRANDA is a multiregion calculation which makes use of a set of collision probability routines to obtain subgroup fluxes for each resonance nuclide in turn, and then calculates resonance integrals. The treatment is restricted to elastic scattering which is spherically symmetric in the centre of mass system. The collision probability routines currently included are reflected slab, translational slab, and a Bonalumi type approximation for cylinders, which were developed by Doherty [1969]. In addition, an approximate cluster routine [Clancy *et al.* 1977] based on the work of Yamamoto & Ishida [1971] is also available. The evaluation of the resonance integral does not depend explicitly on an equivalence relation but an equivalence is implicit in the derivation of the subgroup parameters. A numerical equivalence relation is derived to obtain the outscatters of the resonance nuclide.

A number of corrections are applied to this simple model. The dependence on nuclide mass is included by adapting the extended Hill-Schaeffer method [McKay et al. 1965]. The effect of resonances not being isolated, that is the flux not returning to an asymptotic value between resonances, is included in an indirect manner. The overlap of resonances of different nuclides is treated by a generalisation to the multiregion situation of a standard simple formula. The dependence of the group removal cross section on the resonance escape probability of the group is represented by a region independent factor for each nuclide.

The group reaction rates derived from the corrected resonance integrals are taken as the quantities which must be preserved in deriving effective group cross sections. This is done by iterating on the collision probability formulation of the group equations with an asymptotic source for a set of region dependent factors which, when multiplied by the resonance integrals, give a set of cross sections and consistent region fluxes which reproduce the required reaction rates.

Details of the resonance treatment are given in Section 5, and the results of comparisons with the numerical solution of the PEARLS code are included in Section 6. The agreement between MIRANDA and PEARLS is generally better than 1% in resonance absorption.

3.4 Homogeneous Calculation Using B_L Approximation

A homogeneous model of the lattice is obtained by spatial smearing, using volume weighting only in non-resonance groups, and the fluxes obtained for an asymptotic group source in resonance groups. The calculation is performed in the library group structure using the derived resonance cross sections. The equations solved are either the transport corrected P_0 equations or the B_L equations for any L (except zero). The use of P_0 rather than B_0 is mainly for compatibility with previous methods. A search on critical buckling may be performed. The solution of the equations is by simple Gauss-Seidel iteration, accelerated by few-group scaling applied to the thermal groups.

3.5 Group Condensation and Cross-section Output

The homogeneous group fluxes are combined with the spatial fluxes available in resonance groups in order to energy-condense the cross sections before output. Only limited condensation should be performed in MIRANDA, particularly for large lattice cells, because this flux solution is very approximate. The procedures adopted are quite straightforward, apart from the calculation and condensation of the transport cross section, for which the formulae adopted are based on the use of derived cross sections in reactor leakage calculations. This is also true of condensed P_1 , P_2 , ... matrices if a B_L calculation is performed. It should be noted that the transport cross section of a lattice component which is derived following a B_L calculation may be extremely system dependent (even negative), and it should not be used except to reconstitute the lattice for which it was calculated.

4. MIRANDA AS A MODULE OF AUS

4.1 General

The MIRANDA code has been developed as the general purpose data preparation module of the AUS scheme for use on all reactor types. The codes GYMEA and MURAL are still available for use with AUS, but they were never entirely integrated into the scheme, and their use is no longer recommended in general. However, for any fast reactor calculations which require detailed flux spectra, the MURAL code should be used. Though little experience with MIRANDA in fast reactor calculations has yet been acquired, the intermediate group approach which has been adopted should be satisfactory for most applications, and MIRANDA does have the

advantage of accessing the standard ENDF/B set of data.

In most cases, MIRANDA represents the first phase only of a lattice calculation. The exceptions are homogeneous systems for which MIRANDA alone suffices. To calculate a lattice cell, it is the province of the user to decide what approximations can be made, and which of the available modules should be used. The modular system allows great flexibility but increases the responsibilities of the user. The general approach adopted for complex lattices should be similar to that adopted in the WIMS code. That is, a detailed spectrum calculation in simplified geometry to provide condensation spectra for a fewer-group calculation in a more detailed geometry. A number of such stages may be included before the most detailed spatial representation is reached. In the application of MIRANDA, the fact that the flux calculation is essentially homogeneous must always be borne in mind. This means that in lattices with a marked spectrum variation within the cell, only minimal condensation should be done in MIRANDA, if accurate calculations are required.

4.2 Use of AUS Data Pools

The data pool output of MIRANDA normally consists of :

- (a) a cross-section data pool containing macroscopic cross sections for the materials of the lattice, and any desired microscopic cross sections;
- (b) a geometry data pool giving the lattice geometry and mesh intervals;
- (c) a FLUXB data pool giving a P_0 flux in the spatial mesh of the geometry data pool, for the condensed group structure; and
- (d) additional entries, which include the nuclide compositions of the materials of the lattice, added to the pair of STATUS data pools.

The STATUS data pool is intended to provide information for nuclide editing at any stage of an AUS calculation, or for burnup calculations. For these purposes, cross sections of all nuclides of the lattice may be automatically written either on the same cross-section data pool as the macroscopic cross sections or on an additional data pool. The geometry data pool is intended to supply the geometry required for the next module of the lattice calculation, and the flux data pool provides a flux guess for that module. All data pool output is optional.

The standard associations between data content, FORTRAN logical units and data pools are given in the table below. These default values may be altered by the user.

Data Content	FORTTRAN Unit	DD Name	Symbolic Data Pool Name
Cross-section library - default library AUS.ENDFB	8	DD31	LIB
Macroscopic and microscopic cross-section output	10	DD33	XS1
Microscopic cross-section output	11	DD34	XS2
Geometry of the lattice	6	DD35	GM1
Flux guess for next module	9	DD37	FL2
STATUS data - nuclide compositions, etc.	4	DD38	ST1
Pointer to ST1	5	DD39	ST2

4.3 STATUS Data Pools and Burnup

A full description of the use of STATUS data pools within the AUS system is given by Robinson [1975b]. It is merely noted here that the STATUS data pools play a part in controlling the calculation sequence within the AUS scheme. This control function is intended for use in burnup calculations and does not directly concern the non-burnup user. However, it should be noted that STATUS data sets require initialisation, which is done automatically when a new data set is allocated within the AUS scheme, or which may be done under user direction.

In starting a burnup calculation, MIRANDA may be used to generate a material definition, which includes a minute amount of all nuclides which will be produced in that material during burnup. Once this has been done, all burnup requirements are met automatically.

5. RESONANCE TREATMENT

5.1 Introduction

For ease of presentation, discussion of the resonance treatment has been divided into a number of sections which correspond quite closely to sections of the code. After detailing the data obtained from the cross-section library, the method is introduced under the assumptions of narrow resonance theory. The narrow resonance treatment not only serves to show the basic approach but is also used as part of the solution under all circumstances. The various modifications applied to this simple theory are then given in turn. The final section outlines the derivation of effective group cross sections from the calculated resonance integrals. As the treatment is based on the use of asymptotic group sources, the solution in each energy group is independent of other groups.

5.2 Data Obtained from the Cross-section Library

In the MIRANDA resonance calculation, the only scattering process treated is elastic scattering which is isotropic in the centre of mass system. A further simplification is introduced by ignoring non-resonance absorption. The cross sections in the library are therefore modified to conform with these restrictions. A description of the AUS cross-section data pool is given by Robinson [1975a], and details of library preparation methods are given in Appendix B.

The scattering properties of each nuclide ℓ of the lattice may be obtained from the library value of the atomic mass, A_ℓ , by

$$\alpha_\ell = (A_\ell - A_0)^2 / (A_\ell + A_0)^2, \quad \dots(5.1)$$

$$\xi_\ell = 1 + \alpha_\ell \log \alpha_\ell / (1 - \alpha_\ell), \quad \dots(5.2)$$

where A_0 is the neutron mass, 1.008665, $1 - \alpha_\ell$ is the maximum fractional energy loss, and ξ_ℓ is the average lethargy loss. In addition, the source and removals for the g th energy group are given in terms of

$$\beta_{\ell g} = \begin{cases} \xi_\ell & , \text{ for } \alpha_\ell > E_{g+1}/E_g, \\ (1 - E_{g+1}/E_g - \alpha_\ell \tau_g) / (1 - \alpha_\ell), & \text{ for } \alpha_\ell < E_{g+1}/E_g, \end{cases} \quad \dots(5.3)$$

where E_g is the upper energy boundary of group g , and τ_g is the group lethargy width.

As the library includes moderator nuclides such as H₂O and D₂O, the code allows two atomic masses and an energy independent fractional scattering of each atom to be associated with a non-resonance nuclide. Allowance for these moderator nuclides is made in all mass dependent formulae of the code.

Let M_g denote the set of nuclides for which subgroup data are given in group g . The non-resonance scattering cross section of nuclide ℓ in group g , $\sigma_{p\ell g}$, is taken from the fourth library cross section, which is the total scattering cross section for $\ell \notin M_g$, or the potential scattering cross section for $\ell \in M_g$. The non-resonance macroscopic total cross section for each region i is given by

$$\Sigma_{ig} = \sum_{\ell} N_{\ell i} \sigma_{p\ell g} \quad , \quad \dots(5.4)$$

where $N_{\ell i}$ is the atom density of nuclide ℓ in region i . The non-resonance transport cross section is given by

$$\Sigma_{tig} = \sum_{\ell \notin M_g} N_{\ell i} (\sigma_{t\ell g} - \sigma_{a\ell g}) + \sum_{\ell \in M_g} N_{\ell i} \sigma_{p\ell g} (1 - \bar{\mu}_{\ell}) \quad , \quad \dots(5.5)$$

where $\sigma_{t\ell g}$, $\sigma_{a\ell g}$ are library values of the transport and absorption cross sections respectively, and $\bar{\mu}_{\ell} = 2/(3A_{\ell})$. As any temperature dependence of the above quantities is of no importance in the resonance calculation, values at the lowest temperature are used if they are tabulated against temperature.

Different values of Σ_{ig} in each group require that collision probabilities for each subgroup for each resonance nuclide be re-evaluated in each group. To save computer time, the average values (weighted with the group lethargy width) of Σ_{ig} , Σ_{tig} , and $\sigma_{p\ell g}$ are used for the consecutive groups g to g' which satisfy

$$|\Sigma_{ig} - \Sigma_{ig'}| < 10 \epsilon_{r1} \Sigma_{ig} \quad , \quad \dots(5.6)$$

where ϵ_{r1} , normally 10^{-3} , is an accuracy criterion which may be set by the user.

The subgroup parameters for nuclide ℓ are the total resonance cross section in each subgroup k , $\sigma_{\ell k}$, and the subgroup weights $w_{a\ell k}$, $w_{s\ell k}$, $w_{f\ell k}$, $w_{e\ell k}$, $w_{d\ell k}$ which represent absorption, scattering, fission, fission emission, and flux depression respectively. The weights are obtained by fits to the appropriate quantity as detailed in Appendix B. The form of the fit is

$$I_{x\ell g}(\hat{\sigma}_{pg}) = \sum_k w_{x\ell k} \hat{\sigma}_{pg} / (\hat{\sigma}_{pg} + \sigma_{\ell k}) \quad , \quad \dots(5.7)$$

where $I_{x\ell g}(\hat{\sigma}_{pg})$ represents the group resonance integral per unit lethargy for reaction x , or the ratio of group flux to asymptotic group flux, and $\hat{\sigma}_{pg}$ is the effective potential scattering cross section. The subgroup weights may be tabulated as a function of temperature, and the weights for any temperature are obtained by linear interpolation or extrapolation in \sqrt{T} where T is the temperature in Kelvin. The weights may thus be region dependent in lattices with a region dependent temperature, but this region dependence is not exhibited in the equations given.

Other parameters which may be given in the resonance representation are

- $\langle \sigma_o \rangle_{\ell g}$ the group average value of the peak resonance height σ_o ,
- $\langle 2E_r/\Gamma \rangle_{\ell g}$ the group average value of $2E_r/\Gamma$ (where E_r and Γ are the resonance energy and total width), and
- $\langle D \rangle_{\ell}$ the average spacing between resonances.

The group scattering matrix for a resonance nuclide may be tabulated as a function of $\hat{\sigma}_p$ and T . Temperature interpolation is linear in \sqrt{T} and the required isotropic elastic scattering removal cross section is obtained by

$$\sigma_{r\ell g}(\hat{\sigma}_p) = \left(\sum_{h \neq g} \sigma_{g \rightarrow h, \ell}(\hat{\sigma}_p) - \sigma_{\ell g}^i \right) R_{\ell g} \quad , \quad \dots(5.8)$$

where $\sigma_{g \rightarrow h, \ell}$ is the P_o scattering matrix, $\sigma_{\ell g}^i$ is the inelastic scattering cross section, and $R_{\ell g}$ is the ratio of elastic removals, assuming isotropic scattering, to actual elastic removals. $R_{\ell g}$ has been included in the library only for resonance scatterers, and $\sigma_{\ell g}^i$ is usually zero.

This completes the description of the data on which the resonance treatment is based. The following subsections relate to the calculation of a particular energy group, and the g subscript has been dropped.

5.3 Narrow Resonance Theory

The collision probability formulation of the slowing down equations, under the assumption of isotropic elastic scattering, may be written

$$V_i \Sigma_i(E) \phi_i(E) = \sum_j V_j P_{ji}(E) \sum_m N_{mj} \int_E^{E/\alpha_m} \frac{\sigma_{sm}(E') \phi_j(E') dE'}{E'(1 - \alpha_m)} \quad , \quad \dots(5.9)$$

where V_i is the volume of region i ,
 $\phi_i(E)$ is the neutron flux in region i at energy E ,
 $\Sigma_i(E)$ is the total macroscopic cross section of region i ,
 $P_{ji}(E)$ is the probability that a neutron starting in region j will collide in region i , and
 $\sigma_{sm}(E)$ is the microscopic scattering cross section of nuclide m .

For a resonance which is narrow compared with the scattering ranges, and with an asymptotic flux of ϕ_o/E above the resonance, this reduces to

$$V_i \Sigma_i(E) \phi_i(E) = \sum_j V_j P_{ji}(E) \sum_m N_{mj} \sigma_{pm} \phi_o/E \quad , \quad \dots(5.10)$$

where σ_{pm} is the potential scattering cross section of nuclide m .

For a single resonance nuclide ℓ and no other absorption, Equation 5.10 may be re-written as

$$V_i (\Sigma_i + N_{\ell i} \sigma_{\ell}(E)) \phi_i(E) = \sum_j V_j P_{ji}(E) \Sigma_j \phi_o/E \quad , \quad \dots(5.11)$$

where Σ_i is the non-resonance cross section of region i , and $\sigma_{\ell}(E)$ is the resonance cross section of nuclide ℓ . The absorption resonance integral is then given by

$$R_{ai} = \int \frac{\sigma_{a\ell}(E) \sum_j V_j P_{ji}(E) \Sigma_j}{V_i (\Sigma_i + N_{\ell i} \sigma_{\ell}(E))} \frac{dE}{E}, \quad \dots (5.12)$$

and the resonance escape probability by

$$p = \exp \left(- \sum_i V_i N_{\ell i} R_{ai} \phi_0 \right). \quad \dots (5.13)$$

The definition of resonance integral which has been used in MIRANDA is

$$R_a = \frac{1}{\phi_0} \int \frac{\sigma_a(E) \phi(E) dE}{p(E)}, \quad \dots (5.14)$$

where $p(E)$ is the resonance escape probability to energy E . It is easily seen that this definition leads to the exponential form for p , and that Equation (5.12) is consistent with the definition in that the resonance integrals of a sequence of resonances are additive.

The only energy dependence of Equation (5.12) lies in the cross-section terms and hence the subgroup method becomes most attractive. The subgroup method can be considered to correspond to an approximate Lebesgue integration in Equation (5.12), in which the range of $\sigma_{\ell}(E)$ is divided into a number of subgroups with the k th subgroup having a total cross section $\sigma_{\ell k}$, an absorption cross section $\sigma_{a\ell k}$, and a lethargy width measure $w_{\ell k}$. Rather than attempt to obtain the $w_{\ell k}$ and the $\sigma_{a\ell k}$ directly from the cross sections $\sigma_{\ell}(E)$ and $\sigma_{a\ell}(E)$, the group resonance integrals/lethargy for homogeneous calculations are fitted to subgroup parameters as in Equation (5.7). This approach has the advantage of indirectly removing some of the approximations introduced in the narrow resonance (NR) theory.

The equations solved by the code for each resonance nuclide ℓ using the NR approximation are given by:

$$\Sigma_{ik}'' = \Sigma_i + N_{\ell i} \sigma_{\ell k}, \quad \dots (5.15)$$

$$V_i \Sigma_{ik}'' \phi_{ik} = \sum_j P_{ji} \{ \Sigma_{ik}'' \} V_j \Sigma_j, \quad \dots (5.16)$$

$$I_{x\ell i} = \sum_k w_{x\ell k} \phi_{ik}, \quad \dots (5.17)$$

where ϕ_{ik} is the ratio of the flux for region i and subgroup k to the asymptotic flux ϕ_0/E ,

$P_{ji} \{ \Sigma_{ik}'' \}$ represents the collision probability P_{ji} evaluated for the set of cross sections $\{ \Sigma_{ik}'', \Sigma_{2k}'', \dots \}$, and represents any of the required reactions.

Defining,

$$S_{\ell ik} = \sigma_{\ell k} \phi_{ik} / (1 - \phi_{ik}), \quad \dots (5.18)$$

Equation (5.17) may be re-written as

$$I_{x\ell i} = \sum_k w_{x\ell k} S_{\ell ik} / (S_{\ell ik} + \sigma_{\ell k}). \quad \dots (5.19)$$

Thus $S_{\ell ik}$ is similar to an effective potential scattering cross section.

A value of $\bar{S}_{\ell i}$ which reproduces the calculated absorption integral can be found by iteration. The iteration method used is a simple chord procedure in which $I_{a\ell i}$ is regarded as a function of $\sqrt{\bar{S}_{\ell i}}$. The value of $\bar{S}_{\ell i}$ is accepted if

$$\left| \sum_k w_{\ell k} \bar{S}_{\ell i} / (\bar{S}_{\ell i} + \sigma_{\ell k}) - I_{a\ell i} \right| < \epsilon_{r2} I_{a\ell i} \quad , \quad \dots (5.20)$$

where ϵ_{r2} , normally 0.002, is an accuracy criterion which may be input. The value of $\bar{S}_{\ell i}$ thus established gives a numerical equivalence relation between the multiregion situation and a homogeneous one. In most calculations the $S_{\ell ik}$ are not markedly dependent on k and for homogeneous calculations they reduce to $S_{\ell ik} = \Sigma_1 / N_{\ell 1}$.

5.4 The λ Method

5.4.1 Calculation of λ using the extended Hill-Schaeffer method

The extended Hill-Schaeffer method [McKay *et al.* 1965] was developed for homogeneous calculations using resonance parameters. In this method, a resonance of nuclide ℓ at energy E_r , with a peak height σ_o , total width Γ , absorption width Γ_a , and neutron width Γ_n , has an effective potential scattering cross section $\hat{\sigma}_p$ defined by:

$$\hat{\sigma}_p = \frac{\Gamma}{\Gamma_a + \lambda \Gamma_n} \sum_m \frac{N_m \lambda_m \sigma_{pm}}{N_\ell} \quad . \quad \dots (5.21)$$

The values of λ_m are given by the equations:

$$\lambda_m = 1 - \frac{\alpha_m (C_1 + C_\lambda)}{X_m} \arctan \left(\frac{X_m}{C_1 + \alpha_m C_\lambda} \right) \quad , \quad \dots (5.22)$$

$$\text{where } X_m = 2E_r (1 - \alpha_m) / \Gamma, \quad \text{and} \quad \dots (5.23)$$

$$C_\lambda = (1 + \sigma_o / \hat{\sigma}_p)^{1/2} \quad ; \quad \dots (5.24)$$

these are solved iteratively, together with Equation (5.21). C_1 is the value of C_λ for all $\lambda_m = 1$. The resonance escape probability p_r is given by:

$$p_r = \exp(-\rho N_\ell R \phi_o) \quad , \quad \dots (5.25)$$

$$\rho = 2 / (1 + p_r) \quad , \quad \dots (5.26)$$

where R is the resonance integral obtained by the J-function method, and the first iteration of the equations is usually taken.

The Equations (5.21) to (5.26) are strictly for a homogeneous calculation of one single-level Breit-Wigner resonance without interference scattering, and they require a number of adaptations for use in MIRANDA. Rather than iterating on Equations (5.21) to (5.24), the values of λ_m are obtained from the first iteration with $C_\lambda = C_1$. As previously mentioned, group-averaged values of σ_o and $2E_r / \Gamma$ are stored in the cross-section library;

the averaging method is given in Appendix B. The term $\Gamma/(\Gamma_a + \lambda_\ell \Gamma_n)$ is approximated by $(I_{a\ell}^\infty + I_{s\ell}^\infty)/(I_{a\ell}^\infty + \lambda_\ell I_{s\ell}^\infty)$, where the resonance integrals/lethargy I^∞ are evaluated at infinite dilution. The NR integrals (see Section 5.3) were originally used for this approximation, but this proved unsuitable once interference scattering was included. For negative values of $I_{s\ell}^\infty$, which may occur when a resonance extends over more than one group, $I_{s\ell}^\infty$ is set to zero for heavy nuclides and $I_{a\ell}^\infty$ is set to zero for resonance scatterers.

The extension to multiregion calculations makes use of the NR value obtained for $\bar{S}_{\ell i}$ in Section 5.3. The λ_{mi} , for those regions i which include nuclide ℓ , are thus obtained from:

$$\lambda_{mi} = 1 - \frac{2\alpha_m C_{li}}{X_m} \arctan \frac{X_m}{C_{li}(1 + \alpha_m)}, \quad \dots(5.27)$$

$$X_m = \langle 2E_r/\Gamma \rangle_\ell (1 - \alpha_m), \quad \text{and} \quad \dots(5.28)$$

$$C_{li} = (1 + \langle \sigma_o \rangle_\ell / \bar{S}_{\ell i})^{1/2}. \quad \dots(5.29)$$

For regions j which do not include nuclide ℓ , the values used are

$$\lambda_{mj} = \frac{\sum_i V_i N_{\ell i} \lambda_{mi}}{\sum_i V_i N_{\ell i}}. \quad \dots(5.30)$$

This *ad hoc* treatment of multiregion effects is justified only by the reduction to the required result in simple situations and the accuracy of the final results.

The calculation of a factor p by which the group integrals should be multiplied presents some difficulties as p_r in Equation (5.26) is the escape probability of a resonance. However, as p for a resonance is close to 1 in practical situations, a rather poor approximation will suffice. Indeed, Equations (5.25) and (5.26) are rather approximate as p_r for a pure absorber with hydrogen should be $\exp(-N_\ell R \phi_o)$. The $2/(1 + p)$ factor can be regarded as an empirical correction for which the main justification is the excellent agreement obtained with numerical calculations. The average resonance integral is, therefore, approximated by the NR value at zero temperature; this is given by

$$R_{ri} = \frac{\pi \langle \sigma_o \rangle_\ell}{\langle 2E_r/\Gamma \rangle_\ell} \frac{I_{a\ell}^\infty}{I_{a\ell}^\infty + I_{s\ell}^\infty} \frac{1}{C_{li}}. \quad \dots(5.31)$$

As the calculated group resonance integrals are based on homogeneous calculations of nuclide ℓ and hydrogen, a factor p_ℓ by which the group resonance integrals are to be multiplied is given by

$$p_\ell = \frac{1 + \exp(-\sum_i V_i N_{\ell i} R_{ri} \phi_o^i)}{1 + \exp(-\sum_i V_i N_{\ell i} R_{ri} \phi_o)}, \quad \dots(5.32)$$

where

$$\phi_o = 1 / \sum_i V_i \sum_m N_{mi} \epsilon_m \sigma_{pm}, \quad \dots(5.33)$$

and

$$\phi'_0 = 1 / \sum_i V_i \left(\sum_{m \neq \ell} N_{mi} \sigma_{pm} + N_{\ell i} \epsilon_{\ell} \sigma_{p\ell} \right) \quad \dots (5.34)$$

Thus, at least for hydrogenous systems the factor ρ_{ℓ} is of no concern.

5.4.2 Calculation of λ for very broad resonances

For resonances which are sufficiently wide to extend over several groups (e.g. the 3 keV Na resonance), the λ values derived in Section 5.4.1 for an entire resonance are not very satisfactory. More appropriate values for λ may be obtained from the equation for the group flux in a homogeneous calculation. For an asymptotic group source in a group with constant 'resonance' cross sections for nuclide ℓ of $\sigma_{a\ell}$ and $\sigma_{s\ell}$, a reasonable within group flux is given by

$$\frac{\phi(u)}{p(u)} = \frac{\phi_0 \sum_m N_m \sigma_{pm} \beta_m}{N_{\ell} \sigma_{a\ell} \beta_H + N_{\ell} \sigma_{s\ell} \beta_{\ell} + \sum_m N_m \sigma_{pm} \beta_m} \quad \dots (5.35)$$

where β_m is defined in Equation (5.3), and β_H is the value for hydrogen. The absorption term is not treated correctly, but the flux defined by Equation (5.35) is compatible with the previous treatment, and reduces to the required form of

$$\frac{\phi(u)}{p(u)} = \frac{\phi_0 \sigma_p}{\sigma_a + \sigma_p} \quad \dots (5.36)$$

for hydrogen scattering.

The definition of λ used for very broad resonances is therefore simply

$$\lambda_{mi} = \beta_m / \beta_H \quad \text{for all } i \quad \dots (5.37)$$

The equation equivalent to Equation (5.31) is

$$R_{ri} = \tau I_{a\ell i} \quad \dots (5.38)$$

where $I_{a\ell i}$ is the NR value obtained in Section 5.3. The factor ρ_{ℓ} may be calculated as before.

5.4.3 Subgroup equations

The set of equations for nuclide ℓ to be solved for the subgroup fluxes (equivalent to Equation (5.16) for the NR theory) is given by

$$\begin{aligned} V_i \sum_{ik} \phi_{ik} &= \sum_j P_{ji} \{ \sum_{ik} V_j [\Sigma_{\lambda j} + \phi_{jk} (\Sigma_j - \Sigma_{\lambda j} \\ &+ (1 - \lambda_{\ell j}) N_{\ell j} \sigma_{\ell k} I_{s\ell}^{\infty} / (I_{a\ell}^{\infty} + I_{s\ell}^{\infty})] \} \quad \dots (5.39) \end{aligned}$$

where

$$\Sigma_{\lambda j} = \sum_m N_{mj} \lambda_{mj} \sigma_{pm} \quad \dots (5.40)$$

The collision probabilities $P_{ji}\{\Sigma_{ik}''\}$ have already been computed for the NR treatment and may be re-used. For each subgroup k , Equation (5.39) is solved for the region fluxes ϕ_{ik} using a standard Gauss elimination routine. Values for $l_{x\ell i}$, $S_{\ell ik}$ and $\bar{S}_{\ell i}$ for the λ method can then be computed as for the NR treatment.

5.5 Resonance Scatterers

The treatment of resonance scatterers in MIRANDA is similar to that adopted for the fuel nuclides. The main difference lies in the calculation of overlap of different nuclide resonances. It is clear that a conventional treatment for overlap of the actinide resonances is insufficient to handle, for example, ^{238}U resonances near the 3 keV Na resonance. For light nuclides, the potential scattering cross section is modified to account for resonance scattering. The conventional overlap treatment is given separately in Section 5.7.

The set of resonance nuclides is arranged such that light nuclides are in order of increasing atomic mass and precede all heavy nuclides. The calculation of each resonance nuclide is performed in this order, and the resonance scattering of those light nuclides which have been previously calculated is included in the potential scattering terms of a nuclide calculation. The code also allows more than one pass to be made through the light resonance nuclides.

The calculated resonance integrals of nuclide ℓ may be converted to effective cross sections using the factor $G_{\ell i}$ defined by

$$G_{\ell i} = 1 / \sum_k w_{d\ell k} \phi_{ik} \quad , \quad \dots(5.41)$$

where $w_{d\ell k}$ are the subgroup weights for group flux depression, and ϕ_{ik} are obtained from Equation (5.39) for nuclide ℓ . Defining L_ℓ as the set of light nuclides, excluding nuclide ℓ , which have been calculated before nuclide ℓ , the modifications to the equations previously given may be written as:

$$\Sigma_{ik}'' = \Sigma_i' + N_{\ell i} \sigma_{\ell k} \quad , \quad \dots(5.15a)$$

where

$$\Sigma_i' = \Sigma_i + \sum_{m \in L_\ell} N_{mi} G_{mi} l_{smi} \quad , \quad \dots(5.42)$$

$$V_i \Sigma_{ik}'' \phi_{ik} = \sum_j P_{ji} \{\Sigma_{ik}''\} V_j \Sigma_j' \quad , \quad \dots(5.16a)$$

$$\phi_0 = 1 / \sum_i V_i \left(\sum_m N_{mi} \xi_m \sigma_{pm} + \sum_{m \in L_\ell} N_{mi} (\tau \sigma_{rm}(\bar{S}_{mi}) - \xi_m \sigma_{pm}) \right) \quad , \quad \dots(5.33a)$$

$$\phi_0' = 1 / \sum_i V_i \left(\sum_{m \neq \ell} N_{mi} \sigma_{pm} + N_{\ell i} \xi_\ell \sigma_{p\ell} + \sum_{m \in L_\ell} N_{mi} (\tau \sigma_{rm}(\bar{S}_{mi}) / \xi_m - \sigma_{pm}) \right) \quad , \quad \dots(5.34a)$$

where $\sigma_{rm}(\bar{S}_{mi})$ is the removal cross section of nuclide m which is obtained from the tabulation of $\sigma_{rm}(\hat{\sigma}_p)$ by linear interpolation in $\sqrt{\hat{\sigma}_p}$.

$$\Sigma_{\lambda j} = \sum_m N_{mj} \lambda_{mj} \sigma_{pm} + \sum_{m \in L_\ell} N_{mj} \lambda_{mj} G_{mj} l_{smj} \quad . \quad \dots(5.40a)$$

The collision probabilities are re-evaluated if the fractional change in Σ_1^f is greater than ϵ_{r1} . The equations of the following sections include modifications of this type.

5.6 Non-isolated Resonance Correction

5.6.1 Development of the method for homogeneous calculations

The calculation of resonance integrals given in the previous sections is restricted to a sequence of resonances of a nuclide for which the flux recovers to the asymptotic value, $p(u)\phi_0$, between resonances. At energies in the keV range, this condition is certainly not satisfied for fuel nuclides, as the average resonance spacing is less than the scattering width of the fuel.

For a homogeneous system with a single resonance nuclide ℓ , the function $W(u)$ defined by

$$W(u) = (\sigma_\ell(u) + \sigma_p)\phi(u) / (p(u)\sigma_p\phi_0) \quad , \quad \dots(5.43)$$

gives a measure of the departure of the flux $\phi(u)$ from NR theory for which $W(u)=1$. In PEARLS calculations of ^{238}U and hydrogen used to prepare the cross-section library, significant departures from $W(u)=1$ were observed at high energies where the resonances are narrow. This made it impossible to obtain accurate fits to the deduced resonance integrals. Typical values obtained for the group-averaged value of $W(u)$ for various values of σ_H , the potential scattering due to hydrogen, are given in the following table:

σ_H	2	3	4	10	20	50
$\langle W(u) \rangle$	0.955	1.002	1.029	1.068	1.062	1.039

More extreme values are obtained for mixed moderator systems. Attempts to calculate an average value of $W(u)$ in a direct manner have not proved successful. Therefore, an indirect method which makes use of group cross sections rather than group resonance integrals has been developed.

For a homogeneous system, with \bar{W} defined by

$$\bar{W} = \int W(u) du / \tau \quad , \quad \dots(5.44)$$

we have

$$\begin{aligned} \sigma_p \tau \bar{W} &= \sigma_p \int \frac{\sigma_\ell(u) + \sigma_p}{\sigma_\ell(u) + \sigma_p} W(u) du \quad , \\ &= \int \frac{(\sigma_\ell(u) + \sigma_p)\phi(u)}{\phi_0 p(u)} du \quad , \\ &= \tau I'_{a\ell} + \tau I'_{s\ell} + \sigma_p \int \phi(u) / (\phi_0 p(u)) du, \quad \dots(5.45) \end{aligned}$$

where I' denotes a resonance integral/lethargy which includes the effect on each resonance of higher energy resonances.

Now,

$$\begin{aligned}\sigma_{al} &= \int \sigma_{al}(u) \phi(u) du / \int \phi(u) du \\ &\approx \int \sigma_{al}(u) \phi(u) / p(u) du / \int \phi(u) / p(u) du \\ &= I'_{al} / \{ \bar{W} - (I'_{al} + I'_{sl}) / \sigma_p \} \quad \dots(5.46)\end{aligned}$$

For narrow resonances, \bar{W} is the required non-isolated resonance correction factor, and we may write

$$\begin{aligned}I_{al} &= I'_{al} / \bar{W} \quad , \\ I_{sl} &= I'_{sl} / \bar{W} \quad . \quad \dots(5.47)\end{aligned}$$

In terms of these modified resonance integrals,

$$\sigma_{al} \approx I_{al} / (1 - (I_{al} + I_{sl}) / \sigma_p) \quad , \quad \dots(5.48)$$

and similarly

$$\sigma_{sl} \approx I_{sl} / (1 - (I_{al} + I_{sl}) / \sigma_p) \quad . \quad \dots(5.49)$$

That is, if the effect of the non-asymptotic source is removed from the resonance integrals, group cross sections which are independent of \bar{W} may be obtained from Equations (5.48) and (5.49). At high energies where there are many resonances in a group, the group resonance escape probability may be obtained to high accuracy from σ_{al} and σ_{sl} using

$$p_\ell = 1 - \frac{N_\ell \sigma_{al} \phi_0 \tau \sum_m N_m \sigma_{pm} \beta_m}{N_\ell \sigma_{al} \tau + N_\ell \beta_\ell \sigma_{sl} f_\ell(p_\ell) + \sum_m N_m \beta_m \sigma_{pm} f_m(p_\ell)} \quad , \quad \dots(5.50)$$

where $f_m(p)$ gives the correction to group removals of nuclide m for a group escape probability of p . The approximation used for the function $f_m(p)$ is given in Section 5.8. The value of \bar{W} may then be obtained from

$$\exp(-\bar{W} N_\ell I_{al} \phi_0 \tau) = p_\ell \quad . \quad \dots(5.51)$$

The overall method adopted is:

- (a) given I'_{al} , I'_{sl} from PEARLS calculations of homogeneous mixtures of nuclide ℓ and hydrogen, solve Equations (5.47) to (5.51) for I_{al} and I_{sl} ,
- (b) having calculated I_{al} and I_{sl} in MIRANDA, solve for \bar{W} to obtain a correction factor for I_{al} and I_{sl} .

This method requires modification at lower energies where resonances are neither narrow nor numerous in each group. The effect of the resonance width is excluded from \bar{W} by using values obtained from NR theory throughout the calculation of \bar{W} . That is, for I_{al} and I_{sl}

regarded as functions of $\hat{\sigma}_p$, the values of the integrals at $\hat{\sigma}_p = \sigma_p$ are used in the calculations. In order that the method reduces to a correction factor of unity at low energies, the correction factor \bar{W}^i is actually taken from

$$\bar{W}^i = \begin{cases} 1 + d_\ell (\bar{W} - 1) & , d_\ell > 0, \\ 1 & , d_\ell \leq 0, \end{cases} \quad \dots(5.52)$$

where

$$d_\ell = (E_g - E_{g+1} - 1.5 \langle D \rangle_\ell) / (E_g - E_{g+1}) \quad , \quad \dots(5.53)$$

and \bar{W} is given by Equation (5.51). Equation (5.53) is derived from the fact that the resonance integral is defined for an asymptotic group source.

5.6.2 Application to multiregion calculations

Microscopic absorption and scattering cross sections for nuclide ℓ in region i are given by

$$\sigma_{a\ell i}^W = I_{a\ell i}^N / (1 - (I_{a\ell i}^N + I_{s\ell i}^N) / \bar{S}_{\ell i}^N) \quad , \quad \dots(5.54)$$

and

$$\sigma_{s\ell i}^W = I_{s\ell i}^N / (1 - (I_{a\ell i}^N + I_{s\ell i}^N) / \bar{S}_{\ell i}^N) \quad , \quad \dots(5.55)$$

where $I_{a\ell i}^N$, $I_{s\ell i}^N$ and $\bar{S}_{\ell i}^N$ are obtained from the NR method of Section 5.3. The superscript W denotes a value used in the calculation of the non-isolated resonance correction only. Group fluxes ϕ_i^W are obtained from the solution of the equations:

$$V_i \Sigma_{t i}^W \phi_i^W = \text{Sum}_j V_j P_{j i} \{ \Sigma_{t i}^W \} [T_j^W + (\Sigma_{t j}^W - \Sigma_{r j}^W - \Sigma_{a j}^W) \phi_j^W] \quad , \quad \dots(5.56)$$

where

$$\Sigma_{t i}^W = \Sigma_{t i} + \text{Sum}_{m \in L_\ell} N_{m i} I_{s m i} G_{m i} (1 - \bar{\mu}_m) + N_{\ell i} (\sigma_{a\ell i}^W + \sigma_{s\ell i}^W (1 - \bar{\mu}_\ell)) \quad , \quad \dots(5.57)$$

$$\Sigma_{a j}^W = N_{\ell j} \sigma_{a\ell j}^W \quad , \quad \dots(5.58)$$

$$\begin{aligned} \Sigma_{r j}^W &= \text{Sum}_{m \notin L_\ell} N_{m j} f_m (p_\ell^W) \sigma_{p m} \beta_m / \tau + \text{Sum}_{m \in L_\ell} N_{m j} f_m (p_\ell^W) \sigma_{r m} (\bar{S}_{m j}) \\ &+ N_{\ell j} f_\ell (p_\ell^W) \sigma_{s\ell j}^W \beta_\ell / \tau \quad , \end{aligned} \quad \dots(5.59)$$

$$P_\ell^W = \exp \left(- \text{Sum}_i V_i N_{\ell i} I_{a\ell i}^N \phi_i^W \tau \right) \quad , \quad \dots(5.60)$$

$$T_j^W = \phi_0 \left(\text{Sum}_{m \notin L_\ell} N_{m j} \sigma_{p m} \beta_m + \text{Sum}_{m \in L_\ell} N_{m j} \sigma_{r m} (\bar{S}_{m j}) \tau \right) \quad , \quad \dots(5.61)$$

and ϕ_0 is given by Equation 5.33a. As this correction is not applied to light nuclides, the set L_ℓ is actually the set of all light resonance nuclides. The non-isolated correction factor for nuclide ℓ in region i , $\bar{W}_{\ell i}$, is then given by

$$\bar{W}_{\ell i} = 1 - d_\ell \left(\frac{\sigma_{a\ell i}^W \phi_i^W \log(1 - \text{Sum}_i \Sigma_{a i}^W \phi_i^W V_i)}{I_{a\ell i}^N \phi_0^\tau \text{Sum}_i \Sigma_{a i}^W \phi_i^W V_i} + 1 \right) \quad \dots(5.62)$$

A final set of region-dependent factors $\bar{W}_i^!$ to be applied to the resonance integrals of all nuclides is obtained from

$$\bar{W}_i^! = \prod_\ell \bar{W}_{\ell i} \quad , \quad \dots(5.63)$$

where the product is taken over the resonance integrals for which the non-isolated resonance correction is applicable, i.e. those for which $\langle D \rangle_\ell$ is given.

5.7 Resonance Overlap

The resonance overlap effects considered in this section exclude those overlap effects of resonance scattering of light nuclides which are treated by the method given in Section 5.5.

For calculations which do not include light resonance nuclides, the effect of resonance overlap is included by using

$$I_{x\ell i}^! = \text{Sum}_k w_{x\ell k} S_{\ell i k} / (S_{\ell i k} + \sigma_{\ell k} + \text{Sum}_{m \neq \ell} (G_{mi} - 1) \bar{S}_{\ell i}) \quad , \quad \dots(5.64)$$

where the summation over m is for resonance nuclides excluding ℓ . Equation (5.64) is a generalisation of a standard form for including resonance overlap in calculations for which:

- (a) there is a single fuelled region,
- (b) an average $\bar{S}_{\ell 1}$ is obtained from an equivalence relation, and
- (c) NR theory applies.

The standard form may be written

$$I_{x\ell 1}^! = \text{Sum}_k w_{x\ell k} \bar{S}_{\ell 1} / (\bar{S}_{\ell 1} + \sigma_{\ell k} + \bar{\sigma}) \quad , \quad \dots(5.65)$$

where

$$\bar{\sigma} = \text{Sum}_{m \neq \ell} \frac{N_m}{N_\ell} \frac{I_{am1} + I_{sm1}}{1 - (I_{am1} + I_{sm1}) / \bar{S}_{m1}} \quad . \quad \dots(5.66)$$

Under these conditions $N_m/N_\ell = \bar{S}_{\ell 1} / \bar{S}_{m1}$, and Equation (5.66) becomes

$$\begin{aligned} \bar{\sigma} &= \bar{S}_{\ell 1} \text{Sum}_{m \neq \ell} (I_{am1} + I_{sm1}) / (\bar{S}_{m1} - I_{am1} - I_{sm1}) \\ &= \bar{S}_{\ell 1} \text{Sum}_{m \neq \ell} (G_{m1} - 1) \quad , \quad \dots(5.67) \end{aligned}$$

since, for NR theory,

$$G_{m1} = 1/(1 - (I_{am1} + I_{sm1})/\bar{S}_{m1}) \quad \dots(5.68)$$

The subgroup parameters $w_{d\ell k}$ from which G_{mi} is calculated (Equation (5.41)) have been included in the library specifically for the calculation of resonance overlap effects because, in general, no simple formula, such as Equation (5.68) exists for G_{mi} .

It may also be noted that, if nuclide ℓ is infinitely dilute, Equation (5.64) becomes

$$I'_{x\ell i} = \sum_k w_{x\ell k} / (1 + \sum_{m \neq \ell} (G_{mi} - 1)) \quad \dots(5.69)$$

Then, for a system with two resonance nuclides only,

$$I'_{x\ell i} = \sum_k w_{x\ell k} / G_{mi} = I_{x\ell i} \phi_i / \phi_0 \quad \dots(5.70)$$

which is the required result.

For calculations including light nuclides, Equation (5.64) is modified to become

$$I'_{x\ell i} = \sum_k \frac{w_{x\ell k} \{S_{\ell ik} + \bar{S}_{\ell i} \sum_{m \in M_\ell} (G_{mi} - 1) I_{smi} / (I_{smi} + I_{ami})\}}{S_{\ell ik} + \sigma_{\ell k} + \bar{S}_{\ell i} \{ \sum_{m \neq \ell} (G_{mi} - 1) - \sum_{m \in L_\ell} (G_{mi} - 1) I_{smi} / (I_{smi} + I_{ami}) \}} \quad \dots(5.71)$$

where L_ℓ is the set of light resonance nuclides defined in Section 5.5, and

M_ℓ is the set of remaining light resonance nuclides, not including nuclide ℓ .

That is, the set M_ℓ contains light resonance nuclides with atomic mass greater than ℓ in a one pass calculation, or is the null set in a multipass calculation.

5.8 Correction to Removal Cross Sections

It has already been noted that resonance nuclides may have removal cross sections tabulated as a function of the effective potential scattering cross section $\hat{\sigma}_p$, with interpolation to a value of $\hat{\sigma}_p = \bar{S}_{\ell i}$ being linear in $\sqrt{\hat{\sigma}_p}$. For all other nuclides, the removal cross section in a 1/E flux is given by $\sigma_{p\ell} \beta_\ell / \tau$. It is assumed that the flux dips caused by resonances have no effect on the removal cross sections of such nuclides, but that the removal cross sections of all nuclides require modification to allow for the macroscopic flux shape as represented by the resonance escape probability p . The errors introduced by this assumption are overcome, to some extent, by calculating effective resonance cross sections which reproduce the group reaction rates deduced from resonance integrals, when the removal cross sections have the assumed form.

The function $f_\ell(p_g)$ is defined as the ratio of the removal cross sections of nuclide ℓ for a group resonance escape probability p_g , to that for $p_g=1$, when the scattering cross section of nuclide ℓ is constant. For an assumed within-group flux of $\phi(E)=p(E)/E$, with $p(E)$ linear in E , the following formula is obtained after some manipulation.

$$f_{\ell}(p_g) = \begin{cases} \frac{\tau[(p_g E_g - E_{g+1})\xi_{\ell} - (1 + (\xi_{\ell} - 1)/\alpha_{\ell})(1 - p_g)E_{g+1}]}{\xi_{\ell}[\tau(p_g E_g - E_{g+1}) + (1 - p_g)(E_g - E_{g+1})]}, & \text{for } \alpha_{\ell} > E_{g+1}/E_g, \\ \frac{\tau\{(p_g E_g - E_{g+1})(1 - E_{g+1}/E_g) + \tau[(1 - p_g)E_{g+1} - (p_g E_g - E_{g+1})\alpha_{\ell}] - \alpha_{\ell}(1 - p_g)(E_g - E_{g+1})\}}{[\tau(p_g E_g - E_{g+1}) + (1 - p_g)(E_g - E_{g+1})](1 - E_{g+1}/E_g - \alpha_{\ell}\tau)}, & \text{for } \alpha_{\ell} \leq E_{g+1}/E_g. \end{cases} \quad \dots(5.72)$$

Equation (5.72) is the one originally adopted and is still retained in most cases. However, for highly absorbing systems, the use of $p(E)$ linear in E is unsatisfactory and the form preferred is

$$\phi(u) = \exp((u - u_g) \log p_g / \tau) \quad \dots(5.73)$$

Thus, for $p_g < E_{g+1}/E_g$, the formula used is

$$f_{\ell}(p_g) = \begin{cases} \frac{p_g \log p_g [(1 - \alpha_{\ell} \exp(a \log \alpha_{\ell})) / (1 + a) - \alpha_{\ell} (1 - \exp(a \log \alpha_{\ell})) / a]}{(p_g - 1) \xi_{\ell} (1 - \alpha_{\ell})}, & \text{for } \alpha_{\ell} > E_{g+1}/E_g, \\ \frac{\log p_g [(p_g - E_{g+1}/E_g) / (1 + a) - \alpha_{\ell} (p_g - 1) / a]}{(p_g - 1) (1 - E_{g+1}/E_g - \alpha_{\ell} \tau)}, & \text{for } \alpha_{\ell} \leq E_{g+1}/E_g, \end{cases} \quad \dots(5.74)$$

where $a = \log p_g / \tau$.

The factors $f_{\ell}(p_g)$ are not applied (except in the calculation of \bar{W}) for energies greater than E_p , where E_p (which is normally 50 keV) may be input.

5.9 Cross-section Derivation

The calculated resonance integrals/lethargy for resonance nuclide ℓ in region i with correction factors included are given by

$$I_{x\ell i}'' = \rho_{\ell} \gamma_{\ell} I_{x\ell i}' \quad \dots(5.75)$$

where

$$\gamma_{\ell} = \frac{1/\phi_0}{1/\phi_0 + \sum_i V_i N_{\ell i} (\xi_{\ell} \sigma_{p\ell} - \tau \sigma_{r\ell} (\bar{S}_{\ell i}))} \quad \dots(5.76)$$

for light nuclides ℓ , and $\gamma_{\ell} = 1$ otherwise. The factor γ_{ℓ} arises from the definition of ϕ_0 by

$$\phi_0 = 1 / \sum_i V_i (\sum_{m \in L} N_{mi} \xi_m \sigma_{pm} + \sum_{m \in L} N_{mi} \tau \sigma_{rm} (\bar{S}_{mi})) \quad \dots(5.77)$$

where L is the set of light resonance nuclides.

The overall group resonance escape probability p_g is obtained from

$$p_g = \exp \left(- \sum_i V_i \bar{W}_i \phi_0 \tau \sum_{\ell} N_{\ell i} I''_{a\ell i} \right) \quad \dots (5.78)$$

A reasonable division of resonance absorption A_i in each region is given by

$$A_i = \frac{V_i \bar{W}_i \phi_0 \tau X_{ai} (1-p_g)}{\sum_i V_i \bar{W}_i \phi_0 \tau X_{ai}} \quad \dots (5.79)$$

where

$$X_{ai} = \sum_{\ell} N_{\ell i} I''_{a\ell i} \quad \dots (5.80)$$

To complete the solution, a set of factors F_i is required to represent the inverse of the group flux depression. With effective group cross sections given by

$$\sigma_{x\ell i}^* = F_i I''_{x\ell i} \quad \dots (5.81)$$

and the group flux ψ_i consistent with the $\sigma_{x\ell i}^*$, the equation to be satisfied is

$$A_i = V_i \psi_i F_i X_{ai} \quad \dots (5.82)$$

The solution for F_i and ψ_i is obtained by iteration on the group flux equation in which the source T_i in region i takes the asymptotic value,

$$T_i = \phi_0 \left(\sum_{m \in L} N_{mi} \sigma_{pm} \beta_m + \sum_{m \in L} N_{mi} \tau \sigma_{rm} (\bar{S}_{mi}) \right) \quad \dots (5.83)$$

and the group removal cross section Σ_{ri} in region i is given by

$$\Sigma_{ri} = \sum_{m \in M_1} N_{mi} f_m(p_g) \sigma_{pm} \beta_m / \tau + \sum_{m \in M_2} N_{mi} f_m(p_g) \sigma_{rm} (\bar{S}_{mi}) \quad \dots (5.84)$$

where M_1 is the set of nuclides having a single P_0 scatter matrix, and M_2 is the set of nuclides with a $\hat{\sigma}_p$ -dependent P_0 scatter matrix. The iteration method is given by the equations:

$$\Sigma_i^n = \Sigma_{ti} + F_i^n \left(X_{ai} + \sum_{\ell} N_{\ell i} I''_{s\ell i} (1-\bar{\mu}_{\ell}) \right) \quad \dots (5.85)$$

$$V_i \Sigma_i^n \psi_i^n = \sum_j V_j P_{ji} \{ \Sigma_j^n \} (T_j + \psi_j^n (\Sigma_i^n - \Sigma_{ri} - F_i^n X_{ai})) \quad \dots (5.86)$$

$$F_i^{n+1} = \frac{\sum_i V_i \psi_i^n \Sigma_{ri}}{\sum_i (T_i - A_i)} \times \frac{A_i}{V_i \psi_i^n X_{ai}} \quad \dots (5.87)$$

The first term of Equation (5.87) is a scaling term which is included to improve the convergence. With a collision probability evaluation required for each iteration, an

excessive number of iterations is to be avoided. An initial estimate for F_i is provided by

$$F_i^1 = \prod_{l \notin L} G_{li} \quad \dots(5.88)$$

The convergence test on Equations (5.85) to (5.87) is

$$|F_i^n V_i \psi_i^n X_{ai} - A_i| / A_i < \epsilon_{r3} \quad \dots(5.89)$$

where ϵ_{r3} (normally 10^{-3}) may be input. After solving for F_i , the required effective group cross sections are given immediately by Equation (5.81).

6. COMPARISON OF RESONANCE CALCULATIONS

6.1 Introduction

Comparisons of the MIRANDA resonance treatment with other methods have been restricted to comparisons with the PEARLS code in simple geometries. PEARLS numerically solves the collision probability formulation of the neutron slowing down equations with isotropic elastic scattering, as given by Equation (5.9). The normal point cross-section library used by PEARLS covers the energy range of 19.3 keV to 0.06 eV with 12400 points. Because the evaluation of collision probabilities for this number of points is very time consuming, calculations have been performed for homogeneous and 2-region problems only. Also, the use of a Bonalumi method to approximate collision probabilities in cylindrical geometry means that fuel rods can not be subdivided, as the approximations tend to break down for thin regions of high cross section. In some of the more extreme cases studied, the 2-region representation is far from adequate. However, the same spatial representation is used in the MIRANDA/ICPP calculations as in PEARLS. The AUS collision probability module ICPP [Clancy *et al.* 1977], which includes the same collision probability routines as PEARLS and MIRANDA, has been used in these comparisons to solve the group slowing down equations using group cross sections produced by MIRANDA. All calculations have been performed for an asymptotic source of 1 neutron s^{-1} .

6.2 Cross-section Data

In most of the comparisons, the only resonance nuclide involved is ^{238}U for which the greatest accuracy is required. Initially, a large number of calculations were performed using the ^{238}U library prepared by Doherty (see Section 2). In particular, some 36 PEARLS calculations had been performed with the data for ^{238}U metal rods with graphite or heavy water moderator [Pollard & Harrington, AAEC unpublished report]. Rather than repeat the full range of these results, the majority of the comparisons have been given for these data which are referred to collectively as U238-SCHMIDT. While any reasonable, consistently applied data may suffice for comparison of methods, these data are deficient in that interference scattering is not included. Therefore, additional results have been given for ^{238}U data generated from ENDF/B IV using the methods of Appendix B. A number of cases have been repeated with these data, collectively referred to as U238-ENDFB4, to ensure that the inclusion of resonance scattering has no appreciable effect on the agreement obtained between PEARLS and MIRANDA. A slightly different definition of effective scattering cross section (Section 5.4.1) was used in the U238-SCHMIDT comparisons, but this has no significant effect on the result, because consistency between MIRANDA and subgroup parameter fitting has always been maintained.

A point cross-section library for ^{235}U has not been generated from ENDF/B IV for the full range from 19.3 keV. A complete point cross-section library for ^{235}U generated by Cook & Rose [AAEC unpublished report] from the multilevel resonance parameters of de Saussure *et al.* [1970] in the resolved region, has been used in the resonance overlap comparison. The data generated in the unresolved region proved rather unsatisfactory, but this does not invalidate the comparison. The data for the other resonance nuclides, Na and Fe, used in these comparisons were generated from ENDF/B IV without any such complications.

Apart from the results given in Section 6.7, the MIRANDA calculations were performed with a special purpose AUS library in which moderator nuclides were represented exactly as in PEARLS, *i.e.* isotropic scattering with constant cross section.

6.3 Homogeneous Calculations

Homogeneous calculations have been compared for systems with ^{238}U moderated by either hydrogen or carbon. The results for U238-SCHMIDT are given in Table 1 in terms of the captures in selected groups and the total captures. The agreement for hydrogen moderation is excellent, as one would expect since the subgroup parameters were obtained by fitting to homogeneous $^{238}\text{U}/\text{H}$ mixtures. The agreement to 1 per cent in individual group captures mainly reflects the accuracy of the fit. For carbon moderation the detailed agreement by group is not as good, though the overall agreement is quite acceptable. In the highly absorbing systems, the agreement at lower energies is affected by quite small errors at higher energies. The use of a correction factor Equation (5.32) in the λ method, which depends on the resonance rather than a group, means that detailed agreement is not possible for a resonance covering a number of groups.

Results for two calculations ($^{238}\text{U}/\text{H} = 1/1$ and $^{238}\text{U}/\text{C} = 1/10$) using U238-ENDFB4 are given in Table 2. It can be seen that the agreement between PEARLS and MIRANDA is essentially the same as for the previous data. For the $^{238}\text{U}/\text{C}$ calculation, some values of escape probability for a group, or for a resonance where more appropriate, are also given. The groups which have been combined are those having the same λ parameters in the cross-section library. A comparison of these escape probabilities shows more clearly the accuracy of MIRANDA at low energies. There is a general tendency for MIRANDA to overestimate the escape probability, with the largest error being for the 36.8 eV resonance.

6.4 ^{238}U Metal Rods

Comparisons for ^{238}U metal rods, with diameters in the range 1 to 8 cm, for a range of pitch, with D_2O or graphite moderator, are given in Table 3. These results were obtained with the U238-SCHMIDT data. The results for D_2O are slightly better than for graphite and for both moderators, the resonance capture probabilities agree to 1 per cent except in a few of the more extreme cases. Resonance captures are consistently overestimated by MIRANDA in these cases, but by such a small margin that they are quite acceptable.

Calculations for just two of the cases, with graphite moderator, have been repeated using U238-ENDFB4; the results are given in Table 4. It can be seen that the inclusion of resonance scattering has not affected the comparison, *i.e.* the same errors are obtained for both data sets. The breakdown into four energy groups demonstrates that the agreement is not due to any large cancellation of errors.

6.5 ^{238}U Oxide Rods

Comparisons for ^{238}U oxide rods, mainly of 1 cm diameter, have been made for moderation by H_2O . The results using U238-SCHMIDT (see Table 5) show that MIRANDA underestimates

resonance captures by about 0.5 per cent only. There is very little pitch dependence of the error.

Repeating the standard case, which has a moderator-to-fuel volume ratio of unity, for U238-ENDFB4 gives exactly the same agreement as obtained with U238-SCHMIDT. The results are given in Table 6 in which the second case with a fuel diameter of 2 cm shows that the accuracy of MIRANDA is not dependent on rod size. A possible objection to the approach of fitting subgroup parameters to resonance integrals is that a determination of the temperature coefficient may be inaccurate because it involves the difference of fitted parameters. The calculation of the change in captures with temperature given in Table 6 shows the temperature coefficient to be determined very accurately. Basically, this is because the fits are very accurate and the small errors involved tend to be the same at all temperatures.

6.6 Resonance Overlap

A comparison of MIRANDA and PEARLS in two cases including both ^{235}U and ^{238}U is given in Table 7. The first case is identical with the standard oxide rod case except that the uranium is 5 per cent enriched. The agreement obtained is excellent even at this high enrichment. The second case, a natural uranium metal rod of diameter 2 cm in D_2O , also has high accuracy. The method for calculating the effect of ^{235}U on ^{238}U in these results differed slightly from that given in Section 5. The ^{235}U data were prepared before subgroup parameters fitted to the group flux depression had been included in the library. Therefore, the factor G_{mi} of Equation (5.64), for m representing ^{235}U , was approximated by

$$G_{mi} = \bar{S}_{mi} / (\bar{S}_{mi} - I_{ami} - I_{smi}) \quad , \quad \dots(6.1)$$

which was sufficiently accurate for ^{235}U , but not for ^{238}U when interference scattering was included.

6.7 Resonance Scatterers

Only limited comparisons have been made for typical fast reactor situations involving such resonance scattering nuclides as Na and Fe. Because the PEARLS code is not able to treat many of the effects which become important at high energies, the comparisons have been restricted to homogeneous calculations of simple mixtures over a limited energy range near the major Na and Fe resonances at 3 keV and 28 keV respectively.

The results of the first case with atom densities of $^{238}\text{U}/^{16}\text{O}/^{23}\text{Na} = 0.006/0.015/0.01$ and an asymptotic unit source above 7.1 keV are given in Table 8. The accuracy of MIRANDA is somewhat less than that obtained in thermal reactor calculations. In particular, there are errors of the order of 10 per cent for the group in the range 3.35 to 2.61 keV which includes the resonance peak. The Na resonance has been treated using the wide resonance λ of Section 5.4.2. It is the deficiencies of this method, particularly near the resonance peak, which led to an overestimation of the Na removal cross section, and hence an underestimation of the flux. The accuracy of the calculation of capture rates for the entire energy range considered (7.1 keV to 1.58 keV) is much better at about 1 per cent. The change in the ^{238}U capture rate with temperature is also well predicted.

For the 28 keV Fe resonance, the results obtained for two simple nuclide mixtures are given in Tables 9 and 10. The comparison is restricted to the elastic removal cross section for the group 31.8 to 24.8 keV. It can be seen that the method does not handle this resonance at all well. The major difficulty is that no treatment is included for

the effect of a resonance of one nuclide on the other nuclides of the system. Also, the λ method has not proved adequate to predict the cross sections of Fe in the case where the hole in the cross section is as important as the peak. While the results are poor for this resonance, the overall accuracy of calculations of most fast reactor systems should not be seriously impaired. Improved accuracy could of course be obtained by further refinement of the group structure.

7. HOMOGENEOUS FLUX CALCULATION

7.1 Calculation of Cross Sections

To obtain homogeneous cross sections for a B_L flux calculation, the cross sections of the lattice require spatial smearing. In resonance groups g , the spatial flux ψ_{ig} obtained from Equations (5.85) to (5.87) may be used for this purpose. Setting $\psi_{ig}=1$ in non-resonance groups, the spatial smearing of any cross section σ_x is given by

$$\Sigma_{xg} = \frac{\sum_i V_i \psi_{ig} \sum_{\ell} N_{\ell} \sigma_{x\ell g}}{\sum_i V_i \psi_{ig}} \quad \dots(7.1)$$

This equation is applied to all orders of P_n scattering as well as to cross sections.

The cross-section library includes thermal cross sections and scattering matrices tabulated against temperature. Interpolation (or extrapolation) in these tabulations is linear in $\sqrt{T_i}$ for each region i . For nuclides ℓ which have resonance treatment in group g , effective cross sections $\sigma_{x\ell g}^*$ and equivalent potential scattering $\bar{S}_{\ell ig}$ are available for each region i from the treatment given in Section 5. In this case, the P_n scattering matrices may be tabulated in the library against temperature and potential scattering. Interpolation in these tabulations is again linear in the square root of both variables for each region i . The factors $f_{lg}(p_g)$ obtained in the resonance treatment of a group g are applied as a multiplier to P_0 outscatters from group g for all nuclides. The self-scatter term is adjusted to maintain the total scattering cross section.

The total cross section for a B_L calculation, and the transport cross section for a P_0 flux calculation, require special consideration. The following three cases are distinguished:

A *Groups in which nuclide ℓ does not have resonance treatment.*

The total cross section is obtained from

$$\sigma_{\ell ig} = \sigma_{a\ell g} + \sum_h \sigma_{\ell, g \rightarrow h, 0} \quad \dots(7.2)$$

where $\sigma_{\ell, g \rightarrow h, 0}$ represents the P_0 scatters from group g to h of nuclide ℓ .

The transport cross section, if required, is obtained directly as the first reaction on the library.

B *Light nuclides with resonance treatment.*

The total cross section is obtained from

$$\sigma_{\ell ig} = \sigma_{a\ell g}^* + \sum_h \sigma_{\ell, g \rightarrow h, 0}(T_i, \bar{S}_{\ell ig}) \quad \dots(7.3)$$

that is, as for Equation (7.2) but with region and temperature dependence. For P_0 calculations, the transport cross section is obtained from

$$\sigma_{tlig} = \sigma_{lig} - \sum_h \sigma_{\ell, g \rightarrow h, 1}(T_i, \bar{S}_{lig}) \quad \dots(7.4)$$

C. Heavy nuclides with resonance treatment.

The equations used are:

$$\sigma_{lig} = \sigma_{p\ell} + \sigma_{slig}^* + \sigma_{alig}^* \quad \dots(7.5)$$

$$\sigma_{tlig} = (\sigma_{p\ell} + \sigma_{slig}^*) (1 - \bar{\mu}_\ell) + \sigma_{alig}^* \quad \dots(7.6)$$

The fission spectrum in an AUS library is nuclide dependent but not dependent on the incident neutron energy. The values on the standard library AUS.ENDFB are appropriate for thermal systems. However, these values may be over-ridden by specification of fission spectra in MIRANDA input data. To form an average fission spectrum, the fission spectrum of a nuclide is weighted by the fission emission reaction rate of the nuclide calculated from a group flux estimate. This average spectrum is used only for the MIRANDA flux calculation; the weighting of fission spectra for output uses the calculated flux. The flux estimate may be input, but this should not be necessary for normal calculations.

7.2 The B_L Equations

The B_L approximation is a standard method for applying a uniform buckling to an homogenised lattice [e.g. Weinberg & Wigner 1958]. The derivation below is given merely to illustrate the features of the method and detail its application in MIRANDA.

The multigroup form of the transport equation in uniform plane geometry may be written:

$$\begin{aligned} \mu \frac{\partial \psi_g(x, \mu)}{\partial x} + \Sigma_g \psi_g(x, \mu) \\ = \sum_h \sum_\ell \frac{1}{2}(2\ell + 1) \int_{-1}^1 \Sigma_{h \rightarrow g, \ell} P_\ell(\mu') P_\ell(\mu) \psi_h(x, \mu') d\mu' + \frac{1}{2} S_g(x) \quad \dots(7.7) \end{aligned}$$

where $\psi_g(x, \mu)$ is the flux in group g at position x with direction cosine μ , Σ_g is the total cross section, $S_g(x)$ is the fission source, which is isotropic, $\Sigma_{h \rightarrow g}(\underline{\Omega}' \rightarrow \underline{\Omega})$ is the scattering cross section from group h , direction $\underline{\Omega}'$, to group g direction $\underline{\Omega}$ which has been expanded as

$$\Sigma_{h \rightarrow g}(\underline{\Omega}' \rightarrow \underline{\Omega}) = \sum_\ell \frac{(2\ell + 1)}{4\pi} \Sigma_{h \rightarrow g, \ell} P_\ell(\underline{\Omega} \cdot \underline{\Omega}') \quad \dots(7.8)$$

For positive buckling B^2 , the B_L equations may be obtained by assuming the flux to be separable,

$$\psi_g(x, \mu) = e^{iBx} \psi_g(\mu) \quad \dots(7.9)$$

and expanding $\psi_g(\mu)$ as

$$\psi_g(\mu) = \sum_\ell \frac{1}{2}(2\ell + 1) \psi_{g\ell} P_\ell(\mu) \quad \dots(7.10)$$

Substitution in Equation (7.7) gives

$$(\mu iB + \Sigma_g) \psi_g(\mu) = \sum_h \sum_\ell (2\ell + 1) \Sigma_{h \rightarrow g, \ell} \psi_{h\ell} P_\ell(\mu) + \frac{1}{2} S_g \quad \dots(7.11)$$

where $S_g(x) = e^{iBx} S_g$ follows from the separability of the flux.

This may be rewritten as

$$\sum_g \sum_k \frac{1}{2}(2k+1) \psi_{gk} P_k(\mu) = \sum_h \sum_\ell \frac{1}{2}(2\ell+1) \sum_{h \rightarrow g, \ell} \psi_{h\ell} P_\ell(\mu) / (1 + \eta_g \mu) + \frac{1}{2} S_g P_0(\mu) / (1 + \eta_g \mu) \quad , \quad \dots (7.12)$$

where $\eta_g = iB/\Sigma_g$.

Multiplying by $P_k(\mu)$ and integrating gives

$$\sum_g \psi_{gk} = \sum_h \sum_\ell (2\ell+1) \sum_{h \rightarrow g, \ell} A_{gk\ell} \psi_{h\ell} + A_{gko} S_g \quad , \quad \dots (7.13)$$

where

$$A_{gk\ell} = \frac{1}{2} \int_{-1}^1 \frac{P_k(\mu) P_\ell(\mu)}{1 + \eta_g \mu} d\mu \quad . \quad \dots (7.14)$$

The coefficients $A_{gk\ell}$ may be generated by noting that

$$(\ell+1) A_{k, \ell+1} + \frac{2\ell+1}{\eta} A_{k\ell} + \ell A_{k, \ell-1} = \frac{\delta_{\ell k}}{\eta} \quad , \quad \dots (7.15)$$

$$A_{00} = \frac{1}{2\eta} \log \left(\frac{1+\eta}{1-\eta} \right) \quad , \quad \dots (7.16)$$

$$A_{k1} = \frac{1}{\eta} (\delta_{k0} - A_{k0}) \quad , \quad \dots (7.17)$$

$$A_{k\ell} = A_{\ell k} \quad , \quad \dots (7.18)$$

where the g subscript has been dropped.

Rather than deal with complex quantities, we define

$$\phi_{gk} = \psi_{gk} i^k \quad ,$$

then Equation (7.13) becomes

$$\sum_g \phi_{gk} = \sum_h \sum_\ell (2\ell+1) \sum_{h \rightarrow g, \ell} \bar{A}_{gk\ell} \phi_{h\ell} + \bar{A}_{gko} S_g \quad , \quad \dots (7.19)$$

$$\text{where } \bar{A}_{gk\ell} = A_{gk\ell} i^{k-\ell} \quad . \quad \dots (7.20)$$

The $\bar{A}_{gk\ell}$ are real and are given by:

$$-(\ell+1) \bar{A}_{k, \ell+1} + \frac{(2\ell+1)}{\eta} \bar{A}_{k, \ell} + \ell \bar{A}_{k, \ell-1} = \frac{\delta_{\ell k}}{\eta} \quad \dots (7.21)$$

$$\bar{A}_{00} = \frac{1}{\bar{\eta}} \arctan \bar{\eta} \quad , \quad \dots(7.22)$$

$$\bar{A}_{k1} = -\frac{1}{\bar{\eta}} (\delta_{k0} - \bar{A}_{k0}) \quad , \quad \dots(7.23)$$

$$\bar{A}_{k\ell} = \bar{A}_{\ell k} (-1)^{k-\ell} \quad , \quad \dots(7.24)$$

where $\bar{\eta} = B/\Sigma_g$.

This completes the description of the B_L equations for positive B^2 . For negative B^2 , the flux is assumed separable in the form

$$\Psi_g(x, \mu) = e^{bx} \psi_g(\mu) \quad , \quad \dots(7.25)$$

where $b = |B^2|^{1/2}$. The analysis is exactly as for positive B^2 , and Equations (7.13) to (7.18) apply with $\eta_g = b/\Sigma_g$.

It needs to be stressed that it is the expansion of the scattering matrix in Equation (7.8) which is truncated, by setting $\Sigma_{h \rightarrow g, \ell} = 0$ for $\ell > L$, to obtain the B_L approximation. No truncation of the flux is involved, but $\phi_{g\ell}$ for $\ell \leq L$ are the only components of the flux required, and they do not depend on higher order terms in the flux expansion. In practice, small high-order components of the flux allow the scattering expansion to be truncated.

The B_L equations are strictly applicable only when the spatial variation e^{iBx} is the same in all groups. The code does allow B^2 to be group dependent, giving a set of approximate equations which are analogous to the use of a $D_g B_g^2$ leakage term. The use of B_g^2 of differing sign must be avoided for $L \neq 0$. The code actually uses the P_0 method with the transport approximation when a B_0 calculation is requested. The equations to be solved are then given by:

$$\phi_g (\Sigma_{ag} + B_g^2 / (3\Sigma_{tg})) + \text{Sum}_{h \neq g} \Sigma_{g \rightarrow h, 0} \phi_h = \text{Sum}_{h \neq g} \Sigma_{h \rightarrow g, 0} \phi_h + S_g \quad . \quad \dots(7.26)$$

7.3 Solution of the B_L Equations

The B_L Equations (7.14) or (7.19) may be written in the form

$$\Sigma_g \phi_{gk} = \text{Sum}_{\ell} C_{gk\ell} \text{Sum}_h \Sigma_{h \rightarrow g, \ell} \phi_{h\ell} + C_{gk0} \chi_g \quad , \quad \dots(7.27)$$

$$\text{where } C_{gk\ell} = \begin{cases} (2\ell+1) \bar{A}_{gk\ell} & , B^2 > 0, \\ (2\ell+1) A_{gk\ell} & , B^2 < 0, \end{cases}$$

and the fission source is simply the fission spectrum χ_g . The method of solution is a Gauss Seidel iteration over groups with direct inversion of the angular dependence. The iteration process may be written in matrix form for iteration n as

$$\phi_g^n = D_g^{-1} C_g S_g \quad , \quad \dots(7.28)$$

where the matrices are $L \times L$,

$$\underline{\phi}_g^n \text{ has elements } \phi_{gk}^n ,$$

$$\underline{C}_{\approx g} \text{ has elements } C_{gk\ell} ,$$

$$\underline{D}_{\approx g} \text{ has elements } \sum_g \delta_{k\ell} - C_{gk\ell} \sum_{g \rightarrow g, \ell} , \text{ and}$$

$$\underline{S}_g \text{ has elements } \sum_{h < g} \sum_{h \rightarrow g, \ell} \phi_{h\ell}^n + \sum_{h > g} \sum_{h \rightarrow g, \ell} \phi_{h\ell}^{n-1} + \delta_{\ell o} \chi_g .$$

If the buckling B_g^2 does not change between iterations, the matrices $\underline{C}_{\approx g}$ and $\underline{D}_{\approx g}$ remain fixed so that the matrices $\underline{D}_{\approx g}^{-1} \underline{C}_{\approx g}$ may be computed once and used throughout the iteration over groups.

For groups into which there is no upscattering, the solution (for a given B_g^2) is obtained on the first pass, but the convergence of the thermal groups may be very slow when there is a large number of thermal groups. Therefore a few-group scaling technique is employed for the thermal groups. This amounts to condensing the Equations (7.27) into N_G broad groups using the latest estimate of the flux ϕ_{gk}^n . The resulting $N_G \times L$ equations have the form

$$R_{Gk} \gamma_{Gk} = \sum_{\ell} \sum_H R_{H \rightarrow G, \ell} \gamma_{H\ell} + S_{G\ell} , \quad \dots (7.29)$$

where

$$R_{Gk} = \sum_{g \in G} \sum_g \phi_{gk}^n , \quad \dots (7.30)$$

$$R_{H \rightarrow G, \ell} = \sum_{g \in G} \sum_{h \in H} C_{gk\ell} \sum_{h \rightarrow g, \ell} \phi_{h\ell}^n , \quad \dots (7.31)$$

and $S_{G\ell}$ is the epithermal slowing down source.

The Equation (7.29) is solved directly for γ_{Gk} which then gives

$$\phi_{gk}^n = \gamma_{Gk} \phi_{gk}^n \quad \text{for } g \in G . \quad \dots (7.32)$$

The number of groups N_G may be set in the input data but the default value 3 gives a reasonable compromise between excessive computation in the scaling and the acceleration achieved.

The effective multiplication estimate after each iteration n is given simply by

$$k_{\text{eff}}^n = \sum_g (v \Sigma_f)_g \phi_{go}^n . \quad \dots (7.33)$$

The final convergence criterion on the fluxes is

$$\epsilon^n = \max_g |\phi_{go}^n - \phi_{go}^{n-1}| / \phi_{go}^n < \epsilon_f , \quad \dots (7.34)$$

where ϵ_f may be input (default value 10^{-4}).

The advantages of the group scaling method are most apparent in calculations involving a search for the critical buckling. The fluxes for each buckling estimate need not be converged because the few-group scaling ensures that reasonable estimates of k_{eff} are obtained on each iteration. The buckling search consists of finding an eigenvalue λ such that bucklings λB_g^2 give $k_{\text{eff}} = k_{\text{reqd}}$. The first estimate of λ , λ^1 which may be input (normally 1) is used to give k_{eff}^1 and hence a second estimate of λ from

$$\lambda^2 = \frac{\lambda^1 (k_{\text{eff}}^1/k_{\text{reqd}} - \text{Sum}_g \Sigma_{\text{ag}} \phi_{\text{go}})}{1 - \text{Sum}_g \Sigma_{\text{ag}} \phi_{\text{go}}} \quad \dots(7.35)$$

Successive estimates of λ^m are then given by

$$\lambda^{m+1} = \lambda^m + \frac{\lambda^2 - \lambda^1}{1/k_{\text{eff}}^2 - 1/k_{\text{eff}}^1} (1/k_{\text{reqd}} - 1/k_{\text{eff}}^m) \quad \dots(7.36)$$

The form of Equations (7.35) and (7.36) which is taken simply from

$$k_{\text{eff}}^m = k_{\infty} / (1 + \lambda^m M^2 B^2) \quad ,$$

ensures convergence after a few iterations. For each value of λ^m except λ^1 , the estimate of k_{eff}^m is accepted after one iteration on the fluxes. For λ^1 , the additional criterion

$$\epsilon^n < 2 |k_{\text{eff}}^1 - k_{\text{reqd}}| \quad \dots(7.37)$$

must be satisfied before k_{eff}^1 is accepted.

8. GROUP CONDENSATION AND CROSS-SECTION OUTPUT

8.1 General

Cross sections (or reaction rates) are generated by MIRANDA for defined materials or library nuclides which may or may not be present in the calculated system. In addition, a nuclide which is present in more than one material of the system may have cross sections prepared which are region dependent.

The extraction of cross sections from the data library for output, follows the same prescriptions given in Section 7.1 for the homogeneous flux calculation. The general formula used to condense and/or smear all cross sections, apart from the transport and total cross section, is given by

$$\sigma'_{x\ell ig} = \frac{\text{Sum}_{g \in G} \phi_{go} \text{Sum}_i V_i \rho_i \Psi_{ig} \text{Sum}_{\ell} w_{\ell} \sigma_{x\ell ig}}{\text{Sum}_{g \in G} \phi_{go} \text{Sum}_i V_i \rho_i \Psi_{ig}} \quad , \quad \dots(8.1)$$

where Ψ_{ig} is the spatial flux in group g , $\Psi_{ig} = 1$ in non-resonance groups;
 ϕ_{go} is the homogeneous scalar group flux;
 $\sigma_{x\ell ig}$ is the cross section of library nuclide ℓ in resonance region i for group g ;

- w_ℓ is $\delta_{\ell k}$ if nuclide k is to be formed, or the weight of nuclide ℓ in the definition of a material if a defined material is to be formed; and
- (a) $\rho_i = \delta_{ij}$ if the region j , for which the cross sections are required, is specified by the user;
- (b) $\rho_i = N_{\ell i}$, the concentration of nuclide ℓ in region i , for a nuclide ℓ to be formed with cell averaged cross sections;
- (c) $\rho_i = N_{\ell i} \delta_{M_i, M_j}$ for a nuclide ℓ to be formed for each region j in which $N_{\ell j}$ is non-zero and for which the material M_j in region j is distinct;
- (d) $\rho_i =$ the volume fraction of the region i occupied by the material, for a material explicitly included in the calculated system;
- (e) $\rho_i = \min(N_{\ell i}/w_\ell)$ for a material not explicitly in the calculated system; or
- (f) $\rho_i = 1$ for all i , if all $\rho_i = 0$ under the above conditions.

The formal definition of ρ_i becomes clear when used in conjunction with the input description of Section 9.

For transfer matrices, the condensation and smearing formula becomes

$$\sigma_{G \rightarrow H, k} = \frac{\sum_{g \in G} \phi_{gk} \sum_i V_i \rho_i \psi_{ig} \sum_\ell w_\ell \sum_{h \in H} \sigma_{\ell, i, g \rightarrow h, k}}{\sum_{g \in G} \phi_{gk} \sum_i V_i \rho_i \psi_{ig}} \quad \dots (8.2)$$

If output of scatter matrices with k of higher order than the B_L flux calculation is requested, ϕ_{g0} is substituted for ϕ_{gk} , $k > L$. It must be noted that condensation of scatter matrices for $k \neq 0$ over the appropriate component of the B_L flux, implies that the matrices are to be used in a leakage calculation. If this is not the case, condensation in MIRANDA should be minimal.

8.2 Transport and Total Cross Section

8.2.1 P_0 calculation

The requirements for condensing the transport cross section following a P_0 flux calculation are considered first. In this case, the transport cross sections of the individual nuclides are obtained from the cross section library, and the macroscopic transport cross section of the homogenised system is given by

$$\Sigma_{tg} = \frac{\sum_i V_i \psi_{ig} \Sigma_{tig}}{\sum_i V_i \psi_{ig}} \quad \dots (8.3)$$

where

$$\Sigma_{tig} = \sum_\ell N_{\ell i} \sigma_{tig}$$

That is

$$\Sigma_{tg} = \sum_i \psi_{ig}^i \Sigma_{tig} \quad \dots (8.4)$$

where $\psi_{ig}^i = V_i \psi_{ig} / \sum_i V_i \psi_{ig}$

As it is the leakage which needs to be conserved, a reasonable formula for condensing Σ_{tg} is given by

$$\Sigma'_{tG} = \frac{\text{Sum}_{g \in G} B_g^2 \phi_g}{\text{Sum}_{g \in G} (B_g^2 \phi_g / \Sigma_{tg})} \quad \dots(8.5)$$

In terms of the diffusion coefficient D_g , this may be rewritten

$$\Sigma'_{tG} = \frac{\text{Sum}_{g \in G} D_g B_g^2 \phi_g \text{ Sum}_i \psi'_{ig} \Sigma_{tig}}{\text{Sum}_{g \in G} D_g B_g^2 \phi_g} \quad \dots(8.6)$$

This suggests that in condensing Σ_{tig} the weighting should be $\psi'_{ig} D_g B_g^2 \phi_g$. However, the definition

$$\Sigma'_{tig} = \frac{\text{Sum}_{g \in G} \Sigma_{tig} \psi'_{ig} D_g B_g^2 \phi_g}{\text{Sum}_{g \in G} \psi'_{ig} D_g B_g^2 \phi_g} \quad \dots(8.7)$$

gives a value of Σ'_{tig} such that, if the flux $\psi'_{ig} \phi_g$ were exact, the leakage calculated in the condensed group structure would not be conserved. Therefore, the definition used is

$$\Sigma'_{tig} = \frac{\text{Sum}_{g \in G} \Sigma_{tig} \psi'_{ig} D_g B_g^2 \phi_g \text{ Sum}_{g \in G} \phi_g}{\text{Sum}_{g \in G} D_g B_g^2 \phi_g \text{ Sum}_{g \in G} \psi'_{ig} \phi_g} \quad \dots(8.8)$$

which has the required property that

$$\Sigma'_{tG} = \frac{\text{Sum}_i (\text{Sum}_{g \in G} \psi'_{ig} \phi_g) \Sigma'_{tig}}{\text{Sum}_{g \in G} \phi_g} \quad \dots(8.9)$$

8.2.2 B_1 calculation

Before considering the condensation formula to be employed, a definition of the transport cross section in the library group structure is required. The B_1 equations for group g may be written (from Equation (7.27))

$$\Sigma\phi_0 = C_{00}S_0 + 3C_{01}S_1 \quad \dots(8.10)$$

$$\Sigma\phi_1 = C_{10}S_0 + 3C_{11}S_1$$

where the g subscript has been dropped and S_0 and S_1 represent the source components. Using the recurrence relations, the equations may be rewritten as

$$\Sigma\phi_0 = C_{00}S_0 - (3\Sigma/B)(1-C_{00})S_1$$

$$\Sigma\phi_1 = (\Sigma/B)(1-C_{00})S_0 + (3\Sigma^2/B^2)(1-C_{00})S_1 \quad \dots(8.11)$$

We therefore have

$$\Sigma\phi_0 + B\phi_1 = S_0 \quad \dots(8.12)$$

that is, $B\phi_1$ represents the leakage. After some manipulation we also obtain

$$B\phi_1 = B^2\phi_0 / \left(\frac{C_{00}B^2}{\Sigma(1-C_{00})} - \frac{3S_1}{\phi_1} \right) \quad \dots(8.13)$$

If $B \ll \Sigma_g$,

$$C_{00} = 1 - B^2/(3\Sigma^2),$$

and Equation (8.13) becomes

$$B\phi_1 = B^2\phi_0/(3\Sigma - 3S_1/\phi_1) \quad \dots(8.14)$$

This leads to the definition of the transport cross section as

$$\Sigma_{tg} = \Sigma_g - \sum_h \Sigma_{h \rightarrow g, 1} \phi_{h1}/\phi_{g1} \quad \dots(8.15)$$

The definition (8.15) reproduces the correct leakage only for B_1 calculations with small B^2 . To ensure that leakage is preserved in all cases, the definition required is

$$\Sigma_{tg}^* = \frac{B^2\phi_{g0}}{3(S_{g0} - \Sigma_g\phi_{g0})} \quad \dots(8.16)$$

This does not lead to a definition of the transport cross section for components of the system, but the ratio $\Sigma_{tg}^*/\Sigma_{tg}$ may be used as a correction factor to the transport cross section of system components obtained as in Equation (8.15).

The condensation/mixing rule, equivalent to Equation (8.1), for the transport cross section becomes

$$\sigma'_{tG} = \frac{\sum_{g \in G} \phi_{g0} \sum_{g \in G} D_g B^2 \phi_g \sum_i \Psi_i^! \rho_i \sum_{\ell} w_{\ell} (\sigma_{\ell ig} - \sum_h \sigma_{\ell, i, h \rightarrow g, 1} \phi_{h1}/\phi_{g1})}{\sum_{g \in G} (S_{g0} - \Sigma_g \phi_{g0}) \sum_{g \in G} \phi_{g0} \sum_i \rho_i \Psi_i^!} \quad \dots(8.17)$$

$$\text{where } D_g = 1/3 \{ \sum_i \Psi_i^! \sum_{\ell} N_{\ell i} (\sigma_{\ell ig} - \sum_h \sigma_{\ell, i, h \rightarrow g, 1} \phi_{h1}/\phi_{g1}) \} \quad \dots(8.18)$$

The transport cross section given by Equation (8.17) is appropriate for use in a diffusion theory calculation of the leakage. An input option allowing the transport cross sections to be prepared without the factor $\Sigma_{tg}^*/\Sigma_{tg}$ should be used if the leakage is to be calculated using transport theory with P_0 scattering. Under this option, the term $D_g B^2 \phi_g$ in Equation (8.17) is replaced by $(S_{g0} - \Sigma_g \phi_{g0})$.

The condensation/mixing rule for the total cross section simply uses a leakage weighting, thus:

$$\sigma'_G = \frac{\sum_{g \in G} \phi_{g0} \sum_{g \in G} (S_{g0} - \Sigma_g \phi_{g0}) \sum_i \rho_i \Psi_i^! \sum_{\ell} w_{\ell} \sigma_{\ell ig}}{\sum_{g \in G} (S_{g0} - \Sigma_g \phi_{g0}) \sum_{g \in G} \phi_{g0} \sum_i \rho_i \Psi_i^!} \quad \dots(8.19)$$

On AUS cross-section data pools, the total cross section for use in a transport calculation is obtained from the absorption and the P_0 scattering vector. For P_n output, $n \neq 0$, the P_0 self-scatter term is adjusted by MIRANDA to be consistent with the total cross section σ'_G . For P_0 output, the self-scatter term is transport corrected, but the factor $\Sigma_{tg}^*/\Sigma_{tg}$ is not included.

9. INPUT DATA

9.1 General Layout

Input data to MIRANDA are in free format, with keywords to indicate the data type followed by a string of numeric or alphabetic information. The data are punched in columns 1 to 72 with each keyword starting on a new card. As the data are read with the SCAN input routine [Bennett & Pollard 1967], all the facilities and conventions of SCAN apply. The readability of the data may be improved by including any desired special characters.

Many of the input variables have been given default values. Thus, if the standard value is required, an entire keyword and data may be omitted or trailing data may be left off the end of a data string. There is no set order in which the keywords must be given, but some of the data require information to be previously defined. For example, a material may not be referred to before it is defined. It is, therefore, best to follow the order of keywords given below. When a series of calculations is undertaken, only the data which are to be altered need be given for subsequent calculations.

In the description of keywords given below, those that should suffice for most calculations are indicated by an asterisk. Underlined information should be reproduced exactly.

* 9.2 HEAD Heading Information

<u>HEAD</u>	JOBNAME	HEADING
where	JOBNAME	is a word of 1 to 6 alphanumeric characters which provides a unique label for all output including each material on an output cross-section data pool, and
	HEADING	is a string of characters, including blanks, also used for labelling.

Example:

```
HEAD      SR5      TEST CALCULATION
```

9.3 PRELUDE Problem Size Specification

```
PRELUDE  MDEF = md      MREQD = mr      MAXX = mx      MAXBN = mb
```

with default values

```
PRELUDE  MDEF = 20      MREQD = 0      MAXX = 20      MAXBN = 0
```

where	md	is the maximum number of defined materials,
	mr	is the maximum number of output materials i.e. the number of materials on the REQD card,
	mx	is the maximum number of geometry intervals, and
	mb	is the maximum order of a B_L flux solution.

The PRELUDE values of MREQD, MAXX and MAXBN may be exceeded in the first calculation, which serves to redefine these maxima, so that a PRELUDE card is seldom required. If, however, a subsequent calculation requires a larger value than the first, a PRELUDE card is necessary.

Example:

```
PRELUDE  MAXBN = 3      MDEF = 30
```

is required for a B3 calculation following a B1 calculation with 30 materials defined.

9.4 USE Library Selection

```
USE      lib      nn
```

with default

```
USE      8      10000
```

where lib is the FORTRAN unit number of the input cross-section library, and nn is the maximum number of library nuclides which are to be used; nn would only have application in a burnup calculation, e.g. to discard fission products.

A USE card serves to initialise variables to the standard state, causes a preliminary reading of the cross-section library and causes the STATUS data pool to be read. If a USE card is not given before any input card except HEAD, PRELUDE (or TEST) is given, the code generates the standard USE card.

9.5 SELECT Library Selection

SELECT name, source, mod = newname
 where name is the name of a library nuclide for which a non-standard set of data is required,
 source is the data source of the required data,
 mod if given, selects the appropriate data modification, and
 newname if given, renames the nuclide so that two versions of a nuclide may be included in a calculation.

The nuclides on the library are labelled by 20 characters consisting of an 8-character simple name, an 8-character data source and a 4-character modifier. The library may include more than one version of a nuclide, and the one having the highest update number is normally used. A number of SELECT cards may be used to choose non-standard versions of nuclide data, but they must immediately follow a USE card, or be the first cards apart from HEAD, PRELUDE, or TEST. The nuclide list for AUS.ENDFB is given in Appendix A.

Example:

```
SELECT U233 BNL65PHF MOD2 = U233A
```

selects an old set of U233 data and renames it U233A so that it may be compared with the standard U233 data.

* 9.6 TEMP Default Temperature

TEMP t
 with default
 TEMP 300
 where t is the default temperature (K) for any *following* material definitions which do not include a specific temperature value.

* 9.7 DEFN Material Definition

DEFN matname t name₁, conc₁, name₂, conc₂, ...
 where matname is the 1- to 8-character name to be given to the defined material,
 t is the temperature (K) of the material, which may be omitted,
 name_i is the name of a library nuclide or a previously defined material, and
 conc_i is the quantity of name_i to be included, usually in 10²⁴ atom cm⁻³.

The set of nuclides currently included in the AUS.ENDFB library is given in Appendix A. The names they have been given are the obvious isotope or element name. Though a definition in terms of defined materials is permitted, this is only to avoid duplication of input as in the example:

DEFN	U02	U235	.05	U238	.95	0	2.
DEFN	FUELA	450.	U02	.022			
DEFN	FUELB	600.	U02	.022	B10	1.E-5	

* 9.8 REQD Output Material Selection

REQD name₁ (r₁), name₂ (r₂), ...

where name_j is the name of a library nuclide or a defined material which is required for output, and

r_j if given, selects the resonance geometry interval number for which the nuclide or material is to be produced.

An interval number r_j is not normally given as the code averages over the required region. The following description of the default values should be read in conjunction with the definitions of ρ_i in Equation (8.1). For a defined material, average cross sections are formed over the cell regions occupied by that material (definition (d) for materials explicitly in the system, and definition (e) for intermediate materials such as U02 above) or over the entire cell for materials not in the cell (definition (f)). For a library nuclide in the cell, a choice may be made between one set of average cross sections (definition (b)) or a set of cross sections for each resonance region which includes the nuclide and is filled by a different material (definition (c)). The choice is made using the REQDREG card, with the default being to prepare a number of cross section sets for fuel nuclides only.

If output of a resonance nuclide is requested for a resonance region in which the nuclide concentration is zero, infinite dilution cross sections will be used. Correct cross sections of a resonance nuclide in such regions may be generated by including a small amount, say 1.E-20, of the nuclide in the material definitions. This procedure is useful in preparing cross sections for a reaction rate scan across the lattice.

If the library order is known, a group of nuclides may be selected using:

REQD name₁ TO name₂, ...

Examples:

REQD FUEL, MOD, U235 TO PU241

REQD FUEL, CAN, MOD, REFL(3)

* 9.9 XM or RM Geometry Size Specification

XM ibc x₁, x₂, ... , x_n obc

RM ibc x₁, x₂, ... , x_n obc

where XM implies slab geometry,

RM implies cylindrical geometry,

ibc is the inner boundary condition,

x_i is the width of the ith mesh interval in cm, and

obc is the outer boundary condition.

The boundary condition has the values 0 for reflective and -1 for translational conditions. Either an XM or RM card is always required, and homogeneous cases should be run as a one-region calculation.

Example:

RM 0 0.5 0.25 0

specifies a two-region cylinder with fuel radius of 0.5 cm and an outer radius of 0.75 cm.

* 9.10 REG Geometry Layout Specification

REG {MX/MR} (int₁, ... , int_n, name₁), ...

where MX or MR may be included for compatibility with other AUS modules or omitted,

int₁, ..., int_n are the mesh interval numbers which are filled by the defined material, name₁, and name_j may have the form of a material name, or be M(j) which specifies the jth material on the previously given REQD card.

Examples:

```
REG 1 FUEL 2 MOD
REG MX 1 3 5 7 M(1) MX 2(2)8 M(2)
```

* 9.11 RODSUB and ARRAY Cluster Specification

In cluster geometry, the composition and position of fuel rods within the annular geometry given by the RM and REG cards is specified by sets of RODSUB and ARRAY cards. The material specified by the REG card fills that part of the annulus not occupied by the rods. The cluster geometry is currently limited to equally spaced rods whose centres lie on a circle. The cards have the form:

RODSUB j (dr₁, ... , dr_n), (name₁, ... , name_n)

where j is the number of the ring, numbered from the centre outward,

n is the number of radial subdivisions of a rod in this ring,

dr_i is the width in cm of the ith radial subdivision, and

name_i is the name of the material in the ith subdivision.

ARRAY j, nrod, prod, grad

where j is as defined above,

nrod is the number of rods in the ring,

prod is the radius of the circle on which the rod centres lie, and

grad is the angular displacement of one rod from a reference diameter of the cluster (in radians or degrees).

The angular displacement is not used in MIRANDA but is entered in the AUS geometry data pool.

Example:

```
DEFN FUELA U238 .048 U235 .0048
DEFN FUELB FUELA 1.
DEFN MOD D20 .033
REQD FUELA FUELB MOD U235 U238
RM 0 0.825 0.16 1.62 5.858 0
REG 1 FUELA 2 3 4 MOD
RODSUB 1 0.825 FUELB
ARRAY 1 6 1.875
```

This specifies a 7-rod cluster of unclad fuel pins. Different fuel names are used for the central rod and the rods of the ring, in order that two sets of cross sections will be prepared. Two different sets of U235 and U238 data are also prepared. If one fuel name had been used, average cross sections for the fuel, U235 and U238 would be produced.

* 9.12 RESREG Resonance Geometry Specification

The RESREG card specifies the geometry to be used in the multiregion resonance calculation and must always be included. A blank RESREG card indicates that the geometry is that given by the XM or RM and REG cards. However, there is little point in including a large number of mesh intervals in the resonance calculation. Not only can this become rather expensive in computer time, but the results obtained with a single mesh interval in each physical region should be equally reliable in most cases. The collision probability approximation of a constant source within a mesh interval is completely satisfied for the off-resonance source term of the resonance calculation. Additionally, the Bonalumi approximation used in cylindrical geometry becomes worse as the fuel pin is subdivided. A more accurate collision probability routine will be included, if calculations of resonance reaction rate distributions within a fuel pin are required.

A RESREG card is used to smear the geometry given by the XM or RM and REG card. No provision has been made for smearing the rod subdivisions of cluster geometry. The form of the card is:

RESREG $ibc, \quad x_1, \dots, x_m, \quad obc \quad \underline{\text{SMEAR}} \quad i_1, \dots, i_n$

where $ibc, x_1, \dots, x_m, obc$ specify an m region geometry to be used in the resonance calculation, with the variables having the same meaning as given on the XM or RM card,

i_1, \dots, i_n are the resonance region intervals into which each main geometry interval is to be smeared, and

n is the number of main geometry intervals.

That is the i_j are integers with values between 1 and m .

Example:

```
XM      -1      4*0.5 -1
REG     1      FUELA   3      FUELB   2  4      MOD
RESREG  0      2*0.5   0      SMEAR   1  2  1  2
```

This specifies a 4-region translational slab with 2 different fuel regions, which is treated in the resonance calculation as a 2-region reflected slab in which the fuelled regions are smeared together.

* 9.13 BUCK Group Buckling

BUCK $[B\&] \quad B_1^2, B_2^2, \dots, B_n^2$

with default

BUCK B0 1.E-20

where $B\&$ specifies the order of the $B\&$ flux solution and is optional, and B_i^2 is the buckling for energy group i .

If a short list of B_i^2 is given, the last value in the list is used in the remaining groups. Thus one value is sufficient for a constant group buckling. A transport corrected P_0 calculation is actually performed instead of B_0 .

Example:

```
BUCK   B1   .02
```

* 9.14 SEARCH Search for Critical Buckling

SEARCH OFF BSQ FOR k, δk WITH $\lambda_L, \lambda_1, \lambda_2, \lambda_U$
 ON

with default

SEARCH OFF BSQ FOR 1. .0002 WITH -100. 1. 1.1 100.

where ON,OFF turns the search on or off and the default is 'no search',

k is the value of k_{eff} required,

δk is the accuracy to which k is required,

λ_L is the lower limit on the eigenvalue,

λ_1 is the first estimate of the eigenvalue,

λ_2 does not apply to the present search option, and

λ_U is the upper limit on the eigenvalue.

The module searches for an eigenvalue λ such that λ times input buckling gives a k_{eff} of k. The buckling in any following calculation is λB_g^2 . If λ goes outside the limits, the search is abandoned as an error.

Example:

SEARCH ON BSQ FOR 1.02

9.15 GSCE Group Source

In any calculation which does not include a fissionable nuclide, a ^{235}U fission spectrum is used as the source for the group flux calculation. If this default is not satisfactory a group source may be specified by:

GSCE S_1, S_2, \dots, S_n

where S_i is the source in group i and a short vector is filled out with zero.

The resulting fluxes are normalised to a total source of 1 neutron $\text{cm}^{-3} \text{s}^{-1}$. In fact, the source may be overwritten in this manner in any calculation.

9.16 FSTEMP Nuclide Fission Spectra

The dependence of fission spectra on incident neutron energy is one quantity which is not included in the cross-section library. The library value of the fission spectrum of a nuclide is that appropriate for thermal calculations. Provision has, therefore, been made for fission spectra to be input.

The form is:

FSTEMP name, T_1 , name₂, T_2 , ...

where name_i is the name of a library nuclide whose fission spectrum is to be altered,

T_i is the temperature of the simple Maxwellian form of the fission spectrum in eV.

Example:

FSTEMP U235 1.323E+6

This would have no effect as this is the current library value.

* 9.17 OUTPUT Type of Output Required

OUTPUT XS RR AUS lib FLUX GEOM ZERO Pn

with default of

OUTPUT AUS 10 P₀ FLUX GEOM

A selection may be made of any of the given parameters. The selection process is additive however, so ZERO must be used to stop any output option previously selected. The options

have the meaning:

XS print cross sections,
 RR print reaction rates per unit source,
 AUS write an AUS cross-section data pool on FORTRAN unit lib,
 and add to the STATUS data pool as necessary,
 FLUX write an AUS FLUXB data pool for the main geometry mesh,
 GEOM write an AUS geometry data pool, and
 Pn scattering matrices on the cross section data pool produced up to
 order P_n .

All OUTPUT is for the materials on the REQD card in condensed groups.

Examples:

OUTPUT XS RR

This adds print options to the standard option of writing all data sets.

OUTPUT ZERO RR

This prints reaction rates and nothing else is produced.

* 9.18 GROUPS Condensed Group Structure

GROUPS n, g₁, ... ,g_{n+1}

where n is the number of condensed groups,
 g₁ is the first library group of condensed group 1, and
 g_i for i > 1, is the last library group of
 condensed group i-1.

Example:

GROUPS 13 1 10(10)120 128

9.19 TRANSPORT Transport Cross Section Option

Transport cross sections following a B_L calculation are normally adjusted to give the correct leakage in a diffusion theory calculation of a reactor, that is Equation (8.18) is used. If this is not appropriate, the keyword required is

TRANSPORT P1

* 9.20 ISOTLIB Specification of Output Nuclides

ISOTLIB liba name₁, ... ,name_n BURNUP Pn

with default

ISOTLIB lib ALLMAT P-1

where all quantities are optional,
 liba is the FORTRAN unit on which a nuclide cross-section data pool is written and it may be the same as the main output cross-section data pool,
 lib is the main output cross-section data pool,
 name_i is a defined material whose constituent nuclides are to be produced, or is the keyword ALLMAT which causes the constituent nuclides of all REQD defined materials to be produced,
 BURNUP causes the definitions of the set of materials to be modified to include a small amount of all nuclides produced in that material during burnup, and
 Pn is the order of scattering matrices, with the default being no matrices at all.

nangle is the order of Gaussian quadrature in the collision probability evaluation.

EFOFP E_p
with default

EFOFP 5.E+4

where E_p is the energy in eV above which the removal correction factor $f_{\lambda}(p_g)$ given in Section 5.8 is not applied.

PEARLS ipearl

with default

PEARLS 0

where ipearl takes the values:

- 0 a normal calculation,
- 1 a slowing down calculation in which the source term of the homogeneous flux calculation is an asymptotic slowing down source rather than a fission source, and
- 2 as for 1 but with a neutron mass of unity.

This control card is used for comparisons with the PEARLS code using a special purpose cross-section library which includes nuclide slowing-down distributions in place of fission spectra.

9.24 Flux Options

GFLUX ϕ_1, \dots, ϕ_{NG}

or

GFLUX WESTCOTT r

with default

GFLUX WESTCOTT .08

where ϕ_i is a group flux estimate for the i th library group,
 $r(>0)$ is the ratio of epithermal to thermal flux in a group flux estimate of Westcott form, and
 $r(<0)$ gives an estimated flux/ lethargy of an integrated fission spectrum times $E^{|r|}$.

This flux estimate is normally used only to weight the fission spectra for use in the homogeneous flux calculation, and hence is of no importance.

FLUXPARM limfl, limsea, nscale, ϵ_f

with default

FLUXPARM 40 10 3 1.E-4

where limfl is limit on the number of iterations to converge the group flux calculation,
 limsea is not used at present,
 nscale is the number of broad groups used in scaling the thermal flux to improve convergence, and
 ϵ_f is the required flux accuracy.

If limfl = 0, a flux calculation is not performed and cross sections may be averaged over an input flux spectrum given by GFLUX.

9.25 TEST Print Control of Intermediate Data

TEST n

with default

TEST 0
 where n = 0 for a normal printout of input data, cross-section library contents, material table, k_{eff} , flux and reaction rates in the library groups (see Appendix C),
 = 1 prints, additionally, the cross sections of resonance nuclides,
 = 2 prints, additionally to 1, information on the resonance calculation and the flux convergence which is used in debugging,
 = -1 prevents most normal printout, including the library contents if a TEST card is placed first.

9.26 WRITE GEOMLIB Write Geometry

WRITE GEOMLIB

The card causes a geometry data pool to be written immediately and may be used to create a geometry data pool which is different from the geometry of the MIRANDA calculation.

* 9.27 START Begin Calculation

START

The card causes the calculation which has been set up by the previous control cards to begin.

9.28 READ STATUS

The card causes the STATUS data pool to be read immediately. This will set up a succeeding calculation which is specified by the STATUS data pool.

* 9.29 STOP

STOP

The card causes termination of the module.

9.30 Example

A sample of a lattice calculation using the modules MIRANDA, ANAUSN [Clancy *et al.* 1977] and EDIT [Pollard 1977] is given in Appendix C. The calculation includes:

- (a) MIRANDA - 3-region resonance calculation, B_3 flux calculation and condensation to 26 groups;
- (b) ANAUSN - 26-group k_{inf} spatial calculation in S_6 with P_1 scattering;
- (c) EDIT - edit of ANAUSN fluxes, B_3 flux calculation to give final k_{eff} and two group reaction rates.

10. CONCLUSION

The MIRANDA module provides a fast and accurate method of preparing cross-section data for each region of a lattice cell. The subgroup treatment of resonance events allows a complex cell geometry to be accurately represented through collision probability methods. The resonance treatment has been compared with numerical solution of the few-region slowing down equations for isotropic scattering. These comparisons demonstrate that an accuracy of better than 1 per cent in resonance absorption is obtained over a very wide range of thermal reactor calculations, but the resonance scattering materials for fast reactors are not represented as accurately. Comparisons with both thermal and fast reactor experiments will be given in a later report.

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TABLE 1
HOMOGENEOUS CALCULATIONS WITH U238-SCHMIDT

Atom Ratio		Group Capture											
		$^{238}\text{U}/\text{H}=1/1$		$^{238}\text{U}/\text{H}=1/10$		$^{238}\text{U}/\text{C}=1/2$		$^{238}\text{U}/\text{C}=1/10$		$^{238}\text{U}/\text{C}=1/100$			
Group	Energy	PEARLS	MIRANDA	PEARLS	MIRANDA	PEARLS	MIRANDA	PEARLS	MIRANDA	PEARLS	MIRANDA	PEARLS	MIRANDA
1	19.3-15.0 kev	.00748	.00748	.000827	.008718	.08718	.08749	.02100	.02103	.00226	.00226	.00226	.00226
3	11.7-9.12 kev	.00911	.00912	.001066	.001067	.08714	.08682	.02532	.02530	.00292	.00292	.00292	.00292
5	7.10-5.53 kev	.00915	.00915	.001175	.001174	.06924	.06905	.02522	.02521	.00325	.00325	.00325	.00325
7	4.31-3.36 kev	.00674	.00676	.001018	.001018	.04026	.03990	.01884	.01889	.00290	.00290	.00290	.00290
9	2.61-2.04 kev	.00635	.00635	.001150	.001148	.03128	.03129	.01828	.01829	.00341	.00341	.00341	.00341
11	1.59-1.23 kev	.00643	.00643	.001326	.001328	.02709	.02697	.01870	.01861	.00407	.00407	.00407	.00407
13	961 -749 ev	.00942	.00943	.002245	.002252	.03309	.03313	.02711	.02708	.00725	.00725	.00725	.00725
15	583 -454 ev	.00864	.00865	.002240	.002254	.02474	.02470	.02436	.02426	.00727	.00727	.00727	.00727
17	354 -275 ev	.00677	.00674	.002197	.002193	.01589	.01599	.01908	.01905	.00778	.00778	.00778	.00778
19	215 -167 ev	.00797	.00797	.00376	.00377	.02254	.02228	.02994	.02957	.01444	.01444	.01444	.01444
20	167 -130 ev	.00797	.00797	.00195	.00194	.01459	.01445	.01939	.01938	.00562	.00562	.00562	.00562
21	130 -101 ev	.02047	.02049	.00813	.00813	.02992	.02955	.05349	.05244	.03187	.03187	.03187	.03187
22	101 -78.9 ev	.01348	.01335	.00374	.00374	.01801	.01714	.02949	.02878	.01134	.01134	.01134	.01134
23	78.9-61.4 ev	.01951	.01946	.00775	.00774	.02020	.02045	.04485	.04422	.02975	.02975	.02975	.02975
24	61.4-47.9 ev	.00126	.00125	.000154	.000154	.00157	.00170	.00181	.00187	.00036	.00036	.00036	.00036
25	47.9-37.3 ev	.01667	.01668	.00338	.00337	.01512	.01668	.02969	.03084	.00869	.00869	.00869	.00869
26	37.3-29.0 ev	.03669	.03669	.01774	.01769	.02216	.02056	.07970	.07446	.06585	.06585	.06585	.06585
27	29.0-22.6 ev	.00615	.00615	.00082	.00082	.00370	.00490	.00710	.00809	.00179	.00179	.00179	.00179
28	22.6-17.6 ev	.05391	.05398	.02676	.02661	.01746	.01761	.09138	.09088	.09277	.09277	.09277	.09277
29	17.6-13.7 ev	.00335	.00335	.00046	.00046	.00098	.00134	.00281	.00329	.00095	.00095	.00095	.00095
30	13.7-10.7 ev	.00269	.00270	.00037	.00037	.000736	.000771	.00223	.00230	.00073	.00073	.00073	.00073
31	10.7-9.19 ev	.00389	.00389	.00056	.00056	.000981	.001014	.00330	.00338	.00111	.00111	.00111	.00111
32	9.19-8.32 ev	.00305	.00307	.00044	.00044	.000737	.000777	.00254	.00262	.00085	.00085	.00085	.00085
33	8.32-7.52 ev	.00789	.00787	.00123	.00124	.00165	.00224	.00685	.00899	.00243	.00243	.00243	.00243
34	7.52-6.81 ev	.03292	.03289	.01243	.01251	.00415	.00411	.03930	.04287	.02909	.02909	.02909	.02909
35	6.81-6.16 ev	.04647	.04627	.04107	.04079	.00350	.00311	.06074	.05722	.13746	.13746	.13746	.13746
36	6.16-5.57 ev	.01442	.01435	.00299	.00297	.000983	.00115	.00896	.01095	.00511	.00511	.00511	.00511
37	5.57-5.04 ev	.00618	.00616	.00106	.00106	.000267	.000392	.00264	.00348	.00164	.00164	.00164	.00164
	19.3 keV-1 ev	.48057	.48018	.16726	.16683	.99914	.99906	.9333	.9325	.5360	.5360	.5360	.5360

TABLE 2

HOMOGENEOUS CALCULATIONS WITH U238-ENDFB4

Atom Ratio		Group Capture				Group Escape Probability	
		$^{238}\text{U}/\text{H}=1/1$		$^{238}\text{U}/\text{C}=1/10$		$^{238}\text{U}/\text{C}=1/10$	
Group	Energy	PEARLS	MIRANDA	PEARLS	MIRANDA	PEARLS	MIRANDA
1	19.3-15.0 keV	.00631	.00631	.01765	.01767		
3	11.7-9.12 keV	.00729	.00729	.02025	.02023		
5	7.10-5.53 keV	.00815	.00814	.02254	.02253		
7	4.31-3.36 keV	.00842	.00842	.02334	.02338		
9	2.61-2.04 keV	.00909	.00910	.02535	.02531		
11	1.59-1.23 keV	.00872	.00872	.02390	.02382		
13	961 -749 eV	.01041	.01042	.02959	.02954		
15	583 -454 eV	.00937	.00939	.02580	.02578	.96137	.96134
17	354 -275 eV	.00885	.00884	.02274	.02272	.96322	.96326
19	215 -167 eV	.01584	.01586	.03659	.03643	.93576	.93609
20	167 -130 eV	.00824	.00823	.01998	.01999	.96252	.96252
21	130 -101 eV	.02607	.02613	.06158	.06040	.88041	.88239
22	101 -78.9 eV	.01481	.01471	.02961	.02923	.93396	.93550
23	78.9-61.4 eV	.02254	.02248	.04672	.04610	.88513	.88797
24	61.4-47.9 eV	.00128	.00127	.00173	.00185	.72117	.73814
25	47.9-37.3 eV	.01485	.01485	.02431	.02462		
26	37.3-29.0 eV	.04080	.04068	.07981	.07382		
27	29.0-22.6 eV	.00568	.00567	.00606	.00734		
28	22.6-17.6 eV	.05608	.05625	.08648	.08591	.64670	.65251
29	17.6-13.7 eV	.00341	.00339	.00259	.00317		
30	12.7-10.7 eV	.00225	.00224	.00168	.00174	.99035	.99041
31	10.7-9.19 eV	.00372	.00371	.00284	.00294	.98352	.98362
32	9.19-8.32 eV	.00276	.00276	.00207	.00215	.98787	.98783
33	8.32-7.52 eV	.00705	.00705	.00546	.00702		
34	7.52-6.81 eV	.03008	.03009	.03145	.03438		
35	6.81-6.16 eV	.04585	.04572	.05412	.05167	.39782	.39397
36	6.16-5.57 eV	.01349	.01346	.00759	.00953		
37	5.57-5.04 eV	.00570	.00568	.00223	.00300		
	19.3 keV - 1 eV	.50112	.50083	.94140	.93966		

TABLE 3

TWO-REGION CALCULATIONS OF ^{238}U METAL RODS WITH U238-SCHMIDT

Diameter (cm)		D_2O Moderator		^{12}C Moderator	
Rod	Moderator	PEARLS result for capture probability 19.3 keV to 1 eV	MIRANDA % error	PEARLS result for capture probability 19.3 keV to 1 eV	MIRANDA % error
1.0	2.0	0.6229	+0.2	0.9556	+0.4
1.0	4.0	0.2168	+0.1	0.5256	+0.8
1.0	8.0	0.05882	0.0	0.16667	+0.3
1.0	16.0	0.01493	0.0	0.04408	+0.1
1.0	32.0	0.003742	0.0	0.01117	0.0
1.0	64.0	0.000936	0.0	0.002802	0.0
2.0	4.0	0.5710	+0.4	0.9287	+0.7
2.0	8.0	0.1729	+0.2	0.4366	+0.9
2.0	16.0	0.04467	+0.1	0.12814	+0.3
2.0	32.0	0.01123	+0.1	0.03329	+0.1
2.0	64.0	0.002813	0.0	0.008402	+0.0
4.0	8.0	0.5027	+0.9	0.8818	+1.2
4.0	16.0	0.1356	+0.6	0.3546	+1.2
4.0	32.0	0.03416	+0.5	0.09896	+0.6
4.0	64.0	0.008554	+0.4	0.02541	+0.5
8.0	16.0	0.4236	+1.4	0.8103	+1.5
8.0	32.0	0.1054	+1.1	0.2840	+1.5
8.0	64.0	0.02620	+0.9	0.07647	+1.0

TABLE 4
TWO-REGION CALCULATIONS OF ^{238}U METAL RODS WITH U238-ENDFB4

Energy Range	2 cm diameter rod 16 cm diameter ^{12}C		8 cm diameter rod 64 cm diameter ^{12}C	
	PEARLS captures	MIRANDA % error	PEARLS captures	MIRANDA % error
19.3 - 5.53 keV	.008910	+0.8	.007268	+1.4
5.53 - 0.454 keV	.022689	+1.2	.016382	+1.7
454 - 10.7 eV	.061162	-0.1	.034377	+0.5
10.7 - 1 eV	.042634	+0.4	.023329	+0.7
19.3 keV - 1 eV	.13539	+0.3	.081356	+0.9

TABLE 5
TWO-REGION CALCULATIONS OF ^{238}U OXIDE RODS IN H_2O
1 cm DIAMETER RODS WITH U238-SCHMIDT

Energy Range	Volume ratio Mod/Fuel = 1/1		Volume ratio Mod/Fuel = 3/1		Volume ratio Mod/Fuel = 5/1	
	PEARLS captures	MIRANDA % error	PEARLS captures	MIRANDA % error	PEARLS captures	MIRANDA % error
19.3 - 5.53 keV	.01546	+0.2	.00537	+0.2	.002324	+0.2
5.53 - 0.454 keV	.03336	+0.1	.01258	+0.3	.00556	+0.3
454 - 10.7 eV	.11343	-0.3	.04713	-0.4	.02140	-0.4
10.7 - 1 eV	.08435	-1.4	.03789	-0.8	.01767	-0.6
19.3 keV - 1 eV	.24660	-0.6	.10296	-0.4	.04694	-0.3

TABLE 6
TWO-REGION CALCULATIONS OF ^{238}U OXIDE RODS IN H_2O
MODERATOR/FUEL VOLUME RATIO = 1/1 WITH U238-ENDFB4

Energy Range	1 cm Diameter Rod		2 cm Diameter Rod		1 cm Diameter Rod 300 K to 900 K	
	PEARLS captures ^{238}U	MIRANDA % error	PEARLS captures	MIRANDA % error	PEARLS Δ captures 300 to 900 K	MIRANDA % error
19.3 - 5.53 keV	.01262	+0.1	.01228	+0.3	.00048	-2.0
5.53 - 0.454 keV	.03875	+0.1	.03537	+0.5	.00615	+1.0
454 - 10.7 eV	.12478	-0.3	.10746	-0.1	.01099	-0.2
10.7 - 1 eV	.08106	-1.4	.07005	-2.1	.00038	-16.0
19.3 keV - 1 eV	.25721	-0.6	.22516	-0.6	.01800	-0.2

TABLE 7
TWO-REGION CALCULATIONS OF RESONANCE OVERLAP

Energy Range	5% Enrichment Uranium Oxide 1 cm Diameter Rod in H_2O Mod/Fuel volume = 1/1				Natural Uranium Metal 2 cm Diameter Rod in D_2O 8 cm Diameter Moderator			
	PEARLS captures ^{238}U	MIRANDA % error ^{238}U	PEARLS absorption ^{238}U	MIRANDA % error ^{238}U	PEARLS captures ^{238}U	MIRANDA % error ^{238}U	PEARLS absorption ^{235}U	MIRANDA % error ^{235}U
19.3 - 5.53 keV	.01197	+0.1	.00414	+0.1	.01247	+0.8	.000645	+0.8
5.53 - 0.454 keV	.03657	+0.1	.02032	+0.2	.03138	+1.2	.003227	+1.0
454 - 10.7 eV	.10887	-1.1	.10223	+1.0	.08082	-0.4	.018852	-0.5
10.7 - 1 eV	.06366	+0.5	.04710	-1.8	.05395	+0.3	.009529	-0.6
19.3 keV - 1 eV	.22106	-0.4	.17379	+0.1	.17862	+0.2	.032252	-0.3

TABLE 8

CALCULATION OF 3 keV Na RESONANCE

$${}^{238}\text{U}|{}^{16}\text{O}|{}^{23}\text{Na} = .006|.015|.01$$

Group	Energy Range keV	Group Flux		${}^{238}\text{U}$ Capture Cross Section ⁺		${}^{23}\text{Na}$ Capture Cross Section ⁺	
		PEARLS	MIRANDA	PEARLS	MIRANDA	PEARLS	MIRANDA
1	7.10 - 5.53	16.82	16.74	0.7105	0.7088	.00107	.00109
2	5.53 - 4.31	12.59	12.22	0.7620	0.7555	.00343	.00354
3	4.31 - 3.35	6.415	6.063	0.8597	0.8490	.01692	.01799
4	3.35 - 2.61	1.297	1.198	1.1885	1.1023	.1870	.1954
5	2.61 - 2.03	5.476	5.765	0.9928	1.0139	.05825	.05888
6	2.03 - 1.58	12.504	13.231	0.8374	0.8464	.02033	.01969
+	7.10 - 1.58			0.26706	0.26767	.00986	.01004

Group	${}^{23}\text{Na}$ Removal Cross Section		Change in ${}^{238}\text{U}$ Capture Cross Section. ⁺ 300 to 900 K	
	PEARLS	MIRANDA	PEARLS	MIRANDA
1	2.679	2.650	.05428	.05457
2	4.241	4.274	.07313	.07355
3	10.689	10.947	.07619	.07543
4	61.044	66.332	.04114	.03050
5	10.535	10.811	.10933	.11460
6			.14460	.14280
+			.02365	.02387

+ Last row is reaction rate for the full energy range.

TABLE 9

CALCULATION OF 28 keV Fe RESONANCE

$$\text{Fe} | {}^{23}\text{Na} | {}^{16}\text{O} = .018 | .01 | .015$$

Nuclide		Fe	²³ Na	¹⁶ O	Mixture
Removal Cross Section	PEARLS	0.523	2.21	2.41	.0677
	MIRANDA	0.593	1.33	1.80	.0510
	% error	+13	-40	-25	-25
Scattering Cross Section	PEARLS	13.52			
	MIRANDA	9.25			
	% error	-32			

TABLE 10

CALCULATION OF 28 keV Fe RESONANCE

$$\text{Fe} | {}^{23}\text{Na} | {}^{16}\text{O} = .009 | .01 | .015$$

Nuclide		Fe	²³ Na	¹⁶ O	Mixture
Removal Cross Section	PEARLS	0.460	1.96	2.23	.0572
	MIRANDA	0.554	1.33	1.80	.0453
	% error	+20	-32	-20	-21
Scattering Cross Section	PEARLS	16.99			
	MIRANDA	12.04			
	% error	-29			

APPENDIX A
AUS.ENDFB 128-GROUP LIBRARY

TABLE A1
NUCLIDES AS AT 19/5/76

Nuclide Name	Data Source	Recommended	P _n Order	Temperature	No. of Subgroups	No. of Scat. Tabulations (σ_p)	Note
TH232	ENDFB4		3	300	9	5	
PA233	PHF68		0	300,900	8	-	
U232	NDXD40		0	300	-	-	
U233	BNL65PHF	NO	0	300,900	7	-	
U233	ENDFB4	YES	3	300	-	-	
U234	ENDFB4		3	300	9	4	
U235	ENDFB3	NO	3	300,900	7	-	
U235	ENDFB4	YES	3	300,900	7	4	
U236	ENDFB4		3	300	9	4	
NP237	ENDFB4		3	300	-	-	
U238	ENDFB4	YES	3	300,900	9	8	
U238	ENDFSMDT	NO	3	300,900	8	9	
PU239	ENDFB4		3	300,900	7	4	
PU240	ENDFB4		3	300,900	10	4	
PU241	ENDFB4		3	300,900	8	4	
PU242	ENDFB4		3	300,900	9	4	
CH2	ENDFB3		3	296	-	-	(d)
H20	ENDFB3		3	296,600	-	-	(e)
D20	ENDFB3		3	296,400	-	-	(f)
C	ENDFB4	YES	3	296	-	-	(g)
C	ENDFB3	NO	3	296	-	-	(g)
O	ENDFB3		3	296,600,900,1200	-	-	
BEO	NDXD40		0	300	-	-	
NA	ENDFB3		3	300	7	9	
AL	AEEW69	NO	0	300	-	-	
AL	ENDFB4	YES	3	300	-	-	
CR	ENDFB4		3	300	7	7	
FE	ENDFB4		3	300	7	8	
NI	ENDFB4		3	300	7	7	
ZIRC2	ENDFB4		3	300	-	-	(h)
LI6	AEEW69		-	-	-	-	
HE3	AEEW69		-	-	-	-	
T3	NDXD40		-	-	-	-	
ZZ999	NDXD127G		-	-	-	-	(i)
XX999	NDXD127G		-	-	-	-	(j)
B10	ENDFB4		3	300	-	-	
N	AEEW69		-	-	-	-	
F	AEEW69		-	-	-	-	
CL	AEEW69		-	-	-	-	

APPENDIX A1 (Continued)

Nuclide Name	Data Source	Recommended	P _n Order	Temperature	No. of Subgroups	No. of Scat. Tabulations ($\hat{\sigma}_p$)	Note
CA	AEEW69		-	-	-	-	
TI	AEEW69		-	-	-	-	
MN	ENDFB4		3	300	-	-	
FE56	ENDFB4		-	-	-	-	(k)
CO	NDXD40		-	-	-	-	
CU	ENDFB4		3	300	-	-	
GA	AEEW69		-	-	-	-	
CU63	ENDFB4		-	-	-	-	(l)
RH	ENDFB4		3	300	-	-	
AG107	BNL66		-	-	-	-	
CD	AEEW69		-	-	-	-	
IN115	ENDFB4		-	-	-	-	(m)
DY164	ENDFB4		3	300	-	-	
ER166	BNL73		-	-	-	-	
ER167	BNL73		-	-	-	-	
LUL176	ENDFB4		3	300	-	-	
TA	AEEW69		-	-	-	-	
W	AEEW69		-	-	-	-	
W186	BNL66PHF		-	-	-	-	
AU	ENDFB4		3	300	-	-	
SI	AEEW69		0	300	-	-	

NOTES

- (a) In addition to the above nuclides, the library includes 41 individual fission products and one pseudo fission product from the AAEC fission product library (Bertram et al. 1971). The individual fission products represented may be obtained from the MIRANDA sample output in Appendix C.
- (b) Nuclides whose data source is not ENDFB3 or ENDFB4 have been obtained from the 127-group CYMEA library. AEEW69 indicates the UKAEA nuclear data file (Norton 1968), and BNL66, BNL73 the editions of ENL325.
- (c) Nuclides with a dash for P_n order have no scattering matrix.
- (d) Polythene thermal scattering from ENDF material 1011.
- (e) H₂O thermal scattering from ENDF material 1002.
- (f) D₂O thermal scattering from ENDF material 1004.
- (g) Graphite thermal scattering from ENDF material 1065.
- (h) ZIRC2 is Zircaloy 2 (or 4).
- (i) ZZ999 is a 1/v absorber with cross section of 1 barn at 0.0253 eV.
- (j) XX999 has a resonance integral of 1 barn.
- (k) ⁵⁶Fe (n,p) cross section only, as AUS reaction 7.
- (l) ⁶³Cu (n,γ) cross section, as AUS reaction 7.
- (m) ¹¹⁵In (n,γ) cross section to 54 min and 2.2 s states of ¹¹⁶In only, as AUS reaction 7.

TABLE A2
GROUP BOUNDARIES

Group	Energy	Lethargy	Group	Energy	Lethargy
1	12.84 - 10.00 MeV	-0.25 - 0.0	43	354 - 275 eV	10.25 - 10.50
2	10.00 - 7.79 MeV	0.0 - 0.25	44	275 - 214 eV	10.50 - 10.75
3	7.79 - 6.07 MeV	0.25 - 0.50	45	214 - 167 eV	10.75 - 11.00
4	6.07 - 4.72 MeV	0.50 - 0.75	46	167 - 130 eV	11.00 - 11.25
5	4.72 - 3.68 MeV	0.75 - 1.00	47	130 - 101 eV	11.25 - 11.50
6	3.68 - 2.87 MeV	1.00 - 1.25	48	101 - 78.9 eV	11.50 - 11.75
7	2.87 - 2.23 MeV	1.25 - 1.50	49	78.9 - 61.4 eV	11.75 - 12.00
8	2.23 - 1.74 MeV	1.50 - 1.75	50	61.4 - 47.9 eV	12.00 - 12.25
9	1.74 - 1.35 MeV	1.75 - 2.00	51	47.9 - 37.3 eV	12.25 - 12.50
10	1.35 - 1.05 MeV	2.00 - 2.25	52	37.3 - 29.0 eV	12.50 - 12.75
11	1050. - 821 keV	2.25 - 2.50	53	29.0 - 22.6 eV	12.75 - 13.00
12	821 - 639 keV	2.50 - 2.75	54	22.6 - 17.6 eV	13.00 - 13.25
13	639 - 498 keV	2.75 - 3.00	55	17.6 - 13.7 eV	13.25 - 13.50
14	498 - 388 keV	3.00 - 3.25	56	13.7 - 10.7 eV	13.50 - 13.75
15	388 - 302 keV	3.25 - 3.50	57	10.7 - 9.19 eV	13.75 - 13.9
16	302 - 235 keV	3.50 - 3.75	58	9.19 - 8.31 eV	13.90 - 14.0
17	235 - 183 keV	3.75 - 4.00	59	8.31 - 7.52 eV	14.00 - 14.1
18	183 - 143 keV	4.00 - 4.25	60	7.52 - 6.80 eV	14.10 - 14.2
19	143 - 111 keV	4.25 - 4.50	61	6.80 - 6.16 eV	14.20 - 14.3
20	111 - 86.5 keV	4.50 - 4.75	62	6.16 - 5.57 eV	14.3 - 14.4
21	86.5 - 67.4 keV	4.75 - 5.00	63	5.57 - 5.04 eV	14.4 - 14.5
22	67.4 - 52.5 keV	5.00 - 5.25	64	5.04 - 4.56 eV	14.5 - 14.6
23	52.5 - 40.9 keV	5.25 - 5.50	65	4.56 - 4.13 eV	14.6 - 14.7
24	40.9 - 31.8 keV	5.50 - 5.75	66	4.13 - 3.74 eV	14.7 - 14.8
25	31.8 - 24.8 keV	5.75 - 6.00	67	3.74 - 3.38 eV	14.8 - 14.9
26	24.8 - 19.3 keV	6.00 - 6.25	68	3.38 - 3.06 eV	14.9 - 15.0
27	19.3 - 15.0 keV	6.25 - 6.50	69	3.06 - 2.77 eV	15.0 - 15.1
28	15.0 - 11.7 keV	6.50 - 6.75	70	2.77 - 2.50 eV	15.1 - 15.2
29	11.7 - 9.12 keV	6.75 - 7.00	71	2.50 - 2.27 eV	15.2 - 15.3
30	9.12 - 7.10 keV	7.00 - 7.25	72	2.27 - 2.05 eV	15.3 - 15.4
31	7.10 - 5.53 keV	7.25 - 7.50	73	2.05 - 1.86 eV	15.4 - 15.5
32	5.53 - 4.31 keV	7.50 - 7.75	74	1.86 - 1.68 eV	15.5 - 15.6
33	4.31 - 3.35 keV	7.75 - 8.00	75	1.68 - 1.52 eV	15.6 - 15.7
34	3.35 - 2.61 keV	8.00 - 8.25	76	1.52 - 1.37 eV	15.7 - 15.8
35	2.61 - 2.03 keV	8.25 - 8.50	77	1.37 - 1.24 eV	15.8 - 15.9
36	2.03 - 1.58 keV	8.50 - 8.75	78	1.24 - 1.13 eV	15.9 - 16.0
37	1.58 - 1.23 keV	8.75 - 9.00	79	1.13 - 1.02 eV	16.0 - 16.1
38	1230 - 961 eV	9.00 - 9.25	80	1.02 - .921 eV	16.1 - 16.2
39	961 - 749 eV	9.25 - 9.50	81	.921 - .834 eV	16.2 - 16.3
40	749 - 583 eV	9.50 - 9.75	82	.834 - .754 eV	16.3 - 16.4
41	583 - 454 eV	9.75 - 10.00	83	.754 - .682 eV	16.4 - 16.5
42	454 - 354 eV	10.00 - 10.25	84	.682 - .618 eV	16.5 - 16.6

TABLE A2 (Continued)

Group	Energy (eV)	Lethargy	Group	Energy (eV)	Lethargy
85	.618 - .559	16.6 - 16.7	107	.0684 - .0619	18.8 - 18.9
86	.559 - .506	16.7 - 16.8	108	.0619 - .0560	18.9 - 19.0
87	.506 - .457	16.8 - 16.9	109	.0560 - .0507	19.0 - 19.1
88	.457 - .414	16.9 - 17.0	110	.0507 - .0459	19.1 - 19.2
89	.414 - .375	17.0 - 17.1	111	.0459 - .0415	19.2 - 19.3
90	.375 - .339	17.1 - 17.2	112	.0415 - .0376	19.3 - 19.4
91	.339 - .307	17.2 - 17.3	113	.0376 - .0340	19.4 - 19.5
92	.307 - .278	17.3 - 17.4	114	.0340 - .0307	19.5 - 19.6
93	.278 - .251	17.4 - 17.5	115	.0307 - .0278	19.6 - 19.7
94	.251 - .227	17.5 - 17.6	116	.0278 - .0252	19.7 - 19.8
95	.227 - .206	17.6 - 17.7	117	.0252 - .0228	19.8 - 19.9
96	.206 - .186	17.7 - 17.8	118	.0228 - .0206	19.9 - 20.0
97	.186 - .168	17.8 - 17.9	119	.0206 - .0187	20.0 - 20.1
98	.168 - .152	17.9 - 18.0	120	.0187 - .0169	20.1 - 20.2
99	.152 - .138	18.0 - 18.1	121	.0169 - .0153	20.2 - 20.3
100	.138 - .125	18.1 - 18.2	122	.0153 - .0138	20.3 - 20.4
101	.125 - .113	18.2 - 18.3	123	.0138 - .0125	20.4 - 20.5
102	.113 - .102	18.3 - 18.4	124	.0125 - .0076	20.5 - 21.0
103	.102 - .0924	18.4 - 18.5	125	.0076 - .0046	21.0 - 21.5
104	.0924 - .0836	18.5 - 18.6	126	.0046 - .0028	21.5 - 22.0
105	.0836 - .0756	18.6 - 18.7	127	.0028 - .0017	22.0 - 22.5
106	.0756 - .0684	18.7 - 18.8	128	.0017 - .0010	22.5 - 23.0

APPENDIX B
METHODS OF PREPARATION OF THE AUS.ENDFB LIBRARY

B1 GENERAL

Most of the data taken from ENDF/B have been prepared using the SUPERTOG code [Wright et al. 1969]. SUPERTOG has been run with a weighting spectrum consisting of an integrated fission spectrum joined to a 1/E region joined to a thermal Maxwellian, to prepare group average data with scattering matrices up to order P₃. These SUPERTOG data have been used for all non-resonance data except thermal scattering. For moderator nuclides, thermal scattering data (P₀ and P₁ matrices) have been generated by PIXSE [MacDougall 1963] from ENDF tabulations of S(α,β). The thermal and epithermal data have been smoothly joined using spline fits. For other nuclides, thermal scattering data (P₀ matrix only) have been generated using the gas kernel as in MULGA [Clancy et al. 1963]. The methods used in preparing resonance data are detailed in the following subsections.

B2 CALCULATION OF POINT CROSS SECTIONS FROM RESOLVED RESONANCE PARAMETERS

The standard ENDF/B resonance prescription [Drake 1970] has been followed, but with the inclusion of Doppler broadening. The formulae for a single isotope are given below:

Single-level Breit-Wigner

$$\sigma_Y(E) = \frac{4\pi}{k^2} \sum_{\ell} \sum_J g_J \sum_r \frac{\Gamma_{nr} \Gamma_{Yr}}{\Gamma_r^2} \Psi(\theta_r, x_r)$$

$$\sigma_f(E) = \frac{4\pi}{k^2} \sum_{\ell} \sum_J g_J \sum_r \frac{\Gamma_{nr} \Gamma_{fr}}{\Gamma_r^2} \Psi(\theta_r, x_r)$$

$$\sigma_s(E) = \frac{4\pi}{k^2} \sum_{\ell} \left\{ (2\ell + 1) \sin^2 \phi_{\ell} + \sum_J g_J \sum_r \frac{\Gamma_{nr}}{\Gamma_r} \left[\left(\frac{\Gamma_{nr}}{\Gamma_r} - 2 \sin^2 \phi_{\ell} \right) \Psi(\theta_r, x_r) + (\sin 2\phi_{\ell}) \phi(\theta_r, x_r) \right] \right\}$$

where $\sigma_Y(E)$, $\sigma_f(E)$, $\sigma_s(E)$, are the capture, fission and scattering cross sections at energy E,

the summation on angular momentum state ℓ includes s and p waves only,

the summation on J is over all spin states for a given ℓ ,

the summation on r is over all resonances with a given ℓ and J,

$$g_J = \frac{1}{2}(2J + 1)/(2I + 1),$$

J is the spin of the compound nucleus,

I is the spin of the target nucleus,

$$\Gamma_{nr} \equiv \Gamma_{nr}(E) = P_{\ell}(E) \Gamma_{nr}(|E_r|) / P_{\ell}(|E_r|),$$

E_r is the resonance energy,

$\Gamma_{nr}(|E_r|)$ is the neutron width for the rth resonance evaluated at the resonance energy,

$$\Gamma_r = \Gamma_{nr}(E) + \Gamma_{Yr} + \Gamma_{fr},$$

Γ_{Yr} is the radiation width,

Γ_{fr} is the fission width,

ϕ_{ℓ} is the phase shift, given by

$$\Phi_0 = \hat{\rho},$$

$$\Phi_1 = \hat{\rho} - \tan^{-1}\hat{\rho},$$

$$\hat{\rho} = k\hat{a},$$

\hat{a} is the effective scattering radius,

k is the neutron wave number, given by

$$k = 2.19685 \times 10^{-3} E A' / (A' + 1),$$

A' is the ratio of the isotope mass to that of the neutron,

$P_\ell(E)$ is the penetration factor, given by

$$P_0 = \rho$$

$$P_1 = \rho^3 / (1 + \rho^2),$$

$$\rho = ka,$$

a is the channel radius, given by

$$a = (1.23(A')^{1/3} + 0.8) \times 10^{-1},$$

the resonance energy is displaced using

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

S_ℓ is the shift factor, given by

$$S_0 = 0$$

$$S_1 = -1/(1 + \rho^2),$$

$$x_r = 2(E - E_r') / \Gamma_r',$$

$$\theta_r = \Gamma_r' \left(\frac{A'}{4 \times 8.6164 \times 10^{-5} T E_r'} \right)^{1/2},$$

T is the temperature (K), and

Ψ and ϕ are the Doppler broadened line-shape functions which are calculated using the QUICKW function [Toppel *et al.* 1967].

Because it is rather time-consuming to sum over all resonances for each energy value, a cut-off value Δ is introduced, such that for $|x_r| > \Delta$ the only contribution from the r th resonance to the cross section at energy E is the interference scattering (s wave only) represented by

$$\frac{2\pi}{k^2} g_J \sin 2\phi_\ell \frac{\Gamma_{nr}(E)}{(E - E_r')}$$

Multilevel Breit-Wigner

For $T = 0$, this requires the addition to $\sigma_s(E)$ of the level-level interference term

$$\frac{4\pi}{k^2} \sum_\ell \sum_J g_J \sum_{r \neq l}^{r-1} \sum_{s=1}^{2\Gamma_{nr} \Gamma_{ns}} \frac{\Gamma_r \Gamma_s}{\Gamma_r \Gamma_s} \frac{1 + x_r x_s}{(1 + x_r^2)(1 + x_s^2)}$$

This term has been approximately Doppler broadened by the use of

$$\frac{4\pi}{k^2} \sum_\ell \sum_J g_J \sum_{r \neq l}^{r-1} \sum_{s=1}^{2\Gamma_{nr} \Gamma_{ns}} \frac{\Gamma_r \Gamma_s}{\Gamma_r \Gamma_s} \{ \Psi(\theta_r, x_r) \Psi(\theta_s, x_s) + \phi(\theta_r, x_r) \phi(\theta_s, x_s) \}$$

This may be expressed as

$$\frac{4\pi}{k^2} \sum_{\ell} \sum_J g_J \left\{ \left(\sum_r \frac{\Gamma_{nr}}{\Gamma_r} \psi(\theta_r, x_r) \right)^2 + \left(\sum_r \frac{\Gamma_{nr}}{\Gamma_r} \phi(\theta_r, x_r) \right)^2 \right. \\ \left. - \sum_r \frac{\Gamma_{nr}^2}{\Gamma_r^2} (\psi(\theta_r, x_r)^2 + \phi(\theta_r, x_r)^2) \right\} ,$$

which avoids the double summation over resonances.

B3 CALCULATION OF GROUP RESONANCE INTEGRALS FROM UNRESOLVED RESONANCE PARAMETERS

The average resonance cross sections about an energy E, as a function of temperature and potential scattering, are calculated by an integration over neutron width and fission width, assuming narrow resonance theory to apply and using the J function to integrate over a resonance. The method follows closely that used in MC² [Topell et al. 1967] and SUPERTOG. The average resonance cross sections are given by the formulae :

$$\langle \sigma_Y(E) \rangle = \sum_{\ell} \sum_J \frac{\sigma_p \Gamma_{\gamma s}}{F \langle D_s \rangle} \int_0^{\infty} P_n(r) \int_0^{\infty} P_k(t) J(\theta, \beta) dt dr ,$$

$$\langle \sigma_f(E) \rangle = \sum_{\ell} \sum_J \frac{\sigma_p}{F \langle D_s \rangle} \int_0^{\infty} P_n(r) \int_0^{\infty} P_k(t) t \langle \Gamma_{fs} \rangle J(\theta, \beta) dt dr ,$$

$$\langle \sigma_s(E) \rangle = \sum_{\ell} \sum_J \frac{\sigma_p}{F \langle D_s \rangle} \int_0^{\infty} P_n(r) \int_0^{\infty} P_k(t) (r \langle \Gamma_{ns} \rangle - 2\Gamma_s \sin^2 \phi_{\ell}) J(\theta, \beta) dt dr ,$$

$$F = 1 - \frac{1}{\langle D_s \rangle} \int_0^{\infty} P_n(r) \int_0^{\infty} P_k(t) \Gamma_s (1 - 2 \sin^2 \phi_{\ell}) J(\theta, \beta) dt dr$$

where $\langle \sigma_s(E) \rangle$ is the average resonance scattering cross section,

$$\sigma_p = \sigma_H + \sum_{\ell} \frac{4\pi}{k^2} (2\ell + 1) \sin^2 \phi_{\ell} ,$$

σ_H is the potential scattering excluding the isotope itself,

s represents a particular ℓ, J state,

$\langle D_s \rangle$ is the average level spacing,

$P_n(r)$ is the chi-squared distribution for neutron widths,

$P_k(t)$ is the chi-squared distribution for fission widths,

r is the ratio of neutron width to mean width,

t is the ratio of fission width to mean width,

$\Gamma_{\gamma s}$ is the radiation width,

$\langle \Gamma_{fs} \rangle$ is the mean fission width,

$$\langle \Gamma_{ns} \rangle = \langle \Gamma_{ns}^0 \rangle \sqrt{E} V_{\ell}(E) \mu_{\ell, J} ,$$

$\langle \Gamma_{ns}^0 \rangle$ is the mean reduced neutron width,

$$V_0(E) = 1,$$

$$V_1(E) = \rho^2 / (1 + \rho^2) \quad ,$$

$\mu_{\ell, J}$ = number of degrees of freedom of the neutron width distribution,

$$\Gamma_s = r \langle \Gamma_{ns} \rangle + t \langle \Gamma_{fs} \rangle + \Gamma_{\gamma s} \quad ,$$

$$\theta = \Gamma_s \left(\frac{A^1}{4 \times 8.6164 \times 10^{-5} T E} \right)^{1/2}$$

$$\beta = \sigma_p / \sigma_o \quad ,$$

$$\sigma_o = \frac{4\pi}{k^2} g_J (1 - 2 \sin^2 \phi_{\ell}) \frac{r \langle \Gamma_{ns} \rangle}{\Gamma_s} \quad , \text{ and}$$

$J(\theta, \beta)$ is the J-function, which is evaluated by a double, 4-point Gaussian integration [Nicholson & Grasseschi 1970].

It can be seen that the formulae imply that there is no overlap between resonances of the same ℓ, J state and that the cross sections for each ℓ, J state are additive. These simple assumptions tend to overestimate the cross sections (because of the first assumption) at low values of potential scattering. The more detailed alternative approach (generating an appropriate sequence of resonances from which point cross sections are calculated) is required in order to overcome this deficiency. Unfortunately, the more detailed method has been applied only to ^{238}U to date.

Values for the group resonance integral per unit lethargy, I , are calculated from the average cross sections by a simple 5-point integration over the group. The formula is

$$I_x = \frac{1}{5} \sum_{i=1}^5 \frac{\sigma_p + \langle \sigma_x(E_i) \rangle + \sigma_{Bx}(E_i)}{\sigma_p + \langle \sigma_{\gamma}(E_i) \rangle + \langle \sigma_f(E_i) \rangle + \langle \sigma_s(E_i) \rangle + \sigma_{Btot}(E_i)} \quad ,$$

where I_x is the group resonance integral/lethargy for any of capture, fission or scattering,

$\langle \sigma_x(E_i) \rangle$ is the average cross section for any reaction,

$\sigma_{Bx}(E_i)$ is the background cross section for that reaction,

$\sigma_{Btot}(E_i)$ is the total background cross section, and

the points E_i are on a constant lethargy spacing.

B4 CALCULATION OF GROUP RESONANCE INTEGRALS FROM A POINT CROSS-SECTION LIBRARY

Point cross-section libraries have been generated on an ultra-fine mesh for use in the PEARLS code. The two different mesh structures which have been used for fuel isotopes and light resonance material are given in the following table:

Structure 1		Structure 2	
Lethargy Range	Lethargy Interval	Lethargy Range	Lethargy Interval
6.25 - 8.75	3.90625×10^{-5}	2.0 - 5.0	1.2207×10^{-4}
8.75 - 11.25	7.8125×10^{-5}	5.0 - 6.0	2.4414×10^{-4}
11.25 - 13.75	1.5625×10^{-4}	6.0 - 7.0	4.8828×10^{-4}
13.75 - 16.25	3.125×10^{-4}	7.0 - 10.0	9.7656×10^{-4}
16.25 - 18.75	6.25×10^{-4}		

For all fuel isotopes except ^{238}U , only that part of the first mesh structure which covers the resolved resonance range has been used. The PEARLS code numerically solves the neutron slowing-down equation for isotropic elastic scattering in few-region geometry. In practice, a specialised version of the code, MINI-PEARLS, has been developed to undertake calculations of a single nuclide with hydrogen (with constant scattering cross section) in a homogeneous mixture. This saves computer time lost through the generality of PEARLS. The group resonance integrals/lethargy as a function of potential scattering have been calculated from a series of these homogeneous calculations. The formulae used to derive resonance integrals and other required quantities are given below.

The group resonance integral/lethargy for group g is given by

$$I_{\alpha\ell g} = \frac{F_g \int_g \sigma_{\alpha\ell}(E) \phi(E) / \rho(E) dE}{\tau_g \phi_{0g}}$$

where $\phi(E)$ is the flux obtained by numerical solution of the homogeneous mixture for a unit source,

$\rho(E)$ is the resonance escape probability to energy E ,

τ_g is the group lethargy width,

ϕ_{0g} is the asymptotic flux for group g , given by

$$\phi_{0g} = 1 / (\sigma_H + \xi_\ell \sigma_{p\ell g}) ,$$

σ_H is the potential scattering due to hydrogen,

$\sigma_{p\ell g}$ is the potential scattering due to the resonance nuclide ℓ , and

F_g is a correction factor to account for the deviation of the source into the group from the asymptotic value.

The outscatters from the group are given by

$$\sigma_{\ell, g \rightarrow g+1} = \frac{\int_{E_{g+1}}^{E_{g+1}/\alpha_\ell} \frac{\sigma_{s\ell}(E) \phi(E) (E_{g+1} - \alpha_\ell E) dE}{\rho(E) E (1 - \alpha_\ell)}}{\int_g \phi(E) / \rho(E) dE}$$

where E_{g+1} is the lower energy boundary of group g .

The self scatter term includes an inversely weighted total cross section.

Thus,

$$\sigma_{\ell, g \rightarrow g} = \sigma_{\ell g} - \sigma_{a\ell g} - \sigma_{\ell, g \rightarrow g+1} ,$$

where

$$\sigma_{a\ell g} = \frac{\int_g \sigma_{a\ell}(E) \phi(E) / \rho(E) dE}{\int_g \phi(E) / \rho(E) dE}$$

$$\sigma_{\ell g} = \frac{\int_g \phi(E) / \rho(E) dE}{\int_g \frac{\phi(E)}{\rho(E) (\sigma_H + \sigma_\ell(E))} dE} - \sigma_H .$$

The other quantity required is the depression of the group flux, which is given by

$$R_g = F_g R'_g ,$$

$$R'_g = \frac{\int_g \phi(E)/\rho(E) dE}{\tau_g \phi_{og}} .$$

The correction factor F_g is approximated in terms of other derived quantities by

$$F_g = \frac{\phi_{og} \{ \sigma_H (E_g - E_{g+1}) / E_g + \xi_l \sigma_{plg} \}}{S_g / \rho(E_g)} ,$$

where

$$S_g = \sigma_H (E_g - E_{g+1}) \left\{ \frac{\phi_{oo}}{E_1} + \sum_{h=1}^{g-1} \left(\frac{1}{E_{h+1}} - \frac{1}{E_h} \right) \bar{p}_h R'_h \phi_{oh} \right\} +$$

$$+ \sigma_{l,g-1 \rightarrow g} R'_{g-1} \bar{p}_{g-1} \tau_{g-1} \phi_{o,g-1} ,$$

$$\bar{p}_g = \frac{1}{2} (\rho(E_g) + \rho(E_{g+1})) .$$

B5 FITTING OF SUBGROUP PARAMETERS

λ Parameters

Resonance integrals obtained by the methods B3 or B4 are fitted by subgroup parameters in the cross-section editing module AUSED [Harrington 1976]. For each temperature, the resonance integral is regarded as a function of effective potential scattering cross section $\hat{\sigma}_p$. The value of $\hat{\sigma}_p$ at each tabulated value of the resonance integrals (index i) is given by

$$\sigma_{pi} = (\sigma_{Hi} + \lambda_{li} \sigma_{pl}) \frac{l_a^\infty + l_s^\infty}{l_a^\infty + \lambda_{li} l_s^\infty} ,$$

where l_a^∞, l_s^∞ are the absorption and resonance scattering integrals at infinite dilution,

$$\lambda_{li} = \xi_l E_g / (E_g - E_{g+1}) , \quad \text{or}$$

$$\lambda_{li} = 1 - \frac{2 \alpha_l C_i}{x} \tan^{-1} \left(\frac{x}{C_i (1 + \alpha_l)} \right) ,$$

$$x = \langle 2E_r / \Gamma \rangle_l (1 - \alpha_l) ,$$

$$C_i = \{ 1 + \langle \sigma_o \rangle_l / (\sigma_{Hi} + \sigma_{pl}) \}^{\frac{1}{2}} , \quad \text{and}$$

all quantities, except σ_{Hj} , ξ_{ℓ} , α_{ℓ} are group dependent but the group subscript has been dropped.

For each group, there is a choice between :

- (a) using narrow resonance theory $\lambda_{\ell} = 1$,
- (b) using the very broad λ_{ℓ} (first definition), and
- (c) using the Hill-Schaeffer method.

In the last case, suitable group averaged parameters $\langle 2E_r/\Gamma \rangle_{\ell}$ and $\langle \sigma_o \rangle_{\ell}$ are required.

For a number of resonances in a group, the average parameters $\langle 2E_r/\Gamma \rangle_{\ell}$ and $\langle \sigma_o \rangle_{\ell}$ have been formed in a rather arbitrary manner by weighting the value for each resonance with the total resonance integral at $T = 0$ for a chosen value of σ_p . That is

$$\langle \sigma_o \rangle_{\ell} = \frac{\sum_r \sigma_{or} R_r}{\sum_r R_r} ,$$

$$\langle 2E_r/\Gamma \rangle_{\ell} = \frac{\sum_r R_r}{\sum_r \frac{1}{2} \Gamma_r R_r / E_r} ,$$

where

$$R_r = \frac{\pi \Gamma_r \sigma_{or}}{2 E_r} \left(1 + \frac{\sigma_{or}}{\bar{\sigma}_p} \right)^{-\frac{1}{2}} ,$$

the summation on r is over resonances in the group, and the value $\bar{\sigma}_p$ has been chosen to be :

$$\sigma_p = \begin{cases} 100 & , \text{ for } ^{238}\text{U and } ^{232}\text{Th} \\ 1000 & , \text{ for other fuel isotopes.} \end{cases}$$

The effect of altering this arbitrary weighting has not been investigated. Comparison of the overall results obtained with the numerical solution of the PEARLS code has proved satisfactory.

For fuel isotopes, the choice between (a), (b), and (c) above is reasonably straightforward. Narrow resonance theory is applied when the resonance integrals have been computed by the method B3. A difficulty arises with a low energy resonance which extends over a number of groups, because of a resonance dependent, rather than a group dependent, factor in the MIRANDA theory (Equation (5.32)). The approach adopted has been to use the same resonance parameters for a maximum of two groups on either side of the resonance peak, and to use the very broad λ_{ℓ} for the extreme wings of the resonance.

For light resonance nuclides, the choice is somewhat more arbitrary as none of the methods may be particularly appropriate in some groups. The very wide resonance λ has been found to give the best fit to the resonance integrals in many of the groups.

Non-isolated Resonance Correction

Before fitting subgroup parameters to the resonance integrals, those integrals calculated in MINI-PEARLS are adjusted by removing the non-isolated resonance correction applied in MIRANDA. The treatment has already been given in Section 5.6.1.

Subgroup Fitting

An approximation to the resonance integrals per unit lethargy of the form

$$I_{xli} \approx \sum_k w_{xlk} \hat{\sigma}_{pi} / (\hat{\sigma}_{pi} + \sigma_{lk})$$

is required, where σ_{lk} is independent of group and temperature. The subgroup parameters w_{xlk} are obtained by a least squares fit to minimise

$$Q = \sum_i \left(1 - \sum_k \frac{w_{xlk} \sigma_{pi}}{(\sigma_{pi} + \sigma_{lk}) I_{xli}} \right)^2$$

subject to additional constraints on w_{xlk} . The integrals fitted are absorption, total, fission and the group flux depression (I_{ali} , I_{alsi} , I_{fli} , and R_i). The additional constraint is $w_{xlk} \geq 0$ when fitting I_{ali} , I_{fli} and R_i , while w_{xlk} has the same sign as σ_{lk} when fitting the total resonance integral. The method used in this constrained fit has been described by Doherty [1972]. The additional subgroup weights for scattering and fission emission are then obtained from

$$w_{s lk} = w_{lk} - w_{a lk}, \text{ and}$$

$$w_{e lk} = v w_{f lk}.$$

In the work of Doherty [1972], eight values of σ_{lk} , starting at 0.625 and proceeding in multiples of 4 to 10 240, were used. These values have been retained for all nuclides, but with the upper range extended or contracted depending on the peak resonance height for the nuclide. In addition, a negative value -2.5 has been included for ^{238}U and ^{232}Th to allow for interference scattering effects, while two negative values have generally been included for light resonance nuclides. Thus the number of subgroups varies between 7 and 10. The accuracy of the fits obtained is generally better than 1 per cent, except in some cases where it is the form of the fit which is in error, rather than the values of σ_{lk} .

B6 SCATTERING MATRICES FOR THE RESONANCE GROUPS

Scattering matrices may be tabulated as a function of effective potential scattering cross section $\hat{\sigma}_p$. For heavy nuclides, scattering in resonance groups has been represented by a P_0 matrix only. The P_0 matrix has been obtained as a function of $\hat{\sigma}_p$ from MINI-PEARLS calculations which assume isotropic scattering in the centre of mass system. For those groups treated by the unresolved resonance method given in B3, only the value at infinite dilution obtained from SUPERTO G has been included in the library.

For light resonance nuclides, anisotropic scattering and a P_0, P_1 representation have been prepared by the following approximate treatment. The data obtained from MINI-PEARLS (using isotropic scattering in the centre of mass) as a function of $\hat{\sigma}_p$ have been combined with the infinite dilution values obtained from SUPERTO G. The ratio of SUPERTO G P_0 removal to MINI-PEARLS P_0 removal at infinite dilution has been taken as a constant factor to be applied to all P_0 removals as a function of $\hat{\sigma}_p$. This ratio is also stored in the library for use in the resonance treatment. The P_1 matrix at infinite dilution obtained from SUPERTO G has been shielded by the factors that apply to the total elastic scattering. That is,

$$\sigma_{l, g \rightarrow h, l}(\hat{\sigma}_p) = \sigma_{l, g \rightarrow h, l}(\infty) \frac{\sum_h \sigma_{l, g \rightarrow h, o}(\hat{\sigma}_p)}{\sum_h \sigma_{l, g \rightarrow h, o}(\infty)}.$$

This merely ensures that $\bar{\mu}$ remains constant as $\hat{\sigma}_p$ varies.

B7 TRANSPORT CROSS SECTION

For P_0 calculations in MIRANDA, a library value of the transport cross section is required. For nuclides not classed as moderators, this has been obtained simply from

$$\sigma_{t\ell g} = \sigma_{\ell g} - \sum_h \bar{\mu} \sigma_{\ell, g \rightarrow h, 1} ;$$

that is, total cross section minus $\bar{\mu}$ times scattering cross section. For moderator nuclides, such as H_2O , CH_2 , D_2O and C , the transport cross section is calculated from a B1 calculation of a ^{235}U fission spectrum source in the moderator with an infinitesimal buckling. The calculation is performed in MIRANDA which thus is used in preparing its own library.

APPENDIX C
SAMPLE LATTICE CALCULATION

```

*DD1
STEP *
LINK MIRANDA
LINK ANAUSN(1,3)
LINK EDIT(1,4)
END

STOP
*DD2
HEAD TRX1 REF ENDF-202
DEFN FUEL U235 6.253-4 U238 4.7205-2
DEFN VOID 0 1.-10
DEFN CLAD AL .06025
DEFN MOD H2O .03338
REQD FUEL VOID CLAD MOD U235 U238
RM 0 5*.0983 .0127 .0711 5*.0745836 0
REG 1(1)5 FUEL 6 VOID 7 CLAD 8(1)12 MOD
RESREG 0 .4915 .0838 .372918 0 SMEAR 5*1 2 2 5*3
BUCK B3 5.7-3
OUTPUT P3
GROUPS 26 1 3(2)11(6)41 51 61 71 80(4)128
START
STOP
*DD3
TRX
AUS NL 1 NSN 6 END
*DD4
BUCK B3 5.7-3 SEARCH OFF
GROUPS 2 1 15 26
OUTPUT RR START

```

AUSYS CODE SUPERVISOR * 16 DEC 76*
STEP *

ISN	LIST OF SOURCE STATEMENTS
1	LINK MIRANDA
2	LINK ANAUSN(1,3)
3	LINK EDIT(1,4)
4	END

ERROR LEVEL OF 0

CODE MIRANDA CALLED FROM ISN 1 OF PATH AT TIME 0.02 MINS FROM START

UNIT ASSIGNMENTS

(FT01F001, 'DD 2), (FT03F001, 'DD13), (FT04F001,ST1,DD38), (FT05F001,ST2,DD39), (FT06F001, 'DD21), (FT07F001,GML,DD35),
 (FT08F001,L18,DD31), (FT09F001,FL2,DD37), (FT10F001,XS1,DD33), (FT11F001,XS2,DD34), (FT12F001,XS3,DD40), (
 STORAGE ALLOCATED- 5518 WORDS
 HEAD TRX1 REF ENDF-202
 DEFW FUEL U235 6.253-4 U238 4.7205-2

TRXI REF ENDF-202

MATERIAL TABLE	FUEL	VOID	CLAD	MOO
TEMP.	300.0	300.0	300.0	300.0
8 U235	6.2530E-04	0.0	0.0	0.0
11 U238	4.7205E-02	0.0	0.0	0.0
18 H2O	0.0	0.0	0.0	3.3380E-02
22 C	0.0	1.0000E-10	0.0	0.0
26 Al	0.0	0.0	6.0250E-02	0.0

TIME= 0.028 MINS
 VOLUMES FOR RESONANCE THEORY
 7.58920E-01 2.80851E-01 1.78489E+00

TIME= 0.095 MINS

IGEOM= 9 **CIRCULAR WHITE REFLECTING BOUNDARY BOMALUMI METHOD

TIME= 0.181 MINS

TIME= 0.278 MINS

***** B 3 FLUX SOLUTION

KEFF	ACC	EIGENY	8**2(1)
9.91410D-01	1.0000E+00	1.0000E+00	5.70000D-03
1.00469D+00	1.54318E+00	1.0000E+00	5.70000D-03
1.00607D+00	1.55261E-01	1.0000E+00	5.70000D-03
1.00634D+00	4.96966E-02	1.0000E+00	5.70000D-03
1.00659D+00	1.85499E-02	1.0000E+00	5.70000D-03
1.00640D+00	6.59852E-03	1.0000E+00	5.70000D-03
1.00640D+00	2.18715E-03	1.0000E+00	5.70000D-03
1.00640D+00	6.71434E-04	1.0000E+00	5.70000D-03
1.00640D+00	2.26396E-04	1.0000E+00	5.70000D-03
1.00640D+00	6.88531E-05	1.0000E+00	5.70000D-03

GRP	MU-FISS	ABS	SUM MU-FISS	SUM ABS	FLUX0	FLUX1	FLUX2	FLUX3
1	7.91926D-04	2.31019D-05	7.91926D-04	2.31019D-05	1.55530D-02	3.36217D-03	8.16678D-04	2.06619D-04
2	7.91926D-04	8.46092D-05	3.52190D-03	1.07711D-04	8.83116D-02	1.20061D-02	2.79245D-03	6.77121D-04
3	6.18338D-03	1.48187D-03	9.70529D-03	1.37416D-03	1.66096D-01	3.21252D-02	6.97236D-03	1.56570D-03
4	7.97540D-03	2.97407D-03	1.76807D-02	4.34823D-03	3.42029D-01	6.08794D-02	1.98810D-02	2.38102D-03
5	1.16377D-02	4.60863D-03	2.93184D-02	8.95687D-03	5.37213D-01	8.47264D-02	1.44994D-02	2.44062D-03
6	1.54900D-02	5.74913D-03	4.48084D-02	1.47060D-02	7.69922D-01	1.42260D-01	1.78752D-02	2.71508D-03
7	1.92028D-02	7.53720D-03	6.40112D-02	2.24370D-02	9.84473D-01	1.44373D-01	2.32245D-02	3.61008D-03
8	1.71865D-02	7.20795D-03	8.11948D-02	2.94517D-02	6.17758D-01	1.33345D-01	1.91775D-02	2.62307D-03
9	1.03427D-02	5.04706D-03	9.15376D-02	3.64887D-02	1.01262D+00	1.27890D-01	1.66721D-02	2.05077D-03
10	1.82124D-03	2.04080D-03	9.35588D-02	3.65395D-02	8.09820D-01	1.13582D-01	1.31104D-02	1.31913D-03
11	8.51112D-04	1.83232D-03	9.42099D-02	3.83719D-02	9.60542D-01	9.52372D-02	1.00282D-02	8.23101D-04
12	5.48321D-04	1.78599D-03	9.47583D-02	4.01578D-02	1.01766D+00	1.00059D-01	9.85390D-03	7.70488D-04
13	4.42630D-04	1.44238D-03	9.52009D-02	4.16002D-02	8.77415D-01	8.65862D-02	7.46159D-03	5.02526D-04
14	3.34661D-04	1.06729D-03	9.55355D-02	4.26675D-02	6.64476D-01	5.65662D-02	3.67907D-03	1.47927D-04
15	3.62578D-04	1.16782D-03	9.58981D-02	4.38353D-02	7.05863D-01	5.41293D-02	3.68910D-03	1.62495D-04
16	3.30330D-04	1.11032D-03	9.62285D-02	4.49457D-02	6.14749D-01	4.72690D-02	2.96727D-03	1.16235D-04
17	2.92513D-04	1.08104D-03	9.65210D-02	4.60267D-02	5.29157D-01	3.96980D-02	2.23584D-03	7.44012D-05
18	2.69871D-04	1.03580D-03	9.67008D-02	4.70625D-02	4.58411D-01	3.26709D-02	1.63044D-03	4.39334D-05
19	2.65048D-04	1.07183D-03	9.70559D-02	4.81344D-02	4.26373D-01	2.91422D-02	1.34645D-03	3.40334D-05
20	2.40767D-04	1.03360D-03	9.72590D-02	4.91680D-02	3.71576D-01	2.42590D-02	1.00082D-03	2.12232D-05
21	2.53972D-04	1.17718D-03	9.75506D-02	5.03452D-02	3.61532D-01	2.21498D-02	8.51332D-04	1.80887D-05
22	2.46575D-04	1.37732D-03	9.77972D-02	5.17225D-02	3.27616D-01	2.01293D-02	7.43611D-04	1.67439D-05
23	2.27733D-04	1.50623D-03	9.80240D-02	5.32287D-02	3.04765D-01	1.78788D-02	6.22510D-04	1.40834D-05
24	2.23758D-04	1.55253D-03	9.82487D-02	5.47812D-02	2.81761D-01	1.52585D-02	4.72678D-04	9.45416D-06

25 2-42848D-04 1.77411D-03 9-84915D-02 5-64953D-02 2-84574D-01 1-53939D-02 2-84574D-01 1-53939D-02 4-98436D-04 1-21747D-05
 26 2-39065D-04 1.77050D-03 9-87306D-02 5-82658D-02 2-66981D-01 1-45138D-02 4-64741D-04 1-20542D-05
 27 2-48080D-04 1.87477D-03 9-89787D-02 6-01406D-02 2-58156D-01 1-38264D-02 4-61275D-04 1-19710D-05
 28 2-67970D-04 1.97404D-03 9-92467D-02 6-21147D-02 2-51230D-01 1-32166D-02 4-20517D-04 1-16982D-05
 29 2-92523D-04 2-11401D-03 9-95392D-02 6-42287D-02 2-45526D-01 1-26635D-02 4-01376D-04 1-12808D-05
 30 2-98646D-04 2-15139D-03 9-98390D-02 6-63800D-02 2-41368D-01 1-23354D-02 3-93583D-04 1-12594D-05
 31 3-45379D-04 2-37999D-03 1-00184D-01 6-87580D-02 2-36591D-01 1-18637D-02 3-76388D-04 1-06512D-05
 32 3-41260D-04 2-46182D-03 1-00060D-01 7-36353D-02 2-31455D-01 1-11603D-02 3-51327D-04 1-07481D-05
 33 4-41260D-04 2-46182D-03 1-00060D-01 7-36353D-02 2-31455D-01 1-11603D-02 3-51327D-04 1-07481D-05
 34 4-67916D-04 2-71184D-03 1-01979D-01 7-90327D-02 2-27261D-01 1-09299D-02 3-50157D-04 9-96795D-06
 35 5-05613D-04 2-68533D-03 1-01979D-01 7-90327D-02 2-27261D-01 1-09299D-02 3-50157D-04 9-96795D-06
 36 6-09494D-04 2-70029D-03 1-02589D-01 8-17330D-02 2-25523D-01 1-08607D-02 3-51579D-04 1-00646D-05
 37 6-58174D-04 2-68820D-03 1-03247D-01 8-44210D-02 2-23723D-01 1-09294D-02 3-61191D-04 1-05823D-05
 38 7-55299D-04 3-21244D-03 1-04002D-01 8-76366D-02 2-21474D-01 1-06786D-02 3-51224D-04 1-01918D-05
 39 7-80018D-04 3-28598D-03 1-04782D-01 9-09196D-02 2-20197D-01 1-08587D-02 3-66167D-04 1-09020D-05
 40 1-05935D-03 3-47373D-03 1-05841D-01 9-43930D-02 2-18416D-01 1-06247D-02 3-55968D-04 1-04558D-05
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 42 1-15716D-03 3-03714D-03 1-08305D-01 1-00693D-01 2-15891D-01 1-05867D-02 3-59449D-04 1-06226D-05
 43 1-26493D-03 3-14861D-03 1-09570D-01 1-03842D-01 2-14949D-01 1-04960D-02 3-55571D-04 1-04300D-05
 44 1-89044D-03 3-75454D-03 1-11460D-01 1-07596D-01 2-12218D-01 1-02470D-02 3-40510D-04 9-74729D-06
 45 1-61534D-03 3-22361D-03 1-13075D-01 1-12820D-01 2-09385D-01 9-81459D-03 3-19278D-04 8-80373D-04
 46 1-76069D-03 3-47283D-03 1-14834D-01 1-16293D-01 2-09546D-01 1-03739D-02 3-53739D-04 1-03994D-05
 47 1-71367D-03 3-83010D-03 1-16550D-01 1-24476D-01 1-97915D-01 8-86045D-03 3-17360D-04 9-25034D-06
 48 1-85568D-03 3-99087D-03 1-18405D-01 1-29867D-01 2-03717D-01 1-02448D-02 3-51861D-04 1-04710D-05
 49 1-78428D-03 3-83023D-03 1-20190D-01 1-37297D-01 1-97512D-01 9-36023D-03 3-05324D-04 8-51487D-06
 50 4-41349D-03 3-03764D-03 1-24603D-01 1-49334D-01 2-02128D-01 9-93065D-03 3-37203D-04 9-94700D-06
 51 2-50730D-03 3-83980D-03 1-27110D-01 1-46173D-01 1-93305D-01 8-60095D-03 2-65852D-04 6-89805D-06
 52 3-42490D-03 1-39157D-02 1-30355D-01 1-60089D-01 1-82065D-01 8-74032D-02 2-80701D-04 7-60640D-06
 53 3-43975D-03 3-81144D-03 1-33975D-01 1-63901D-01 1-93317D-01 9-34359D-03 3-10588D-04 8-93557D-06
 54 3-33776D-03 1-95931D-02 1-37312D-01 1-83494D-01 1-64819D-01 7-63791D-03 2-32730D-04 5-81195D-06
 55 2-49852D-03 2-73471D-03 1-39811D-01 1-86228D-01 1-88889D-01 9-28491D-03 3-17460D-04 9-25034D-06
 56 3-14786D-03 3-95902D-03 1-42959D-01 1-90187D-01 1-86041D-01 9-09350D-03 3-07998D-04 9-12494D-06
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 59 1-58235D-04 2-45383D-03 1-49787D-01 1-98437D-01 7-18004D-02 3-40413D-03 1-12209D-04 3-19343D-06
 60 4-11200D-04 1-05867D-02 1-50198D-01 2-09024D-01 5-79181D-02 2-52441D-03 7-17409D-05 1-62926D-06
 61 2-92450D-04 1-59634D-02 1-50491D-01 2-24987D-01 4-64621D-02 2-02672D-03 5-26477D-05 9-90011D-07
 62 4-82187D-04 5-34867D-03 1-50973D-01 2-30336D-01 6-32510D-02 3-10188D-03 9-91036D-05 2-63385D-06
 63 2-81916D-04 2-30787D-03 1-51255D-01 2-32643D-01 6-82379D-02 3-36522D-03 1-10776D-04 3-12986D-06
 64 2-42059D-04 1-90327D-03 1-51497D-01 2-34547D-01 6-84021D-02 3-40682D-03 1-13273D-04 3-27468D-06
 65 8-55472D-05 1-92668D-03 1-51582D-01 2-35573D-01 7-08141D-02 3-49676D-03 1-18367D-04 3-52299D-06
 66 9-11943D-05 8-75409D-04 1-51674D-01 2-36449D-01 7-14871D-02 3-52460D-03 1-20151D-04 3-62270D-06
 67 1-26949D-03 1-49251D-03 1-52943D-01 2-37941D-01 7-04359D-02 3-46243D-03 1-17669D-04 3-53409D-06
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 78 2-08904D-03 1-73821D-03 1-60036D-01 2-48342D-01 7-20127D-02 3-46348D-03 1-14410D-04 3-25887D-06
 79 2-67742D-03 1-95573D-03 1-62713D-01 2-50297D-01 7-28205D-02 3-46021D-03 1-13253D-04 3-18244D-06
 80 1-91857D-03 1-53983D-03 1-64432D-01 2-51837D-01 7-37354D-02 3-40839D-03 1-16279D-04 3-25138D-06
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 85 2-22173D-03 1-88744D-03 1-74195D-01 2-60145D-01 7-89069D-02 3-58611D-03 1-13330D-04 3-08001D-06

86 2-500710-03 2-070790-03 1-766950-01 2-623150-01 7-977480-02 3-588930-03 1-109920-04 2-970310-06
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91 5-783160-03 4-097810-03 1-973450-01 2-775460-01 8-052610-02 3-080720-03 8-518550-05 1-940370-06
92 6-481920-03 4-570340-03 2-038270-01 2-821160-01 8-203080-02 3-018400-03 8-114070-05 1-785820-06
93 6-560440-03 4-717250-03 2-103870-01 2-868340-01 8-466600-02 2-988150-03 7-802160-05 1-664470-06
94 6-591960-03 4-860340-03 2-169790-01 2-916940-01 8-901760-02 3-001250-03 7-631100-05 1-587800-06
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96 7-418730-03 5-601370-03 2-312240-01 3-024180-01 1-021840-01 3-123790-03 7-505340-05 1-501190-06
97 8-313770-03 6-283470-03 2-359580-01 3-087020-01 1-166620-01 3-234700-03 7-546780-05 1-484050-06
98 9-038660-03 7-239330-03 2-491420-01 3-159410-01 1-235870-01 3-389910-03 7-670620-05 1-485490-06
99 1-128680-02 8-454930-03 2-604290-01 3-239660-01 1-378990-01 3-581500-03 7-882060-05 1-507030-06
100 1-333090-02 9-920580-03 2-737600-01 3-431600-01 1-536540-01 3-801590-03 8-161710-05 1-547610-06
101 1-575560-02 1-163980-02 2-895160-01 3-495600-01 1-705650-01 4-013490-03 8-394060-05 1-571580-06
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105 2-685980-02 1-936210-02 3-802670-01 4-117890-01 2-278170-01 4-434490-03 8-448930-05 1-543880-06
106 2-945220-02 2-178800-02 4-097190-01 4-328670-01 2-319330-01 4-346270-03 8-069540-05 1-368970-06
107 3-161900-02 2-250940-02 4-413880-01 4-523760-01 2-335760-01 4-170400-03 7-534350-05 1-235510-06
108 3-333390-02 2-361300-02 4-746710-01 4-789890-01 2-311200-01 3-907990-03 6-827890-05 1-070740-06
109 3-451780-02 2-434160-02 5-091890-01 5-033300-01 2-248670-01 3-612100-03 6-112390-05 9-137270-07
110 3-512140-02 2-466730-02 5-443100-01 5-279980-01 2-151530-01 3-297320-03 5-414990-05 7-715160-07
111 3-520310-02 2-463370-02 5-795130-01 5-526310-01 2-030000-01 2-959200-03 4-596210-05 6-308840-07
112 3-476000-02 2-424520-02 6-142740-01 5-768770-01 1-888350-01 2-626680-03 4-030640-05 5-088810-07
113 3-388970-02 2-356850-02 6-481630-01 6-004450-01 1-736020-01 2-313160-03 3-430650-05 4-046750-07
114 3-265950-02 2-245450-02 6-808230-01 6-231000-01 1-578780-01 2-028760-03 2-913610-05 3-195250-07
115 3-110970-02 2-132300-02 7-119320-01 6-446330-01 1-820090-01 1-770320-03 2-871900-05 2-522340-07
116 3-936980-02 2-028900-02 7-413020-01 6-649220-01 1-266900-01 1-549020-03 2-106680-05 1-996670-07
117 2-744620-02 1-892950-02 7-687480-01 6-838510-01 1-119550-01 1-359960-03 1-815210-05 1-612270-07
118 2-545930-02 1-753490-02 7-942080-01 7-013860-01 9-825890-02 1-204290-03 1-585740-05 1-338650-07
119 2-346200-02 1-613710-02 8-176700-01 7-175230-01 8-569200-02 1-080200-03 1-425560-05 1-185040-07
120 2-144060-02 1-473170-02 8-391100-01 7-322350-01 7-417950-02 9-852970-04 1-325880-05 1-141360-07
121 1-951220-02 1-339340-02 8-586220-01 7-856480-01 6-394830-02 9-194270-04 1-291370-05 1-227780-07
122 1-762790-02 1-208950-02 8-762500-01 7-577380-01 5-474870-02 8-720000-04 1-311740-05 1-448180-07
123 1-585670-02 1-086820-02 8-921070-01 7-886060-01 4-670430-02 8-254940-04 1-331220-05 1-703230-07
124 5-706180-02 3-006140-02 9-491690-01 8-076370-01 1-455300-01 3-542820-03 7-648950-05 1-595350-06
125 3-050440-02 2-082730-02 9-796730-01 8-284850-01 6-011540-02 1-655510-03 3-780340-05 8-681970-07
126 1-547450-02 1-055060-02 9-951480-01 8-390350-01 2-364780-02 5-857040-04 6-593880-06-3-529370-08
127 7-589100-03 5-169820-03 1-002740+00 8-442050-01 9-008910-03 1-760790-04-4-820870-06-2-987590-07
128 3-660310-03 2-491310-03 1-006400+00 8-466960-01 3-374820-03 4-979570-05-1-839230-05-5-087640-07

TIME= 0.450 MINS

TIME= 0.597 MINS

AUSYS CODE SUPERVISOR * 16 DEC 76*

CODE ANAUSN CALLED FROM ISN 2 OF PATH AT TIME 0.64 MINS FROM START

UNIT ASSIGNMENTS
(FT01F001, '00 3), (FT02F001, 'DD12), (FT03F001, 'DD13), (FT08F001, 'DD21), (FT09F001, XS1, DD33), (FT10F001, 6M1, DD35),
(FT11F001, FL2, DD37), (FT12F001, 'DD22), (FT22F001, XS2, DD34), (FT23F001, XS3, DD40), (

44526 WORDS REQUESTED THROUGH " DARRAY "

TRX

4.2 MINUTES ALLOWED

DATA CARDS AS READ

1 2 3 4 5 6 7
12345678901234567890123456789012345678901234567890123456789012

AUS NL 1 NSN 6 END

INTEGR PARAMETERS FROM AUS LIBRARIES

KEYWORD AUS PROCESSED, 0 ITEMS READ, IC= 4
KEYWORD NL PROCESSED, 1 ITEMS READ, IC= 9
KEYWORD NSN PROCESSED, 1 ITEMS READ, IC= 15

AUS GFOM LIB
TRX1 REF ENDF-202

AUS XS LIB
AUSDATA NXSCAT TRX1 REF ENDF-202
MATT 1 IS FUEL TRX10001DRIG
MATT 2 IS VOID TRX10002DRIG
MATT 3 IS CLAD TRX10002DRIG
MATT 4 IS MOD TRX10003DRIG

FL2 REJECTED
KEYWORD END PROCESSED, 0 ITEMS READ, IC= 19

13984 WORDS NEEDED FOR THIS PROBLEM

TRX

ID 1 PROBLEM IDENTIFICATION
 NL 1 MAXIMUM SCATTERING ANISOTROPY
 IEVT 1 PROBLEM TYPE(0,1,2-6 Q,K,SEARCH)
 JOM 1 SLAB(0),CYLINDER(1),SPHERE(2)
 IBR 3 RIGHT B.C. OPTIONS LIKE IBL
 NHAT 4 NUMBER OF MATERIALS
 NOV 0 NUMBER OF INTERVALS WITH VOLUME SOURCE
 NG 26 NUMBER OF GROUPS

 EV 0.0 EIGENVALUE GUESS
 EV2 0.0 " " GUESS 2
 EPS 5.00000E-04 " " ACCURACY REQUESTED
 EPSPNT 5.00000E-04 POINT FLUX ACCURACY REQUESTED

IADJ 0 REGULAR(0),ADJOINT(1)
 NSN 6 SN ORDER
 NMIX 0 LENGTH OF MIXING TABLES
 IBL 1 LEFT B.C. FREE(0),REFL(1),PERIODIC(2),WHITE(3)
 NZ 4 NUMBER OF ZONES
 NI 12 NUMBER OF INTERVALS
 NOA 0 NUMBER OF INTERVALS WITH SHELL SOURCE
 MAXOUT 100 MAX. NUMBER OF OUTERS

MONITOR PRINT

OUTERS	INNER	EIGENV	FISSIONS	N.BALANCE	LAMBDA	MAX(D Ø/ Ø)	DDM. RATIO	FD. ERROR
1	489	1.166390E+00	1.166390E+00	1.00000E+00	1.166390E+00	5.664470E+00	0.0	1.08159E-01
2	624	1.166920E+00	1.166920E+00	9.99996E-01	1.000450E+00	5.103640E-03	5.66036E-03	6.21389E-04
3	650	1.166960E+00	1.166960E+00	9.99996E-01	1.00040E+00	2.739500E-03	6.32709E-03	3.93253E-06
4	676	1.166970E+00	1.166970E+00	9.99995E-01	1.000010E+00	2.521310E-05	-1.13106E-01	4.44794E-07

SUM OVER ALL GROUPS

BALANCE TABLE

LAST LINE IS SUM OVER ALL ZONES

ACTIVATIONS	ABSORPTIONS	NU.FISSIONS	COLLISIONS	L. LEAKAGE	R. LEAKAGE
1	2	3	4	5	6
1	8.88616E+00	9.09516E-01	1.16697E+00	4.88320E+00	0.0
2	4.65598E-01	1.08251E-13	0.0	1.63429E-10	-9.04902E-02
3	2.81872E+00	6.63345E-03	0.0	4.44804E-01	-9.04974E-02
4	2.10110E+01	8.36536E-02	0.0	2.88889E+01	-8.38683E-02
++++	3.31815E+01	9.99802E-01	1.16697E+00	3.42169E+01	0.0

FINAL PRINT

OUTERS	INNER	EIGENV	FISSIONS	N.BALANCE	LAMBDA	MAX(D Ø/ Ø)	DDM. RATIO	FD. ERROR
5	702	1.166980E+00	1.166980E+00	9.99994E-01	1.000010E+00	2.145060E-05	0.0	1.56044E-07

TIME FOR THIS CASE = 1.41 MINUTES

AUSYS CODE SUPERVISOR * 16 DEC 76*

CODE EDIT CALLED FROM ISN 3 OF PATH AT TIME 2.06 MINS FROM START

UNIT ASSIGNMENTS

(FT01F001, .DD 4), (FT02F001, .DD12), (FT03F001, .DD13), (FT04F001,ST1,DD38), (FT05F001,ST2,DD39), (FT06F001, .DD21), (FT07F001,GML,DD35), (FT09F001,FL2,DD37), (FT10F001,XSL,DD33), (FT11F001,XS2,DD34), (FT12F001,XS3,DD40), (FT14F001, .DD54), (FT15F001, .DD22), (

EDIT OF AUS RUNS 16 DEC 76 19 HRS 36 MIN 29.88 SEC

PRELUDE (STANDARD)
USE 10,0 ## PRELUD OF LIB FOR NG,ETC
IGM=7 ## UNIT FOR GEOM DATA
IFLUX=9 ## UNIT FOR FLUX DUMP
NREAC=0 ## MAX OF THIS WITH LIB VALUES TAKEN
MAXBN=0 ## MAX OF THIS WITH LIB VALUES TAKEN
NIXS=200 ## LIB MAT NAMES ETC
NJS=2000 ## STATUS LIB INFO RELATED TO LIB MATS
NIWH=100 ## WHERE-ABOUTS NAMES AND POINTERS
NJMH=1000 ## WHERE-ABOUTS ACTUAL INTERVALS
NJDF=200 ## DEPN NAMES AND POINTERS
NJRD=1000 ## DEPN ACTUAL RHS
NJRD=200 ## REO EXPANDED OUT (POINTERS TO DEFNS)
NIMW=100 ## REO OVERFLOW FOR MULTIPLE DEFNS
MNGC=400 ## MAX THIS WITH MAXX, ETC USED FOR WORKING ARRAY
MNGA=129 ## COLLECTION OF GROUP COLLAPSE DATA
NID=200 ## NGC TABLE POINTER FOR GROUP NGD+1
MIST=30 ## ENTRIES OF (WHEREABOUTS,REO) FOR PRESENT LIB MAT
END ## ERROR DUMP LIST LENGTH
* KEYWORD PRINT IN USERS PRELUDE CAUSES COMMON AND TABLES TO PRINT
END

8UCK B3 5.7-3 SEARCH OFF
*STANDARD DATA FOLLOWS
BUCK 3000*1--3 GROUPS #NG,0,1(1)1000,NGD#NG ##NORMALLY STARTS 1 IN DATA
TIME=0,NAME 0,0,1 ##DEFAULT FOR STATUS LIB USE
SCANWT=1000*1, NSCALE=3 SMALLN=1,-25
SEARCH ON 850 FOR KEFF=1,2,-4 WITH LAMDA=-1,+2,1,-1,1,-1,+2
LIRSEA=20 LIMFL=50 FLUXAC=1,-4 CELLNAME CELL PRINT 2
IGNORE=1 #DON'T IGNORE U235,0 ETC TYPE DEFNS
IDMP 20*0
END

*4 ORDIN COMMON USED 223 000000DF (BASE 10 AND BASE 16 RESP)
*4 DYNAM COMMON USED 42598 00004666
*4 COMMON WORDS LEFT 0 000000000

GROUPS 2 1 15 26
OUTPUT RR START

Table with columns: GROUP, LETHARGY, ENERGY, VELOCITY. Rows 1-4 showing numerical values for each parameter.

UPD= 1 MN= 6 NG= 26 NREAC= 8 P3 SCAT

LAST VAR SEARCH
LAST VAR GROUPS

LAST VAR \$OPT
LAST VAR USE
LAST VAR ICM
LAST VAR IFLUX
LAST VAR NREAC
LAST VAR MAXBN
LAST VAR NIXS
LAST VAR NJXS
LAST VAR NIWH
LAST VAR NJMH
LAST VAR NJDF
LAST VAR NJRD
LAST VAR NIWD
LAST VAR NIWH
LAST VAR MNGC
LAST VAR MNGA
LAST VAR NINO
LAST VAR MIST
LAST VAR MIST
LAST VAR END
LAST VAR \$OPT
LAST VAR \$OPT
LAST VAR NGD
LAST VAR NAME
LAST VAR SMALLN
LAST VAR WITH
LAST VAR PRINT
LAST VAR IGNORE
LAST VAR RELXE
LAST VAR IDMP

5 2.50000E+00 8.20850E+05 1.41739E+01
 6 4.00000E+00 1.83156E+05 8.80829E+00
 7 5.50000E+00 4.08677E+04 4.09826E+00
 8 7.00000E+00 9.11882E+03 1.90040E+00
 9 8.50000E+00 2.03468E+03 8.91308E-01
 10 1.00000E+01 4.53999E+02 4.20309E-01
 11 1.25000E+01 3.72665E+01 1.49761E-01
 12 1.43000E+01 6.16011E+00 5.29081E-02
 13 1.53000E+01 2.26618E+00 2.63674E-02
 14 1.62000E+01 9.21363E-01 1.64794E-02
 15 1.66000E+01 6.17603E-01 1.19913E-02
 16 1.70000E+01 4.13994E-01 9.82415E-03
 17 1.74000E+01 2.77510E-01 8.03669E-03
 18 1.78000E+01 1.86019E-01 6.56021E-03
 19 1.82000E+01 1.24693E-01 5.35647E-03
 20 1.86000E+01 8.35834E-02 4.39329E-03
 21 1.90000E+01 5.60280E-02 3.61279E-03
 22 1.94000E+01 3.75596E-02 2.97002E-03
 23 1.98000E+01 2.51749E-02 2.43874E-03
 24 2.02000E+01 1.68753E-02 2.00065E-03
 25 2.10000E+01 7.58254E-03 1.51243E-03
 26 2.30000E+01 1.02619E-03 9.06767E-04

CONTENTS OF XS-LIB(S).... NAME, SOURCE, MOD, MODIFIER, PN-DATA

THEN NO OF LIB MAT CONTAINING NAME, CONC IN MAT- OR VOL RATIO IF -VE ... FROM STL \$DATA.....TIME\$CELL/ 0.0 TRX1 1

1 FUEL * 1 (TRX10001,ORIG) P3 IN 0
 2 VOID * 1 (TRX10002,ORIG) P3 IN 0
 3 CLAD * 1 (TRX10003,ORIG) P3 IN 0
 4 MOD * 1 (TRX10003,ORIG) P3 IN 0
 5 U235 * 1 (TRX10001,ORIG) P3 IN 1 6.25300E-04
 6 U238 * 1 (TRX10001,ORIG) P3 IN 1 4.72050E-02

GEOM LIB... TRX

GEOM LIB GENERATED WHERE-ABOUTS....

WHERE#FUEL = 1 2 3 4 5
 WHERE#VOID = 6
 WHERE#CLAD = 7
 WHERE#MOD = 8 9 10 11 12
 WHERE#ALL = 1 2 3 4 5 6 7 8 9 10 11 12

GENERATED DEFNS....

DEFN FUEL * 1 P3= FUEL * 1#FUEL
 DEFN VOID * 1 P3= VOID * 1#VOID
 DEFN CLAD * 1 P3= CLAD * 1#CLAD
 DEFN MOD * 1 P3= MOD * 1#MOD
 DEFN U235 * 1 P3= U235 * 1#FUEL
 DEFN U238 * 1 P3= U238 * 1#FUEL
 DEFN TRX1 * 0 P3= FUEL * 1#FUEL

FL2 WDSN-TYPE FLUX DUMP

TRX
 KEFF= 1.166976D+00 FROM REAL P1 DUMP. ACCEPTS TO P0 FLUX
 SETUP FROM DATAPDBLS COMPLETED

DIM= 1 GEOM= 1 LAYOUTS= 1 MAXX= 12

READ -1 FUEL , 1 VOID , 1 CLAD , 1 MOD , 1 U235 , 1 U238 , 1

***** B3 FLUX SOLUTION (ACTUALLY P0 SOLUTION IS TAKEN IF B0 IS SPECIFIED)

KEFF ACC EIGENV B#2(1)
9.86703D-01 1.77039E-01 1.00000E+00 5.70000D-03
9.85715D-01 1.00972E-01 1.00000E+00 5.70000D-03
9.85778D-01 9.24388E-03 1.00000E+00 5.70000D-03
9.85785D-01 8.35864E-04 1.00000E+00 5.70000D-03
9.85786D-01 9.70906E-05 1.00000E+00 5.70000D-03

Table with 7 columns: GRP, NU, FISS, ABS, SUM, NU, FISS, SUM, ABS, FLUX0, FLUX1, FLUX2, FLUX3. It contains 26 rows of numerical data representing flux solution results for various groups and nuclides.

TRX10002 REF ENDF-202 16 DEC 76 19 HRS 36 MIN 29.88 SEC
 **FOR RR(M) LAST GROUP IS TOTAL AND IN NSFV,ETC N=CONC,S=XS,F=FLUX,V=VOL TAKEN OVER REGION AND GROUPS

RR NSFV FOR FUEL , 1 (FUEL ,TRX10001,MOD1) VOL OF REGION= 7.58921E-01 VOL FRACTION= 2.68677E-01 REAC 9-
 GROUP ENERGY TRANSPORT ABSORPTION NU-FISSION SCATTERING TOTAL CAPTUREI CAPTURE2 'FLUX' REAC 9-
 1 6.17603E-01 2.26723E+00 2.58959E-01 1.79419E-01 2.86456E+00 3.124480E+00 6.83005E-02 1.89708E-01 2.14826E-03 6.345160+00
 2 1.02619E-03 1.01907E+00 5.14774E-01 8.06367E-01 6.21907E-01 1.136688E+00 3.33375E-01 1.81397E-01 0.0 1.441240+00
 3.28629E+00 7.06633E+00 4.26148E+00 4.01676E-01 3.71105E-01 2.14826E-03 7.786400+00

RR NSFV FOR VOID , 1 (VOID ,TRX10002,MOD1) VOL OF REGION= 3.97265E-02 VOL FRACTION= 1.40642E-02 REAC 9-
 GROUP ENERGY TRANSPORT ABSORPTION NU-FISSION SCATTERING TOTAL CAPTUREI CAPTURE2 'FLUX' REAC 9-
 1 6.17603E-01 9.38830E-11 9.50759E-14 0.0 1.12321E-10 1.12416E-10 0.0 7.39037E-17 0.0 3.258730-01
 2 1.02619E-03 2.95425E-11 9.95108E-16 0.0 3.08049E-11 3.08079E-11 0.0 9.95108E-16 0.0 8.154880-02
 1.23424E-10 9.60703E-14 0.0 1.43128E-10 1.43224E-10 0.0 1.06901E-15 0.0 4.074220-01

RR NSFV FOR CLAD , 1 (CLAD ,TRX10002,MOD1) VOL OF REGION= 2.41125E-01 VOL FRACTION= 8.53642E-02 REAC 9-
 GROUP ENERGY TRANSPORT ABSORPTION NU-FISSION SCATTERING TOTAL CAPTUREI CAPTURE2 'FLUX' REAC 9-
 1 6.17603E-01 2.88560E-01 7.34422E-04 0.0 3.44683E-01 3.45417E-01 0.0 3.61760E-05 1.84413E-04 1.962840+00
 2 1.02619E-03 4.40882E-02 4.84285E-03 0.0 4.08137E-02 4.61291E-02 0.0 0.0 0.0 5.027320-01
 3.32648E-01 5.57727E-03 0.0 3.85496E-01 3.91546E-01 0.0 3.61760E-05 1.84413E-04 2.465570+00

RR NSFV FOR MOD , 1 (MOD ,TRX10003,MOD1) VOL OF REGION= 1.78489E+00 VOL FRACTION= 6.31894E-01 REAC 9-
 GROUP ENERGY TRANSPORT ABSORPTION NU-FISSION SCATTERING TOTAL CAPTUREI CAPTURE2 'FLUX' REAC 9-
 1 6.17603E-01 4.30968E+00 5.55649E-03 0.0 1.28395E+01 1.28880E+01 0.0 4.20952E-03 0.0 1.425580+01
 2 1.02619E-03 6.99327E+00 6.46030E-02 0.0 6.99563E+00 1.19061E+01 0.0 6.46030E-02 0.0 4.094290+00
 1.13029E+01 7.01594E-02 0.0 1.89341E+01 2.47941E+01 0.0 6.88125E-02 0.0 1.835010+01

RR NSFV FOR U235 , 1 (U235 ,TRX10001,ORIG) VOL OF REGION= 7.58921E-01 VOL FRACTION= 2.68677E-01 REAC 9-
 GROUP ENERGY TRANSPORT ABSORPTION NU-FISSION SCATTERING TOTAL CAPTUREI CAPTURE2 'FLUX' REAC 9-
 1 6.17603E-01 5.37865E-02 4.8448E-02 8.18263E-02 3.51419E-02 8.36169E-02 3.36041E-02 1.48573E-02 1.29892E-05 3.967630-03
 2 1.02619E-03 3.13515E-01 3.90962E-01 8.06367E-01 1.56306E-02 4.04590E-01 3.33375E-01 5.75845E-02 0.0 9.012080-04
 3.67302E-01 4.39410E-01 8.88192E-01 4.88207E-01 3.66979E-01 7.24417E-02 1.29892E-05 4.868830-03

RR NSFV FOR U238 , 1 (U238 ,TRX10001,ORIG) VOL OF REGION= 7.58921E-01 VOL FRACTION= 2.68677E-01 REAC 9-
 GROUP ENERGY TRANSPORT ABSORPTION NU-FISSION SCATTERING TOTAL CAPTUREI CAPTURE2 'FLUX' REAC 9-
 1 6.17603E-01 2.21344E+00 2.07411E-01 9.75939E-02 2.82942E+00 3.04118E+00 3.46965E-02 1.74851E-01 2.13528E-03 2.995230-01
 2 1.02619E-03 7.05552E-01 1.23812E-01 0.0 6.08276E-01 7.32092E-01 0.0 1.23812E-01 0.0 6.803380-02
 2.91899E+00 3.31224E-01 9.75939E-02 3.43769E+00 3.77327E+00 3.46965E-02 2.98663E-01 2.13528E-03 3.675570-01

ENDOFFILE

LAST VAR

STOP. END OF DATA FOR EDIT TRX10002 REF ENDF-202 16 DEC 76 19 HRS 36 MIN 29.88 SEC

