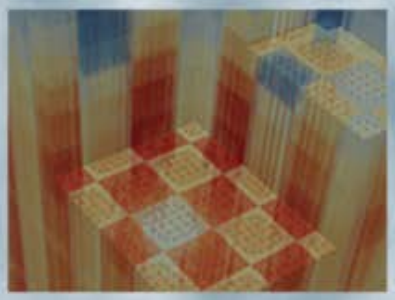
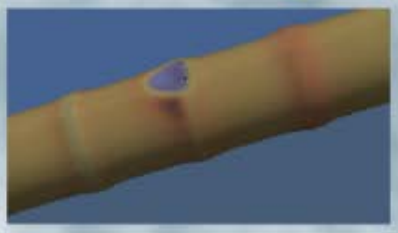
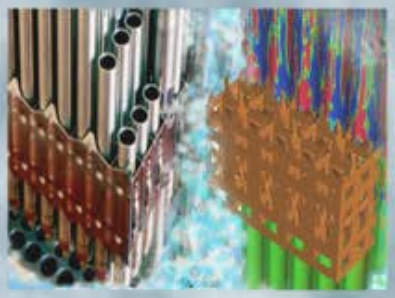
CASL-X-2015-1013-000

Procedure to Generate the MPACT Multigroup Library

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EXECUTIVE SUMMARY

The CASL neutronics simulator MPACT is under development for the neutronics and T-H coupled simulation for the light water reactor. The objective of this document is focused on reviewing the current procedure to generate the MPACT multigroup library. Detailed methodologies and procedures are included in this document for further discussion to improve the MPACT multigroup library.

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ACRONYMS

0D	Zero-Dimensional (Homogeneous)
1D	One-Dimensional
2D	Two-Dimensional
CASL	Consortium for Advanced Simulation of Light Water Reactors
CE	Continuous Energy (as in cross sections)
ESSM	Embedded Self-Shielding Method
IR	Intermediate Resonance
MG	Multi-group (as in cross sections)
MOC	Method of Characteristics
NR	Marrow Resonance
ORNL	Oak Ridge National Laboratory
PW	Pointwise
PWR	Pressurized Water Reactor
RI	Resonance Integral
URR	Unresolved resonance
WR	Wide Resonance

1. INTRODUCTION

The main neutronic simulator in the Consortium for Advanced Simulation of Light Water Reactors (CASL) is the MPACT code which is being developed collaboratively by Oak Ridge National Laboratory and University of Michigan. The key characteristics of the MPACT code includes the subgroup method [Hel03] and the embedded self-shielding method (ESSM) [Wil12] for resonance self-shielding calculation, and a whole core solver with a 2D/1D synthesis method on the frame of 3D coarse mesh finite difference (CMFD) method for which axial and radial correction factors are obtained from 1D nodal expansion method (NEM) or Simplified P_N and 2D method of characteristics (MOC), respectively. The multigroup (MG) cross section library for MPACT has been generated with significant extensions of the AMPX [Wia14] and SCALE [Sca09] code packages developed at Oak Ridge National Laboratory for which the AMPX code package has been significantly improved especially for the Bondarenko approach of resonance self-shielding calculation such as the subgroup method and ESSM used in MPACT.

The objective of this document is focused on reviewing the current procedure to generate the MPACT MG library. Detailed methodologies and procedures for the generation of the MPACT MG library are included in this document for further discussion to improve the library. This document includes the followings.

- MG cross section processing by AMPX (Chapter 2)
- Improvement of resonance data (Chapter 3)
- Resonance self-shielding methods (Chapter 4)
- Generation of miscellaneous data (Chapter 5)
- Generation of the MPACT MG library (Chapter 6)
- Challenging technical issues (Chapter 7)

2. MULTIGROUP CROSS SECTION PROCESSING BY AMPX

2.1 Conventional AMPX procedure

AMPX-6 [Wia14] is a modular system of FORTRAN computer programs to generate the MG and continuous energy (CE) cross section libraries for modern deterministic and Monte Carlo transport codes by processing the ENDF/B libraries. Since the CASL neutronics simulator MPACT is a deterministic transport code, only the AMPX MG library generation procedure is discussed.

The AMPX MG library includes various neutron reactions of the Bondarenko F-factors as a function of background cross section for all energy groups including resolved and unresolved resonances. The resolved resonance F-factors have been generated by the narrow resonance (NR) approximation and the unresolved ones by the J-function method [Lee11] based on the NR approximation. And MG 1D and 2D cross section data have been obtained by using a weighting function of Maxwellian spectrum + 1/E + fission spectrum. At low energies, the weighting function is a Maxwellian spectrum which has a flux shape that assumes the neutron scatters into a region with a free gas scatterer that has no absorption. The Maxwellian flux spectrum has the following formula.

$$\phi(E) = M(E) = Ee^{-\frac{E}{kT}}, \tag{2.1.1}$$

where E, k, T denote neutron energy, Boltzmann constant and temperature of the material in Kelvin, respectively. In the slowing down range, 0.125 eV < E < E_{cut}, the weighting spectrum is assumed to be $\phi(E) = 1/E$. The cutoff energy E_{cut} for the slowing down range must be selected and is typically 55 keV by default in the AMPX modules. In the region, E_{cut} < E < 10^7 eV, where fission neutrons are born, the following fission spectrum is used.

$$\phi(E) = \chi(E) = E^{0.5}e^{-\frac{E}{\theta}}, \tag{2.1.2}$$

where θ is temperature of the fission spectrum (e.g., 1.2 × 10^6 eV). For energies above 10^7 eV, the particles are considered to be in another slowing down region; hence, the spectrum is assumed to have a $1/E$ shape.

MG self-shielded cross sections of reaction type i (Bondarenko F-factors) as a function of background cross sections (σ_0) and material temperature (T)are calculated by using the following equation based on narrow resonance approximation.

$$\sigma_{i,g}(T,\sigma_0) = \frac{\int_g \frac{\sigma_i(T,E)\sigma_0\phi(E)}{\sigma_t(T,E)+\sigma_0}dE}{\int_g \frac{\sigma_0\phi(E)}{\sigma_t(T,E)+\sigma_0}dE}, \tag{2.1.3}$$

where T denotes temperature and σ_t is total cross section. The MG scattering matrix can be obtained by

$$\sigma_{s,l,gg'} = \frac{1}{\int_g \phi(E)dE} \int_g y(E)\sigma_s(E)\phi(E)dE \int_{g'} f_l(E,E')dE', \quad (2.1.4)$$

where *y(E)* is a multiplicity which is unity for scattering and $f_l(E,E')$ a normalized double differential distribution. It should be noted that the 2-D scattering data (not for 2-D thermal scattering) are temperature independent in the AMPX MG library.

2.2 Practical weighting function

In the standard SCALE sequences (e.g. TRITON), self-shielded MG 1D and 2D data for resolved resonance and thermal energy groups are determined by performing the problem-dependent CENTRM slowing down transport calculation for each pin cell type with eq. (2.2.1), and thus the resolved resonance data in the AMPX MG library are not used.

$$\hat{\Omega}\cdot\nabla\psi + \Sigma_t(\vec{r},u)\psi(\vec{r},u,\hat{\Omega}) = \int_{4\pi} d\Omega' \int_0^\infty du' \Sigma_s(\vec{r},u'\to u,\hat{\Omega}'\cdot\hat{\Omega})\psi(\vec{r},u',\hat{\Omega}') + q(\vec{r},u,\hat{\Omega}), \quad (2.1.1)$$

where

- $\hat{\Omega}$: neutron direction
- $\vec{r}$: space coordinate
- u : neutron lethargy
- ψ : angular flux
- Σ_t : macroscopic total cross section
- Σ_s : double differential scattering cross section
- q : external source.

However, since Bondarenko approach for resonance self-shielding calculation does not include any problem-dependent pointwise slowing down calculation, weighting function would make a significant impact on the accuracy mostly through 2-D scattering matrix. The weighting function of Maxwellian spectrum + 1/E + fission spectrum is far from a realistic weighting function. Practical weighting functions for various temperatures can be obtained by performing the CENTRM MG/PW calculations for a typical PWR fuel pin. Figure 2.2.1 provides a sample of pointwise neutron spectra obtained by CENTRM. This would be performed using the XSProc sequence with “parm=centrm”. The weight functions need to be generated to include various temperatures.

There are several pending issues associated with the pointwise weighting function. Since resonance self-shielded cross sections are independently estimated, 1D cross sections are independent upon the pointwise weighting function. However, in reality since the current MPACT procedure includes resonance data only for the specified energy groups, 1D cross

sections of non-resonance groups should be dependent on the weighting functions. MG scattering matrices are obtained by simple flux weighting and renormalization is applied only to total scattering, within-group and out-scattering components. Therefore, this procedure may introduce wrong neutron fluxes resulting in some errors in reaction rates. Pointwise neutron spectra are very changeable according to ^{235}U enrichment, moderator-to-fuel ratio, burnup and void fraction. Therefore, selection of weighting function would be another challenging issue.

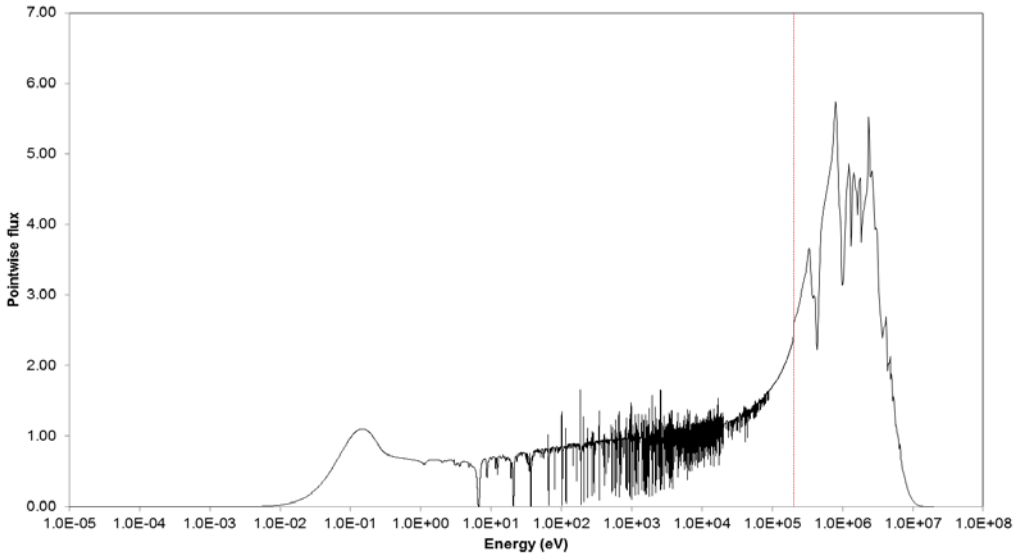


Figure 2.2.1 Pointwise neutron spectra

3. GENERATION OF IMPROVED RESONANCE DATA

Although the AMPX MG library includes MG resonance self-shielded cross sections (Bondarenko F-factors) as a function of background cross sections generated by eq. (2.1.3), they cannot guarantee accurate result due to significant approximations such as coarse energy group, weighting functions and resonance interferences. Therefore, the MG resonance self-shielded data need to be improved in accordance with resonance self-shielding method. This chapter describes several methods to improve the resonance self-shielded cross section data.

3.1 Slowing down equation

The time-independent Boltzmann equation is as follows:

$$\hat{\Omega}\cdot\nabla\psi+\Sigma_t(\vec{r},u)\psi(\vec{r},u,\hat{\Omega})=\int_{4\pi}d\Omega'\int_0^{\infty}du'\Sigma_s(\vec{r},u'\rightarrow u,\hat{\Omega}'\cdot\hat{\Omega})\psi(\vec{r},u',\hat{\Omega}')+q(\vec{r},u,\hat{\Omega}), \quad (3.1.1)$$

where

- $\hat{\Omega}$: neutron direction
- $\vec{r}$: space coordinate
- u : neutron lethargy
- ψ : angular flux
- Σ_t : macroscopic total cross section
- Σ_s : double differential scattering cross section
- q : external source.

The continuous scalar flux can be obtained by solving eq. (3.1.1) using the point-wise cross sections. The effective group self-shielded cross section of the resonance isotope can be obtained using the equation (3.1.2):

$$\sigma_{x,g}=\frac{\int_{\Delta u_g}\sigma_x(u)\phi(u)du}{\int_{\Delta u_g}\phi(u)du}. \quad (3.1.2)$$

In the SCALE code package CENTRM and PMC perform the above calculations to obtain the group self-shielded cross sections for various geometrical models including infinite medium, slab, 1D cylinder and sphere and 2D square pin.

A flowchart of the SCALE modules executed for self-shielding is shown in Figure 3.1.1. First, the fast-executing Bondarenko method is applied to all energy groups for the total, elastic, capture, and fission cross sections of all materials by using BONAMI. In this method MG data at problem-specific conditions are interpolated from the tabulated self-shielding factors in the MG library. While the analytical flux expression used to process Bondarenko shielding factors is reasonable for higher energy groups, it tends to break down at lower energies. SCALE 6

provides other approaches to generate problem-dependent MG data directly from PW data within the energy range in which the Bondarenko method is not desirable - typically the resolved resonance and thermal ranges for criticality safety and reactor physics applications. As shown in Figure 3.1.2, the energy range of interest is divided into the upper multigroup (UMR), PW, and lower multigroup (LMR) ranges, as defined by the input energy boundaries E_{max} and E_{min}, which have default values of 20 keV and 10^{-3} eV, respectively, in SCALE 6. Generally it is recommended that the PW energy range should encompass the resolved resonance ranges of all nuclides that impact the spectral fine-structure; however MG data in the UMR and LMR are always self-shielded with the Bondarenko method. Thus it is not necessary to perform a PW calculation within the energy range where the Bondarenko approximation is adequate. This is done by the CENTRM code, which computes neutron spectra on a fine energy mesh within the PW energy range using various approximations to the Boltzmann equation. In the energy region outside the specified PW range, CENTRM performs an MG calculation so that a full energy range solution is obtained.

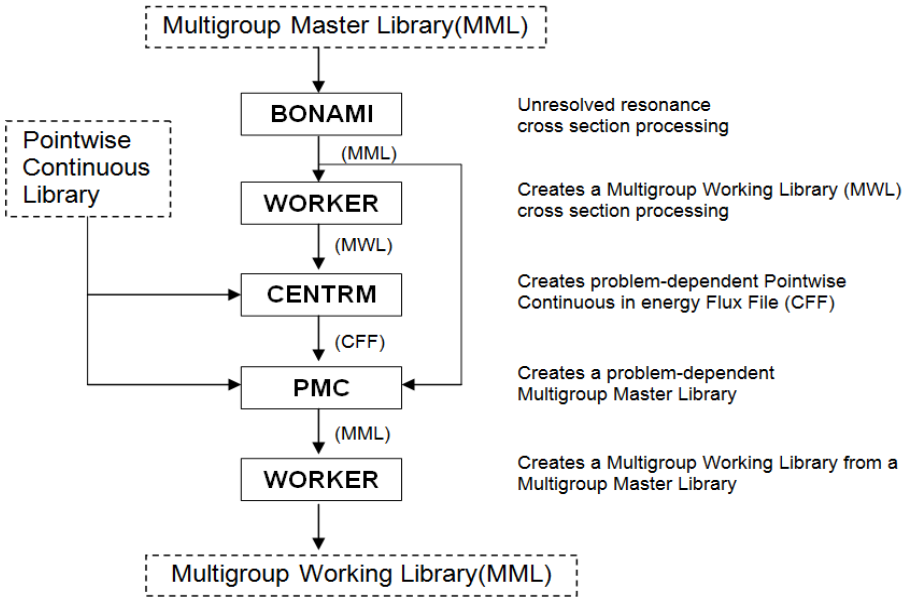


Figure 3.1.1 Flowchart of modules used to generate problem-dependent MG data

The PMC module computes problem-specific MG data for groups within the PW energy range of the CENTRM calculation and replaces the more approximate values from BONAMI. PMC uses the CENTRM spectra for each spatial region as a problem-dependent weight function for averaging energy-dependent data in the PW libraries into MG data. The resulting problem-specific cross-section library is passed to higher-dimensional MG transport calculations performed with other SCALE modules.

Exact same procedure can be utilized in improving MG resonance data in the AMPX MG library. The only difference is to additionally introduce the following assumptions to exclude resonance interference effect according to a user option.

a. Only one resonant nuclide is assumed in the mixture with a constant potential scattering cross section (σ_p), a resonance scattering cross section ($\sigma_{rs}(u)$) and a resonance absorption cross section ($\sigma_{ra}(u)$).
b. The non-resonant nuclides are considered to have negligible absorption and constant potential scattering cross sections.

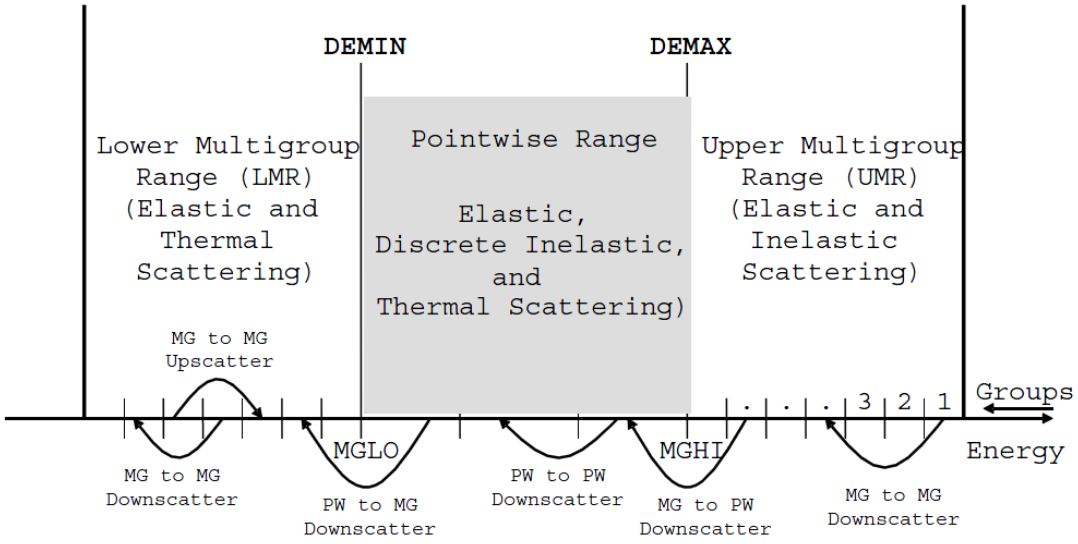


Figure 3.1.2 Definition of UMR, PW, and LMR energy ranges

Exact same procedure by using CENTRM can be utilized in improving resonance data. Several methods are available to improve resonance data which include homogeneous or heterogeneous models, and multiple absorber model to pre-consider resonance interferences or single absorber model to exclude resonance interference. A new procedure using I-CRAWDIUS has been developed to provide potential cross sections or pointwise cross sections to CENTRM for the background nuclides to exclude or include resonance interference between resonance nuclides according to user option.

3.2 Intermediate resonance (IR) approximation

To cast the scattering source term in eq. (3.1.6) into a more tractable form, the intermediate resonance (IR) approximation is introduced.

In this approximation, the fraction λ_i of the scattering for each isotope i is assumed to be so effective that the maximum lethargy gain per collision is significantly greater than the practical resonance width (i.e., the narrow resonance scattering)[Hel03, Sta83]. A resonance affects only a small interval of the integration range from u-Δ_i to u, and its contribution to the scattering source $Q(u)$ is negligible. Since outside the resonances $\Sigma_{si}(u)=\Sigma_{pi}$ and $\phi(u)=constant$, the contribution

of isotope i to $Q(u)$ is $\lambda_i \Sigma_{pi}$. This is the unperturbed slowing down source. Conversely, the remaining fraction $(1-\lambda_i)$ is assumed to be so ineffective that neutrons gain a negligible amount of lethargy compared with Δu_g (i.e., the wide resonance scattering). The resonances are so wide that the integrand can be replaced by its average value, which leads to the $(1-\lambda_i)\Sigma_{si}(u)\phi(u)$ contribution to the source $Q(u)$. Thus, this fraction of scattering does not provide source neutrons from outside the resonance widths but it should be considered as due to self-scattering which neither adds nor removes neutrons. With these approximations, eq. (3.1.6) can be rewritten for the coarse energy groups:

$$\hat{\Omega}\cdot\nabla\psi_{g,k}+\sum_i \Sigma^k_{i,g,t}\psi_{g,k}(\hat{\Omega})=\sum_i \lambda_{i,g}\Sigma^k_{i,p}+\sum_i (1-\lambda_{i,g})\Sigma^k_{i,g,s}\phi_{g,k}. \tag{3.2.1}$$

Eq. (3.2.1) can be rewritten by assuming isotropic angular flux as

$$\hat{\Omega}\cdot\nabla\psi_{g,k}+\sum_i (\Sigma^k_{i,g,a}+\lambda_{i,g}\Sigma^k_{i,p})\psi_{g,k}(\hat{\Omega})=\sum_i \lambda_{i,g}\Sigma^k_{i,p}. \tag{3.2.2}$$

For the homogeneous mixture, the self-shielded flux can be obtained from eq. (3.2.2) as

$$\phi_g=\frac{\sum_i \lambda_{i,g}\Sigma_{i,p}}{\sum_{i=resonance}\Sigma_{i,g,a}+\sum_i \lambda_{i,g}\Sigma_{i,g,s}}=\frac{\lambda_g\Sigma_p}{\Sigma_{g,a}+\lambda_g\Sigma_{g,s}}. \tag{3.2.3}$$

3.3 Intermediate resonance parameters

Let us assume there is only one resonance isotope having an atomic number density N_R. In a homogeneous system, the background cross section of this mixture is defined by

$$\sigma_b=\frac{\sum_{i=all} N_i\lambda_i\sigma_{i,p}}{N_R}. \tag{3.3.1}$$

Eq. (3.2.1) can be rewritten by using eq. (3.3.1) as

$$\phi_g=\frac{\sigma_{g,b}}{\sigma_{g,a}+\sigma_{g,b}+\lambda_g\sigma_{g,rs}}. \tag{3.3.2}$$

Since the atomic mass of hydrogen (^1H) is very close to unity, lethargy gain of any neutron colliding with hydrogen is very big and the neutron can scatter beyond a resonance without any collision. This is essentially the same as the narrow resonance approximation. Therefore, for hydrogen, the intermediate resonance parameter is defined as unity. For other isotopes, the intermediate resonance parameter is obtained by comparing results of various $^{238}U/^1H$ mixtures

where the hydrogen is partly replaced by the other isotopes. This is often referred to as a hydrogen-equivalence parameter.

For homogeneous mixtures including ^{238}U and ^{1}H, eq. (3.2.1) can be written as follows:

$$(N^{238}\sigma_{g,a}^{238} + N^{238}\sigma_{g,rs}^{238} + N^{238}\lambda_g^{238}\sigma_p^{238} + N^1\lambda_g^1\sigma_p^1)\phi_g = N^{238}\lambda_g^{238}\sigma_p^{238} + N^1\lambda_g^1\sigma_p^1. \quad (3.3.3)$$

In order to obtain the hydrogen-equivalence parameter for a nuclide, a part of hydrogen (N^1) is replaced with a certain nuclide (N^X). The amount of the hydrogen atomic number density replaced by another isotopic atomic number density can be adjusted to obtain the same $\sigma_{g,a}^{238}$ from the slowing down calculation by using eq. (3.1.6). The balance equation will be

$$\begin{aligned}(N^{238}\sigma_{g,a}^{238} + N^{238}\sigma_{g,rs}^{238} + N^{238}\lambda_g^{238}\sigma_p^{238} + (N^1 - N^x)\lambda_g^1\sigma_p^1 + N^x\lambda_g^x\sigma_p^x)\phi_g = \\ N^{238}\lambda_g^{238}\sigma_p^{238} + (N^1 - N^x)\lambda_g^1\sigma_p^1 + N^x\lambda_g^x\sigma_p^x.\end{aligned} \quad (3.3.4)$$

By comparing these two equations, the unknown intermediate resonance parameter ($\lambda^x{}_g$) can be obtained as follows:

$$\lambda_g^x = \frac{\Sigma_{g,b} - N^{238}\lambda_g^{238}\sigma_p^{238} - (N^1 - N^x)\lambda_g^1\sigma_p^1}{N^x\sigma_p^x}, \quad (3.3.5)$$

where

$$\Sigma_{g,b} = N^{238}\lambda_g^{238}\sigma_p^{238} + N^1\lambda_g^1\sigma_p^1. \quad (3.3.6)$$

In the actual application, it is too time consuming to determine the fraction of the hydrogen atomic number density that needs to be replaced with a target nuclide. Therefore, the following procedure can be used instead using data derived from ^{238}U data.

(a) Compute a $\sigma_{g,a}^{238}$ table as a function of $\sigma_{g,b}^{238}$ by changing the particle number density of hydrogen for a homogeneous mixture at the fixed ^{238}U (N^{238}) particle number density.
(b) Compute the slowing down calculation for a mixture of ^{238}U (N^{238}), ^{1}H (N^1) and a target nuclide x (N^x), and obtain a new $\sigma_{g,a}^{238}$.
(c) Read the corresponding $\sigma_{g,b}^{238}$ from the prepared $\sigma_{g,a}^{238}$ table.
(d) Calculate the hydrogen equivalent parameter using the following equation.

$$\lambda_g^x = \frac{\sigma_{g,b}^{238}N^{238} - N^{238}\lambda_g^{238}\sigma_p^{238} - N^1\lambda_g^1\sigma_p^1}{N^x\sigma_p^x}. \quad (3.3.7)$$

Intermediate resonance parameters can be also calculated for the other resonance nuclide such as ^{235}U, ^{239}Pu and others.

3.4 Resonance self-shielded data by homogeneous models

The energy dependence of the cross sections in the library has been discretized by dividing the energy range of interest, 10^{-5}eV~10MeV, into a number of broad groups. These cross sections have been obtained by flux-averaging point XS – some-times more than 10^5 points with typical reactor spectra. However, it is unfortunate that this procedure is impractical for the resonance isotopes in the range from 100KeV~1eV[4,5]. In this range, the cross sections exhibit many resonances and hence so that thousands of energy groups would be required for a satisfactory discretization. In general, the number of resonance groups is limited to 5~30 for very coarse group structures including 50~60 energy groups, though SCALE generally uses well over 150. The objective of the resonance treatment is to evaluate the effective cross section for the resonance isotopes in the all resonance energy groups:

$$\sigma_{x,g} = \frac{\int_{\Delta u_g} \sigma_x(u)\phi(u)du}{\int_{\Delta u_g} \phi(u)du} \quad . \tag{3.4.1}$$

In eq. (3.4.1), the lethargy ($u=ln(E_0/E)$, E_0=10MeV) is used instead of the neutron energy and x represents a reaction type. However, the library data available for this purpose are tables of group-dependent resonance integrals (RI) (i.e., the numerator of eq. (3.4.1)) versus temperatures and background cross sections. In CENTRM, the flux in eq. (3.4.1) is calculated by solving the neutron slowing down equation for homogeneous or heterogeneous system.

To describe the slowing down equation in homogeneous infinite system containing a mixture of isotopes, indexed i, of which one is a resonance absorber, the following three assumptions are used:

1) Non-resonance isotopes have negligible absorption and a constant potential scattering cro ss section for the resonance energy range.
2) Resonance isotopes have resonance absorption ($\sigma_{ai}(u)$) and scattering ($\sigma_{rs,i}(u)$) cross sect ions in addition to the potential scattering cross section (σ_{pi}). However, apart from the re sonance energy region, these resonance absorption and scattering cross sections are negli gible.
3) The resonances are so well-separated that the flux between them has its constant asympto tic value (i.e., set to 1).

With these assumptions, the slowing down equation at resonance energy region, and away from fission sources is given by

$$\begin{aligned} &\Sigma(u)\phi(u) = Q(u), \\ &Q(u) = \sum_i \int_{u-\Delta_i}^{u} \Sigma_{si}(u')\phi(u')\frac{\exp(u'-u)}{1-\alpha_i}du', \end{aligned} \tag{3.4.2}$$

where

$$
\begin{aligned}
&\Sigma_{xi} = N_i \sigma_{xi}, \\
&\Sigma_{si}(u) = \Sigma_{pi} + \Sigma_{rs,i}(u), \\
&\Sigma_i(u) = \Sigma_{si}(u) + \Sigma_{ai}(u), \\
&\Sigma(u) = \sum_i \Sigma_i(u), \\
&\alpha_i = (A_i - 1)^2 / (A_i + 1)^2, \\
&\Delta_i = -\ln(\alpha_i).
\end{aligned}
\tag{3.4.3}
$$

In eq. (3.4.3), $\Sigma(u)$ and N are the total macroscopic cross section and atomic number density, respectively and A_i and Δ_i are the atomic mass and the maximum lethargy gain per collision with isotope i, respectively. $1\text{-}\alpha_i$ is the maximum fractional energy loss per collision with isotope i.

In a homogeneous system, for a given composition the self-shielded cross section can be calculated using equations (3.4.1) through (3.4.3) and the corresponding background cross section can be calculated using eq. (3.4.5).

$$
\sigma_b = \frac{\sum_{i=all} N_i \lambda_i \sigma_{i,p}}{N_R}. \tag{3.4.5}
$$

Different background cross sections can be obtained by using various composition mixtures (typically a mixture of ^{1}H and target resonance nuclide), creating a self-shielded cross-section table as a function background cross section. Therefore, for a given composition, the corresponding background cross section can be easily calculated using eq. (3.4.5) and the self-shielded cross section can be read from the table directly.

3.5 Resonance self-shielded data by heterogeneous models

In a heterogeneous system, for a given composition and geometry the self-shielded cross section can also be calculated using equations (3.4.1) through (3.4.3). However, since there is a leakage effect in equation (3.1.1); equation (3.3.1) cannot be used to obtain the corresponding background cross section. Thus, the equivalence theory between the infinite homogeneous and heterogeneous problems was devised by introducing an equivalence cross section (Σ_e) as follows:

$$
\Sigma_b = \lambda \Sigma_p \quad \rightarrow \quad \Sigma_b = \lambda \Sigma_p + \Sigma_e. \tag{3.5.1}
$$

The balance equation with an equivalence theory and an elimination of the scattering resonance ($\lambda \Sigma_{rs}$) thus becomes:

$$
(\Sigma_a + \lambda \Sigma_p + \Sigma_e)\phi = \lambda \Sigma_p + \Sigma_e. \tag{3.5.2}
$$

The background cross section is not a physical quantity but an artificial one used to retrieve the correct self-shielded cross section at a given composition and geometry. It is only important to be consistent in the procedures between its generation and its use. Therefore, the elimination of the scattering resonance is possible as long as consistency is maintained. In a heterogeneous system, the self-shielded scalar flux can be obtained by solving eq. (3.2.1) with a self-shielded absorption cross section obtained by solving eq. (3.1.1). The corresponding background cross section is obtained as follows:

$$\sigma_{g,b} = \frac{\Sigma_{g,b}}{N_R} = \frac{\sum_i N_i \lambda_i \sigma_{i,g,p} + \Sigma_{g,e}}{N_R} = \frac{\sigma_{g,a}\phi_g}{1-\phi_g}. \tag{3.5.3}$$

The following is a procedure to obtain the self-shielded cross section table.

(a) Compute the pointwise slowing down calculations, eq. (3.1.1), by using CENTRM/PMC for the heterogeneous models.
(b) Edit various MG self-shielded cross sections including absorption ($\sigma_{g,a}$), fission ($\sigma_{g,f}$) and scattering ($\sigma_{g,s}$).
(c) Solve the MG fixed source eq. (3.5.4) with $\sigma_{g,a}$ from step (b) to obtain the scalar flux (ϕ_g).

$$\hat{\Omega}\cdot\nabla\psi_{g,k} + \sum_i (\Sigma^k_{i,g,a} + \lambda_{i,g}\Sigma^k_{i,p})\psi_{g,k}(\hat{\Omega}) = \sum_i \lambda_{i,g}\Sigma^k_{i,p} \tag{3.5.4}$$

(d) Obtain the corresponding background cross section ($\sigma_{g,b}$) using eq. (3.5.3) for the heterogeneous model.
(e) Repeat the procedures (a) through (d) by changing the geometry and composition configurations to obtain different background cross sections.
(f) Add infinite dilution cross sections and complete the self-shielded cross section tables as a function of background cross section for $\sigma_{g,a}$, $\sigma_{g,f}$ and $\sigma_{g,s}$.
(g) Repeat the above procedures for various temperatures.

In eq. (3.4.1) the numerator is defined as a resonance integral (RI) with the flux and cross section a function of lethargy instead of Energy. In reference [Sta83], the self-shield cross section is approximated using the background cross section (σ_b) and the resonance integral:

$$\sigma_{g,a}(\sigma_b) = \frac{R_{g,a}(\sigma_b)}{1 - R_{g,a}(\sigma_b)/\sigma_b}, \tag{3.5.5}$$

and

$$\nu\sigma_{g,f}(\sigma_b) = \frac{R_{g,\nu f}(\sigma_b)}{1 - R_{g,a}(\sigma_b)/\sigma_b}, \tag{3.5.5}$$

where $\sigma_{g,a}$ is an absorption cross section, $\sigma_{g,f}$ a fission cross section, ν the number of neutrons released from a fission, and $R_{g,a}$ and $R_{g,\nu f}$ are absorption and ν*fission resonance integrals, respectively. Using equations (3.5.5) and (3.5.6), the self-shield cross section table can be converted into the resonance integral table.

Various background cross sections can be achieved by changing geometrical and compositional configurations as shown in Table 3.5.1.

Table 3.5.1 Example of variations for ^{238}U

Case		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
Volume	Fuel	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	Clad	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	Mod	1.0	1.0	1.0	1.0	1.0	2.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0
Fuel	^{235}U	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.5	0.25	0.125	0.0625	0.03125	0.01	0.01	0.01	0.01
	^{238}U	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.5	0.25	0.125	0.0625	0.03125	0.01	0.001	1.0E-6	1.0E-7
	^{16}O	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.5	0.25	0.125	0.0625	0.03125	0.01	0.01	0.01	0.01
H_2O	^{1}H	2.5E-3	0.2	0.5	0.75	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	^{16}O	2.5E-3	0.2	0.5	0.75	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0

3.6 Resonance self-shielded data by Monte Carlo code

Conceptually this procedure is almost same with the deterministic procedure introduced in Sections 3.4 and 3.5. The only difference is to perform Monte Carlo CE calculations to edit MG self-shielded cross sections instead of performing pointwise slowing down calculation with a deterministic transport code. Either eigenvalue or fixed source Monte Carlo calculations can be performed.

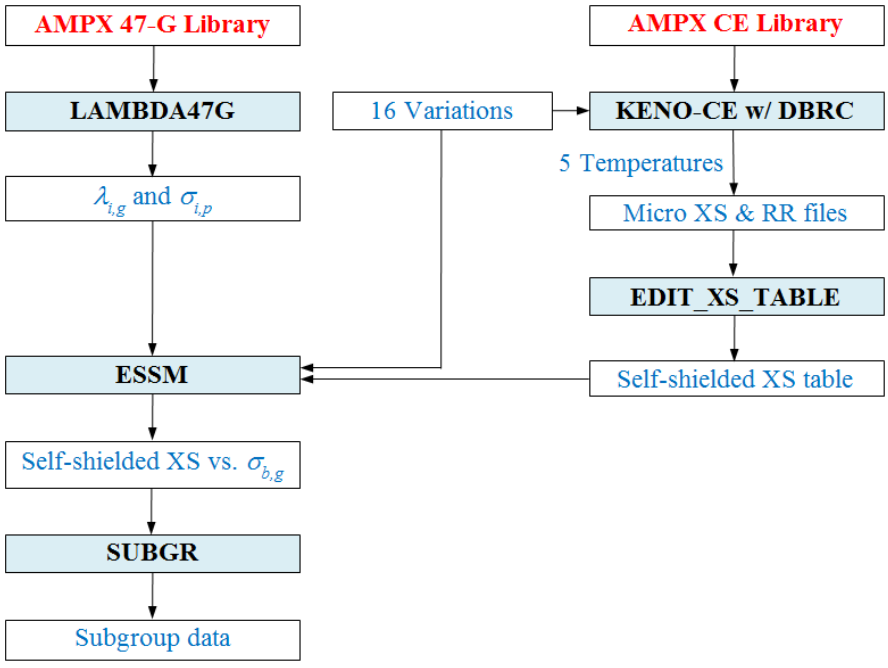


Figure 3.6.1 Procedure to generate resonance data with epithermal upscattering

No deterministic slowing down program is available to consider epithermal upscattering (>5.0 eV). Therefore the Bondarenko f-factor (self-shielded cross section) tables must be generated by performing the continuous energy Monte Carlo calculations and evaluating the corresponding background cross sections [Kim03]. The F-factor tables can be generated by using either homogeneous or heterogeneous models. The key feature of this procedure is to perform the Monte Carlo calculations to obtain MG self-shielded cross sections instead of solving deterministic PW slowing down calculations. In this study, the KENO CE calculations were performed to edit effective microscopic cross sections rather than the CENTRM slowing down calculations. The corresponding background cross sections can be obtained by the same method described in Sections 3.4 and 3.5. The Bondarenko F-factors have been obtained by performing the KENO CE calculations without and with the Doppler Broadening Rejection Correction (DBRC) [Bec10] option to consider the resonance upscattering effect. Figure 3.6.1 provides the procedure to generate resonance data with epithermal upscattering by using KENO-CE.

3.7 Unresolved resonance self-shielded data

In the conventional MG procedure, the Bondarenko f-factor tables at the URR energy groups are generated by using a narrow resonance approximation with a J-function method [Lee11] for which arbitrary background cross-sections are provided. The background cross-section is estimated for the specified composition and geometry, and the self-shielded 1-D cross-sections are read from the f-factor table. This procedure introduces some bias in the self-shielded cross-sections at the URR groups. We are going to solve this problem by improving the overall procedure including a new generation of the f-factor tables for the URR groups.

Typically narrow resonance approximation could be a good solution for the URR energy range in which PW neutron spectrum could be approximated in terms of total and background cross-sections. Since the probability tables are provided at the URR energy range which include cross-section levels and weights, multi-group self-shielded cross-section tables (f-factor table) could be obtained by using a narrow resonance approximation with probability table as follows:

$$\sigma_{x,g}(\sigma_0) = \frac{\int_g \sum_m p^m \sigma_x^m(E)\phi^m(E,\sigma_0)dE}{\int_g \sum_m p^m \phi^m(E,\sigma_0)dE}, \tag{3.7.1}$$

$$\phi^m(E,\sigma_0) = \frac{\sigma_0}{\sigma_t^m(E)+\sigma_0}W(E), \tag{3.7.2}$$

where

σ_0 = background cross-section,
σ_x^m = a cross-section level of the level *m* and reaction *x*,
σ_t^m = a total cross-section level of the level *m*,

p^m = a probability of the level *m*,
$\sigma_{x,g}$ = a self-shielded cross-section of reaction *x*.

3.8 Self-shielded data for within-group elastic scattering

The AMPX MG library does include temperature independent elastic scattering matrix which results in temperature bias when performing self-shielding calculation based on Bondarenko approach. Recently new MT=2022 has been added to consider removal correction to generate temperature dependent elastic scattering matrix. DECLIB has been modified to generate temperature dependent temperature dependent elastic scattering matrix by using pre-obtained temperature dependent background cross sections.

The new MT=2022 is for within-group cross section (σ_g^{within}) for elastic scattering which includes Bondarenko F-factors and 1D data. If background cross section is determined by ESSM or subgroup method, total elastic and within-group elastic cross sections can be obtained through interpolation. Temperature dependent elastic scattering matrix at temperature *T* can be obtained by using the following equations.

$$\tilde{\sigma}_{gg}^{elastic}(T) = \sigma_g^{within}(T)\,. \tag{3.8.1}$$

$$\tilde{\sigma}_{gg'}^{elastic}(T) = \sigma_{gg'}^{elastic}(T_0)\cdot\frac{\sigma_g^{elastic}(T)-\sigma_g^{within}(T)}{\sum_{g'}\sigma_{gg'}^{elastic}(T_0)-\sigma_{gg}^{elastic}(T_0)}\,. \tag{3.8.2}$$

The DECLIB program has been modified to estimate temperature dependent elastic scattering matrix by using eqs. (3.8.1) and (3.8.2) with the nuclide-wise background cross sections.

4. RESONANCE SELF-SHIELDING METHODS

4.1 Subgroup method

Figure 4.1.1 shows the coarse energy group including resonances. Effective self-shielded cross section for this group can be obtained by the following flux weighting:

$$\sigma_{x,g} = \frac{\int_{\Delta u_g} \sigma_x(u)\phi(u)du}{\int_{\Delta u_g} \phi(u)du}, \tag{4.1.1}$$

where $\sigma_{x,g}$ denotes the effective cross section of reaction x at the energy group g, u is lethargy, and $\phi(u)$ the continuos or pointwise sclar flux. Continuous scalar flux can be obtained by solving the slowing down equation with the point-wise cross sections.

In the subgroup method, the resonances are divided by the subgroup levels and the corresponding probability for each subgroup level (σ_{xn}) is defined as the subgroup weight (w_{xn}) as shown in Figure 4.1.1. [Hel03] Therefore, eq. (4.1.1) can be approximated with removing the coarse group index as follows:

$$\sigma_x = \frac{\sum_n w_{xn}\sigma_{xn}\phi_n}{\sum_n w_{an}\phi_n}, \tag{4.1.2}$$

where the summation of the subgroup weights is unity.

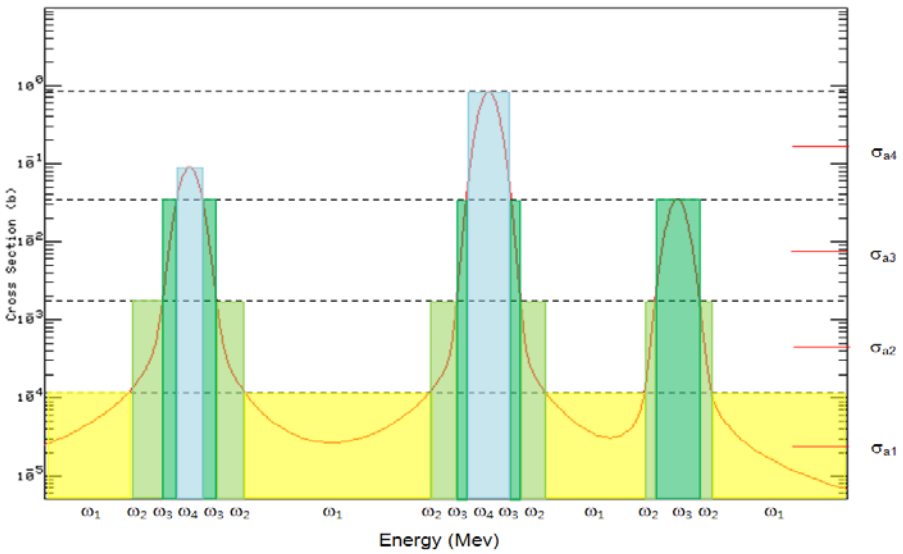


Figure 4.1.1 Resonances and subgroups

In the transport lattice calculation, the final goal of the resonance treatment is to construct a procedure such that the self-shielded cross section estimated by eq. (4.1.2) will be identical to the self-shielded cross section by eq. (4.1.1). The self-shielded sclar flux ϕ_n in eq. (4.1.2) should be estimated from the fixed source transport calculation. If there is only one resonant nuclide, the fixed source transport equation will be

$$\hat{\Omega}\cdot\nabla\psi_n + (N_r\sigma_{an} + \sum_i \lambda_i \Sigma_p^i)\psi_n = \sum_i \lambda_i \Sigma_p^i \,, \tag{4.1.3}$$

and

$$\phi_n = \int \psi_n d\hat{\Omega} \,, \tag{4.1.4}$$

where N_r denotes the particle number density for the resonant nuclide, Σ_p a potential cross section, and ψ_n an angular flux. Equivalence theory enforces that the self-shielded scalar flux is expressed with the absorption (σ_{an}) and the background cross sections (σ_{bn}).

$$\phi_n = \frac{\sigma_{bn}}{\sigma_{an} + \sigma_{bn}} \,. \tag{4.1.5}$$

Typically the background cross section in the heterogeneous model is divided into two parts as follows:

$$\sigma_{bn} = \lambda\sigma_p + \sigma_{en}(\sigma_{an}) \,, \tag{4.1.6}$$

where λ denotes an intermediate resonance parameter, σ_p a potential cross section, and σ_{en} an equivalence cross section. By using eq. (4.1.5), eq. (4.1.2) can be written as follows:

$$\sigma_x = \frac{\sum_n w_{xn}\sigma_{xn}\dfrac{\sigma_{bn}}{\sigma_{an}+\sigma_{bn}}}{1-\sum_n w_{an}\dfrac{\sigma_{an}}{\sigma_{an}+\sigma_{bn}}} \,. \tag{4.1.7}$$

Therefore, if the subgroup levels and weights are given for a certain nuclide, the effective self-shielded cross section can be obtained by estimating the corresponding background cross sections (σ_{bn}) in the lattice calculation. Since the equivalence cross section is not sensitive to the absorption cross section, but to the geometrical configuration, σ_{bn} is often approximated by a single background cross section σ_b. Eq. (4.1.7) can be written as follows:

$$\sigma_x = \frac{\sum_n w_{xn}\sigma_{xn}\dfrac{\sigma_b}{\sigma_{an}+\sigma_b}}{1-\sum_n w_{an}\dfrac{\sigma_{an}}{\sigma_{an}+\sigma_b}}. \tag{4.1.8}$$

If there are several resonant nuclides, there will be a resonant interference between the resonant nuclides. Since this interference will affect on the self-shielded scalar flux, eq. (4.1.8) can be written as follows:

$$\sigma_x = \frac{\sum_n w_{xn}\sigma_{xn}\dfrac{\sigma_b}{\sigma_{an}+\hat{\sigma}_a+\sigma_b}}{1-\sum_n w_{an}\dfrac{\sigma_{an}}{\sigma_{an}+\hat{\sigma}_a+\sigma_b}}, \tag{4.1.9}$$

where $\hat{\sigma}_a$ is the total absorption cross section of the other resonant nuclides. The effective self-shielded cross sections are estimated iteratively.

4.2 Subgroup data generation

The resonance integral (RI_x) is defined as the numerator of eq. (4.1.1), and the resonance integral divided by lethargy width is also called resonance integral (R_x). The resonance integral can be written by using the subgroup weights and levels from eq. (4.1.7) as follows:

$$R_x = \sum_n w_n\sigma_{xn}\frac{\sigma_{bn}}{\sigma_{an}+\sigma_{bn}} \approx \sum_n w_n\sigma_{xn}\frac{\sigma_b}{\sigma_{an}+\sigma_b}. \tag{4.2.1}$$

Since the denominator of eq. (4.1.1) can be understood as a scalar flux (ϕ) for the coarse energy group, eq. (4.1.1) can be rewritten as follows:

$$\sigma_x = \frac{R_x}{\phi}. \tag{4.2.2}$$

As described in Section 3.5, the constituent compositions and the geometrical configurations are varied to obtain various background cross sections to complete the resonance integral table. Index '*k*' for the variation cases can be added to eq. (4.2.2).

$$\sigma_{x,k} = \frac{R_{x,k}}{\phi_k} \quad (k = 1, 2, \ldots, K). \tag{4.2.3}$$

The resonance integral ($R_{x,k}$) can be estimated directly from the IRFFACTOR program for the variation cases. The subgroup levels and weights can be obtained from eqs. (4.2.1) by the least

square fitting to minimize the difference between the original resonance integral and the reconstructed resonance integral using eq. (4.2.1).

Subgroup levels are arbitrary given and the corresponding subgroup weights are obtained by minimizing the following function *f*.

$$f(w_1,\ldots,w_K)=\sum_k \frac{1}{R_{x,k}^2}\left(R_{x,k}-\sum_n w_{xn}\sigma_{xn,k}\frac{\sigma_{bn,k}}{\sigma_{an,k}+\sigma_{bn,k}}\right)^2. \tag{4.2.4}$$

$$f(w_1,\ldots,w_K)=\sum_k \frac{1}{R_{x,k}^2}\left(R_{x,k}-\sum_n w_{xn}\sigma_{xn,k}\frac{\sigma_{b,k}}{\sigma_{an,k}+\sigma_{b,k}}\right)^2. \tag{4.2.5}$$

Subgroup levels are to be automatically adjusted to minimize the difference between the original resonance integral and the reconstructed resonance integral using the subgroup levels and weights. The resonance integral table from the IRFFACTOR calculation includes the background cross sections as a function of absorption cross section at each variation *k* to cover all the subgroup levels. Although the subgroup levels are varied at iterations, the corresponding background cross section($\sigma_{bn,k}$) can be obtained through the interpolation of the given table. SUBGR includes two options to generate the subgroup weights and levels by using eqs. (4.2.4) and (4.2.5) which use the level dependent and constant background cross sections, respectively.

When the resonance interference is neglected, errors in estimating the effective self-shielded cross section come mainly from the subgroup levels and weights themselves, and the scalar flux estimation. In the real application the self-shielded scalar flux is estimated by the following equation.

$$\hat{\phi}_k = 1-\sum_n w_{an}\frac{\sigma_{an,k}}{\sigma_{an,k}+\sigma_{bn,k}}, \tag{4.2.6}$$

where the subgroup weights and levels are given and the corresponding background cross sections ($\sigma_{bn,k}$) are obtained by the fixed source transport calculations of the transport lattice code using eq. (4.1.3). The difference between the scalar flux(ϕ_k) in eq. (4.2.3) and the scalar flux($\hat{\phi}_k$) in eq. (4.2.6) causes a difference in the effective self-shielded cross section.

In order to remove this error a new method [Joo09] has been proposed recently to generate the subgroup weights, in which the subgroup weights are to be estimated to conserve the self-shielded cross sections as follows:

$$f(w_1,\ldots,w_K)=\sum_k \frac{1}{R_{x,k}^2}\left(\hat{R}_{x,k}-\sum_n w_{xn}\sigma_{xn,k}\frac{\sigma_{bn,k}}{\sigma_{an,k}+\sigma_{bn,k}}\right)^2, \tag{4.2.7}$$

where

$$\hat{R}_{x,k}=\sigma_{x,k}\hat{\phi}_k=\sigma_{x,k}\left(1-\sum_n w_{an}\frac{\sigma_{an,k}}{\sigma_{an,k}+\sigma_{bn,k}}\right). \tag{4.2.8}$$

4.3 Subgroup method for non-uniform temperature distribution

In a heterogeneous system, the self-shielded resonance cross sections are estimated from the self-shielded scalar fluxes obtained by the following fixed source transport equation.

$$\hat{\Omega}\cdot\nabla\psi_{g,m}+\sum_i(\Sigma^m_{i,a,g}+\lambda_{i,g}\Sigma_{i,p})\psi_{g,m}(\hat{\Omega})=\sum_i\lambda_{i,g}\Sigma_{i,p}\,, \tag{4.3.1}$$

where subscript *m* denotes a problem case with different absorption cross section levels at energy group *g*. In eq. (4.3.1), $\Sigma_{i,a,g}$ and $\Sigma_{i,p}$ denote macroscopic absorption and potential cross sections of nuclide *i*, respectively, and $\lambda_{i,g}$ intermediate resonance parameter.

Eq. (4.3.1) should be modified for the resonance transport calculations involving non-uniform temperature distribution in which the macroscopic absorption cross sections should include the temperature distribution as follows:

$$\Sigma^m_{i,a,g}=N_i\sigma^m_{i,a,g}(T_{ave.})\frac{\sigma^m_{i,a,g}(T)}{\sigma^m_{i,a,g}(T_{ave.})}\approx N_i\sigma^m_{i,a,g}(T_{ave.})\,f_{i,a,g}(T)\,, \tag{4.3.2}$$

where *T* and $T_{ave.}$ are local and volume-averaged temperatures, respectively. While the function *f(T)* was approximated by the following equation [Wem07].

$$f_{i,a,g}(T)=\frac{R_{i,a,g}(T,\sigma_p)}{R_{i,a,g}(T_{ave.},\sigma_p)}\cdot\frac{\sigma_p-R_{i,a,g}(T_{ave.},\sigma_p)}{\sigma_p-R_{i,a,g}(T,\sigma_p)}\,, \tag{4.3.3}$$

where

$$\sigma_p\approx\frac{\sum_{j=all}N_j\lambda_{j,g}\sigma_{j,p}}{N_i}\,, \tag{4.3.4}$$

N_i is the particle number density of nuclide *i*, and $R_{i,a,g}$ resonance integral. Eq. (4.3.4) can be rewritten without any approximation as follows:

$$\sigma^m_{b,g}=\frac{\sum_{j=all}N_j\lambda_{j,g}\sigma_{j,p}+\Sigma^m_{e,g}}{N_i}\,. \tag{4.3.5}$$

Therefore the explicit equation will be

$$f^m_{i,a,g}(T)=\frac{\sigma^m_{i,a,g}(T)}{\sigma^m_{i,a,g}(T_{ave})}=\frac{R_{i,a,g}(T,\sigma^m_{b,g})}{R_{i,a,g}(T_{ave.},\sigma^m_{b,g})}\cdot\frac{\sigma^m_{b,g}-R_{i,a,g}(T_{ave.},\sigma^m_{b,g})}{\sigma^m_{b,g}-R_{i,a,g}(T,\sigma^m_{b,g})}\,. \tag{4.3.6}$$

When performing a MPACT calculation with T-H feedback, $\Sigma^m_{e,g}$ can be obtained from the previous outer iteration.

Another better approximation is to get the correction factor from the previous step as follows:

$$\Sigma_{i,a,g}^{m(\ell+1)} = N_i \sigma_{i,a,g}^{m}(T_{ave.}) \frac{\sigma_{i,a,g}^{m}(T)}{\sigma_{i,a,g}^{m}(T_{ave.})} \approx N_i \sigma_{i,a,g}^{m}(T_{ave.}) \frac{\sigma_{i,a,g}^{(\ell)}(T)}{\sigma_{i,a,g}^{(\ell)}(T_{ave.})}. \quad (4.3.7)$$

4.4 Embedded self-shielding method (ESSM)

ESSM [Hon11, Wil12] has been developed for the resonance self-shielding calculation which requires the fixed source transport calculations in estimating background cross sections. When estimating resonance self-shielded cross section by ESSM, absorption cross sections ($\Sigma_{i,a,g}$) at fuel and cladding are iteratively determined by solving the fixed source transport eq. (4.4.1).

$$\hat{\Omega} \cdot \nabla \varphi_g(\hat{\Omega}_m) + \sum_j (\Sigma_{j,a,g} + \lambda_{j,g} \Sigma_{j,p}) \varphi_g(\hat{\Omega}_m) = \sum_j \lambda_{j,g} \Sigma_{j,p}, \quad (4.4.1)$$

$$\hat{\Omega} \cdot \nabla \varphi_g(\hat{\Omega}_m) + \Sigma_{t,g} \varphi_g(\hat{\Omega}_m) = S_g, \quad (4.4.2)$$

where φ_g is an angular flux of group g, $\Sigma_{j,a,g}$ a macroscopic absorption cross section of nuclide j, $\Sigma_{j,p}$ a macroscopic potential cross section and $\lambda_{j,g}$ an intermediate resonance parameter. The corresponding macroscopic and microscopic background cross sections can be obtained by using the following eq. (4.4.3).

$$\Sigma_{i,b,g} = \frac{\Sigma_{i,a,g} \phi_{i,g}}{1 - \phi_{i,g}} \quad \rightarrow \quad \sigma_{i,b,g}^{j} = \frac{\Sigma_{i,b,g}}{N_{i,j}}. \quad (4.4.3)$$

Self-shielded absorption cross sections for each nuclide can be read from the Bondarenko F-factor tables in the AMPX MG library [Dun02], and the absorption cross sections are utilized in updating $\Sigma_{j,a,g}$. And then the same ESSM calculation will be performed. This iteration procedure will be continued until the macroscopic background cross sections ($\Sigma_{i,b,g}$) are converged.

There are several issues associated with ESSM as follows:

- Counter influence between cladding and fuel in ESSM
- ESSM with correction factors for non-uniform temperature distribution

The above issues are discussed in detail and probable solutions are proposed for some issues.

5. GENERATION OF MISCELLANEOUS DATA

5.1 Transport cross sections for ^{1}H

The MOC eigenvalue calculation with high order ($\geq P_2$) scattering requires 2 times longer computing time compared to the P_0 calculation. Typically most of transport lattice codes are utilizing out-scattering based transport corrected P_0 (TCP_0) scattering matrix in which diagonal terms of P_0 scattering matrix are subtracted by total P_1 scattering cross sections. The P_1 corrected P_0 scattering matrix for ^{1}H may include negative value in the diagonal components which causes negative flux resulting in convergence error. Another issue of out-scattering based transport correction does show significant global power tilt for whole core problems including reflector. Therefore a proper transport correction method is needed to have reasonable neutron leakage as high order scattering is considered and to guarantee no negative flux.

The Neutron Leakage Conservation method ($NLCP_0$) [Her13] used in the CASMO series for long time has been used to generate transport cross sections for ^{1}H. The goal of $NLCP_0$ is to obtain diffusion coefficients to have same neutron leakage as obtained in the high order scattering transport calculation as follows:

$$\hat{\Omega}\cdot\nabla\varphi_g(\hat{\Omega}) = -D_g\nabla^2\phi_g\,. \tag{5.1.1}$$

When we have a 1D model, neutron leakages at the specified surfaces can be obtained from the high order scattering transport calculation.

$$Leakage = J_{right} - J_{left}\,. \tag{5.1.2}$$

We can determine diffusion coefficients to have same leakage in the diffusion calculation by using the following derivation.

$$-D\nabla^2\phi + \Sigma_a\phi = \frac{1}{k_{eff}}\nu\Sigma_f\phi\,. \tag{5.1.3}$$

$$\nabla^2\phi + B^2\phi = 0 \rightarrow \frac{\partial^2}{\partial x^2}\phi(x) + B^2\phi(x) = 0\,. \tag{5.1.4}$$

$$\phi(x) = \cos(Bx)\,. \tag{5.1.5}$$

$$J_{right} - J_{left} = \int_0^W dx(-D\frac{\partial^2}{\partial x^2}\phi(x)) = \int_0^W dxDB^2\phi(x) = DB^2\int_0^W dx\phi(x) = DB^2\hat{\phi}\,. \tag{5.1.6}$$

$$D = \frac{J_{right} - J_{left}}{B^2\hat{\phi}}. \tag{5.1.7}$$

$$B^2_{geom} = \left(\frac{\pi}{W}\right)^2. \tag{5.1.8}$$

When performing the multigroup transport calculation with high order scattering, it is required to check if the group-wise bucklings are constant independently upon energy group. This work can be completed by drawing normalized neutron spectrum shape for each group.

$$B_{geom}^2 = B^2 = B_g^2 . \tag{5.1.9}$$

We can obtain multi-group diffusion coefficients and transport cross sections.

$$D_g = \frac{J_{g,right} - J_{g,left}}{B^2 \hat{\phi}_g} . \tag{5.1.10}$$

$$\Sigma_{tr,g} = \frac{1}{3D_g} . \tag{5.1.11}$$

The computational model was from the reference paper [Her13] as follows:

- 1-D slab 100 cm w/ vacuum boundary, 0.005 cm mesh size
- All ^{1}H with 4.780E+23 atom/cm^3
- 9 temperatures : 293.6, 350.0, 400.0, 450.0, 500.0, 550.0, 600.0, 650.0, 800.0 K
- Source : ^{235}U fission spectrum with buckled Cosine spatial distribution

This work can be done by using either continuous energy Monte Carlo or multigroup deterministic transport codes. A new 1D MOC code including high order scattering capability has been developed to generate transport corrected ^{1}H cross sections. Figure 5.1.1 provides the 47-group transport correction factors for ^{1}H with various temperatures.

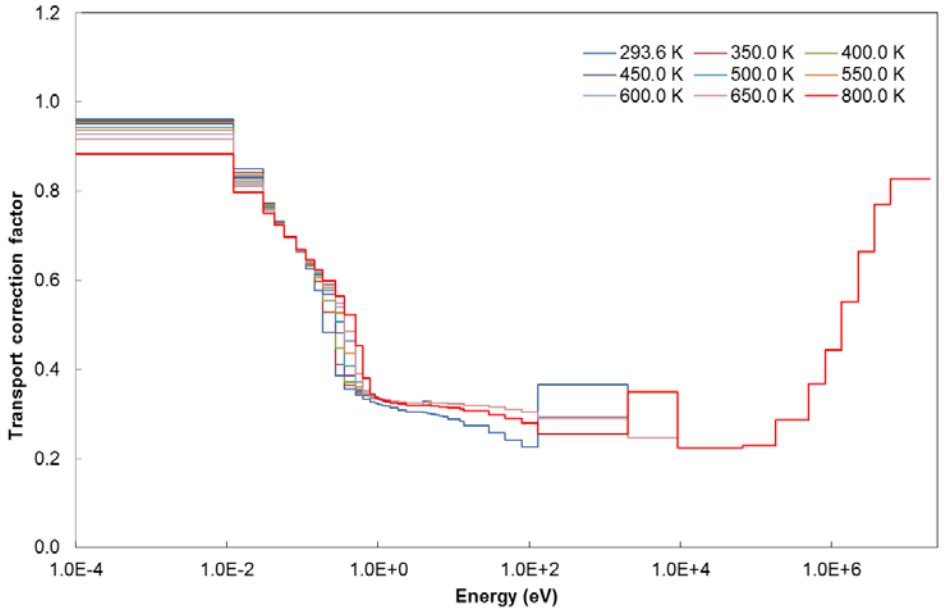


Figure 5.1.1 47-group transport correction factors for ^{1}H

5.2 Transient data

Since the ORNL AMPX code package [Wia14] does not support to generate transient data such as decay constants and delayed neutron fractions, the NJOY program [Mac94] developed at LANL has been utilized to generate the transient data. Since there was no information for the ENDF/B nuclides including transient data, the NJOY input files were generated for all 37 heavy nuclides in the MPACT library. Tape 24 from the GROUPR module includes 47-group neutron data including transient data. A simple editing program has been developed to edit transient data such as decay constants and delayed neutron fractions. In order to obtain total number of neutrons released per fission to be used in obtaining delayed neutron fraction, typical 47-group PWR spectrum has been obtained from the VERA progression problem 1b as shown Figure 5.2.1.

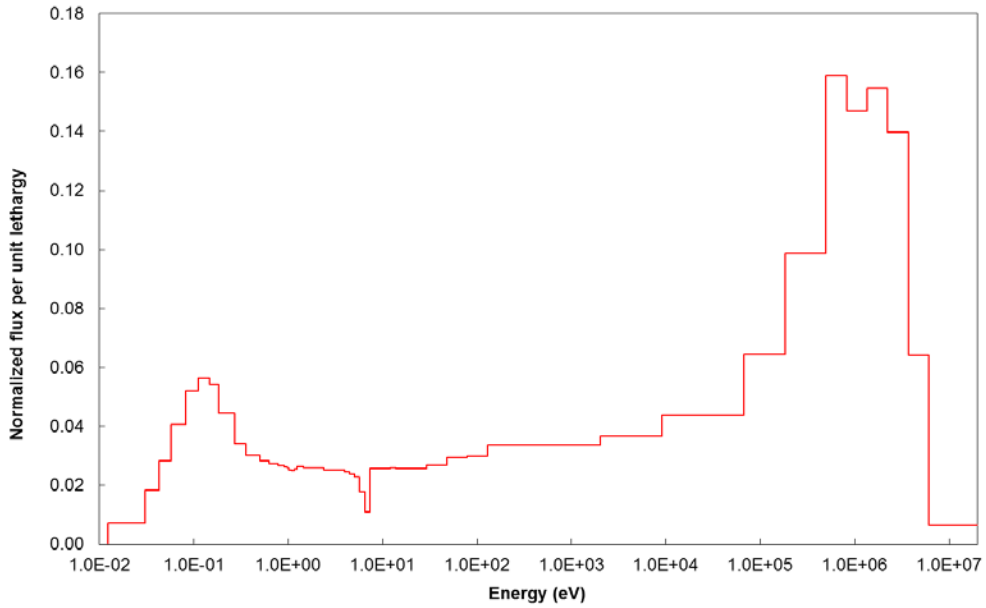


Figure 5.2.1 47-group weighting function

The ENDF/B-7.0 and 7.1 neutron data include transient data only for 21 nuclides. Figure 5.2.2 provides transient data including nuclide identification, total number of neutrons released per fission, decay constants and delayed neutron fractions for each nuclide.

```
       90232  2.417105E+00
1.240000E-02  3.340000E-02  1.210000E-01  3.210000E-01  1.210000E+00  3.290000E+00
8.237550E-04  2.839532E-03  3.391569E-03  9.961879E-03  3.760367E-03  1.827437E-03
       91231  2.429466E+00
1.240000E-02  3.340000E-02  1.210000E-01  3.210000E-01  1.210000E+00  3.290000E+00
3.772028E-04  1.018876E-03  7.348728E-04  1.774840E-03  4.798565E-04  1.831329E-04
       91233  2.429815E+00
1.240000E-02  3.340000E-02  1.210000E-01  3.210000E-01  1.210000E+00  3.290000E+00
7.746643E-04  2.092295E-03  1.509164E-03  3.645136E-03  9.855432E-04  3.761569E-04
       92233  2.500074E+00
```

```
 1.247938E-02  3.227449E-02  1.046448E-01  2.941518E-01  1.242443E+00  1.022323E+01
 2.567975E-04  7.701037E-04  5.537597E-04  1.142208E-03  2.146458E-04  2.239787E-05
        92234  2.633240E+00
 1.248240E-02  3.129530E-02  1.074630E-01  3.032230E-01  1.288730E+00  1.044220E+01
 2.754770E-04  1.165225E-03  8.999964E-04  2.034102E-03  4.624642E-04  6.164186E-05
        92235  2.438879E+00
 1.249056E-02  3.182406E-02  1.093753E-01  3.169898E-01  1.353983E+00  8.636377E+00
 2.183402E-04  1.136937E-03  1.102438E-03  3.142815E-03  9.126013E-04  3.225451E-04
        92236  2.585205E+00
 1.248999E-02  3.068560E-02  1.091980E-01  3.224705E-01  1.378583E+00  1.021014E+01
 2.294104E-04  1.726554E-03  1.473179E-03  3.893188E-03  1.382420E-03  2.693897E-04
        92237  2.556079E+00
 1.249577E-02  3.037978E-02  1.068975E-01  3.240317E-01  1.334253E+00  9.544175E+00
 2.081865E-04  2.419830E-03  2.019126E-03  6.103966E-03  2.421639E-03  5.043196E-04
        92238  2.788314E+00
 1.249423E-02  3.025520E-02  1.159376E-01  3.414764E-01  1.318630E+00  9.979027E+00
 1.631869E-04  1.811873E-03  2.016816E-03  7.130047E-03  3.684767E-03  9.734561E-04
        93237  2.943373E+00
 1.248610E-02  3.077587E-02  1.065464E-01  3.139911E-01  1.334211E+00  1.050869E+01
 1.169523E-04  7.177156E-04  6.106869E-04  1.677948E-03  4.688961E-04  8.045746E-05
        94238  2.992942E+00
 1.332500E-02  3.117100E-02  1.161500E-01  2.888400E-01  8.561400E-01  2.713800E+00
 5.261947E-05  3.337788E-04  2.202819E-04  4.974348E-04  2.221220E-04  7.038188E-05
        94239  2.867711E+00
 1.248110E-02  2.994667E-02  1.071553E-01  3.176193E-01  1.352380E+00  1.069116E+01
 7.441243E-05  6.029267E-04  4.208394E-04  8.788662E-04  2.338068E-04  3.832867E-05
        94240  3.081800E+00
 1.332900E-02  3.051000E-02  1.151600E-01  2.974000E-01  8.476600E-01  2.879600E+00
 9.336029E-05  7.385726E-04  4.404519E-04  9.638943E-04  5.243305E-04  1.597601E-04
        94241  2.946479E+00
 1.359900E-02  2.996600E-02  1.167300E-01  3.069100E-01  8.701000E-01  3.002800E+00
 9.923741E-05  1.233243E-03  7.840723E-04  1.920227E-03  1.086294E-03  3.750161E-04
        94242  3.146448E+00
 1.360300E-02  3.023800E-02  1.154300E-01  3.041900E-01  8.272100E-01  3.137200E+00
 1.229591E-04  1.449077E-03  7.864419E-04  2.042159E-03  1.412084E-03  4.483058E-04
        95241  3.236158E+00
 1.333800E-02  3.079800E-02  1.130500E-01  2.867700E-01  8.653600E-01  2.643000E+00
 4.687282E-05  3.351367E-04  2.062589E-04  4.438472E-04  2.274633E-04  5.988720E-05
        95243  3.564782E+00
 1.349900E-02  2.975900E-02  1.137700E-01  2.985900E-01  8.820200E-01  2.811100E+00
 5.213651E-05  6.568510E-04  3.428585E-04  7.020686E-04  3.694160E-04  1.071179E-04
        96242  3.753388E+00
 1.295600E-02  3.124500E-02  1.129100E-01  2.783400E-01  8.710400E-01  2.196900E+00
 2.760101E-05  1.027275E-04  5.117072E-05  1.024804E-04  6.385763E-05  1.359061E-05
        96245  3.597515E+00
 1.340000E-02  3.070000E-02  1.130000E-01  3.001000E-01  8.340000E-01  2.768600E+00
 3.942668E-05  3.180151E-04  2.974124E-04  6.592391E-04  3.654310E-04  9.948328E-05
        98249  3.888388E+00
 1.351700E-02  2.945000E-02  1.053200E-01  2.929800E-01  8.474900E-01  2.469800E+00
 1.709062E-05  2.721421E-04  9.365231E-05  1.804290E-04  1.120952E-04  1.896568E-05
        98251  4.140665E+00
 1.569700E-02  2.883000E-02  1.076900E-01  3.245800E-01  8.837100E-01  2.631400E+00
 9.953225E-06  6.522987E-04  3.156976E-04  4.898075E-04  3.069656E-04  4.397731E-05
```

Figure 5.2.2 Transient data from ENDF/B-7.0

5.3 Effective recoverable energy per fission

The energy release per fission is required for burnup calculations, and is usually defined without the kinetic energy of the incident neutrons and the energy carried away by neutrinos. However, the energy release per fission includes the contributions from the kinetic energy of incident neutrons and from the decay of the capture products:

$$W^i_{fiss} = E^i_r + Q^i_c + W^i_n , \tag{5.3.1}$$

where W^i_{fiss} is the effective energy release in fission, E^i_r is the energy release in fission excluding the energy carried away by neutrinos and the kinetic energy of the incident neutrons, Q^i_c is the contribution from the decay of the capture products, and W^i_n is the kinetic energy of the incident neutrons. Index *i* refers to a fissionable nuclide in all cases.

E^i_r values are extracted from the MF=1/MT=458 section of an evaluated nuclear data file, while the kinetic energy of the incident neutron is obtained by approximately averaging the energy with the fission reaction rate. The averaging process involved the multi-group approximation and the cross sections obtained from the MCNP calculations based on ENDF/B cross section data:

$$W^i_n = \frac{\sum_g \overline{E}_g \sigma^i_{f,g} \phi_g}{\sum_g \sigma^i_{f,g} \phi_g}, \tag{5.3.2}$$

where $\sigma^i_{f,g}$ is the microscopic fission cross section of the fissionable nuclide *i* in the energy group *g*, ϕ_g is the neutron spectrum, and E_g is the average group energy. A typical PWR fuel pin was used in this calculation.

The average group energy was a simple mean of the group boundary values, except for the highest energy groups for which more accurate values were adopted to give the average energy in a Maxwellian fission spectrum at a temperature corresponding to 1.4 MeV:

$$E_g = \frac{\int_g E\sqrt{E} \cdot \exp(-E/T) dE}{\int_g \sqrt{E} \cdot \exp(-E/T) dE}. \tag{5.3.3}$$

The additional energy released due to gamma activation is calculated from

$$Q_c = (\overline{\nu} - 1) Q , \tag{5.3.4}$$

where ($\overline{\nu}$ -*1*) represents the average number of neutrons that are captured, and *Q*=6.1 MeV [Jam99].

5.4 Effective background cross sections

While the AMPX MG library includes resonance data for all nuclides and energy groups, the MPACT library includes resonance data for the specified nuclides and energy groups. For example, 49 nuclides include subgroup data and resonance integral tables and 191 nuclides out of 295 include IR parameters only for groups 10~26. If infinitely dilute cross sections are provided in the MPACT MG library, the MPACT results would underestimate the multiplication

factors at very high burnup points due to higher capture cross sections. Therefore, pre-self-shielded cross sections need to be included in the MPACT MG library.

At low burnup points heavy and fission product nuclides produced by decay and neutron reactions do not significantly contribute on the multiplication factor due to tiny amount of atomic number densities. It is reasonable to determine high burnup point at which background cross sections are estimated to be used in obtaining 1D self-shielded cross sections. This work can be done by the MPACT single pin depletion calculation to obtain atomic number density at high burnup point (50 MWD/kgU) and then effective microscopic background cross sections can be obtained from the MPACT subgroup or ESSM calculations.

6. GENERATION OF THE MPACT MG LIBRARY

6.1 Generation of the initial AMPX MG library

The AMPX MG library can be generated by using the program EXSITE by which all the AMPX module input files for all nuclides can be automatically prepared through expanding a template shown in Figure 6.1.1. Figure 6.1.2 provides the AMPX procedure to generate the AMPX MG library where the left side of flow chart is for the conventional procedure and the right side for new procedure to improve the Bondarenko resonance data. The following data are required in generating the AMPX MG library.

- ENDF/B-VII neutron cross section data
- ENDF/B-VII listing file
- ENDF/B-VII Doppler broadening data files
- ENDF/B-VII probability table files
- Pointwise weighting function

```
=neutron_mg
master=result/neut_
temperature=293
broaden=/home/c31/exsite/result/broaden_
neutgroups=47
thermalgroups=26 neutuserdef=yes
neutbounds=<1.000000E-6 1.239596E-2 3.061288E-2 4.275520E-2 5.692194E-2 8.196816E-2 1.115699E-1
1.457206E-1 1.844302E-1 2.705213E-1 3.576701E-1 5.032318E-1 6.250621E-1 7.820830E-1 9.099967E-1
9.710043E-1 1.013699E+0 1.072203E+0 1.125397E+0 1.166404E+0 1.235105E+0 1.457402E+0 1.855391E+0
2.382393E+0 3.927903E+0 4.450897E+0 5.043477E+0 5.715008E+0 6.476017E+0 7.338215E+0 8.315287E+0
1.209903E+1 1.371000E+1 2.902291E+1 4.785117E+1 7.889325E+1 1.300704E+2 2.034700E+3 9.118801E+3
6.737900E+4 1.831601E+5 4.978702E+5 8.208500E+5 1.353400E+6 2.231299E+6 3.678800E+6 6.065300E+6
2.000000E+7>
weightuser=yes
weighttab1=/home/dw8/libraries/endf7.1/mg/252/casl_lib_flux
makeyield=no
thermcut=5.05 thermsplice=5 thinthermal=yes
makethermal=yes
thermaltemp=<293.0 600.0 900.0 1200.0 2400.0>
input=input/neut_
evals=/neptune/home02/ykk/libraries/endf7.0/endf7.0.xml
end

=bondarenko_prob
master=result/bond_
broaden=/home/c31/exsite/result/broaden_
n1d=result/neut_ temperature=293
prob=/home/c31/exsite/result/ptable_
weightuser=yes
weighttab1=/home/dw8/libraries/endf7.1/mg/252/casl_lib_flux
sig0=<1.0E8 1000000.0 100000.0 10000.0 5000.0 2000.0 1000.0 640.0 320.0 160.0 120.0 80.0 40.0 20.0
10.0 4.0 1.0 1.0E-6>
temps=<293.0 600.0 900.0 1200.0 2400.0>
input=input/bond_
evals=/neptune/home02/ykk/libraries/endf7.0/endf7.0.xml
end

=bind_mg
master=result/master_ neutron=result/neut_
addfree=yes addbond=yes bond=result/bond_
input=input/bind_
evals=/neptune/home02/ykk/libraries/endf7.0/endf7.0.xml
end
```

Figure 6.1.1 Sample template to generate the AMPX input files

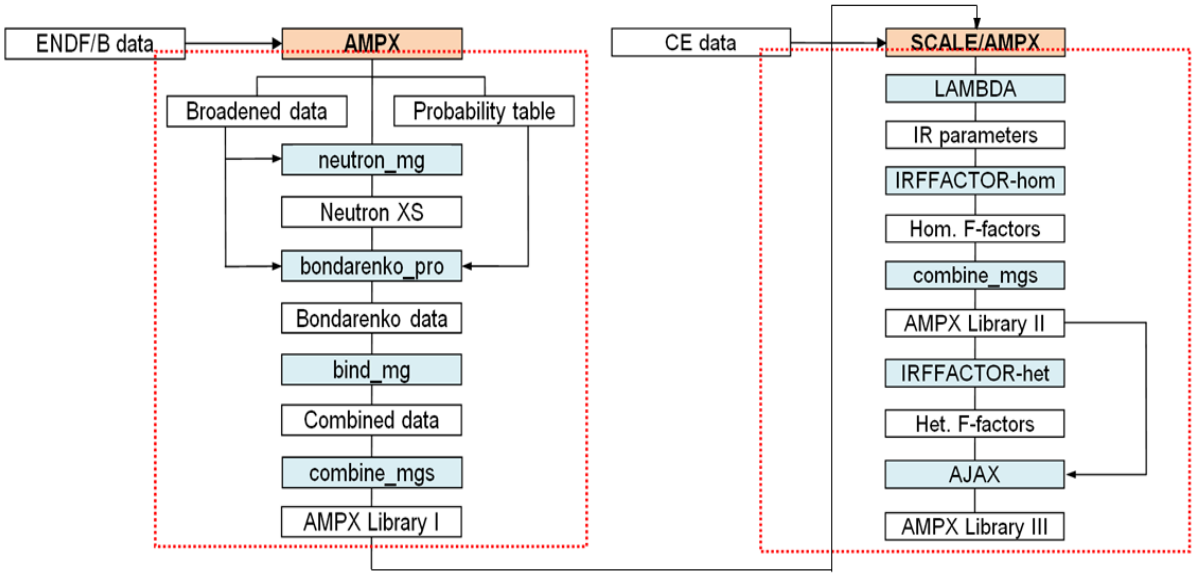


Figure 6.1.2 Flow chart of the AMPX procedure

After completing the AMPX calculations for all nuclides, individual MG data files can be merged into an AMPX MG library (I) by the AMPX AJAX module.

6.2 Intermediate resonance parameters and Homogeneous F-factors

The intermediate resonance (IR) parameters are generated for all nuclides by using the AMPX-LAMBDA module with a procedure introduced in Section 3.3 in which the IR parameters are estimated only for the specified energy groups (for example, the 47-g library for groups 10~46) and unity is assigned to other energy groups. In addition homogeneous F-factors are generated for the same energy groups for the IR parameters by the AMPX-IRFFACTOR-hom module with a procedure described in Section 3.4 which are substituted for the original F-factors.

Figure 6.2.1 provides a template to be expanded to generate the LAMBDA and IRFFACTOR-hom input files for all nuclides. An expanded sample input for ^{235}U is shown in Appendix A.1. Figure 6.2.2 provides a flow chart of the resonance data generation procedure in which pointwise slowing down calculations are performed by CENTRM. The following data are included in the AMPX MG master library.

- Intermediate resonance parameters : all nuclides, all energy groups
- Homogeneous F-factors : Nuclides Atomic number $\geq$ 40 (Zr)

```
=ffactors
master=/home/ykk/libraries/endf7.0/mg/47g/ampx47g_70_07182014_00_ykk.bin
cedesc=/scale/scale_dev_data/ce_v7.0_endf
cedatadir=ln -fs /scale/scale_dev_data/cekenolib_7.0
kernels=/scale/scale_dev_data/endf_b/vers7
low=10 high=46
out=irflib/irf
input=input/in_
evals=/neptune/home02/ykk/libraries/endf7.0/endf7.0.xml
end
```

Figure 6.2.1 Sample template to generate the IR parameters and homogeneous F-factors

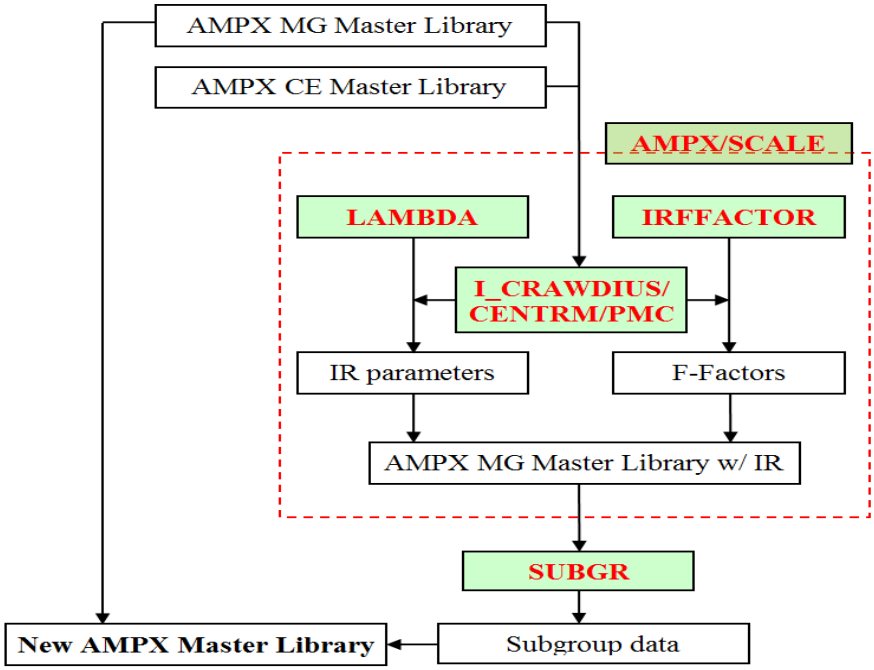


Figure 6.2.1 Flow chart of the resonance data generation procedure

6.3 Heterogeneous F-factors

Only selected nuclides include heterogeneous F-factors which are very important resonance nuclides significantly impacting on the neutronics result. The following 20 nuclides have been selected to have heterogeneous F-factors. Option for level dependent background cross sections has been used for all nuclides except for Ag, In and Cd nuclides.

- ^{107}Ag, ^{109}Ag, ^{113}Cd, ^{113}In, ^{115}In, ^{155}Gd, ^{156}Gd, ^{157}Gd, ^{158}Gd, ^{232}Th, ^{233}U, ^{235}U, ^{236}U, ^{238}U, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am

The IRFFACTOR-het input file for ^{238}U to generate heterogeneous F-factors is shown in Figure 6.3.1 and a companion input file for various geometrical and compositional configurations is provided in Appendix B.1. Since typically Bondarenko approach is not able to consider resonance interference effect explicitly, heterogeneous F-factors can be generated in two different ways with or without considering explicit resonance interference. 'Single' and 'Multiple' indicate without and with resonance interference, respectively. Both models are applied only to 5 heavy nuclides including ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, and ^{241}Pu.

The Heterogeneous IRFFACTOR results in two F-factor tables of which the first one can be incorporated by the AMPX-AJAX and the second one (subgrpdata) is for SUBGR to generate subgroup data. The first one (or the AMPX MG master library) also can be utilized in the subgroup data generation. However, in order to generate subgroup data by using eq. (4.2.7) to conserve cross sections, subgroup level dependent background cross sections should be added to the F-factor tables (self-shielded cross section table). The AMPX MG library does not include the subgroup level dependent background cross sections, but the 'subgrpdata' file includes them.

```
' ------------------------------------------------------------------------
' Heterogeneous irffactor for U-238 :: multiple absorber ENDF/B-VII.0
' ------------------------------------------------------------------------
=shell
ln -sf $RTNDIR/../cases/U238-HetCases-new.inp het_input
ln -sf /home/ykk/libraries/endf7.0/mg/47g/ffactor/ampx47g_70_07182014_01_ykk.bin  ft88f001
end

=irffactor
 in=88 out=92 fnuc=92238 medit=3 essm=yes nterp=1
 absopt=1 mopt=3  removal=yes
 cellfil="het_input"
 ehres=20.0E+03
 subgrxs= 1.0 5.0 10.0 50.0 100.0 500.0 1000.0 5000.0 10000.0 20000.0  end
end

=shell
mv  ft92f001 $RTNDIR/U238_ffactors_multiple_m3
mv  subgrpdata $RTNDIR/subgrpdata_U238_m3
end
```

Figure 6.3.1 Sample input to generate the heterogeneous F-factors

6.4 Generation of subgroup data

At first Bondarenko F-factors in the AMPX MG library should be converted into resonance integral tables to be used in the subgroup data generation. And then subgroup data are generated by using SUBGR. Subgroup data including weights and levels have been generated for important 49 resonance nuclides as shown in Table 6.4.1 and for all energy groups. Figures 6.4.1 and 6.4.2 provide the standard subgroup level and the SUBGR input files, respectively.

Table 6.4.1 List of nuclides including subgroup data

No	Nuclide	ID	Method	σ_a	$\nu\sigma_f$	No	Nuclide	ID	Method	σ_a	$\nu\sigma_f$
1	^{91}Zr	40091	RI	o	x	26	^{163}Dy	66163	RI	o	x
2	^{96}Zr	40096	RI	o	x	27	^{164}Dy	66164	RI	o	x
3	^{95}Mo	42095	RI	o	x	28	^{166}Er	68166	RI	o	x
4	^{99}Tc	43099	RI	o	x	29	^{167}Er	68167	RI	o	x
5	^{103}Rh	45103	RI	o	x	30	^{176}Hf	72176	RI	o	x
6	^{108}Pd	46108	RI	o	x	31	^{177}Hf	72177	RI	o	x
7	^{107}Ag	47107	RI	o	x	32	^{178}Hf	72178	RI	o	x
8	^{109}Ag	47109	RI	o	x	33	^{179}Hf	72179	RI	o	x
9	^{113}In	49113	RI	o	x	34	^{180}Hf	72180	RI	o	x
10	^{115}In	49115	RI	o	x	35	^{182}W	74182	RI	o	x
11	^{131}Xe	54131	RI	o	x	36	^{183}W	74183	RI	o	x
12	^{133}Cs	55133	RI	o	x	37	^{184}W	74184	RI	o	x
13	^{152}Sm	62152	RI	o	x	38	^{186}W	74186	RI	o	x
14	^{151}Eu	63151	RI	o	x	39	^{232}Th	90232	XS	o	x
15	^{152}Eu	63152	RI	o	x	40	^{233}U	92233	XS	o	o
16	^{153}Eu	63153	RI	o	x	41	^{235}U	92235	XS	o	o
17	^{154}Eu	63154	RI	o	x	42	^{236}U	92236	XS	o	o
18	^{155}Eu	63155	RI	o	x	43	^{238}U	92238	XS	o	x
19	^{155}Gd	64155	XS	o	x	44	^{238}Pu	94238	XS	o	o
20	^{156}Gd	64156	XS	o	x	45	^{239}Pu	94239	XS	o	o
21	^{157}Gd	64157	XS	o	x	46	^{240}Pu	94240	XS	o	o
22	^{158}Gd	64158	XS	o	x	47	^{241}Pu	94241	XS	o	o
23	^{160}Dy	66160	RI	o	x	48	^{242}Pu	94242	XS	o	o
24	^{161}Dy	66161	RI	o	x	49	^{241}Am	95241	XS	o	o
25	^{162}Dy	66162	RI	o	x						

RI : Resonance Integral conservation
XS: Cross section conservation

```
$TIT:
  AMPX 47-G LIBRARY
$DIM:
      54      7      4
$NUC:    0
  00000
  L7A    0  -2.0  2.0  4.800000E+00  4.000000E+01  2.500000E+02  7.500000E+02  2.000000E+03  7.000000E+03  2.000000E+04
  L4A    0  -5.0  5.0  1.000000E+01  5.000000E+02  2.000000E+03  1.000000E+04
$NUC:    1
  40090
  L7A    0  -2.0  2.0  4.800000E+00  4.000000E+01  2.500000E+02  7.500000E+02  2.000000E+03  7.000000E+03  2.000000E+04
  L4A    0  -5.0  5.0  1.000000E+01  5.000000E+02  2.000000E+03  1.000000E+04


$NUC:   40
  92235
  L7A    0  -2.0  2.0  4.800000E+00  4.000000E+01  2.500000E+02  7.500000E+02  2.000000E+03  7.000000E+03  2.000000E+04
  L4A    0  -5.0  5.0  1.000000E+01  5.000000E+02  2.000000E+03  1.000000E+04
$NUC:   41
  92236
  L7A    0  -2.0  2.0  4.800000E+00  4.000000E+01  2.500000E+02  7.500000E+02  2.000000E+03  7.000000E+03  2.000000E+04
  L4A    0  -5.0  5.0  1.000000E+01  5.000000E+02  2.000000E+03  1.000000E+04
$NUC:   42
  92238
  L7A    0  -2.0  2.0  4.800000E+00  4.000000E+01  2.500000E+02  7.500000E+02  2.000000E+03  7.000000E+03  2.000000E+04
  L4A    0  -5.0  5.0  1.000000E+01  5.000000E+02  2.000000E+03  1.000000E+04
$END:
```

Figure 6.4.1 Sample of the initial subgroup level

```
%TITL
  SUBGROUP DATA GENERATION
%IOPT
  iop  0         !0/1/2: constant/variable(RI)/variable(sig)
  con  0.05 0.005 0.005
  grp   1  51
%FILE
  sub  .\lib\subgr_51g_70s.lev
  rit  .\lib\ssxs_51g_70s_10012015.dat
%RESO
   nuc     1    40091   0   1  !
   nuc     2    40096   0   1  !
   nuc     3    42095   0   1  !
   nuc     4    43099   0   1  !
   nuc     5    45103   0   1  !
   nuc     6    46108   0   1  !
   nuc     7    47107   0   1  !
   nuc     8    47109   0   1  !
   nuc     9    49113   0   1  !
   nuc    10    49115   0   1  !
   nuc    11    54131   0   1  !
   nuc    12    55133   0   1  !
   nuc    13    62152   0   1  !
   nuc    14    63151   0   1  !
   nuc    15    63152   0   1  !
   nuc    16    63153   0   1  !
   nuc    17    63154   0   1  !
   nuc    18    63155   0   1  !
   nuc    19    64155   2   1  !
   nuc    20    64156   2   1  !
   nuc    21    64157   2   1  !
   nuc    22    64158   2   1  !
   nuc    23    66160   0   1  !
   nuc    24    66161   0   1  !
   nuc    25    66162   0   1  !
   nuc    26    66163   0   1  !
   nuc    27    66164   0   1  !
   nuc    28    68166   0   1  !
   nuc    29    68167   0   1  !
   nuc    30    72176   0   1  !
   nuc    31    72177   0   1  !
   nuc    32    72178   0   1  !
   nuc    33    72179   0   1  !
   nuc    34    72180   0   1  !
   nuc    35    74182   0   1  !
   nuc    36    74183   0   1  !
   nuc    37    74184   0   1  !
   nuc    38    74186   0   1  !
   nuc    39    90232   2   1  !
   nuc    40    92233   2   2  !
   nuc    41    92235   2   2  !
   nuc    42    92236   2   2  !
   nuc    43    92238   2   1  !
   nuc    44    94238   2   2  !
   nuc    45    94239   2   2  !
   nuc    46    94240   2   2  !
   nuc    47    94241   2   2  !
   nuc    48    94242   2   2  !
   nuc    49    95241   2   2  !
%FINE
```

Figure 6.4.2 Sample of the SUBGR input

6.5 Generation of the MPACT MG library

Appendices A and B provide the detailed data information for the MPACT MG library and the DECLIB input to generate the ENDF/B-7.1 based V4.0 MPACT 47-group library. The following data files are required for DECLIB to generate the MPACT MG library.

- The AMPX 47-g library
- ENDF/B files : Neutron data, decay constants, fission product yields
- Subgroup data and resonance integral table (49 nuclides, groups 10-26)
- Transport correction factors (^{1}H)
- Pre-determined background cross sections (105 nuclides)

- Transient data (21 nuclides)
- Subgroup data with epithermal upscattering (^{238}U)

Figure 6.5.1 provides a flow diagram of DECLIB to generate the MPACT MG library of which data structure is shown in Appendix C.

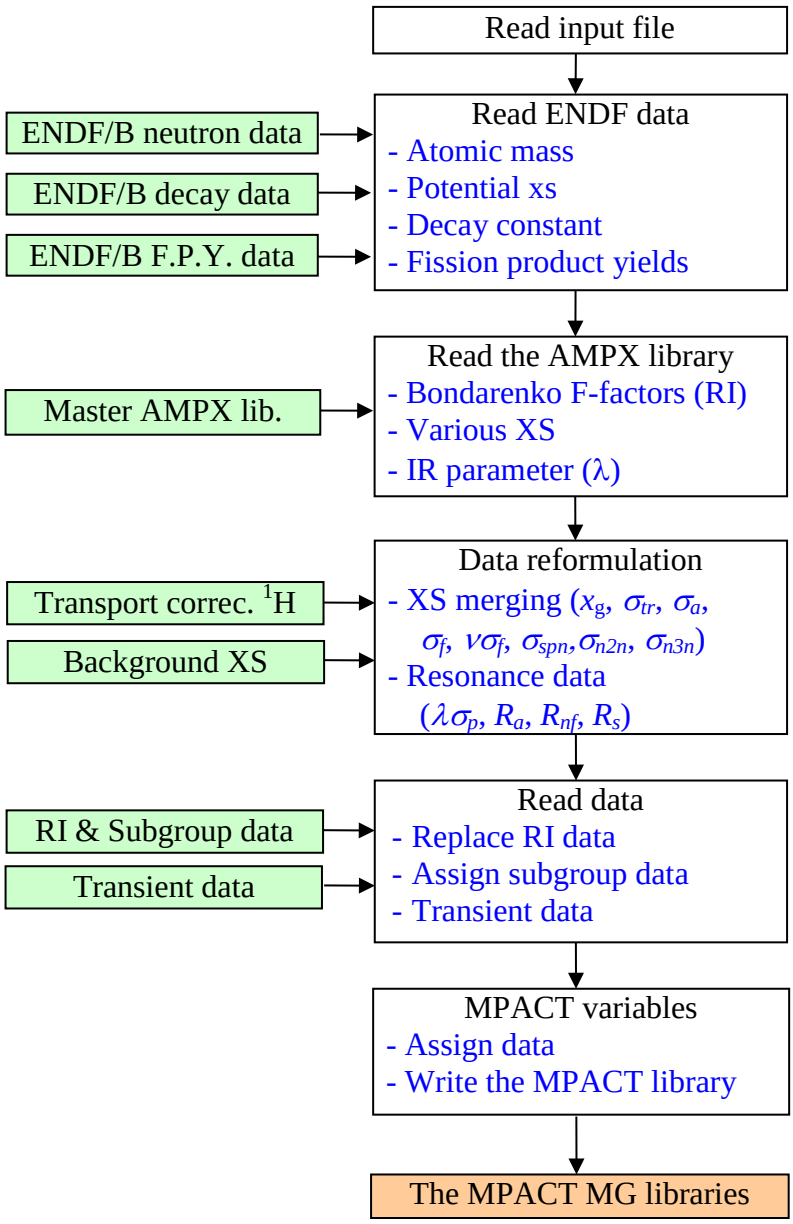


Figure 6.5.1 DECLIB calculation flow

Multigroup cross sections are directly edited from the AMPX master library. MPACT solves the time-independent Boltzmann equation as follows:

$$\hat{\Omega}\cdot\nabla\psi_g + \Sigma_{tr,g}(\vec{r})\psi_g(\vec{r},\hat{\Omega}) = \sum_{g'}\Sigma_{sg'g}\phi_{g'} + \frac{1}{k_{eff}}\chi_g\sum_{g'}\nu\Sigma_{fg'}\phi_{g'}, \qquad (6.5.1)$$

where

$\hat{\Omega}$: neutron direction
$\vec{r}$: space coordinate
g : neutron energy group
ψ_g : angular flux
ϕ_g : scalar flux
$\Sigma_{tr,g}$: macroscopic transport cross section
$\Sigma_{s,g'g}$: transport corrected scattering matrix
ν : the number of neutrons released from a fission
$\Sigma_{f,g'}$: fission cross section
χ_g : fission spectrum
k_{eff} : fffective multiplication factor.

The required data for the transport calculation are transport cross section, fission cross section, the number of neutrons released from a fission, and fission spectrum for each nuclide. Since the absorption and fission cross sections are modified through the resonance treatment and are needed for the depletion calculation, those cross sections should be included. And (n,2n) and (n,3n) cross sections are required for the depletion cross sections. High order (P_1~ P_3) scattering matrices are to be included for the future use. Therefore, the multigroup data required in the library are as follows:

a. Total cross section (σ_t)
b. Absorption cross section ($\sigma_{a=}\ \sigma_{c+}\sigma_f$)
c. Fission cross section (σ_f)
d. Neutrons released from a fission (ν)
e. Scattering cross sections ($\sigma_{s0\sim3}$)
f. (n,2n) cross section ($\sigma_{n,2n}$)
g. (n,3n) cross section ($\sigma_{n,3n}$)
h. $P_{0\sim3}$ scattering matrix ($\sigma_{sngg'}$)
i. Fission spectrum (χ_g)

Since the AMPX master library includes cross section data for various reactions, it is required to merge cross sections to generate the above underlined data. Table 6.5.1 provides which MT numbers are to be merged for the required data.

(n,2n) and (n,3n) cross sections are not treated explicitly, but included in the absorption cross section and scattering matrix as follows:

$$\sigma_{a,g}^{c} = \sigma_{c,g} + \sigma_{f,g} - \sigma_{n2n,g} - 2\sigma_{n3n,g}, \tag{6.5.2}$$

and

$$\sigma_{s,gg'}^{c} = \sigma_{s,gg'} + 2\sigma_{n2n,gg'} + 3\sigma_{n3n,gg'}. \tag{6.5.3}$$

The effective fission spectrum needs to be re-estimated by using MT=18, 452, 455, 1055 and 1099 by using the following formula.

$$\chi_g = \frac{\chi_g^{prompt}\sum_{g'}\nu_{g'}^{prompt}\sigma_{g'}\phi_{g'} + \chi_g^{delayed}\sum_{g'}\nu_{g'}^{delayed}\sigma_{g'}\phi_{g'}}{\sum_{g'}\nu_{g'}^{prompt}\sigma_{g'}\phi_{g'} + \sum_{g'}\nu_{g'}^{delayed}\sigma_{g'}\phi_{g'}}. \tag{6.5.4}$$

Table 6.5.1 MT numbers to be merged

Cross section	MT numbers in the AMPX master library		
	F-factors	1-D cross section	2-D cross section
σ_t	1	-	-
σ_c	102	103~117	-
σ_f	18	-	-
ν	-	452	-
σ_{s0}	2	4	-
$\sigma_{n,2n}$	-	11, 16	11, 16
$\sigma_{n,3n}$	-	17	17
$\sigma_{sngg'}$	-	-	2, 50~91, 1007, 1008
χ_g*	-	18, 452, 455, 1055, 1056, 1099	-
λ	-	2000	-
$\sigma_{s,g}^{within}$	2022	-	-

*Since MT=1018 is just for prompt neutron, χ_g is internally recalculated.

7. CHALLENGING ISSUES

7.1 Drawbacks of the MPACT MG library

The current MPACT 47-group library includes the following drawbacks.

- 49 nuclides include full resonance data such as subgroup data, RI table and IR parameters
- Groups 10 through 26 include resonance data.
- Pre-self-shielded cross sections should be utilized for non-resonance nuclides and non-resonance energy groups.
- Temperature independent elastic scattering matrices are available. (This is a drawback of the AMPX MG library.)
- Although the ENDF/B-7.0 AMPX MG library includes 419 nuclides, the MPACT MG library include 295 nuclides and in addition some of nuclides are duplicated for activation and fission product nuclides.
- Many of fission product nuclides include only absorption cross sections.
- There are many duplicated nuclides at activation and fission product nuclides.
- High order scattering matrices ($\geq P_2$) are available only for important nuclides.

7.2 Resonance interference

Self-shielded cross section table can be generated by considering resonance interference effect between resonance nuclides such as ^{238}U and ^{235}U for the CENTRM pointwise slowing down calculation. This method may be able to provide better agreement for the specific cases in MG 1D self-shielded cross sections or reaction rates between reference solution and the MPACT result. However, resonance interferences are doubly considered due to the Bondarenko iteration of subgroup method for resonance interference, and this procedure would introduce significant ^{235}U enrichment bias resulting in radial power tilt at the whole core calculation.

Resonance interference could not be considered explicitly in the conventional Bondarenko resonance self-shielding methods such as subgroup method, ESSM and Dancoff based methods when using coarse energy group structure. There can be several solutions as follows:

a. Pre-calculated resonance interference factor tables [Kim11]
b. ESSM+0D slowing down [Kim12]
c. ESSM-X [Liu15]

However, these methods are still under development and include various pending technical issues associated with computing time and accuracy. These will be discussed later.

7.3 Resonance self-shielding effect on scattering matrix

In deterministic transport calculation, the accuracy is determined by quality of both 1D and 2D cross section data. Recently new F-factor table for removal correction has been included to

adjust scattering matrix in the AMPX MG master library. It is noted that this approach is very successful in resolving temperature bias problem due to temperature independent scattering matrix. At first a new functionality to utilize the F-factor table for removal correction needs to be incorporated into MPACT. However, since this approach is based on Bondarenko method, there should be some bias in estimating self-shielding effect in scattering matrix. New resonance self-shielding method is based on quasi 1D slowing down calculation. Therefore, removal correction factor for 2D data can be explicitly estimated simultaneously with an estimation of 1D data. These removal correction factors can be applied to scattering matrix.

7.4 Intra pin self-shielding effect in ESSM

When estimating resonance self-shielded cross section by ESSM, absorption cross sections ($\Sigma_{i,a,g}$) at fuel and cladding are iteratively determined by solving the fixed source transport eq. (7.4.1).

$$\hat{\Omega}\cdot\nabla\psi_g + \sum_i(\Sigma_{i,a,g} + \lambda_{i,g}\Sigma_{i,p})\psi_g(\hat{\Omega}) = \sum_i \lambda_{i,g}\Sigma_{i,p}\ . \tag{7.4.1}$$

Typical PWR and BWR fuel pins include UO_2 fuel and zirconium alloy fuel cladding in which ^{235}U, ^{238}U, ^{91}Zr and ^{95}Zr are important resonant nuclides requiring explicit resonance treatment. Since Zr nuclides are located at different zone from fuel, there is no direct resonance interference effect with fuel nuclides.

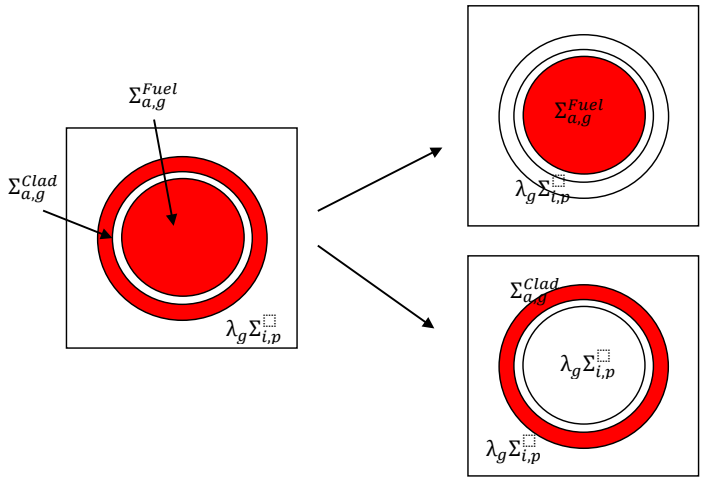
When generating F-factor tables by using homogeneous or heterogeneous models by the SCALE and AMPX procedures, only one resonant nuclide is considered to have absorption cross section and other background nuclides include only potential or scattering cross sections in slowing down and ESSM calculations. Multigroup cross sections are obtained from the slowing down calculations and the corresponding background cross sections are obtained by solving eq. (7.4.1) and then by using eq. (7.4.2).

$$\Sigma_{b,g} = \frac{\Sigma_{a,g}\phi_g}{1-\phi_g} \quad\rightarrow\quad \sigma^i_{b,g} = \frac{\Sigma_{b,g}}{N_i}\ . \tag{7.4.2}$$

When performing multigroup ESSM calculation, absorption cross sections at fuel and cladding are estimated simultaneously. Since the scalar flux (ϕ_g) at fuel is influenced by the cladding absorption cross section and vice versa, self-shielded cross sections at fuel and cladding introduce some bias because of inconsistency between how to generate F-factor table and how to use it.

In order to avoid this problem, the AMPX 56-group master library includes two sets of cross section data for ^{91}Zr and ^{96}Zr. The first set of F-factor table was prepared by using a conventional procedure, and the second set of F-factor table was generated by using a model shown in Figure

7.4.1 (a). The second set of F-factor tables cannot be utilized in other composition except for fuel cladding. While the impact on Zr nuclides of cladding by fuel is significant, the impact on U nuclides of fuel by cladding is not. In order to have the highest quality of self-shielded cross sections and a simplified procedure, this impact should be considered for both cladding and fuel with a utilization of only one set of F-factor table.



(a) (b)

Figure 7.4.1 Counter influence between fuel and cladding

In order to solve this problem category concept in the subgroup method can be utilized. Or if fuel and cladding regions are separated from each other which is somewhat similar with category concept, this problem can be resolved which may be called a geometrical category.

Another idea is to include a special option to generate a table of macroscopic cross sections as a function of temperature for which resonance self-shielding effect, if necessary, can be considered by using a simple model such as single pin and homogeneous mixture. This option can be applied to cladding, detector and moderator. Similar approach can be applied to the subgroup method.

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REFERENCE

[Ald03] D. L. Aldama and et. al., "WIMS-D Library Update," IAEA (2003).

[Bec10] B. Becker, "On the influence of the Resonance Scattering Treatment in Monte Carlo Codes on High Temperature Reactor Characteristics," Ph. D. Thesis, University Stuttgart, June, 2010 (2010).

[Dud76] James J. Duderstadt and Louis J. Hamilton, "Nuclear Reactor Analysis," John Wiley & Sons, Inc. (1976).

[Hel03] HELIOS Methods, Studsvik Scandpower, 20 November 2003.

[Hon11] Ser Gi Hong, Kang Seog Kim, "Iterative Resonance Treatment Methods Using Resonance Integral Table in Heterogeneous Transport Lattice Calculations," Ann. Nucl. Energ., 38, 32-43 (2011).

[Jam99] M. F. James, "Energy Release in Fission of Th-232, U-233, U-234, U-236, Np-237, Pu-238, Pu-240 and Pu-242," J. Nucl. Energy, 23, 1999.

[Joo09] H. G. Joo and et al., "Subgroup Weight Generation Based on Shielded Pin-Cell Cross Section Conservation," *Ann. nucl. Energy,* 36, 859 (2009).

[Kim03] Kang Seog Kim et al., "Monte Carlo Resonance Treatment for the Deterministic Transport Lattice Codes," Journal of the Korean Nuclear Society, 35, No.6, 581-595 (2003).

[Kim11] Kang-Seog Kim, Ser Gi Hong, "A New Procedure to Generate Resonance Integral Table with an Explicit Resonance Interference for Transport Lattice Codes," Ann. Nucl. Ener., 38, 118-127 (2011).

[Kim12] Kang-Seog Kim, Mark L. Williams, "Preliminary Assessment of Resonance Interference Treatment by Using 0-D Slowing Down Calculation in the Embedded Self-Shielding Method," Trans. Am. Nucl. Soc., 107, 1128-1131 (2012).

[Lee11] C. H. Lee and W. S. Yang, "MC^2-3: Multigroup Cross Section Generation Code for Fast Reactor Analysis," ANL-NE-11-41, Argonne National Laboratory (2011).

[Liu14] Yuxuan Liu, William Martin, Mark L. Williams, Kang-Seog Kim, "Resonance Self-shielding Method for Fuel Annular Subdivisions Using Quasi-1D Slowing down Solutions," (In preparation) (2014).

[Mat05] H. Matsumoto, M. Ouisloumen and T. Takeda, "Development of Spatially Dependent Resonance Shielding Method," *J. Nucl. Sci Technol.*, **42**, 688 (2005).

[Sca09] "SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation," ORNL-TM/2005/39, Version 6, Vols. I–III, Oak Ridge National Laboratory, Oak Ridge, Tennessee (2009). (Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-750.)

[Sta83] Rudi J.J. Stamm'ler and Maximo J. Abbate, "Methods of Steady-State Reactor Physics in Nuclear Design," Academic Press (1983).

[Sto96] C. Stoker and Z. Weiss, "Spatially Dependent Resonance Cross Sections in a Fuel Rod," *Ann. Nucl. Energy.*, **23**, 765 (1996).

[Wem07] C. A. Wemple, et al., "Improved Temperature-Dependent Resonance Treatment in HELIOS-1.9," Trans. Am. Nucl. Soc., 96, 657-659 (2007).

[Wia14] D. Wiarda, S. Goluoglu, M.E. Dunn, N.M. Green and L. M. Petrie, "AMPX-6: A Modular Code System for Processing ENDF/B Evaluations," in preparation (2014).

[Wil06] Mark L. Williams, M. Asgari, D. F. Hollenbach, "CENTRM: A One-Dimensional Neutron Transport Code For Computing Pointwise Energy Spectra," ORNL/TM-2005/39, Version 5.1, Vol. II, Book 4, Sect. F18 (2006).

[Wil11] Mark L. Williams, "Resonance Self-Shielding Methodologies in SCALE 6," *Nuclear Technology*, **174**, 149-168 (2011).

[Wil12] Mark L. Williams and Kang-Seog Kim, "The Embedded Self-Shielding Method," PHYSOR 2012, Knoxville, Tennessee, USA (2012).

Appendix A.1 Sample input of LAMBDA and IRFFACTOR-hom for ^{235}U

```
=shell
ln -fs /home/ykk/libraries/endf7.0/mg/47g/ampx47g_70_07182014_00_ykk.bin ft77f001
cp /scale/scale_dev_data/ce_v7.0_endf .
ln -fs /scale/scale_dev_data/cekenolib_7.0
cp /scale/scale_dev_data/endf_b/vers7//1-0 .
end
=ajax
0$$  20  e
1$$  1  e t
2$$  77  4  e t
3$$ 92238 1001 92235 92235 e t
end
=lambda
in=20  out=44 bnuc=1001  fnuc=92238
iddens=0.0238333 bdens=0.0357499 dens=0.00743805
low=10 high=46
temp=600.0
end
=ajax
0$$ 46 e 1$$ 1 e t
2$$ 44 1 e t
3$$ 92235    e t
end
=shell
cp ft46f001 ${RTNDIR}/../irflib/irf_lambda_u235
end
=irffachomo
in=44 out=45 fnuc=92235 bnuc=1001
dens=1.0 ehres=2.25000E+03
low=10 high=46
end
=ajax
0$$ 48 e 1$$ 1 e t
2$$ 45 1 e t
3$$ 92235   e t
end
=shell
cp ft48f001 ${RTNDIR}/../irflib/irf_irf_u235
end
```

Appendix B.1 Sample input of IRFFACTOR-het for ^{238}U

```
=csas1x  parm=centrm
hetrocells to compute f-factors of U238;
 ft88f001
read composition

'
' ***CELL-1 Composition
'
u-235 1  0  9.39468E-04  293  end
u-238 1  0  2.22624E-02  293  end
o-16  1  0  4.64223E-02  293  end
al-27 2  0  6.02620E-02  293  end
h-1   3  0  1.17012E-04  293  end
o-16  3  0  5.85142E-05  293  end

'
' ***CELL-2 Composition
'
u-235 4  0  9.39468E-04  293  end
u-238 4  0  2.22624E-02  293  end
o-16  4  0  4.64223E-02  293  end
al-27 5  0  6.02620E-02  293  end
h-1   6  0  9.36093E-03  293  end
o-16  6  0  4.68114E-03  293  end

'
' ***CELL-3 Composition
'
u-235 7  0  9.39468E-04  293  end
u-238 7  0  2.22624E-02  293  end
o-16  7  0  4.64223E-02  293  end
al-27 8  0  6.02620E-02  293  end
h-1   9  0  2.34023E-02  293  end
o-16  9  0  1.17028E-02  293  end

'
' ***CELL-4 Composition
'
u-235 10  0  9.39468E-04   293  end
u-238 10  0  2.22624E-02   293  end
o-16  10  0  4.64223E-02   293  end
al-27 11  0  6.02620E-02   293  end
h-1   12  0  3.51035E-02   293  end
o-16  12  0  1.75543E-02   293  end

'
' ***CELL-5 Composition
'
u-235 13  0  9.39468E-04   293  end
u-238 13  0  2.22624E-02   293  end
o-16  13  0  4.64223E-02   293  end
al-27 14  0  6.02620E-02   293  end
h-1   15  0  4.68046E-02   293  end
o-16  15  0  2.34057E-02   293  end

'
' ***CELL-6 Composition
'
u-235 16  0  9.39468E-04   293  end
```

```
u-238 16  0  2.22624E-02   293  end
o-16  16  0  4.64223E-02   293  end
al-27 17  0  6.02620E-02   293  end
h-1   18  0  4.68046E-02   293  end
o-16  18  0  2.34057E-02   293  end

'
' ***CELL-7 Composition
'
u-235 19  0  9.39468E-04   293  end
u-238 19  0  2.22624E-02   293  end
o-16  19  0  4.64223E-02   293  end
al-27 20  0  6.02620E-02   293  end
h-1   21  0  4.68046E-02   293  end
o-16  21  0  2.34057E-02   293  end

'
' ***CELL-8 Composition
'
u-235 22  0  9.39468E-04   293  end
u-238 22  0  2.22624E-02   293  end
o-16  22  0  4.64223E-02   293  end
al-27 23  0  6.02620E-02   293  end
h-1   24  0  4.68046E-02   293  end
o-16  24  0  2.34057E-02   293  end

'
' ***CELL-9 Composition
'
u-235 25  0  4.69734E-04   293  end
u-238 25  0  1.11312E-02   293  end
o-16  25  0  2.32111E-02   293  end
al-27 26  0  6.02620E-02   293  end
h-1   27  0  4.68046E-02   293  end
o-16  27  0  2.34057E-02   293  end

'
' ***CELL-10 Composition
'
u-235 28  0  2.34867E-04   293  end
u-238 28  0  5.56561E-03   293  end
o-16  28  0  1.16056E-02   293  end
al-27 29  0  6.02620E-02   293  end
h-1   30  0  4.68046E-02   293  end
o-16  30  0  2.34057E-02   293  end

'
' ***CELL-11 Composition
'
u-235 31  0  1.17434E-04   293  end
u-238 31  0  2.78280E-03   293  end
o-16  31  0  5.80278E-03   293  end
al-27 32  0  6.02620E-02   293  end
h-1   33  0  4.68046E-02   293  end
o-16  33  0  2.34057E-02   293  end

'
' ***CELL-12 Composition
'
u-235 34  0  5.87168E-05   293  end
u-238 34  0  1.39140E-03   293  end
o-16  34  0  2.90139E-03   293  end
al-27 35  0  6.02620E-02   293  end
```

```
h-1   36  0  4.68046E-02   293  end
o-16  36  0  2.34057E-02   293  end

'
' ***CELL-13 Composition
'
u-235 37  0  2.93584E-05   293  end
u-238 37  0  6.95701E-04   293  end
o-16  37  0  1.45070E-03   293  end
al-27 38  0  6.02620E-02   293  end
h-1   39  0  4.68046E-02   293  end
o-16  39  0  2.34057E-02   293  end

'
' ***CELL-14 Composition
'
u-235 40  0  9.39468E-06   293  end
u-238 40  0  2.22624E-05   293  end
o-16  40  0  4.64223E-04   293  end
al-27 41  0  6.02620E-02   293  end
h-1   42  0  4.68046E-02   293  end
o-16  42  0  2.34057E-02   293  end

'
' ***CELL-15 Composition
'
u-235 43  0  9.39468E-06   293  end
u-238 43  0  2.22624E-08   293  end
o-16  43  0  4.64223E-04   293  end
al-27 44  0  6.02620E-02   293  end
h-1   45  0  4.68046E-02   293  end
o-16  45  0  2.34057E-02   293  end

'
' ***CELL-16 Composition (infinitely dilute; Homo mixture)
'
u-235 70  0  9.3947E-05 293  end
u-238 70  0  1.0E-12    293  end
o-16  70  0  0.046422   293  end
al-27 70  0  0.060262   293  end
h-1   70  0  4.4183E-02 293  end
o-16  70  0  2.2095E-02 293  end
'-------------------------------------------------------

end composition

read celldata

'
' ***CELL-1 Geometry
 latticecell  squarepitch  pitch=1.2620 3 fuelr=0.4025 1
              cladr=0.4759 2   end
 centrmdata  demin=.0001  demax=9.E3 iup=15 npxs=6 end centrmdata

'
' ***CELL-2 Geometry
 latticecell  squarepitch  pitch=1.2620 6  fuelr=0.4025 4
              cladr=0.4759 5   end
 centrmdata  demin=.0001  demax=9.E3 iup=15 npxs=6 end centrmdata

'
' ***CELL-3 Geometry
 latticecell  squarepitch  pitch=1.2620 9  fuelr=0.4025 7
```

```
             cladr=0.4759 8   end
 centrmdata  demin=.0001  demax=9.E3 iup=15 npxs=6 end centrmdata

'
' ***CELL-4 Geometry
 latticecell  squarepitch  pitch=1.2620 12  fuelr=0.4025 10
             cladr=0.4759 11   end
 centrmdata  demin=.0001  demax=9.E3 iup=15 npxs=6 end centrmdata

'
' ***CELL-5 Geometry
 latticecell  squarepitch  pitch=1.2620 15  fuelr=0.4025 13
             cladr=0.4759 14   end
 centrmdata  demin=.0001  demax=9.E3 iup=15 npxs=6 end centrmdata

'
' ***CELL-6 Geometry
 latticecell  squarepitch  pitch=1.5728 18  fuelr=0.4025 16
             cladr=0.4759 17   end
 centrmdata  demin=.0001  demax=9.E3 iup=15 npxs=6 end centrmdata

'
' ***CELL-7 Geometry
 latticecell  squarepitch  pitch=2.0581 21  fuelr=0.4025 19
             cladr=0.4759 20   end
 centrmdata  demin=.0001  demax=9.E3 iup=15 npxs=6 end centrmdata

'
' ***CELL-8 Geometry
 latticecell  squarepitch  pitch=2.2621 24 fuelr=0.4025 22
             cladr=0.4759 23   end
 centrmdata  demin=.0001  demax=9.E3 iup=15 npxs=6 end centrmdata

'
' ***CELL-9 Geometry
 latticecell  squarepitch  pitch=2.2621 27  fuelr=0.4025 25
             cladr=0.4759 26   end
 centrmdata  demin=.0001  demax=9.E3 iup=15 npxs=6 end centrmdata

'
' ***CELL-10 Geometry
 latticecell  squarepitch  pitch=2.2621 30  fuelr=0.4025 28
             cladr=0.4759 29   end
 centrmdata  demin=.0001  demax=9.E3 iup=15 npxs=6 end centrmdata

'
' ***CELL-11 Geometry
 latticecell  squarepitch  pitch=2.2621 33  fuelr=0.4025 31
             cladr=0.4759 32   end
 centrmdata  demin=.0001  demax=9.E3 iup=15 npxs=6 end centrmdata

'
' ***CELL-12 Geometry
 latticecell  squarepitch  pitch=2.2621 36  fuelr=0.4025 34
             cladr=0.4759 35   end
 centrmdata  demin=.0001  demax=9.E3 iup=15 npxs=6 end centrmdata

'
' ***CELL-13 Geometry
 latticecell  squarepitch  pitch=2.2621 39  fuelr=0.4025 37
             cladr=0.4759 38   end
 centrmdata  demin=.0001  demax=9.E3 iup=15 npxs=6 end centrmdata
```

```
'
' ***CELL-14 Geometry
 latticecell  squarepitch  pitch=2.2621 42 fuelr=0.4025 40
              cladr=0.4759 41   end
 centrmdata  demin=.0001  demax=9.E3 iup=15 npxs=6 end centrmdata

'
' ***CELL-15 Geometry
 latticecell  squarepitch  pitch=2.2621 45  fuelr=0.4025 43
              cladr=0.4759 44   end
 centrmdata  demin=.0001  demax=9.E3 iup=15 npxs=6 end centrmdata

'
' ***CELL-16 Geometry (infinitely dilute; Homo mixture)
infhommedium  70   end
 centrmdata  demin=.0001  demax=9.E3 iup=15 end centrmdata

'-------------------------------------------------------
end celldata

end
```

Appendix C.1 Data information in the MAPCT 47-group library

NO1 0 non depletable
>0 depletable (w/ decay constant)
2 RI-a only (fissionable w/ kappa, beta, FPY)
3 RI -a & RI-vf (fissionable w/ kappa, beta, FPY)
NO2 NFPY (Ordering no. of FPY) (+/- : cumulative/direct yield)
NO3 Indicator for fission spectrum (0/>0 : no/yes)
NO4 Indicator for (n,2n) & (n,3n) XS (0/1/2/3 : no/(n,2n)/(n,3n)/both)
NO5 The number of temperatures for XS
NO6 The number of temperatures for RI
NO7 The number of temperatures for p2~p3
NO8 The number of sig-0's for RI

1 – 49: Full XS + subgroup data
50 – 191: Full XS + resonance data such as IR parameter, potential XS
192 – end: Part XS

No	NID	Amass	NO1	NO2	NO3	NO4	NO5	NO6	NO7	NO8	AID
1	40091	90.9056	1	0	0	0	3	5	0	16	Zr-91
2	40096	95.9083	1	0	0	0	3	5	0	16	Zr-96
3	42595	94.9059	1	17	0	0	3	5	0	16	Mo-95
4	43599	99.0005	1	23	0	1	3	5	0	16	Tc-99
5	45103	102.9050	1	0	0	0	3	5	0	16	Rh-103
6	46608	107.9039	1	37	0	0	3	5	0	16	Pd-108
7	47107	106.9054	0	0	0	3	3	5	0	16	Ag-107
8	47109	108.9045	0	0	0	3	3	5	0	16	Ag-109
9	49113	112.9039	0	0	0	0	3	5	0	16	In-113
10	49115	114.9041	0	0	0	0	3	5	0	16	In-115
11	54631	130.9055	1	57	0	3	3	5	0	16	Xe-131
12	55633	132.9057	1	63	0	1	3	5	0	16	Cs-133
13	62152	151.9201	0	0	0	3	5	5	0	16	Sm-152
14	63151	150.9195	0	0	0	3	5	5	0	16	Eu-151
15	63152	151.9251	1	0	0	3	5	5	0	16	Eu-152
16	63153	152.9217	0	0	0	3	5	5	0	16	Eu-153
17	63154	153.9223	1	0	0	3	5	5	0	16	Eu-154
18	63155	154.9229	1	0	0	3	5	5	0	16	Eu-155
19	64155	154.9229	0	0	0	1	5	5	0	16	Gd-155
20	64156	155.9225	0	0	0	1	5	5	0	16	Gd-156
21	64157	156.9241	0	0	0	1	5	5	0	16	Gd-157
22	64158	157.9236	0	0	0	1	5	5	0	16	Gd-158
23	66160	159.9248	0	0	0	0	3	5	0	16	Dy-160
24	66161	160.9274	0	0	0	0	3	5	0	16	Dy-161
25	66162	161.9270	0	0	0	0	3	5	0	16	Dy-162
26	66163	162.9286	0	0	0	0	3	5	0	16	Dy-163
27	66164	163.9282	0	0	0	3	3	5	0	16	Dy-164
28	68166	165.9304	0	0	0	0	3	5	0	16	Er-166
29	68167	166.9320	0	0	0	0	5	5	0	16	Er-167
30	72176	175.9414	0	0	0	1	3	5	0	16	Hf-176
31	72177	176.9430	0	0	0	1	3	5	0	16	Hf-177
32	72178	177.9436	0	0	0	1	3	5	0	16	Hf-178
33	72179	178.9462	0	0	0	1	3	5	0	16	Hf-179
34	72180	179.9468	0	0	0	1	3	5	0	16	Hf-180
35	74182	181.9531	0	0	0	1	3	5	0	16	W-182
36	74183	182.9517	0	0	0	1	3	5	0	16	W-183
37	74184	183.9502	0	0	0	1	3	5	0	16	W-184
38	74186	185.9575	0	0	0	1	3	5	0	16	W-186

39	90232	232.0333	2	0	1	3	5	5	5	16	Th-232
40	92233	233.0450	3	0	2	3	5	5	5	16	U-233
41	92235	235.0441	3	0	3	3	5	5	5	16	U-235
42	92236	236.0458	3	0	4	3	3	5	3	16	U-236
43	92238	238.0510	2	0	5	3	5	5	5	16	U-238
44	94238	238.0495	3	0	6	3	3	5	0	16	Pu-238
45	94239	239.0522	3	0	7	3	5	5	5	16	Pu-239
46	94240	240.0542	3	0	8	3	5	5	5	16	Pu-240
47	94241	241.0487	3	0	9	3	5	5	5	16	Pu-241
48	94242	242.0584	3	0	10	3	3	5	3	16	Pu-242
49	95241	241.0568	3	0	0	3	3	5	0	16	Am-241
50	1001	1.0078	0	0	0	0	8	0	8	0	H-1
51	1002	2.0141	0	0	0	1	5	0	5	0	H-2
52	1006	1.0078	0	0	0	0	3	0	3	0	H-1
53	1040	1.0078	0	0	0	0	3	0	3	0	H-1
54	3006	4.0026	0	0	0	0	5	0	5	0	Li-6
55	3007	6.0151	0	0	0	1	3	0	3	0	Li-7
56	4009	7.0160	0	0	0	1	3	0	0	0	Be-9
57	5000	9.0122	0	0	0	0	3	0	0	0	B-Nat
58	5010	10.8120	1	0	0	0	3	0	0	0	B-10
59	5011	10.0129	1	0	0	0	3	0	0	0	B-11
60	6000	11.0093	0	0	0	0	5	0	5	0	C-Nat
61	6001	12.0011	0	0	0	0	10	0	10	0	C-Nat
62	7014	12.0011	0	0	0	1	3	0	0	0	N-14
63	8001	14.0031	0	0	0	0	5	0	5	0	O-UO2
64	8016	15.9905	0	0	0	0	5	0	5	0	O-16
65	9019	15.9905	0	0	0	0	3	0	0	0	F-19
66	11023	18.9982	0	0	0	0	5	0	0	0	Na-23
67	12000	22.9895	0	0	0	0	3	0	0	0	Mg-Nat
68	13027	24.3051	0	0	0	0	3	0	3	0	Al-27
69	14000	26.9818	0	0	0	0	3	0	0	0	Si-Nat
70	15031	28.0853	0	0	0	0	3	0	0	0	P-31
71	16000	30.9741	0	0	0	0	3	0	0	0	S-Nat
72	17000	32.0636	0	0	0	0	3	0	0	0	Cl-Nat
73	19000	35.4526	0	0	0	0	3	0	0	0	K-Nat
74	20000	39.1019	0	0	0	0	3	0	0	0	Ca-Nat
75	22000	40.0803	0	0	0	0	3	0	0	0	Ti-Nat
76	23000	47.8789	0	0	0	0	3	0	0	0	V-Nat
77	24000	50.9416	0	0	0	1	3	0	0	0	Cr-Nat
78	24050	51.9957	0	0	0	0	3	0	0	0	Cr-50
79	24052	49.9461	0	0	0	0	3	0	0	0	Cr-52
80	24053	51.9402	0	0	0	0	3	0	0	0	Cr-53
81	24054	52.9408	0	0	0	0	3	0	0	0	Cr-54
82	25055	53.9394	0	0	0	1	3	0	0	0	Mn-55
83	26000	54.9381	0	0	0	1	3	0	0	0	Fe-Nat
84	26054	55.8446	0	0	0	0	3	0	0	0	Fe-54
85	26056	53.9394	0	0	0	0	3	0	0	0	Fe-56
86	26057	55.9345	0	0	0	0	3	0	0	0	Fe-57
87	26058	56.9351	0	0	0	0	3	0	0	0	Fe-58
88	27059	57.9337	0	0	0	1	3	0	0	0	Co-59
89	28000	58.9332	0	0	0	1	3	0	0	0	Ni-Nat
90	28058	58.6936	0	0	0	0	3	0	0	0	Ni-58
91	28060	57.9357	0	0	0	0	3	0	0	0	Ni-60
92	28061	59.9308	0	0	0	0	3	0	0	0	Ni-61
93	28062	60.9314	0	0	0	0	3	0	0	0	Ni-62
94	28064	61.9280	0	0	0	0	3	0	0	0	Ni-64
95	29063	63.9282	0	0	0	0	3	0	0	0	Cu-63
96	29065	62.9296	0	0	0	0	3	0	0	0	Cu-65
97	40000	64.9278	0	0	0	1	3	0	3	0	Zr-Nat

98	40001	91.2196	0	0	0	1	8	0	8	0	Zr-Zrh2
99	40090	91.2196	0	0	0	0	3	0	0	0	Zr-90
100	40092	89.9043	0	0	0	0	3	0	0	0	Zr-92
101	40094	91.9050	0	0	0	0	3	0	0	0	Zr-94
102	41093	93.9063	0	0	0	0	5	0	0	0	Nb-93
103	42000	92.9032	0	0	0	3	3	0	0	0	Mo-Nat
104	44601	95.9402	1	25	0	0	3	0	0	0	Ru-101
105	45103	100.9058	0	0	0	0	3	0	0	0	Rh-103
106	45603	102.9050	1	31	0	1	3	0	0	0	Rh-103
107	45605	104.9062	1	32	0	0	3	0	0	0	Rh-105
108	46605	104.9052	1	34	0	0	3	0	0	0	Pd-105
109	46607	106.9054	1	36	0	0	3	0	0	0	Pd-107
110	47609	108.9045	1	38	0	3	3	0	0	0	Ag-109
111	48000	112.4258	0	0	0	0	3	0	0	0	Cd-Nat
112	48110	109.9031	0	0	0	0	3	0	0	0	Cd-110
113	48111	110.9047	0	0	0	0	3	0	0	0	Cd-111
114	48112	111.9033	0	0	0	0	3	0	0	0	Cd-112
115	48113	112.8999	0	0	0	1	3	0	0	0	Cd-113
116	48114	113.9035	0	0	0	0	3	0	0	0	Cd-114
117	49000	114.9071	0	0	0	0	3	0	0	0	In-Nat
118	49615	114.9071	1	44	0	0	3	0	0	0	In-115
119	50000	118.7107	0	0	0	0	3	0	0	0	Sn-Nat
120	50112	111.9013	0	0	0	0	3	0	0	0	Sn-112
121	50114	113.8984	0	0	0	0	3	0	0	0	Sn-114
122	50115	114.9031	0	0	0	0	3	0	0	0	Sn-115
123	50116	115.9017	0	0	0	0	3	0	0	0	Sn-116
124	50117	116.9033	0	0	0	0	3	0	0	0	Sn-117
125	50118	117.9018	0	0	0	0	3	0	0	0	Sn-118
126	50119	118.9035	0	0	0	0	3	0	0	0	Sn-119
127	50120	119.9020	0	0	0	0	3	0	0	0	Sn-120
128	50122	121.9032	0	0	0	0	3	0	0	0	Sn-122
129	50124	123.9054	0	0	0	0	3	0	0	0	Sn-124
130	51000	121.7577	0	0	0	0	3	0	0	0	Sb-Nat
131	51121	120.9036	0	0	0	0	3	0	0	0	Sb-121
132	51123	122.9038	0	0	0	0	3	0	0	0	Sb-123
133	54634	133.9053	1	60	0	3	3	0	0	0	Xe-134
134	60643	142.9097	1	81	0	3	3	0	0	0	Nd-143
135	60645	144.9129	1	83	0	3	3	0	0	0	Nd-145
136	61647	146.9151	1	88	0	3	3	0	0	0	Pm-147
137	61748	147.9177	1	92	0	0	3	0	0	0	Pm-148m
138	62153	152.9217	1	0	0	0	3	0	0	0	Sm-153
139	62647	146.9151	1	93	0	3	3	0	0	0	Sm-147
140	62649	148.9173	1	95	0	3	3	0	0	0	Sm-149
141	62650	149.9169	1	96	0	1	3	0	0	0	Sm-150
142	62651	150.9195	1	97	0	3	3	0	0	0	Sm-151
143	62652	151.9201	1	98	0	3	3	0	0	0	Sm-152
144	63156	155.9245	1	0	0	0	3	0	0	0	Eu-156
145	63157	156.9251	1	0	0	0	3	0	0	0	Eu-157
146	63653	152.9217	1	102	0	3	3	0	0	0	Eu-153
147	63654	153.9223	1	103	0	3	3	0	0	0	Eu-154
148	63655	154.9229	1	104	0	3	3	0	0	0	Eu-155
149	64152	151.9201	0	0	0	1	3	0	0	0	Gd-152
150	64154	153.9213	0	0	0	1	3	0	0	0	Gd-154
151	64160	159.9268	0	0	0	1	3	0	0	0	Gd-160
152	64655	154.9229	1	108	0	1	3	0	0	0	Gd-155
153	64656	155.9225	1	109	0	1	3	0	0	0	Gd-156
154	64657	156.9241	1	110	0	1	3	0	0	0	Gd-157
155	64658	157.9236	1	111	0	1	3	0	0	0	Gd-158
156	68168	167.9414	0	0	0	0	3	0	0	0	Er-166

157	71176	175.9414	0	0	0	0	3	0	0	0	Lu-176
158	72174	173.9402	0	0	0	1	3	0	0	0	Hf-174
159	73181	180.9545	0	0	0	3	3	0	0	0	Ta-181
160	73182	181.9500	0	0	0	3	3	0	0	0	Ta-182
161	74000	183.8564	0	0	0	3	3	0	0	0	W-Nat
162	79197	196.9660	0	0	0	0	3	0	0	0	Au-197
163	82206	205.9694	0	0	0	0	3	0	0	0	Pb-206
164	82207	206.9780	0	0	0	0	3	0	0	0	Pb-207
165	82208	207.9766	0	0	0	0	3	0	0	0	Pb-208
166	83209	208.9803	0	0	0	3	3	0	0	0	Bi-209
167	90230	230.0361	3	0	0	3	3	0	0	0	Th-230
168	91231	231.0347	3	0	0	3	3	0	0	0	Pa-231
169	91233	233.0399	3	0	0	3	5	0	0	0	Pa-233
170	92232	232.0333	3	0	0	3	3	0	0	0	U-232
171	92234	234.0405	3	0	11	3	3	0	3	0	U-234
172	92237	237.0484	3	0	0	3	3	0	0	0	U-237
173	93237	237.0482	3	0	12	3	3	0	0	0	Np-237
174	93238	238.0510	3	0	0	0	3	0	0	0	Np-238
175	93239	239.0526	3	0	13	3	3	0	0	0	Np-239
176	94236	236.0458	3	0	14	3	3	0	0	0	Pu-236
177	95242	242.0594	3	0	0	0	3	0	0	0	Am-242
178	95342	242.0594	3	0	0	3	3	0	0	0	Am-242m
179	95243	243.0610	3	0	0	3	3	0	0	0	Am-243
180	96242	242.0584	3	0	0	3	3	0	0	0	Cm-242
181	96243	243.0610	3	0	0	3	3	0	0	0	Cm-243
182	96244	244.0626	3	0	0	3	3	0	0	0	Cm-244
183	96245	245.0652	3	0	0	3	3	0	0	0	Cm-245
184	96246	246.0668	3	0	0	3	3	0	0	0	Cm-246
185	96247	247.0725	3	0	0	3	3	0	0	0	Cm-247
186	96248	248.0721	3	0	0	3	3	0	0	0	Cm-248
187	97249	249.0797	3	0	0	3	3	0	0	0	Bk-249
188	98249	249.0797	3	0	0	3	3	0	0	0	Cf-249
189	98250	250.0763	3	0	0	3	3	0	0	0	Cf-250
190	98251	251.0799	3	0	0	3	3	0	0	0	Cf-251
191	98252	252.0815	3	0	0	3	3	0	0	0	Cf-252
192	1003	3.0160	0	0	0	0	3	0	0	0	T-3
193	2003	3.0149	0	0	0	0	3	0	0	0	He-3
194	35581	80.9163	1	1	0	0	1	0	0	0	Br-81
195	36582	81.9135	1	2	0	1	1	0	0	0	Kr-82
196	36583	82.9141	1	3	0	3	1	0	0	0	Kr-83
197	36584	83.9114	1	4	0	1	1	0	0	0	Kr-84
198	36585	84.9125	1	5	0	0	1	0	0	0	Kr-85
199	36586	85.9106	1	6	0	3	1	0	0	0	Kr-86
200	38589	88.9075	1	7	0	0	1	0	0	0	Sr-89
201	38590	89.9078	1	8	0	0	1	0	0	0	Sr-90
202	39589	88.9058	1	9	0	1	1	0	0	0	Y-89
203	39590	89.9072	1	10	0	0	1	0	0	0	Y-90
204	39591	90.9074	1	11	0	0	1	0	0	0	Y-91
205	40591	90.9029	1	12	0	1	1	0	0	0	Zr-91
206	40593	92.9064	1	13	0	0	1	0	0	0	Zr-93
207	40595	94.9080	1	14	0	0	1	0	0	0	Zr-95
208	40596	95.9049	1	15	0	1	1	0	0	0	Zr-96
209	41595	94.9068	1	16	0	0	1	0	0	0	Nb-95
210	42095	94.9059	0	0	0	0	1	0	0	0	Mo-95
211	42596	95.9047	1	18	0	0	3	0	0	0	Mo-96
212	42597	96.9061	1	19	0	0	1	0	0	0	Mo-97
213	42598	97.9055	1	20	0	0	1	0	0	0	Mo-98
214	42599	98.9078	1	21	0	0	1	0	0	0	Mo-99
215	42600	99.9075	1	22	0	0	1	0	0	0	Mo-100

216	44600	99.9042	1	24	0	0	1	0	0	0	Ru-100
217	44602	101.9044	1	26	0	0	1	0	0	0	Ru-102
218	44603	102.9060	1	27	0	0	1	0	0	0	Ru-103
219	44604	103.9056	1	28	0	0	1	0	0	0	Ru-104
220	44605	104.9082	1	29	0	0	1	0	0	0	Ru-105
221	44606	105.9078	1	30	0	0	1	0	0	0	Ru-106
222	46604	103.9036	1	33	0	0	1	0	0	0	Pd-104
223	46606	105.9038	1	35	0	0	1	0	0	0	Pd-106
224	47710	109.9061	1	39	0	0	1	0	0	0	Ag-110m
225	47611	110.9057	1	40	0	0	1	0	0	0	Ag-111
226	48610	109.9031	1	41	0	0	1	0	0	0	Cd-110
227	48611	110.9047	1	42	0	0	1	0	0	0	Cd-111
228	48613	112.8999	1	43	0	1	1	0	0	0	Cd-113
229	50125	124.9080	0	0	0	0	1	0	0	0	Sn-125
230	51621	120.9087	1	45	0	0	1	0	0	0	Sb-121
231	51625	124.9050	1	46	0	0	1	0	0	0	Sb-125
232	51627	126.9069	1	47	0	0	1	0	0	0	Sb-127
233	52727	126.9052	1	48	0	0	1	0	0	0	Te-127m
234	52729	128.9074	1	49	0	0	1	0	0	0	Te-129m
235	52632	131.9082	1	50	0	0	1	0	0	0	Te-132
236	53627	126.9042	1	51	0	3	1	0	0	0	I-127
237	53629	128.9054	1	52	0	0	1	0	0	0	I-129
238	53631	130.9066	1	53	0	0	1	0	0	0	I-131
239	53635	134.9100	1	54	0	0	1	0	0	0	I-135
240	54628	127.9038	1	55	0	3	1	0	0	0	Xe-128
241	54630	129.9039	1	56	0	3	1	0	0	0	Xe-130
242	54632	131.9041	1	58	0	3	1	0	0	0	Xe-132
243	54633	132.9057	1	59	0	0	1	0	0	0	Xe-133
244	54635	134.9069	1	61	0	0	1	0	0	0	Xe-135
245	54636	135.9075	1	62	0	3	1	0	0	0	Xe-136
246	55634	133.9073	1	64	0	0	1	0	0	0	Cs-134
247	55635	134.9059	1	65	0	0	1	0	0	0	Cs-135
248	55636	135.9075	1	66	0	0	1	0	0	0	Cs-136
249	55637	136.9071	1	67	0	0	1	0	0	0	Cs-137
250	56634	133.9043	1	68	0	0	1	0	0	0	Ba-134
251	56637	136.9051	1	69	0	0	1	0	0	0	Ba-137
252	56640	139.9109	1	70	0	0	1	0	0	0	Ba-140
253	57639	138.9063	1	71	0	0	1	0	0	0	La-139
254	57640	139.9099	1	72	0	0	1	0	0	0	La-140
255	58640	139.9059	1	73	0	0	1	0	0	0	Ce-140
256	58641	140.9085	1	74	0	0	1	0	0	0	Ce-141
257	58642	141.9091	1	75	0	0	1	0	0	0	Ce-142
258	58643	142.9127	1	76	0	0	1	0	0	0	Ce-143
259	58644	143.9133	1	77	0	0	1	0	0	0	Ce-144
260	59641	140.9075	1	78	0	3	1	0	0	0	Pr-141
261	59643	142.9107	1	79	0	0	1	0	0	0	Pr-143
262	60642	141.9081	1	80	0	0	1	0	0	0	Nd-142
263	60644	143.9103	1	82	0	0	1	0	0	0	Nd-144
264	60646	145.9135	1	84	0	3	1	0	0	0	Nd-146
265	60647	146.9161	1	85	0	0	1	0	0	0	Nd-147
266	60648	147.9167	1	86	0	3	1	0	0	0	Nd-148
267	60650	149.9209	1	87	0	3	1	0	0	0	Nd-150
268	61648	147.9177	1	89	0	0	1	0	0	0	Pm-148
269	61649	148.9183	1	90	0	0	1	0	0	0	Pm-149
270	61651	150.9215	1	91	0	0	1	0	0	0	Pm-151
271	62648	147.9147	1	94	0	0	1	0	0	0	Sm-148
272	62653	152.9217	1	99	0	0	1	0	0	0	Sm-153
273	62654	153.9223	1	100	0	0	1	0	0	0	Sm-154
274	63651	150.9195	1	101	0	3	1	0	0	0	Eu-151

275	63656	155.9245	1	105	0	0	1	0	0	0	Eu-156
276	63657	156.9251	1	106	0	0	1	0	0	0	Eu-157
277	64654	153.9213	1	107	0	1	1	0	0	0	Gd-154
278	64660	159.9268	1	112	0	1	1	0	0	0	Gd-160
279	65159	158.9252	0	0	0	0	1	0	0	0	Tb-159
280	65160	158.9273	1	0	0	0	1	0	0	0	Tb-160
281	65161	160.9276	1	0	0	0	1	0	0	0	Tb-161
282	65659	158.9252	1	113	0	0	1	0	0	0	Tb-159
283	65660	158.9273	1	114	0	0	1	0	0	0	Tb-160
284	65661	160.9276	1	115	0	0	1	0	0	0	Tb-161
285	66660	159.9248	1	116	0	0	1	0	0	0	Dy-160
286	66661	160.9274	1	117	0	0	1	0	0	0	Dy-161
287	66662	161.9270	1	118	0	0	1	0	0	0	Dy-162
288	66663	162.9286	1	119	0	0	1	0	0	0	Dy-163
289	66664	163.9282	1	120	0	3	1	0	0	0	Dy-164
290	67165	164.9298	0	0	0	3	1	0	0	0	Ho-165
291	67665	164.9298	1	121	0	3	1	0	0	0	Ho-165
292	77191	190.9781	0	0	0	0	1	0	0	0	Ir-191
293	77193	192.9803	0	0	0	0	1	0	0	0	Ir-193
294	91232	232.0386	1	0	0	0	1	0	0	0	Pa-232
295	91234	234.0433	1	0	0	0	1	0	0	0	Pa-234

Appendix C.2 DECLIB input to generate the ENDF/B-7.1 V4.0 MPACT 47-group library

```
%TITL
  DATE::FEBRUARY 26, 2015; GROUP::47; MASTER::ENDF/B-VII R1; SUBGROUP::YES; TRC::YES
%IOPT
! LIBRARY VERSION
  VER  4.0
! 0: Unformatted master library -> Formatted master library
! 1: Formatted master library -> Unformatted master library
! 2: Unformatted master library -> DeCART library
! 3: Formatted master library -> DeCART library
  LIB   2
! 0: lambda*sig-p is not included in sig-b
! 1: lambda*sig-p is included in sig-b
  BXS   0
! 0: No transport corrected total XS
! 1: Transport corrected total XS
! 2: Transport correction is applied to p1 scattering matrix only for testing.
  XST   1
%FILE
  AMP  ..\lib\ampx47g_71_07202014_02m_ykk.bin    lib47_HetFfactors_VII.1.fmt
  DEC  mpact47g_71s_v4.1m1_03102015.fmt   mpact47g_71s_v4.1m1_03102015.bin
  END  ..\lib\n-endfb7.1
  DCY  ..\lib\dec-endfb7.1
  FPY  ..\lib\fpy-endfb7.1
  SUB  ..\lib\subgr_47g_71s_02252015_merge.sub              !Subgroup data
  TRC  ..\lib\trcorr_47g_71_10242014_5n.dat                 !Transport correction
  XSB  ..\lib\backxs_47g_03022015_final.dat                 !Background XS
  DLY  ..\lib\totbeta_e71_10062014.dat                      !Transient data
  DBR  ..\lib\subgr_47g_71s_10312014_u238epi.sub            !Epithermal upscattering
%COLL
  FLX  ..\lib\fluxcur_47g_fa.dat
  SUB  e:\ornl\declib\lib\subgr.sub_moc49g_mod
  LAM  e:\ornl\declib\lib\rilamb.irp_e705_49g
%RESO  !# of fast / end of reso.
  GRP    9  26
%NUCL
! NRES  NELR   NELT  NYLD
  49    191    295   121
!  48    191    295   121
!
! ------------------------------------------------------------------------------------------
! NID    NUCLIDE ID  1000*Z+500*A+100*B+A
!        A=0: ACTIVATION & HEAVY NUCLIDES / A=1: F.P. NUCLIDES
!        B=0: STABLE / B=1: METASTABLE
! AMASS  ATOMIC MASS
! AID    ALPHANUMERIC NUCLIDE ID.
! NO0    1/2/3  COLLAPSING SPECTRA (MODERATOR/FUEL/STRUCTURE)
! NO1    0  NON DEPLETABLE
!       >0  DEPLETABLE (W/ DECAY CONSTANT)
!        1
!        2 RI-A ONLY (FISSIONABLE W/ KAPPA, BETA, FPY)
!        3 RI-A & RI-NF (FISSIONABLE W/ KAPPA, BETA, FPY)
! NO2    NFPY  (ORDERING NO. OF FPY) (+/- : CUMULATIVE/DIRECT YIELD)
! NO3    NPI   (WITH P1/P2/P3)
! NO4    NCHIX (WITH FISSION SPECTRA)
! NO5    N2N   (WITH N2N)
! NO6    N3N   (WITH N3N)
! NO7    EPU   (WITH EPITHERMAL UPSCATTERING RESONANCE DATA)
! NO8    TRC   (TRANSPORT CORRECTION) (0/1/2 : OUTSCATT/NLC/INSCATT)
! AMPX   # OF AMPX NUCLIDES TO BE MERGED
! #T     # OF TEMPERATURES
! ------------------------------------------------------------------------------------------
! NO     NID      AMASS       AID    NO0 NO1 NO2 NO3 NO4 NO5 NO6 NO7 NO8 AMPX  #T  TEMPERATURE(K)
! ------------------------------------------------------------------------------------------------
   1   40091    90.9056   'Zr-91  '    3   1   0   0   0   0   0   0   0    1   3  293  900 2000
           1   40091  100.0
   2   40096    95.9083   'Zr-96  '    3   1   0   0   0   0   0   0   0    1   3  293  900 2000
           1   40096  100.0
   3   42595    94.9059   'Mo-95  '    2   1  17   0   0   0   0   0   0    1   3  293  900 2000
           1   42095  100.0
   4   43599    99.0005   'Tc-99  '    2   1  23   0   0   2   0   0   0    1   3  293  900 2000
           1   43099  100.0
   5   45103   102.9050   'Rh-103 '    3   1   0   0   0   0   0   0   0    1   3  293  900 2000
           1   45103  100.0
   6   46608   107.9039   'Pd-108 '    2   1  37   0   0   0   0   0   0    1   3  293  900 2000
           1   46108  100.0
   7   47107   106.9054   'Ag-107 '    3   0   0   0   0   3   1   0   0    1   3  293  900 2000
           1   47107  100.0
   8   47109   108.9045   'Ag-109 '    3   0   0   0   0   4   2   0   0    1   3  293  900 2000
           1   47109  100.0
   9   49113   112.9039   'In-113 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
           1   49113  100.0
  10   49115   114.9041   'In-115 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
           1   49115  100.0
  11   54631   130.9055   'Xe-131 '    2   1  57   0   0   5   3   0   0    1   3  293  900 2000
           1   54131  100.0
  12   55633   132.9057   'Cs-133 '    2   1  63   0   0   6   0   0   0    1   3  293  900 2000
           1   55133  100.0
  13   62152   151.9201   'Sm-152 '    3   0   0   0   0   7   4   0   0    1   5  293  600  900 1200 2400
           1   62152  100.0
  14   63151   150.9195   'Eu-151 '    3   0   0   0   0   8   5   0   0    1   5  293  600  900 1200 2400
           1   63151  100.0
```

```
  15   63152   151.9251   'Eu-152 '    3   1   0   0   0   9   6   0   0    1   5  293  600  900 1200 2400
          1   63152  100.0
  16   63153   152.9217   'Eu-153 '    3   0   0   0   0  10   7   0   0    1   5  293  600  900 1200 2400
          1   63153  100.0
  17   63154   153.9223   'Eu-154 '    3   1   0   0   0  11   8   0   0    1   5  293  600  900 1200 2400
          1   63154  100.0
  18   63155   154.9229   'Eu-155 '    3   1   0   0   0  12   9   0   0    1   5  293  600  900 1200 2400
          1   63155  100.0
  19   64155   154.9229   'Gd-155 '    2   0   0   0   0  13   0   0   0    1   5  293  600  900 1200 2400
          1   64155  100.0
  20   64156   155.9225   'Gd-156 '    2   0   0   0   0  14   0   0   0    1   5  293  600  900 1200 2400
          1   64156  100.0
  21   64157   156.9241   'Gd-157 '    2   0   0   0   0  15   0   0   0    1   5  293  600  900 1200 2400
          1   64157  100.0
  22   64158   157.9236   'Gd-158 '    2   0   0   0   0  16   0   0   0    1   5  293  600  900 1200 2400
          1   64158  100.0
  23   66160   159.9248   'Dy-160 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   66160  100.0
  24   66161   160.9274   'Dy-161 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   66161  100.0
  25   66162   161.9270   'Dy-162 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   66162  100.0
  26   66163   162.9286   'Dy-163 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   66163  100.0
  27   66164   163.9282   'Dy-164 '    3   0   0   0   0  17  10   0   0    1   3  293  900 2000
          1   66164  100.0
  28   68166   165.9304   'Er-166 '    2   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   68166  100.0
  29   68167   166.9320   'Er-167 '    2   0   0   0   0   0   0   0   0    1   5  293  600  900 1200 2400
          1   68167  100.0
  30   72176   175.9414   'Hf-176 '    3   0   0   0   0  18   0   0   0    1   3  293  900 2000
          1   72176  100.0
  31   72177   176.9430   'Hf-177 '    3   0   0   0   0  19   0   0   0    1   3  293  900 2000
          1   72177  100.0
  32   72178   177.9436   'Hf-178 '    3   0   0   0   0  20   0   0   0    1   3  293  900 2000
          1   72178  100.0
  33   72179   178.9462   'Hf-179 '    3   0   0   0   0  21   0   0   0    1   3  293  900 2000
          1   72179  100.0
  34   72180   179.9468   'Hf-180 '    3   0   0   0   0  22   0   0   0    1   3  293  900 2000
          1   72180  100.0
! ------------------------------------------------------------------------------------------------- Newly added on 05/22/2013(b)
  35   74182   181.9531   'W-182  '    3   0   0   0   0  23   0   0   0    1   3  293  900 2000
          1   74182  100.0
  36   74183   182.9517   'W-183  '    3   0   0   0   0  24   0   0   0    1   3  293  900 2000
          1   74183  100.0
  37   74184   183.9502   'W-184  '    3   0   0   0   0  25   0   0   0    1   3  293  900 2000
          1   74184  100.0
  38   74186   185.9575   'W-186  '    3   0   0   0   0  26   0   0   0    1   3  293  900 2000
          1   74186  100.0
! ------------------------------------------------------------------------------------------------- Newly added on 05/22/2013(e)
  39   90232   232.0333   'Th-232 '    2   2   0  18   1  27  11   0   0    1   5  293  600  900 1200 2400
          1   90232  100.0
  40   92233   233.0450   'U-233  '    2   3   0  19   2  28  12   0   0    1   5  293  600  900 1200 2400
          1   92233  100.0
  41   92235   235.0441   'U-235  '    2   3   0  21   3  29  13   0   0    1   5  293  600  900 1200 2400
          1   92235  100.0
  42   92236   236.0458   'U-236  '    2   3   0  22   4  30  14   0   0    1   3  293  900 2000
          1   92236  100.0
  43   92238   238.0510   'U-238  '    2   2   0  23   5  31  15   1   0    1   5  293  600  900 1200 2400
          1   92238  100.0
  44   94238   238.0495   'Pu-238 '    2   3   0   0   6  32  16   0   0    1   3  293  900 2000
          1   94238  100.0
  45   94239   239.0522   'Pu-239 '    2   3   0  24   7  33  17   0   0    1   5  293  600  900 1200 2400
          1   94239  100.0
  46   94240   240.0542   'Pu-240 '    2   3   0  25   8  34  18   0   0    1   5  293  600  900 1200 2400
          1   94240  100.0
  47   94241   241.0487   'Pu-241 '    2   3   0  26   9  35  19   0   0    1   5  293  600  900 1200 2400
          1   94241  100.0
  48   94242   242.0584   'Pu-242 '    2   3   0  27  10  36  20   0   0    1   3  293  900 2000
          1   94242  100.0
  49   95241   241.0568   'Am-241 '    2   3   0   0   0  37  21   0   0    1   3  293  900 2000
          1   95241  100.0
! ------------------------------------------------------------------------------------------------------------------------
  50    1001     1.0078   'H-1    '    1   0   0   1   0   0   0   0   1    1   9  293.6  350  400  450  500  550  600  650  800
          1    1001  100.0
  51    1002     2.0141   'H-2    '    1   0   0   2   0  38   0   0   0    1   5  293  600  900 1200 2400
          1    1002  100.0
  52    1006     1.0078   'H-1    '    1   0   0   3   0   0   0   0   0    1   3  293  900 2000
          1 5001001  100.0
  53    1040     1.0078   'H-1    '    1   0   0   4   0   0   0   0   0    1   3  296  400  500  600  700  800 1000 1200
          1 7001001  100.0
 54     2004     4.0026   'He-4   '    1   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1    2004  100.0
 55     3006     6.0151   'Li-6   '    1   0   0   7   0   0   0   0   0    1   5  293  600  900 1200 2400
          1    3006  100.0
 56     3007     7.0160   'Li-7   '    1   0   0   8   0  39   0   0   0    1   3  293  900 2000
          1    3007  100.0
 57     4009     9.0122   'Be-9   '    1   0   0   0   0  40   0   0   0    1   3  293  900 2000
          1    4009  100.0
 58     5000    10.8120   'B-nat  '    1   0   0  28   0   0   0   0   0    2   5  293  600  900 1200 2400
          1    5010   19.90
          2    5011   80.10
 59     5010    10.0129   'B-10   '    1   1   0  29   0   0   0   0   0    1   5  293  600  900 1200 2400
          1    5010  100.0
 60     5011    11.0093   'B-11   '    1   1   0  30   0   0   0   0   2    1   5  293  600  900 1200 2400
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          1    5011  100.0
 61     6000    12.0011   'C-nat  '    1   0   0   9   0   0   0   0   2    1   5  293  600  900 1200 2400
          1    6000  100.0
 62     6001    12.0011   'C-nat  '    1   0   0   0   0   0   0   0   0    1  10  296  400  500  600  700  800 1000 1200 1600
2000
          1 3006000  100.0
 63     7014    14.0031   'N-14   '    1   0   0   0   0  41   0   0   0    1   3  293  900 2000
          1    7014  100.0
 64     8001    15.9905   'O-uo2  '    2   0   0  11   0   0   0   0   0    2   5  293  600  900 1200 2400
          1    8016   99.762
          2    8017    0.238
 65     8016    15.9905   'O-16   '    1   0   0  12   0   0   0   0   2    1   5  293  600  900 1200 2400
          1    8016  100.0
 66     9019    18.9982   'F-19   '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1    9019  100.0
 67    11023    22.9895   'Na-23  '    3   0   0   0   0   0   0   0   0    1   5  293  600  900 1200 2400
          1   11023  100.0
 68    12000    24.3051   'Mg-nat '    3   0   0   0   0   0   0   0   0    3   3  293  900 2000
          1   12024   78.99
          2   12025   10.0
          3   12026   11.01
 69    13027    26.9818   'Al-27  '    3   0   0  13   0   0   0   0   0    1   5  293  600  900 1200 2400
          1   13027  100.0
 70    14000    28.0853   'Si-nat '    3   0   0   0   0   0   0   0   0    3   3  293  900 2000
          1   14028   92.23
          2   14029    4.67
          3   14030    3.10
 71    15031    30.9741   'P-31   '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   15031  100.0
 72    16000    32.0636   'S-nat  '    3   0   0   0   0   0   0   0   0    4   3  293  900 2000
          1   16032   95.02
          2   16033    0.75
          3   16034    4.21
          4   16036    0.02
 73    17000    35.4526   'Cl-nat '    3   0   0   0   0   0   0   0   0    2   3  293  900 2000
          1   17035   75.77
          2   17037   24.23
 74    19000    39.1019   'K-nat  '    3   0   0   0   0   0   0   0   0    3   3  293  900 2000
          1   19039   93.26
          2   19040    0.01
          3   19041    6.73
 75    20000    40.0803   'Ca-nat '    3   0   0   0   0   0   0   0   0    6   3  293  900 2000
          1   20040  96.941
          2   20042   0.647
          3   20043   0.135
          4   20044   2.086
          5   20046   0.004
          6   20048   0.187
 76    22000    47.8789   'Ti-nat '    3   0   0   0   0   0   0   0   0    5   3  293  900 2000
          1   22046   8.0
          2   22047   7.3
          3   22048  73.8
          4   22049   5.5
          5   22050   5.4
 77    23000    50.9416   'V-nat  '    3   0   0   0   0   0   0   0   0    2   3  293  900 2000
          1   23050    0.25
          2   23051   99.75
 78    24000    51.9957   'Cr-nat '    3   0   0   0   0  42   0   0   0    4   3  293  900 2000
          1   24050    4.345
          2   24052   83.789
          3   24053    9.501
          4   24054    2.365
 79    24050    49.9461   'Cr-50  '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   24050  100.0
 80    24052    51.9402   'Cr-52  '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   24052  100.0
 81    24053    52.9408   'Cr-53  '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   24053  100.0
 82    24054    53.9394   'Cr-54  '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   24054  100.0
 83    25055    54.9381   'Mn-55  '    3   0   0   0   0  43   0   0   0    1   3  293  900 2000
          1   25055  100.0
 84    26000    55.8446   'Fe-nat '    3   0   0   0   0  44   0   0   0    4   3  293  900 2000
          1   26054    5.845
          2   26056   91.754
          3   26057    2.119
          4   26058    0.282
 85    26054    53.9394   'Fe-54  '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   26054  100.0
 86    26056    55.9345   'Fe-56  '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   26056  100.0
 87    26057    56.9351   'Fe-57  '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   26057  100.0
 88    26058    57.9337   'Fe-58  '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   26058  100.0
 89    27059    58.9332   'Co-59  '    3   0   0   0   0  45   0   0   0    1   3  293  900 2000
          1   27059  100.0
 90    28000    58.6936   'Ni-nat '    3   0   0   0   0  46   0   0   0    5   3  293  900 2000
          1   28058   60.077
          2   28060   26.223
          3   28061    1.140
          4   28062    3.634
          5   28064    8.926
 91    28058    57.9357   'Ni-58  '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   28058  100.0
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92    28060    59.9308   'Ni-60  '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   28060  100.0
93    28061    60.9314   'Ni-61  '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   28061  100.0
94    28062    61.9280   'Ni-62  '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   28062  100.0
95    28064    63.9282   'Ni-64  '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   28064  100.0
96    29063    62.9296   'Cu-63  '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   29063  100.0
97    29065    64.9278   'Cu-65  '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   29065  100.0
98    40000    91.2196   'Zr-nat '    3   0   0  14   0  47   0   0   0    5   3  293  900 2000
          1   40090  51.45
          2   40091  11.22
          3   40092  17.15
          4   40094  17.38
          5   40096   2.80
99    40001    91.2196   'Zr-zrh2'    3   0   0  15   0  48   0   0   0    5   8  296  400  500  600  700  800 1000 1200
          1   1040090  51.45
          2   1040091  11.22
          3   1040092  17.15
          4   1040094  17.38
          5   1040096   2.80
100   40090    89.9043   'Zr-90  '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   40090  100.0
101   40092    91.9050   'Zr-92  '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   40092  100.0
102   40094    93.9063   'Zr-94  '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   40090  100.0
103   41093    92.9032   'Nb-93  '    3   0   0   0   0   0   0   0   0    1   5  293  600  900 1200 2400
          1   41093  100.0
104   42000    95.9402   'Mo-nat '    3   0   0   0   0  49  22   0   0    7   3  293  900 2000
          1   42092  14.84
          2   42094   9.25
          3   42095  15.92
          4   42096  16.68
          5   42097   9.55
          6   42098  24.13
          7   42100   9.63
105   44601   100.9058   'Ru-101 '    2   1  25   0   0   0   0   0   0    1   3  293  900 2000
          1   44101  100.0
106   45603   102.9050   'Rh-103 '    2   1  31   0   0  50   0   0   0    1   3  293  900 2000
          1   45103  100.0
107   45605   104.9062   'Rh-105 '    2   1  32   0   0   0   0   0   0    1   3  293  900 2000
          1   45105  100.0
108   46605   104.9052   'Pd-105 '    2   1  34   0   0   0   0   0   0    1   3  293  900 2000
          1   46105  100.0
109   46607   106.9054   'Pd-107 '    2   1  36   0   0   0   0   0   0    1   3  293  900 2000
          1   46107  100.0
110   47609   108.9045   'Ag-109 '    2   1  38   0   0  51  23   0   0    1   3  293  900 2000
          1   47109  100.0
111   48000   112.4258   'Cd-nat '    3   0   0   0   0   0   0   0   0    8   3  293  900 2000
          1   48106   1.25
          2   48108   0.89
          3   48110  12.49
          4   48111  12.80
          5   48112  24.13
          6   48113  12.22
          7   48114  28.73
          8   48116   7.49
112   48110   109.9031   'Cd-110 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   48110  100.0
113   48111   110.9047   'Cd-111 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   48111  100.0
114   48112   111.9033   'Cd-112 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   48112  100.0
115   48113   112.8999   'Cd-113 '    3   0   0   0   0  52   0   0   0    1   3  293  900 2000
          1   48113  100.0
116   48114   113.9035   'Cd-114 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   48114  100.0
117   49000   114.9071   'In-nat '    3   0   0   0   0   0   0   0   0    2   3  293  900 2000
          1   49113   4.30
          2   49115  95.70
118   49615   114.9071   'In-115 '    2   1  44   0   0   0   0   0   0    1   3  293  900 2000
          1   49115  100.000
119   50000   118.7107   'Sn-nat '    3   0   0   0   0   0   0   0   0   10   3  293  900 2000
          1   50112    0.970
          2   50114    0.650
          3   50115    0.340
          4   50116   14.540
          5   50117    7.680
          6   50118   24.220
          7   50119    8.580
          8   50120   32.600
          9   50122    4.630
         10   50124    5.790
120   50112   111.9013   'Sn-112 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   50112  100.0
121   50114   113.8984   'Sn-114 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   50114  100.0
122   50115   114.9031   'Sn-115 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   50115  100.0
123   50116   115.9017   'Sn-116 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   50116  100.0
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124   50117   116.9033   'Sn-117 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   50117  100.0
125   50118   117.9018   'Sn-118 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   50118  100.0
126   50119   118.9035   'Sn-119 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   50119  100.0
127   50120   119.9020   'Sn-120 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   50120  100.0
128   50122   121.9032   'Sn-122 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   50122  100.0
129   50124   123.9054   'Sn-124 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   50124  100.0
130   51000   121.7577   'Sb-nat '    3   0   0   0   0   0   0   0   0    2   3  293  900 2000
          1   51121  57.210
          2   51123  42.790
131   51121   120.9036   'Sb-121 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   51121  100.0
132   51123   122.9038   'Sb-123 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   51123  100.0
133   54634   133.9053   'Xe-134 '    2   1  60   0   0  53  24   0   0    1   3  293  900 2000
          1   54134  100.0
134   60643   142.9097   'Nd-143 '    2   1  81   0   0  54  25   0   0    1   3  293  900 2000
          1   60143  100.0
135   60645   144.9129   'Nd-145 '    2   1  83   0   0  55  26   0   0    1   3  293  900 2000
          1   60145  100.0
136   61647   146.9151   'Pm-147 '    2   1  88   0   0  56  27   0   0    1   3  293  900 2000
          1   61147  100.0
137   61748   147.9177   'Pm-148m'    2   1  92   0   0   0   0   0   0    1   3  293  900 2000
          1 1061148  100.0
138   62153   152.9217   'Sm-153 '    3   1   0   0   0   0   0   0   0    1   3  293  900 2000
          1   62153  100.0
139   62647   146.9151   'Sm-147 '    2   1  93   0   0  57  28   0   0    1   3  293  900 2000
          1   62147  100.0
140   62649   148.9173   'Sm-149 '    2   1  95   0   0  58  29   0   0    1   3  293  900 2000
          1   62149  100.0
141   62650   149.9169   'Sm-150 '    2   1  96   0   0  59   0   0   0    1   3  293  900 2000
          1   62150  100.0
142   62651   150.9195   'Sm-151 '    2   1  97   0   0  60  30   0   0    1   3  293  900 2000
          1   62151  100.0
143   62652   151.9201   'Sm-152 '    2   1  98   0   0  61  31   0   0    1   3  293  900 2000
          1   62152  100.0
144   63156   155.9245   'Eu-156 '    3   1   0   0   0   0   0   0   0    1   3  293  900 2000
          1   63156  100.0
145   63157   156.9251   'Eu-157 '    3   1   0   0   0   0   0   0   0    1   3  293  900 2000
          1   63157  100.0
146   63653   152.9217   'Eu-153 '    2   1 102   0   0  62  32   0   0    1   3  293  900 2000
          1   63153  100.0
147   63654   153.9223   'Eu-154 '    2   1 103   0   0  63  33   0   0    1   3  293  900 2000
          1   63154  100.0
148   63655   154.9229   'Eu-155 '    2   1 104   0   0  64  34   0   0    1   3  293  900 2000
          1   63155  100.0
149   64152   151.9201   'Gd-152 '    3   0   0   0   0  65   0   0   0    1   3  293  900 2000
          1   64152  100.0
150   64154   153.9213   'Gd-154 '    3   0   0   0   0  66   0   0   0    1   3  293  900 2000
          1   64154  100.0
151   64160   159.9268   'Gd-160 '    3   0   0   0   0  67   0   0   0    1   3  293  900 2000
          1   64160  100.0
152   64655   154.9229   'Gd-155 '    2   1 108   0   0  68   0   0   0    1   3  293  900 2000
          1   64155  100.0
153   64656   155.9225   'Gd-156 '    2   1 109   0   0  69   0   0   0    1   3  293  900 2000
          1   64156  100.0
154   64657   156.9241   'Gd-157 '    2   1 110   0   0  70   0   0   0    1   3  293  900 2000
          1   64157  100.0
155   64658   157.9236   'Gd-158 '    2   1 111   0   0  71   0   0   0    1   3  293  900 2000
          1   64158  100.0
156   68168   167.9414   'Er-166 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   68168  100.0
157   71176   175.9414   'Lu-176 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   71176  100.0
158   72174   173.9402   'Hf-174 '    3   0   0   0   0  72   0   0   0    1   3  293  900 2000
          1   72174  100.0
159   73181   180.9545   'Ta-181 '    3   0   0   0   0  73  35   0   0    1   3  293  900 2000
          1   73181  100.0
160   73182   181.9500   'Ta-182 '    3   0   0   0   0  74  36   0   0    1   3  293  900 2000
          1   73182  100.0
161   74000   183.8564   'W-nat  '    3   0   0   0   0  75  37   0   0    4   3  293  900 2000
          1   74182  26.62
          2   74183  14.31
          3   74184  30.64
          4   74186  28.43
162   79197   196.9660   'Au-197 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   79197  100.0
163   82206   205.9694   'Pb-206 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   82206  100.0
164   82207   206.9780   'Pb-207 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   82207  100.0
165   82208   207.9766   'Pb-208 '    3   0   0   0   0   0   0   0   0    1   3  293  900 2000
          1   82208  100.0
166   83209   208.9803   'Bi-209 '    3   0   0   0   0  76  38   0   0    1   3  293  900 2000
          1   83209  100.0
167   90230   230.0361   'Th-230 '    2   3   0   0   0  77  39   0   0    1   3  293  900 2000
          1   90230  100.0
168   91231   231.0347   'Pa-231 '    2   3   0   0   0  78  40   0   0    1   3  293  900 2000
          1   91231  100.0
169   91233   233.0399   'Pa-233 '    2   3   0   0   0  79  41   0   0    1   5  293  600  900 1200 2400
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         1   91233  100.0
 170   92232   232.0333   'U-232  '    2   3   0   0   0  80  42   0   0    1   3  293  900 2000
         1   92232  100.0
 171   92234   234.0405   'U-234  '    2   3   0  20  11  81  43   0   0    1   3  293  900 2000
         1   92234  100.0
 172   92237   237.0484   'U-237  '    2   3   0   0   0  82  44   0   0    1   3  293  900 2000
         1   92237  100.0
 173   93237   237.0482   'Np-237 '    2   3   0   0  12  83  45   0   0    1   3  293  900 2000
         1   93237  100.0
 174   93238   238.0510   'Np-238 '    2   3   0   0   0   0   0   0   0    1   3  293  900 2000
         1   93238  100.0
 175   93239   239.0526   'Np-239 '    2   3   0   0  13  84  46   0   0    1   3  293  900 2000
         1   93239  100.0
 176   94236   236.0458   'Pu-236 '    2   3   0   0  14  85  47   0   0    1   3  293  900 2000
         1   94236  100.0
 177   95242   242.0594   'Am-242 '    2   3   0   0   0   0   0   0   0    1   3  293  900 2000
         1   95242  100.0
 178   95342   242.0594   'Am-242m'    2   3   0   0   0  86  48   0   0    1   3  293  900 2000
         1 1095242  100.0
 179   95243   243.0610   'Am-243 '    2   3   0   0   0  87  49   0   0    1   3  293  900 2000
         1   95243  100.0
 180   96242   242.0584   'Cm-242 '    2   3   0   0   0  88  50   0   0    1   3  293  900 2000
         1   96242  100.0
 181   96243   243.0610   'Cm-243 '    2   3   0   0   0  89  51   0   0    1   3  293  900 2000
         1   96243  100.0
 182   96244   244.0626   'Cm-244 '    2   3   0   0   0  90  52   0   0    1   3  293  900 2000
         1   96244  100.0
 183   96245   245.0652   'Cm-245 '    2   3   0   0   0  91  53   0   0    1   3  293  900 2000
         1   96245  100.0
 184   96246   246.0668   'Cm-246 '    2   3   0   0   0  92  54   0   0    1   3  293  900 2000
         1   96246  100.0
 185   96247   247.0725   'Cm-247 '    2   3   0   0   0  93  55   0   0    1   3  293  900 2000
         1   96247  100.0
 186   96248   248.0721   'Cm-248 '    2   3   0   0   0  94  56   0   0    1   3  293  900 2000
         1   96248  100.0
 187   97249   249.0797   'Bk-249 '    2   3   0   0   0  95  57   0   0    1   3  293  900 2000
         1   97249  100.0
 188   98249   249.0797   'Cf-249 '    2   3   0   0   0  96  58   0   0    1   3  293  900 2000
         1   98249  100.0
 189   98250   250.0763   'Cf-250 '    2   3   0   0   0  97  59   0   0    1   3  293  900 2000
         1   98250  100.0
 190   98251   251.0799   'Cf-251 '    2   3   0   0   0  98  60   0   0    1   3  293  900 2000
         1   98251  100.0
 191   98252   252.0815   'Cf-252 '    2   3   0   0   0  99  61   0   0    1   3  293  900 2000
         1   98252  100.0
!   ------------------------------------------------------------------------------------------
 192   1003     3.0160   'T-3    '    1   0   0   0   0   0   0   0   0    1   3  293  900 2000
         1    1003  100.0
 193   2003     3.0149   'He-3   '    1   0   0   0   0   0   0   0   0    1   3  293  900 2000
         1    2003  100.0
 194   35581   80.9163   'Br-81  '    2   1   1   0   0   0   0   0   0    1   1 1100
         1   35081  100.0
 195   36582   81.9135   'Kr-82  '    2   1   2   0   0 100   0   0   0    1   1 1100
         1   36082  100.0
 196   36583   82.9141   'Kr-83  '    2   1   3   0   0 101  62   0   0    1   1 1100
         1   36083  100.0
 197   36584   83.9114   'Kr-84  '    2   1   4   0   0 102   0   0   0    1   1 1100
         1   36084  100.0
 198   36585   84.9125   'Kr-85  '    2   1   5   0   0   0   0   0   0    1   1 1100
         1   36085  100.0
 199   36586   85.9106   'Kr-86  '    2   1   6   0   0 103  63   0   0    1   1 1100
         1   36086  100.0
 200   38589   88.9075   'Sr-89  '    2   1   7   0   0   0   0   0   0    1   1 1100
         1   38089  100.0
 201   38590   89.9078   'Sr-90  '    2   1   8   0   0   0   0   0   0    1   1 1100
         1   38090  100.0
 202   39589   88.9058   'Y-89   '    2   1   9   0   0 104   0   0   0    1   1 1100
         1   39089  100.0
 203   39590   89.9072   'Y-90   '    2   1  10   0   0   0   0   0   0    1   1 1100
         1   39090  100.0
 204   39591   90.9074   'Y-91   '    2   1  11   0   0   0   0   0   0    1   1 1100
         1   39091  100.0
 205   40591   90.9029   'Zr-91  '    2   1  12   0   0 105   0   0   0    1   1 1100
         1   40091  100.0
 206   40593   92.9064   'Zr-93  '    2   1  13   0   0   0   0   0   0    1   1 1100
         1   40093  100.0
 207   40595   94.9080   'Zr-95  '    2   1  14   0   0   0   0   0   0    1   1 1100
         1   40095  100.0
 208   40596   95.9049   'Zr-96  '    2   1  15   0   0 106   0   0   0    1   1 1100
         1   40096  100.0
 209   41595   94.9068   'Nb-95  '    2   1  16   0   0   0   0   0   0    1   1 1100
         1   41095  100.0
 210   42095   94.9059   'Mo-95  '    3   0   0   0   0   0   0   0   0    1   1 1100
         1   42095  100.0
 211   42596   95.9047   'Mo-96  '    2   1  18   0   0   0   0   0   0    1   3  293  900 2000
         1   42096  100.0
 212   42597   96.9061   'Mo-97  '    2   1  19   0   0   0   0   0   0    1   1 1100
         1   42097  100.0
 213   42598   97.9055   'Mo-98  '    2   1  20   0   0   0   0   0   0    1   1 1100
         1   42098  100.0
 214   42599   98.9078   'Mo-99  '    2   1  21   0   0   0   0   0   0    1   1 1100
         1   42099  100.0
 215   42600   99.9075   'Mo-100 '    2   1  22   0   0   0   0   0   0    1   1 1100
         1   42100  100.0
 216   44600   99.9042   'Ru-100 '    2   1  24   0   0   0   0   0   0    1   1 1100
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        1   44100  100.0
217   44602   101.9044   'Ru-102 '    2   1  26   0   0   0   0   0   0    1   1 1100
        1   44102  100.0
218   44603   102.9060   'Ru-103 '    2   1  27   0   0   0   0   0   0    1   1 1100
        1   44103  100.0
219   44604   103.9056   'Ru-104 '    2   1  28   0   0   0   0   0   0    1   1 1100
        1   44104  100.0
220   44605   104.9082   'Ru-105 '    2   1  29   0   0   0   0   0   0    1   1 1100
        1   44105  100.0
221   44606   105.9078   'Ru-106 '    2   1  30   0   0   0   0   0   0    1   1 1100
        1   44106  100.0
222   46604   103.9036   'Pd-104 '    2   1  33   0   0   0   0   0   0    1   1 1100
        1   46104  100.0
223   46606   105.9038   'Pd-106 '    2   1  35   0   0   0   0   0   0    1   1 1100
        1   46106  100.0
224   47710   109.9061   'Ag-110m'    2   1  39   0   0   0   0   0   0    1   1 1100
        1 1047110  100.0
225   47611   110.9057   'Ag-111 '    2   1  40   0   0   0   0   0   0    1   1 1100
        1   47111  100.0
226   48610   109.9031   'Cd-110 '    2   1  41   0   0   0   0   0   0    1   1 1100
        1   48110  100.0
227   48611   110.9047   'Cd-111 '    2   1  42   0   0   0   0   0   0    1   1 1100
        1   48111  100.0
228   48613   112.8999   'Cd-113 '    2   1  43   0   0 107   0   0   0    1   1 1100
        1   48113  100.0
229   50125   124.9080   'Sn-125 '    3   0   0   0   0   0   0   0   0    1   1 1100
        1   50125  100.0
230   51621   120.9087   'Sb-121 '    2   1  45   0   0   0   0   0   0    1   1 1100
        1   51121  100.0
231   51625   124.9050   'Sb-125 '    2   1  46   0   0   0   0   0   0    1   1 1100
        1   51125  100.0
232   51627   126.9069   'Sb-127 '    2   1  47   0   0   0   0   0   0    0   1 1100
233   52727   126.9052   'Te-127m'    2   1  48   0   0   0   0   0   0    1   1 1100
        1 1052127  100.0
234   52729   128.9074   'Te-129m'    2   1  49   0   0   0   0   0   0    1   1 1100
        1 1052129  100.0
235   52632   131.9082   'Te-132 '    2   1  50   0   0   0   0   0   0    1   1 1100
        1   52132  100.0
236   53627   126.9042   'I-127  '    2   1  51   0   0 108  64   0   0    1   1 1100
        1   53127  100.0
237   53629   128.9054   'I-129  '    2   1  52   0   0   0   0   0   0    1   1 1100
        1   53129  100.0
238   53631   130.9066   'I-131  '    2   1  53   0   0   0   0   0   0    1   1 1100
        1   53131  100.0
239   53635   134.9100   'I-135  '    2   1  54   0   0   0   0   0   0    1   1 1100
        1   53135  100.0
240   54628   127.9038   'Xe-128 '    2   1  55   0   0 109  65   0   0    1   1 1100
        1   54128  100.0
241   54630   129.9039   'Xe-130 '    2   1  56   0   0 110  66   0   0    1   1 1100
        1   54130  100.0
242   54632   131.9041   'Xe-132 '    2   1  58   0   0 111  67   0   0    1   1 1100
        1   54132  100.0
243   54633   132.9057   'Xe-133 '    2   1  59   0   0   0   0   0   0    1   1 1100
        1   54133  100.0
244   54635   134.9069   'Xe-135 '    2   1  61   0   0   0   0   0   0    1   1 1100
        1   54135  100.0
245   54636   135.9075   'Xe-136 '    2   1  62   0   0 112  68   0   0    1   1 1100
        1   54136  100.0
246   55634   133.9073   'Cs-134 '    2   1  64   0   0   0   0   0   0    1   1 1100
        1   55134  100.0
247   55635   134.9059   'Cs-135 '    2   1  65   0   0   0   0   0   0    1   1 1100
        1   55135  100.0
248   55636   135.9075   'Cs-136 '    2   1  66   0   0   0   0   0   0    1   1 1100
        1   55136  100.0
249   55637   136.9071   'Cs-137 '    2   1  67   0   0   0   0   0   0    1   1 1100
        1   55137  100.0
250   56634   133.9043   'Ba-134 '    2   1  68   0   0   0   0   0   0    1   1 1100
        1   56134  100.0
251   56637   136.9051   'Ba-137 '    2   1  69   0   0   0   0   0   0    1   1 1100
        1   56137  100.0
252   56640   139.9109   'Ba-140 '    2   1  70   0   0   0   0   0   0    1   1 1100
        1   56140  100.0
253   57639   138.9063   'La-139 '    2   1  71   0   0   0   0   0   0    1   1 1100
        1   57139  100.0
254   57640   139.9099   'La-140 '    2   1  72   0   0   0   0   0   0    1   1 1100
        1   57140  100.0
255   58640   139.9059   'Ce-140 '    2   1  73   0   0   0   0   0   0    1   1 1100
        1   58140  100.0
256   58641   140.9085   'Ce-141 '    2   1  74   0   0   0   0   0   0    1   1 1100
        1   58141  100.0
257   58642   141.9091   'Ce-142 '    2   1  75   0   0   0   0   0   0    1   1 1100
        1   58142  100.0
258   58643   142.9127   'Ce-143 '    2   1  76   0   0   0   0   0   0    1   1 1100
        1   58143  100.0
259   58644   143.9133   'Ce-144 '    2   1  77   0   0   0   0   0   0    1   1 1100
        1   58144  100.0
260   59641   140.9075   'Pr-141 '    2   1  78   0   0 113  69   0   0    1   1 1100
        1   59141  100.0
261   59643   142.9107   'Pr-143 '    2   1  79   0   0   0   0   0   0    1   1 1100
        1   59143  100.0
262   60642   141.9081   'Nd-142 '    2   1  80   0   0   0   0   0   0    1   1 1100
        1   60142  100.0
263   60644   143.9103   'Nd-144 '    2   1  82   0   0   0   0   0   0    1   1 1100
        1   60144  100.0
264   60646   145.9135   'Nd-146 '    2   1  84   0   0 114  70   0   0    1   1 1100
```

```
         1   60146  100.0
 265   60647   146.9161   'Nd-147 '    2   1  85   0   0   0   0   0   0    1   1 1100
         1   60147  100.0
 266   60648   147.9167   'Nd-148 '    2   1  86   0   0 115  71   0   0    1   1 1100
         1   60148  100.0
 267   60650   149.9209   'Nd-150 '    2   1  87   0   0 116  72   0   0    1   1 1100
         1   60150  100.0
 268   61648   147.9177   'Pm-148 '    2   1  89   0   0   0   0   0   0    1   1 1100
         1   61148  100.0
 269   61649   148.9183   'Pm-149 '    2   1  90   0   0   0   0   0   0    1   1 1100
         1   61149  100.0
 270   61651   150.9215   'Pm-151 '    2   1  91   0   0   0   0   0   0    1   1 1100
         1   61151  100.0
 271   62648   147.9147   'Sm-148 '    2   1  94   0   0   0   0   0   0    1   1 1100
         1   62148  100.0
 272   62653   152.9217   'Sm-153 '    2   1  99   0   0   0   0   0   0    1   1 1100
         1   62153  100.0
 273   62654   153.9223   'Sm-154 '    2   1 100   0   0   0   0   0   0    1   1 1100
         1   62154  100.0
 274   63651   150.9195   'Eu-151 '    2   1 101   0   0 117  73   0   0    1   1 1100
         1   63151  100.0
 275   63656   155.9245   'Eu-156 '    2   1 105   0   0   0   0   0   0    1   1 1100
         1   63156  100.0
 276   63657   156.9251   'Eu-157 '    2   1 106   0   0   0   0   0   0    1   1 1100
         1   63157  100.0
 277   64654   153.9213   'Gd-154 '    2   1 107   0   0 118   0   0   0    1   1 1100
         1   64154  100.0
 278   64660   159.9268   'Gd-160 '    2   1 112   0   0 119   0   0   0    1   1 1100
         1   64160  100.0
 279   65159   158.9252   'Tb-159 '    3   0   0   0   0   0   0   0   0    1   1 1100
         1   65159  100.0
 280   65160   158.9273   'Tb-160 '    3   1   0   0   0   0   0   0   0    1   1 1100
         1   65160  100.0
 281   65161   160.9276   'Tb-161 '    3   1   0   0   0   0   0   0   0    0   1 1100
 282   65659   158.9252   'Tb-159 '    2   1 113   0   0   0   0   0   0    1   1 1100
         1   65159  100.0
 283   65660   158.9273   'Tb-160 '    2   1 114   0   0   0   0   0   0    1   1 1100
         1   65160  100.0
 284   65661   160.9276   'Tb-161 '    2   1 115   0   0   0   0   0   0    0   1 1100
 285   66660   159.9248   'Dy-160 '    2   1 116   0   0   0   0   0   0    1   1 1100
         1   66160  100.0
 286   66661   160.9274   'Dy-161 '    2   1 117   0   0   0   0   0   0    1   1 1100
         1   66161  100.0
 287   66662   161.9270   'Dy-162 '    2   1 118   0   0   0   0   0   0    1   1 1100
         1   66162  100.0
 288   66663   162.9286   'Dy-163 '    2   1 119   0   0   0   0   0   0    1   1 1100
         1   66163  100.0
 289   66664   163.9282   'Dy-164 '    2   1 120   0   0 120  74   0   0    1   1 1100
         1   66164  100.0
 290   67165   164.9298   'Ho-165 '    3   0   0   0   0 121  75   0   0    1   1 1100
         1   67165  100.0
 291   67665   164.9298   'Ho-165 '    2   1 121   0   0 122  76   0   0    1   1 1100
         1   67165  100.0
 292   77191   190.9781   'Ir-191 '    3   0   0   0   0   0   0   0   0    1   1 1100
         1   77191  100.0
 293   77193   192.9803   'Ir-193 '    3   0   0   0   0   0   0   0   0    1   1 1100
         1   77193  100.0
 294   91232   232.0386   'Pa-232 '    2   1   0   0   0   0   0   0   0    1   1 1100
         1   91232  100.0
 295   91234   234.0433   'Pa-234 '    2   1   0   0   0   0   0   0   0    0   1 1100
%FINE
```

Appendix C.3 Structure of the V4.0 MPACT MG library

[Structure]

%VERSION:
[iversion, adte]

%DIM:
[nog, nofg, norg, nchi, nelt, nelr, nres, nyld, nsubg, nflxhel]

%GRP:
[enbhel(ig)]$_{ig=1,nog}$

%CHI:
[chix(ig)]$_{ig=1,nog}$

%DIR:
do i=1,nelt
[ix, nid, amass, ityp, ifpy, ichi, inmn, ntemp, nrtemp, np1temp, npot, aid]
enddo

%NUC: [i, nid, amass, ityp, ifpy, ichi, inmn, ntemp, nrtemp, np1temp, npot, aid]
["TP1+"]
[temp(it)] $_{it=1, ntemp}$
["XSD+"]
do ig=1,nog
do it=1,ntemp
[ig, it, siga, {sigf, signf, sigtr, sigs, ib,ie, sm(jg)$_{jg= ib, ie}$}]
enddo
enddo
[" SP1+"]
do ig=1,nog
do it=1,np1temp
[ig, it, sigsp1(ig,it), ib, ie, smp1(jg,it)$_{jg= ib, ie}$]
enddo
enddo
["POT+"]
{[lamsigp(ig)] $_{ig=igresb,igrese}$
[sigsres(ig)] $_{ig=igresb,igrese}$
[nu(ig)] $_{ig=igresb,igrese}$
[" TP2+"]
[rtemp(it)] $_{it=1,nrtemp}$
[" XS0+"]
[sigpot(ip)] $_{ip=1,npot}$
[" RIA+"]
do ig=igresb,igrese
do it=1,ldiso(i)%nrtemp
[ig, it, ria(ip,it,ig)$_{ip=1, npot}$]
enddo
enddo
["RIS+"]
do ig=igresb,igrese
do it=1,ldiso(i)%nrtemp
[ig, it, ris(ip,it,ig)$_{ip=1, npot}$]
enddo

```
    enddo
["RNF+"]
    do ig=igresb,igrese
      do it=1,ldiso(i)%nrtemp
        [ig, it, rinf(ip,it,ig)ip=1, npot]
      enddo
    enddo
["SA7+"]
    do ig=igresb,igrese
      [ig, sgsa(ix,ig)ix=1,nsubg]
    enddo
    do ig=igresb,igrese
      do it=1,ldiso(i)%nrtemp
        [ig, it, sgwa(ix,it,ig)ix=1,nsubg]
      enddo
    enddo
["SF7+"]
    do ig=igresb,igrese
      [ig, sgsnf(ix,ig)ix=1,nsubg]
    enddo
    do ig=igresb,igrese
      do it=1,ldiso(i)%nrtemp
        [ig, it, sgwnf(ix,it,ig)ix=1,nsubg]
      enddo
    enddo
["SA4+"]
    do ig=igresb,igrese
      [ig, sgsafsp(ix,ig)ix=1,nflx]
    enddo
    do ig=igresb,igrese+1
      do it=1,ldiso(i)%nrtemp
        [ig, it, sgwafsp(ix,it,ig)ix=1,nflx]
      enddo
    enddo
["CHI+"]
    [chi(ig)] ig=1,nog
["CHI-"]
    [chid(ig)] ig=1,nog
[" FIS+"]
    [kappa, kappa0]
    [beta(ib)] ib=0,6
    [dcybeta(ib)] ib=1,6
    [yield(iy)] iy=1,nyld
[" DCY+"]
    [ldiso(i)%dcy]
[" TP3+"]
   [ldiso(i)%p1temp(it)] it=1,np1temp
[" SP2+"]
    do ig=1,nog
      do it=1,np1temp
        [ig, it, sigsp1(ig,it), ib, ie, smp2(jg,it)jg= ib, ie]
      enddo
    enddo
[" SP3+"]
    do ig=1,nog
      do it=1,np1temp
```

[ig, it, sigsp1(ig,it), ib, ie, smp3(jg,it)$_{jg= ib, ie}$]
enddo
enddo
[" N2N+"]
[ldiso(i)%sign2n(ig)]$_{ig=1,nog}$
[" N3N+"]
[ldiso(i)%sign3n(ig)]$_{ig=1,nog}$
Repeat **%NUC: for nelt nuclides.

%END:

Variables	Type	Description
nog	I	The number of energy groups
nofg	I	The number of fast energy groups
norg	I	The number of resonance energy groups
nchi	I	The number of energy groups w/ fission spectra
nelt	I	The total number of nuclides
nelr	I	The number of nuclides w/ full xs sets
nyld	I	The number of fission product nuclides
nres	I	The number of resonant nuclides
nsubg	I	The number of subgroup levels
nflx	I	The number of coarse subgroup levels
igresb	I	Starting group for resonance (=nofg+1)
igrese	I	Ending group for resonance (=nofg+norg)
u(ig)	R	Lethargy energy group boundaries (ig=1,nog)
enb(ig)	R	Energy group boundaries (ig=1,nog)
chix(ig)	R	Common fission spectrum (ig=1,nog)
sm(p?)(i,j)%	T	[scatmat] P0~p3 scattering matrix
%ib	I	Stating energy group (in)
%ie	I	Ending energy group (in)
%ioutsb	I	Stating energy group (out)
%ioutse	I	Ending energy group (out)
%from(k)	R	Scattering matrix (k=%ib,%ie)
ldiso(i)%	T	[libdata] Nuclidewise multigroup data (i=1,nelt)
%nid	I	Nuclide id.
%ityp	I	Indicator for data type 0 non depletable >0 depletable (w/ decay constant) 2 ri-a (fissionable w/ kappa, beta, fpy) 3 ri-a & ri-nf (same as above)
%ichi	I	Indicator for fission spectrum (0/>0 : no/yes)
%ifpy	I	Indicator & ordering no. for f.p.y.
%inmn	I	Indicator for (n,2n) & (n,3n) xs (0/1/2/3 : no/(n,2n)/(n,3n)/both)
%ntemp	I	The number of temperatures for xs
%nrtemp	I	The number of temperatures for ri
%npot	I	The number of sig-0's for ri
%np1temp	I	The number of temperatures for p1~p3
%aid	A8	Alphanumeric nuclide id.
%aw	R	Atomic mass
%kappa	R	Energy release per fission (w/sec) only w/o neutrino energy
%kappa0	R	Energy release per fission (w/sec) w/o decay and neutron kinetic energy
%crit_nd	R	Critical pnd
%dcy	R	Decay constant (/sec)

%chi(j)	R	Fission spectrum (j=1,nog)
%chid(j)	R	Delayed neutron spectrum (j=1,nog)
%beta(j)	R	Delayed neutron yields (j=1,6)
%dcybeta(j)	R	Delayed neutron decay constant (j=1,6)
%rtemp(j)	R	Square root temperatures for ri (j=1,%nrtemp)
%sigpot(j)	R	Square root sig-0's for ri (j=1,%npot)
%temp(j)	R	Temperatures for xs (j=1,%ntemp)
%p1temp(j)	R	Temperatures for p1~p3 (j=1,%np1temp)
%lamsigp(j)	R	Lambda*potential xs (j=igresb,igrese)
%sigsres(j)	R	Scattering xs (j=igresb,igrese)
%nu(j)	R	The number of neutrons released (j=igresb,igrese)
%yield(j,k)	R	Fission product yields (j=1, ;k=1,)
%siga(j,k)	R	Absorption xs (j=1,nog; k=1,%ntemp)
%sigf(j,k)	R	Fission xs (j=1,nog; k=1,%ntemp)
%signf(j,k)	R	Nu*fission xs (j=1,nog; k=1,%ntemp)
%sigtr(j,k)	R	Transport xs (j=1,nog; k=1,%ntemp)
%sigs(j,k)	R	Scattering xs (j=1,nog; k=1,%ntemp)
%sigstr(j,k)	R	Transport correct scattering xs (j=1,nog; k=1,%ntemp)
%sigsp1(j,k)	R	P1 scattering xs (j=1,nog; k=1,%np1temp)
%sigsp2(j,k)	R	P2 scattering xs (j=1,nog; k=1,%np1temp)
%sigsp3(j,k)	R	P3 scattering xs (j=1,nog; k=1,%np1temp)
%sign2n(j)	R	(n,2n) xs (j=1,nog)
%sign3n(j)	R	(n,3n) xs (j=1,nog)
%sm(j,k)%	T	[scatmat] P0 corrected scattering matrix (j=1,nog; k=1,%np1temp)
%smp1(j,k)%	T	[scatmat] P1 scattering matrix (j=1,nog; k=1,%np1temp)
%smp2(j,k)%	T	[scatmat] P2 scattering matrix (j=1,nog; k=1,%np1temp)
%smp3(j,k)%	T	[scatmat] P3 scattering matrix (j=1,nog; k=1,%np1temp)
%ria(j,k,l)	R	Absorption ri (j=1,%npot; k=1,%nrtemp; l=igresb,igrese)
%rinf(j,k,l)	R	Nu*fission ri (j=1,%npot; k=1,%nrtemp; l=igresb,igrese)
%ris(j,k,l)	R	Scattering ri (j=1,%npot; k=1,%nrtemp; l=igresb,igrese)
%sgsa(j,k)	R	Subgroup levels of absorption ri (j=1,nsubg; k=igresb,igrese)
%sgsnf(j,k)	R	Subgroup levels of nu*fission ri (j=1,nsubg; k=igresb,igrese)
%sgsafsp(j,k)	R	Subgroup levels of absorption ri (j=1,nflx; k=igresb,igrese+1)
%sgwa(j,k,l)	R	Subgroup weights of absorption ri (j=1,nsubg; k=1,%nrtemp; k=igresb,igrese)
%sgwnf(j,k,l)	R	Subgroup weights of nu*fission ri (j=1,nsubg; k=1,%nrtemp; k=igresb,igrese)
%sgwafsp(j,k,l)	R	Subgroup weights of absorption ri (j=1,nflx; k=1,%nrtemp; k=igresb,igrese+1)