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# CONSTRUCTION OF FAST NEUTRON GROUP STRUCTURES USING CPXSD FOR SHIELDING PROBLEMS

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## ABSTRACT

The accuracy of multigroup cross-section libraries has an important role in the accuracy of deterministic neutron transport calculations. Currently, there are several multigroup libraries available for specific applications. However, there is no publicly available group structure construction methodology that can be used for generating problem-dependent libraries; thus we have developed the CPXSD (Contributon and Point-wise Cross-Section Driven) methodology for this purpose. In this paper, we used the CPXSD methodology to construct fine- and broad-group structures for fast neutron cavity dosimetry problems. For the fine-group, we constructed a 450-group structure that contains 449 groups above 0.1MeV, and one group below 0.1MeV. We generated the 450-group (fine-group) LIB450 library and compared it to a reference 492-group LIB492 library by calculating reaction rates at the cavity dosimeter. The 492-group structure of the LIB492 library was derived from an "ad-hoc" procedure, for fast neutron dosimetry calculations, for the TMI-1 reactor. We demonstrated that the two fine-group libraries gave comparable reaction rates. Furthermore, we constructed broad-group structures from the 450-group structure, and generated two broad-group libraries: the 16-group LIB16 and 15-group LIB15, derived from scalar flux and bi-linear adjoint techniques, respectively. The LIB16 and LIB15 libraries have almost half the number of groups of the Oak Ridge National Laboratory's BUGLE library groups above 0.1MeV. These new broad-group libraries and the BUGLE-96 library were compared to continuous energy library calculations. LIB16 and LIB15 yield reaction rates which are in better agreement to the Monte Carlo predictions than those obtained using the BUGLE-96 library. For example, the LIB15 library is ~4% closer to the continuous energy reaction rate, compared to BUGLE-96.

*Key Words*: multigroup structure, multigroup cross sections, contributon, fast neutron dosimetry

## 1. INTRODUCTION

The discrete ordinates method ($S_N$ method) [1] is widely used for deterministic neutron transport calculations. For a time-independent problem, the $S_N$ method requires discretization of the spatial, angular and energy dependencies of particles. This study concerns the energy discretization.

The dicretization of energy is introduced to the neutron transport equation by partitioning the energy interval into groups, and integrating the transport equation over these energy groups. The multigroup form of the transport equation is obtained by preserving reaction rates. Such formulations lead to deriving multigroup cross sections. Multigroup cross sections represent point-wise cross sections that have an effective average value in a group.

The standard procedure for generating broad-group libraries can be given in three steps [2]:

Step i) Point-wise cross sections are processed to obtain fine-group cross sections (generally in the order of hundreds).

Step ii) Fine-group cross sections are self-shielded.

Step iii) Fine-group cross sections are collapsed to broad groups.

In step i), cross sections that are obtained via experimental and theoretical means in point-wise form are processed to generate fine-group cross sections in a homogeneous infinite medium. The NJOY code [3] is commonly used for this purpose. Examples of the tasks in NJOY are: reconstruction of point-wise cross sections, calculation of energy self-shielded cross sections, and collapsing point-wise cross sections to fine-group cross sections. Reconstruction provides a linear interpolation between neighboring point-wise cross sections within a specified tolerance. Energy self-shielding corrects fine-group cross sections in the resonance structure region, and collapsing cross sections uses a weighting function to generate fine-group cross sections.

In step ii), further energy self-shielding calculations are conducted to account for material compositions. Therefore, when self-shielded cross sections are calculated for an isotope of interest, the effect of other isotopes in a medium are included.

Finally, in step iii), isotopic cross sections are mixed to form mixture cross sections, and a fine-group transport calculation is performed for a simplified one-dimensional reactor model. Fine-group scalar fluxes are computed and used as weighting functions to collapse fine-group cross sections to broad groups.

There are several multigroup libraries that contain cross sections for different isotopes generated for specific applications. For example, for Light Water Reactor shielding and pressure vessel dosimetry calculations, multigroup libraries such as BUGLE [4] and SAILOR [5] exist. These libraries have 47-neutron and 20-gamma groups, and are referred to as broad-group libraries. Note that broad-group libraries are prepared generally in the order of tens.

One of the factors that cause inaccuracies in a multigroup library generation is the group structure. Hence, we developed the CPXSD (Contributon and Point-wise Cross Section Driven) methodology [6] that constructs effective fine- and broad-group structures for a problem and objective of interest. This iterative methodology uses i) “contributons” [7], i.e., the important particles that contribute to an objective, to identify the important groups, and ii) point-wise cross sections of an important isotope/material in a problem, for constructing multigroup structures.

This paper is organized as follows: Section 2 discusses group construction methodologies, and Section 3 discusses the CPXSD methodology. Section 4 presents the construction of effective fine- and broad-group structures for the Three Mile Island Unit 1 (TMI-1) reactor, for fast neutron dosimetry problems. Lastly, Section 5 gives conclusions.

## 2. GROUP CONSTRUCTION METHODOLOGIES

There is no publicly available group construction methodology. However, Haghighat and Hanshaw [8] used the response flux formulation to derive a fine-group structure for the TMI-1 reactor for fast neutron dosimetry problems (i.e., for neutron energies greater than 0.1MeV). The energy dependent response flux is given by:

$$C(E) = \int_V dr \int_{4\pi} d\Omega \Psi(\vec{r}, E, \hat{\Omega}) \Psi^+(\vec{r}, E, \hat{\Omega}) . \quad (1)$$

In Equation (1), $\Psi(\vec{r}, E, \hat{\Omega})$ is the angular flux and $\Psi^+(\vec{r}, E, \hat{\Omega})$ is the adjoint function dependent on position $\vec{r}$, energy E and direction $\hat{\Omega}$. Considering spherical harmonics expansion of flux and its adjoint, and using orthogonality, the group-dependent response flux can be written by:

$$C_g = \sum_{s \in D} V_s \sum_{l=0}^{L} \sum_{m=0}^{l} \frac{2l+1}{4\pi} \Psi^m_{l,g,s} \Psi^{m,+}_{l,g,s} . \quad (2)$$

In Equation (2), s refers to a materially uniform sub-domain in domain D, $V_s$ is the volume of the sub-domain, l and m are polar and azimuthal indices, and g refers to energy group. Equation (2) represents the importance of particles in group g, for an objective.

In order to generate a fine-group structure for the TMI-1 reactor using the response flux formulation, Haghighat and Hanshaw used the 199-group VITAMIN-B6 [9] structure developed at the Oak Ridge National Library (ORNL) as their starting group structure. They generated 199-group cross sections, performed self-shielding and forward and adjoint transport calculations using the radial, 1-D TMI-1 reactor model. Using the flux and adjoint function moments computed from the transport calculations, they calculated the 199-group $C_g$'s. Depending on the magnitude of the $C_g$'s per group, they performed an "ad hoc" refinement/coarsening on the 199-group VITAMIN-B6 structure. The groups corresponding to large $C_g$'s were partitioned into more groups, so that these groups could be represented more accurately. Due to computer memory limitations, group refinement was performed such that the total number of groups would not exceed 500. The group that had the highest $C_g$ was sub-divided into 20 evenly partitioned groups and the remaining groups were similarly evenly divided to fewer groups based on the ratio of their $C_g$ to the maximum $C_g$. Through this process, a 492-group structure was obtained. This 492-group structure was used in NJOY with the Evaluated Nuclear Data File Version VI (ENDF/B-VI) library, and a new 492-fine-group library, LIB492, was generated.

The number of groups added per VITAMIN-B6 group that gives the 492-group structure is shown in Figure 1. The 492-group structure has significantly more energy groups above 0.1MeV compared to the VITAMIN-B6 group structure; there are 489 groups in LIB492 while there are only 104 groups in the VITAMIN-B6 library above 0.1MeV.

The group structure construction procedure developed by Haghighat and Hanshaw that led to the derivation of the LIB492 library is an "ad hoc" approach because i) it uses a well-known group structure as the starting point (i.e., the VITAMIN-B6 group structure), and ii) group refinement is performed in an arbitrary manner (i.e., even partitioning). Hence, we developed a new, problem-

dependent, iterative methodology that remedies these shortcomings. The discussion of the CPXSD methodology is presented in Section 3.

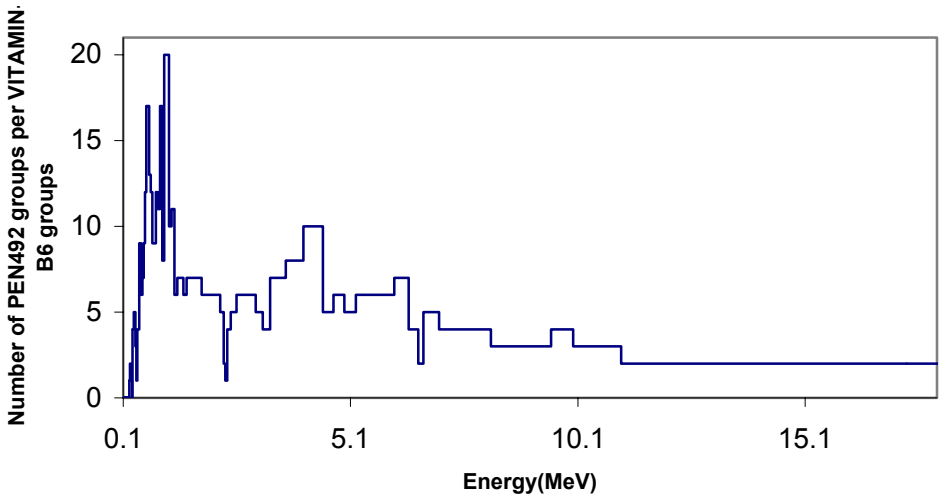


**Figure 1. Number of groups added per VITAMIN-B6 group that forms the LIB492 group structure.**

## 3. DISCUSSION ON THE CPXSD (CONTRIBUTON AND POINT-WISE CROSS-SECTION DRIVEN) METHODOLOGY

The CPXSD methodology is an iterative method that constructs effective fine- and broad-group structures for a problem of interest, depending on the objectives of the problem. This new methodology constructs group structures by refining an initial arbitrary group structure, e.g., an evenly partitioned group structure. Refinement of the initial group structure is performed according to i) the importance of groups in the initial group structure, and ii) point-wise cross sections of an important isotope/material in the problem.

### 3.1. Procedure of the CPXSD Methodology

Figure 2 shows the process for fine-group structure construction using the CPXSD methodology, and fine-group library generation. The procedure is explained as follows:

i) An initial group structure is selected. The initial group structure can be arbitrary, e.g., evenly partitioned.
ii) Cross sections are processed for the initial group structure (e.g., with NJOY).
iii) Self-shielding calculations are performed.
iv) Mixture cross sections are calculated and used in a 1-D reactor model for neutron transport calculations.
v) Objectives of the problem are calculated.
vi) The importance of groups in the initial group structure is calculated.
vii) The group that has the maximum importance is identified.

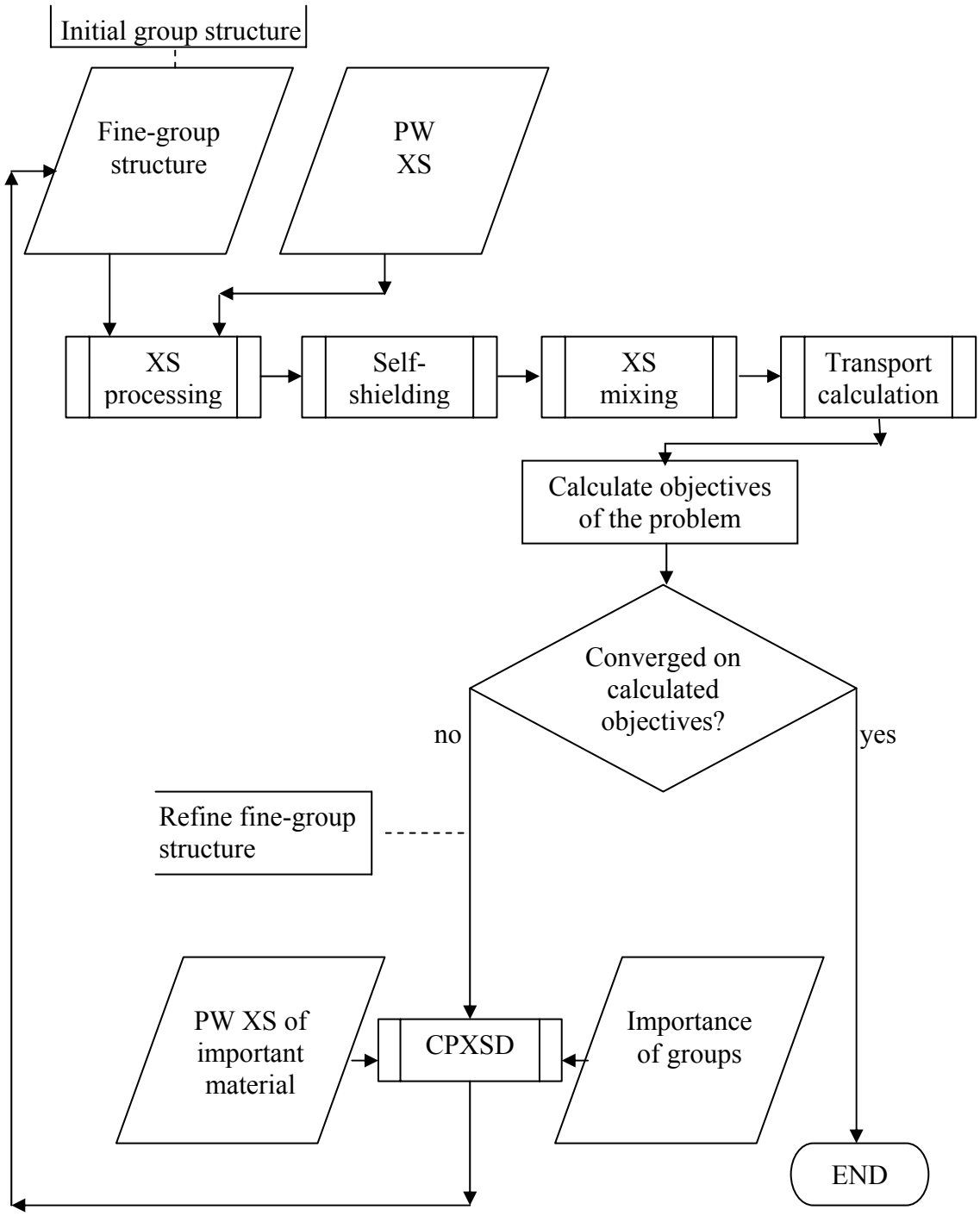


**Figure 2. Process for fine-group structure construction using the CPXSD methodology (XS and PW refer to cross-section and point-wise, respectively).**

viii) The group that has the maximum importance is refined depending on the point-wise cross sections of the important isotope/material of interest. If the important isotope/material point-wise cross sections have a resonance structure, resonance and non-resonance parts are determined, and their areas are calculated. The resonance that has the largest area is selected, and one sub-group is placed that encloses this resonance. Figure 3 illustrates point-wise cross sections that have a resonance structure. Sub-groups are placed in other resonance and non-resonance parts depending on their areas with respect to the largest resonance area. With this refinement process, the number of sub-groups in the most important group is determined. If the point-wise cross sections do not have a resonance structure, the group is evenly partitioned in energy, based on a user defined number.

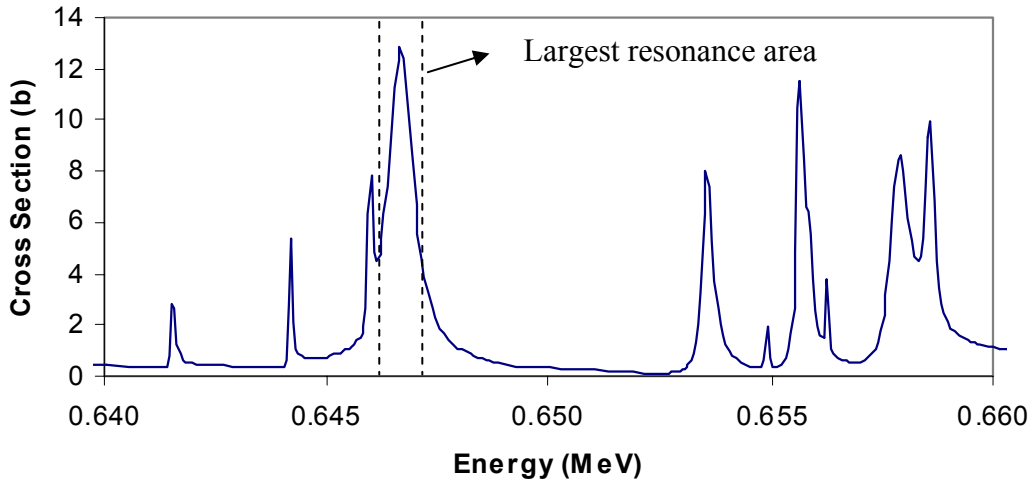


**Figure 3. Resonance structure in a group**

ix) The number of sub-divisions in other groups is set based on their importance compared to the maximum importance.

x) Refinement within other groups is performed similar to the refinement process performed in the most important group. However, since the number of sub-groups to be placed in each group is already set, resonance areas in descending order are used as the reference area and refinement is performed until the number of sub-divisions set for that group is closely matched.

xi) After the refinement process is completed for all groups, and the new group structure is constructed, a new multigroup library is generated and utilized, considering steps ii) to v).

xii) If the calculated objectives obtained from the two succeeding group structures are within a specified tolerance, the procedure ends. Otherwise steps vii) through xii) are repeated for construction of a finer group structure, with the exception that in step viii), one group is enclosed in the next largest resonance area, and sub-divisions are performed accordingly.

## 4. CONSTRUCTION OF A GROUP STRUCTURE FOR THE TMI-1 REACTOR FOR SHIELDING APPLICATIONS

In this section a group structure is constructed for the 1-D TMI-1 reactor for pressure vessel dosimetry problems. The TMI-1 reactor consists of twenty-seven nuclides: $^{27}$Al, $^{10}$B, C, Ca, $^{50}$Cr, $^{52}$Cr, $^{53}$Cr, $^{54}$Cr, $^{54}$Fe, $^{56}$Fe, $^{57}$Fe, $^{58}$Fe, $^{1}$H, K, Mg, $^{55}$Mn, $^{23}$Na, $^{58}$Ni, $^{60}$Ni, $^{61}$Ni, $^{62}$Ni, $^{64}$Ni, $^{16}$O, Si, Zr, $^{235}$U and $^{238}$U.

In generating an effective fine-group library for the TMI-1 reactor, the NJOY code is used for cross-section processing. NJOY version 94.15 is used for $^{27}$Al and $^{235}$U, and NJOY version 91.94m is used for the remaining isotopes. ENDF/B-VI release 3 is used for $^{235}$U, and ENDF/B-VI release 2 is used for the remaining isotopes. The choice of the NJOY versions and ENDF data for the twenty-seven isotopes are taken considering the NJOY versions and ENDF data in generating the BUGLE-96 library. Note that the BUGLE-96 library uses ENDF/B-VI release 3 data for $^{27}$Al; however we use ENDF/B-VI release 2 for this isotope because of the difficulty we encountered in processing the release 3 data file.

The AMPX modules [10] from the SCAMPI code package [11] are used for post-processing of cross sections. The modules used from the SCAMPI code package, and their functions in the cross-section library generation procedure for this study, are listed in Table I. The 1-D option of the two-dimensional DORT code [12] is used for neutron transport calculations.

**Table I. AMPX Modules that are used in the Generation of Fine-Group Libraries**

| Module Name | Function |
|---|---|
| **SMILER** | Converts NJOY Group-wise Evaluated Nuclear Data Files (GENDF) to AMPX master library format |
| **AJAX** | Gathers AMPX master libraries |
| **BONAMI** | Performs self-shielding calculations |
| **NITAWL** | Converts AMPX master libraries to AMPX working library format (the code may also be utilized to use the Nordheim Integral method for resonance self-shielding) |

Since the purpose of this study is to generate a group structure for fast neutron dosimetry applications, six dosimetry reactions that are sensitive to energies above 0.1MeV are selected. These are $^{63}$Cu(n,α), $^{54}$Fe(n,p), $^{58}$Ni(n,p), $^{46}$Ti(n,p), $^{237}$Np(n,f), and $^{238}$U(n,f). The normalized cross sections of these dosimetry isotopes and their sum are shown in Figure 4. The objective is to calculate reaction rates accurately, using a formulation:

$$R = \sum_g \sigma_g \cdot \Phi_g \,. \tag{3}$$

In Equation (3), $\sigma_g$ is the microscopic cross-section, and $\Phi_g$ is the scalar flux, in group g.

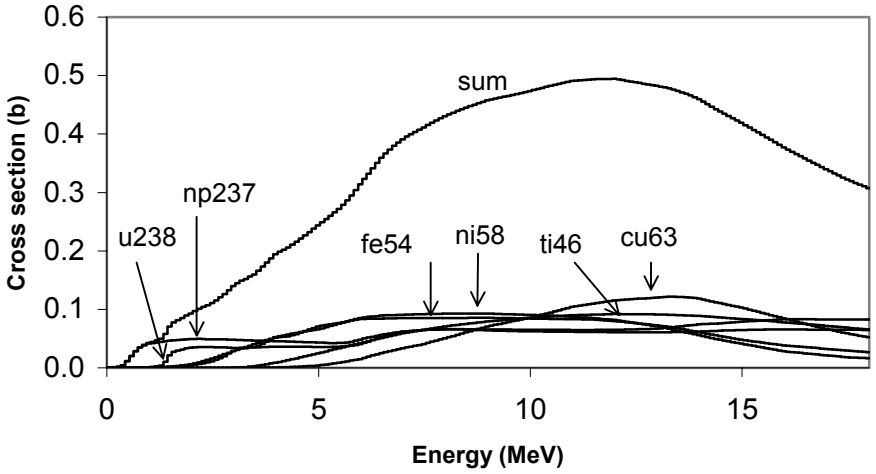


**Figure 4. Normalized dosimetry cross sections and their sum.**

### 4.1. Fine-Group Structure Construction

The fine-group structure construction process begins by selecting an initial fine-group structure. For the initial group structure, the energy range between 0.1MeV and 18MeV is partitioned into even energy intervals of 0.1MeV; i.e., 180 groups are placed above 0.1MeV, and one group is placed below 0.1MeV. Cross sections are processed in NJOY, and are post-processed using the AMPX modules, leading to the generation of the 181-group LIB181 library. The 181-group DORT calculations are performed to obtain fluxes in the TMI-1 reactor, and reaction rates of the six dosimeter isotopes are calculated at the cavity dosimeter.

Next, the 181-group structure is refined, and a new library is generated to calculate reaction rates. For the refinement process, two items are determined: i) importance of groups and ii) an important isotope/material in the system.

In order to calculate the importance of groups in the 181-group structure, the group-wise response flux formulation is used. Figure 5 shows the normalized LIB181 response fluxes per unit energy. This figure illustrates that the most important groups are between 0.1 and 2MeV; this is due to the sensitivity of $^{237}$Np(n,f) cross sections, and large magnitude of fluxes in that energy range, as shown in Figure 6.

The important isotope in the problem is selected as $^{56}$Fe since this isotope has an important impact on the fluxes computed at the cavity dosimeter. Figure 7 shows the $^{56}$Fe cross sections from 0.1 to 10MeV. There is a significant resonance structure, especially between 0.1 to 2MeV.

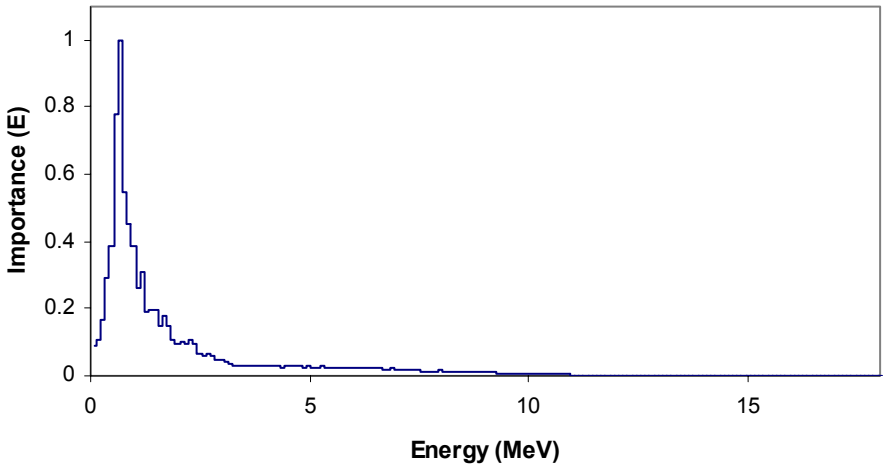


**Figure 5. The 180-group response fluxes per unit energy.**

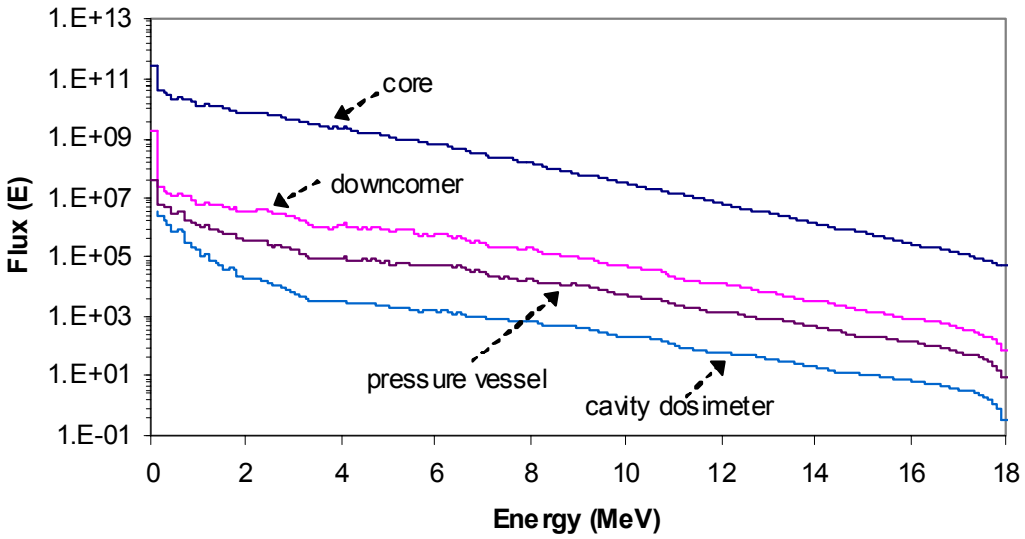


**Figure 6. The 180-group flux spectra in the core, downcomer, pressure vessel and cavity dosimeter regions.**

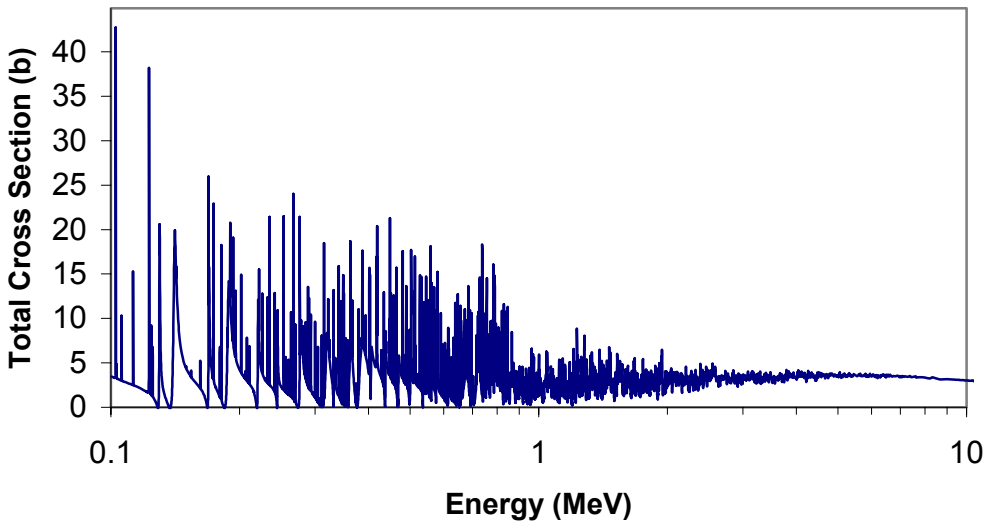


**Figure 7: $^{56}$Fe point-wise cross sections.**

Using the CPXSD methodology, we constructed the 246, 282, 450, 497 and 659-group structures. We generated libraries for these group structures, and obtained reaction rates at the cavity dosimeter. Considering a 1% convergence criterion on reaction rates, the 450-group structure was chosen as the converged group structure, and the LIB450 library was generated. The LIB450 library has 449 groups above 0.1MeV, and one group below 0.1MeV. The importance of groups in LIB450 and LIB181 are plotted in Figure 8, between 0.1 and 2MeV. The importance of groups in LIB450 shows a resonance structure, which is the reflection of the significant resonance structure in cross sections in the pressure vessel region within that energy range.

Next, reaction rates were calculated for the six dosimeter isotopes at the cavity dosimeter using LIB450 and LIB492. The LIB450 to LIB492 reaction rate ratios are given in Table II. The ratios of the two libraries are very close to 1, i.e., the two libraries are comparable. In order to compare the differences in reaction rates with the 199-group VITAMIN-B6-like library, with the finer group libraries that we generate, we compute VITAMIN-B6-like to LIB492 reaction rates. The VITAMIN-B6-like library is also generated with the BUGLE-96 procedure. The results are listed in Table II. We observe that the $^{237}$Np(n,f) reaction rate calculated by theVITAMIN-B6-like library has ~4% difference compared to that calculated by LIB492. Since the $^{237}$Np(n,f) reaction is sensitive between 0.1 and 2MeV, the additional groups placed in this energy range in LIB492 and LIB450 provide improvement for this isotope.

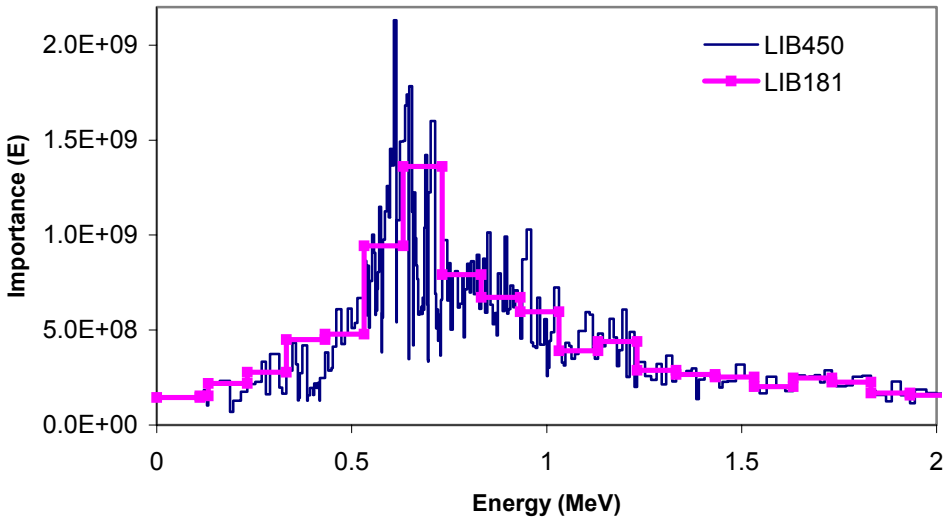


**Figure 8. Importance of groups calculated with the LIB181 and LIB450 libraries.**

**Table II. LIB450 and VITAMIN-B6-like to LIB492 Reaction Rate Ratios**

| Reaction | LIB450 / LIB492 | VITAMIN-B6-like / LIB492 |
|---|---|---|
| $^{63}$Cu(n,α) | .9974 | .9846 |
| $^{54}$Fe(n,p) | .9985 | .9801 |
| $^{58}$Ni(n,p) | .9982 | .9790 |
| $^{46}$Ti(n,p) | .9977 | .9820 |
| $^{237}$Np(n,f) | .9916 | .9593 |
| $^{238}$U(n,f) | .9973 | .9780 |

## 4.2. Broad-Group Structure Construction

Effective broad-group structures were constructed by the CPXSD methodology by refining an initial broad-group structure consisting of five groups above 0.1MeV. The initial broad-group boundaries were selected from the threshold energies of the six dosimeter isotopes. Similar to the fine-group construction, $^{56}$Fe was selected as the important isotope in the problem. Sub-groups were added one at a time to construct new broad-group structures and libraries. Reaction rates at the cavity dosimeter were calculated for each broad-group library generated, and calculations proceeded until a convergence criterion of 1% was achieved in reaction rates.

Two broad-group structures were constructed with the CPXSD methodology. These libraries were generated from scalar flux and bi-linear adjoint collapsing, and are referred to as the LIB16 and LIB15 libraries, respectively. LIB16 and LIB15 have only one group below 0.1MeV.

Table III gives ratios of the LIB16 and LIB15 reaction rates to those from the fine-group LIB450 library. These ratios indicate that the broad-group libraries yield results which are in close agreement (within 1%) with those obtained from the fine-group library.

**Table III. LIB16 and LIB15 to LIB450 Reaction Rate Ratios**

| Reaction | LIB16 / LIB450 | LIB15 / LIB450 |
|---|---|---|
| $^{63}$Cu(n,α) | .9882 | 1.006 |
| $^{54}$Fe(n,p) | .9884 | .9924 |
| $^{58}$Ni(n,p) | .9888 | .9946 |
| $^{46}$Ti(n,p) | .9896 | 1.005 |
| $^{237}$Np(n,f) | .9996 | 1.012 |
| $^{238}$U(n,f) | .9992 | 1.003 |

### 4.3. Multigroup to Continuous Energy Library Comparisons

In order to examine the effectiveness of the broad-group structures constructed by the CPXSD methodology, LIB492, LIB16, LIB15, and the ORNL BUGLE-96 ($B96_{ORNL}$) libraries were compared to continuous energy libraries. Continuous energy libraries were used in the $A^3$MNCP (Automated Adjoint Accelerated MCNP) code [13] for computing reaction rates at the cavity dosimeter.

Table IV gives the reaction rate ratios of the multigroup to the continuous energy libraries. In comparing multigroup with continuous energy reaction rates, we observe that the accuracy of the CPXSD generated libraries is either similar to, or better than the BUGLE-96 library. For example, for the $^{237}$Np(n,f) reaction, LIB15 is ~4% closer to the continuous energy reaction rate. Note that even though some reaction rates calculated with LIB16 and LIB15 are similar to those of $B96_{ORNL}$, the LIB16 and LIB15 libraries have almost half the number of groups of the $B96_{ORNL}$ library (i.e., 26 groups above 0.1MeV) that results in significant saving in computing time especially for multidimensional calculations.

**Table IV. Multigroup to Continuous Energy (CE) Reaction Rate Ratios**

| Reaction | LIB492 / CE | LIB16 / CE | LIB15 / CE | $B96_{ORNL}$ / CE |
|---|---|---|---|---|
| $^{63}Cu(n,\alpha)$ | .9312 | .9301 | .9056 | .9111 |
| $^{54}Fe(n,p)$ | .9385 | .9196 | .9152 | .9006 |
| $^{58}Ni(n,p)$ | .9376 | .9167 | .9168 | .9000 |
| $^{46}Ti(n,p)$ | .9357 | .9255 | .9059 | .9074 |
| $^{237}Np(n,f)$ | .9423 | .9052 | .9380 | .8984 |
| $^{238}U(n,f)$ | .9337 | .9063 | .9219 | .8990 |

## 5. CONCLUSIONS

In this paper, we introduced the CPXSD methodology that was developed to construct effective group structures for a problem of interest. We applied the methodology to construct fine- and broad-group structures for the TMI-1 reactor for fast neutron dosimetry, i.e., for energies above 0.1MeV. For fine-group calculations, we constructed a 450-group structure, and generated a LIB450 library. We demonstrated that the LIB450 reaction rates are in close agreement with a reference 492-group library (LIB492). Furthermore, we compared reaction rates using the VITAMIN-B6-like and LIB492 libraries, and showed that using the finer group structure improved reaction rates, especially for $^{237}Np(n,f)$ (~4%). For broad-group calculations, two effective broad-group libraries were generated from LIB450: a 16-group LIB16 derived from the scalar flux weighting technique, and a 15-group LIB15 derived from the bi-linear adjoint weighting technique. These two libraries have almost half the number of groups of the BUGLE-96 library above 0.1MeV. Comparing with the reference continuous energy Monte Carlo results, LIB15 and LIB16 yield reaction rates which are at least as accurate as those obtained from the BUGLE-96 library. For example, for $^{237}Np(n,f)$, comparing with BUGLE-96, the LIB15 library with only 15 groups yields a reaction rate which is ~4% closer to the continuous energy reaction rate.

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