ADVANCED METHODOLOGY FOR SELECTING GROUP STRUCTURES FOR MULTIGROUP CROSS SECTION GENERATION

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ABSTRACT

Multigroup ("broad-group") cross section libraries are required for neutronic calculations. Since multigroup cross sections are one of the major factors affecting the accuracy of deterministic neutronic calculations, it is important to reduce their uncertainties. Cross section libraries include uncertainties caused by three major factors including energy group structure, self-shielding method, and collapsing technique. This paper addresses two of these factors: i) selection of group structure ii) collapsing technique. For the selection of group structure, we develop the CPXSD (Contributon and Point-wise Cross Section Driven) methodology. For the collapsing methodology, we utilize a recently developed bilinear adjoint weighting formulation. We apply the CPXSD for a pressure vessel neutron dosimetry problem. We demonstrate that CPXSD can result in an effective fine-group structure that has relatively fewer groups than a finer, reference group structure. We also demonstrate that the bilinear adjoint weighting methodology gives superior results compared to other collapsing approaches.

1. INTRODUCTION

To improve the accuracy of neutronic calculations, it is necessary to reduce the uncertainties associated with the cross sections. There are three major factors that affect the accuracy of cross section generation. These include energy group structure, self-shielding method, and collapsing methodology. This paper focuses on reducing the uncertainties associated with two of these factors: i) energy group structure ii) collapsing methodology. We develop a new methodology

that selects effective energy group structures for multigroup cross section generation that will enable achieving better results in transport calculations. Although the methodology is general, this paper focuses on the Light Water Reactor (LWR) shielding and pressure vessel neutron dosimetry applications. These type of applications are important for fast neutrons having energies above ~0.1MeV. Further, we demonstrate the significance of the bilinear adjoint collapsing methodology in order to weight cross sections effectively.

The standard approach for generation of broad-group libraries is given in three steps[1].
Step i) Processing point-wise cross sections to obtain fine-group (in the order of hundreds) cross sections,
Step ii) Performing resonance self-shielding calculations,
Step iii) Performing transport calculations for a simplified model and obtaining scalar fluxes for collapsing cross sections from a fine- into a broad-group structure.

In step i, neutron and/or photon cross sections are commonly processed with the NJOY code[2] considering a homogeneous medium. Cross-section processing involves several tasks, for example: reconstructing point-wise cross sections by using a piece-wise linear interpolation approach, calculating point-wise cross sections depending on the temperature of the medium, and generating fine-group cross sections (i.e., group constants). The fine-group cross sections are obtained by averaging the group constants with an infinite medium spectrum, or a user-supplied spectrum.

In step ii, cross sections in the resolved resonance region are corrected. In the resonance energy regions, corresponding to the peaks in the cross section distribution, we observe dips in the flux distribution. Consequently, the medium is self-shielded (in energy) from particles that have energies corresponding to the peak cross section values[3].

In step iii, self-shielded cross sections are used in transport calculations to obtain a fine-group flux spectrum in order to collapse cross sections from fine- to broad-group structure. The common approach of collapsing cross sections uses the scalar flux for weighting; this method is referred to as the "scalar flux weighting"[4,5].

The fine- and broad-group structures used in generating multigroup libraries are selected based on experience or some heuristic methodology. There is no standard methodology available for selecting fine- and broad-group structures. However, using an appropriate energy group structure is of at most importance for obtaining accurate solutions for any multigroup neutronic calculation.

Haghighat and Hanshaw[6] used the "contributon" theory[7] for selecting a fine-group structure for pressure vessel cavity dosimetry calculations. Furthermore, they developed a new collapsing methodology[6,8], the bilinear adjoint collapsing method, and demonstrated that this is a superior

methodology compared to other available techniques including the scalar flux weighting and the consistent P_N (Ref. 9) techniques.

This paper addresses group structure selection procedure and collapsing methodology. On the group structure, we develop a new general methodology by extending the "ad hoc" procedure used by Haghighat and Hanshaw. On the collapsing methodology, we examine the effectiveness of the new bilinear adjoint technique.

Section 2 gives information on the theory of selection of energy group structure and collapsing methodologies. Section 3 includes work performed on establishing the standard methodology for multigroup cross section generation. Section 4 analyzes fine- and broad-group structures. In this section we analyze different fine group structures, the effect of fine-group structure to broad-group collapsing, and the bilinear adjoint collapsing methodology. In Section 5, the new methodology for generation of group structure is used to generate a cross section library. The new methodology is applied to a pressure vessel cavity dosimetry problem. Finally, Section 6 gives conclusions.

2. THEORY

2.1 SELECTION OF ENERGY GROUP STRUCTURE

Here, we develop a new general methodology for selection of problem-dependent group structures. We extend the "ad hoc" procedure developed by Haghighat and Hanshaw based on the "contributon" theory. The "contributon" theory is given by

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

where $\Psi(\vec{r}, E, \hat{\Omega})$ 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 "contributon" can be obtained as

$$C_g = \sum_{s \in D} V_s \sum_{l=0}^{L} \sum_{m=0}^{l} \frac{2l+1}{4\pi} \Psi_{l,g,s}^{m} \Psi_{l,g,s}^{m,+} \tag{2}$$

where 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 for a spherical harmonic polynomial, and *g* refers to energy group.

The group-dependent "contributon" in equation (2) gives the importance of a neutron at an energy group g to a response (detector). Haghighat and Hanshaw used this formulation to obtain a new fine-group structure starting from the 199-group VITAMIN-B6 library[10]. They performed 199-group forward and adjoint transport calculations for a one-dimensional radial Three Mile Island Unit-1 (TMI-1) reactor model, and calculated the corresponding 199-group C_g 's. The groups that showed large C_g 's were partitioned into more groups, so that these groups could be represented more accurately. Due to 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 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 ENDF/B-VI library to prepare a new 492-fine-group library.

The above procedure is an "ad hoc" approach because it uses a well-known group structure as the starting point, and its group partitioning is quite arbitrary. Hence, we have developed a new general methodology that remedies above shortcomings.

2.1.1 DISCUSSION ON THE CPXSD (CONTRIBUTON AND POINT-WISE CROSS SECTION DRIVEN) METHODOLOGY

As we discussed in Section 2.1, Haghighat and Hanshaw developed an "ad hoc" procedure with two shortcomings: i) starting group structure ii) group partitioning procedure. We have developed an iterative methodology that overcomes the above shortcomings. For the starting group structure, we consider an arbitrary structure, e.g., evenly partitioned. To refine the group structure, depending on problem objectives, we use the cross section information of one or a group of materials that have significant impact. For example, for the pressure vessel cavity dosimetry, iron is the most important element that affects the response at the cavity dosimeter. Important isotopes of iron have significant resonance behavior between 0.1 and ~6MeV. Figure1 shows the total cross section of Fe-56. In the resonance energy region, adjacent energy groups exhibit significantly different probability of interactions. As this result, the neutron population in different energy groups is significantly different; higher values of cross sections indicate lower neutron population and vice versa. Since our interest is in neutrons that reach the detector, we wish to represent the resonance minima effectively in an energy group structure. For this reason, we sub-divide groups, depending on the locations of resonance minima. Since resonances are dense and may have a wide energy range, it is not practical to select all the minima for group partitioning. Therefore, we calculate the "contributon" for an arbitrary group structure for the problem of interest. We identify the range with the highest 'contributon" and determine the number of minima in this range to set the maximum value of sub-divisions. Then we set the

number of sub-divisions for other regions relative to their magnitude of their “contributon” to the maximum “contributon” value. Following sub-division of the starting group structure, we recalculate C(E) for the refined group structure and perform transport calculation to obtain C(E) and the objectives of the problem. If the accuracy of the calculated objectives is not adequate, we iterate on the above procedure.

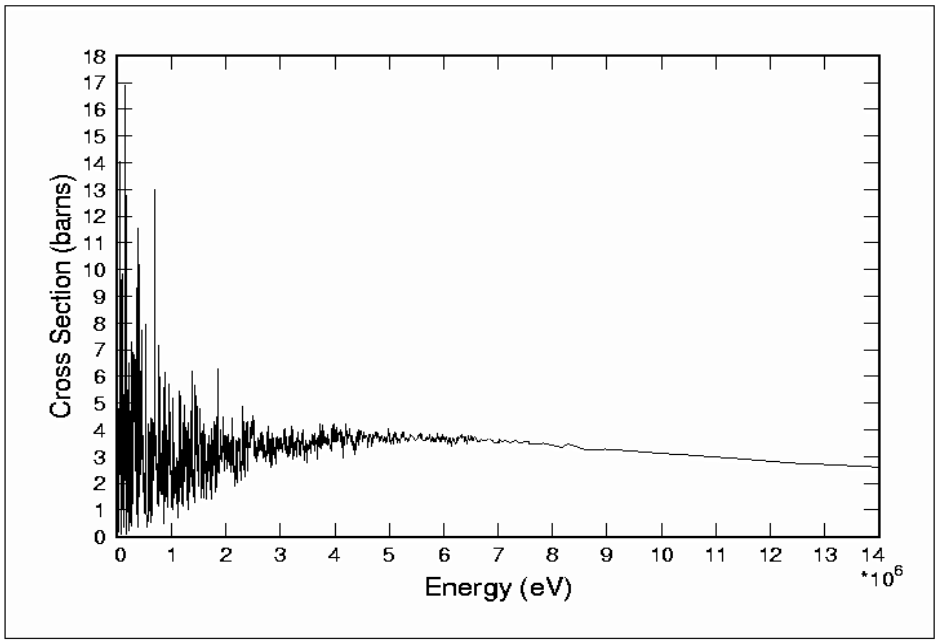

Figure 1. Total Cross Section of Fe-56

Above methodology that uses both contributon formulation and point-wise cross section information is referred to as the CPXSD (Contributon and Point-wise Cross Section Driven) methodology.

2.2 COLLAPSING METHODOLOGIES

The last step in a broad-group library generation is collapsing fine- to broad-group cross sections. Collapsing can be done based on three different methods including “scalar flux”, “consistent P_N”, and the recently developed “bilinear adjoint” weighting. Scalar flux weighting does not account for angular variations, and all scattering moments are weighted with the same scalar flux. The consistent P_N approximation in 1-D uses Legendre moments of the flux to weight multigroup scattering cross section moments. This method, however, requires further approximation when extended to a multidimensional geometry. The bilinear adjoint weighting method, however, includes angular dependencies in any dimensionality order without introducing approximations. The method evaluates multigroup constants by using forward flux and the importance function to weight cross sections. Weighting with spatial and angular

variables is performed according to the important particles that are contributing to a detector. The bilinear adjoint weighting has been shown to be superior compared to the two other methods, especially when angular dependencies are important, for example, the fast neutron cavity dosimetry. The formulations for the total and scattering cross sections are expressed by:

$$\sigma_{t,g} = \frac{\int_g dE \sigma_t(E) \int_{D_s} dr \left(\sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \sum_{m=-l}^{l} \Psi_l^m(\vec{r},E) \Psi_{l,g}^{m,+}(\vec{r}) \right)}{\int_g dE \int_{D_s} dr \left(\sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \sum_{m=-l}^{l} \Psi_l^m(\vec{r},E) \Psi_{l,g}^{m,+}(\vec{r}) \right)} \tag{3}$$

$$\sigma_{s,l,g' \to g} = \frac{\int_g dE \int_{g'} dE' \sigma_{s,l}(E' \to E) \int_{D_s} dr \left(\sum_{m=-l}^{l} \Psi_l^m(\vec{r},E) \Psi_{l,g}^{m,+}(\vec{r}) \right)}{\int_j dE' \int_{D_s} dr \left(\sum_{m=-l}^{l} \Psi_l^m(\vec{r},E) \Psi_{l,g}^{m,+}(\vec{r}) \right)} \tag{4}$$

The scalar flux and bilinear adjoint weighting methodologies will be utilized and analyzed in collapsing calculations in Section 4.

3. ESTABLISHMENT OF THE EXISTING STANDARD METHODOLOGY FOR GENERATION OF MULTIGROUP CROSS SECTIONS

The BUGLE cross-section libraries[4] are commonly being used for the LWR shielding and pressure vessel dosimetry applications. These libraries are chosen as the standard libraries. In order to examine the new CPXSD methodology, we first establish the standard approach available for multigroup cross section generation. The BUGLE-93 and BUGLE-96 libraries are generated from the VITAMIN-B6 library that has 199-neutron and 42-gamma energy group structures. These libraries use ENDF/B-VI data: BUGLE-93 is generated from release 2 and BUGLE-96 from release 3. The NJOY code is used to process cross sections and finally obtain multigroup, i.e., fine group cross sections. BUGLE-93 uses NJOY version 91.94m. BUGLE-96 uses NJOY version 94.15 for the isotopes H-2, N-14, Al-27, Ba-138, U-235, Pu-241, Am-241, and version 91.94m for the remaining isotopes. BUGLE-93 uses AMPX-77 (Ref. 11) and BUGLE-96 uses the SCAMPI (Ref. 12) code package for self-shielding and collapsing. For example, self-shielding is performed using the BONAMI code[13]. Cross sections are mixed and used in a 1-D reactor model for transport calculations with the XSDRNPM code[14]. The fluxes obtained in the reactor are used to collapse the fine-group cross sections to broad group by scalar flux weighting using the MALOCS code[11].

The procedure for generating BUGLE-96 was modified for improving accuracy and versatility. These modifications are listed below[15]:

i) Iterations for performing upscattering sources and obtaining a converged flux distribution in the thermal range in 1-D transport calculations with fine group structure were performed,
ii) The temperature dependence of cross sections in the thermal range was corrected,
iii) The choice of using a cross section library that contains upscattering cross sections was added,
iv) The effect of water in the treatment of iron self-shielding was not included,
v) An error in MALOCS was corrected.

With this work, we have generated the BUGLE-93 and BUGLE-96 libraries. For comparison, we analyze 199-group spectrum obtained from a 1-D transport calculation of a PWR, and collapsed (i.e., 47-group) total cross sections of hydrogen in water generated in the core.

Figures 2 and 3 show the relative difference between the PSU and ORNL generated 199-neutron group fluxes for BUGLE-93 and BUGLE-96, respectively. Group numbers from 1 to 104 represent the energy range between 0.1 to19.64MeV. The thermal energy range is defined from group 164 to group 199 (1.0E-05 to 5.0435eV). The relative differences are plotted at four locations including the core, downcomer, 1/4T PV and concrete regions. The maximum relative difference is ~2.4% in generating BUGLE-93, and 2.6% in generating BUGLE-96 fluxes at the core region. These maximum differences occur at the thermal energy range. We attribute these differences to computer round-off errors or precision.

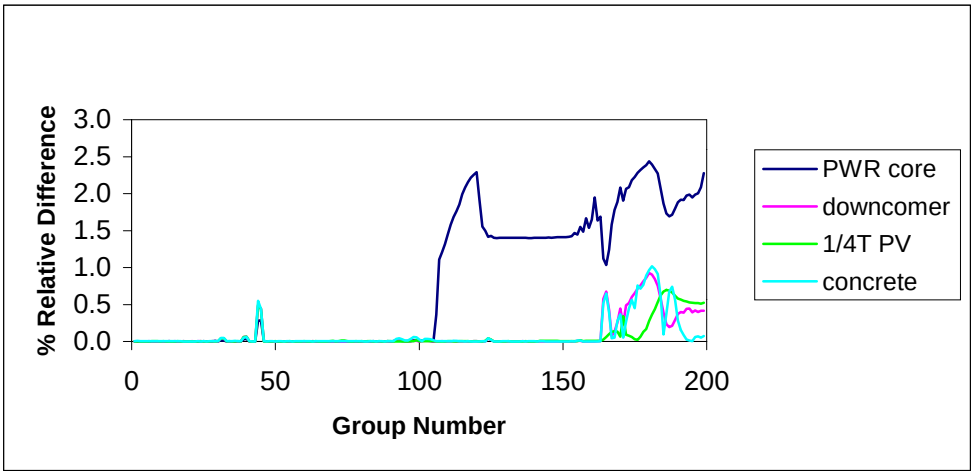

Figure 2. Percent Discrepancy of 199-Neutron Group Fluxes in Generating BUGLE-93

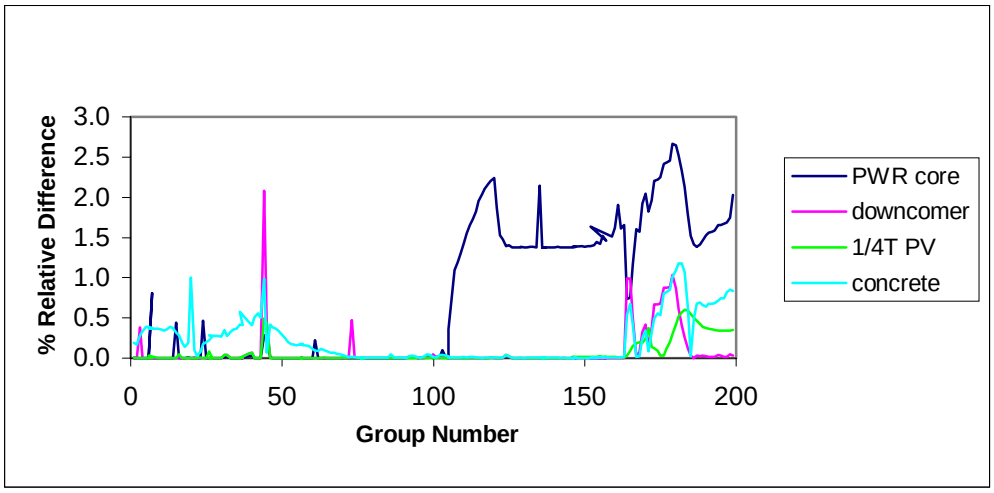

Figure 3. Percent Discrepancy of 199-Neutron Group Fluxes in Generating BUGLE-96

Table I compares the PSU and ORNL generated 26-group total cross sections of hydrogen in water in the core region. We selected the first 26 groups since this is the range corresponding to energies above 0.1MeV that we are interested in. The maximum differences are in the order of 10^{-3} %. Similar results are obtained for BUGLE-96, hence, for brevity they are not presented here.

In summary, we have installed and benchmarked the existing state-of-the-art code system for generation of multigroup cross sections at Penn State.

Table I. Comparison of BUGLE-93 Generated by ORNL and PSU for the Total Cross Section of H-1

Group Number	ORNL Generated	PSU Generated	Difference (%)
1	6.3731E-01	6.3732E-01	7.85E-04
2	7.4106E-01	7.4107E-01	6.75E-04
3	8.7667E-01	8.7667E-01	3.42E-04
4	1.0108E+00	1.0108E+00	3.96E-03
5	1.1454E+00	1.1454E+00	1.75E-03
6	1.3225E+00	1.3225E+00	3.02E-03
7	1.5334E+00	1.5334E+00	6.52E-04
8	1.8305E+00	1.8305E+00	5.46E-04
9	2.1596E+00	2.1596E+00	1.85E-03
10	2.3586E+00	2.3586E+00	4.24E-04
11	2.5050E+00	2.5050E+00	7.98E-04
12	2.6131E+00	2.6131E+00	7.65E-04
13	2.6515E+00	2.6516E+00	1.89E-03
14	2.6962E+00	2.6962E+00	1.85E-03
15	2.8569E+00	2.8569E+00	1.05E-03
16	3.1159E+00	3.1159E+00	6.42E-04
17	3.4322E+00	3.4322E+00	0.00E+00
18	3.9189E+00	3.9189E+00	5.10E-04
19	4.5076E+00	4.5076E+00	0.00E+00
20	4.8599E+00	4.8599E+00	8.23E-04
21	5.2570E+00	5.2570E+00	5.71E-04
22	5.8389E+00	5.8389E+00	3.43E-04
23	6.6513E+00	6.6513E+00	1.50E-04
24	7.5922E+00	7.5922E+00	1.32E-04
25	8.9649E+00	8.9649E+00	1.12E-04
26	1.1142E+01	1.1142E+01	3.59E-03

4. ANALYSIS OF FINE- AND BROAD-GROUP STRUCTURES

This section includes results obtained from transport calculations with 492-, 199- and 25-energy group structures. The 492-group structure (PEN492) is developed by Haghighat and Hanshaw, 199-group corresponds to the VITAMIN-B6 group structure (PEN199) developed by RSIC, ORNL, and 25-group structure (PEN25) is a subset of the 47-neutron-group BUGLE library group structure. Groups 3 to 489 in PEN492, 2 to 104 in PEN199, and 1 to 24 in PEN25 are between 0.1 to 17MeV. This energy range will be considered for calculations in this section.

We use the 1-D TMI-1 cycle 7 reactor model in this study. The regions and dimensions of this model are given in Table II. We use 27 nuclides for this model: Al-27, B-10, C, Ca, Cr-50, Cr-

52, Cr-53, Cr-54, Fe-54, Fe-56, Fe-57, Fe-58, H-1, K, Mg, Mn-55, Na-23, Ni-58, Ni-60, Ni-61, Ni-62, Ni-64, O-16, Si, Zr, U-235 and U-238. We use ENDF/B-VI rel.3 data for these nuclides. Similar to BUGLE-96, we use NJOY version 94.15 for U-235, and NJOY version 91.94m for the remaining nuclides. We utilize the SCAMPI code system to self-shield, and compute mixture cross sections. The self-shielding of iron cross sections are performed without the presence of water. We use the S_N code DORT (Ref. 14) for calculation of multigroup flux distribution for the TMI-1 cycle 7 reactor with two different models. Model 1 uses 606 spatial meshes, P_7 order of scattering, and an S_{16} quadrature set. Model 2 uses 122 spatial meshes, P_7 order of scattering, and an S_8 quadrature set.

Table II. Dimensions of the 1-D Radial TMI-1 Reactor

Region	Outer radius (cm)
Core	163.82
Baffle plate	166.0
Former	179.07
Core barrel	184.15
Gap water	186.71
Thermal shield	191.79
Downcomer water	216.694
Pressure vessel clad	217.170
Pressure vessel	238.603
Cavity	287.02
Insulation	298.45
Cavity	348.758
Guide Tube + Aluminum	350.5
Cavity	351.542
Aluminum + Guide Tube	353.284
Cavity	375.92
Concrete	420.0

We calculate the reaction rates for six dosimeters including ^{63}Cu(n,α), ^{46}Ti(n,p), ^{58}Ni(n,p), ^{54}Fe(n,p), ^{237}Np(n,f), and ^{238}U(n,f) at the cavity dosimeter. All of these reactions are important in fast energy ranges, i.e., energies above 0.1MeV.

Table III shows the ratios of PEN199 to PEN492 reaction rates at the cavity dosimeter, within the energy range of 0.1 to 17MeV. This means that we have calculated reaction rate ratios for groups 2 to 104 for PEN199, and for groups 3 to 489 for PEN492. Table III gives results for both models. We may consider the PEN492 reaction rates as the reference case since it has the finest group structure. The maximum differences between PEN492 and PEN199 for the two models are 4.6% and 4.5%, respectively. ^{237}Np(n,f) reaction has the maximum difference in both models.

Table III. Reaction Rate Ratios, PEN199 to PEN492

RESPONSE	Ratio	
	Model 1 (P_7, S_{16}, 606 meshes)	Model 2 (P_3, S_8, 122 meshes)
^{63}Cu(n,a)	.98582	.98574
^{54}Fe(n,p)	.98389	.98386
^{58}Ni(n,p)	.98189	.98190
^{46}Ti(n,p)	.98424	.98417
^{237}Np(n,f)	.95421	.95501
^{238}U(n,f)	.97898	.97910

In order to analyze the effect of fine-group structures on group collapsing, we perform scalar flux collapsing from PEN492 to PEN25 ($PEN25_{492}$), and from PEN199 to PEN25 ($PEN25_{199}$), using model 1 within the energy range of 0.1 to 17MeV. We collapse cross sections by using the code we developed for scalar flux collapsing approach. Reaction rate ratios of $PEN25_{492}$ to PEN492, $PEN25_{199}$ to PEN199, and $PEN25_{199}$ to PEN492 are calculated. Table IV gives these ratios for six responses. The reaction rates obtained for $PEN25_{199}$ are in excellent agreement with those obtained from PEN199. The reason for this excellent agreement is due to the fact that we are not loosing much when we collapse from PEN199 to $PEN25_{199}$. If we examine the reaction rates ratios of $PEN25_{199}$ to the reference PEN492, and $PEN25_{492}$ to PEN492, we see that there is a difference of ~1% in the two calculations. This indicates that there is a slight difference between the $PEN25_{199}$ $PEN25_{492}$ libraries for this application. The broad-group results are not very sensitive to the original fine-group structure (e.g. PEN492 vs. PEN199).

The final analysis in this section is the comparison of scalar flux and bilinear adjoint collapsing methodologies. We use the codes we developed for scalar flux and bilinear adjoint collapsing methodologies. We collapse the PEN492 library to 25 groups with the two approaches using model 2 for the energy range of 0.1 to 17MeV. Table V shows the broad- to fine-group reaction rate ratios for six responses. The bilinear adjoint collapsing method gives superior results compared to scalar flux collapsing, especially for the ^{237}Np(n,f) reaction. For this nuclide, the difference from the reference calculation is 3.8% with the scalar flux collapsing method, whereas we obtain a difference of 0.002 from the reference calculation using the bilinear adjoint collapsing method.

Table IV. Broad- to Fine-Group Reaction Rate Ratios for Model 1 (P_7, S_{16}, 606 meshes) Using Scalar Flux Collapsing Methodology

RESPONSE	$PEN25_{492}$/PEN492	$PEN25_{199}$/PEN199	$PEN25_{199}$/PEN492
^{63}Cu(n,a)	.98748	.98951	.97548
^{54}Fe(n,p)	.98364	.98931	.97337
^{58}Ni(n,p)	.98284	.99104	.97310
^{46}Ti(n,p)	.98864	.99218	.97655
^{237}Np(n,f)	.96064	.99411	.94859
^{238}U(n,f)	.98062	.99683	.97588

Table V. $PEN25_{492}$ to PEN492 Reaction Rate Ratios for Model 2 (P_3, S_8, and 122 meshes) Using Scalar Flux and Bilinear Adjoint Collapsing Methodologies

RESPONSE	$PEN25_{492}$/PEN492	
	Scalar flux collapsing	Bilinear adjoint collapsing
^{63}Cu(n,a)	.98724	.98926
^{54}Fe(n,p)	.98374	.99619
^{58}Ni(n,p)	.98302	.99695
^{46}Ti(n,p)	.98867	.99089
^{237}Np(n,f)	.96203	.99795
^{238}U(n,f)	.98090	.99984

5. APPLICATION OF THE CPXSD METHODOLOGY

The CPXSD (Contributon and Point-wise Cross Section Driven) methodology is used to select an effective group structure for the TMI-1 cycle 7 reactor for fast neutron dosimetry calculations. We start with an evenly partitioned, i.e., arbitrary group structure. We consider energy intervals of 0.1MeV between 0.1 to 18MeV in the partitioning process. We end up with 180 groups in this fast energy range, and place only one group below 0.1MeV.

First we generate cross sections with NJOY for the 27 nuclides given in Section 4 with the 181-group structure. We use the SCAMPI code package to self-shield and mix cross sections. The DORT code is used for 1-D transport calculations with this 181-group library (PEN181). We perform both forward and adjoint calculations in order to calculate the group-dependent "contributon", C_g. To determine the adjoint function distribution for the adjoint calculation, six dosimeter responses are considered: ^{63}Cu(n,α), ^{46}Ti(n,p), ^{58}Ni(n,p), ^{54}Fe(n,p), ^{237}Np(n,f), and ^{238}U(n,f). These six response cross sections are normalized and summed. By this mean, we include the effect of the six responses in one adjoint source. Thus, instead of applying "contributon" theory for six adjoint sources and generating six different group structures, we generate only one group structure that uses an adjoint source representative of the six response functions. The 181-group response cross sections are shown in Figure 4.

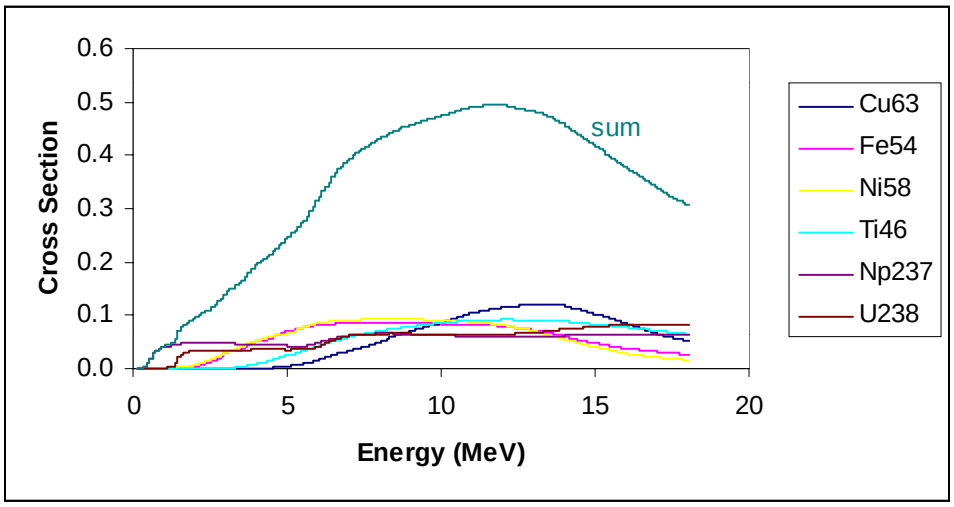

Figure 4. The 181-Group Normalized Response Cross Sections

The 181-group C(E)'s are calculated and presented in Figure 5. The C(E)'s have large magnitudes within an energy range 0.1 to 2MeV. The peaks, i.e., high C(E)'s point the energy groups that contribute more to the detector. Figures 6 through 8 show the C(E)'s plotted at energy ranges of 0.1 to 2MeV, 2 to 9.5MeV, and 9.5 to 20MeV. The C(E) shows resonance structure for energies from 0.1 to ~9.5MeV and is a smooth function of energy above ~9.5MeV. The different C(E) distributions reflect the behavior of iron cross sections in different energy ranges.

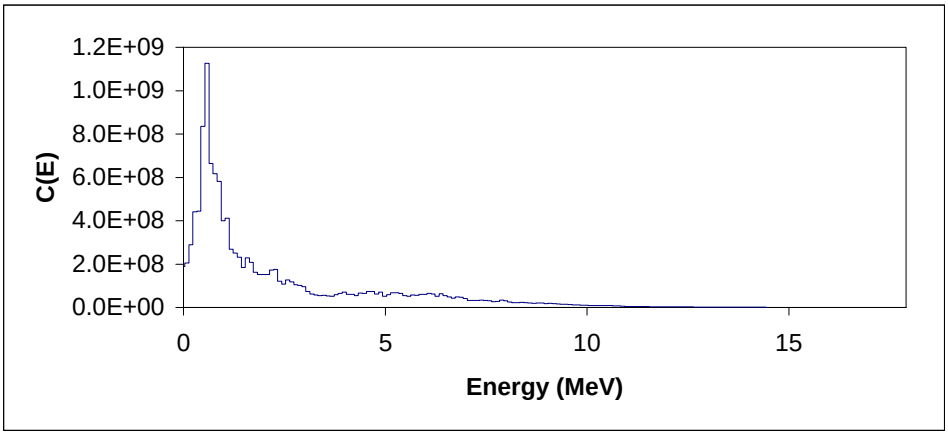

Figure 5. The C(E) Distribution Above 0.1MeV Using the PEN181 Library

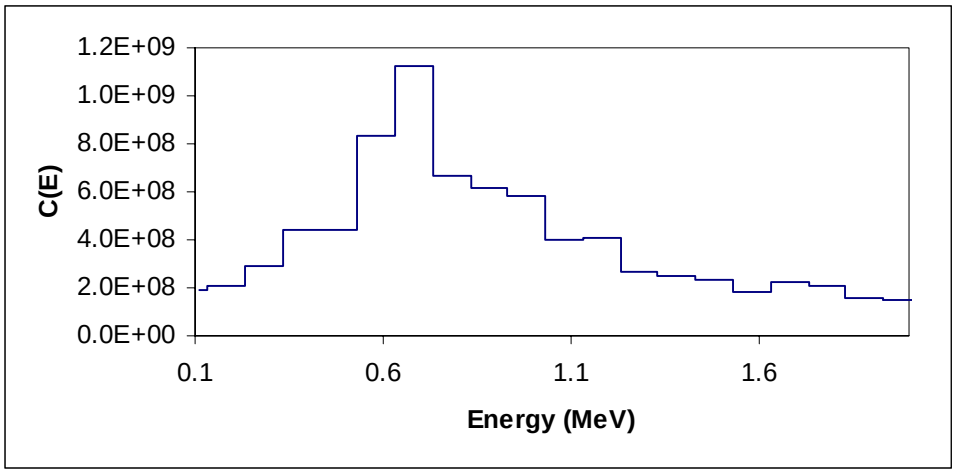

Figure 6. The C(E) Distribution Between 0.1 and 2MeV Using the PEN181 Library

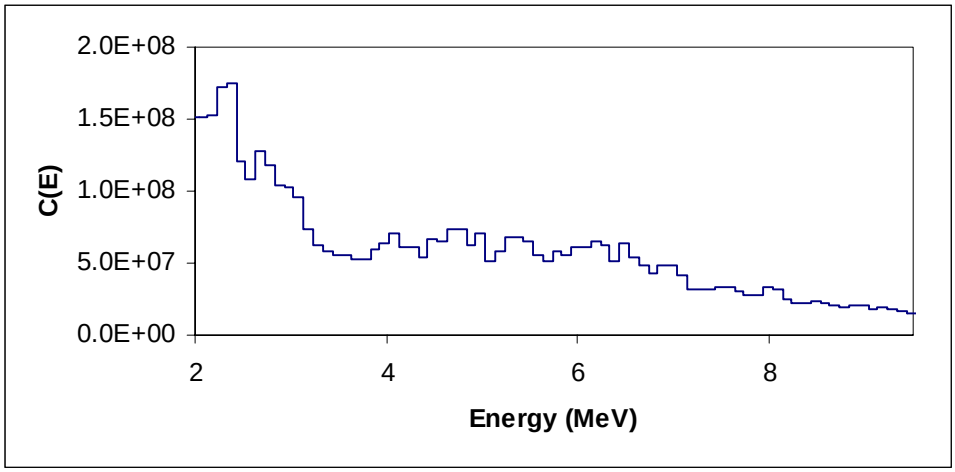

Figure 7: The C(E) Distribution Between 2 and 9.5MeV Using the PEN181 Library

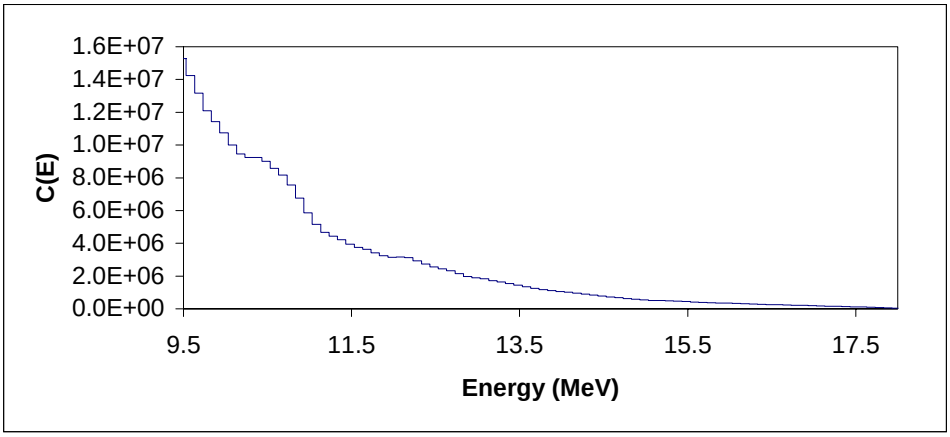

Figure 8: The C(E) Distribution Above 9.5MeV Using the PEN181 Library

In order to apply CPXSD to select an effective group structure for this problem, we select iron the "important" material in our system. Total cross section of Fe-56 has many resonances above 0.1MeV. Since the maximum contribution of neutrons to the detector is between 0.1 to ~2.MeV, we start our refinement in this energy range. This energy region contains 20 groups of PEN181. We extract the locations of all the minima between 0.1 to 2MeV from the point-wise ENDF data. The next step is to find the energy group that has the highest C(E). For this problem, the highest C(E) is between 0.632 to 0.732MeV. For this energy range we represent all Fe-56 minima by placing sub-groups such that each sub-group contains a Fe-56 minima. Between 0.632 to 0.732MeV we place 20 sub-groups. For other energy groups we set the number of sub-divisions relative to the region of highest C(E). With this method, we end up with a total of 301 energy groups. From these, 140 groups are between 0.1 to 2.MeV. Using this new group structure, we generate a new 301-group cross section library (PEN301), and calculate 301-group C(E)'s. In Figure 9, the 140-group (from PEN301) and 20-group (from PEN181) C(E)'s representing the energy range between 0.1 to 2MeV are presented. It is interesting to note that CPXSD methodology effectively identified the important peaks that were not present in PEN181.

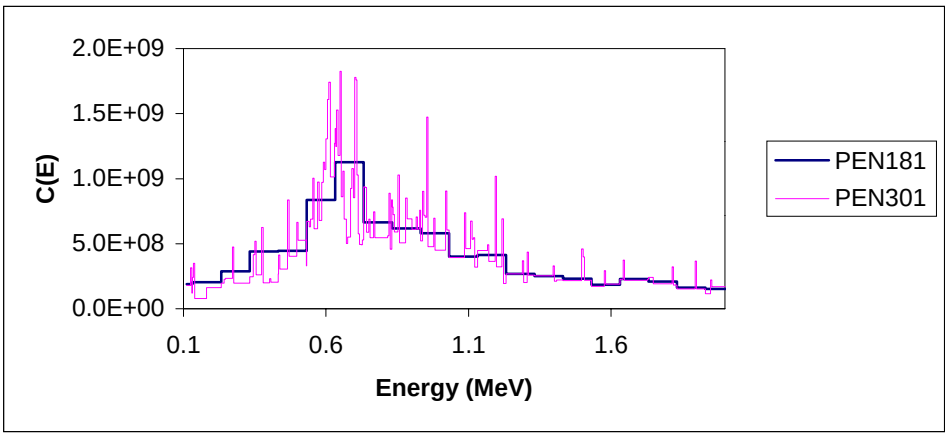

Figure 9. The C(E) Distribution in PEN181 and PEN301 Between 0.1 to 2MeV

We next analyze the PEN199, PEN181, and PEN301 group structures with PEN492 based on selected reactions in the range of 0.1 to 2MeV, choosing reactions important in the range of 0.11109 to 2.032MeV. We consider ^{54}Fe(n,p), ^{58}Ni(n,p), ^{237}Np(n,f) and ^{238}U(n,f) reactions that are sensitive in energy ranges of ~1.732-2.032MeV, ~1.232-2.032MeV, ~0.432-2.032MeV, ~1.332-2.032MeV, respectively. Table VI gives the reaction rate ratios of PEN199, PEN181, and PEN301 to PEN492 for these reactions. We observe that PEN301 library calculations are in well agreement (with 1-2%) with PEN492. The differences of PEN181 and PEN199 compared to PEN492 are within 2-4% and 4-12%, respectively.

Table VI. Reaction Rate Ratios of Different Fine-Group Structures

RESPONSE	PEN301/PEN492	PEN181/PEN492	PEN199/PEN492
^{54}Fe(n,p)	.98376	.95596	.87721
^{58}Ni(n,p)	.98822	.97622	.95681
^{237}Np(n,f)	.99067	.96406	.94472
^{238}U(n,f)	.98695	.97562	.94790

6. SUMMARY AND CONCLUSIONS

The accuracy of a broad-group library generation depends on fine- and broad-group structures, self-shielding method and collapsing methodology. We address the issues related to the selection of effective group structures and collapsing methodology. We apply the new CPXSD (Contributon and Point-wise Cross Section Driven) methodology for pressure vessel cavity dosimetry problem, and we demonstrate the effectiveness of bilinear adjoint collapsing.

BUGLE-like libraries are generated for the validation of methodology. Consequently, we benchmark the state-of-the-art code system for multigroup cross section generation. Fine- and broad-group analysis is performed using PEN199 and PEN492 fine-group structures. These group structures are collapsed to 25 group. The effect of the fine- to the broad-group cross sections are examined. We show that the fine-group structure does not have a significant effect on scalar flux weighted collapsing. By performing scalar flux and bilinear adjoint collapsing, we demonstrate that the bilinear adjoint weighting approach gives better results. For example, there is relative difference of 3.6% between the two collapsing methodologies in the computation of the ratio of $PEN25_{492}$ to PEN492 for the ^{237}Np(n,f) reaction.

The CPXSD (Contributon and Point-wise Cross Section Driven) methodology is used for the generation of an effective group structure for a reactor dosimetry problem. Starting with an arbitrary i.e. evenly partitioned group structure above 0.1MeV (PEN181), the CPXSD resulted in a 301-group structure (PEN301). Based on the comparison of several dosimetry interactions, it is demonstrated that PEN301 is in excellent agreement (1-2%) with the reference PEN492, while the standard 199-group (PEN199) library differs from PEN492 as much as 12%. It is worth to note that the CPXSD yields accurate results comparable to a library with significantly larger number of groups, e.g., for the test problem, CPXSD resulted in 301 groups as compared to a reference library of 492 groups. Currently, we are applying the CPXSD to other applications, e.g., for boiling water reactor core shroud neutron and gamma dose calculations. We are also examining other approaches (e.g., using cross section information) for the selection of the starting energy group structure.

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