

**IMPROVEMENTS TO THE POOL CRITICAL ASSEMBLY  
BENCHMARK USING 3-D DISCRETE ORDINATE TRANSPORT  
WITH ADAPTIVE DIFFERENCE**

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To my beautiful wife, Ashley, thank you for all the encouragement, support, and affection over all these years in college. You have always shared my dreams and encouraged my pursuit of them.

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## SUMMARY

The internationally circulated Pool Critical Assembly (PCA) Pressure Vessel Benchmark was analyzed using the PENTRAN Parallel  $S_N$  code system for the geometry, material, and source specifications as described in the PCA Benchmark documentation. Improvements to the benchmark are proposed through the application of more representative flux and volume weighted homogenized cross sections for the PCA reactor core, which were obtained from a rigorous heterogeneous modeling of all fuel assembly types in the core. A new source term definition is also proposed based on calculated relative power in each core fuel assembly with a spectrum based on the Uranium-235 fission spectra. This research focused on utilizing the BUGLE-96 cross section library and accompanying reaction rates, while examining both adaptive differencing on a coarse mesh basis, as well as the sole use of Directional Theta-Weighted (DTW)  $S_N$  differencing scheme in order to compare the calculated PENTRAN results to measured data. The results show good comparison with the measured data, which suggests PENTRAN is a viable and reliable code system for calculation of light water reactor neutron shielding and dosimetry calculations. Furthermore, the improvements to the benchmark methodology resulting from this work provide a 6 percent increase in accuracy of the calculation (based on the average of all calculation points), when compared with experimentally measured results at the same spatial location in the PCA pressure vessel simulator.

# CHAPTER 1

## INTRODUCTION

The Pool Critical Assembly (PCA) Pressure Vessel Benchmark, initially developed and performed by Oak Ridge National Laboratory, is an industry standard benchmark problem which can be performed for partial establishment of the qualification of a radiation transport methodology for pressure vessel neutron fluence calculations.<sup>[1]</sup> The geometry presented in the PCA benchmark is well representative of the shielding methods used to reduce neutron fluence in the pressure vessel in a modern light water reactor (LWR). The system geometry, source definition, and material specifications are generally well characterized in the PCA benchmark documentation. Measured results for various foil sample interactions at specific locations varying in distance from the face of the reactor core are provided in terms of equivalent fission fluxes per PCA core fission neutron, and are used for comparison to calculated results obtained with a transport code. Good agreement between the experimentally measured data and transport calculated equivalent fission fluxes provided the basis for validation of the user's transport methodology for pressure vessel fluence calculations.

As originally implemented, the PCA benchmark was performed with the DORT 2-D  $S_n$  computer code and the multigroup cross sections libraries BUGLE-93, SAILOR-95, and BUGLE-96.<sup>[2, 3, 4]</sup> The 2-D flux synthesis method was utilized to combine one and two-dimensional transport calculations to obtain an approximate three-dimensional result using the DOTSYN code.<sup>[5]</sup> The benchmark was performed in this research using the 3-D Parallel Environment Neutral-Particle TRANsport  $S_N$  code (PENTRAN). The PENTRAN code system was developed by Sjoden and Haghghat, and can be used for fully decomposed (angle, energy, spatial) parallel 3-D Cartesian multigroup forward or adjoint discrete ordinates ( $S_N$ ) simulations.<sup>[6]</sup> The  $S_N$  method is a deterministic approach

that discretizes the angle, energy, and physical spatial variables into a finite number of discrete angular ordinates, energy groups, and spatial grids over the entire phase space system; the PENTRAN code uses a spatial discretization scheme where coarse meshes contain fine meshes in a block-adaptive Cartesian mesh structure. <sup>[6]</sup> Thus, the use of flux synthesis was not required.

The scope of this research was limited to the use of BUGLE-96 cross sections only, and the PCA Benchmark was evaluated with PENTRAN as described. After which, a rigorous modeling of the heterogeneous fuel assemblies was undertaken to obtain flux and volume weighted homogenized cross sections for two different types of fuel assemblies, and an assembly containing a control rod, which had been neglected in the original benchmark evaluation methodology. The flux and volume weighted cross sections were used to obtain a 3-D PENTRAN transport solution for the reactor core, in an effort to obtain an accurate representation for the fixed source of the PCA reactor core. The benchmark was then re-evaluated using this improved benchmark methodology in an effort to reduce the overall modeling related errors and provide calculations which were as close to the experimentally measured data as possible.

## **CHAPTER 2**

### **POOL CRITICAL ASSEMBLY BENCHMARK**

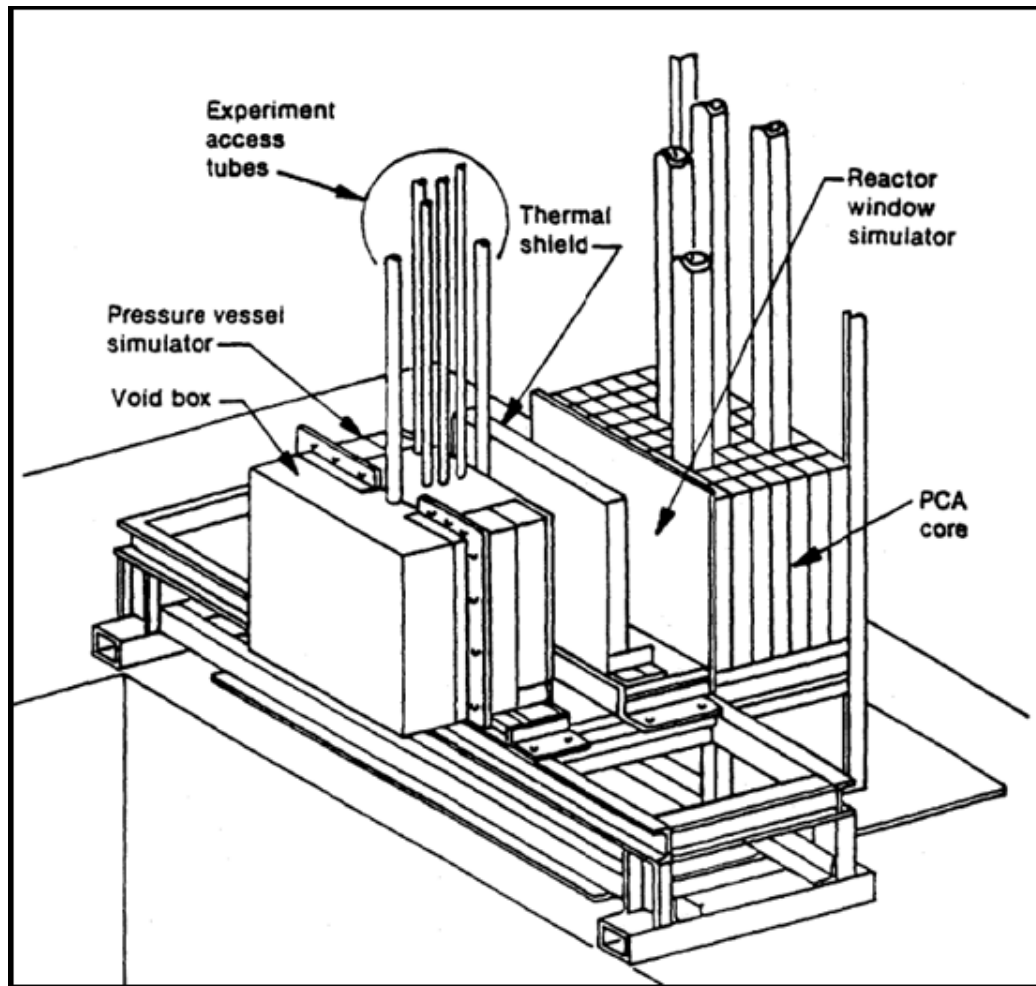
#### **PROBLEM IN DETAIL**

This chapter defines the Pool Critical Assembly (PCA) pressure vessel benchmark, present computational results from previous benchmark analyses, and provides results for the benchmark being performed based on the problem definition but using the 3-D discrete ordinates transport solver PENTRAN. Analysis of the PCA benchmark can be used in partial fulfillment requirements for the validation of a transport calculation methodology for pressure vessel neutron fluence calculations, which are required by the United States Nuclear Regulatory Commission (NRC).<sup>[1]</sup> The PCA benchmark provides measured reaction rates at several locations, inside, within, and beyond the pressure vessel simulator in terms of the equivalent  $^{235}\text{U}$  fission fluxes. To complete the benchmark, one must compare the results of calculations using the transport methodology of choice to the experimentally measured data.

#### **2.1 General Benchmark Geometry**

The geometry presented in the PCA benchmark is well representative of the shielding methods used to reduce neutron fluence in the pressure vessel in a modern pressurized water reactor (PWR). The geometry, source definition, and material specifications are generally well characterized in the PCA Benchmark documentation, as are the supplied measured results for various interactions at specific locations varying in distance from the face of the reactor core. A 3-D sketch of the PCA benchmark facility is shown in Fig. 2.1 and consists of the reactor core and various components which allow for the simulation of a typical Light Water Reactor (LWR). The components present in the PCA benchmark facility are the reactor core, reactor window also referred to as the core face simulator, thermal shield, pressure vessel simulator and void box. The thermal

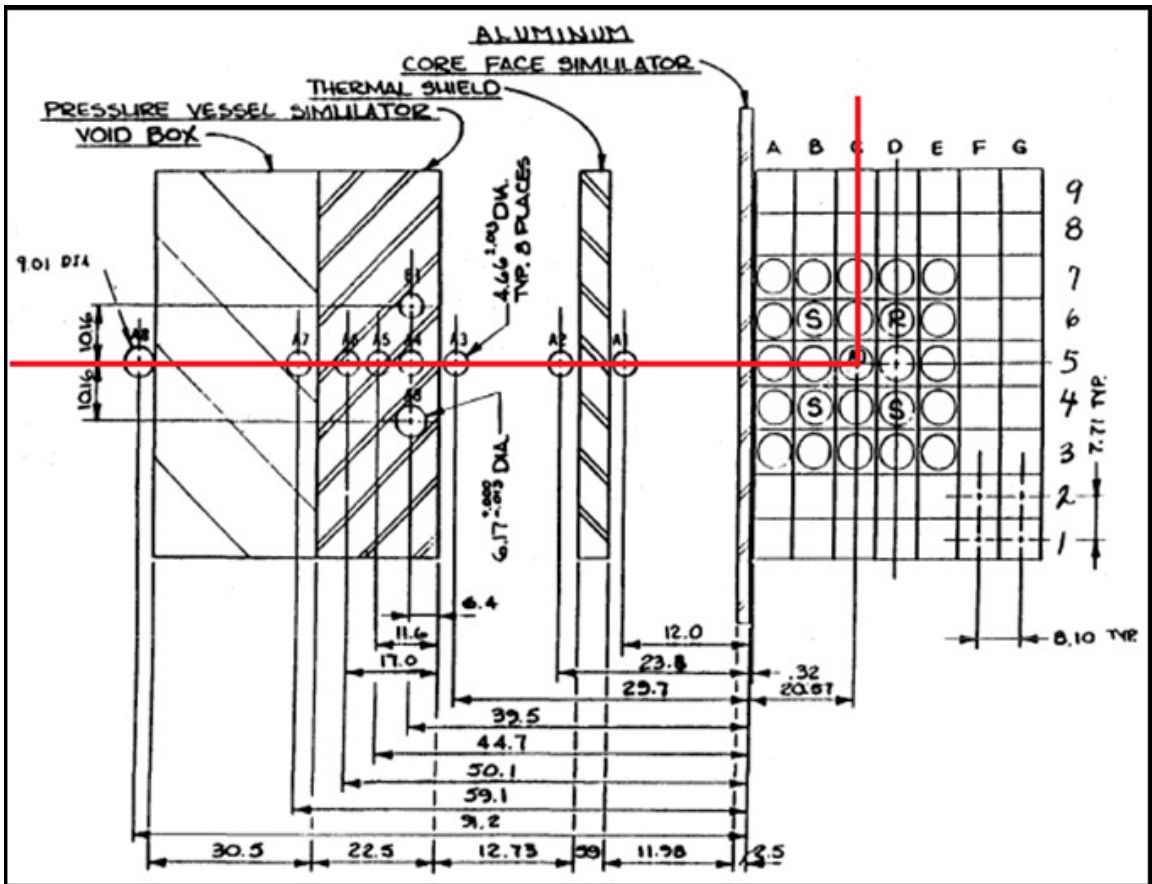
shield is a movable component, and for the experiments run in which results for the PCA benchmark were obtained, the distance from the reactor window to the thermal shield was 12 cm, and the distance from the pressure vessel simulator to the thermal shield was 13 cm. The facility was submerged in a large pool of water, which provided cooling for the reactor core as well as moderation and shielding of neutrons.



**Figure 2.1:** PCA Pressure Vessel Benchmark Facility (Image from NUREG/CR-6454).<sup>[1]</sup>

Fig. 2.2 depicts a horizontal cross section of the PCA benchmark facility through the core midplane. The PCA reactor core consisted of 25 fuel assemblies, arranged in a symmetric 5 by 5 lattice. Quarter core symmetry was maintained. Thus, in an effort to

conserve computation time and increase computational efficiency only one quarter of the core was simulated. This resulted in modeling the region above and to the left of the red lines shown in Fig. 2.2. It is important to note, the original authors of the PCA benchmark also undertook the same simplification, so a one-to-one comparison can still be made between the two computational methodologies, as both modeled the geometry of the system in the same manner. Locations marked as A1-A8 in Fig. 2.2 represent experiment tubes (also depicted in Fig. 2.1) and mark the locations in the pressure vessel simulator where the measured reaction rates were obtained for comparison of the resulting computer calculations.

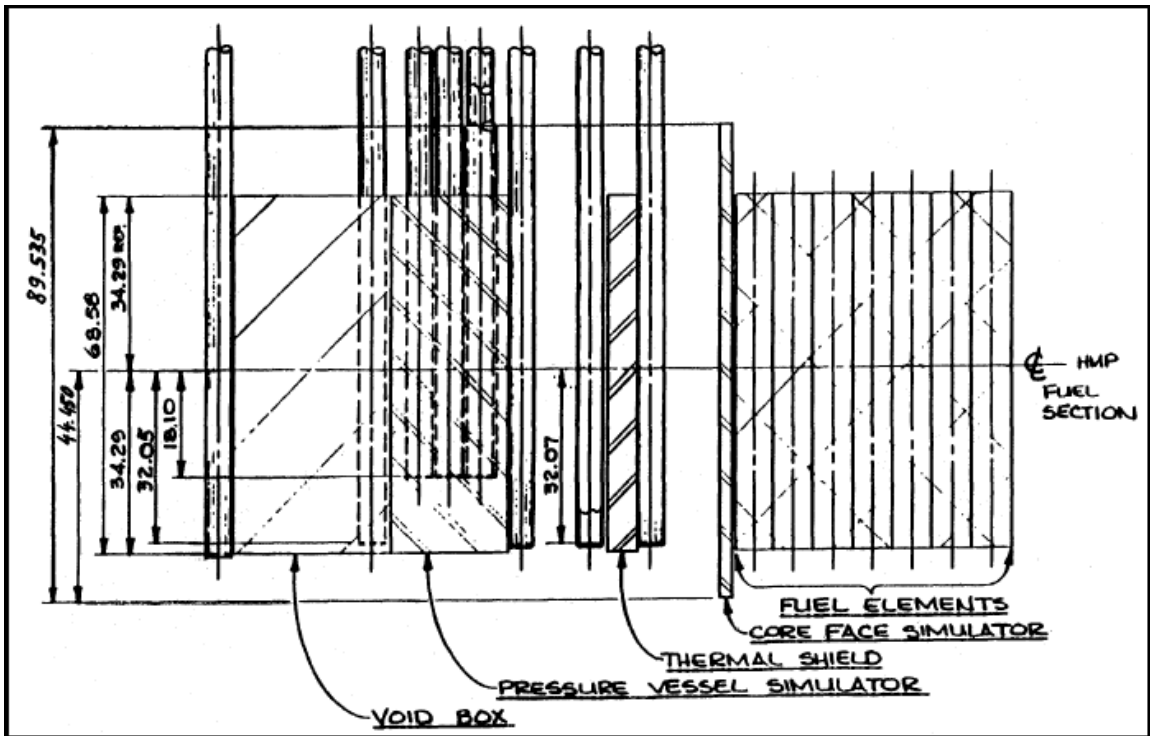


**Figure 2.2:** Horizontal cross section of the PCA Pressure Vessel Benchmark Facility

(Image from NUREG/CR-6454).<sup>[1]</sup> All dimensions are in centimeters.



Fig. 2.3 provides a vertical cross section of the PCA benchmark facility, complete with measurements in centimeters for the height of various core components based on the centerline of the fuel. Some of these measurements provide insight into the depth of the experiment tubes, within which the experiments were performed. It becomes important to note that all measurements presented in the PCA benchmark documentation were obtained at the core centerline. Moreover, the experiment tubes were also backfilled with material consistent with the surrounding material; thus in computational models, the physical presence of the tubes can be neglected since the backfill provides little to no change in neutron behavior compared to the material present around these tubes.



**Figure 2.3:** Vertical cross section of the PCA Pressure Vessel Benchmark Facility

(Image from NUREG/CR-6454).<sup>[1]</sup> All dimensions are in centimeters.

## 2.2 Out of Core Components

The out of core components of the PCA benchmark facility are the components which combine to form the pressure vessel simulator portion of the facility; the core face simulator, thermal shield, pressure vessel simulator, and void box. Dimensions and material specifications of each of these components are addressed in the following subsections. As mentioned previously, the reactor and simulator is situated in a large pool of light water, at an average temperature of 37.7 °C, though temperatures were noted to fluctuate by 5 °C from summer to winter. <sup>[1]</sup>

### 2.2.1 Core Face Simulator (CFS)

The CFS or reactor window is a 2.5 cm thick, 89.535 cm high, and 91.44 cm wide aluminum plate which is located 0.32 cm from the edge of the reactor fuel (shown in Figs. 2.2 and 2.3). Material specifications for the aluminum were taken as Al 6061-T6, consisting entirely of <sup>27</sup>Al with a density of 2.7 g/cm<sup>3</sup>.

### 2.2.2 Thermal Shield (TS)

The TS is a 5.9 cm thick, 68.58 cm wide and 68.58 cm high movable piece of stainless steel (SS 304L) which was placed between the CFS and the pressure vessel simulator. The exact location is more precisely depicted in Figs. 2.2 and 2.3. The density of SS 304L was 8.0 g/cm<sup>3</sup>; with an isotopic composition of 0.03% C, 2.00% Mn, 1.00% Si, 19.00% Cr, 9.50% Ni and 68.47% Ni (percents are weight percent, all elements were taken to be the natural composition of the element).

### 2.2.3 Pressure Vessel Simulator (PVS)

The PVS is a 22.5 cm thick, 68.58 cm wide and 68.58 cm tall piece of carbon steel (SA-36). Experiment tubes were located at ¼, ½, and ¾ thickness in order to observe the drop-off and deposition of neutron flux as a function of pressure vessel thickness (see Figs. 2.2 and 2.3). The isotopic composition of SA-36 was defined to be 0.04% P, 0.05% S, 0.25% C, and 99.66% Fe. Elements assumed to be the natural composition of the element, isotopic breakdowns are reported in weight percent.

#### **2.2.4 Void Box (VB)**

The VB is a large aluminum clad box which sits just beyond the PVS with the function of acting like the air which is typically beyond the pressure vessel in a LWR. Since the PCA benchmark facility is a pool reactor, the air box was required as light water will moderate neutrons, while air typically has little to no effect on neutron behavior. The dimensions of the VB were noted at 30.48 cm thick, 68.58 cm high and 68.58 cm wide. A 0.3175 cm thick aluminum walled box filled with air essentially made up the VB, however since aluminum is effectively transparent to neutrons and the wall thickness was so small, the wall was neglected in the computer models and air was put in its place to reduce the overall number of Cartesian meshes. The air inside the void box was assumed to have a density of  $1.203 \times 10^{-3} \text{ g/cm}^3$ , with isotopic breakdown of 76.90%  $^{14}\text{N}$ , 22.93%  $^{16}\text{O}$ , and 0.17%  $^1\text{H}$  (in weight percent).

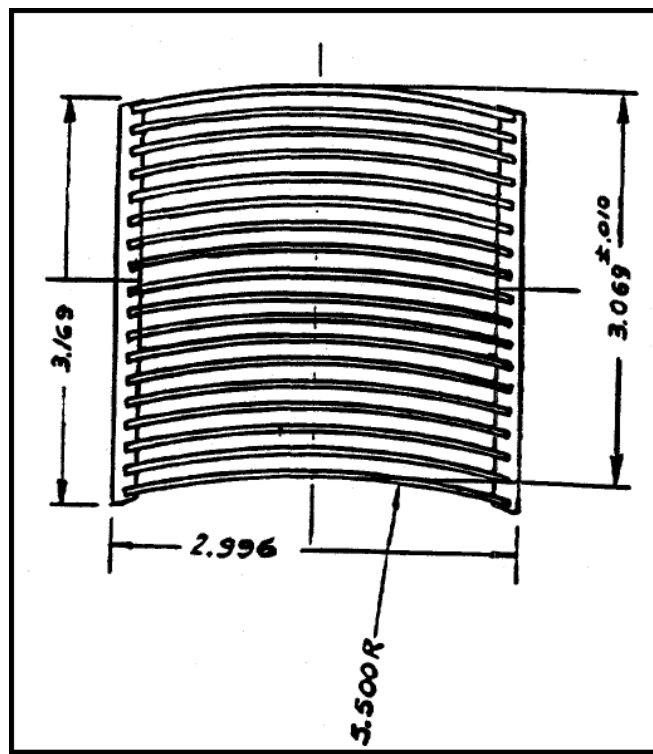
### **2.3 Core Components**

As described, the within core components consist of three types of fuel assemblies; the standard fuel assembly, ORR fuel assembly, and control rod assembly. The fuel assemblies contained various numbers of curved fuel plates, containing aluminum cladding, with 93 weight percent enriched  $^{235}\text{U}$  dispersed in an aluminum matrix as the reactor fuel. Fuel assembly pitch was consistent between assembly types and defined to be 8.100 cm between rows (horizontal direction of Fig. 2.2) and 7.709 cm between columns (vertical direction of Fig. 2.2).<sup>[1]</sup> Cross sections for fuel assemblies were homogenized, per benchmark instructions, using a volume fraction approach.

#### **2.3.1 Standard Fuel Assembly**

The standard PCA fuel assembly contains 18 curved fuel plates, where each plate and a 0.051 cm thick fuel region (U-Al alloy) contained within aluminum cladding which was 0.051 cm thick on both sides. Water passed between the fuel plated in channels which were 0.297 cm thick and the entire assembly was held together by aluminum side plates. Due to the complex nature of the curved fuel plate geometry (Fig. 2.4), the

benchmark instructed the user to homogenize the fuel region based on the volume fraction of each material within. Volume homogenizations were performed based on the provided volumes of the fuel assembly (3747 cm<sup>3</sup>), aluminum (1515.9 cm<sup>3</sup>) and water (2231.1 cm<sup>3</sup>) present in the standard fuel assembly. It was noted that 140 g of 93 weight percent enriched <sup>235</sup>U was present in the entire assembly. The density of water was then assumed to be 1.00 g/cm<sup>3</sup> and the aluminum density was assumed to be consistent with the aluminum defined for the CFS (2.7 g/cm<sup>3</sup>). These densities allowed for the volumes provided to be converted into mass, which was then used to find the weight percent of each isotope present, including the 140 g of <sup>235</sup>U, noting that the 140 g only refers to the 93% of the U mass present, the balance was assumed to be <sup>238</sup>U. These assumptions, combined with the directives in the benchmark lead to the isotopics and density of the standard PCA fuel assembly, presented in Table 2.1.



**Figure 2.4:** Horizontal cross section of a standard PCA fuel assembly (Image from NUREG/CR-6454).<sup>[1]</sup> All dimensions are in inches.

**Table 2.1:** Standard PCA fuel assembly isotopics and density based on volume fraction homogenization of neutron cross sections.

<b>Isotope</b>	<b>Weight Percent</b>
<sup>1</sup> H	3.856500
<sup>16</sup> O	30.602900
<sup>27</sup> Al	63.215500
<sup>235</sup> U	2.162343
<sup>238</sup> U	0.162757
<b>Density</b>	<b>1.73256 g/cm<sup>3</sup></b>

### 2.3.2 ORR Fuel Assembly

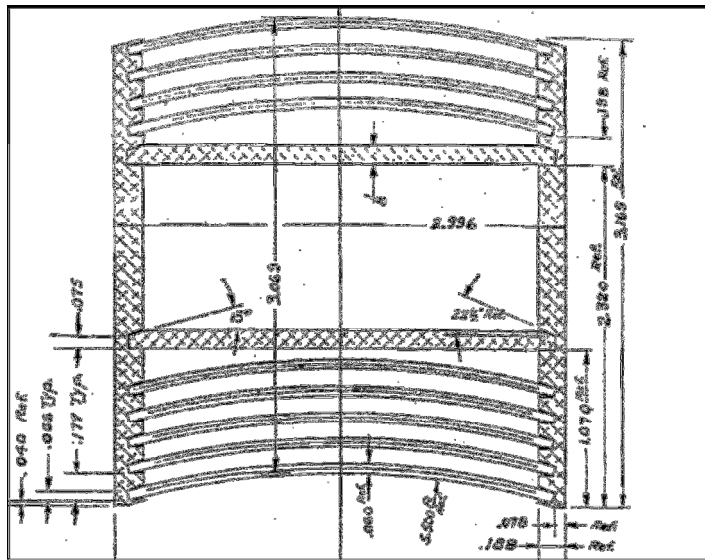
The ORR fuel assembly contains 19 curved fuel plates, in a similar geometry as the standard fuel assembly. However, there are some differences. While the fuel thickness in each plate is still 0.051 cm, the clad thickness on both sides of the end plates is 0.057 cm, and the clad thickness on the non-end fuel plates is 0.038 cm. The water thickness between fuel plates was 0.295 cm and there was a total of 200 g of 93 weight percent enriched <sup>235</sup>U in the fuel assembly. The homogenization process was performed identically to the process described for the standard fuel assembly, and the resulting isotopics and density of the ORR fuel assembly can be found in Table 2.2, below.

**Table 2.2:** ORR PCA fuel assembly isotopics and density based on volume fraction homogenization of neutron cross sections.

<b>Isotope</b>	<b>Weight Percent</b>
<sup>1</sup> H	3.818500
<sup>16</sup> O	30.301000
<sup>27</sup> Al	62.598100
<sup>235</sup> U	3.058491
<sup>238</sup> U	0.230209
<b>Density</b>	<b>1.74982 g/cm<sup>3</sup></b>

### 2.3.3 Control Rod Fuel Assembly

The fuel assembly which contains the control rod is essentially a standard PCA fuel assembly, but with 9 fuel plates removed from the center of the assembly, resulting in a total of 9 fuel plates and a hole for the control rod to be inserted into, as shown in Fig. 2.5. The mass of 93 weight percent enriched  $^{235}\text{U}$  in the control rod assembly totaled 70 g, dispersed in an aluminum matrix amongst the 9 fuel plates. Additional aluminum plates were added to provide a guide for the control rod to pass through. The control rod geometry (not depicted in this section) was again complex in nature, containing several curved surfaces and concentric cylinders, containing  $\text{B}_4\text{C}$  as the absorber, aluminum cladding, and a lead weight. [7] Although the control rod was inserted 11.74 cm into the fuel assembly from the top of the core, the control rod itself was not included in the cross section development for the benchmark. Instead, the benchmark developers accounted for the control rod's effect on the neutron population when calculating the source term; therefore there is no boron carbide present in the isotopics of the control rod assembly, which are depicted in Table 2.3.



**Figure 2.5:** Horizontal cross section of a PCA control rod fuel assembly (Image from NUREG/CR-6454). [1] All dimensions are in inches.

**Table 2.3:** PCA control rod fuel assembly isotopics and density based on volume fraction homogenization of neutron cross sections.

<b>Isotope</b>	<b>Weight Percent</b>
<sup>1</sup> H	3.901900
<sup>16</sup> O	30.962900
<sup>27</sup> Al	63.959000
<sup>235</sup> U	1.093866
<sup>238</sup> U	0.082334
<b>Density</b>	<b>1.71242 g/cm<sup>3</sup></b>

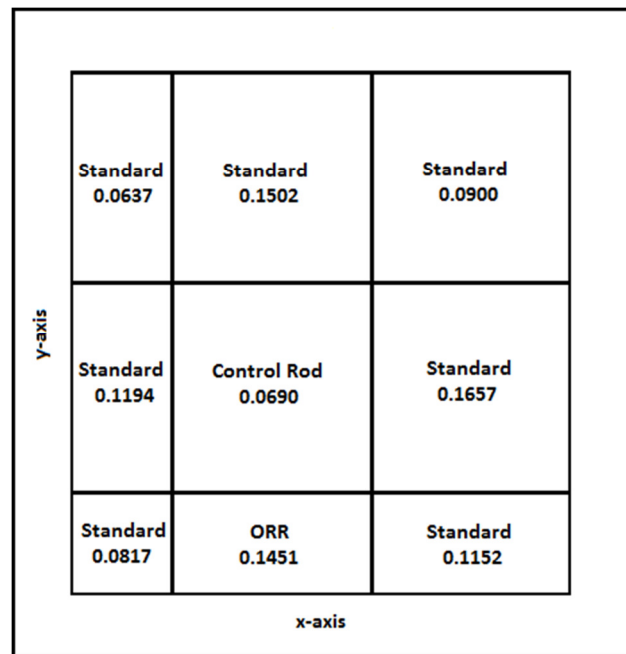
## 2.4 Source Term Definition

In order to obtain calculated solutions to the benchmark, a fixed source must be defined which is well representative of the reactor core in the critical configuration. The fuel loading pattern for the PCA core was chosen to specifically ensure several requirements were met. These include demanding the fuel elements contain no fission products (i.e. fresh fuel), fuel assemblies facing the experiment (pressure vessel simulator) must be a consistent type of fuel assembly with the same mass of <sup>235</sup>U, and quarter core symmetry must be maintained. <sup>[1]</sup> To define a well representative fixed source, the benchmark power distribution was characterized using a combination of fission chamber measurements and a two-dimensional transport calculation. A three-dimensional profile was then assembled by applying a core averaged buckling weight, accounting for the axial distribution being slightly below the core midplane due to the control rod being partially inserted; where the three-dimensional power profile is characterized by Eq. 2.1.

$$p(x, y, z) = \frac{1}{C} p(x, y) \cos[B_z(z - z_0)] \quad (2.1)$$

In Eq. 2.1, the average core buckling  $B_z$  was set equal to  $4.42 \times 10^{-2} \text{ cm}^{-1}$ ,  $z_0$  is the displacement of the vertical power distribution from the core midplane, taken to be -4.20 cm, and  $C$  is an arbitrary normalization constant which allows for the core power to be normalized. Fig. 2.6 provides the normalized PCA reactor source term for the quarter

core. The source was normalized to equal one over the quarter core of the reactor, where the pressure vessel simulator would be located beyond the top of Fig. 2.6. Fig. 2.6 also provides the type of fuel assembly in each location. Since the core was arranged with a 5 by 5 assembly fuel loading pattern, the model contains 4 assemblies which are  $\frac{1}{2}$  fuel assemblies and one assembly which is a  $\frac{1}{4}$  fuel assembly. Reflective boundary conditions were applied on the  $-x$  and  $-y$  axes, allowing for the model to maintain quarter core symmetry. It becomes important to note that since the quarter core power was normalized to one fission neutron per second, the final resulting fluxes must then be divided by 4, since the model is effectively providing results for a reactor core normalized to 4 fission neutrons per second due to the specular reflective boundary conditions. The normalization process was performed, rather than simply modeling the actual source magnitude present in the reactor, due to the reporting of experimental results and their associated uncertainties in units of equivalent fission fluxes per PCA core fission neutron per second (experimental results are shown in section 2.5).<sup>[1]</sup>



**Figure 2.6:** Normalized source strength by PCA fuel assembly.



## 2.5 Experimental Results of Fission Chamber and Radiometric Measurements

Experimental results, from a combination of fission chamber measurements and foil activation analyses were used as the comparison basis for the validation of the user's transport methodology. These results were obtained at seven locations at various distances from the reactor core face and within, before, and after several components of the LWR pressure vessel simulator setup, listed in Table 2.4, and shown in Fig. 2.2. <sup>[1]</sup>

**Table 2.4:** Experimental measurement locations in the PCA benchmark.

<b>Location</b>	<b>Distance from Core Face (cm)</b>	<b>Description of Location</b>
<b>A1</b>	12.0	Before Thermal Shield
<b>A2</b>	23.8	Past Thermal Shield
<b>A3</b>	29.7	In front of Pressure Vessel
<b>A4</b>	39.5	Pressure Vessel (1/4 Thickness)
<b>A5</b>	44.7	Pressure Vessel (1/2 Thickness)
<b>A6</b>	50.1	Pressure Vessel (3/4 Thickness)
<b>A7</b>	59.1	Void Box

Six different radiation interactions were included as part of this benchmark, though each interaction was not necessarily determined at every experimental location in the PCA pressure vessel simulator. The experimental results were provided in the benchmark documentation in terms of equivalent fission fluxes per PCA core fission neutron per second. <sup>[1]</sup> Since the experimental results, shown in Table 2.5, are based on actual measurements, uncertainties were provided. These uncertainties accounted for foil size corrections (if relevant), counting statics, detector pileup and dead time, background correction and corrections for interference reactions, run-to-run monitoring, and positional uncertainties in the experimental channel. <sup>[1]</sup> Uncertainties provided in Table 2.5, account for all applicable uncertainties. A transport methodology can be considered validated for pressure vessel neutron fluence calculations if the resulting calculated results lie within the uncertainty of the measurement.

**Table 2.5:** Experimental results for fission chamber and radiometric measurements of equivalent fission fluxes per 1 PCA core fission neutron per second. <sup>[1]</sup> †

Location	<sup>237</sup> Np (n,f)	<sup>238</sup> U (n,f)	<sup>27</sup> Al (n,α)	<sup>58</sup> Ni (n,p)	<sup>115</sup> In (n,n')	<sup>103</sup> Rh (n,n')
A1	6.64E-06 ± 6.2%	--	7.87E-06 ± 1.0%	5.83E-06 ± 1.4%	5.61E-06 ± 1.0%	5.54E-06 ± 1.0%
A2	--	--	1.02E-06 ± 2.0%	6.18E-07 ± 2.0%	6.06E-07 ± 2.0%	--
A3	2.27E-07 ± 6.3%	--	4.48E-07 ± 1.0%	2.31E-07 ± 1.4%	1.99E-07 ± 1.0%	--
A4	9.27E-08 ± 5.5%	6.11E-08 ± 6.9%	1.02E-07 ± 2.0%	5.30E-08 ± 1.0%	5.87E-08 ± 0.7%	7.74E-08 ± 1.5%
A5	5.18E-08 ± 5.7%	2.74E-08 ± 6.8%	4.10E-08 ± 2.2%	2.09E-08 ± 1.8%	2.76E-08 ± 1.5%	4.35E-08 ± 5.0%
A6	2.70E-08 ± 5.8%	1.12E-08 ± 7.1%	1.54E-08 ± 2.2%	7.43E-09 ± 2.2%	1.17E-08 ± 3.0%	2.19E-08 ± 5.0
A7	7.25E-09 ± 9.2%	--	--	--	--	--

† For <sup>237</sup>Np and <sup>235</sup>U equivalent fission fluxes, combined uncertainties are given. For other interactions, experimental precision is provided. Experimental precision was defined by foil size corrections, counting statics, dead time, pileup, background corrections, interfering reaction corrections, run-to-run monitoring, and positional uncertainties.

## 2.6 Calculation of Equivalent Fission Fluxes

The measured data was provided in terms of equivalent fission fluxes per 1 PCA core fission neutron which were calculated using Eq. 2.2, where  $\bar{\phi}$  is the “equivalent fission flux,”  $\phi_g$  is the flux in group  $g$  at the experiment location,  $\sigma_{rx,g}$  is the reaction rate for group  $g$ ,  $\sigma_{ref}$  is the reaction cross section averaged over the <sup>235</sup>U fission spectrum and  $S_0$  is the total number of source particles.

$$\bar{\phi} = \frac{\sum_{g=1}^G \phi_g \sigma_{rx,g}}{\sigma_{ref} S_0} \quad (2.2)$$

As previously noted, since the quarter core result was normalized to one,  $S_0$  must be multiplied by 4 to obtain the appropriate equivalent fission flux. Values for  $\sigma_{ref}$  were defined in the PCA benchmark documentation, verified via hand calculation, and are shown in Table 2.6. Reaction rates can be found in Appendix A.

**Table 2.6:** Reaction cross sections averaged over the  $^{235}\text{U}$  fission spectra, in mbarns.

$^{237}\text{Np}$ (n,f)	$^{238}\text{U}$ (n,f)	$^{27}\text{Al}$ (n, $\alpha$ )	$^{58}\text{Ni}$ (n,p)	$^{115}\text{In}$ (n,n')	$^{103}\text{Rh}$ (n,n')
1312	305	0.705	109	189	773
$\pm 50$	$\pm 9$	$\pm 0.040$	$\pm 6$	$\pm 8$	$\pm 38$

## CHAPTER 3

### THE DISCRETE ORDINATES METHOD

This chapter will address the Discrete Ordinates ( $S_N$ ) Method and its application to obtain solutions to the linear Boltzmann equation. The discretized form of the transport equation will be presented in a 3-D Cartesian geometry as the scope of this thesis is limited to computations specifically in the Cartesian coordinate system. In the  $S_N$  method, the linear Boltzmann equation (Eq. 3.1) is discretized in all of its independent variables (space, energy, and angle) as discussed in the upcoming sections.

$$\begin{aligned}
 \widehat{\Omega} \cdot \vec{\nabla} \psi(\vec{r}, E, \widehat{\Omega}) + \sigma(\vec{r}, E) \psi(\vec{r}, E, \widehat{\Omega}) &= q^{ext}(\vec{r}, E, \widehat{\Omega}) \\
 + \int_0^\infty dE' \int d\widehat{\Omega}' \sigma_s(\vec{r}, E' \rightarrow E, \widehat{\Omega} \cdot \widehat{\Omega}') \psi(\vec{r}, E', \widehat{\Omega}') & \\
 + \frac{\chi(\vec{r}, E)}{k} \int_0^\infty dE' \int d\widehat{\Omega}' \nu \sigma_f(\vec{r}, E') \psi(\vec{r}, E', \widehat{\Omega}') &
 \end{aligned} \tag{3.1}$$

#### 3.1 Discretization of the Energy Variable

The energy variable of the Boltzmann transport equation is partitioned into a number of discrete energy ranges, or “groups.”<sup>[8]</sup> Starting with the highest energy particles ( $g=1$ ) and ending with the lowest energy particles ( $g=G$ ). Thus, particles in energy group  $g$  are defined as having energies between  $E_{g-1}$  and  $E_g$ . The overall result of this discretization is an approximation to the transport equation in terms of the angular flux of each energy group where the group angular flux is defined by Eq. 3.2.

$$\psi_g(\vec{r}, \widehat{\Omega}) = \int_{E_g} dE \psi(\vec{r}, E, \widehat{\Omega}) = \int_{E_g}^{E_{g-1}} dE \psi(\vec{r}, E, \widehat{\Omega}) \tag{3.2}$$

The energy integrals can be further divided to represent the contribution from each energy group

$$\int_0^\infty dE' \approx \sum_{g'=1}^G \int_{g'} dE' \quad (3.3)$$

and integrating Eq. 3.1 over energies between  $E_{g-1}$  and  $E_g$ , one obtains the following.

$$\begin{aligned} & \widehat{\Omega} \cdot \vec{v} \int_g dE \psi(\vec{r}, E, \widehat{\Omega}) + \int_g dE \sigma(\vec{r}, E) \psi(\vec{r}, E, \widehat{\Omega}) \\ &= \int_g dE q^{ext}(\vec{r}, E, \widehat{\Omega}) \\ &+ \sum_{g'=1}^G \int_g dE \int_{g'} dE' \int d\widehat{\Omega} \sigma_s(\vec{r}, E' \rightarrow E, \widehat{\Omega} \cdot \widehat{\Omega}') \psi(\vec{r}, E', \widehat{\Omega}') \\ &+ \int_g dE \frac{\chi(\vec{r}, E)}{k} \sum_{g'=1}^G \int_{g'} dE' \int d\widehat{\Omega} \nu \sigma_f(\vec{r}, E') \psi(\vec{r}, E', \widehat{\Omega}') \end{aligned} \quad (3.4)$$

Given that multigroup cross-sections for an arbitrary reaction process  $rxn$  are defined by

$$\sigma_{rxn,g}(\vec{r}) = \frac{\int_{E_g}^{E_{g-1}} dE \int_{4\pi} d\widehat{\Omega} \sigma_{rxn}(\vec{r}, E) \psi(\vec{r}, E, \widehat{\Omega})}{\int_{E_g}^{E_{g-1}} dE \int_{4\pi} d\widehat{\Omega} \psi(\vec{r}, E, \widehat{\Omega})}. \quad (3.5)$$

Based on the definition provided in Eq. 3.5, the group cross-sections representing total, fission and scattering reaction processes can be subsequently defined by Eqs. 3.6-3.8.

$$\sigma_{t,g}(\vec{r}) = \frac{\int_{E_g}^{E_{g-1}} dE \int_{4\pi} d\widehat{\Omega} \sigma_t(\vec{r}, E) \psi(\vec{r}, E, \widehat{\Omega})}{\int_{E_g}^{E_{g-1}} dE \int_{4\pi} d\widehat{\Omega} \psi(\vec{r}, E, \widehat{\Omega})} \quad (3.6)$$

$$\sigma_{f,g}(\vec{r}) = \frac{\int_{E_g}^{E_{g-1}} dE \int_{4\pi} d\widehat{\Omega} \sigma_f(\vec{r}, E) \psi(\vec{r}, E, \widehat{\Omega})}{\int_{E_g}^{E_{g-1}} dE \int_{4\pi} d\widehat{\Omega} \psi(\vec{r}, E, \widehat{\Omega})} \quad (3.7)$$

$$\begin{aligned} & \sigma_{s,gg'}(\vec{r}, \widehat{\Omega} \cdot \widehat{\Omega}') \\ &= \frac{\int_{E_{g'}}^{E_{g-1}} dE' \int_{4\pi} d\widehat{\Omega}' \sigma_s(\vec{r}, E' \rightarrow E, \widehat{\Omega} \cdot \widehat{\Omega}') \psi(\vec{r}, E', \widehat{\Omega}')}{\int_{E_g}^{E_{g-1}} dE \int_{4\pi} d\widehat{\Omega} \psi(\vec{r}, E, \widehat{\Omega})} \end{aligned} \quad (3.8)$$

Combining the definition of multigroup cross-sections with the form of the transport equation shown in Eq. 3.4 and the representation of the angular flux given in Eq. 3.2, the multigroup form of the transport equation becomes

$$\begin{aligned} \widehat{\Omega} \cdot \vec{\nabla} \psi_g(\vec{r}, \widehat{\Omega}) + \sigma_{t,g}(\vec{r}) \psi_g(\vec{r}, \widehat{\Omega}) &= q_g^{ext}(\vec{r}, \widehat{\Omega}) \\ + \sum_{g'=1}^G \int_{4\pi} d\widehat{\Omega} \sigma_{s,gg'}(\vec{r}, \widehat{\Omega} \cdot \widehat{\Omega}') \psi_{g'}(\vec{r}, \widehat{\Omega}') & \\ + \frac{\chi_g(\vec{r})}{k} \sum_{g'=1}^G \nu \sigma_{f,g'}(\vec{r}) \phi_{g'}(\vec{r}) & \end{aligned} \quad (3.9)$$

where  $q_g^{ext}(\vec{r}, \widehat{\Omega})$  is the angular dependent fixed source, and the scalar flux is defined as

$$\phi_g(\vec{r}) = \int_{4\pi} d\widehat{\Omega} \psi_g(\vec{r}, \widehat{\Omega}). \quad (3.10)$$

The angular variable in Eq. 3.9 is normalized over the unit sphere so integration over  $\widehat{\Omega}$  is expressed in terms of the azimuthal angle  $\phi$  and polar angle cosine  $\mu$ .

$$\int_{4\pi} d\widehat{\Omega} = \int_{-1}^1 \frac{d\mu}{2} \int_0^{2\pi} \frac{d\phi}{2\pi} = 1 \quad (3.11)$$

The angular dependency of the scattering cross-section can be expanded using spherical harmonics (Eqs. 3.12 and 3.13). The scattering cross-section is assumed to only be dependent on the cosine of the scattering angle. Thus,  $\mu_0 = \widehat{\Omega} \cdot \widehat{\Omega}'$ , where  $\widehat{\Omega}$  and  $\widehat{\Omega}'$  represent the directions of a particle before and after the scattering interaction. This assumption implies that the probability of scattering into a direction  $\widehat{\Omega}'$  with energy group  $g'$  is independent of the initial direction of the particle. It is thus important to note that at very low energies (i.e. ‘‘cold neutrons’’), this assumption becomes an approximation.

$$\sigma_{s,g' \rightarrow g}(\vec{r}, \mu_0) \cong \sum_{l=1}^L (2l+1) \sigma_{sl,g' \rightarrow g}(\vec{r}) P_l(\mu_0) \quad (3.12)$$

$$\sigma_{sl,g' \rightarrow g}(\vec{r}) = \int_{-1}^1 \frac{d\mu_0}{2} \sigma_{s,g' \rightarrow g}(\vec{r}, \mu_0) P_l(\mu_0) \quad (3.13)$$

The direction cosine between the initial and scattered direction of the particle can be given by

$$\mu_0 = \mu\mu' + (1 - \mu^2)^{1/2}(1 - \mu'^2)^{1/2}\cos(\phi - \phi'). \quad (3.14)$$

Using the Legendre Addition Theorem, the Legendre polynomial  $P_l(\mu_0)$  can be expressed in terms of orthogonal spherical surface harmonics.

$$P_l(\mu_0) = \frac{1}{(2l+1)} \sum_{k=-l}^l Y_{l,k}^*(\theta', \phi') Y_{l,k}(\theta, \phi) \quad (3.15)$$

The spherical surface harmonics,  $Y_{l,k}^*$  and  $Y_{l,k}$  can be defined in terms of the Associated Legendre polynomials.

$$Y_{l,k}(\theta, \phi) = \sqrt{(2l+1) \frac{(l-k)!}{(l+k)!}} P_l^k(\mu) \exp(ik\phi) \quad (3.16)$$

$$Y_{l,-k}(\theta, \phi) = (-1)^k Y_{l,k}^*(\theta, \phi) \quad (3.17)$$

Combining Eqs. 3.15-3.17,  $P_l(\mu_0)$  can be rewritten as follows,

$$P_l(\mu_0) = P_l(\mu)P_l(\mu') + 2 \sum_{k=1}^l \frac{(l-k)!}{(l+k)!} P_l^k(\mu) P_l^k(\mu') \cos(k(\phi - \phi')). \quad (3.18)$$

By Subtraction Theorems of Trigonometry:

$$\cos(k(\phi - \phi')) = \cos(k\phi)\cos(k\phi') + \sin(k\phi)\sin(k\phi') \quad (3.19)$$

The directional vector  $\widehat{\Omega}$  can be expressed as a set of directional cosines along the x, y, and z axes,  $\langle \mu, \eta, \xi \rangle$ . Where  $\eta$  and  $\xi$  can further be expressed in terms of  $\mu$  and  $\phi$  as follows:

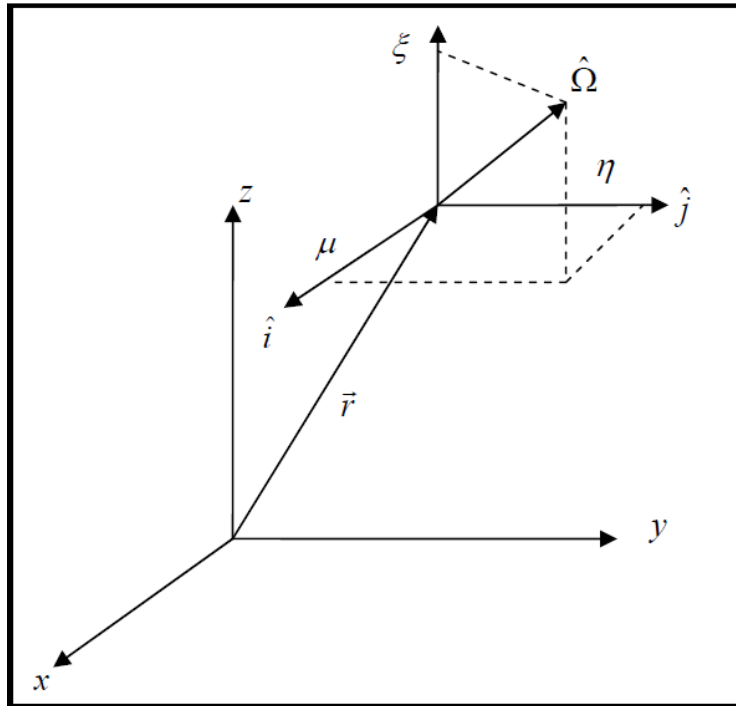
$$\eta = \sqrt{(1 - \mu^2)} \cos(\phi) \quad (3.20)$$

$$\xi = \sqrt{(1 - \mu^2)} \sin(\phi) \quad (3.21)$$

In 3-D Cartesian coordinates, the streaming operator ( $\widehat{\Omega} \cdot \vec{\nabla}$ ) in Eq. 3.9 becomes:

$$\widehat{\Omega} \cdot \vec{\nabla} = \mu \frac{d}{dx} + \eta \frac{d}{dy} + \xi \frac{d}{dz} \quad (3.22)$$

Figure 3.1 depicts the 3-D Cartesian coordinate system, where the position vector ( $\vec{r}$ ) represents the  $(x,y,z)$  location of a particle traveling in direction  $\hat{\Omega}$ , projected into  $\langle \mu, \eta, \xi \rangle$ .



**Figure 3.1:** 3-D Cartesian coordinate system.



Substituting Eqs. 3.12, 3.18, 3.19, and 3.22 into Eq. 3.9, one obtains the multigroup form of the transport equation expanded in Legendre in Cartesian coordinates: <sup>[6]</sup>

$$\begin{aligned}
& \left( \mu \frac{d}{dx} + \eta \frac{d}{dy} + \xi \frac{d}{dz} + \sigma_{t,g}(x, y, z) \right) \psi_g(x, y, z, \mu, \phi) \\
& = q_g^{ext}(x, y, z, \mu, \phi) \\
& + \sum_{g'=1}^G \sum_{l=0}^L (2l+1) \sigma_{sl,g' \rightarrow g}(x, y, z) \{ P_l(\mu) \phi_{l,g'}(x, y, z) + \\
& 2 \sum_{k=1}^l \frac{(l-k)!}{(l+k)!} P_l^k(\mu) [ \phi_{cl,g'}^k(x, y, z) \cos(k\phi) + \phi_{sl,g'}^k(x, y, z) \sin(k\phi) ] \} \\
& + \frac{\chi_g(x, y, z)}{k} \sum_{g'=1}^G \nu \sigma_{f,g'}(x, y, z) \phi_{0,g'}(x, y, z)
\end{aligned} \tag{3.23}$$

where,

$\mu$  : direction cosine along the x-axis

$\eta$  : direction cosine along the y-axis

$\xi$  : direction cosine along the z-axis

$\sigma_{t,g}$  : group total macroscopic cross-section

$\psi_g$  : angular flux in energy group g

$\phi$  : azimuthal angle, constructed by taking  $\arctan(\xi/\eta)$

$q_g^{ext}$  : group external source

$\sigma_{sl,g' \rightarrow g}$  :  $l^{th}$  moment of the macroscopic scattering cross-section

$P_l(\mu)$  :  $l^{th}$  Legendre Polynomial

$\phi_{l,g'}$  :  $l^{th}$  scalar flux moment for group g'

$P_l^k(\mu)$  : associated  $l^{th}$ ,  $k^{th}$  Legendre Polynomial

$\phi_{cl,g'}^k$  : cosine associated  $l^{th}$ ,  $k^{th}$  scalar flux moment for group g'

$\phi_{sl,g'}^k$  : sine associated  $l^{th}$ ,  $k^{th}$  scalar flux moment for group g'

$\chi_g$  : fission spectrum constant for group g

$k$  : criticality eigenvalue

$\nu \sigma_{f,g'}$  : group fission production

The scalar flux moments present in Eq. 3.23 are defined as follows:

$$\phi_{l,g'}(x, y, z) = \int_{-1}^1 \frac{d\mu'}{2} P_l(\mu') \int_0^{2\pi} \frac{d\phi'}{2\pi} \psi_{g'}(x, y, z, \mu', \phi') \quad (3.24)$$

$$\phi_{cl,g'}^k = \int_{-1}^1 \frac{d\mu'}{2} P_l^k(\mu') \int_0^{2\pi} \frac{d\phi'}{2\pi} \cos(k\phi') \psi_{g'}(x, y, z, \mu', \phi') \quad (3.25)$$

$$\phi_{sl,g'}^k = \int_{-1}^1 \frac{d\mu'}{2} P_l^k(\mu') \int_0^{2\pi} \frac{d\phi'}{2\pi} \sin(k\phi') \psi_{g'}(x, y, z, \mu', \phi') \quad (3.26)$$

### 3.2 Discretization of the Angular Variable

The angular component of the transport equation,  $\widehat{\Omega}$ , is discretized by considering a finite number of discrete directions, where the angular flux is only evaluated along these ordinates. Each discrete direction corresponds to a point on the surface of a unit sphere with an associated surface area that mathematically corresponds to the integration weight of the scheme: often referred to as a quadrature set. However, quadrature sets must satisfy the following properties: <sup>[9]</sup>

$$\sum_{m=1}^M w_m = 1.0 \quad (3.27)$$

$$\sum_{m=1}^M w_m \mu_m^n = \sum_{m=1}^M w_m \eta_m^n = \sum_{m=1}^M w_m \xi_m^n = 0.0, \quad \text{for } n \text{ odd} \quad (3.28)$$

$$\sum_{m=1}^M w_m \mu_m^n = \sum_{m=1}^M w_m \eta_m^n = \sum_{m=1}^M w_m \xi_m^n = \frac{1}{n+1}, \quad \text{for } n \text{ even} \quad (3.29)$$

Since the net current  $J_{net}$  in an isotropic flux is absolutely equal to zero, Eqs. 3.27-3.28 must hold true, where Eq. 3.27 implies the associated weights must be positive and normalized to a constant, generally chosen to be one. Eq. 3.28, known as the “*odd moment conditions*,” must be satisfied for the quadrature set to be symmetric on the unit sphere for each set of directions, regardless of 90-degree axis rotations. While, Eq. 3.29, known as the “*even moment conditions*,” are required to insure proper integration of the

Legendre functions in order to obtain accurate results for the angular flux (and thus scalar flux, currents, etc.).

### 3.2.1 Level Symmetric Quadrature

A common method for generating quadrature sets is the level-symmetric technique. In this method, the ordinates are symmetric in each octant of the unit sphere, and ordered along the z-axis with  $N/2$  distinct levels. The number of directions on each level can be calculated as follows:

$$\frac{N}{2} - i + 1, \quad \text{for } i = 1, N/2 \quad (3.30)$$

where  $N$  is the order of the  $S_N$  method and in a 3-D geometry, the total number of directions  $M$  is

$$M = N(N + 2). \quad (3.31)$$

Since, for any angular direction vector the ordinate must lie on the surface of the unit sphere, where  $i, j, k$  are the indices of the direction cosines:

$$\mu_i^2 + \eta_j^2 + \xi_k^2 = 1.0 \quad (3.32)$$

Due to the rotational symmetry requirement of level-symmetric quadrature, coupled with Eq. 3.32, one can derive the following recursion relationship for directions in level-symmetric quadrature sets:

$$\mu_i^2 = \mu_1^2 + C(i - 1) \quad (3.33)$$

where,

$$C = \frac{2}{N-2}(1 - 3\mu_1^2), \quad \text{for } 2 \leq i \leq \frac{N}{2}. \quad (3.34)$$

The weights associated with each individual direction, often referred to as “*point weights*,” can then be determined with another set of equations. In the case of  $S_8$  level-symmetric quadrature set, this condition can be satisfied by Eqs. 3.35a-d.

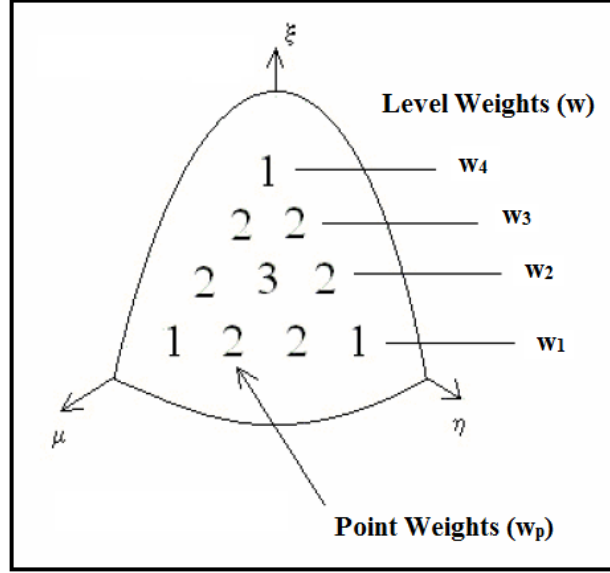
$$2w_{p1} + 2w_{p2} = w_1 \quad (3.35a)$$

$$2w_{p2} + w_{p3} = w_2 \quad (3.35b)$$

$$2w_{p2} = w_3 \quad (3.35c)$$

$$1w_{p1} = w_4 \quad (3.35d)$$

Where  $w_1, w_2, w_3,$  and  $w_4$  are weights associated with each level, and  $w_{p1}, w_{p2},$  and  $w_{p3}$  are the point weights associated with each direction, as depicted in Figure 3.2.



**Figure 3.2:** Point and level weight pattern for  $S_8$  level-symmetric quadrature set.

It is important to note that level-symmetric quadrature sets are limited to order  $S_{20}$ . Beyond  $S_{20}$ , unphysical negative weights appear, which has prompted the development of Legendre-Chebyshev ( $P_n-T_n$ ) quadratures which have mitigated the nonphysical negative weights of level-symmetric quadrature sets. <sup>[10]</sup>

### 3.3 Discretization of the Spatial Variable

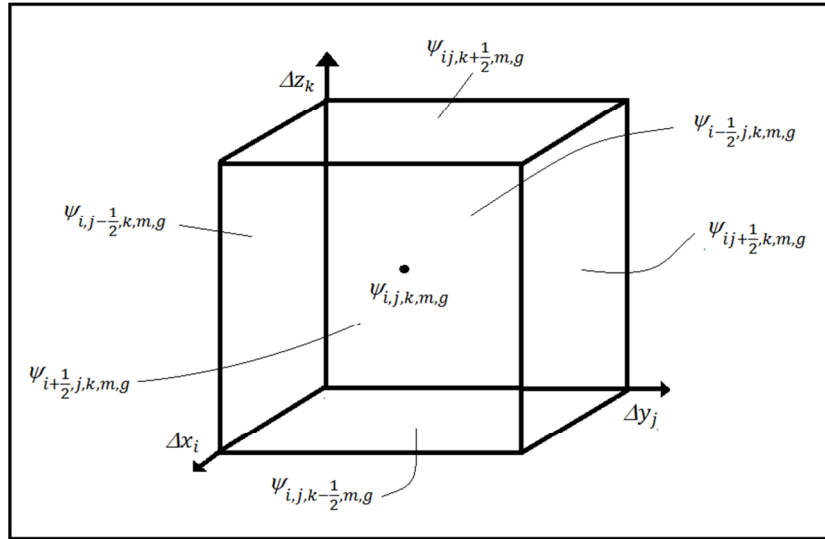
The linear Boltzmann equation, as depicted in Eq. 3.23 can be recast in as abbreviated form as follows,

$$\left( \mu_m \frac{d}{dx} + \eta_m \frac{d}{dy} + \xi_m \frac{d}{dz} + \sigma_g(\vec{r}) \right) \psi_{m,g}(\vec{r}) = Q_{m,g}(\vec{r}). \quad (3.36)$$

The angular dependence in Eq. 3.36 is denoted by  $m$ , which references a particular discrete ordinate direction of the angular flux from  $m = 1, M$  and with energy dependence  $g$ , for energy group  $g = 1, G$ . The right hand side of Eq. 3.36 represents the scattering, external source, and fission source terms, lumped together as an overall source  $Q_{m,g}$  at each discrete spatial location  $\vec{r}$ . The spatial domain is partitioned into computational cells or “*meshes*” inside of which material cross-sections and source terms are considered to be constant within each cell. Integrating Eq. 3.36 over the cell volume  $V_{i,j,k} = \Delta x_i \Delta y_j \Delta z_k$ , and then dividing by the cell volume, one obtains the volume and surface averaged angular flux values, which reduces Eq. 3.36 to

$$\begin{aligned} & \frac{\mu_m}{\Delta x_i} \left( \psi_{i+\frac{1}{2},j,k,m,g} - \psi_{i-\frac{1}{2},j,k,m,g} \right) + \frac{\eta_m}{\Delta y_j} \left( \psi_{ij+\frac{1}{2},k,m,g} - \psi_{ij-\frac{1}{2},k,m,g} \right) \\ & + \frac{\xi_m}{\Delta z_k} \left( \psi_{ij,k+\frac{1}{2},m,g} - \psi_{ij,k-\frac{1}{2},m,g} \right) + \sigma_{i,j,k} \psi_{i,j,k,m,g} = Q_{i,j,k,m,g}. \end{aligned} \quad (3.37)$$

The indices  $i, j$ , and  $k$  in Eq. 3.37 refer to cell or mesh center values, while  $i \pm 1/2, j \pm 1/2$  and  $k \pm 1/2$  represent mesh surface values. Figure 3.3 depicts the location of surface and volume averaged angular flux values for each spatial mesh as referenced in Eq. 3.37.



**Figure 3.3:** Spatial cell/mesh volume element with locations of surface and volume averaged angular flux values.

# CHAPTER 4

## DIFFERENCING SCHEMES, BOUNDARY CONDITIONS, AND ITERATIVE METHODS

The solution of the discrete ordinate transport equations is obtained through a process called a “*transport sweep*;” by which the solutions are calculated by marching along the ordinates in each octant of the unit sphere. <sup>[9]</sup> For each computational mesh or cell, in a three dimensional system, the incoming angular flux is known on three sides from either boundary conditions or calculation results from previous cells. Thus, relationships between these three incoming angular fluxes and cell averaged volumetric source (assumed to be known from previous source iterations), to the three outgoing angular fluxes are required for each discrete ordinate and are known as “*differencing schemes*.”

### 4.1 Differencing Schemes

Various types of differencing schemes can be implemented in order to obtain solutions using the  $S_N$  method, and can be either weighted differencing schemes or higher-order differencing schemes. Weighted schemes require only the angular fluxes, whereby the cell average flux is related to the cell boundary angular fluxes. Higher order schemes require higher order angular flux moments, which can be linear or non-linear, discontinuous, characteristic, and/or exponential. <sup>[11]</sup> For weighted spatial differencing schemes Eq. 4.1a-c are assumed to be valid between cell average and boundary angular fluxes (in the  $x, y, z$  or  $i, j, k$  directions).

$$\psi_{i,j,k,m,g} = a_{i,j,k,m,g} \left( \psi_{i+\frac{1}{2},j,k,m,g} + \left( \frac{1}{a_{i,j,k,m,g}} - 1 \right) \psi_{i-\frac{1}{2},j,k,m,g} \right) \quad (4.1a)$$

$$\psi_{i,j,k,m,g} = b_{i,j,k,m,g} \left( \psi_{i,j+\frac{1}{2},k,m,g} + \left( \frac{1}{b_{i,j,k,m,g}} - 1 \right) \psi_{i,j-\frac{1}{2},k,m,g} \right) \quad (4.1b)$$

$$\psi_{i,j,k,m,g} = c_{i,j,k,m,g} \left( \psi_{i,j,k+\frac{1}{2},m,g} + \left( \frac{1}{c_{i,j,k,m,g}} - 1 \right) \psi_{i,j,k-\frac{1}{2},m,g} \right) \quad (4.1c)$$

Values for  $a_{i,j,k,m,g}$ ,  $b_{i,j,k,m,g}$ , and  $c_{i,j,k,m,g}$  are selected based on the type of weighted differencing scheme utilized, while the  $m$  subscript refers to the discrete ordinate and  $g$  refers to the energy group.

#### 4.1.1 Diamond Differencing Scheme

In the traditional diamond differencing scheme, the cell average angular flux is treated as the mathematical average of any two opposite cell boundary fluxes. Thus the constants  $a_{i,j,k,m,g}$ ,  $b_{i,j,k,m,g}$ , and  $c_{i,j,k,m,g}$  in Eqs. 4.1a-c are all set equal to one half. This allows for Eqs. 4.1a-c to be rewritten as follows:

$$\psi_{i,j,k,m,g} = \frac{1}{2} \left( \psi_{i+\frac{1}{2},j,k,m,g} + \psi_{i-\frac{1}{2},j,k,m,g} \right) \quad (4.2a)$$

$$\psi_{i,j,k,m,g} = \frac{1}{2} \left( \psi_{i,j+\frac{1}{2},k,m,g} + \psi_{i,j-\frac{1}{2},k,m,g} \right) \quad (4.2b)$$

$$\psi_{i,j,k,m,g} = \frac{1}{2} \left( \psi_{i,j,k+\frac{1}{2},m,g} + \psi_{i,j,k-\frac{1}{2},m,g} \right) \quad (4.2c)$$

In order to obtain the cell center angular flux, we must eliminate the outgoing angular fluxes in Eq. 3.37; since we are guaranteed to have the incoming angular flux on three surfaces from either previous cell calculations or boundary conditions. In doing so we arrive at the following:

$$\begin{aligned} & \psi_{i,j,k,m,g} \\ &= \frac{\frac{2\mu_m}{\Delta x_i} \psi_{i-\frac{1}{2},j,k,m,g} + \frac{2\eta_m}{\Delta y_j} \psi_{i,j-\frac{1}{2},k,m,g} + \frac{2\xi_m}{\Delta z_k} \psi_{i,j,k-\frac{1}{2},m,g} + Q_{i,j,k,m,g}}{\sigma_{i,j,k,g} + \frac{2\mu_m}{\Delta x_i} + \frac{2\eta_m}{\Delta y_j} + \frac{2\xi_m}{\Delta z_k}} \end{aligned} \quad (4.3)$$

The outgoing angular fluxes can then be evaluated by recasting Eqs. 4.2a-c in terms of cell averaged angular flux and incoming angular flux on each ordinate, taking into account which octant the current ordinate is located in. For example, if one was

located in the positive octant ( $\mu_m > 0$ ,  $\eta_m > 0$ , and  $\xi_m > 0$ ), outgoing angular fluxes are determined by Eqs. 4.4a-c.

$$\psi_{i+\frac{1}{2},j,k,m,g} = 2\psi_{i,j,k,m,g} - \psi_{i-\frac{1}{2},j,k,m,g} \quad (4.4a)$$

$$\psi_{i,j+\frac{1}{2},k,m,g} = 2\psi_{i,j,k,m,g} - \psi_{i,j-\frac{1}{2},k,m,g} \quad (4.4b)$$

$$\psi_{i,j,k+\frac{1}{2},m,g} = 2\psi_{i,j,k,m,g} - \psi_{i,j,k-\frac{1}{2},m,g} \quad (4.4c)$$

The diamond differencing scheme is accurate to second order, but may result in negative solutions.<sup>[9]</sup> To rectify this nonphysical situation, the negative fluxes are set to zero and the cell average flux is then recalculated to maintain the balance of particles in the cell. This approach is commonly referred to as “*negative flux fixup*” or “*Diamond Zero*.” Though, it is important to note that the use of Diamond Zero (DZ) differencing has proven to be a source of load imbalance in parallel processing, thus it is not an optimum choice of differencing scheme for large scale geometries which require the use of parallel computing.<sup>[12]</sup> It is also important to note that non-physical oscillations are inherent in solutions obtained by diamond differencing schemes, which occur due to the mismatch between the direction of particles and the spatial axis. These oscillations are caused by a forced relationship between the cell average angular flux to the boundary fluxes, since there is not a directionally dependent boundary contribution relative to each axis.<sup>[13, 14]</sup> This, coupled with diamond difference’s issues with negative fluxes, provide for poor convergence.

#### 4.1.2 Directional Theta-Weighted Differencing Scheme

In order to mitigate boundary condition induces oscillations, the Directional Theta-Weighted differencing scheme (DTW) was developed by Petrovic and Haghghat; whereby, to insure flux positivity, fixed theta-weighted parameters are introduced and one can solve for the cell average angular flux using Eqs. 4.1a-c.<sup>[15, 16]</sup> Assuming the diamond relationships hold in the y- ad z-directions, and that the lower bound of the



angular flux in the outgoing direction is absolutely zero, the weight  $a_{i,j,k,m,g}$  is determined to be:

$$a_{i,j,k,m,g} = 1 - \frac{Q_{i,j,k,m,g} + \frac{|\mu_m|}{\Delta x_i} \psi_{i-\frac{1}{2},j,k,m,g} + \theta \left( \frac{|\eta_m|}{\Delta y_j} \psi_{i,j-\frac{1}{2},k,m,g} + \frac{|\xi_m|}{\Delta z_k} \psi_{i,j,k-\frac{1}{2},m,g} \right)}{\left( \frac{2|\eta_m|}{\Delta y_j} + \frac{2|\xi_m|}{\Delta z_k} + \sigma_{ij,k,g} \right) \psi_{i-\frac{1}{2},j,k,m,g}} \quad (4.5)$$

Following the same methodology along the other two axes, one arrives at weights for  $b_{i,j,k,m,g}$  and  $c_{i,j,k,m,g}$ :

$$b_{i,j,k,m,g} = 1 - \frac{Q_{i,j,k,m,g} + \frac{|\eta_m|}{\Delta y_j} \psi_{i,j-\frac{1}{2},k,m,g} + \theta \left( \frac{|\mu_m|}{\Delta x_i} \psi_{i-\frac{1}{2},j,k,m,g} + \frac{|\xi_m|}{\Delta z_k} \psi_{i,j,k-\frac{1}{2},m,g} \right)}{\left( \frac{2|\mu_m|}{\Delta x_i} + \frac{2|\xi_m|}{\Delta z_k} + \sigma_{ij,k,g} \right) \psi_{i,j-\frac{1}{2},k,m,g}} \quad (4.6)$$

$$c_{i,j,k,m,g} = 1 - \frac{Q_{i,j,k,m,g} + \frac{|\xi_m|}{\Delta z_k} \psi_{i,j,k-\frac{1}{2},m,g} + \theta \left( \frac{|\mu_m|}{\Delta x_i} \psi_{i-\frac{1}{2},j,k,m,g} + \frac{|\eta_m|}{\Delta y_j} \psi_{i,j-\frac{1}{2},k,m,g} \right)}{\left( \frac{2|\mu_m|}{\Delta x_i} + \frac{2|\eta_m|}{\Delta y_j} + \sigma_{ij,k,g} \right) \psi_{i,j,k-\frac{1}{2},m,g}} \quad (4.7)$$

In order to minimize oscillations, the theta parameters must be dependent of the characteristic of the incident radiation. Thus, the  $\theta$  in Eqs. 4.5-4.7 must be substituted by the result of Eq. 4.8a-c, depending on the direction cosine of the x-, y-, and z-axes (i.e.  $\mu_m, \eta_m, \xi_m$ ).

$$\theta(\mu_m) = \mu_m^2 \quad (4.8a)$$

$$\theta(\eta_m) = \eta_m^2 \quad (4.8b)$$

$$\theta(\xi_m) = \xi_m^2 \quad (4.8c)$$

Thus, the DTW cell averaged angular flux can be shown to equal:

$$\psi_{i,j,k,m,g} = \frac{\frac{|\mu_m|}{a_{i,j,k,m,g}\Delta x_i} \psi_{i-\frac{1}{2},j,k,m,g} + \frac{|\eta_m|}{b_{i,j,k,m,g}\Delta y_j} \psi_{i,j-\frac{1}{2},k,m,g} + \frac{|\xi_m|}{c_{i,j,k,m,g}\Delta z_k} \psi_{i,j,k-\frac{1}{2},m,g} + Q_{i,j,k,m,g}}{\sigma_{i,j,k,g} + \frac{|\mu_m|}{a_{i,j,k,m,g}\Delta x_i} + \frac{|\eta_m|}{b_{i,j,k,m,g}\Delta y_j} + \frac{|\xi_m|}{c_{i,j,k,m,g}\Delta z_k}} \quad (4.9)$$

The DTW scheme is clearly nonlinear, and the weight constants  $a_{i,j,k,m,g}$ ,  $b_{i,j,k,m,g}$ , and  $c_{i,j,k,m,g}$  are guaranteed to range from  $\frac{1}{2}$  to 1. It is important to note that the truncation error of the DTW differencing scheme, can result in either an overestimate or underestimate of the angular flux. Though, since one is typically interested in the scalar flux, the truncation errors often cancel when the angular fluxes are integrated together. Since the DTW scheme guarantees flux positivity and is free of oscillations caused by directional weighting, it is typically much more accurate than DZ, performing especially well in areas of the reactor core where flux gradients are smaller.

#### 4.1.3 Exponential Directional-Weighted Differencing Scheme

The Exponential Directional-Weighted (EDW) differencing scheme, developed by Sjoden and Haghghat, is a predictor corrector differencing scheme which utilizes the DTW scheme's solution to predict a solution for the angular flux, and then corrects it using an exponential fit.<sup>[17]</sup> The EDW scheme is inherently positive and derived as follows:

$$\psi_{i,j,k,m,g} = a_0 \exp\left(\frac{\lambda_i P_1(x)}{|\mu_m|}\right) \exp\left(\frac{\lambda_j P_1(y)}{|\eta_m|}\right) \exp\left(\frac{\lambda_k P_1(z)}{|\xi_m|}\right) \quad (4.10)$$

The DTW differencing scheme is utilized in order to calculate the angular fluxes (denoted  $\tilde{\psi}$ ), which are required in order to estimate the coefficients  $\lambda_i$ ,  $\lambda_j$ , and  $\lambda_k$ , as shown in Eqs. 4.11 a-c, respectively.

$$\lambda_i \approx \frac{\left(\tilde{\psi}_{i+\frac{1}{2},j,k,m,g} - \tilde{\psi}_{i-\frac{1}{2},j,k,m,g}\right) |\mu_m|}{2\tilde{\psi}_{i,j,k,m,g}} \quad (4.11a)$$

$$\lambda_j \approx \frac{\left( \tilde{\psi}_{i,j+\frac{1}{2},k,m,g} - \tilde{\psi}_{i,j-\frac{1}{2},k,m,g} \right) |\eta_m|}{2\tilde{\psi}_{i,j,k,m,g}} \quad (4.11b)$$

$$\lambda_k \approx \frac{\left( \tilde{\psi}_{i,j,k+\frac{1}{2},m,g} - \tilde{\psi}_{i,j,k-\frac{1}{2},m,g} \right) |\xi_m|}{2\tilde{\psi}_{i,j,k,m,g}} \quad (4.11c)$$

The cell averaged angular flux can then be calculated for the EDW differencing scheme, and is given in Eq. 4.12.

$$\begin{aligned} \psi_{i,j,k,m,g} = & \left[ \exp\left(\frac{2\lambda_i}{|\mu_m|}\right) - 1 \right] \left[ \exp\left(\frac{2\lambda_j}{|\eta_m|}\right) - 1 \right] \left[ \exp\left(\frac{2\lambda_k}{|\xi_m|}\right) - 1 \right] \\ & \cdot \frac{1}{\beta} \left( \frac{|\mu_m|}{\Delta x_i} \psi_{i-\frac{1}{2},j,k,m,g} + \frac{|\eta_m|}{\Delta y_j} \psi_{i,j-\frac{1}{2},k,m,g} + \frac{|\xi_m|}{\Delta z_k} \psi_{i,j,k-\frac{1}{2},m,g} \right. \\ & \left. + Q_{i,j,k,m,g} \right) \end{aligned} \quad (4.12)$$

where  $\beta$  is calculated using Eqs. 4.11a-c, and is defined in Eq. 4.13, below. <sup>[6]</sup>

$$\begin{aligned} \beta = & \frac{2\lambda_i}{\Delta x_i} \left[ \exp\left(\frac{2\lambda_i}{|\mu_m|}\right) \right] \left[ \exp\left(\frac{2\lambda_j}{|\eta_m|}\right) - 1 \right] \left[ \exp\left(\frac{2\lambda_k}{|\xi_m|}\right) - 1 \right] \\ & + \frac{2\lambda_j}{\Delta y_j} \left[ \exp\left(\frac{2\lambda_i}{|\mu_m|}\right) - 1 \right] \left[ \exp\left(\frac{2\lambda_j}{|\eta_m|}\right) \right] \left[ \exp\left(\frac{2\lambda_k}{|\xi_m|}\right) - 1 \right] \\ & + \frac{2\lambda_k}{\Delta z_k} \left[ \exp\left(\frac{2\lambda_i}{|\mu_m|}\right) - 1 \right] \left[ \exp\left(\frac{2\lambda_j}{|\eta_m|}\right) - 1 \right] \left[ \exp\left(\frac{2\lambda_k}{|\xi_m|}\right) \right] \\ & + \sigma_{i,j,k,g} \left[ \exp\left(\frac{2\lambda_i}{|\mu_m|}\right) - 1 \right] \left[ \exp\left(\frac{2\lambda_j}{|\eta_m|}\right) - 1 \right] \left[ \exp\left(\frac{2\lambda_k}{|\xi_m|}\right) - 1 \right] \end{aligned} \quad (4.13)$$

The EDW differencing scheme should provide a stable and more accurate solution for the angular flux in regions where higher angular flux gradients are observed; since at its core the scheme corrects the angular flux solution which was predicted by the DTW scheme.

#### 4.1.4 Exponential Directional Iterative Differencing Scheme

The Exponential Directional Iterative (EDI) differencing scheme, which also utilizes a predictor-corrector scheme following the same exponential basis provided in the EDW scheme. However, the EDI scheme possesses an iterative refinement of the exponential constants, which are held constant in the EDW scheme, and thus can provide increased accuracy over the EDW basis.<sup>[6]</sup> Each exponential constant is solved for in a manner consistent with Eqs. 4.11a-c, however, in this case, instead of using the DTW solution for the angular fluxes, one establishes a fixed point iteration based on the previous EDW iteration in order to refine the constant; resulting in the *successive iteration* (I-1, I, I+1...) of each exponential constant, as follows in Eqs. 4.14a-c.

$$\lambda_{i,I} = \frac{\left( \psi_{i+\frac{1}{2},j,k,m,g}(\lambda_{i,I-1}) - \psi_{i-\frac{1}{2},j,k,m,g}(\lambda_{i,I-1}) \right) |\mu_m|}{2 \psi_{i,j,k,m,g}(\lambda_{i,I-1})} \quad (4.14a)$$

$$\lambda_{j,I} = \frac{\left( \psi_{i,j+\frac{1}{2},k,m,g}(\lambda_{j,I-1}) - \psi_{i,j-\frac{1}{2},k,m,g}(\lambda_{j,I-1}) \right) |\eta_m|}{2 \psi_{i,j,k,m,g}(\lambda_{j,I-1})} \quad (4.14b)$$

$$\lambda_{k,I} = \frac{\left( \psi_{i,j,k+\frac{1}{2},m,g}(\lambda_{k,I-1}) - \psi_{i,j,k-\frac{1}{2},m,g}(\lambda_{k,I-1}) \right) |\xi_m|}{2 \psi_{i,j,k,m,g}(\lambda_{k,I-1})} \quad (4.14c)$$

The EDI scheme then solves for the cell average angular flux following the same methodology laid out for the EDW scheme, whereby Eq. 4.12 can be applied, though instead of using Eqs. 4.11a-c for all exponential constants, these equations are utilized as the starting basis for the iterative sequence (i.e. the first iteration), after which Eqs. 4.14a-c are used for refinement and convergence in order to obtain more accurate exponential constants. The overall efficiency and accuracy gain of the EDI differencing scheme over the EDW scheme is variant, depending on the geometry of the system modeled and the severity of the angular flux gradients. In regions with high angular flux gradients, one can expect an increased accuracy with the EDI scheme, over the EDW and DTW differencing

schemes. However, the computational overhead of the EDI scheme is more significant, since it inherently adds an iterative process where a direct process exists for EDW and DTW schemes.

## 4.2 Adaptive Differencing

The adaptive differencing strategy allows for a computer code to automatically select the best differencing scheme available in order to obtain the most accurate solution for the cell averaged angular flux, based on specific “*upgrade criteria*” metrics which are calculated by the code.<sup>[18]</sup> The PENTRAN code system functions models geometries using coarse and fine meshes, where fine meshes are contained inside of each coarse mesh, and allow for refinement of the fine meshing in regions of higher importance or areas where curved geometries require enhanced meshing to resolve structures. Taylor projections are used to couple discrepancies in fine mesh size on coarse mesh borders, which insures the balance of particles between adjacent fine meshes of dissimilar size.<sup>[19]</sup> PENTRAN selects the differencing scheme from the DZ, DTW, and EDI schemes, whereby DZ is upgraded to DTW, which is then upgraded to EDI if necessary.

At the beginning of each new in-group transport sweep, PENTRAN resets the differencing scheme in each fine mesh of every coarse mesh to the scheme originally prescribed by the user, then the code adapts to the most appropriate scheme on a coarse mesh basis. The adaptive difference strategy is implemented in the following manner: assuming the user assigns the DZ scheme as the starting basis in each coarse mesh, PENTRAN automatically upgrades to the DTW scheme in a particular coarse mesh should negative flux fixup in anywhere any fine mesh contained within that coarse mesh. This is then followed by another upgrade from DTW to the EDI scheme if any linear weight factor (shown in Eqs. 4.5-4.7), exceed the user maximum allowable weight, typically taken to be 0.95. It is important to note that the user assigns the starting basis differencing scheme, so should the user start by assigning the DTW scheme, PENTRAN will only upgrade from DTW to EDI and DZ will not be used.

PENTRAN also allows for the user to lock a differencing scheme in any particular coarse mesh, forcing it to implement the user assigned scheme in all fine meshes contained within that coarse mesh. This approach can save on computational run time, since the computer is not using time to corroborate via message passing among processors and select the best differencing scheme, but can lead to solution discrepancies or convergence errors, should the user select a scheme which is not ideal for the region of choice.

### 4.3 Flux Moments

The various flux moments required for the solution to the transport equation are derived based on the cell averaged angular flux calculated with any differencing scheme, following the general scheme presented in Eq. 4.15, where  $l$  refers to the  $l^{\text{th}}$  flux moment.

$$\phi_{i,j,k,g,l} = \frac{1}{8} \sum_{m=1}^M w_m \psi_{i,j,k,m,g} P_l(\mu_m) \quad (4.15)$$

Note that the  $1/8$  term on the right side of Eq. 4.15 is included to account for the requirement that level-symmetric quadrature weights were derived to sum to exactly one in each of the eight octants of the unit sphere. By setting  $l$  in Eq. 4.15 to zero, one would obtain the scalar flux at the location  $i, j, k$  in energy group  $g$ . In a similar fashion, the Associated Legendre moments can be calculated as follows:

$$\phi_{i,j,k,g,C,l}^k = \frac{1}{8} \sum_{m=1}^M w_m \psi_{i,j,k,m,g} P_l^k(\mu_m) \cos\left(k \tan^{-1}\left(\frac{\xi_m}{\eta_m}\right)\right) \quad (4.16)$$

$$\phi_{i,j,k,g,S,l}^k = \frac{1}{8} \sum_{m=1}^M w_m \psi_{i,j,k,m,g} P_l^k(\mu_m) \sin\left(k \tan^{-1}\left(\frac{\xi_m}{\eta_m}\right)\right) \quad (4.17)$$

#### 4.4 Boundary Conditions

The three standard boundary conditions, albedo, specular reflective, and vacuum (zero return current), can be expressed by the general formula presented in Eq. 4.18.

$$\psi_g(\vec{r}_s, \hat{\Omega}_m) = a\psi_g(\vec{r}_s, \hat{\Omega}'_m) \quad (4.18)$$

Where  $\hat{\Omega}_m \cdot \hat{n} = -\hat{\Omega}'_m \cdot \hat{n}$  and  $a$  is defined based on the type of boundary condition as follows:

$a = 1$ , specular reflective boundary condition

$a = 0$ , vacuum (zero return current) boundary condition

$a = \alpha$ , albedo boundary condition (can be energy group dependent).

#### 4.5 Iterative Methods

Due to the integro-differential nature of the Boltzmann transport equation, the solution of the multigroup discrete ordinates equations can be obtained through the use of an iterative process. If the user is trying to obtain the solution to a fixed source problem, only the application of the Source Iteration Method is required. However, if an eigenvalue solution is needed, both the Source Iteration Method and Power Iteration Method are required to obtain both a converged flux as well as accurate and converged eigenvalue.

##### 4.5.1 Source Iteration Method

The Source Iteration Method or “*source iteration*” refers to the process of guessing a source (generally the in-group scattering source), and then sweeping through the angular, spatial and energy domains of the discretized system.<sup>[9]</sup> Upon completion of the transport sweep, scalar flux and flux moment solutions are obtained from the angular flux and a new in-group scattering source is calculated. This process is repeated until the convergence criteria (or tolerance) is met for each cell averaged angular flux solution,

along each ordinate, for every energy group, and at every spatial location, as shown in Eq. 4.19.

$$\epsilon_{\psi} > \frac{|\psi^i - \psi^{i-1}|}{\psi^{i-1}} \quad (4.19)$$

Typical values for  $\epsilon_{\psi}$  vary from problem to problem, and depending on the importance of a particular region's solution to the rest of the problem, but are generally taken to be  $10^{-3}$  to  $10^{-4}$ .

#### 4.5.2 Power Iteration Method

Criticality eigenvalue problems are solved using the Power Iteration Method, in which the eigenvalue of the system is associated with the fission distribution (which is nonnegative). Typically source iterations are performed based on an initial guess of the angular flux and converged, after which a power iteration is performed to obtain the eigenvalue. This process is then repeated until both the source iteration and power iteration have converged within the designated tolerance levels. Eq. 4.20 depicts how to calculate the eigenvalue of the  $i^{\text{th}}$  power iteration.

$$k^i = k^{i-1} \frac{\int dE \int d\vec{r} \nu \sigma_f(\vec{r}, E) \phi^i(\vec{r}, E)}{\int dE \int d\vec{r} \nu \sigma_f(\vec{r}, E) \phi^{i-1}(\vec{r}, E)} \quad (4.20)$$

A typical starting guess for the eigenvalue  $k$ , is one, though if the eigenvalue of the system can be guessed more precisely at the problem onset, faster convergence may be observed. The convergence criteria  $\epsilon_k$ , for the eigenvalue is shown in Eq. 4.21, where tolerances are generally taken to be  $10^{-5}$  at a minimum.

$$\epsilon_k > \frac{|k^i - k^{i-1}|}{k^{i-1}} \quad (4.21)$$

It is important to note that power iterations are often referred to as “*outer iterations*,” while source iterations are referred to as “*inner iterations*” in a computational framework for reactor physics criticality solvers.



## CHAPTER 5

### PCA BENCHMARK ANALYSIS

As originally implemented, the PCA benchmark was performed with the DORT 2-D  $S_N$  computer code and the multigroup cross sections libraries BUGLE-93, SAILOR-95, and BUGLE-96. <sup>[2, 3, 4]</sup> The 2-D flux synthesis method was utilized to combine one and two-dimensional transport calculations to obtain an approximate three-dimensional result using the DOTSYN code. <sup>[5]</sup> Transport calculations were performed with  $S_8$  level symmetric quadrature set and  $P_3$  anisotropic scattering cross sections. Although the benchmark documentation provides results using BUGLE-93, SAILOR-95, and BUGLE-96 cross sections, this research addressed the use of only BUGLE-96 cross sections. Therefore, only the BUGLE-96 previous transport methodology results will be presented in this thesis.

#### **5.1 Results of Previous Transport Methods Presented in the Benchmark**

In order to obtain values for calculated equivalent fission fluxes for the various interactions listed at different locations in the PCA benchmark facility, the authors of the benchmark (Remec and Kam) followed the process explained in Chapter 2, in which the scalar flux at each experiment location, in each energy group is multiplied by the reaction rate (found in Appendix A), summed over all energy groups. That quantity was then divided by the reaction cross section averaged over the  $^{235}\text{U}$  fission spectrum and the total number of source neutrons. By following that process, the authors obtained calculated results, which they then divided by the experimentally measured reaction rates (shown in Table 2.5) to obtain calculated-to-measured (C/M) equivalent fission fluxes. <sup>[1]</sup> Remec and Kam then go on to conclude that “it is expected that the agreements of the calculations with the measurements, similar to those shown [in Table 5.1], should typically be obtained when the discrete ordinates method and [BUGLE-96] libraries are

used for the PCA benchmark analysis.”<sup>[1]</sup> While these C/M ratios provide a good comparison to determine if a transport methodology is better suited than the one prescribed by the authors, it is important to note that only the  $^{237}\text{Np}(n,f)$  interaction at A3 location fell within uncertainty of the experimentally measured data. All other locations provided calculation results which differed from the measurement by more than the uncertainty of the measurement. Results obtained from the flux synthesis method consistently under predicted the reaction rate at all experimental locations.

**Table 5.1:** Calculated-to-measured equivalent fission fluxes obtained by benchmark authors using DORT/DOTSYN flux synthesis (average C/M of  $0.92 \pm 0.03$ ).<sup>[1]</sup>

Location	$^{237}\text{Np}$ (n,f)	$^{238}\text{U}$ (n,f)	$^{27}\text{Al}$ (n, $\alpha$ )	$^{58}\text{Ni}$ (n,p)	$^{115}\text{In}$ (n,n')	$^{103}\text{Rh}$ (n,n')
A1	0.89	--	0.94	0.90	0.91	0.93
A2	--	--	0.93	0.91	0.91	--
A3	0.97	--	0.98	0.93	0.95	--
A4	0.93	0.90	0.96	0.91	0.97	0.96
A5	0.92	0.86	0.95	0.90	0.94	0.92
A6	0.89	0.84	0.95	0.94	0.95	0.91
A7	0.89	--	--	--	--	--

## 5.2 PENTRAN Computational Model of PCA Benchmark Facility

The PENTRAN code system was developed by Sjoden and Haghigat, and can be used for fully decomposed (angle, energy, spatial) parallel 3-D Cartesian multigroup forward or adjoint discrete ordinates simulations. The  $S_N$  method is a deterministic approach that discretizes the angle, energy, and physical spatial variables into a finite number of discrete angular ordinates, energy groups, and spatial grids over the entire phase space system; the PENTRAN code uses a spatial discretization scheme where coarse meshes contain fine meshes in a block-adaptive Cartesian mesh structure.<sup>[6]</sup> Thus, the use of flux synthesis was not required in order to obtain a 3-D solution for the PCA benchmark problem.

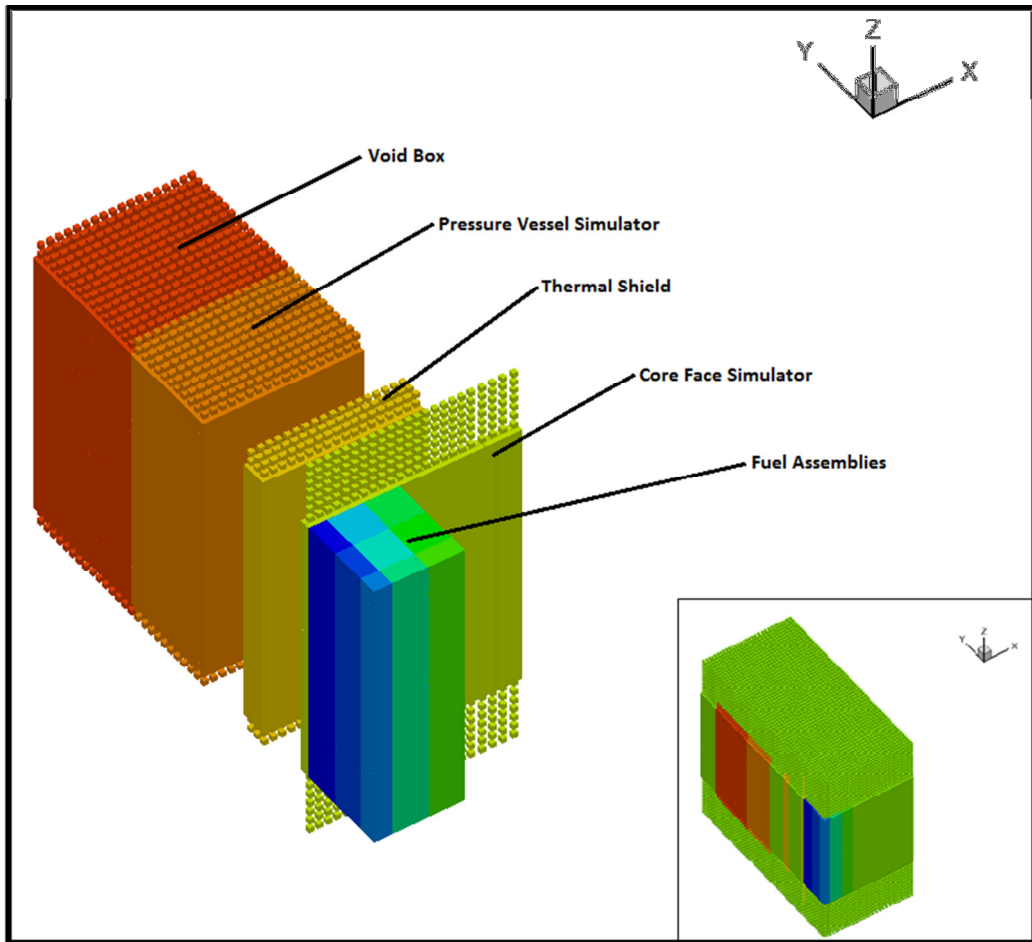
### 5.2.1 Description of Model Geometry

The model geometry was designed using a 3-D Cartesian mesh and provided an exact representation of the problem geometry with a few small changes, as described partially in Chapter 2, but included here for completeness. The void box consisted of an aluminum box of wall thickness 0.3175 cm containing air, and to simplify the number of meshes the aluminum was ignored and the void box was modeled as air only. The second simplification was the removal of 0.32 cm of water between the core face and the core face simulator (CFS) to reduce the number of meshes. The models were run at  $S_8$  quadrature (80 directions per mesh) and the DTW differencing scheme was locked in all coarse meshes. The models were also executed enabling the adaptive differencing option allowing PENTRAN to automatically select the appropriate differencing scheme in each coarse mesh basis.

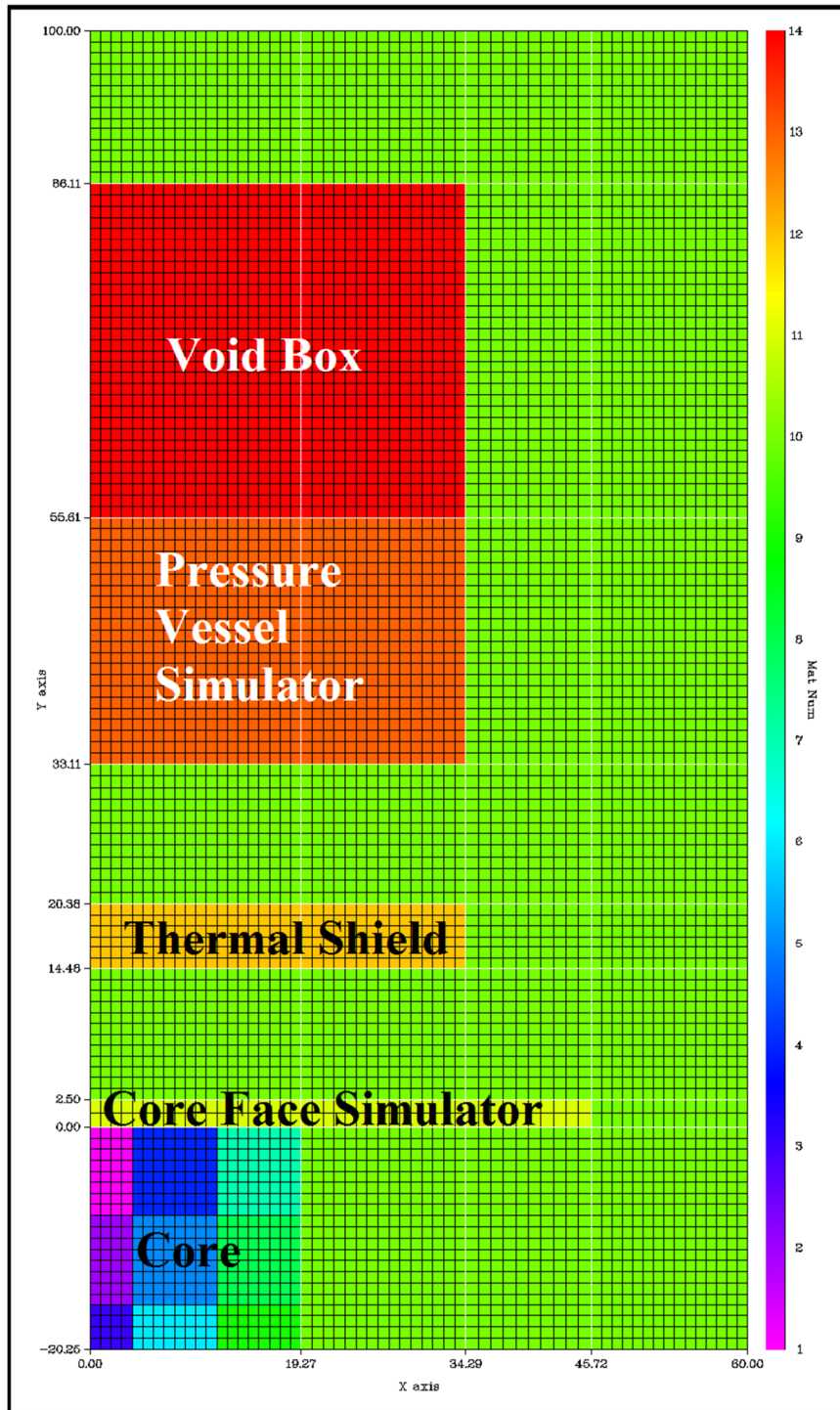
The 3-D model (Fig. 5.1) extends 25 cm above and below the fuel (in the axial direction), 100 cm from the core face in the y-direction, and 60 cm from the center of the core outward in the x-direction. All fine meshes on the same axial plane where fuel is present are 1 cm x 1 cm x 1 cm, and in the extended areas above and below the core, a 2 cm x 2 cm x 2 cm mesh is used. Specular reflective boundary conditions were applied to the  $-y$  and  $-x$  direction boundaries, while vacuum boundary conditions were applied to the other boundaries. This resulted in a total of 468,696 fine meshes in the model. Fig. 5.1, depicts the geometry, as described, presenting a large figure where the water pool material was “blanked” or peeled away so the PCA reactor core and pressure vessel simulator components could be shown with more clarity. The image on the lower right hand side of Fig. 5.1 depicts the complete geometry plot, with the water in place. Fig. 5.2 depicts the same geometry, as a two-dimensional slice through the reactor core midplane, and can be used as a reference material map for flux plots presented later in this Chapter.

The parallel decomposition allowed by the PENTRAN code system includes angular, spatial, and energy decomposition. Given that the PCA Benchmark problem

consisted of 47 energy groups, with 9 different source regions (one for each fuel assembly), 320 coarse meshes,  $S_8$  quadrature and  $P_3$  anisotropic cross section scattering order (which match the  $S_N$  and  $P_n$  orders used by the authors of the benchmark with the DORT/DOTSYN approach), a choice of a parallel decomposition of 80 processors in the spatial domain was selected based on the per processor memory of the computer and the desire for the quickest problem convergence. [20]



**Figure 5.1:** PCA benchmark geometry for PENTRAN calculations, the larger representation depicts the PCA Experiment with the water “blanked” from the plot, the smaller image (box) on the lower right shows the same model with the water included.



**Figure 5.2:** 2-D slice through the core midplane of the PCA Benchmark geometry for PENTRAN calculations.

### **5.2.2 Source Term Treatment and Cross Section Development**

A total of 9 different fixed sources were defined, one to represent each fuel assembly, with source normalization performed to match the relative source contribution from each full, half or quarter fuel assembly modeled in the quarter core as described in the PCA benchmark documentation (shown in Fig. 2.6). The only difference between the source definition process explained in Chapter 2, and the source defined for PENTRAN calculations, was that the source magnitude was set to a total of  $10^6$  neutrons per second being emitted from the quarter core. This was done to prevent numerical issues with convergence of neutron fluxes in regions far away from the source. To correct for this, when calculating equivalent fission fluxes one would now divide by  $4 \times 10^6$  instead of just 4; recalling that the division by 4 is required due to the specular reflective boundary conditions on the  $-y$  and  $-x$  axes.

Cross sections for each material component outside the reactor core, as well as for the different fuel assembly types were performed using GMIX (and in house cross section mixing code) with the weight percent and densities of each material, as described in Chapter 2, using the 47 neutron energy group BUGLE-96 cross section library.<sup>[21, 4]</sup>

### **5.3 Results of Benchmark Analysis using PENTRAN**

Following the described model methodology, two PENTRAN runs were executed and results for calculated-to-measured equivalent fission fluxes were obtained. The two runs were performed with identical geometries, convergence criteria, and cross sections. However, in the first case the DTW differencing scheme was locked for all coarse meshes in the problem, forcing PENTRAN to use the DTW scheme at all fine mesh locations. In the second case, the adaptive differencing option was utilized. DTW was set as the basis for starting and the code was allowed to upgrade to EDI if the weight of any ordinate in a coarse mesh exceeded 0.95.

### 5.3.1 Results Obtained with DTW Differencing Scheme

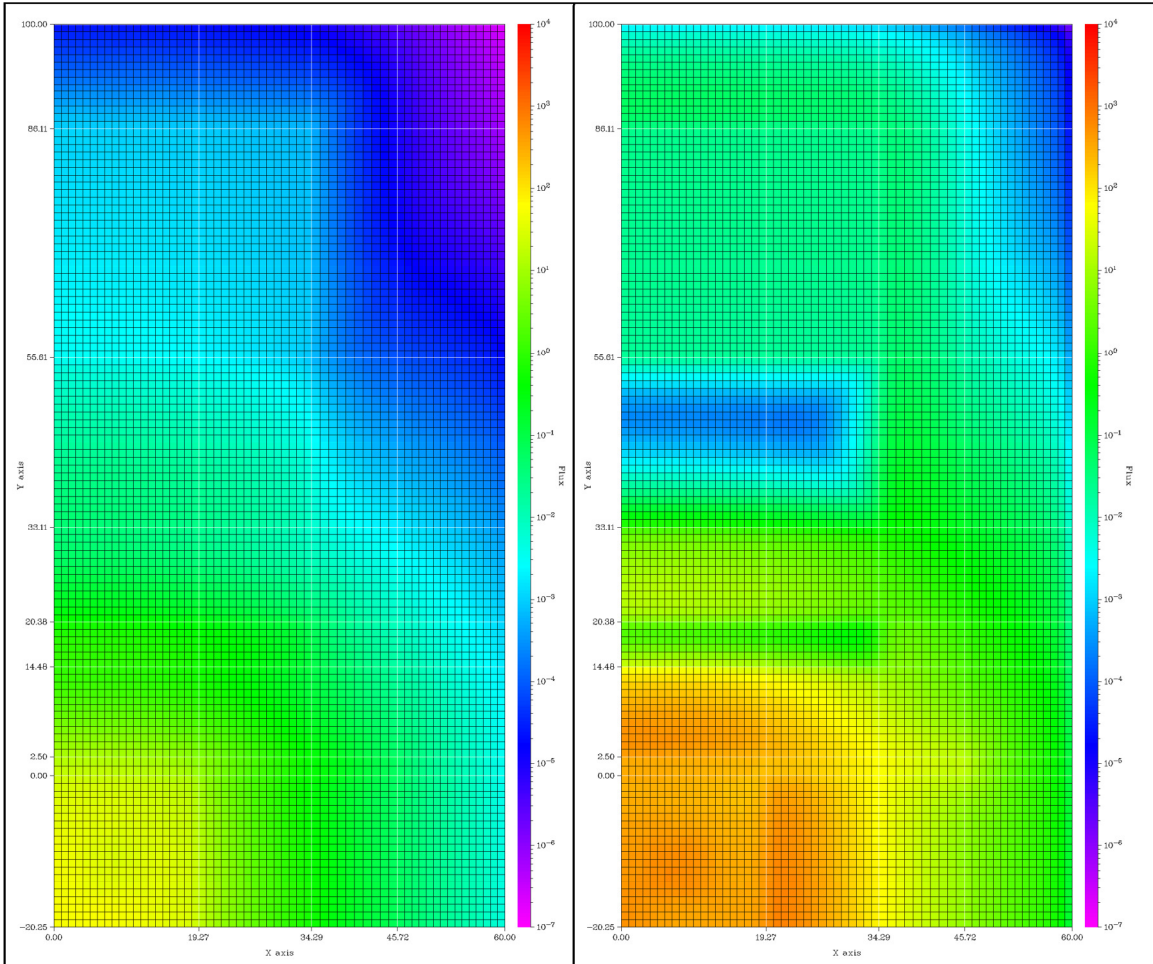
Results obtained for calculated-to-measured equivalent fission fluxes at the different measurement locations can be seen in Table 5.2. The C/M ratios are consistent with levels obtained by calculations provided in the benchmark (Table 5.1). However, there are some distinct differences between the two results; first, PENTRAN both over- and under-predicts solution whereas the previous code methodology only under-predicted the reaction rates. Secondly, PENTRAN with the DTW differencing scheme provided calculated results within the experimental uncertainty for four of the reaction rates ( $^{237}\text{Np}(n,f)$  at A3,  $^{27}\text{Al}(n,\alpha)$  at A3 and A6, and  $^{115}\text{In}(n,n')$  at A3), whereas previous methods only achieved this for one reaction at a single location.

**Table 5.2:** Calculated-to-measured (C/M) equivalent fission fluxes obtained from 3-D transport with PENTRAN and DTW differencing scheme (average C/M of  $0.92 \pm 0.05$ ).

Location	$^{237}\text{Np}(n,f)$	$^{238}\text{U}(n,f)$	$^{27}\text{Al}(n,\alpha)$	$^{58}\text{Ni}(n,p)$	$^{115}\text{In}(n,n')$	$^{103}\text{Rh}(n,n')$
A1	0.89	--	0.91	0.89	0.89	0.92
A2	--	--	0.87	0.85	0.85	--
A3	1.04	--	1.00	0.98	1.00	--
A4	0.92	0.86	0.91	0.88	0.94	0.95
A5	0.91	0.84	0.93	0.89	0.92	0.92
A6	0.90	0.86	0.99	0.97	0.96	0.93
A7	0.89	--	--	--	--	--

The scalar flux distribution calculated by PENTRAN with the DTW differencing scheme can be seen in Fig. 5.3, for 1.0026 MeV and 0.1 eV neutrons on a log scale, where Fig. 5.2 can be utilized to determine the location of core components. These plots are consistent with what one would expect the neutron plot to look like given the components present in the model. The location of the pressure vessel simulator and thermal shield are clearly defined in the 0.1 eV plot (right side of Fig. 5.3), where thermal absorption is occurring. The cumulative parallel run time on 80 processors was 10.45

hours and fluxes in all 47 groups were converged within  $10^{-3}$  at all locations, except in the lowest energy group in coarse meshes near the vacuum boundaries of the problem (away from locations of interest).



**Figure 5.3:** Flux plots of 1.0026 MeV (left) and 0.1 eV (right) through the PCA core midplane, log scale. See Fig. 5.2 for relative location of core and out of core components.

### 5.3.2 Results Obtained with Adaptive Differencing

Results obtained for calculated-to-measured equivalent fission fluxes at the different measurement locations for PENTRAN calculations using adaptive differencing can be seen in Table 5.3. The C/M ratios are consistent with levels obtained by



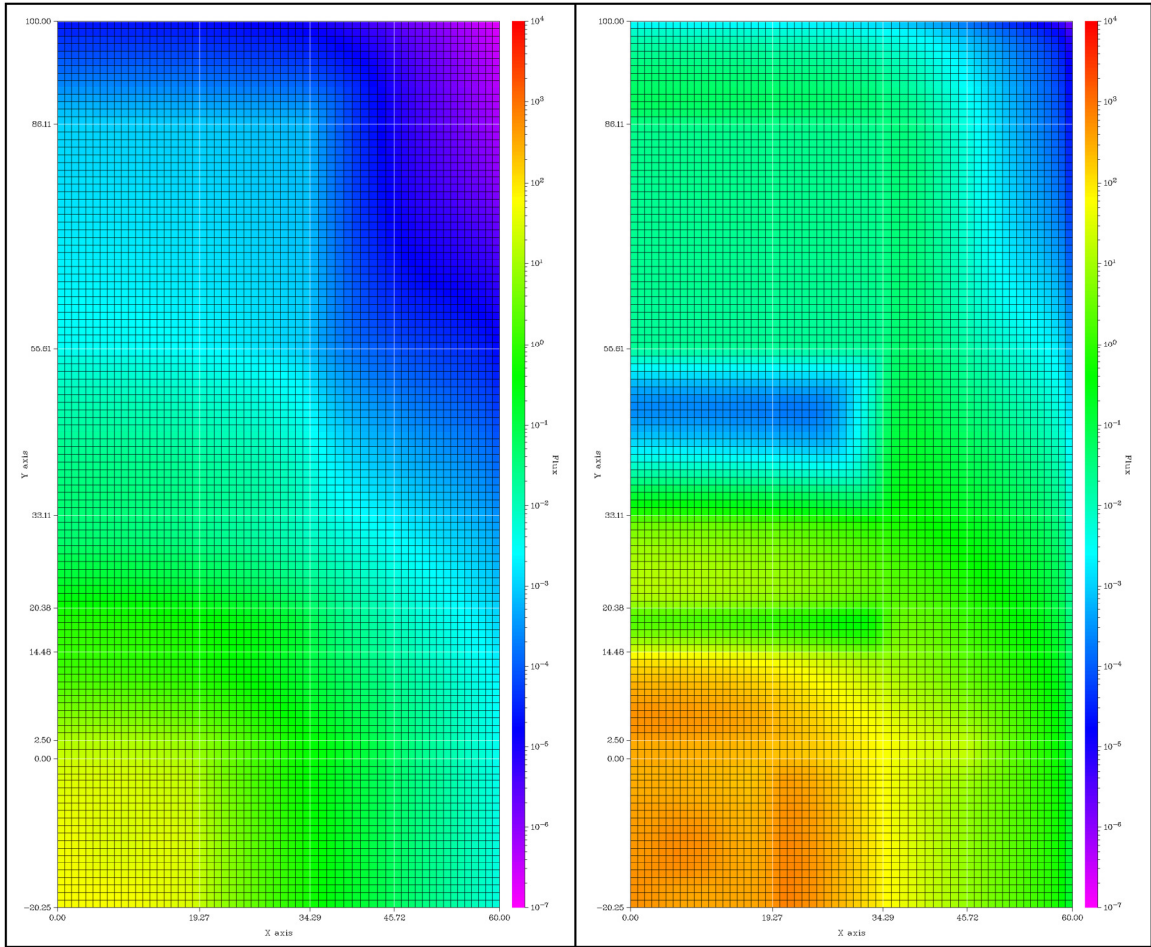
calculations provided in the benchmark (Table 5.1) and those obtained by PENTRAN with the DTW differencing scheme locked (Table 5.2). Again, with adaptive differencing PENTRAN both over- and under-predicts the solution for the scalar flux (and thus the calculated equivalent fission flux), whereas the previous code methodology only under-predicted the reaction rates. PENTRAN's adaptive differencing scheme provided calculated results within the experimental uncertainty for four reaction rates ( $^{237}\text{Np}(n,f)$  at A3,  $^{27}\text{Al}(n,\alpha)$  at A3 and A6, and  $^{115}\text{In}(n,n')$  at A3).

**Table 5.3:** C/M equivalent fission fluxes obtained from 3-D PENTRAN calculation using the adaptive differencing scheme (average C/M  $0.92 \pm 0.05$ ).

Location	$^{237}\text{Np}(n,f)$	$^{238}\text{U}(n,f)$	$^{27}\text{Al}(n,\alpha)$	$^{58}\text{Ni}(n,p)$	$^{115}\text{In}(n,n')$	$^{103}\text{Rh}(n,n')$
A1	0.89	--	0.91	0.89	0.89	0.92
A2	--	--	0.87	0.85	0.85	--
A3	1.04	--	1.01	0.98	1.00	--
A4	0.92	0.86	0.92	0.88	0.94	0.96
A5	0.91	0.84	0.94	0.89	0.92	0.92
A6	0.90	0.86	1.00	0.97	0.96	0.93
A7	0.90	--	--	--	--	--

The scalar flux distribution calculated by PENTRAN with the adaptive differencing scheme can be seen in Fig. 5.4, for 1.0026 MeV and 0.1 eV neutrons on a log scale, where Fig. 5.2 can again be utilized to determine the location of core components. These plots are consistent with flux plots obtained with the DTW differencing scheme, but appear to show smoother transitions in regions with higher flux gradients. Thermal peaking coming out of the void box and into the water appears to be better defined. The cumulative parallel run time on 80 processors was 26.33 hours, which represented 2.52 times more computing time than the DTW solution. The increase in computation time can be directly related to the iterative nature of the EDI scheme, which requires an extra iterative loop over the DTW scheme. Fluxes were converged to  $10^{-3}$  in

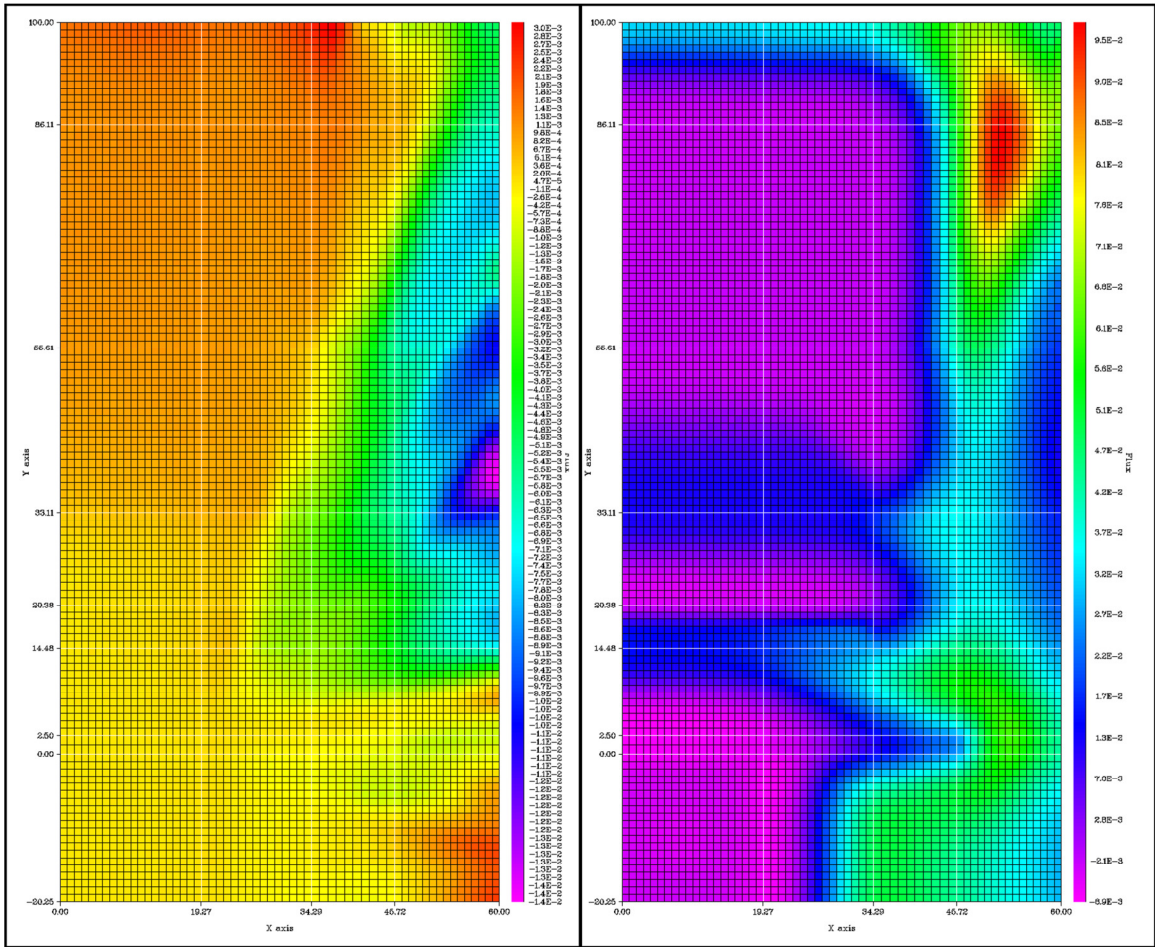
most groups; however the high energy groups (above 7 MeV) beyond the void box and the thermal groups near vacuum boundaries were converged to  $5 \times 10^{-3}$ . Since the iterative errors in these coarse meshes were all within  $5 \times 10^{-3}$ , and these regions did not contain locations where calculations and measurements were being compared, the model was considered converged overall.



**Figure 5.4:** PENTRAN flux plots using adaptive differencing scheme for 1.0026 MeV (left) and 0.1 eV (right) energy group through the PCA core midplane on log scale. See Fig. 5.2 for relative location of core and out of core components.

Fig. 5.5 depicts the difference between the scalar flux obtained by PENTRAN using the DTW and adaptive differencing schemes (i.e. DTW minus adaptive). The

1.0026 MeV plot (left) ranged from -1.4% to 0.3% difference, while the 0.1 eV plot (right) ranged from -0.7% to 9.5%. When looking at the figure it becomes clear that areas of higher discrepancy between DTW and adaptive differencing schemes are located in regions on the vacuum boundaries of the problem, or where the thermal flux undergoes larger flux gradients.



**Figure 5.5:** Plot of difference in scalar flux obtained with DTW and adaptive differencing schemes (for 1.0026 MeV (left) and 0.1 eV (right)). Both differencing schemes provide solutions with the same order of magnitude throughout the model.

#### 5.4 Discussion of PENTRAN Results using Benchmark Prescribed Methodology

The overall results of the PENTRAN calculations were consistent with what the benchmark authors described as expected values for validation of a transport methodology for pressure vessel fluence calculations. Therefore, one can conclude that PENTRAN has passed the benchmark. For both the DTW and adaptive differencing schemes, the average calculated-to-measured result was 0.92 with a standard deviation of 0.05, which is the same average C/M for the calculations performed by the authors. However, the standard deviation of the author's calculations was only 0.03. The difference in standard deviation can be directly related to PENTRAN both over- and under-predicting the C/M values, while the DORT/DOTSYN approach only provided solutions which under-predicted the equivalent fission flux. Thus, more of the C/M ratios were closer to the average, which was below a C/M of 1.00.

When comparing the results obtained by PENTRAN from the DTW case and adaptive differencing cases, the adaptive differencing scheme seems to perform in a comparable manner; providing results slightly closer to measured values at 3 locations. C/M ratios for the  $^{238}\text{U}(n,f)$  reaction, while consistent with calculated results provided in the benchmark, were significantly lower than the rest of the C/M ratios on the whole. This can be attributed to a combination of two factors, first the location of the measurements were at  $\frac{1}{4}$ ,  $\frac{1}{2}$ , and  $\frac{3}{4}$  pressure vessel thickness and second, the  $^{238}\text{U}(n,f)$  reaction rate has a probability of occurrence in all 47 energy groups, while the other interactions (with the exception of  $^{237}\text{Np}(n,f)$ ) only occur at higher energies. Given the material specification of the pressure vessel, coupled with the high flux gradient of neutrons entering the pressure vessel, hyper accurate results may be difficult to obtain in that region as the scattering between the lowest 17 energy groups now becomes important. This was illustrated by the  $^{27}\text{Al}(n,\alpha)$  reaction, which provided relatively accurate C/M results through the pressure vessel, but the reaction only occurs in the

highest 7 energy groups (above 4.9659 MeV) and the fast flux in the pressure vessel was not subject to the same gradient observed in lower energy groups.

Though the overall results, per benchmark specifications passed the benchmark, given the larger than desired discrepancy from an actual calculation, sources of error in the benchmark model development process were explored in an effort to justify and mitigate any errors arising from model development, cross section mixing, etc. These proposed improvements, which include a flux and volume weighting homogenization of in core components, as well as a more refined fixed source term for the reactor core will be explained in detail in chapter 6.

## **CHAPTER 6**

### **IMPROVEMENTS TO THE PCA BENCHMARK**

In an effort to obtain more accurate computational results in comparison to the measured experimental data, the process for calculation was further investigated, and two main areas were targeted for potential improvement could allow for increased accuracy in computational results. As originally implemented, the PCA benchmark suggested a volume fraction approach to weighting cross sections in the reactor core, which ignored the control rod when obtaining cross sections. This process will be replaced by a flux and volume weighting, as an improvement which includes the control rod being partially inserted into the reactor core. Secondly, the original source term, which was generated using fission chamber measurements coupled with 3-D flux synthesis (where needed), will now be replaced by a quarter core power distribution obtained from a 3-D discrete ordinate transport solution for a 47 group eigenvalue calculation. This chapter explains this process in detail and provides the updated source term and cross sections for use in the improved PCA benchmark.

#### **6.1 Flux and Volume Weighted Homogenized Cross Sections for PCA Reactor**

Cross section weighting is an important part of the homogenization process and was identified as a potential source of error in the original model. This was due to the assumption with volume weighting a cross section, which does not account for spectral effects or larger neutron populations in certain materials before they are homogenized. In the case of the PCA core, where uranium, aluminum and water are present in the fuel assemblies, this approach is not ideal. By adding flux weighting, now the effects of the flux spectra on the individual materials can be accounted for in the overall homogenized cross section. The PCA reactor core contained a standard fuel assembly, ORR fuel assembly and a control rod fuel assembly. As originally implemented, the cross section

development neglected to account for the presence of the control rod inserted, as such a control rod out and control rod in fuel assembly will be homogenized as an improvement in order to capture the effects of the control rod on the neutron population in the core.

To perform the flux weighted homogenization, the in house computer code HMIX was utilized. HMIX allows for the user to homogenize selected materials in a heterogeneous transport model into a single material, following the process in Eq. 6.1. [22]

$$\begin{aligned} \Sigma_{hom,g} \\ = \frac{\Sigma_{fuel,g}V_{fuel}\bar{\phi}_{fuel,g} + \Sigma_{clad,g}V_{clad}\bar{\phi}_{clad,g} + \Sigma_{mod,g}V_{mod}\bar{\phi}_{mod,g}}{V_{fuel}\bar{\phi}_{fuel,g} + V_{clad}\bar{\phi}_{clad,g} + V_{mod}\bar{\phi}_{mod,g}} \end{aligned} \quad (6.1)$$

where,

$\Sigma_{hom,g}$  is the homogenized macroscopic cross section in group  $g$

$\Sigma_{x,g}$  is the macroscopic cross section for material  $x$ , in group  $g$

$V_x$  is the volume of material  $x$

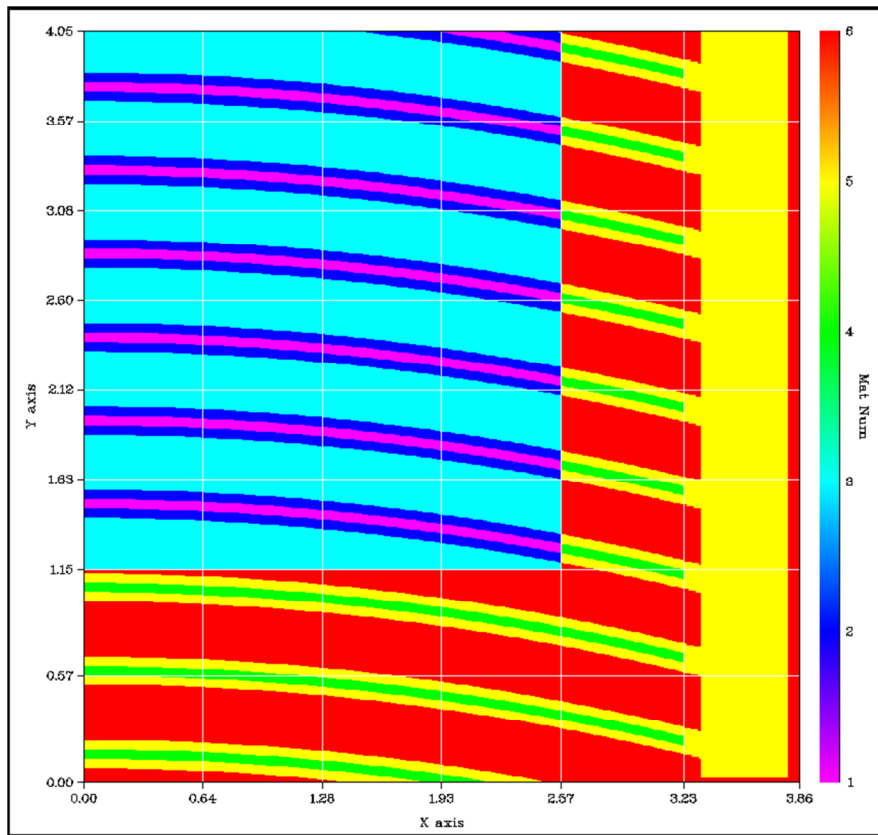
$\bar{\phi}_{x,g}$  is the average scalar flux in material  $x$ , in group  $g$ .

Eq. 6.1, is simply a generalization of the process undertaken for a typical fuel, clad, moderator homogenization. Should other heterogeneous materials be present there would simply be more terms in the numerator and denominator of Eq. 6.1. This process is applied to each cross section, whether it is absorption, fission, total, scatter, or group to group scatter; which results in a new cross section table that is representative of the material region homogenized.

### 6.1.1 Standard Fuel Assembly

To obtain homogenized cross sections for the PCA standard fuel assembly, a rigorous modeling of the curved fuel plate geometry (laid out in the benchmark documentation) was undertaken, accounting for quarter assembly symmetry, as depicted in Fig. 6.1. Due to the curved nature of the fuel plates, if one looks at the bottom of Fig. 6.1, it can be observed that the top fuel plate of another fuel assembly would be present in

the model, which accounts for the missing portion of the fuel plate at the top of the model. Cross sections were developed using GMIX with the BUGLE-96 library and material specifications shown in Table 6.1. [4, 21] Due to the presence of the large aluminum support plate which held the fuel assembly together on both sides, two homogenized regions were created from this model. They represented the “*Inner Standard Fuel Assembly*” and “*Outer Standard Fuel Assembly*.” The inner assembly consisted of the water, clad, and fuel on the inner portion of the fuel assembly (depicted by the light blue, dark blue, and purple regions of Fig. 6.1), while the outer assembly consisted of water, clad, aluminum side plate, and fuel (depicted by the red, yellow, and green regions of Fig. 6.1). Since the clad and side plated were both constructed of aluminum, only a single material was defined to represent both components.



**Figure 6.1:** PENTRAN model of PCA standard fuel assembly.

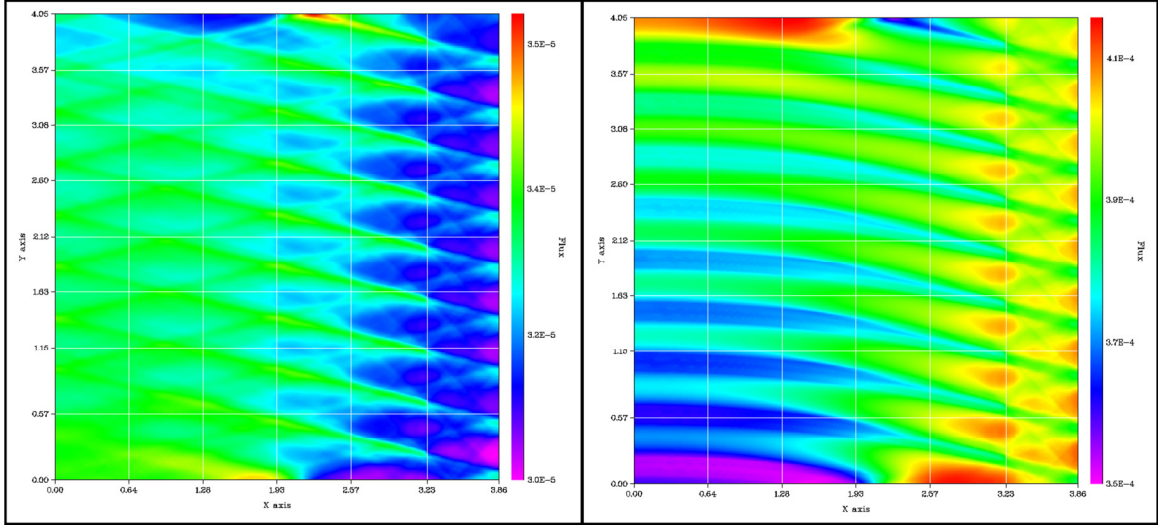


**Table 6.1:** Material specifications for the PCA Standard Fuel Assembly in PENTRAN.

Material	Isotope	Weight Percent	Density (g/cm <sup>3</sup> )
Fuel	<sup>27</sup> Al	85.0584	2.880193
	<sup>235</sup> U	13.8957	
	<sup>238</sup> U	1.0459	
Clad/Side Plate	<sup>27</sup> Al	100.0000	2.700000
Water	<sup>1</sup> H	11.1881	1.000000
	<sup>16</sup> O	88.8119	

The fuel density calculated in Table 6.1, was determined based on the procedure for UAl<sub>x</sub>-Al dispersed fuel defined by the IAEA, and assumed 7% porosity, based on volume. [23] The U mass was assumed to be dispersed evenly throughout the aluminum which was part of the fuel mass, with the density of uranium metal assumed to be 19.0 g/cm<sup>3</sup> for calculations based on the IAEA protocol. After obtaining macroscopic cross sections for the PENTRAN model, the model was run on 192 processors with S<sub>8</sub> level symmetric quadrature and P<sub>3</sub> anisotropic scattering, taking a total of 35.3 wall clock hours to complete. Due to presence of the curved fuel plates, which had a thickness of around 5 mm, the PENTRAN model was a 2-D assembly with specular reflective boundary conditions on all axes. This resulted in a total of 404,120 fine meshes present in the model in order to conserve the mass and volume of each material present in the fuel assembly. The result of the 47 group eigenvalue calculation was a  $k_{eff}$  of 1.569568 with an iterative error of  $8.37 \times 10^{-5}$ . Although, typically the iterative error is desired to be less than  $1.0 \times 10^{-5}$ , in this case as the small size of fine meshing can lead to difficulties with numerics since the code divides by numbers that are near zero when mesh size approaches  $5 \times 10^{-3}$  cm, as was the case with this model. Flux profiles for the PCA standard fuel assembly are depicted in Fig. 6.2, for the 1.0026 MeV and 0.1 eV energy groups and values for the homogenized standard fuel assembly cross sections can be found in Appendix B. Ray effect is present in the higher energy flux plot, due to the lower quadrature utilized but since the benchmark requires a 47 group calculation, going

to a higher quadrature was not feasible due to memory constraints on the supercomputer, at lower energies the ray effects were not present, as shown in Fig. 6.2.

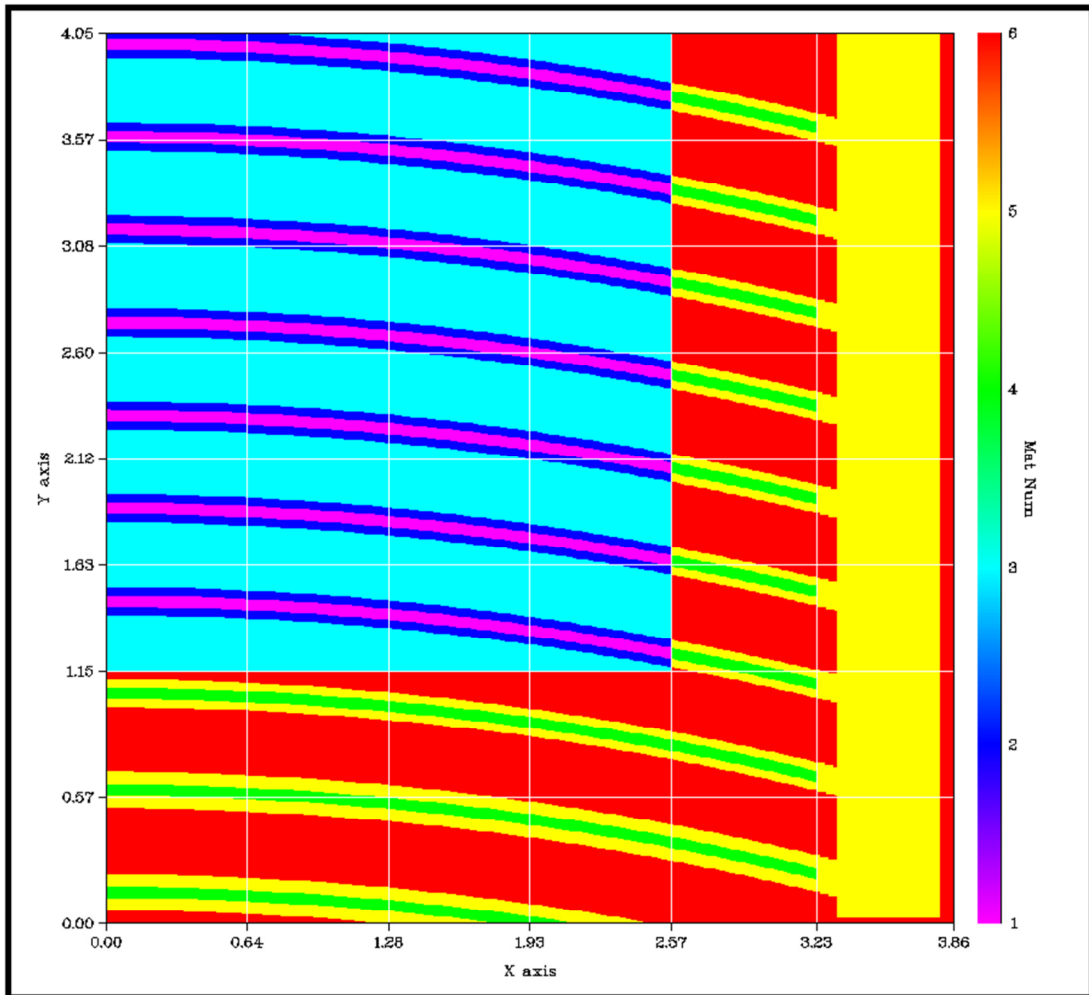


**Figure 6.2:** Flux profiles of the PCA standard fuel assembly obtained by a PENTRAN eigenvalue calculation for the 1.0026 MeV (left) and 0.1 eV (right) energy groups.

### 6.1.2 ORR Fuel Assembly

The approach undertaken to obtain flux and volume weighted homogenized cross sections for the ORR fuel assembly was identical to the process used in the standard fuel assembly. The geometry was again modeled in PENTRAN based on the parameters defined in the benchmark documentation, accounting for the difference in thickness of the end fuel plates in the ORR fuel assembly. Quarter assembly symmetry was maintained, with specular reflective boundary conditions on all sides of the 2-D assembly model. The same coarse and fine mesh structure was again utilized, with a minimum mesh size of around  $5 \times 10^{-3}$  cm in a single direction, which prompted similar numerical issues, resulting in slightly elevated iterative errors in the eigenvalue. Fig. 6.3 depicts the material map of the PENTRAN model for the ORR fuel assembly, where again an inner and outer fuel zone was homogenized. The inner fuel consisted of fuel, clad and water

(shown as purple, dark blue and light blue, respectively), while the outer fuel contained fuel, clad, aluminum side plate, and water (green, yellow, and red respectively). Material specifications for each component are shown in Table 6.2, where IAEA protocol was again applied to calculate the fuel density, assuming 7% porosity on a volume basis. The fuel density is higher than the standard fuel assembly, since the ORR assembly has 200 g of  $^{235}\text{U}$ , as opposed to the standard assembly's 140 g  $^{235}\text{U}$ , which accounts for 93% of U mass in the model.

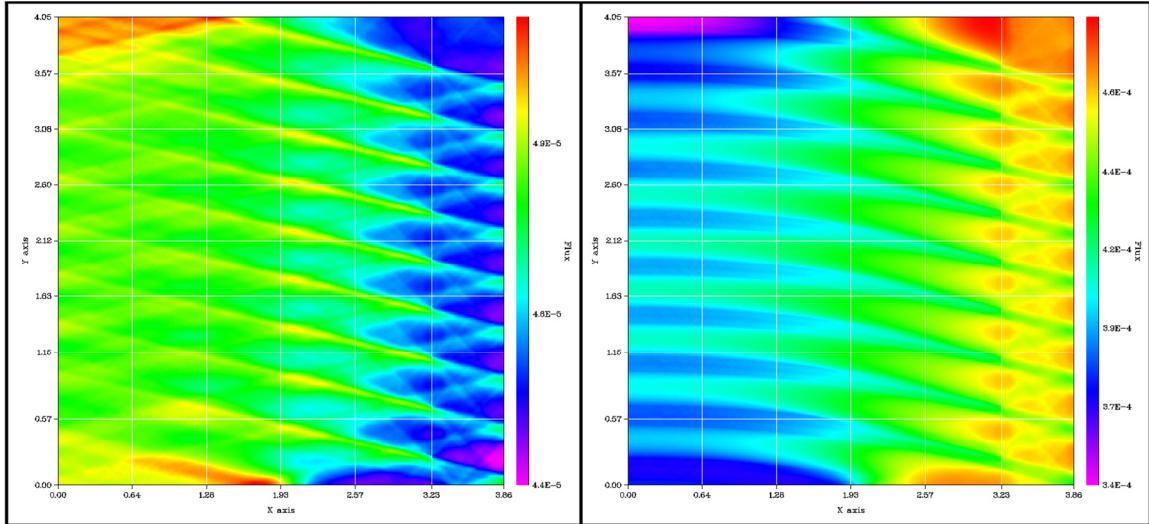


**Figure 6.3:** PENTRAN model of PCA ORR fuel assembly.

**Table 6.2:** Material specifications of the PENTRAN PCA ORR fuel assembly model.

Material	Isotope	Weight Percent	Density (g/cm <sup>3</sup> )
Fuel	<sup>27</sup> Al	80.6545	3.010660
	<sup>235</sup> U	17.9913	
	<sup>238</sup> U	1.3542	
Clad/Side Plate	<sup>27</sup> Al	100.0000	2.700000
Water	<sup>1</sup> H	11.1881	1.000000
	<sup>16</sup> O	88.8119	

The PENTRAN model was executed on 192 processors in parallel, with  $S_8$  level symmetric quadrature, and  $P_3$  anisotropic scattering. There were a total of 404,120 fine meshes present in the 2-D slice of the ORR assembly, which resulted in a cumulative run time of 39.28 wall clock hours. The resulting  $k_{eff}$  was 1.675106 with an iterative error of  $8.52 \times 10^{-5}$ . The eigenvalue is higher than the standard assembly; which is as expected due to the increased amount of high enriched uranium present in the fuel plates. Flux profiles for the 1.0026 MeV and 0.1 eV energy groups are shown in Fig. 6.4, below. The increased rate of thermal absorption in the fuel is more drastic than the standard fuel assembly, and the population of fast neutrons is flatter across the center of the fuel assembly as opposed to the standard assembly (shown in Fig. 6.2). The resulting homogenized cross sections for the inner and outer ORR fuel assembly can be found in Appendix B.



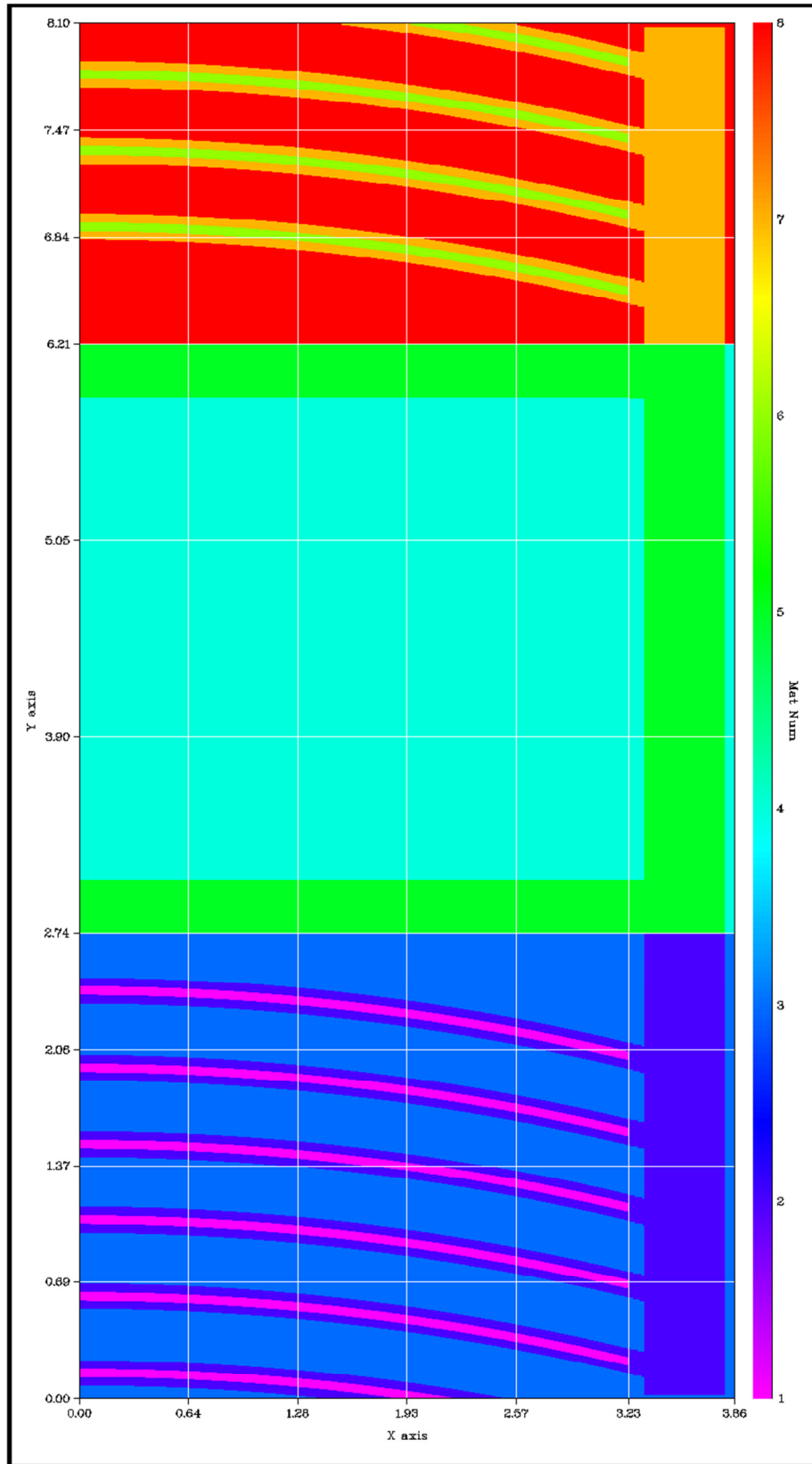
**Figure 6.4:** Flux profiles of the PCA ORR fuel assembly obtained by a PENTRAN eigenvalue calculation for the 1.0026 MeV (left) and 0.1 eV (right) energy groups.

### 6.1.3 Control Rod Out Fuel Assembly

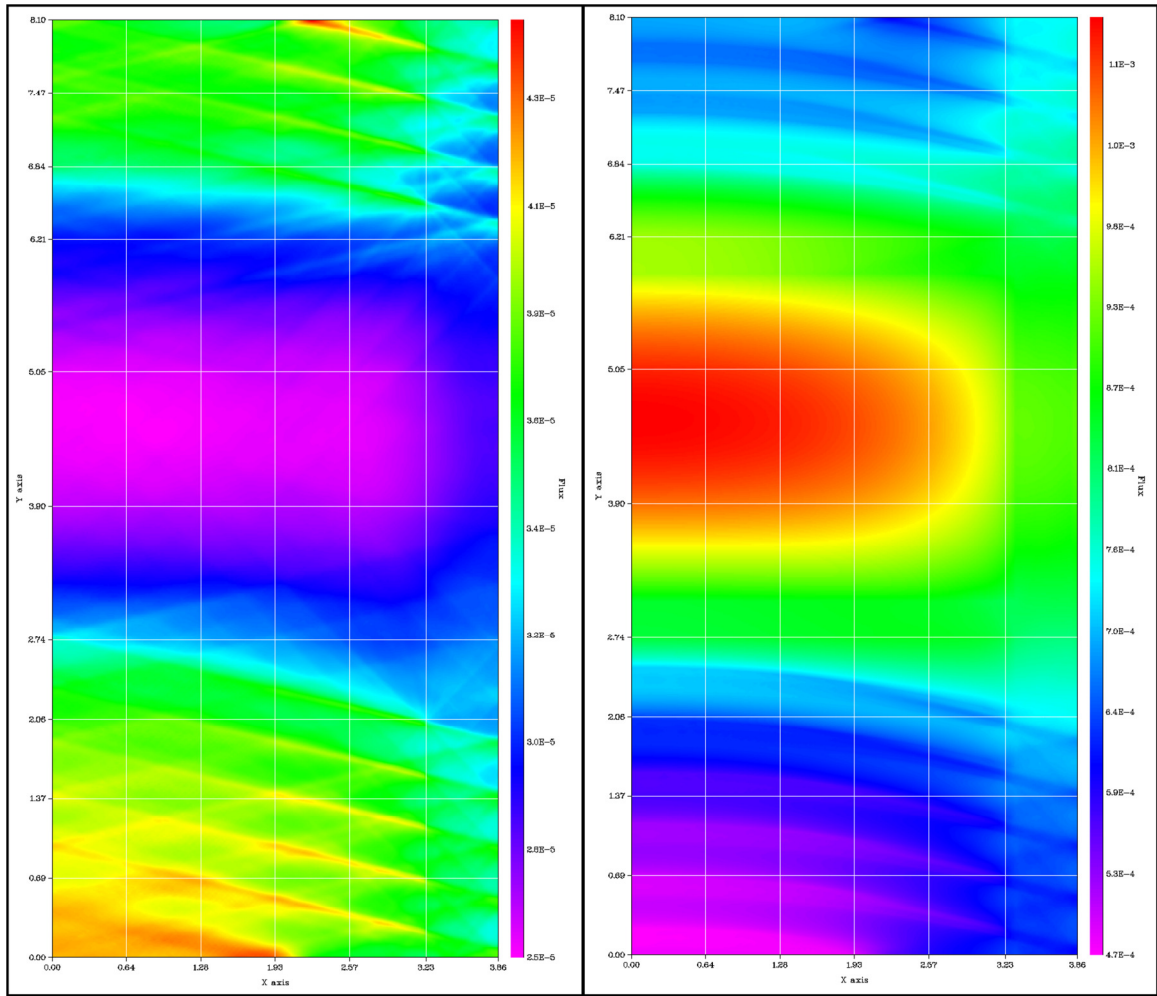
The geometry of the fuel assembly containing the control rod was well defined by a technical sketch (see Fig. 2.5) in the benchmark documentation. The control rod assembly was essentially a PCA standard fuel assembly with 9 of the center plates removed, leaving a total of 5 fuel plates below and 4 fuel plates above the control rod. Aluminum guide bars were placed across the assembly to provide additional support and defined channel for the control rod to be inserted into. The heterogeneous PENTRAN model (Fig. 6.5) was divided into 3 regions for cross section homogenization; lower fuel, control rod guide, and upper fuel. The lower fuel consisted of the bottom 5 fuel plates, clad, aluminum side plate, and top of the previous fuel assembly (denoted by the purple, dark blue and blue regions of Fig. 6.5). The control rod guide consisted of the aluminum side plates, aluminum guide/support plates, and water backfill for where the control rod would be inserted (green and light blue in Fig. 6.5). The upper fuel contained the top 4 fuel plates in the assembly, their cladding, aluminum side plate and water moderator (depicted by the yellow, orange and red areas of Fig. 6.5). Material compositions of the

components were identical to the definitions for the PCA standard fuel assembly listed in Table 6.1, as this geometry is simply an adaptation of that assembly type. Half assembly symmetry was maintained and specular reflective boundary conditions were applied on all sides of this 2-D assembly model.

The PENTRAN model contained 501,765 fine meshes and was run with  $S_8$  quadrature and  $P_3$  anisotropic scattering, taking a total of 30.10 wall clock hours on 120 processors in parallel to execute. Very small fine mesh size of  $5 \times 10^{-3}$  cm, again led to difficulties with convergence since the code was dividing by numbers approaching zero. A  $k_{eff}$  of 1.150994 was calculated with an iterative error of  $1.45 \times 10^{-5}$ . The eigenvalue was lower than the standard fuel assembly, which was as expected since this assembly contained half of the fuel of a standard assembly. Scalar flux profiles for the 1.0026 MeV and 0.1 eV energy groups are shown in Fig. 6.6. Ray effect is again noted in the higher energy groups, but due to the high memory demand of running 47 energy groups an increase in quadrature was not feasible from the computational standpoint. However, flux profiles look excellent for the more thermal groups, where the thermal peaking in the water backfill and absorption in the fuel are apparent in Fig. 6.6. Homogenized cross sections for the upper and lower fuel regions and the control rod guide region can be found in Appendix B for the control rod out fuel assembly model.



**Figure 6.5:** PENTRAN model of PCA control rod out fuel assembly.



**Figure 6.6:** Flux profiles of the PCA control rod out fuel assembly from a PENTRAN eigenvalue calculation for the 1.0026 MeV (left) and 0.1 eV (right) energy groups.

#### 6.1.4 Control Rod In Fuel Assembly

The geometry for the control rod in fuel assembly (Fig. 6.7) was identical to the control rod out assembly, however this time the control rod was included in the control rod guide region. The technical specifications of the control rod (geometry, material composition, etc.) were not included as part of the benchmark documentation, however design drawings of the actual PCA reactor control rods were obtained after corresponding with the benchmark's original author, and the geometry was modeled appropriately in Fig. 6.7. <sup>[7]</sup> The small circle of green in Fig. 6.7 contains a lead weight, surrounded by



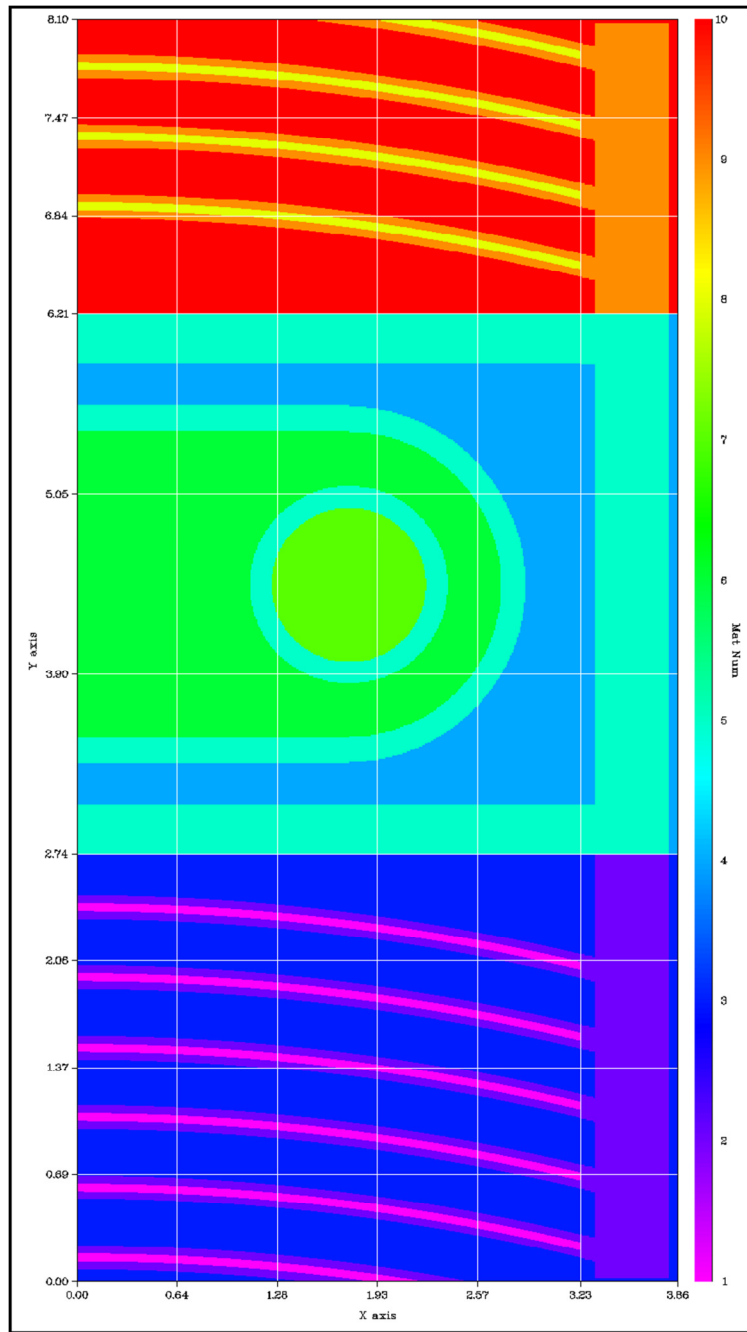
aluminum cladding (light blue in Fig. 6.7), and the absorber was B<sub>4</sub>C (light green in Fig. 6.7) which was encased in aluminum. Isotopic composition and density for these components can be found in Table 6.3, while all other components (fuel, cladding, water, aluminum support plate) are identical to the control rod out assembly which used the cross sections for the standard PCA fuel assembly. The control rod was again homogenized into upper and lower control rod in fuel, and a central control rod in region which contained the control rod (aluminum clad, B<sub>4</sub>C, lead), the surrounding water, the control rod guide structure, and the aluminum support plate. Half assembly symmetry was utilized in this 2-D control rod in fuel assembly, with specular reflective boundary conditions on all sides.

**Table 6.3:** Material specifications of the PENTRAN PCA control rod.

Material	Isotope	Weight Percent	Density (g/cm <sup>3</sup> )
B <sub>4</sub> C	<sup>10</sup> B	14.3802	1.60
	<sup>11</sup> B	57.8823	
	<sup>12</sup> C	27.7375	
Lead	<sup>206</sup> Pb	24.1000	11.34
	<sup>207</sup> Pb	22.1000	
	<sup>208</sup> Pb	53.8000	

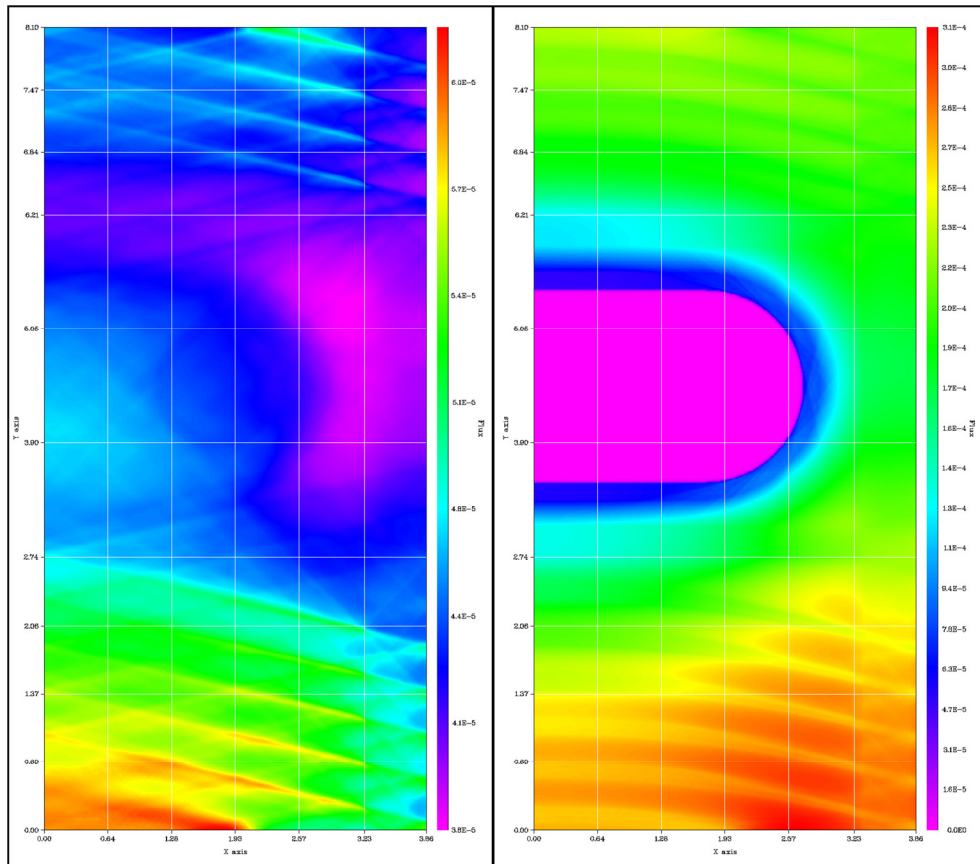
The fine mesh structure of the PENTRAN model was identical to that of the control rod out model, resulting in 501,765 fine meshes, S<sub>8</sub> quadrature, and P<sub>3</sub> anisotropic scattering cross sections. The model was run on 120 processors in parallel, for a total wall clock runtime of 39.08 hours, which was longer than the control rod out case, but as expected since the presence of the control rod causes more drastic flux gradients which require additional computational time to resolve in some energy groups. Since the same fine mesh structure was utilized, numerics were also an issue due to mesh size (5x10<sup>-3</sup> cm). Nevertheless, the  $k_{eff}$  was calculated to be 0.436709 with an iterative error of 2.20x10<sup>-5</sup>. The eigenvalue is substantially subcritical, which is as expected with the presence of the control rod inserted into the assembly. With the development of the

control rod in and out cross sections, the presence of the control rod axially can be accounted for by inputting the control rod in cross sections up to the point where the rod was inserted, and then using the control rod out cross sections for the rest of the fuel assembly when modeling the quarter core of the PCA reactor.



**Figure 6.7:** PENTRAN model of PCA control rod in fuel assembly.

Scalar flux profiles for the 1.0026 MeV and 0.1 eV energy groups can be found in Fig. 6.8. Ray effect is prominent in the 1.0026 MeV plot, while thermal absorption in the control rod is visibly observed, as well as an overall depression of the thermal flux (compared to the control rod out assembly) in the 0.10 eV plot. Again, due to limitations on computer processor availability at the time of this simulation, computer memory was constrained to 2 GB per core. Coupled with the 47 energy group requirement, increasing quadrature to reduce ray effect was not feasible, however the lower energy neutron groups showed little to no ray effect in plots of the scalar flux. Homogenized cross sections for the upper and lower fuel regions and the control rod region can be found in Appendix B for the control rod in fuel assembly.



**Figure 6.8:** Flux profiles of the PCA control rod in fuel assembly from a PENTRAN eigenvalue calculation for the 1.0026 MeV (left) and 0.1 eV (right) energy groups.

## 6.2 Development of Updated Source Term for PCA Reactor Core

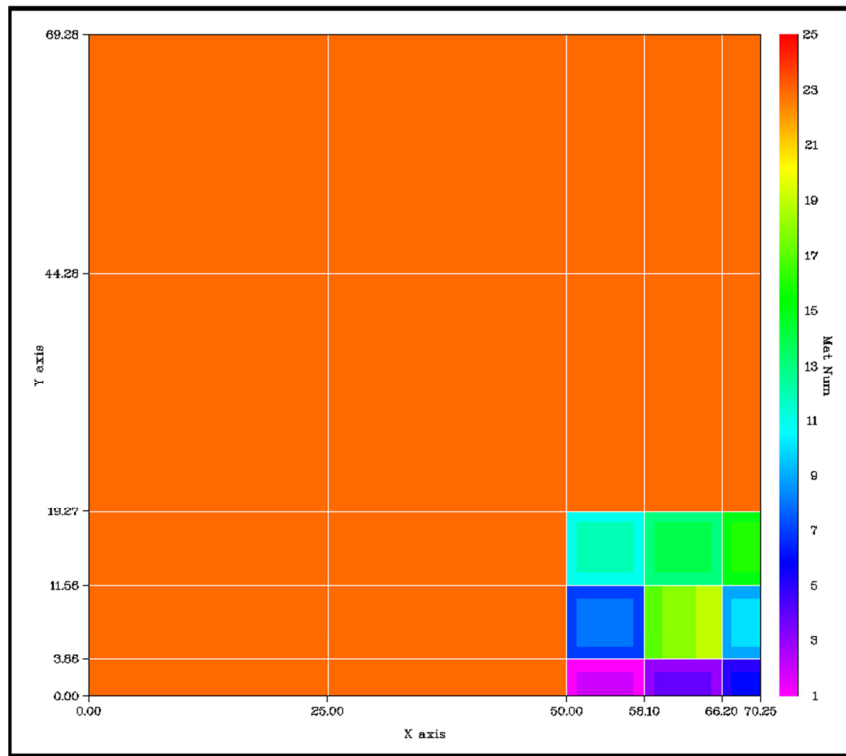
The accuracy of the fixed source term defined in the benchmark to represent the PCA reactor core was another potential source of error in the calculated-to-measured, since originally the power profile was characterized by a combination of fission chamber measurements and flux synthesis calculations using DORT/DOTSYN. In an effort to correct for errors based on flux synthesis calculations and the omission of the control rod in the reactor core, a new source term was developed using a 3-D  $S_N$  eigenvalue calculation with PENTRAN to obtain an accurate power profile from a true transport solution.

### 6.2.1 Source Term Development Methodology

In order to obtain a more accurate source term, the PCA reactor core was modeled, in a pool of water without the pressure vessel simulator components. The homogenized cross sections developed for the standard, ORR, control rod in, and control rod out fuel assemblies were used to assemble a quarter core model, where the control rod was inserted to the appropriate level as defined in the benchmark documentation. A 47 group eigenvalue simulation was performed and the relative power contribution from each portion of each fuel assembly was calculated, using the in house code POWERPACK. <sup>[24]</sup> This solution for the relative power in each section of each fuel assembly (2 sections per assembly for the standard and ORR assemblies, 6 sections for the control rod assembly) was then used as the relative source magnitude in the updated source term, while the source spectrum was set to be the  $^{235}\text{U}$  fission spectrum. Since the fuel in the reactor is  $^{235}\text{U}$ , the power profile should mimic the fission spectrum for  $^{235}\text{U}$  and while the power on a group dependent basis is available for each region in POWERPACK's output, it was decided to continue to use the fission spectrum as the source spectrum since the normalized power and fission spectrum values differed minimally in most places.

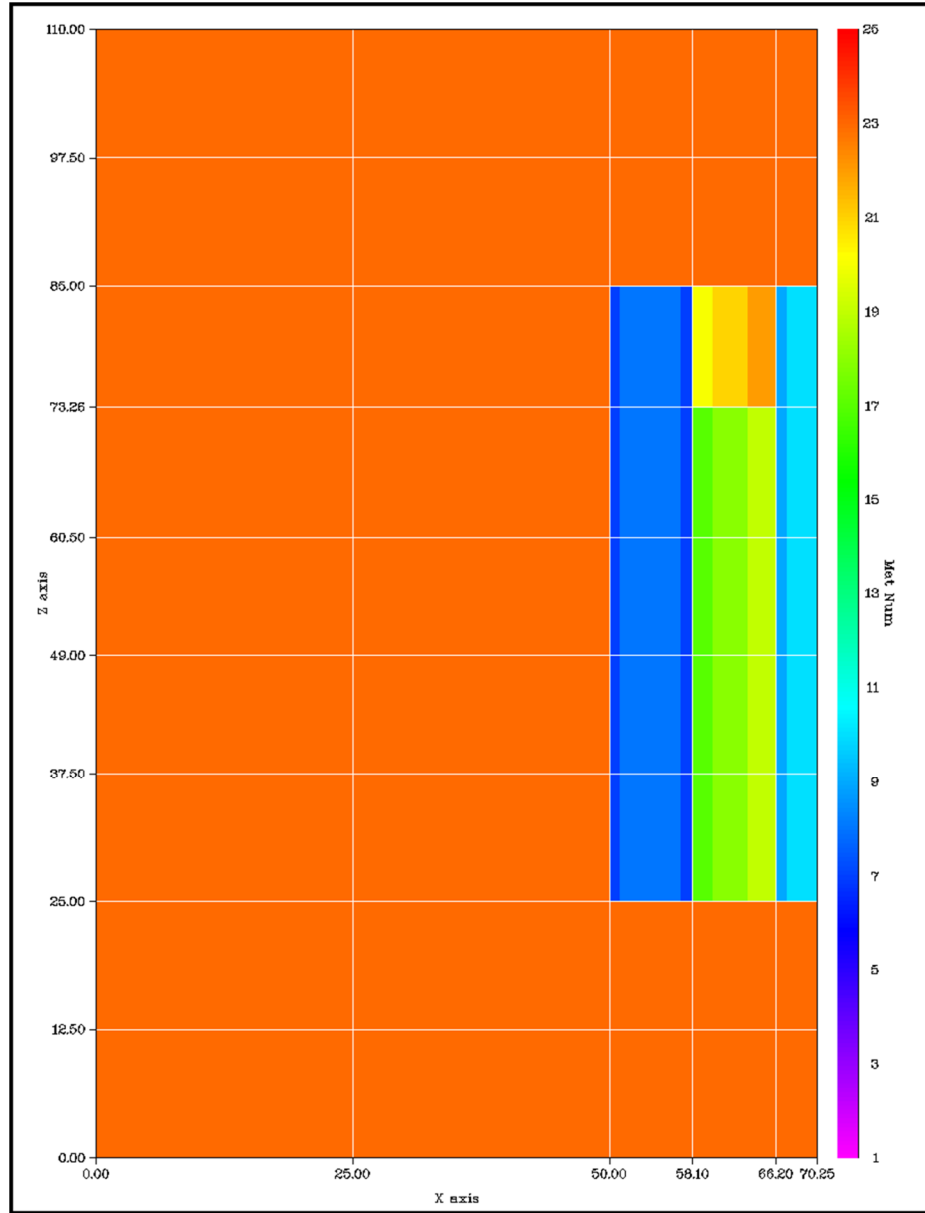
## 6.2.2 PCA Reactor Quarter Core Eigenvalue Model

PENTRAN homogenized reactor core model consisted of 345,438 fine meshes, with a  $S_8$  level symmetric quadrature, and the flux and volume weighted homogenized material cross sections developed for the in core components. The reactor was surrounded by 50 cm of water in the x- and y- directions, representing approximately 5 mean free paths of the highest energy neutron group in water, and 35 cm of water above and below the reactor core, which was consistent with the fixed source simulation. Specular reflective boundary conditions were used on  $-x$  and  $+y$  boundaries of Fig. 6.9, while vacuum boundaries were set on all other sides in order to maintain quarter core symmetry. Fig. 6.9 depicts the material map setup for the inner and outer fuel zones through the core midplane, defined for each assembly in order to calculate the relative contribution of power of each region in every assembly to the total power.



**Figure 6.9:** Horizontal cross section of PENTRAN PCA quarter core eigenvalue model, used to calculate the improved PCA core source term.

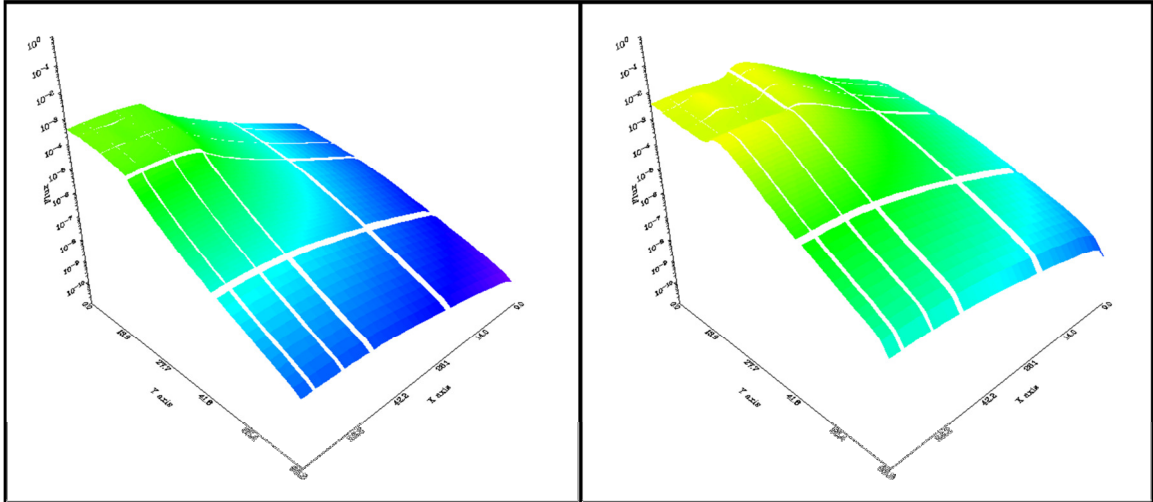
The depth of control rod insertion was taken into account by using the control rod in homogenized cross sections for the region the rod was inserted, while the remainder of the control rod assembly was composed of the control rod out homogenized cross sections, as shown in Fig. 6.10, which depicts slice through the control rod fuel assembly.



**Figure 6.10:** Vertical cross section of PENTRAN PCA quarter core eigenvalue model through the control rod fuel assembly, used to calculate the improved PCA core source term.

The use of homogenized cross sections allowed for modeling with a larger fine mesh size, which explains the relatively small number of fine meshes required to model the system, when comparing to the mesh requirement for the heterogeneous fuel assemblies. With the increased mesh size, there were no issues with the numerics, and the quarter core eigenvalue model converged to a  $k_{eff}$  of 1.041303 with an iterative error of  $3.66 \times 10^{-6}$ . To execute to completion, the model was placed on 90 processors in parallel and ran for 51.34 wall clock hours. Though it is important to note, the 90 processors in this case had 4 GB of RAM each, while the models executed of the fuel assemblies were performed on machines with only 2 GB of RAM each. The increase in RAM allowed for a decrease in the amount of message passing and overhead just to run the process (~1 GB per processor), which allowed for the shorter computation time. Had this been run using only 2 GB per core, over 200 processors would have been required and the CPU time would have increased significantly due to the increased message pass requirements.

The adaptive differencing option was used in PENTRAN, with DTW set as the basis, allowing for the code to automatically upgrade to the EDI differencing scheme where it deemed DTW to be insufficient. Iterative tolerances were defined to be  $1.0 \times 10^{-3}$  for the flux and  $1.0 \times 10^{-5}$  for the eigenvalue. Scalar flux profiles for the 1.0026 MeV and 0.1 eV energy groups are shown in Fig. 6.11, plotted on a log scale, as a horizontal cross section through the core midplane. The thermal plot clearly displays the thermal peaking of neutrons in the water just outside the core boundaries as well as in the water region of the control rod assembly (the control rod is only inserted ~12 cm, while the core midplane is 30 cm from the top of the core).

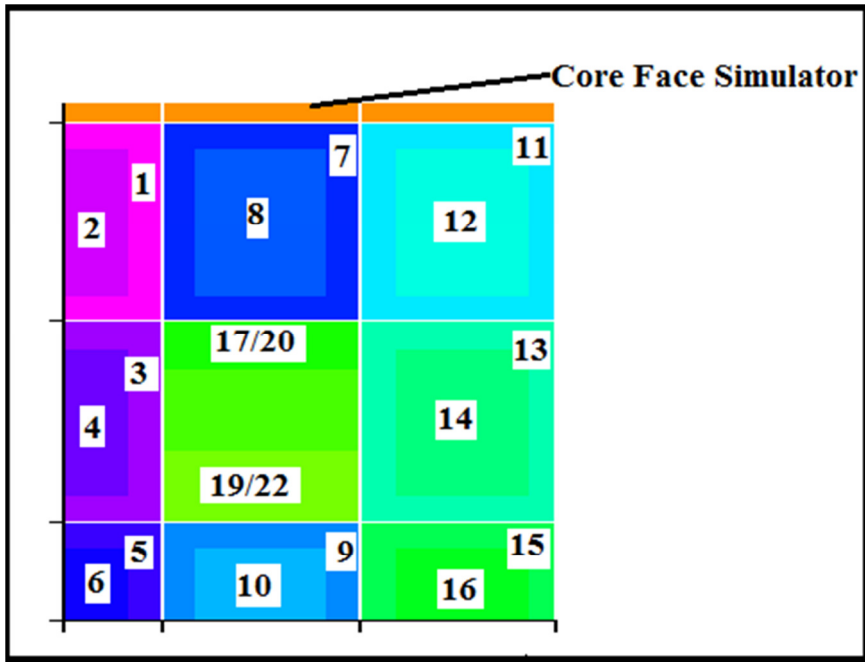


**Figure 6.11:** Flux profiles of the PCA quarter core obtained by a PENTRAN eigenvalue calculation for the 1.0026 MeV (left) and 0.1 eV (right) energy groups.

### 6.2.3 Updated PCA Core Source Term

After obtaining solutions for the scalar flux at all fine mesh locations in the PENTRAN quarter core eigenvalue model and running POWERPACK to obtain the normalized power in each region, the updated source term was obtained for each region in all core coarse meshes. <sup>[24]</sup> Following the zone numbering scheme displayed in Fig. 6.12, the relative source magnitude based on power contribution is shown in Table 6.4. The numbering scheme was setup so all odd numbers correspond to the outer fuel region of the standard or ORR fuel assemblies, while the even numbers correspond to the inner fuel region of the standard or ORR fuel assemblies (1-8 and 11-16 are standard, 9-10 are ORR). The zones labeled 17/20 and 19/22 represent the control rod top and bottom fuel, respectively (rod out/rod in). Table 6.4 presents the resulting relative power contribution for each zone number and the homogenized material used in that zone. It is important to note that the control rod in normalized source magnitudes are an order of magnitude lower, since that region only accounted for approximately 20% of the fuel assembly height.



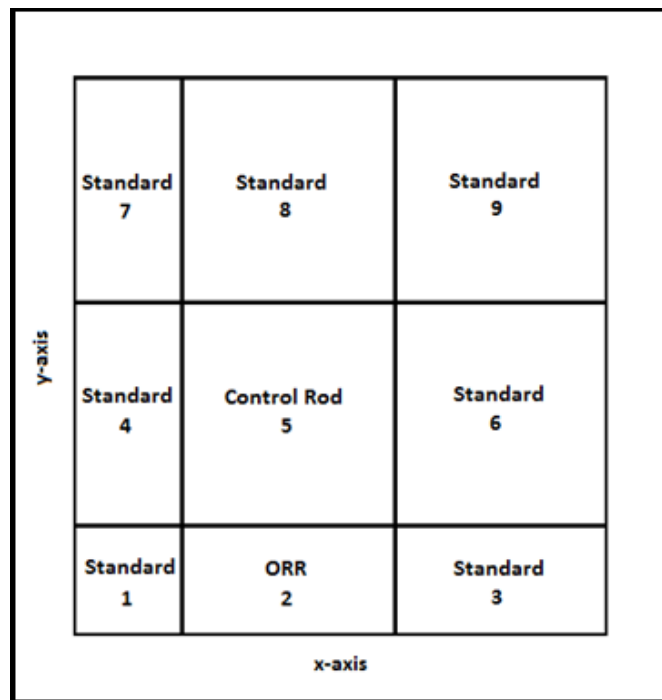


**Figure 6.12:** Updated PCA quarter core fixed source numbering scheme.

**Table 6.4:** Updated PCA core fixed source term based on 3-D PENTRAN calculation.

Zone Number	Homogenized Material	Source Magnitude (% of Source per Zone Number)
1	Standard Outer Fuel	5.048480
2	Standard Inner Fuel	3.335550
3	Standard Outer Fuel	6.490410
4	Standard Inner Fuel	4.541180
5	Standard Outer Fuel	3.351820
6	Standard Inner Fuel	2.454820
7	Standard Outer Fuel	9.265850
8	Standard Inner Fuel	6.085260
9	ORR Outer Fuel	8.265610
10	ORR Inner Fuel	5.023220
11	Standard Outer Fuel	7.308530
12	Standard Inner Fuel	4.497680
13	Standard Outer Fuel	9.679350
14	Standard Inner Fuel	6.225790
15	Standard Outer Fuel	5.123730
16	Standard Inner Fuel	3.404020
17	Control Rod Out Top Fuel	3.511510
19	Control Rod Out Bottom Fuel	5.614010
20	Control Rod In Top Fuel	0.279077
22	Control Rod In Bottom Fuel	0.494092

When normalized source magnitude calculated by PENTRAN/POWERPACK was calculated per assembly and compared with the normalized source magnitude provided in the PCA benchmark documentation, drastic differences are observed in several locations. Using Fig. 6.13 (a copy of Fig. 2.6, with a numbering scheme overlaid on the image), coupled with the results of the comparison, shown in Table 6.5, it becomes clear that the use of flux synthesis to estimate the 3-D flux provides poor performance near specular reflective boundaries or material transitions. With the percent difference in the source term exceeding 23% in 5 fuel assemblies based on full three-dimensional transport calculations, the proposition of inaccuracies in the source term provided in the benchmark appear to be correct. Thus, it was anticipated that the use of the updated source term, coupled with the improved flux and volume weighted cross sections for the core, and accounting for the control rod's partial insertion would result in calculated-to-measured equivalent fluxes which are closer to unity.



**Figure 6.13:** Numbering scheme for comparison of updated source term to original source term.

**Table 6.5:** Comparison of updated source term to original source term.

<b>Zone Number</b>	<b>Original Source Term (Flux Synthesis and Fission Chamber)</b>	<b>Updated Source Term (PENTRAN/POWERPACK)</b>	<b>Difference</b>
<b>1</b>	0.0817	0.0581	40.70%
<b>2</b>	0.1451	0.1329	9.19%
<b>3</b>	0.1152	0.0853	35.09%
<b>4</b>	0.1194	0.1103	8.23%
<b>5</b>	0.0690	0.0990	30.29%
<b>6</b>	0.1657	0.1591	4.18%
<b>7</b>	0.0637	0.0838	24.02%
<b>8</b>	0.1502	0.1535	2.16%
<b>9</b>	0.0900	0.1191	23.77%

# CHAPTER 7

## IMPROVED BENCHMARK RESULTS, DISCUSSION, AND CONCLUSIONS

Combining the improved flux and volume homogenized cross sections, accounting for the control rod insertion in the reactor core, and utilizing the improved source term developed based on a core power profile obtained with 3-D transport, this chapter depicts how these changes have impacted the overall calculated-to-measured equivalent fission fluxes for both the DTW and adaptive differencing schemes.

### 7.1 PENTRAN Results with Improvements to PCA Benchmark

The same overall PENTRAN model geometry was utilized to calculate results with the improved PCA benchmark as the original benchmark methodology. However, with the addition of the improved cross sections and the new inner and outer zone fuel, the fine meshing in the reactor core had to be increased in order to maintain balance of mass and volume for all fuel types in each assembly. Similar mesh size was maintained in the pressure vessel simulator, only the few coarse meshes near the core required additional fine meshing, in order to conserve less than a 3:1 ratio of fine mesh size between coarse meshes. Additional coarse meshes were added so each fuel assembly was contained in its own coarse mesh in order to prevent load imbalance. This resulted in a PENTRAN model with 600 coarse meshes (60 per z- level, with 10 z- levels in the model) for a total of 808,634 fine meshes, with  $S_8$  level symmetric quadrature,  $P_3$  anisotropic scattering cross sections, and 47 energy groups. The same input deck was run for both the DTW and adaptive differencing cases; the only change between the two setups was to account for the differencing scheme. The models were run on 30 processors in parallel, with 8 GB of RAM per processor. The decrease in number of processors was allowed since the amount of RAM per processor was increased from 4 GB per core to 8

GB per core, and the phase space was decomposed only in the spatial dimension, with 20 coarse meshes on each processor and load balancing turned on. Automatic load balance (a PENTRAN selectable option) allows for the highest and lowest memory demand coarse meshes to be sorted and paired on the same processor, effectively balancing the total workload so that all processors have approximately the same amount of computational work to perform.

### 7.1.1 Results Obtained with DTW Differencing Scheme

Results obtained with PENTRAN and DTW differencing achieved numerical convergence in all coarse meshes for all groups. The maximum number of iterations per group was set at 1500, but only the most thermal group required more than 350 iterations to converge. The model ran to completion on 30 parallel processors in 15.96 wall clock hours, after which the scalar flux was obtained at each measurement location and calculated-to-measured equivalent fission fluxes were obtained on a per fission neutron basis, resulting in the ratios displayed in Table 7.1. The results are much closer to unity than results previously obtained with the original benchmark methodology, with an average C/M of 0.97 and a standard deviation of 0.04. PENTRAN both over- and under-predicted the solution, with a total of 12 calculated solutions falling within the experimental uncertainty. These 12 reaction rates ( $^{237}\text{Np}(n,f)$  at A1, A4, A5, A7;  $^{27}\text{Al}(n,\alpha)$  at A1, A5;  $^{58}\text{Ni}(n,p)$  at A6;  $^{115}\text{In}(n,n')$  at A4, A6;  $^{103}\text{Rh}(n,n')$  at A4, A5, A6) are a significant improvement over the original benchmark methodology, where only 4 reaction rates achieved calculated results within measurement uncertainty, and is immensely better than the 1 reaction rate achieved by the flux synthesis approach described in the benchmark documentation.

**Table 7.1:** C/M equivalent fission fluxes obtained with PENTRAN and DTW

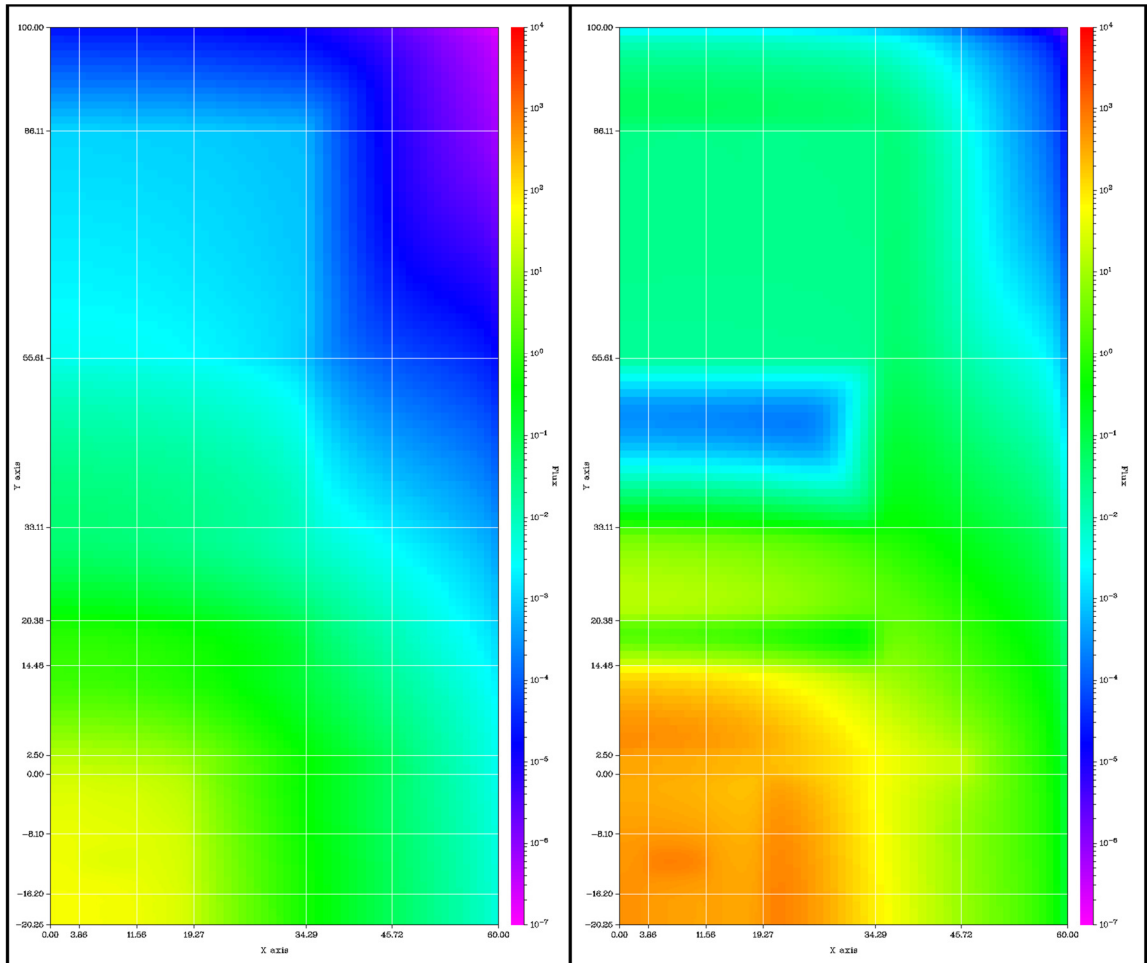
differencing, using the improved benchmark methodology (average C/M of  $0.97 \pm 0.04$ ).

Location	$^{237}\text{Np}$ (n,f)	$^{238}\text{U}$ (n,f)	$^{27}\text{Al}$ (n, $\alpha$ )	$^{58}\text{Ni}$ (n,p)	$^{115}\text{In}$ (n,n')	$^{103}\text{Rh}$ (n,n')
A1	0.95	--	0.99	0.95	0.95	0.98
A2	--	--	0.94	0.93	0.93	--
A3	1.08	--	1.05	1.02	1.05	--
A4	0.97	0.92	0.97	0.94	1.00	1.01
A5	0.96	0.89	0.98	0.94	0.98	0.98
A6	0.94	0.90	1.03	1.02	1.00	0.97
A7	0.94	--	--	--	--	--

The improved benchmark methodology with DTW differencing, provided a 5% increase in C/M accuracy (based on the average of all data points) when compared to the results obtained with PENTRAN and DTW for the original benchmark methodology. Table 7.2 depicts the increase or decrease in accuracy of C/M between the improved and original benchmark methodologies using PENTRAN and the DTW differencing scheme. Scalar flux plots of the 1.0026 MeV and 0.1 eV energy groups are shown in Fig. 7.1, on a log scale; where the plot of thermal neutron flux depicts more noticeable changes across the reactor core when compared to the original methods flux plot (Fig. 5.3) and the thermal shield and pressure vessel are clearly depicted by the change in flux in those components.

**Table 7.2:** Increase (+) or decrease (-) in accuracy of C/M results using DTW differencing between original and improved methodologies for each measurement.

Location	$^{237}\text{Np}$ (n,f)	$^{238}\text{U}$ (n,f)	$^{27}\text{Al}$ (n, $\alpha$ )	$^{58}\text{Ni}$ (n,p)	$^{115}\text{In}$ (n,n')	$^{103}\text{Rh}$ (n,n')
A1	+0.06	--	+0.08	+0.06	+0.06	+0.06
A2	--	--	+0.07	+0.08	+0.08	--
A3	-0.04	--	-0.05	+0.00	-0.05	--
A4	+0.05	+0.06	+0.06	+0.06	+0.06	+0.04
A5	+0.05	+0.05	+0.05	+0.05	+0.06	+0.06
A6	+0.04	+0.04	-0.02	+0.01	+0.04	+0.04
A7	+0.05	--	--	--	--	--



**Figure 7.1:** PENTRAN flux plots of 1.0026 MeV (left) and 0.1 eV (right) through the PCA core midplane, log scale, using the improved benchmark methodology and DTW differencing.

### 7.1.2 Results Obtained with Adaptive Differencing

The final case studied allowed PENTRAN to use the adaptive differencing scheme, starting with DTW and upgrading to EDI if need be. The maximum number of iterations per group was set at 1500. The top 6 energy groups (energies above 7.40 MeV) hit the maximum number of iterations, which was due to not being able to converge such high energy fluxes in coarse meshes which bordered vacuum boundaries. Coarse meshes containing locations for C/M evaluations were converged within the specified tolerance. The model was run on 30 processors in parallel, taking a total of 121.29 hours to complete. This time is inflated, since if the maximum number of iterations had been set to around 400, the upper energy groups would not have utilized so much computer time (due to numerical truncation in some coarse meshes bordering the vacuum boundaries) and would likely reduced the computation time to around 24 hours.

Table 7.3, displays the resulting C/M equivalent fission fluxes obtained with adaptive differencing, resulting in an average C/M of 0.98 and a standard deviation of 0.04. The adaptive differencing scheme provided consistent results with the DTW scheme for the improved benchmark methodology; however, on average it performed 1% closer to unity, with a smaller standard deviation than the DTW scheme. Suggesting the adaptive difference does provide slightly more accurate solutions in areas where DTW has a difficult time resolving the flux gradient. PENTRAN both over- and under-predicted the solution, with a total of 13 calculated solutions falling within the experimental uncertainty. These 13 reaction rates ( $^{237}\text{Np}(n,f)$  at A1, A4, A5, A7;  $^{27}\text{Al}(n,\alpha)$  at A1, A4, A5;  $^{58}\text{Ni}(n,p)$  at A6;  $^{115}\text{In}(n,n')$  at A4, A6;  $^{103}\text{Rh}(n,n')$  at A4, A5,A6) showed significant improvement over the original benchmark methodology, where only 4 reaction rates achieved calculated results within measurement uncertainty with a PENTRAN calculation, and was a massive performance increase compared to the 1 reaction rate achieved by the flux synthesis approach described in the benchmark documentation. Table 7.4 provides the increase in accuracy obtained with the improved



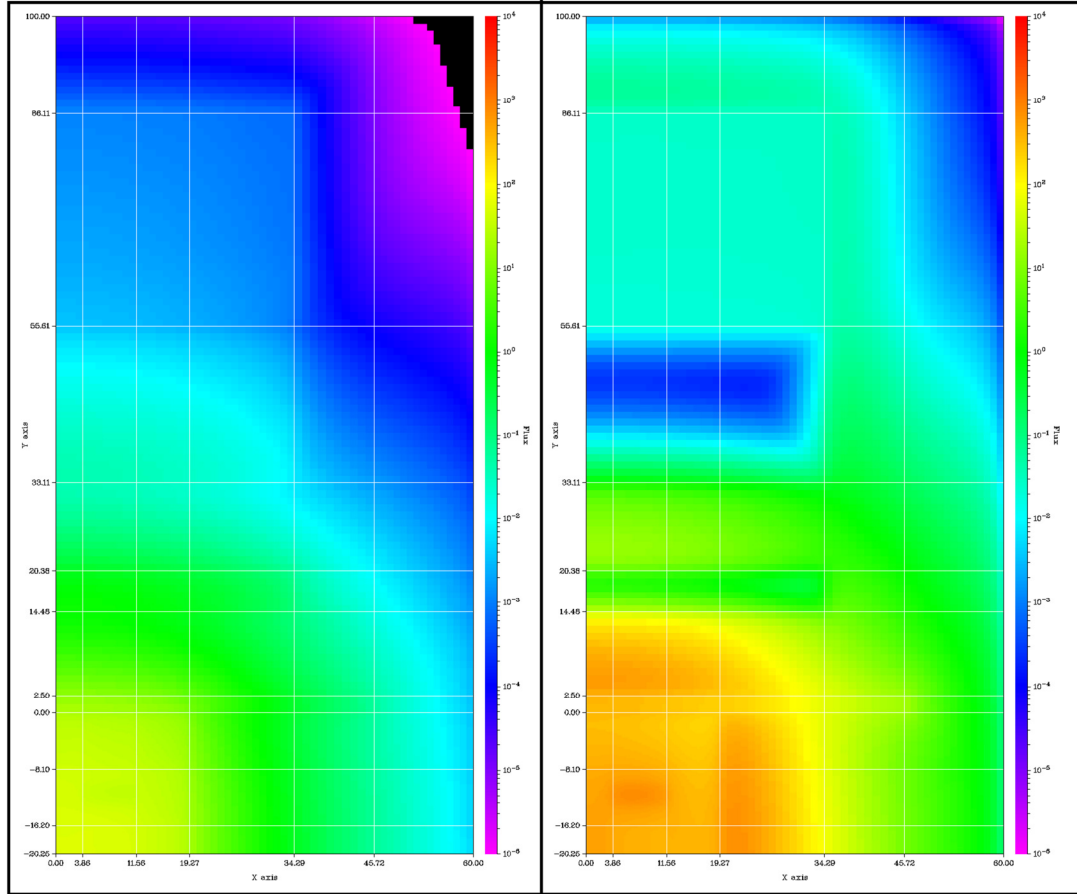
benchmark methodology, over the original benchmark methodology when using the adaptive differencing scheme. Scalar flux plots of the 1.0026 MeV and 0.1 eV energy groups are shown in Fig. 7.2, on a log scale. The 1.0026 MeV plot depicts a black region on the vacuum-vacuum corner boundary, where the flux dropped off below the log scale minimum, Fig. 7.2 was plotted on the same scale as Fig. 7.1, and this region highlights one of the main differences between the DTW and adaptive differencing solutions.

**Table 7.3:** C/M equivalent fission fluxes obtained with PENTRAN and adaptive differencing, using the improved benchmark methodology (average C/M of  $0.98 \pm 0.04$ ).

Location	$^{237}\text{Np}$ (n,f)	$^{238}\text{U}$ (n,f)	$^{27}\text{Al}$ (n, $\alpha$ )	$^{58}\text{Ni}$ (n,p)	$^{115}\text{In}$ (n,n')	$^{103}\text{Rh}$ (n,n')
A1	0.95	--	0.99	0.95	0.95	0.98
A2	--	--	0.94	0.93	0.93	--
A3	1.08	--	1.05	1.03	1.05	--
A4	0.97	0.92	0.98	0.94	1.00	1.01
A5	0.96	0.89	0.99	0.95	0.98	0.98
A6	0.94	0.90	1.04	1.02	1.01	0.98
A7	0.94	--	--	--	--	--

**Table 7.4:** Increase (+) or decrease (-) in accuracy of C/M results using adaptive differencing between original and improved methodologies for each measurement.

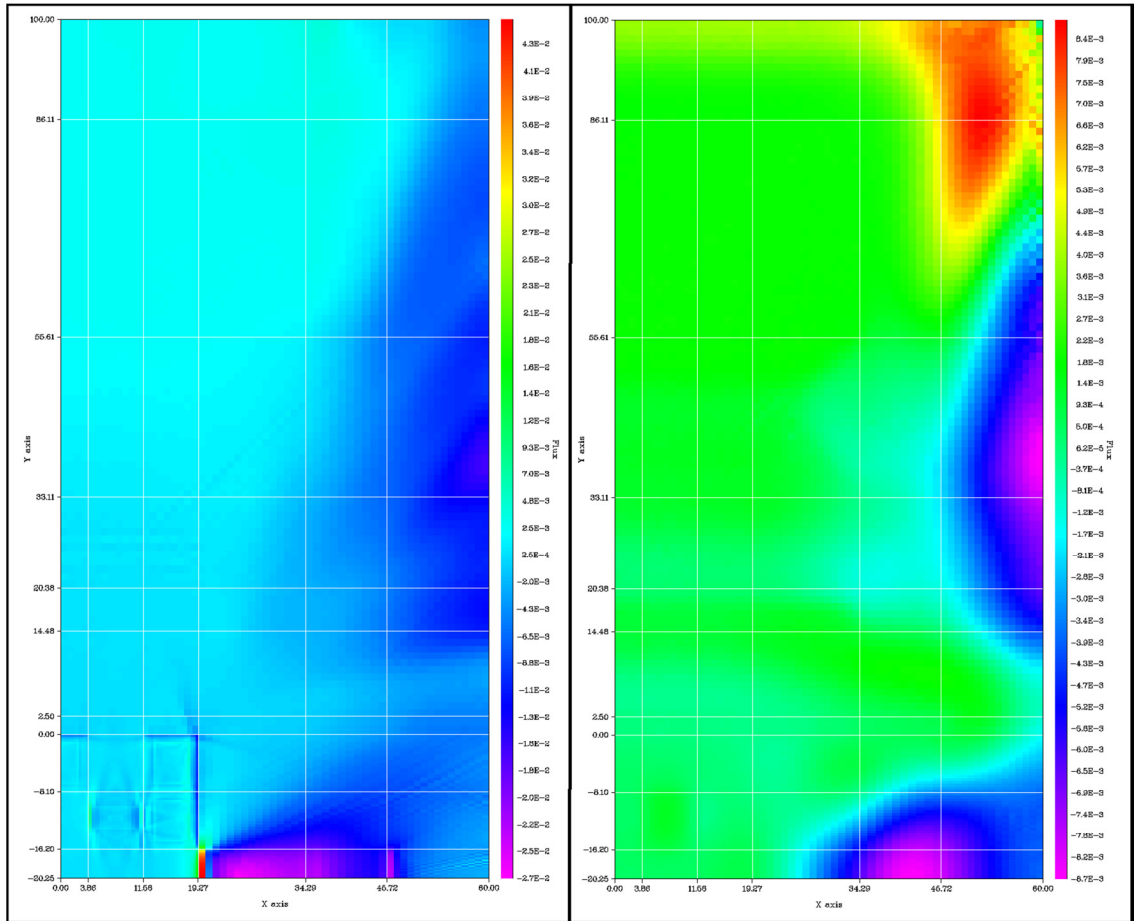
Location	$^{237}\text{Np}$ (n,f)	$^{238}\text{U}$ (n,f)	$^{27}\text{Al}$ (n, $\alpha$ )	$^{58}\text{Ni}$ (n,p)	$^{115}\text{In}$ (n,n')	$^{103}\text{Rh}$ (n,n')
A1	+0.06	--	+0.08	+0.06	+0.06	+0.06
A2	--	--	+0.07	+0.08	+0.08	--
A3	-0.04	--	-0.04	-0.01	-0.05	--
A4	+0.05	+0.06	+0.06	+0.06	+0.06	+0.03
A5	+0.05	+0.05	+0.05	+0.06	+0.06	+0.06
A6	+0.04	+0.04	-0.04	+0.01	+0.03	+0.04
A7	+0.04	--	--	--	--	--



**Figure 7.2:** PENTRAN flux plots of 1.0026 MeV (left) and 0.1 eV (right) through the PCA core midplane, log scale, using the improved benchmark methodology and adaptive differencing.

Fig. 7.3 depicts the difference between scalar flux results obtained with the DTW and adaptive differencing schemes (DTW result minus adaptive). The 1.0026 MeV plot (left) ranged from -0.27% to 0.42%, while the 0.1 eV plot (right) ranged from -0.87% to 0.84%. Similarities between Figs. 7.1 and 7.2 justify the small range of difference between the DTW and adaptive difference scalar flux solutions. However, when looking at the vacuum-vacuum boundary in the upper right hand corner of each plot, one observes a difference between the solutions obtained with the two differencing schemes. The 1.0026 MeV plot suggests a larger difference, however it is also noticeable in the 0.1 eV

plot as well. Furthermore, the boundary of the pressure vessel simulator also shows some differences in the 0.1 eV plot. These differences suggest that PENTRAN required upgrading to the EDI differencing scheme in these regions in order to provide a more accurate solution for the angular fluxes (see Appendix C for differencing scheme selected for each coarse mesh, using adaptive difference).



**Figure 7.3:** Plot of difference in scalar flux obtained with DTW and adaptive differencing schemes using the improved benchmark methodology (for 1.0026 MeV (left) and 0.1 eV (right)).

## 7.2 Discussion of Results using Improved Benchmark Methodologies

Overall the improved benchmark methodology provided a significant increase in calculated equivalent fission flux accuracy over the original benchmark methodology. The inclusion of well representative core cross sections based on a flux and volume weighting, accounting for the effect of the control rod in transport calculations, and utilizing a true 3-D transport calculated source term, provided a massive increase in accuracy (on average) for both the DTW and adaptive differencing PENTRAN solutions. The DTW calculations provided a 5% improvement of C/M equivalent fission fluxes (compared to the ideal solution of a C/M of 1.00), while maintaining the same standard deviation. Using adaptive differencing, a 6% improvement in calculation (on average) was observed (again compared to a C/M of 1.00), coupled with a reduction in the standard deviation from 0.05 originally, to 0.04 with the improved benchmark methodology.

With 12 of the DTW calculated reaction rates and 13 of the adaptive differencing calculated reaction rates being within the experimental error of the measurements with the improved benchmark methodology; PENTRAN coupled with the benchmark improvements indeed provided hyper-accurate solutions for equivalent fission fluxes compared to the original methodology with PENTRAN, which achieved this for only 4 reaction rates for both the DTW and adaptive differencing scheme based solutions and showed a significant improvement over the TORT/DOTSYN approach, which attained that accuracy for only 1 reaction rate. The benchmark improvements provided in Chapter 6 delivered a definitive improvement of the transport solution, when comparing the calculated equivalent fission fluxes to the measurements and their associated errors, reported in the benchmark documentation and provided in Table 2.5 of this document. Although following the original benchmark methodology, PENTRAN was validated (based on criteria presented in the PCA benchmark documentation) as a transport methodology capable of calculating pressure vessel fluence calculations with accuracy,

the use of the improved benchmark methods provided results which were over one standard deviation more accurate to measurement.

### 7.3 Conclusions

Overall, the PENTRAN code system performed well and was validated for calculations of pressure vessel fluence, based on the original implementation of the PCA Benchmark. By allowing for flux and volume weighted cross sections to be used for the fuel assemblies, accounting for the control rod, and using an updated fixed source term, derived from the power profile obtained via a 3-D transport quarter core eigenvalue simulation, using the  $^{235}\text{U}$  fission spectra as the source spectra. The overall average of calculated-to-measured equivalent fission fluxes increased from 0.92 (original benchmark methodology) to 0.98 (improved benchmark methodology), representing a 6% improvement to measurement (based on the average), when using the adaptive differencing scheme incorporated in the PENTRAN discrete ordinate transport code. It may be interesting for future researchers to consider the effect of using an increased number of energy groups (i.e. a cross section library which is more refined than the BUGLE-96 47 group library, possibly 200 energy groups), since the increased number of groups should provide a better treatment of the resonance regions for the  $^{238}\text{U}(n,f)$  interaction, which could result in an improved agreement between calculations and measurements.

Since the result of a transport calculation is compared to an experimentally measured values for validation of a transport methodology for pressure vessel fluence calculations, it would be advantageous for individuals attempting to benchmark their transport methodology to utilize the most accurate material cross sections and source term available, which based on the results presented in this research, provide a significant increase in accuracy. Thus, the use of the improved cross sections and fission source term developed as part of this research by future investigators attempting to validate their transport codes for pressure vessel fluence calculations would enable increased

calculation accuracy for comparison to measured data in the Pool Critical Assembly  
Pressure Vessel Benchmark.

## APPENDIX A

### REACTION RATES FOR PCA BENCHMARK ANALYSIS

Energy Group	Upper MeV	<sup>237</sup> Np(n,f) [barns]	<sup>238</sup> U(n,f) [barns]	<sup>27</sup> Al(n,α) [barns]	<sup>58</sup> Ni(n,p) [barns]	<sup>115</sup> In(n,n') [barns]	<sup>103</sup> Rh(n,n') [barns]
1	1.7332E+01	2.2070E-24	1.1980E-24	1.0650E-25	2.6810E-25	5.8360E-26	2.4790E-25
2	1.4191E+01	2.0840E-24	1.0290E-24	1.2380E-25	4.7680E-25	1.0100E-25	4.0700E-25
3	1.2214E+01	2.1024E-24	9.8470E-25	1.0210E-25	5.9370E-25	2.1610E-25	7.8440E-25
4	1.0000E+01	2.1727E-24	9.9530E-25	7.4550E-26	6.2350E-25	2.8560E-25	1.0670E-24
5	8.6071E+00	2.2398E-24	9.9080E-25	3.9010E-26	6.2530E-25	3.1270E-25	1.1180E-24
6	7.4082E+00	1.9757E-24	8.3090E-25	9.8300E-27	6.0490E-25	3.3800E-25	1.1510E-24
7	6.0652E+00	1.4947E-24	5.5850E-25	3.8350E-28	5.0550E-25	3.3770E-25	1.1260E-24
8	4.9659E+00	1.5306E-24	5.4620E-25	0.0000E+00	3.7500E-25	3.2160E-25	1.0890E-24
9	3.6788E+00	1.6083E-24	5.2580E-25	0.0000E+00	2.4690E-25	3.3650E-25	1.0360E-24
10	3.0119E+00	1.6505E-24	5.2350E-25	0.0000E+00	1.7050E-25	3.4290E-25	1.0150E-24
11	2.7253E+00	1.6634E-24	5.3290E-25	0.0000E+00	1.2380E-25	3.4320E-25	9.7650E-25
12	2.4660E+00	1.6605E-24	5.3680E-25	0.0000E+00	9.6100E-26	3.3460E-25	9.3890E-25
13	2.3653E+00	1.6697E-24	5.3780E-25	0.0000E+00	8.7790E-26	3.3090E-25	9.2610E-25
14	2.3457E+00	1.6826E-24	5.3830E-25	0.0000E+00	7.9470E-26	3.2600E-25	9.0850E-25
15	2.2313E+00	1.6822E-24	5.2930E-25	0.0000E+00	5.0540E-26	2.8480E-25	8.3730E-25
16	1.9205E+00	1.6471E-24	4.7480E-25	0.0000E+00	2.8000E-26	2.2450E-25	8.0360E-25
17	1.6530E+00	1.5863E-24	3.0950E-25	0.0000E+00	1.4640E-26	1.6840E-25	7.1140E-25
18	1.3534E+00	1.4744E-24	4.5370E-26	0.0000E+00	5.8400E-27	1.0140E-25	6.3930E-25
19	1.0026E+00	1.3412E-24	1.2420E-26	0.0000E+00	1.3160E-27	5.0160E-26	5.7750E-25
20	8.2085E-01	1.1937E-24	3.6770E-27	0.0000E+00	8.7690E-28	2.5670E-26	4.7850E-25
21	7.4274E-01	9.3756E-25	1.5260E-27	0.0000E+00	5.5250E-28	1.4540E-26	3.3640E-25
22	6.0810E-01	6.0967E-25	6.2210E-28	0.0000E+00	1.7320E-28	4.6440E-27	2.0780E-25
23	4.9787E-01	2.6358E-25	2.7660E-28	0.0000E+00	0.0000E+00	1.8940E-27	1.4170E-25
24	3.6883E-01	9.3229E-26	1.5540E-28	0.0000E+00	0.0000E+00	1.6800E-28	9.8250E-26
25	2.9721E-01	4.5853E-26	7.8110E-29	0.0000E+00	0.0000E+00	0.0000E+00	5.9390E-26
26	1.8316E-01	2.3444E-26	5.9250E-29	0.0000E+00	0.0000E+00	0.0000E+00	2.8740E-26
27	1.1109E-01	1.4804E-26	5.6020E-29	0.0000E+00	0.0000E+00	0.0000E+00	1.3080E-26
28	6.7379E-02	1.1892E-26	5.9670E-29	0.0000E+00	0.0000E+00	0.0000E+00	3.5610E-27
29	4.0868E-02	1.0683E-26	6.7000E-29	0.0000E+00	0.0000E+00	0.0000E+00	3.1420E-29
30	3.1828E-02	1.0170E-26	7.7870E-29	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
31	2.6058E-02	9.9114E-27	8.1540E-29	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
32	2.4176E-02	9.7686E-27	8.4180E-29	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
33	2.1875E-02	9.5420E-27	9.2440E-29	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
34	1.5034E-02	9.1273E-27	1.0760E-28	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
35	7.1017E-03	8.7778E-27	1.3310E-29	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
36	3.3546E-03	9.3038E-27	8.5930E-33	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
37	1.5846E-03	1.3803E-26	1.0730E-27	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
38	4.5400E-04	2.5233E-26	1.1830E-29	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
39	2.1445E-04	3.1615E-26	1.6300E-29	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
40	1.0130E-04	5.2978E-26	3.5600E-29	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
41	3.7266E-05	2.9404E-26	1.4000E-28	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
42	1.0677E-05	7.7527E-27	7.7260E-29	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
43	5.0435E-06	3.9276E-27	5.8300E-30	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
44	1.8554E-06	9.9693E-27	7.3120E-30	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
45	8.7643E-07	9.4049E-27	1.0130E-29	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
46	4.1399E-07	5.3464E-27	1.7850E-29	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
47	1.0000E-07	1.4700E-26	7.4480E-28	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

## APPENDIX B

### IMPROVED FLUX AND VOLUME WEIGHTED PCA CORE CROSS SECTIONS

Appendix B contains the flux and volume weighted homogenized cross sections which were developed as part of this thesis research. These cross sections are consistent with the BUGLE-96 47 group neutron library structure, and were developed with the BUGLE-96 library as the cross section basis. Anisotropic scattering moments are provided for  $P_0$  through  $P_3$ , allowing for consistency between the original benchmark method's use of  $P_3$  cross sections. Cross sections are in the standard format for downscatter cross sections, consistent with the example below:

```

siga1 rnsigf1 sigt1 sig1->1      0      0      0      0      0      0
siga2 rnsigf2 sigt2 sig2->2 sig1->2      0      0      0      0      0
siga3 rnsigf3 sigt3 sig3->3 sig2->3 sig1->3      0      0      0      0
siga4 rnsigf4 sigt4 sig4->4 sig3->4 sig2->4 sig1->4      0      0      0
siga5 rnsigf5 sigt5 sig5->5 sig4->5 sig3->5 sig2->5 sig1->5      0      0
siga6 rnsigf6 sigt6 sig6->6 sig5->6 sig4->6 sig3->6 sig2->6 sig1->6      0
siga7 rnsigf7 sigt7 sig7->7 sig6->7 sig5->7 sig4->7 sig3->7 sig2->7 sig1->7

```

This example is for a 7 group case, but can be extended for the 47 group library, line entry for each group is slightly indented, as 47 groups caused text to wrap over more than one line. The  $P_n$  order is noted in the comment lines which begin each cross section block, and the name of each homogenized material type has been abbreviated as follows:

Standard Fuel Assembly Inner Fuel	STDinF
Standard Fuel Assembly Outer Fuel	STDoutF
ORR Fuel Assembly Inner Fuel	ORRinF
ORR Fuel Assembly Outer Fuel	ORRoutF
Control Rod Out Upper Fuel	CROUTtopF
Control Rod Guide Region	CROUT
Control Rod Out Lower Fuel	CROUTbotF
Control Rod In Upper Fuel	CROUTtopF
Control Rod Region	CRIN
Control Rod In Lower Fuel	CRINbotF





1.5639E-04 3.1455E-04 3.6797E-01 7.1142E-02 7.6526E-02 1.6449E-02 8.2018E-03 7.4956E-03 5.2476E-03 4.1436E-03 3.9640E-03 3.8159E-03 3.4097E-03 2.9440E-03 3.1730E-03 1.9233E-03 1.3158E-03 1.1838E-03  
1.1679E-03 6.3741E-04 5.6601E-04 4.5871E-04 4.7637E-04 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00  
0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00  
1.6002E-04 3.1460E-04 3.7208E-01 9.6360E-02 1.2405E-01 4.9840E-02 2.0390E-02 1.4677E-02 1.3409E-02 8.3662E-03 7.1521E-03 6.8380E-03 6.5858E-03 5.8851E-03 5.9603E-03 5.1916E-03 3.2324E-03 2.2683E-03  
2.1087E-03 1.8203E-03 1.0728E-03 9.5037E-04 7.6827E-04 8.1127E-04 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00  
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1.6528E-04 3.1641E-04 4.1797E-01 1.2210E-01 9.6749E-02 3.3019E-02 2.5149E-02 1.6712E-02 1.2994E-02 9.7857E-03 6.8406E-03 5.8655E-03 5.6108E-03 5.4023E-03 4.8264E-03 5.8847E-03 3.8030E-03 2.5062E-03  
1.8611E-03 1.7393E-03 1.2995E-03 8.4507E-04 7.4127E-04 5.9740E-04 6.4650E-04 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00  
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1.7494E-04 3.2899E-04 5.6197E-01 2.3623E-01 1.1926E-01 4.7044E-02 3.6120E-02 2.9463E-02 1.9905E-02 1.5592E-02 1.0287E-02 8.0157E-03 6.8745E-03 6.5751E-03 6.3295E-03 6.2387E-03 6.4117E-03 4.6771E-03  
2.6925E-03 2.1743E-03 1.9134E-03 1.3946E-03 9.5236E-04 8.1346E-04 6.5466E-04 7.2393E-04 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00  
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1.8026E-04 3.3972E-04 4.9847E-01 1.0483E-01 1.1925E-01 3.4272E-02 2.5597E-02 2.0102E-02 1.6390E-02 1.1329E-02 8.4202E-03 5.7223E-03 4.4608E-03 3.8248E-03 3.6572E-03 3.5216E-03 4.0896E-03 2.7923E-03  
2.6205E-03 1.4790E-03 1.1842E-03 9.7465E-04 7.4325E-04 5.0349E-04 4.1660E-04 3.3827E-04 3.8000E-04 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00  
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1.9538E-04 3.5907E-04 5.5535E-01 2.0907E-01 2.0259E-01 8.0146E-02 5.4586E-02 4.0788E-02 3.2018E-02 2.6120E-02 1.8506E-02 1.2248E-02 9.1169E-03 7.1066E-03 6.0924E-03 5.8273E-03 5.6777E-03 6.3926E-03  
4.3064E-03 4.1203E-03 2.3691E-03 1.7762E-03 1.4183E-03 1.1149E-03 7.5642E-04 6.0860E-04 5.0145E-04 5.5875E-04 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00  
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2.5146E-04 3.9573E-04 6.9801E-01 2.6654E-01 1.5332E-01 7.5106E-02 4.9828E-02 3.4553E-02 2.5811E-02 2.0270E-02 1.6563E-02 1.1632E-02 7.5708E-03 5.7677E-03 4.4953E-03 3.8544E-03 3.6858E-03 4.3830E-03  
3.4457E-03 2.8338E-03 2.4474E-03 1.4889E-03 1.0402E-03 8.1853E-04 6.5236E-04 4.4290E-04 3.5576E-04 2.8944E-04 3.1032E-04 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00  
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2.8191E-04 4.3902E-04 8.1830E-01 3.1688E-01 1.8861E-01 7.5930E-02 4.5565E-02 3.0237E-02 2.0966E-02 1.5663E-02 1.2300E-02 1.0135E-02 6.8656E-03 4.5926E-03 3.4989E-03 2.7267E-03 2.3414E-03 2.5299E-03  
2.6846E-03 1.9235E-03 1.7253E-03 1.4122E-03 8.8898E-04 6.0974E-04 4.5600E-04 3.6733E-04 2.5685E-04 2.0400E-04 1.6311E-04 1.6531E-04 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00  
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3.1042E-04 4.9137E-04 8.2945E-01 2.4624E-01 2.1332E-01 9.5603E-02 4.6137E-02 2.7686E-02 1.8373E-02 1.2738E-02 9.5167E-03 7.4721E-03 6.1521E-03 4.1131E-03 2.7902E-03 2.1254E-03 1.6563E-03 1.4751E-03  
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6.1933E-04 5.2682E-04 1.1614E+00 3.5308E-01 1.5597E-01 6.4204E-02 3.2802E-02 1.5830E-02 9.4994E-03 6.3042E-03 4.3704E-03 3.2652E-03 2.5637E-03 2.1061E-03 1.4005E-03 9.5722E-04 7.2912E-04 5.6817E-04  
5.1774E-04 5.5270E-04 4.4851E-04 4.0075E-04 3.4994E-04 2.8489E-04 1.8176E-04 1.2249E-04 8.9964E-05 6.9748E-05 5.1593E-05 3.9657E-05 3.1207E-05 2.8232E-05 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00  
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4.1464E-04 5.8528E-04 8.8594E-01 1.3193E-01 2.5969E-01 7.6856E-02 4.0392E-02 2.0636E-02 9.9577E-03 5.9763E-03 3.9657E-03 2.7494E-03 2.0541E-03 1.6127E-03 1.3246E-03 8.7971E-04 6.0219E-04 4.5870E-04  
3.5742E-04 3.2903E-04 3.0489E-04 2.8214E-04 2.5210E-04 2.1951E-04 1.7853E-04 1.1409E-04 7.6752E-05 5.6601E-05 4.3440E-05 3.2542E-05 2.4765E-05 1.9568E-05 1.7414E-05 0.0000E+00 0.0000E+00 0.0000E+00  
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4.0238E-04 5.9312E-04 8.9084E-01 4.6880E-02 8.0377E-02 4.1076E-02 2.5265E-02 1.3279E-02 6.7837E-03 3.2737E-03 1.9647E-03 1.3037E-03 9.0388E-04 6.7522E-04 5.3018E-04 4.3522E-04 2.8891E-04 1.9795E-04  
1.5078E-04 1.1749E-04 1.0764E-04 9.6329E-05 9.2744E-05 8.2869E-05 7.1974E-05 5.8475E-05 3.7436E-05 2.5144E-05 1.8564E-05 1.4157E-05 1.0670E-05 8.0737E-06 6.3669E-06 5.5799E-06 0.0000E+00 0.0000E+00  
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3.5808E-03 3.4870E-03 1.9738E-03 1.4992E-03 1.1934E-03 9.3411E-04 6.3110E-04 5.0847E-04 4.2604E-04 4.8366E-04 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00  
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9.6933E-08 7.4431E-08 5.6022E-08 5.0068E-08 3.7246E-08 2.7839E-08 3.1010E-08 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00  
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2.8747E-03 -2.4602E-03 -2.1280E-03 -1.7314E-03 -1.1486E-03 -7.7303E-04 -5.5443E-04 -4.1013E-04 -3.1210E-04 -2.3411E-04 -1.6672E-04 -1.2278E-04 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00  
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2.5217E-03 -1.6656E-03 -1.5688E-03 -1.3509E-03 -1.0921E-03 -7.1965E-04 -4.8147E-04 -3.4690E-04 -2.5417E-04 -1.9246E-04 -1.4470E-04 -1.0008E-04 -7.6377E-05 0.0000E+00 0.0000E+00 0.0000E+00  
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**APPENDIX C**

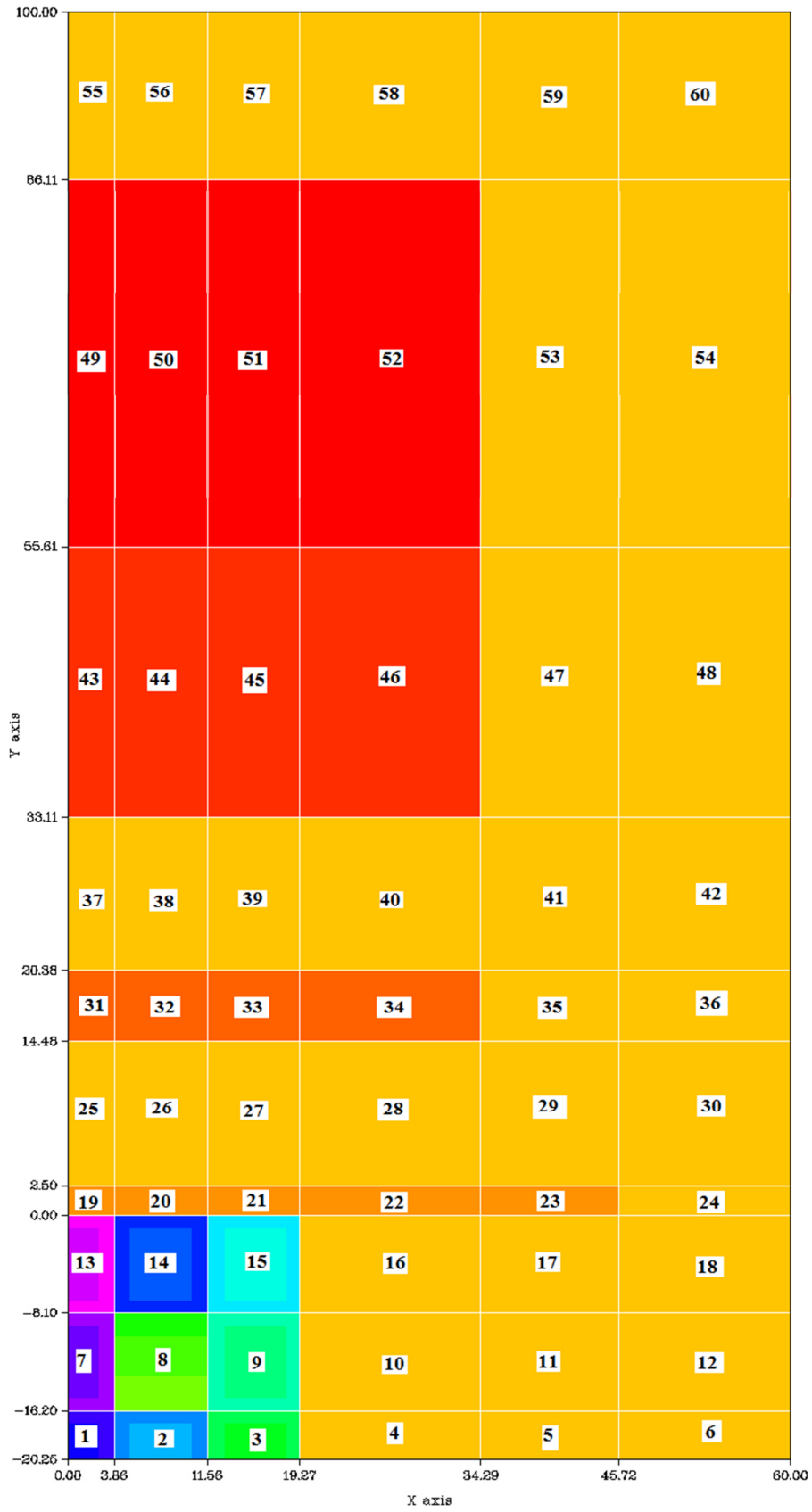
**DIFFERENCING SCHEME SELECTED BY PENTRAN'S**

**ADAPTIVE DIFFERENCE OPTION**

Coarse meshes were numbered from 1 to 600, with 60 coarse meshes per z-level, with z-level boundaries as follows:

<b>z-level</b>	<b>Lower Boundary</b>	<b>Upper Boundary</b>
<b>1</b>	0.00 cm	10.55 cm
<b>2</b>	10.55 cm	20.71 cm
<b>3</b>	20.71 cm	25.00 cm
<b>4</b>	25.00 cm	41.00 cm
<b>5</b>	41.00 cm	57.00 cm
<b>6</b>	57.00 cm	73.26 cm
<b>7</b>	73.26 cm	85.00 cm
<b>8</b>	85.00 cm	89.29 cm
<b>9</b>	89.29 cm	99.45 cm
<b>10</b>	99.45 cm	110.00 cm

The reactor core spanned z-levels 4-7, and the control rod was inserted in z-level 7, based on a slice through the reactor core midplane, the coarse mesh numbering scheme was as follows:





The differencing scheme selected using PENTRAN's adaptive difference option for the improved PCA benchmark methodology is shown below.

Coarse Mesh	z-level 1	z-level 2	z-level 3	z-level 4	z-level 5	z-level 6	z-level 7	z-level 8	z-level 9	z-level 10
1	EDI	EDI	EDI	DTW	DTW	DTW	DTW	EDI	EDI	EDI
2	EDI	EDI	EDI	EDI	DTW	DTW	DTW	EDI	EDI	EDI
3	EDI	EDI	EDI	DTW	DTW	DTW	DTW	EDI	EDI	EDI
4	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
5	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
6	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
7	EDI	EDI	EDI	DTW	DTW	DTW	DTW	EDI	EDI	EDI
8	EDI	EDI	EDI	DTW	EDI	EDI	EDI	EDI	EDI	EDI
9	EDI	EDI	EDI	DTW	DTW	DTW	DTW	EDI	EDI	EDI
10	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
11	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
12	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
13	EDI	EDI	EDI	EDI	DTW	DTW	DTW	EDI	EDI	EDI
14	EDI	EDI	DTW	EDI	DTW	DTW	DTW	EDI	EDI	EDI
15	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
16	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
17	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
18	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
19	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
20	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
21	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
22	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
23	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
24	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
25	EDI	EDI	EDI	EDI	EDI	EDI	EDI	DTW	EDI	EDI
26	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
27	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
28	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
29	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
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33	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
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47	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
48	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI

<b>49</b>	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
<b>50</b>	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
<b>51</b>	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
<b>52</b>	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
<b>53</b>	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
<b>54</b>	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
<b>55</b>	EDI	EDI	EDI	DTW	EDI	EDI	EDI	EDI	EDI	EDI
<b>56</b>	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
<b>57</b>	EDI	EDI	EDI	DTW	EDI	EDI	EDI	EDI	EDI	EDI
<b>58</b>	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
<b>59</b>	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI
<b>60</b>	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI	EDI

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